DISPERSION MODELLING TECHNIQUES FOR CARBON DIOXIDE PIPELINES IN AUSTRALIA

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ABBREVIATIONS

3D	Three-Dimensional
ACT	Australian Capital Territory
AEGL	Acute Emergency Guideline Level
AIChE	American Institute of Chemical Engineers
ALARP	As Low As Reasonably Practicable
ALOHA	Areal Locations of Hazardous Atmospheres
ANLEC R&D	Australian National Low Emissions Coal Research and Development
Ar	Argon
AS	Australian Standard
BCIA	Brown Coal Innovation Australia Ltd
BLEVE	Boiling Liquid Expanding Vapour Explosion
CAD	Computer-Aided Design
CAMEO	Computer-Aided Management of Emergency Systems
CCPS	Center for Chemical Process Safety
CCS	Carbon Capture and Storage
CERC	Cambridge Environmental Research Consultants
CFD	Computational Fluid Dynamics
CH_4	Methane
CHARM	Complex Hazardous Air Release Model
CMAQ	Community Multi-scale Air Quality Model
CO	Carbon Monoxide
CO_2	Carbon Dioxide
CONCAWE	Conservation of Clean Air and Water in Europe
DBFM	Dynamic Boundary Fracture Model
DEGADIS	Dense Gas Dispersion
DISPLAY	Dispersion using Shallow Layer Modelling
DNV-GL	Det Norske Veritas - Germanischer Lloyds[1]
DOD	Department of Defence (US)
EGIG	European Gas Pipeline Incident Data Group
ENVIRON	ENVIRON Australia Pty Ltd
EOR	Enhanced Oil Recovery
EPCRC	Energy Pipelines Cooperative Research Centre
EPRI	Electric Power Research Institute
ERP	Equivalent Roughness Pattern
ERPG	Emergency Response Planning Guideline
EU	European Union

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[1] The merger to form DNV-GL was relatively recent, however, in this document DNV-GL is taken to mean either the new organisation or the separate companies of DNV and GL.

FAC2	Factor of two
FB	Fractional Bias
FLACS	Flame Acceleration Simulator
FRED	Fire Release Explosion Dispersion
GB	Great Britain
GUI	Graphical User Interface
H2	Hydrogen
H_2S	Hydrogen Sulphide
HF	Hydrogen Fluoride
HPAC	Hazard Prediction and Assessment Capability
HSE	Health and Safety Executive (GB)
HSL	British Health & Safety Laboratory
IDLH	Immediately Dangerous to Life and Health
IEA	International Energy Agency
IEAGHG	International Energy Agency Green House Gas research and development program
IPCC	Intergovernmental Panel on Climate Change
ISO	International Organisation for Standardisation
JIP	Joint Industry Program
LANL	Los Alamos National Laboratory
LC_{50}	Lethal Concentration (50%)
LFL	Lower Flammable Limit
LNG	Liquefied Natural Gas (methane)
LPG	Liquefied Petroleum Gas
MAOP	Minimum Allowable Operating Pressure
MDA	Modellers Data Archive
MEP	Model Evaluation Protocol
MSS	MicroSwiftSpray
Mtpa	Million tons per Annum
MVK	Model Validation Kit
N_2	Nitrogen
NAD	Normalised Absolute Difference
NB	Nominal Bore
NH_3	Ammonia
NIOSH	US National Institute for Occupational Safety and Health
NMSE	Normalised Mean Square Error
NO	Nitrogen Monoxide
NOAA	US National Oceanic and Atmospheric Administration
NSW	New South Wales
NT	Northern Territory

NWP	Numerical Weather Prediction
O_2	Oxygen
Pa	Pascals
PAC	Protective Action Criteria
PDF	Probability Density Function
PE	Polyethylene
PERF	Petroleum Environmental Research Forum
PHAST	Process Hazard Analysis Screening Tool
PHMSA	Pipeline and Hazardous Materials Safety Administration (US)
ppm	parts per million
ppmv	parts per million volume
Qld	Queensland
QRA	Quantitative Risk Assessment
QUIC	Quick Urban & Industrial Complex
RIVM	National Institute for Public Health and the Environment (Netherlands)
SA	South Australia
SCF	Supercritical Fluid
SCIPUFF	Second-order Closure Integrated PUFF (software)
SF_6	Sulphur Hexafluoride
Sherpa	Sherpa Consulting Pty Ltd
SLAM	Shallow Layer Model
SLOD	Significant Likelihood of Death
SLOT	Specified Level of Toxicity
SMEDIS	Scientific Model Evaluation of Dense Gas Dispersion Models
SO_2	Sulphur Dioxide
STEL	Short Term Exposure Limit
TAPM	The Air Pollution Model
Tas	Tasmania
TEEL	Temporary Emergency Exposure Limit
TIC	Toxic Industrial Chemicals
TL	Toxic Load
TNO	Netherlands Organisation for Applied Scientific Research
TRACE	Toxic Release Analysis of Chemical Emissions
TWA	Total Weighted Average
TWODEE	TWO Dimensional Shallow Layer Model
UK	United Kingdom
UKOPA	United Kingdom Onshore Pipeline Operators’ Association
URA	Uniform Roughness Array
US DOE	US Department of Energy

US EPA	US Environmental Protection Department
US(A)	United States of America
Vic	Victoria
WA	Western Australia

Terminology

Accident	An **accident** is an unplanned event or sequence of events that results in undesirable consequences. An incident with specific safety consequences.
As Low As Reasonably Practicable (ALARP)	**ALARP** is the risk level at which further steps to reduce risk will incur costs that are grossly disproportionate to the benefits gained. In the Australian context under the Work Health and Safety Act, a person conducting a business or undertaking has the duty to eliminate risk or reduce it so far as is reasonably practicable (SFAIRP).
Consequence	A **consequence** is defined as the direct, undesirable result of an accidental sequence usually involving a fire, explosion or release of toxic material. **Consequence** descriptions may be qualitative or quantitative estimates of the effects of an accident in terms of factors such as health impacts, economic loss or environmental impact.
Hazard	A **Hazard** is something with the potential to cause harm. For example CO_2 under pressure.
Likelihood	A measure of the expected probability or frequency of an event's occurrence.
Risk	**Risk** is a combination of the expected frequency (events/year) and consequence (effects/event) of a single accident or group of accidents.
Natural gas	The common name for methane, and is used in AS 2885. In this document, methane will be used, except in direct quotes or references.
bar	Unit of measurement for pressure, where 1 bar = 100,000 Pa; atmospheric pressure is 101,325 Pa.

AS 2885 (2012) terminology:

High Consequence Area	A location where pipeline failure can be expected to result in multiple fatalities or significant environmental damage.
Primary Location Class	The classification of an area according to its general geographic and demographic characteristics, reflecting both the threats to the pipeline from the land usage and the consequences for the population should the pipeline suffer a loss of containment. Definitions as follows:
R1	Rural - Land that is unused, undeveloped or is used for rural activities. Population nearby is within isolated dwelling.
R2	Rural Residential – Land that is occupied by single residence blocks in the range 1 ha to 5 ha.
T1	Residential – Land that is developed for community living. Multiple dwellings in proximity to each other.
T2	High Density - Land that is developed for high density community use.
Threat	Any activity or condition that can adversely affect the pipeline if not adequately controlled.

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1 EXECUTIVE SUMMARY

1.1 Overview

This report details the findings of an investigation into the modelling of carbon dioxide (CO_2) dispersion, as it applies to new CO_2 pipeline infrastructure in Australia. It provides a critical review of current Australian and international literature regarding CO_2 pipeline design standards, as well as determining 'fit-for-purpose' CO_2 dispersion modelling techniques.

The goal was to understand whether available modelling techniques are capable of reliably simulating the release and dispersion of CO_2 from a pipeline, either as a result of an accidental release or during the planned use of venting systems.

This understanding will help to inform the design and deployment of large scale carbon capture and storage (CCS) infrastructure, which will be essential to preserve the value of fossil fuel reserves in Australia and allow deep reductions in emissions from heavy manufacturing industries.

The investigation addressed two key topics:

- A critical review of current pipeline design standards. On this point, the investigation found that further regulation covering risk assessment of releases from CO_2 pipelines in Australia, beyond those outlined in Australian Standard (AS) 2885 and this document, is not required.
- Identification of a fit-for-purpose CO_2 dispersion model. In this regard, the findings provide guidance for pipeline designers, specifically in Australia but with relevance elsewhere, to make decisions regarding pipeline design and safety.

1.2 Critical review of current pipeline design standards

Any new CO_2 pipeline built in Australia will be subject to the regulatory requirements of the relevant State and Territory government(s).

AS 2885 'Pipelines - Gas and liquid petroleum' specifies the requirements for the safe design, construction, inspection, testing, operation and maintenance of a land or a submarine pipeline. Although not currently mandatory in every State and Territory, AS 2885 is recognised as the appropriate standard for the design of pipelines in Australia and its use is widely accepted.

AS 2885 is primarily applicable to pipelines carrying flammable gas, especially natural gas (methane). While it does make allowance for pipelines carrying hazardous materials other than natural gas, its guidance is less specific in this context, and is generally limited to the requirement that the fundamental principles of the Standard be used to develop alternatives that meet the overall safety objectives. In such cases, a *gap analysis* is required to identify the differences between the proposed fluid and those of gas and liquid petroleum products defined in the standard.

AS 2885.1 adopts a 'safety management study' approach to risk minimisation. This requires a qualitative risk assessment to identify potential threats and appropriate risk mitigation measures, and must be employed at various stages throughout the life of the pipeline.

As such, this investigation reviewed the requirements of a qualitative risk assessment according to AS 2885, and identified knowledge gaps relating specifically to CO_2 pipelines.

In order to apply the AS 2885.1 safety management study approach to CO_2 pipelines, an understanding of the difference between methane and CO_2, in terms of both physical properties and implications for human health is key. A significant difference between natural gas and CO_2 pipelines is in the *mechanism for harm* in the event of an accidental rupture. A natural gas pipeline rupture can create an initial fireball that is extremely dangerous to people and property, with potential effects distances of several hundred metres. Human exposure to CO_2 can increase blood acidity, triggering adverse effects on the respiratory, cardiovascular and central nervous systems, and is called CO_2 intoxication. The impact distances associated with rupture of a CO_2 pipeline would be influenced by wind speed, direction and terrain effects, which would potentially result in a smaller affected area.

AS 2885.1 defines *threshold levels of harm* on the basis of exposure to radiant energy from burning gas. For pipelines carrying methane, these thresholds are (for injury) 4.7 kW/m^2 and (for fatality) 12.6 kW/m^2. Given that loss of containment from CO_2 pipelines has significantly different consequences from methane pipelines, this report recommends that equivalent levels of harm be defined for AS 2885.1 safety management studies concerned with CO_2 pipelines. As a guide, this report concludes the following levels may be considered appropriate:

- 'Severe' = threshold of injury = 3 vol% CO_2 in air for 60 minutes
- 'Major' = threshold of fatality = 5 vol% CO_2 in air for 60 minutes.

The investigation made the following conclusions in relation to the applicability of AS 2885 for safe design and operation of CO_2 pipelines:

- For the **preliminary design stage** of a new CO_2 pipeline in Australia, the design tools provided in AS 2885.1 are applicable. It should be possible to gain regulatory approval to proceed to the detailed design stage without the need for additional detailed modelling. In particular, this report supports the current recommendation in Appendix BB of AS 2885.1 that, for CO_2 pipelines, 'the measurement length for definition of the location class limits shall be estimated on the basis that the pipeline is transporting natural gas'.

- For the subsequent **detailed design stage**, consequence analysis will be necessary to help identify the measurement length, to select locations for isolation valves and vent stations along the length of the pipeline, and to determine the maximum allowable discharge rate in high consequence locations.
- During the **working life of the pipeline**, AS 2885.1 also specifies that the safety management study process must continue, and that an appropriate emergency response plan be developed.

For both the detailed design phase and pipeline working life, the design tools provided in AS 2885.1 are not adequate. Modelling tools suitable for simulating the dispersion characteristics of dense, cold clouds of CO_2 gas must be used. This finding leads into the second key topic of the investigation – identifying a 'fit for purpose' model.

1.3 Identification of a 'fit for purpose' CO_2 dispersion model

The investigation considered a series of modelling tools that may be regarded as ‘fit for purpose’ for simulating the dispersion characteristics of CO_2 gas. The assessment was based on a number of criteria:

- Availability, ease of use, access to technical support
- Ability to calculate appropriate source terms for different CO_2 release scenarios
- Validation history, particularly with CO_2
- Ability to account for complex terrain and variable atmospheric conditions
- Applicability to different stages of the design process
- Acceptability to Australian regulators.

Modelling of a release of dense phase CO_2 from a pipeline requires consideration of a number of aspects, including transient pipeline depressurisation, multi-phase jet release, and dispersion of both dense and neutral gas.

A range of dense gas dispersion models were investigated, including empirical correlations, integral models, Lagrangian particle and plume dispersion models and computational fluid dynamics (CFD) models. Selected models were reviewed and evaluated against the various criteria to determine if they could be considered ‘fit for purpose’.

Only two dense gas dispersion models include the ability to simulate pipeline depressurisation: the DNV-GL model PHAST and the TNO model EFFECTS. All other models would require input from a separate modelling tool to perform this simulation. Additionally, both DNV-GL and TNO have participated in recent major research projects (CO_2PipeTrans, CO_2PipeHaz and COOLTRANS), all of which aimed to improve understanding of the phenomena that occur when dense phase CO_2 is released to atmospheric conditions.

PHAST version 6.6 and later and the forthcoming EFFECTS 10 are the only two commercial packages that can account for both a wide range of source terms and the formation of solid CO_2 particles. While other modelling approaches can be used to achieve a similar outcome, they would require greater effort to assemble and interface the various model components.

From a regulatory perspective, based on the experience in the United States and Europe, the models DEGADIS, HGSYSTEM, SLAB (including EFFECTS), ALOHA, PHAST and SCIPUFF may all be acceptable to Australian regulators. Of these, PHAST version 6.6 and later and the forthcoming EFFECTS 10 have been subject to the greatest refinement using CO_2 release data. This does not preclude a case being made, in principle, for other models considered in this report, depending on the specific requirements of the project.

PHAST and EFFECTS are both types of integral models, which are generally designed to simulate dense gas dispersion over flat terrain. Conversely, Lagrangian and CFD models have the added ability to incorporate complex terrain effects. However, a review of the issues involved found that terrain effects can usually be ignored, as they generally tend to increase dispersion of the dense gas cloud, and therefore reduce the hazard distance. For this reason, flat terrain models can generally be considered fit-for-purpose because they tend to define the worst case at any downwind distance.

The more complex Lagrangian models cannot be recommended as primary design tools. Their lack of field trial validation presents a significant limitation.

CFD models need to be properly validated and their limitations understood. Their sensitivity to user-selected input conditions is an issue that has yet to be adequately resolved. However, their ability to model complex physical situations and low wind conditions means that they are likely to play an increasing role in the future.

Integral models may be regarded as fit for purpose in most circumstances. However, integral models may not be appropriate in situations where the local terrain has the potential to be significantly larger than the size of the gas plume. Where such conditions are a possibility, common sense should be used to determine the applicability of any modelling approach.

The strengths and weaknesses of each model are summarised in Table 1.1. The ‘best’ choice in any instance will depend on a variety of additional factors, such as cost and acceptability to regulators, and the pipeline engineer will need to take these additional factors into account.

One of the main issues identified during this analysis was that predictions from acceptable dense gas models had a ‘factor of two’ margin of error. This has implications for the hazard distance calculated using the models. To account for this margin of error, this report recommends that a conservative hazard distance be calculated, either by:

- using a concentration profile equivalent to half the ‘threshold of injury (or fatality)’ value; or
- using the ‘threshold of injury (or fatality)’ value to calculate a hazard distance, and then increasing this distance by 50%.

Table 1.1: Summary of evaluation criteria for selected models

Model Category	Model Name	Free?	Availability of Graphical User Interface	Complexity of Inputs	Validated against dense gas experiments	Validated against CO_2 experiments	Able to represent a range of source configurations	Ability to account for complex terrain and obstructions	Ability to account for complex meteorology
Integral	SLAB	Yes	Purchase	Medium	Yes	Low	Medium	None	Low
	DEGADIS	Yes	Purchase	Medium to High	Yes	Medium	Low	None	Low
	HGSYSTEM	Yes	No	Medium to High	Yes	Medium	High	Low	Low
	ALOHA	Yes	Free	Low	Yes	Low	Low	None	Low
	EFFECTS (v10)	No	Purchase	Medium	Yes	High	High	None	Low
	SAFER/TRACE	No	Purchase	Medium	Yes	Low	High	None	Low
	GASTAR	No	Purchase	Medium	Yes	Low	High	Medium	Medium
	PHAST	No	Purchase	Medium	Yes	High	High	None	Low
Lagrangian	*QUIC*(b)	*Yes*	*Free*	*Medium*	*Yes*	*Low*	*High*	*High*	*High*
	SCIPUFF	Yes	Free	High	Yes	Low	High	Medium	Medium
	ArRisk(a)	No	Purchase	Medium	Yes	Low	High	High	High
	CHARM (flat terrain)	No	Purchase	Medium	Yes	Low	High	None	Medium
	CHARM (complex terrain)	No	Purchase	Medium	No	Low	High	High	Medium
FD	FLUENT, PANACHE, FLACS, ANSYS-CFX	No	Purchase	High	Yes	Low	High	High	High
	OpenFOAM	Yes	Purchase	High	Yes	Low	High	High	High

(a) Includes MicroSWIFT-SPRAY

(b) Currently only available for non-profit research purposes.

1.4 Summary of major findings

The main findings of this study provide a basic primer in CO_2 dispersion modelling and guidance in selection of a modelling approach that is ‘fit for purpose’ for CO_2 pipeline design in Australia. The guidance provided in this report represents the current international best practice in modelling CO_2 dispersion, specifically for application in the context of AS 2885.

This report has shown that the design tools provided in AS 2885.1 can be used in the preliminary design phase for a new CO_2 pipeline in Australia, and that there are a number of high quality dispersion modelling tools available for use in subsequent design and operational phases.

The selection of an appropriate, fit-for-purpose modelling tool in various instances, drawing on the guidance provided in this report, will allow the risks associated with new CO_2 pipelines to be reduced to as low as reasonably practicable, equivalent to the community expectations for natural gas pipelines.

2 INTRODUCTION

2.1 Overview

This report has been written to provide guidance on international best practise in modelling carbon dioxide (CO_2) dispersion, as it would be applied to new CO_2 pipeline infrastructure in Australia. The scope of issues that this report is intended to address is as follows:

- To review and critique Australian and international literature on dense gas dispersion modelling techniques applicable to CO_2 pipelines, including both controlled venting and unintended release due to rupture or damage by third parties. This includes a review of current international efforts to define critical release volumes and rates, and any associated implications for dispersion modelling. It also includes a comparison of the performance of different modelling approaches under CO_2 release scenario(s) involving complex topography/atmospheric conditions. This work serves to identify international best practice and highlight any gaps that exist in particular approaches or more generally.
- To consider how the CO_2 dispersion modelling results can be utilised in an As Low As Reasonable Practicable (ALARP) risk assessment (or other appropriate normalised approach used by industry and regulators) as applied to the development of a CO_2 pipeline in Australia. The aim is to demonstrate how CO_2 dispersion modelling can be used, in association with other risk mitigation measures (i.e. burial, taint/odorant), for pipeline risk minimisation. This risk assessment approach includes any uncertainties in the modelling analysis in a manner that is both scientifically sound and understandable to stakeholders.
- To compare the international safety and hazard records of both CO_2 and natural gas pipework infrastructure, to help address community concerns about the development of CO_2 pipework infrastructure in Australia. This is new to Australia but not to the world, so a comparison of the unknown CO_2 pipeline with the more familiar natural gas pipeline should provide a valuable tool for community engagement and education.

2.2 Rationale

Implementation of large-scale carbon capture and storage (CCS) technologies will require the deployment of high-pressure pipelines to transport compressed CO_2 from the point of capture to the storage site. In most respects, the processes to design such pipelines are well known, based on long experience in the oil and gas processing industries. In some, respects, however, CO_2 presents some unique challenges because of its specific physical and chemical properties:

- It is heavier than air, so leaks will not disperse as quickly as methane (natural gas).
- It is not flammable, but high concentrations of CO_2 in the blood can trigger adverse physiological effects. Depending on the CO_2 concentration inhaled and the exposure duration, toxicological symptoms range from headaches, increased respiratory and heart rate, dizziness, muscle twitching, confusion, unconsciousness, coma and death.
- It is transported as a dense-phase fluid, not in the gaseous state.
- Fluid leaking from the supercritical state will flash directly to gas, and may additionally form a solid phase of dry ice.
- Releases of dense-phase CO_2 will produce very low temperatures (-78°C or lower), which may lead to problems with embrittlement of infrastructure and harm to anyone exposed.

To date, almost all the existing onshore CO_2 pipelines have been built in the USA, where the CO_2 is predominantly used in enhanced oil recovery. These pipelines are typically routed through sparsely populated regions, where the risk of human injury from a pipeline failure is very low. In most cases, the CO_2 is transported as a compressed gas, and compressed further to the supercritical state close to the injection point.

Conversely, implementation of large-scale CCS at an acceptable cost will require transport of CO_2 in the supercritical state, and it may be necessary to route pipelines through more densely populated areas. Over a decade ago it was recognised that there was insufficient understanding of the behaviour of CO_2 in the supercritical state, or its effects on pipeline materials, to allow the design of CO_2 pipelines with the necessary degree of confidence. Issues requiring further understanding included the rapid corrosion that can occur if water enters a CO_2 system, the very cold temperatures that can occur if a CO_2 system is depressurised, the effect of impurities, the difficulties associated with modelling leaks, and the toxicological effects on humans when air with a high CO_2 concentration is inhaled.

Since that time, a great deal of work has been done to address these knowledge gaps, especially in Europe. At the time of this report (mid 2015), most of this work had only recently been completed and key findings published.

The aim of this report is to compile this information, specifically in relation to the modelling of dispersion of CO_2 released from the supercritical state, and place it in the context of the pipeline design standards that apply in Australia. This report will provide state of the art guidance for pipeline designers, specifically in Australia but with relevance elsewhere, to help facilitate the deployment of large-scale CCS technologies. Dense gas dispersion modelling is a specialised and highly technical subject, and there are no recent reviews that can provide guidance on range of modelling software available. A key objective of this report is to provide a basic primer on CO_2 dispersion modelling and guidance in selection of a modelling approach that is 'fit for purpose' for CO_2 pipeline design in Australia.

2.2.1 Key studies

There were a number of established documents available to provide guidance on CO_2 pipeline design issues. These are described in Table 2.1.

Table 2.1: Established guidance documents

'Latrobe Valley CO_2 storage assessment' (Hooper et al. 2005)	Includes an assessment of the infrastructure risks associated with a new CO_2 pipeline in Victoria's Latrobe Valley.
'State-of-the-art overview of CO_2 pipeline transport with relevance to offshore pipelines' (Oosterkamp and Ramsen 2008)	While written specifically for offshore pipelines, much of the information is relevant to onshore pipelines as well.
'Technical guidance on hazard analysis for onshore carbon capture installations and onshore pipelines' (Energy Institute 2010b)	This document represents the state of the art in the application of dispersion modelling to CO_2 pipeline design in 2010 and remains a useful reference document. The current report covers similar ground, but aims to give a broader coverage with a specific emphasis on Australian regulatory requirements.
'Good plant design and operation for onshore carbon capture installations and onshore pipelines' (Energy Institute 2010a)	Provides an overview of the hardware elements of a CCS system, and guidance on design and operational issues.
'Design and operation of CO_2 pipelines' (DNV 2010).	This is a reference for design of CO_2 pipelines but provides limited guidance on dispersion modelling.
'Guidance on CCS CO_2 safety and environment major accident hazard risk management' (DNV 2013).	Level 4, Section 3.4.1 provides a comprehensive listing of measures that can be adopted to increase the safety of CO_2 pipelines.
'CO_2 pipelines good practice guidelines' (Wilday and Saw 2013).	An up-to-date compilation of international best practice.
'CO_2 pipeline infrastructure' (IEAGHG 2013).	A compendium of public information on CO_2 pipelines worldwide.
'The global status of CCS: 2014' (Global CCS Institute 2012).	Provides an overview of international CO_2 pipeline infrastructure, international design codes and standards, and describes progress on developing an ISO Standard for CO_2 pipeline design.

Since 2010, there have been four separate research programmes under way in Europe and the UK, with the findings being released progressively over that time:

- COOLTRANS
- CO_2PIPETRANS

- CO_2PipeHaz
- CO_2Quest

Each of these are summarised briefly below.

2.2.1.1 COOLTRANS

This programme was commissioned by National Grid to provide the technical foundations for the design and operation of CO_2 pipelines in the UK. A key part of this programme was a series of large shock tube, burst, venting, puncture, rupture and full scale fracture propagation tests, to provide information on how CO_2 behaves in a buried pipeline, how it escapes and how it disperses. The participants had the following roles:

- GL Noble Denton (now DNV-GL) conducted field-scale CO_2 release experiments and provided predictions using consequence models used in risk assessments.
- Nottingham University conducted laboratory experiments to develop an equation of state for CO_2 (with and without impurities) as well as field experiments to examine the environmental effects of fugitive CO_2 emissions.
- University College London, University of Leeds and Kingston University created Computational Fluid Dynamics (CFD) models of, respectively, the release rate, near-field and far-field dispersion behaviour of CO_2.
- The Health and Safety Laboratory developed a Model Evaluation Protocol (MEP) and to conducted some limited tests using the DNV consequence modelling package, PHAST.
- Atkins developed and validated models for crack-propagation in CO_2 pipelines.
- Newcastle University, HH Risk and Pipeline Integrity Engineers (PIE) developed a new failure frequency model for CO_2 pipelines.
- Manchester University/Tyndall Centre examined the public perception of risk as relating to CO_2 pipelines.

The COOLTRANS programme ran from 2011 to December 2013. A summary report of the programme was released in October 2014 (Barnett and Cooper 2014).

2.2.1.2 CO_2PIPETRANS

This was a Joint Industry Project led by DNV[2] that involved three key areas of investigation:

- Experimental medium-scale CO_2 release experiments, to allow development and validation of robust models for dense phase CO_2 depressurization, release, and dispersion.

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[2] https://www.dnvgl.com/oilgas/innovation-development/joint-industry-projects/co2pipetrans.html

- Full scale experiments on pipeline rupture, to improve the design theory for fracture arrest.
- The mechanism and rate of pipeline corrosion in dense phase CO_2, particularly in the presence of impurities such as O_2, SO_x, NO_x and H_2S.

The experimental results have been utilised by the project participants and the CO_2PipeHaz project (Section 2.2.1.3). It is anticipated that an updated industry guidance document will be developed using this data, but it is not yet available.

2.2.1.3 *CO_2PipeHaz*

The CO_2PipeHaz project was funded by the European Commission FP7 Energy Programme, and involved collaboration between University College London, University of Leeds, GEXCON AS, Institut National de l'Environnement et des Risques (INERIS), NCSR, Dalian University of Technology and the Health and Safety Laboratory (HSL).

The objective of the project was to develop improved predictions of fluid phase, discharge rate and atmospheric dispersion during accidental releases from pressurised CO_2 pipelines (Mahgerefteh et al. 2011).

The CO_2PipeHaz project was completed in 2014, and a summary report has been published (Woolley et al. 2014a). Based on the project findings, recommended good practice guidelines for CO_2 pipelines have also been published (Wilday and Saw 2013).

2.2.1.4 *CO_2Quest*

The CO_2Quest project is funded by the European Commission FP7 Energy Programme. Coordinated by University College London, the CO_2QUEST project involves the collaboration of 12 industrial and academic partners in Europe, China and Canada.

The project focuses on the development of state-of-the-art mathematical models along with the use of large scale experiments to identify the impact of CO_2 stream composition on the different parts of the CCS chain. These include the pipeline pressure drop and compressor power requirement, pipeline propensity to ductile and brittle facture propagation, corrosion, geochemical interactions within the storage site, and the ensuing health and environmental hazards[3].

CO_2Quest began in March 2013 and is scheduled for completion in February 2016.

The present report will highlight the utility of the research outcomes from these research programmes, where appropriate, in the context of CO_2 pipeline design in Australia.

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[3] http://www.co2quest.eu

2.3 Structure of the report

The above topics have been addressed in this report as follows:

Chapter 3	provides the justification for undertaking this report. It explains why CO_2 pipelines are needed in Australia, as an essential part of CCS infrastructure. It describes the CO_2 pipeline infrastructure that has been established elsewhere in the world, and the typical operating conditions for such pipelines.
Chapter 4	explains the regulations that would apply to the design and construction of a new CO_2 pipeline in Australia, especially Australian Standard 2885.1. It describes the ALARP risk minimisation approach used in AS 2885.1, and compares this with the quantitative risk assessment approach used in other countries. This Chapter outlines the need for dense gas dispersion modelling at various stages in the design and operation of a CO_2 pipeline in Australia, and discusses how such modelling would be applied during ALARP risk minimisation.
Chapter 5	describes the hazardous aspects of CO_2 transport, and the risks to which the community may be exposed. It describes the effects of exposure to increasing levels of CO_2, and the associated standards established in different countries.
Chapter 6	reviews the factors that can contribute toward community acceptance of a new CO_2 pipeline. It highlights the similarities and differences between natural gas and CO_2 pipelines, and identifies the technical issues that need to be addressed in order to ensure that the risks associated with a CO_2 pipeline are acceptable.
Chapter 7	describes the main components of a CCS system, and the type of CO_2 release scenarios that might be anticipated to arise, either deliberately or accidentally, during pipeline operations. This provides an overview of the range of scenarios that would need to be considered as part of a risk consequence analysis. This Chapter also highlights the recent international research efforts that have sought to provide better information on the consequences of a large-scale CO_2 release.
Chapter 8	considers what is necessary for a dense gas dispersion model to be considered ‘fit for purpose’ in the design of a CO_2 pipeline in Australia. It reviews the different types of models that have been developed, their validation, their limitations, their suitability for different stages of the design process, and their availability.

It discusses the ability of different models to calculate the 'source terms' specific to a CO_2 release, and their ability to account for complex terrain and variable atmospheric conditions. This Chapter also discusses the uncertainties associated with the predictions of dense gas dispersion models, and how these can be taken into account during consequence analysis. Finally, this Chapter reviews the regulatory status of dense gas dispersion models, both overseas and in Australia, and provide examples of the previous use of specific models in the design of commercial CO_2 pipelines. This overview allows a recommendation of models that may be considered 'fit for purpose' for CO_2 pipeline design in Australia.

Chapter 9	describes the additional strategies that comprise international best practice for reducing the risks associated with CO_2 pipelines.

3 CO_2 PIPELINES

3.1 Summary

A substantial and sustained reduction in CO_2 emissions has been identified by the Intergovernmental Panel on Climate Change (IPCC) as being the key mechanism to combat climate change. Energy derived from fossil fuels contributes to the vast majority of CO_2 emissions, so reductions in this sector are essential.

Carbon Capture and Storage (CCS) is regarded as the key to maintaining the viability of fossil fuel utilisation into the future. In Australia there are CCS projects in development, which when deployed at full scale CCS is deployed in Australia, will require an associated CO_2 pipeline infrastructure.

Currently, CO_2 pipelines are most extensively developed in the USA, where CO_2 has been used for enhanced oil recovery for over 40 years. Recently, additional infrastructure has been added to transport CO_2 captured from power stations in the USA and Canada. In other parts of the world, CO_2 pipeline infrastructure is much more limited, although a number of CCS projects are under way.

CO_2 is a gas that is heavier than air at ambient conditions. For CCS applications, CO_2 is transported as a dense phase[4] fluid. In this state, small changes in temperature, pressure or impurity concentration can have a large impact on the density of the fluid.

3.2 The need for CO_2 pipelines in Australia

According to the International Energy Agency (IEA), in 2011 energy production contributed to 83% of anthropogenic greenhouse gas emissions (IEA-EP 2013). Figure 3.1 shows a rising trend in global emissions of CO_2 from energy production, reaching approximately 31 gigatonnes in 2011 (IEA-EP 2013). The IPCC has linked the increase in global CO_2 concentrations with global temperature and sea level rise, stating 'limiting climate change will require substantial and sustained reduction in greenhouse gas emissions.' (IPCC 2013).

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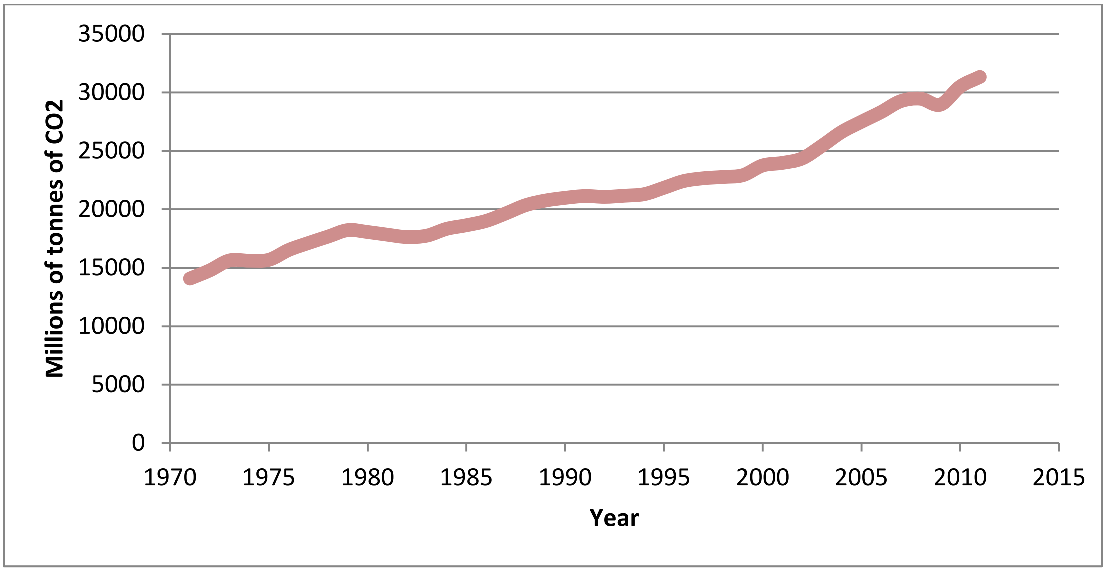
[4] The term ‘dense phase’ is a collective term for CO_2 when it is in either the supercritical or liquid states.

Figure 3.1: Global CO_2 emissions



There are many mechanisms available to reduce greenhouse gas emissions such as:

- reducing energy demand through energy efficiency improvements
- reducing reliance on carbon-intensive fuels, e.g. by switching to nuclear power and renewable energy sources
- reducing the quantity of CO_2 emitted from existing fossil fuel based power production via CCS
- increasing the quantity and efficiency of biological sinks
- reducing non-CO_2 greenhouse gas emissions.

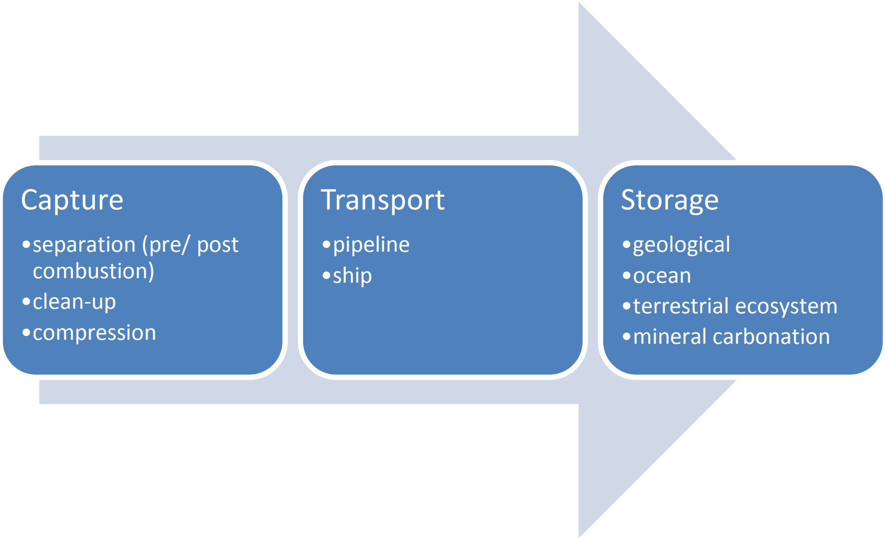
IEA puts forward two key benefits of CCS (IEA 2013):

> *CCS is the only technology available today that has the potential to protect the climate while preserving the value of fossil fuel reserves and existing infrastructure.*
>
> *CCS is currently the only large-scale mitigation option available to make deep reductions in the emissions from industrial sectors such as cement, iron and steel, chemicals and refining.*

CCS is a process consisting of the separation of CO_2 from industrial and energy-related sources, transport to a storage location and long-term isolation from the atmosphere. CCS covers processes used to reduce the quantity of CO_2 emitted to the atmosphere when extracting hydrocarbons, e.g. from the methane purification process, as well as reducing the amount of CO_2 emitted when combusting hydrocarbons, e.g. to generate electricity.

In the context of power generation, the process is described diagrammatically in Figure 3.2. Separation of CO_2 may be done either pre- or post-combustion, usually by chemical absorption. The captured CO_2 is then compressed to a dense phase state and transported by pipeline to a suitable repository. Geological storage, i.e. injection into permeable rock formations, is the main method applied on a commercial scale, however, there is an operating system in The Netherlands that elevates CO_2 levels in commercial greenhouses (OCAP CO_2 v.o.f. 2012).

Figure 3.2: Carbon capture and storage



According to (CO_2CRC 2014), CCS schemes are under way in Australia, focussing on capture technologies, pipeline feasibility and storage options. The location and type of schemes are presented in Figure 3.3.

The largest operational CO_2 pipeline in Australia is currently operated by the Alcoa alumina refinery in Kwinana, Western Australia (WA). The 8 km pipeline transports around 70,000 tonnes of waste CO_2 (>95% purity) per year in gaseous form from the CSBP Kwinana ammonia plant to the Alcoa refinery, where it is used to treat bauxite residue. The 150 mm nominal bore (NB) pipeline has an operating pressure up to 2,000 kPa, and has been in use since 2007[5].

The Otway research project, in Victoria is the first geological CO_2 storage facility in Australia. During Stage 1 of the project, between 2008 and 2011, over 65,000 tonnes of CO_2 from a natural gas well were transported in gaseous form by a 2.25 km pipeline for storage in an onshore depleted gas field[6].

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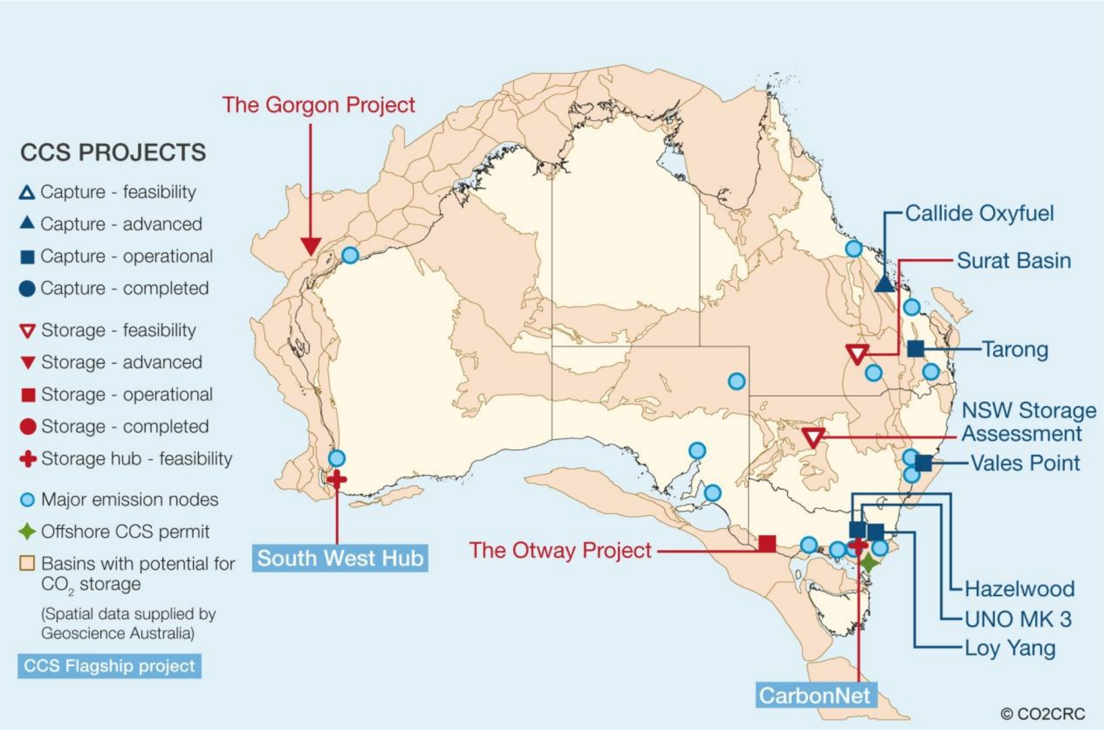
[5] http://www.globalccsinstitute.com/files/project/descriptions/AustraliaAlcoaCarbonationPlant.pdf

[6] http://www.globalccsinstitute.com/files/project/descriptions/AustraliaOtway.pdf

Figure 3.3: CCS in Australia



Chevron’s Gorgon liquefied natural gas (LNG) project will be the first commercial geological CO_2 storage operation in Australia. Due to begin operations in late 2015, the system will use CO_2 extracted during methane purification and re-inject it into a formation 2 km below Barrow Island, WA. The onshore pipeline is 7.3 km in length and 269 – 319 mm in diameter, and will carry 3.4 – 4.0 million tonnes CO_2 per year (Chevron Australia Pty Ltd 2008).

Two other CO_2 storage hubs are currently at the feasibility stage. The CarbonNet Project in Victoria is working to develop common use infrastructure to transport CO_2 from sources (power stations) in the Gippsland region to an offshore geological storage facility[7]. The South West CO_2 Geosequestration Hub in WA is investigating the feasibility of storing CO_2 from industry and power stations in a porous sandstone formation in the onshore Perth Basin[8].

The other CCS systems highlighted in Figure 3.3 represent pilot to demonstration-scale trials of individual elements of a CCS system, including oxyfuel combustion with CO_2 compression as well as trials of post-combustion CO_2 capture technologies. None of these projects require CO_2 transportation pipelines of any significant length.

Large-scale deployment of such CCS technologies in Australia, in response to tightening greenhouse gas regulations, is expected to require a CO_2 transportation

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[7] http://www.energyandresources.vic.gov.au/energy/carbon-capture-and-storage/the-carbonnet-project

[8] http://southwesthub.com.au/

infrastructure of substantially increased size. The scale of such operations may be gauged from the systems that are already in place overseas.

3.3 Overseas infrastructure

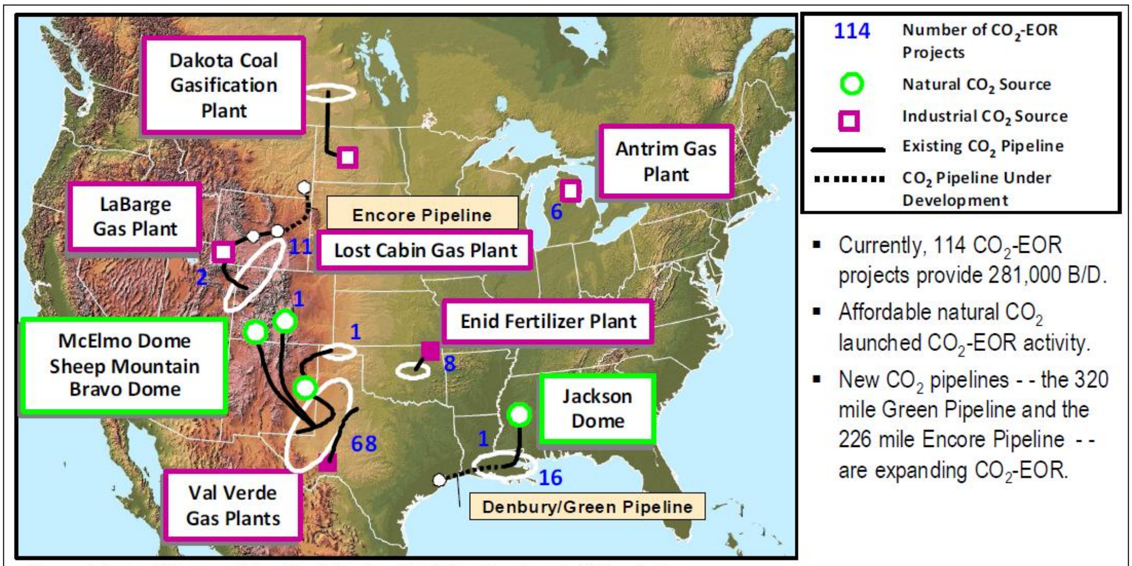
Worldwide, there are currently about 7,200 km of CO_2 pipelines in operation, in North America, Asia, Africa and Europe (Nahas and Mohitpour 2010). The majority are in the USA, which has over 6,500 km of high pressure CO_2 pipelines. There are currently around 50 operational CO_2 pipelines, transporting approximately 68 Mtpa (Global CCS Institute 2014). Almost all of this is related to enhanced oil recovery (EOR) projects.

EOR involves injecting CO_2 into oil reservoirs as they near the end of their working life, to extend oil production. CO_2 injection was first implemented in 1972 in Scurry County, Texas and was then used successfully throughout the Permian Basin in west Texas. In 2010, there were approximately 114 active commercial CO_2 injection projects that together injected over 2 billion cubic feet of CO_2 and produced over 280,000 barrels of oil per day.

Experience over the past 40 years has shown that virtually all of the CO_2 that is injected remains contained in the oil reservoir (Office of Fossil Energy 2014). Consequently, CO_2-EOR is regarded as a suitable storage mechanism for CCS. The economic benefit from enhanced oil production creates a market value for CO_2 used in this manner.

The EOR activity in the USA is summarised in Figure 3.4 (Advanced Resources International Inc 2011).

Figure 3.4: CO_2-EOR activity in the USA



- Currently, 114 CO_2-EOR projects provide 281,000 B/D.
- Affordable natural CO_2 launched CO_2-EOR activity.
- New CO_2 pipelines - - the 320 mile Green Pipeline and the 226 mile Encore Pipeline - - are expanding CO_2-EOR.

Source: Advanced Resources International, Inc., based on Oil and Gas Journal, 2010 and other sources.

Details of some of the main North American CO_2 pipelines used for EOR are shown in Table 3.1, extracted from (Global CCS Institute 2014). A complete listing of CO_2 pipelines in the USA is provided in Appendix C of (Global CCS Institute 2014).

Table 3.1: Main North American EOR CO_2 pipelines

Name of pipeline	Operator	Length (km)	Diameter (mm)	Capacity (Mtpa)
Coffeyville-Burbank	Chaparral Energy	110	200	1.6
TransPetco	TransPetco	177	200	1.6
West Texas	Trinity CO_2	97	300	1.6
Val Verde	Kinder Morgan	134	255	2.1
Weyburn	Dakota Gasification Co.	330	355	2.6
Powder River Basin	Anadarko	201	406	4.3
Canyon Reef Carriers	Kinder Morgan	224	406	4.3
Central Basin	Kinder Morgan	230	406	4.3
Raven Ridge	Chevron	257	406	4.3
Choctaw (NEJD)	Denbury Resources	294	508	7.0
Bravo	Oxy Permian	351	508	7.0
Greencore	Denbury Greencore Pipeline	373	508	14.0
Delta	Denbury Onshore	174	610	11.4
Sheep Mountain	Oxy Permian	656	610	11.4
Green Line I	Denbury Green Pipeline	441	610	18.0
Cortez	Kinder Morgan	808	762	23.6

The majority of the existing CO_2 infrastructure in the USA was built to connect natural CO_2 sources in Colorado and New Mexico to the Permian Basin, where the CO_2 is used for EOR. Over the past 5 years, three new pipelines have been built to transport CO_2 from industrial sources for use in EOR – the Green pipeline in the Gulf Coast, the Greencore pipeline in the Rockies, and the Coffeyville to Burbank pipeline in Kansas (Global CCS Institute 2014).

Development of CCS without the financial benefits of EOR has developed more slowly. The first commercial non-EOR CCS operation in the USA will be the Illinois Industrial CCS Project, which will capture CO_2 from the ADM owned corn-to-ethanol plant in Decatur, Illinois and store it deep underground in a saline reservoir. From November 2011 to January 2015, one million tonnes of CO_2 was successfully captured and stored[9]. Commercial-scale operation (around one million tonnes per annum) is scheduled to begin later in 2015. The length of the CO_2 pipeline involved is only 1.6 km (Gollakota and McDonald 2014).

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[9] http://www.globalccsinstitute.com/project/illinois-industrial-carbon-capture-and-storage-project

In Canada, CO_2 is sourced from the Great Plains Synfuels Plant in North Dakota, and transported via a 330 km pipeline to the Weyburn oil field in Saskatchewan, which has been operating since 2000. This is identified in Figure 3.4 as the 'Dakota Coal Gasification Plant'.

The operator of the Weyburn oil field, Cenovus, has recently constructed the 66 km Rafferty pipeline to transport 1 Mtpa CO_2 for EOR from the SaskPower Boundary Dam power station[10]. Production of CO_2 commenced in October 2014 (IChemE 2014). Excess CO_2 will be transported via a 2 km pipeline for storage in a deep saline aquifer[11].

In Brazil, CO_2-EOR has been carried out by Petrobras since 1987 in the Recôncavo Basin (Bahia) oil fields. In Trinidad, four CO_2-EOR pilot floods were implemented by Petrotrin over the period 1973 to 1990. In Turkey, CO_2-EOR has been used at the Bati Raman field since 1986. CO_2-EOR pilots have apparently been implemented in China, although details are scant (Advanced Resources International Inc 2011).

Overseas infrastructure for purposes other than EOR is limited, and is generally at a small scale. Examples are:

- Snøhvit in Norway, which comprises a 153 km pipeline transporting 0.7 Mtpa of CO_2 from an LNG facility to a deep offshore saline aquifer (IEAGHG 2013).
- OCAP in the Netherlands, which comprises a 97 km pipeline transporting 0.3 Mtpa CO_2 from various sources to approximately 1700 hectares of glass houses (IEAGHG 2013).
- Lacq in France, which comprises a 27 km pipeline transporting 0.06 Mtpa CO_2 from a refinery to a depleted methane reservoir (IEAGHG 2013).
- In Salah, in the southern Saharan Desert in Algeria, which was a demonstration CCS scheme which captured CO_2 from purification of methane (natural gas), transported it for 14 km and captured it in a deep onshore saline aquifer. Injection was carried out from 2004 to 2011 (IEAGHG 2013).

There are currently 22 large-scale CCS projects around the world, representing a total CO_2 capture capacity of 40 Mtpa. Of these, 13 are operational and 9 are under construction. There are a further 14 projects in the Define stage, the most advanced stage of development planning (Global CCS Institute 2014). These include the White Rose and Peterhead CCS projects in the UK, which are two of six demonstration plants that are being supported by the European Commission and certain EU member State governments, with the aim of commercialising CCS by 2020 (Neele et al. 2013).

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[10] www.cenovus.com/operations/oil/docs/rafferty-landowner.pdf

[11] http://www.globalccsinstitute.com/project/boundary-dam-integrated-carbon-capture-and-sequestration-demonstration-project

The COOLTRANS, CO_2PIPETRANS, CO_2PipeHaz and CO_2Quest projects were intended to fill key knowledge gaps and support the development of large-scale CO_2 transportation infrastructure in Europe.

3.4 Typical operating conditions for CO_2 pipelines

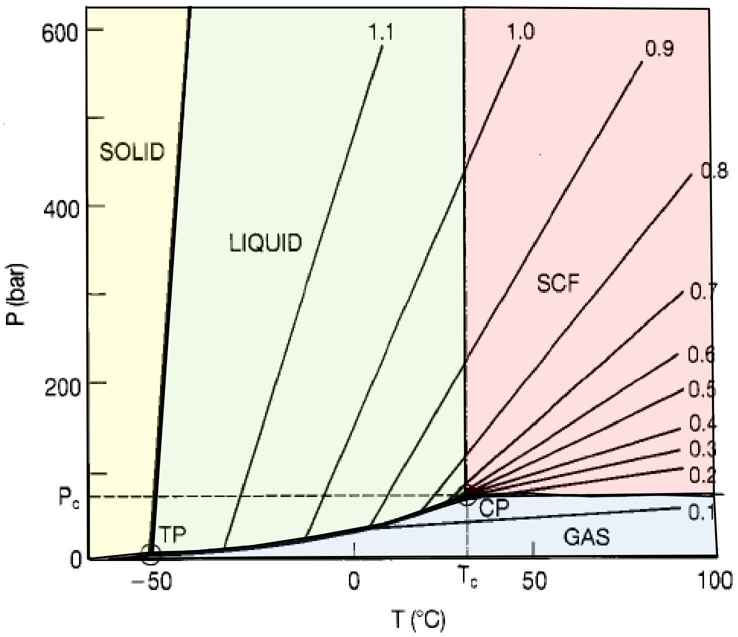
The fundamental physical properties of pure CO_2 are listed in Table 3.2.

Table 3.2: Selected physical properties of pure CO_2 (DNV 2010)

Property	Unit	Value
Molecular Weight	g/mol	44.01
Critical Pressure	bar	73.8
Critical Temperature	ºC	31.1
Triple point pressure	bar	5.18
Triple point temperature	ºC	-56.6
Aqueous solubility at 25°C, 1 bar	g/L	1.45
Gas density at 0°C, 1 bar	kg/ m^3	1.98
Density at critical point	kg/ m^3	467
Liquid density at 0°C, 70 bar	kg/ m^3	995
Sublimation temp, 1 bar	ºC	-79
Latent heat of vaporization (1 bar at sublimation temperature)	kJ/kg	571
Solid density at freezing point	kg/ m^3	1562
Colour	-	None

CO_2 can exist in the gas, liquid, solid (‘dry ice’) and supercritical phases, as shown in Figure 3.5. CO_2 in the supercritical phase has properties of both a gas and a liquid, in that it occupies all available volume, but it can dissolve materials like a liquid. Small changes in temperature or pressure can have a large impact on the state and density of the fluid.

Figure 3.5: Pressure-temperature phase diagram for CO_2 showing lines of constant density (g/cm^3)



Note: SCF= Supercritical Fluid, CP = Critical Point, TP = Triple point.

For economical transport over long distances, CO_2 is usually compressed to a dense single phase – either liquid or SCF. Above 7.4 MPa (74 bar), CO_2 exists as a single dense phase over a wide range of temperatures. A transmission pipeline must be designed to ensure that a single phase is maintained along its entire length. Frictional pressure drop must be taken into account, as well as changes in ambient temperature and elevation. The most widely used operating pressure is between about 7.4 MPa and 21 MPa (Barrie et al. 2004).

As can be seen from the list of CO_2 pipelines in Table 3.1, increasing capacity requires larger diameter pipe. In addition, longer pipelines generally (but not always) tend to be larger diameter. This is because longer pipelines are more expensive, and need to carry larger volumes in order to be economically viable (IEAGHG 2013).

CO_2 pipelines exhibit a broad range of physical characteristics, as shown in Table 3.3.

Table 3.3: Physical characteristics of CO_2 pipelines

	Low	Medium	High
Length (km)	1.9 - 97	116 -380	656 - 808
External diameter (mm)	152 - 270	305 – 508	600 - 921
Wall thickness (mm)	5.2 – 9.5	10 - 13	19 - 27
Capacity (Mtpa)	0.06 - 2	2.6 - 7	10 - 28
Pressure min (MPa)	0.3 – 1.0	3.1 – 3.5	7.2 - 151
Pressure max (MPa)	2.1 – 4.0	9.8 – 14.5	15.1 – 20.0
Initial feed Compressor capacity (MW)	0.2 - 8	15 - 17	43 - 68

This data summarises the results of a survey of 139 CO_2 pipelines in North America (IEAGHG 2013). The wide range of characteristics reflects the inclusion of demonstration projects (typically covering comparatively short distances) as well as commercial EOR projects over long distances.

3.5 The effect of impurities on operating conditions

Depending on the source and technology used for capturing the CO_2 stream, it may contain impurities of various kinds. Indicative compositions of CO_2 streams are presented in Table 3.4 for coal and gas fired power plants using different capture technologies (IPCC 2005). The different techniques for capturing the CO_2 from combustion power plants are commonly characterised as pre-combustion, post combustion, or oxy-fuel processes.

Table 3.4: Indicative composition of carbon dioxide streams

Component	Impurity Concentration, ppmv					
	Coal Fired Power Plant			Gas Fired Power Plant		
	Post	Pre	Oxy-fuel	Post	Pre	Oxy-fuel
Ar/ N_2/ O_2	0.01	0.03-0.6	3.7	0.01	1.3	4.1
H_2S	0	0.01-0.6	0	0	<0.01	0
H_2	0	0.8-2.0	0	0	1	0
SO_2	<0.01	0	0.5	<0.01	0	<0.01
CO	0	0.03-0.4	0	0	0.04	0
NO	<0.01	0	0.01	<0.01	0	<0.01
CH_4+	0	0.01	0	0	2.0	0

Notes: Based on use of coal with a sulphur content of 0.86%, consistent with the typical sulphur content of Victorian Brown Coal (<1%). The concentrations would be directly proportional to the fuel sulphur content. 'Post' and 'Pre' refer to post-combustion and pre-combustion.

Table 3.4 is intended only to indicate the typical impurities that may be present in a CO_2 pipeline, but the concentration data may be regarded as dated. There are currently no widely accepted standards governing the quality of CO_2 for CCS (de Visser et al. 2008). As many as 55 different CO_2 specifications have been identified in the literature (NETL 2013).

The International Organization for Standardization (ISO) is currently working to develop an international standard for the transportation of CO_2 by pipelines. The new standard will consider issues such as the composition and quality of the CO_2 stream and the associated health, safety and environmental issues. It is expected that the new standard will be finalised in 2016-17, and may then become mandatory (Global CCS Institute 2014).

Gaseous impurities present in the CO_2 stream are extremely important for pipeline design and operation, affecting the range of operation, safety considerations, fracture control, cracking, corrosion control, dispersion in the event of a release, fluid density, operating pressure and temperature and the quantity of CO_2 that can be transported (Wetenhall et al. 2014).

The presence of impurities can alter the physical properties of CO_2, including the location of the phase boundaries, density, speed of sound, Joule-Thomson coefficient, viscosity and thermal conductivity. The presence of impurities shifts the boundary of the two-phase region towards higher pressure, so that higher operating pressures are required to keep CO_2 in the supercritical phase. This would have a number of flow-on effects, e.g. on the cost of CO_2 compression and pipeline design for fracture control. Consequently, pipeline design parameters such as materials selection, diameter, wall thickness, inlet pressure, minimum operating pressure and the distance between booster stations may all be affected (Wetenhall et al. 2014).

The CO_2PipeHaz and CO_2Quest projects have involved experimental studies and development of appropriate equation of state models for use in CO_2 pipeline design. This work is currently in progress. The commercial model packages that are available for use in CO_2 pipeline design are discussed in Section 8.9.

From a corrosion perspective, the most important impurity to consider is water. CO_2 will react with water to form carbonic acid, which is highly corrosive to carbon steels. This is discussed further in Section 6.3.1.1.

Recent studies have shown that even small amounts of impurities can significantly increase the saturation pressure of CO_2, making the pipeline more susceptible to fracture propagation and catastrophic, long-running ductile fractures. This issue is discussed further in Section 6.3.1.2.

The potential impact of impurities on the health risks associated with a CO_2 release is discussed in Section 5.5.

4 CO_2 PIPELINE DESIGN IN AUSTRALIA

4.1 Summary

This Chapter provides an overview of the State legislations that regulate the design, construction and operation of onshore pipelines in Australia. A license is generally required for each pipeline, for which the process required is broadly as follows:

- Submitting a pipeline licence application to the regulatory authority. This includes details of the pipeline's design and construction process, the relevant design standards, as well as some form of pipeline safety management study.
- Planning approval, usually including some form of environmental impact assessment, and in some States requiring quantitative analysis of safety risks to the surrounding land-uses from the pipeline.
- Issue of a pipeline licence and associated planning approvals by the relevant regulatory authorities.

Some States mandate conformance with Australian Standard AS 2885 *Pipelines - Gas and liquid petroleum* as a condition for meeting the provisions of the pipeline regulations. Even if AS 2885 is not mandatory, it is common practice in Australia to adopt this standard.

AS 2885 requires a 'safety management study' approach for each pipeline, to identify threats to the pipeline system and apply controls to them, to ensure that residual risk is reduced to an acceptable level. As part of this, the residual risks of identified threats to the pipeline are assessed using a *qualitative* risk matrix analysis. This approach to risk minimisation was developed in Australia and is not used anywhere else in the world.

The design tools and guidance provided in AS 2885 have been developed specifically for methane (natural gas) pipelines. AS 2885 does make allowance for pipelines carrying hazardous materials other than natural gas but the guidance provided is less specific. In 2012 a revision to AS 2885 was issued, recognising that CO_2 pipelines could also be designed according to this Standard. An 'Informative' appendix was added, providing some general information on the properties of CO_2, and highlighting differences in properties and design considerations for CO_2 compared to methane pipelines. However, it noted that:

> *Methods and quantitative prediction of the behaviour of* CO_2 *released from a pipeline are limited and subject to current research. The best available methods shall be used, and estimates and judgements made where necessary. Engineers designing* CO_2 *pipelines shall keep up to date with research in this area as knowledge is expected to evolve rapidly.*

For fluids other than methane, AS 2885 requires that the fundamental principles of the Standard be used to develop alternatives that meet the safety objectives. In such cases, a ‘gap analysis’ is required to identify the differences between the proposed fluid and those of gas and liquid petroleum products.

This Chapter reviews the information needed to undertake a safety management study for a CO_2 pipeline. Analysis of the risk ranking of potential failure events and selection of suitable control measures involves consideration of the following:

- Measurement length – the distance to safety in the event of a catastrophic pipeline failure.
- Location class – a reflection of the population density and the associated risk of multiple fatalities in the event of a loss of containment.
- Isolation valve spacing – which sets a limit on the maximum volume of gas released.
- Maximum discharge rate – which must be limited in particularly sensitive areas.
- Depressurisation – both unintended accidental release and planned release during scheduled system blowdown
- Additional risk mitigation measures
- Emergency response planning.

For many of these areas, the guidance provided in AS 2885 cannot be directly applied to CO_2 pipelines. The differences arise because of the differences in physical properties and health hazards of CO_2 and methane, differences in the consequences of a pipeline failure event, and differences in the dispersion behaviour of a released gas cloud.

This Chapter will identify the knowledge gaps relating to application of AS 2885 to CO_2 pipelines, while the following chapters will review the current state of the art in CO_2 dispersion modelling and provide guidance on appropriate tools for use in the design of CO_2 pipelines in Australia.

This Chapter will also review the state of the art in *quantitative* risk assessment of CO_2 pipelines, which may also be required to meet regulatory requirements for land-use planning in some States in Australia.

4.2 Regulations

The regulatory regimes governing CO_2 pipeline infrastructure in Europe and North America are summarised in (IEAGHG 2013).

In Australia onshore pipelines are regulated under State legislation as summarised in Table 4.1. A pipeline generally requires a licence, although there are some exceptions under the various State regulations.

Some states also identify AS 2885 as a mandatory standard that must be applied to meet the provisions of the pipeline regulations, but even if AS 2885 is not mandatory, it is common practice in Australia to adopt this standard.

Table 4.1: Summary of Australian pipeline regulations

State	Relevant Legislation	CO_2 included	Requires AS 2885 - management	Requires AS 2885 - design	Additional analysis requirements
NSW	Pipelines Act 1967/ Regulation 2013	Yes - as part of a mixture with hydrocarbons (Section 3)	11. Yes - all. A licensee must implement a pipeline management system that relates to the pipeline operated under the licence and is in accordance with the relevant provisions of AS 2885.	10. A licensee must ensure that the design, construction, operation and maintenance of any pipeline operated under the licence are in accordance with the relevant provisions of: (a) in the case of pipelines for high-pressure gas and liquid petroleum—AS 2885, or (b) in any other case—AS 2885 or a standard in respect of which an approval is in force under this clause in relation to the licensee concerned.	Normally a Development Application including a high pressure pipeline would be determined to be 'potentially hazardous and thus require a Preliminary Hazard Analysis. This would normally require a quantitative risk assessment to be developed for the pipeline in order to compare the risk against quantitative criteria.(NSW-DPE 2011).
Vic	Pipelines Act 2005 / Regulation 2011	Yes - included in the definition for petroleum (Section 7)	Partially - Safety Management Plans are covered under specific requirements in Part 6 of the Regulation. Regulation 34 requires construction and operation safety plans in accordance with AS 2885.1 and AS 2885.3 respectively.	No references to AS 2885 requirements for the pipeline design in the Act or Regulations.	Vic may require a quantitative risk assessment to determine the risk levels for comparison with risk criteria relevant to the nature of the development. For example a QRA was conducted for Tarrone Power Station in Vic; a gas pipeline was included in the scope.(Nilsson 2011b)

State	Relevant Legislation	CO_2 included	Requires AS 2885 - management	Requires AS 2885 - design	Additional analysis requirements
SA	Petroleum and Geothermal Energy Act/ Regulations 2013	CO_2 is included as a regulated substance (Section 11).	Yes	Yes 29—Pipelines and flowlines Unless otherwise approved by the Minister, the design, manufacture, construction, operation, maintenance, testing and abandonment of pipelines and flowlines must be carried out in accordance with the relevant requirements of AS 2885 Pipelines—Gas and Liquid Petroleum as in force from time to time.	No requirements found
Qld	Petroleum and Gas (Production and Safety) Act 2004/ Regulations 2004	Regulation Clause 5(3) states that *for Section 10(1)(e) of the Act, carbon dioxide is prescribed to be petroleum.*	Yes (for transmission pipelines only)	Regulation Schedule 1 and 2 Mandatory only for transmission pipelines; preferred for steel pipelines transporting 'petroleum'. CO_2 is defined as 'petroleum', but may not meet the definition of a transmission pipeline, i.e. *a pipeline operated, or to be operated, for the primary purpose of conveying petroleum directly to a market after it has been processed, whether or not it is subsequently processed or reprocessed.*	Normally a Development Application including a high pressure pipeline would be determined to be 'potentially hazardous and thus require a Preliminary Hazard Analysis. This would normally require a quantitative risk assessment to be developed for the pipeline in order to compare the risk against quantitative criteria.(QLD-DOJ 2014)

State	**Relevant Legislation**	**CO_2 included**	**Requires AS 2885 - management**	**Requires AS 2885 - design**	**Additional analysis requirements**
WA	Petroleum Pipelines Act 1969	In Pipeline Act CO_2 is identified as part of a mixture with hydrocarbons (Section 4.1.c) In Western Australia, the Barrow Island Act 2003 (WA) integrates ' CO_2' into the definition of 'petroleum' under the Petroleum Pipelines Act 1969 (WA).	No requirements found.	No requirements found.	WA has objectives for management of risk, generally requiring a quantitative risk assessment to determine the risk levels for comparison with the EPA risk criteria relevant to the nature of the development. This has been applied to gas pipelines and is described in Planning Bulletin 87.(WAPC 2007).

4.3 Australian standard AS 2885 - *'Pipelines - gas and liquid petroleum'*

The AS 2885 series of Standards establishes requirements for the safe design, construction, inspection, testing, operation and maintenance of a land or a submarine pipeline. AS 2885 comprises the following:

- AS 2885.0 General Requirements
- AS 2885.1 Design and Construction
- AS 2885.2 Welding
- AS 2885.3 Operation and Maintenance
- AS 2885.5 Pipelines - Gas and liquid petroleum - Field pressure testing.

AS 2885.0 sets out the fundamental principles, and AS 2885.1, AS 2885.2, AS 2885.3 and AS 2885.5 provide practical rules and guidelines. Where the Standards do not provide detailed requirements appropriate to a specific issue, an engineering assessment based on the guidelines in AS 2885:1-3 can be made.

New pipelines built to carry CO_2 in Australia would be regulated under the relevant location pipeline regulatory instrument. Since AS 2885 is the Australian Standard applicable to gas and petroleum pipelines, it may be expected that any new CO_2 pipeline will be designed and constructed in accordance with AS 2885.

4.4 AS 2885.1 Guidance for CO_2 pipelines

The key issue being addressed in this report is that CO_2 is a very different kind of gas than those specifically treated in AS 2885. The Standard is most directly applicable to pipelines carrying flammable gas, especially natural gas (methane).

The key issue being addressed in this report is that CO_2 is a very different kind of gas compared with that normally considered in AS 2885. The Standard is normally used for pipelines carrying flammable gases and liquids, especially natural gas (methane). The consequence of loss of containment considered is therefore normally a fire. CO_2 has very different properties, as it is not flammable and thus has different safety considerations.

Chapter 6 of this report provides a comparison between natural gas and CO_2 pipelines, highlighting the similarities and differences.

AS 2885 does make allowance for pipelines carrying hazardous materials other than natural gas[12], but the guidance provided is less specific. It requires that the fundamental principles of the Standard be used to develop alternatives that meet the safety objective of the Standard. In such cases, a gap analysis is required to identify the differences between the proposed fluid and those of gas and liquid petroleum

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[12] AS 2885.1 – 2012 Section 1.3

products. Appropriate activities would then be conducted to address those differences, including undertaking a safety management study.

A revision to AS 2885.1 was issued in 2012, which included guidance for design of CO_2 pipelines is in the form of an 'Informative' appendix (Appendix BB), which provides some general information on the properties of CO_2, and highlights differences in properties and design considerations for CO_2 compared to methane pipelines. It provides guidance on how the unique properties of CO_2 may impact on aspects of pipeline design, including the effects of contaminant gases, materials selection, temperature effects and fracture control.

Being ‘Informative’, though, the guidance provided in Appendix BB is not mandatory but should be reviewed in light of any better information. Appendix BB was written at a time when research into CO_2 pipeline design was intensifying in Europe and the UK. Reflecting the evolving state of knowledge, Appendix BB states that:

- *The specific behaviour and effects of released* CO_2 *shall be considered in the safety management study for a* CO_2 *pipeline.*
- *Methods and quantitative prediction of the behaviour of* CO_2 *released from a pipeline are limited and subject to current research. The best available methods shall be used, and estimates and judgements made where necessary. Engineers designing* CO_2 *pipelines shall keep up to date with research in this area as knowledge is expected to evolve rapidly*[13]*.*

The present report is intended to provide an update on the outcomes of relevant research in the intervening years, to assist in preparation of a gap analysis and to provide guidance on the best available methods for engineers to use.

4.5 Approach to risk minimisation in AS 2885.1

AS 2885.1 adopts the ‘safety management study’ approach to risk minimisation. The safety management study is based on a cause-and-control model of risk management, in which potential causes of pipeline failure is identified and then targeted measures are implemented to control each individual threat (Tuft et al. 2012).

A safety management study must be employed at various stages throughout the entire life of the pipeline. AS 2885.1 specifies that, as a minimum, a safety management study shall be undertaken during the following stages:

- Preliminary design and approval
- Detailed design
- Pre-construction review
- Pre-commissioning review.

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[13] AS 2885.1 – 2012 Appendix BB2.1 & BB2.2

The pipeline safety management process consists of the following steps[14]:

(a) Threat identification

(b) Application of physical, procedural and design measures to identified threats

(c) Review and control of failure threats

(d) Assessment of residual risk from failure threats.

Potential risks are assessed using a qualitative method, in which the frequency and severity of failure are estimated on the basis of informed judgement. In contrast, quantitative risk assessment requires these parameters to be quantified on the basis of statistical data. This approach used in AS 2885.1 is intended to be straightforward and user-friendly, requiring minimal specialist input (Tuft et al. 2012).

AS 2885.1 requires that the hazards associated with all potential risks be reduced to As Low As Reasonably Practicable (ALARP). ALARP is achieved when the cost of further risk reduction measures is grossly disproportionate to the benefit gained from the reduced risk that would result[15].

The majority of published risk assessment studies for CO_2 pipelines have used a quantitative, not qualitative, risk assessment methodology (e.g. (Hooper et al. 2005) (Energy Institute 2010b)). Consequently, it can be difficult to see how the findings can be applied in the Australian context.

Therefore, one of the objectives of this report is to present the latest research outcomes in a way that can be readily applied to CO_2 pipeline design according to AS 2885.1.

4.6 Qualitative risk assessment for application to CO_2 pipelines

The procedure for undertaking a qualitative risk assessment is specified in Appendix F of AS 2885.1. For each potential pipeline failure event that is identified, the severity of the consequences (Trivial through to Catastrophic) must be assessed and a frequency of occurrence (Remote through to Frequent) must be assigned.

This information is used to generate a risk score (as shown in Figure 4.1), to determine the risk ranking of each failure event. The risk is acceptable if it has been reduced to low or negligible levels. Intermediate risks must be shown to be reduced to ALARP. High or extreme risks are unacceptable.

AS 2885.1 recognises that the safety risks associated with a pipeline failure are dependent on the population density in the affected area. For example, the safety consequences will be lower in sparsely populated areas. Therefore, the pipeline

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[14] AS 2885.1 – 2012 Section 2.3.1

[15] AS 2885.1 – 2012 Appendix F

route must be analysed to divide it into safety management sections where the land use and population density are consistent[16].

Analysis of the risk ranking of potential failure events and selection of suitable control measures involves consideration of the following:

- Measurement length – the distance to safety in the event of a catastrophic pipeline failure.
- Location class – a reflection of the population density and the associated risk of multiple fatalities in the event of a loss of containment.
- Isolation valve spacing – which sets a limit on the maximum volume of gas released.
- Maximum discharge rate – which must be limited in particularly sensitive areas.
- Depressurisation – both unintended accidental release and planned release during scheduled system blowdown.
- Additional risk mitigation measures
- Emergency response planning.

AS 2885.1 provides guidance on each of these topics, with specific design tools to assist in determining the severity of consequences for a natural gas pipeline failure:

- Threshold levels of harm are defined on the basis of exposure to radiant energy from a burning gas fireball, i.e. injury (4.7 kW/m^2) and fatality (12.6 kW/m^2). These may be mapped on to the risk matrix severity categories as 'severe', 'major' or 'catastrophic'.
- Appendix Y provides guidance on the potential level of harm that may be expected as a function of distance from a ruptured pipeline, based on the typical range of natural gas operating conditions.

However, the guidance provided for CO_2 pipelines is much less specific. The following sections give consideration to the design issues listed above and highlight the knowledge gaps that need to be filled.

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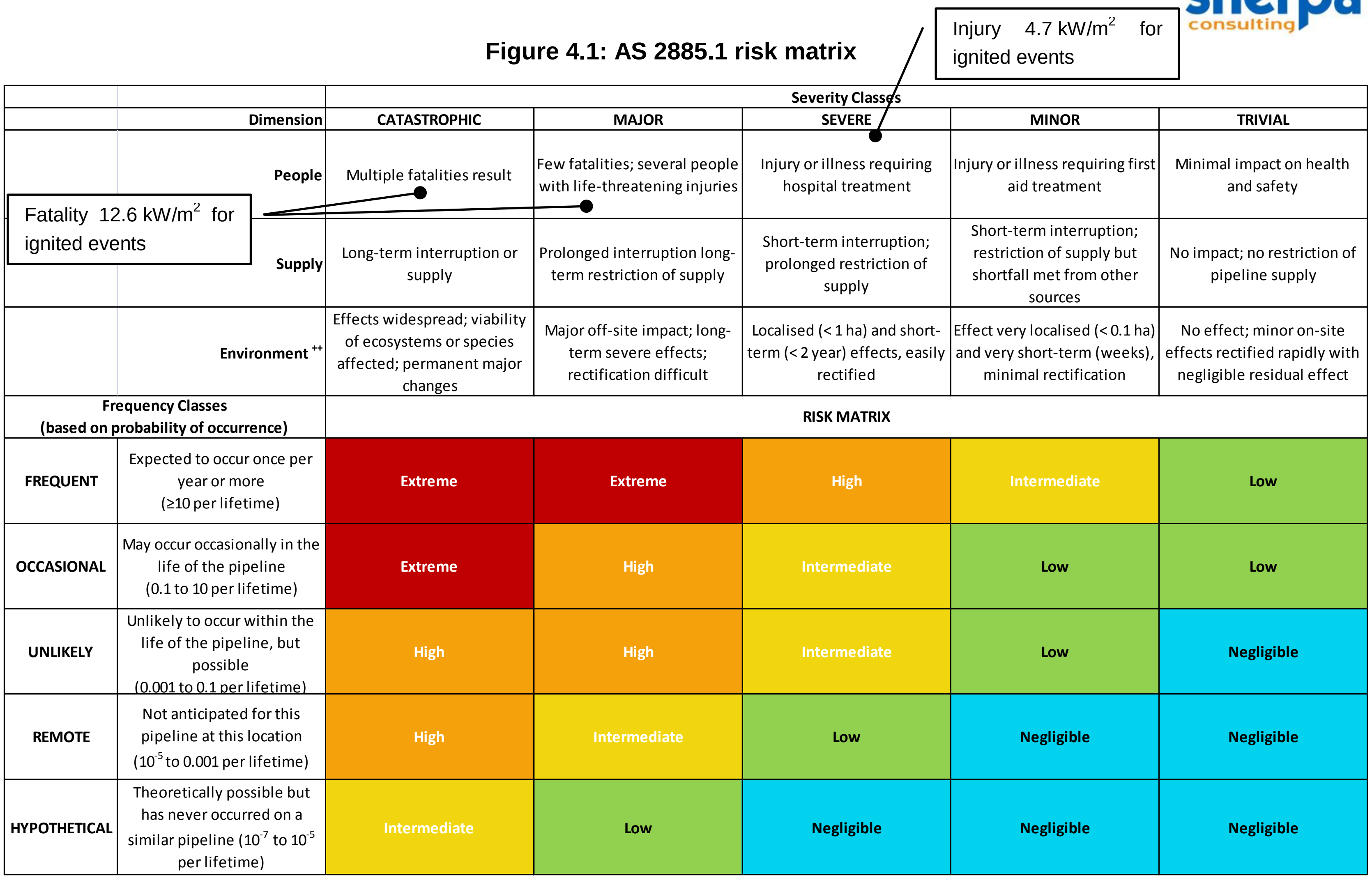
[16] AS 2885.1 – 2012 Section 2.3.2.2

Figure 4.1: AS 2885.1 risk matrix



Injury 4.7 kW/m^2 for ignited events

Fatality 12.6 kW/m^2 for ignited events

		Severity Classes				
	Dimension	CATASTROPHIC	MAJOR	SEVERE	MINOR	TRIVIAL
	People	Multiple fatalities result	Few fatalities; several people with life-threatening injuries	Injury or illness requiring hospital treatment	Injury or illness requiring first aid treatment	Minimal impact on health and safety
	Supply	Long-term interruption or supply	Prolonged interruption long-term restriction of supply	Short-term interruption; prolonged restriction of supply	Short-term interruption; restriction of supply but shortfall met from other sources	No impact; no restriction of pipeline supply
	Environment^{++}	Effects widespread; viability of ecosystems or species affected; permanent major changes	Major off-site impact; long-term severe effects; rectification difficult	Localised (< 1 ha) and short-term (< 2 year) effects, easily rectified	Effect very localised (< 0.1 ha) and very short-term (weeks), minimal rectification	No effect; minor on-site effects rectified rapidly with negligible residual effect
Frequency Classes (based on probability of occurrence)		RISK MATRIX				
FREQUENT	Expected to occur once per year or more (≥10 per lifetime)	Extreme	Extreme	High	Intermediate	Low
OCCASIONAL	May occur occasionally in the life of the pipeline (0.1 to 10 per lifetime)	Extreme	High	Intermediate	Low	Low
UNLIKELY	Unlikely to occur within the life of the pipeline, but possible (0.001 to 0.1 per lifetime)	High	High	Intermediate	Low	Negligible
REMOTE	Not anticipated for this pipeline at this location (10^{-5} to 0.001 per lifetime)	High	Intermediate	Low	Negligible	Negligible
HYPOTHETICAL	Theoretically possible but has never occurred on a similar pipeline (10^{-7} to 10^{-5} per lifetime)	Intermediate	Low	Negligible	Negligible	Negligible

4.6.1 Measurement length

AS 2885.1 defines a distance on either side of the pipeline, known as the ‘measurement length’, which denotes the demarcation boundary of the safety management study.

AS 2885.1 defines the measurement length specifically for natural gas pipelines, as the radius of the 4.7 kW/m^2 radiation contour in the event of a full bore rupture from a pipeline containing methane. This is effectively an estimate of the distance from the pipeline within which a person in the vicinity would be at risk of 'injury' in the event of a catastrophic pipeline failure.

This definition of measurement length is not directly applicable to CO_2 pipelines. Strictly speaking, in order to apply the AS 2885.1 approach, it would be necessary to establish an appropriate parameter to quantify human injury from CO_2 exposure, and to undertake detailed CO_2 dispersion modelling calculations. Chapter 5 of this report provides information on the human health effects of CO_2 concentration and exposure time, and provides guidance on appropriate exposure limits. Chapter 8 describes the dense gas dispersion models that may be regarded as suitable for use.

However, the British Health and Safety Laboratory (HSL) has already undertaken a direct comparison of the risks associated with methane and CO_2 pipelines, using a quantitative risk assessment approach. PHAST (commercial consequence modelling software) and TPRAM (HSE land-use planning software) were used to perform dispersion and risk modelling respectively for a CO_2 release. MISHAP (HSE land-use planning software) was used to obtain the associated risks for methane with similar inputs to the CO_2 modelling. It was concluded that distances to equivalent levels of risk are roughly comparable between CO_2 and natural gas for the same pressure, temperature and hole size (McGillivray and Wilday 2009).

Appendix BB of AS 2885.1 provides the following guidance for CO_2 pipelines:

> *Until further research on dispersion of* CO_2 *releases is completed, the measurement length for definition of the location class limits shall be estimated on the basis that the pipeline is transporting natural gas (see Clause 4.3.2 and Appendix Y).*

Thus, the Appendix BB recommendation for estimation of measurement length is consistent with the conclusions of the HSL study. In the absence of any other studies providing evidence to the contrary, it is recommended that it is appropriate to estimate the measurement length on the basis that the pipeline is transporting natural gas.

Appendix BB continues:

> *However the measurement length shall be extended locally wherever the landform suggests that spread of the gas cloud in a particular direction may be promoted by gravity drainage.*

This statement is misleading because:

a) It implies that the measurement length is strongly dependent on the topography. This is discussed in detail in Section 8.8, where it is shown that the flow of a cold, dense gas cloud is more strongly dependent on the volume and concentration of the release, and the local wind speed and direction. Topography has a relatively minor influence on the dispersion pattern, except under specific circumstances. Section 8.8 also discusses the modelling approaches that can be used to account for terrain effects.

b) It implies that it may be necessary to extend the measurement length in any situation where there is a 'possibility' that the flow might be promoted by gravity drainage, and yet no guidance is provided on how this might be accomplished. Guidance for determining whether or not this is necessary is provided in Section 8.8.

4.6.2 Location class

The pipeline designer is required to consider the risks to people, property and the environment within the 'measurement length' on either side of the pipeline, along its entire length. This is done by allocation of one or more primary ‘location class(es)’ that reflect the predominant land use in the broad area traversed by the pipeline, accounting for population density and the associated risk of multiple fatalities in the event of a loss of containment. Primary location classes are defined as ‘Rural’, ‘Rural Residential’, ‘Residential’ or ‘High Density’.[17]

Within the primary location class, it may be appropriate to allocate one or more secondary location classes, to reflect special land use at certain locations along the route. Secondary location classes may include ‘Industrial’, ‘Heavy Industrial’, ‘Common Infrastructure Corridor’, ‘Submerged’ and ‘Sensitive Use’ (where the societal risk associated with a loss of containment is the dominant consideration (e.g. schools, hospitals, aged care facilities, prisons) and areas of high environmental sensitivity to pipeline failure).[18]

The procedure for determination of location class for CO_2 pipelines is the same as that for natural gas pipelines.

The initial safety management study must then identify any high consequence events that impose major risks to the project, community and environment, and their proposed controls[19]. Potential risks include typical threats in typical locations, as well as location-specific threats, particularly in high consequence areas.

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[17] AS 2885.1 – 2012 Section 4.3.4

[18] AS 2885.1 – 2012 Section 4.3.5

[19] AS 2885.1 – 2012 Appendix B2.1.1

AS 2885.1 does not provide any guidance on how the potential consequences of major risks are to be assessed, or on how the effectiveness of potential risk mitigation measures are to be established.

For CO_2 pipelines, it is necessary to characterise both the nature of the initial release (the 'source term') and the subsequent dispersion behaviour. Guidance on appropriate source terms is provided in Chapter 7, while 'fit for purpose' dispersion modelling techniques are discussed in Chapter 8.

4.7 Isolation valve spacing

Part of the detailed design work will involve selecting suitable spacing and location of pipeline isolation valves. Valves are required to isolate the pipeline in segments for maintenance, operation, repair and for the protection of the environment and the public in the event of loss of pipeline integrity. AS 2885.1 provides nominal guidance on the spacing of valves, but the final selection must be based on a consideration of the consequences of fluid release, and must be approved by the regulator.

The graphical design tools provided in AS 2885.1 for estimating the measurement length are based on an assumed mainline isolation valve spacing distance in a methane pipeline of 50 km. However, this spacing distance is only appropriate for Rural locations with a low population density. In 'Rural Residential', 'Residential' and 'High Density' locations, spacing distances down to 15 km are recommended, but the basis for the final design selection must be approved by the regulator.

Selection of appropriate isolation valve locations and spacing for a CO_2 pipeline will require detailed analysis of the volume contained between the isolation points and the consequences of CO_2 release. The distance between isolation valves will vary along the pipeline route, depending on the location class of each segment. An analysis of the worldwide CO_2 pipeline infrastructure found that the distance between isolation valves typically varies between 10 to 20 km (IEAGHG 2013).

Selection of isolation valve spacing will involve a trade-off between the cost to install and maintain the valves on the one hand, and the consequences of pipeline failure on the other. A method to solve this optimisation problem was presented by (Brown et al. 2014), for a pipeline of 610 mm diameter carrying supercritical CO_2 at 150 bar initial gauge pressure. The area covered by the 7% CO_2 concentration was used to parameterise the hazard associated with a full bore pipeline failure. The cost of the valves decreased hyperbolically for spacings between 5 km and 40 km. The hazard area was very low at the 5 km spacing, and increased linearly to about 25 km. It then fell off slightly and remained fairly constant between 30 to 40 km. The optimum range was found to occur at valve spacings between 10 to 20 km, which is consistent with current practice.

Atmospheric dispersion models are used to calculate a maximum safe volume of CO_2 that could be released in the event of either accidental or controlled discharge

(IEAGHG 2013). Guidance on appropriate source terms is provided in Chapter 7, while ‘fit for purpose’ dispersion modelling techniques are discussed in Chapter 8.

4.8 Restriction of maximum discharge in high consequence areas

AS 2885.1 specifies that the energy release rate of volatile, flammable fluids must be limited in high consequence locations. The limits are:

- no more than 10 GJ/s in ‘Residential’ and ‘Industrial’ locations or
- no more than 1 GJ/s in ‘High Density’ and ‘Sensitive’ locations.[20]

For pipelines carrying other combustible fluids, the Standard states only that 'the maximum allowable discharge rate shall be determined by the safety management study specified in this Standard'.

For a pipeline carrying CO_2, Appendix BB offers the following guidance:

> *Where the pipeline must pass through or near populated areas, the pipeline design shall limit the release rate to the maximum that can be tolerated should a sustained release occur. Specific limits for maximum release rate (Clause 4.7.3) shall be developed as part of the design basis and considered in the safety management study.*

AS 2885.1 specifies that in ‘Residential’, ‘High Density’, ‘Industrial’ and ‘Sensitive’ location classes, the pipeline shall be designed such that rupture is not a credible failure mode.[21] Thus, in these location classes, the pipeline must be designed to ensure that the discharge rate of CO_2 is limited to a safe maximum in the event of continuous release from the largest credible *equivalent defect length produced by the threats identified in that location*.[22]

For determination of the radiation contour corresponding to a particular discharge rate, in the case of natural gas AS 2885.1 specifies that the fluid flow rate be calculated as

> *the quasi-steady state 30 seconds after the initiating event, determined by a suitable unsteady state hydraulic analysis model, and the relevant equivalent hole size. The calculation shall assume that the pipeline is at Maximum Allowable Operating Pressure (MAOP) at the time of gas release*. [23]

The current recommended guidance for CO_2 pipelines

> *is to approximate (in a suitable modelling software package) the time-varying flowrate from the long pipeline with the average release rate over 20 seconds. This gives what is believed to be a conservative set of results. Where more accurate and less conservative results are required, and there is a rapid variation in the release rate of*

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[20] AS 2885.1 – 2012 Section 4.7.3

[21] AS 2885.1 – 2012 Section 4.7.2

[22] Ibid.

[23] AS 2885.1 – 2012 Section 4.10

> *carbon dioxide, then the more rigorous time varying along-wind-diffusion method should be used.* (Energy Institute 2010b).

For consequence analysis of CO_2 pipelines in accordance with AS 2885.1, the choice of whether to use a release rate averaged over the first 20 or 30 seconds of release is somewhat arbitrary. There is likely to be little practical difference between the two values, so either method would seem to be appropriate.

In high consequence locations, AS 2885.1 requires that the penetration resistance of the pipeline be increased to limit maximum size of a puncture hole in the event of accidental damage. It regards the most likely mode of accidental damage to be puncture by the tines of heavy excavation equipment during maintenance operations. Appendix M of the AS 2885.1 provides a method for calculating the equivalent diameter of likely puncture holes, as a function of pipe thickness, for typical bucket excavators ranging from 5 to 55 tonnes. This method has been validated experimentally for pipes with thickness up to 12.5 mm and external diameter up to 355 mm (Brooker 2003) (Brooker 2005).

Chapter 7 provides additional information on historical natural gas pipeline puncture data, to help inform safety management studies for new CO_2 pipelines.

For CO_2 pipelines in high consequence locations, atmospheric dispersion modelling is required to calculate the maximum allowable discharge rate to prevent injury in the event of an accidental puncture. With a fixed MAOP, the main variable is the pipe thickness. The maximum allowable discharge rate must be calculated with the use of an appropriate dense gas dispersion model, as part of the safety management study, to the satisfaction of the regulator.

Guidance on appropriate source terms is provided in Chapter 7, while ‘fit for purpose’ dispersion modelling techniques are discussed in Chapter 8.

4.8.1 Pipeline venting

In addition to accidental gas releases, AS 2885.1 also requires consideration of threats that arise during the course of normal pipeline operations. For CO_2 pipelines, this would include venting or blowdown of sections for maintenance purposes. Design of blowdown facilities for CO_2 pipelines should consider aspects that facilitate safe dispersion, such as discharge at a safe location, height, discharge velocity and concentration. This is discussed in detail in Section 7.3.1.2.

(DNV 2010) provides guidelines for the design of vent stations, which require the use of dispersion simulations and a suitable model for pipeline decompression. Guidance on models that are suitable for use in this application is provided in Chapter 8.

4.8.2 Additional risk mitigation measures

AS 2885.1 requires that the pipeline design should include a range of different measures to mitigate the risk of pipeline damage and improve operational safety, including[24]:

- Additional wall thickness may be required to provide protection against damage by external interference and for resistance to other load conditions and failure mechanisms or to provide allowance for loss of wall thickness due to corrosion, erosion or other causes.
- The pipelines shall be protected against corrosion and external interference. For example, by:
  - Both active and passive corrosion protection;
  - Separation by burial and other physical barriers;
  - Separation by exclusion; and
  - Procedural controls.
- The pipeline shall be designed to be pressure-tested to verify that it is leak tight and has the required strength.
- A pipeline may be telescoped where the design pressure decreases progressively along the pipeline and a suitable pressure control is provided.
- The pipeline should be designed so that its integrity can be monitored by the use of internal testing devices without taking the pipeline out of service.

In addition to these general measures, accumulated international experience in the operation of CO_2 pipelines has produced good practice guidelines for CO_2-specific risk mitigation strategies. These are reviewed in Chapter 9.

4.8.3 Emergency response planning

AS 2885.1 requires that CO_2 pipeline operators will develop an emergency response plan, to ensure an effective response in the event of any unplanned release of CO_2[25]. Modelling software is often used as an emergency response planning tool, for use in desktop simulations of potential incidents and response planning [26].

In such applications, the modelling software is required to be user-friendly and provide quick answers. This potentially creates a different set of ‘fitness for purpose’ criteria than needed for other applications. Guidance on dispersion models suitable for use in emergency response planning for CO_2 pipelines is provided in Chapter 8.

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[24] AS 2885.1 – 2012 Section 5

[25] AS 2885.1 – 2012 Section 5.5.1

[26] AS 2885.3 – 2012 Section 11.2

4.9 Quantitative Risk Assessment for pipelines in Australia

AS 2885.1 recognises that QRA methods may be used under specific circumstances, e.g. to allow comparison of alternative risk mitigation methods, or if required in particular regulatory jurisdictions.

In some cases a planning or approval authority may also require that a quantitative risk assessment is undertaken. This would be an additional requirement and does not eliminate the need for an AS 2885.1 safety management study including the qualitative risk assessment.

In New South Wales (NSW), QRA is often required for development applications identified as being 'potentially hazardous'. A number of pipeline developments have been assessed in this way:

- Natural gas delivery pipeline between Young and Bomen in NSW (Nilsson 2009)
- AGL's proposed Dalton Power Station (Nilsson 2011a)
- Hunter Pipeline (Sherpa 2008).

Queensland has used NSW guidelines, but has recently developed guidelines for use in Queensland (QLD-DOJ 2014). Examples of pipeline developments that used QRA methods are:

- Arrow Energy Bowen Gas Project (Sherpa 2012)
- Santos GLNG Gas Field Development Project (Santos 2014).

As the name suggests, the accuracy of quantitative risk assessment relies on the ability to accurately quantify of all the individual risk factors that are involved in a particular incident. This requires a statistical approach, using data collected from historical records of similar incidents. For CO_2 pipelines, where there has been a very good safety record, there is insufficient data to draw upon, so natural gas pipeline statistics are usually used as a proxy.

(Koornneef et al. 2010) presented a systematic evaluation of the impact of methodological choices and uncertainties in input parameters on the results of QRA for CO_2 pipelines. A sensitivity analysis showed that the existing knowledge gaps and uncertainties have a large effect on the accuracy of the assessed risks.

(Energy Institute 2010b) is a very good reference to consult on QRA for CO_2 pipelines. It provides a helpful explanation of the basics of QRA and illustrative examples for CO_2 using the integral dispersion modelling software, PHAST. This study recognised that the source term data for CO_2 releases was inadequate, and recommended a programme of work to develop improved source terms and improved dispersion models that could manage the solid/vapour transition more effectively.

The EU-funded CO_2PipeHaz project was established to undertake such a research programme. It successfully developed and validated improved predictions of fluid phase, discharge rate and atmospheric dispersion (using CFD modelling) for accidental releases from pressurised CO_2 pipelines (Woolley et al. 2014b).

The CO_2PipeHaz project also developed guidance specifically for use in integral consequence modelling for CO_2 and its use in QRA. This guidance, presented in (McGillivray et al. 2014), includes CO_2 harm criteria, pipeline release scenarios, failure rates, dispersion modelling and risk calculation. The guidance provided in this paper represents the current state of the art in the use of QRA for CO_2 pipelines.

4.10 Conclusions

Onshore gas pipelines in Australia are subject to State regulations, and vary from one jurisdiction to another. Some states also require AS 2885.1 as the mandatory standard to be applied. Even if AS 2885.1 is not mandatory, it is common practice in Australia to adopt this standard. AS 2885.1 requires the use of a safety management study to identify threats to the pipeline system and apply controls to them, using a qualitative risk matrix methodology.

The foregoing sections have identified a number of knowledge gaps which currently make it difficult to design CO_2 pipelines in accordance with AS 2885..1 Issues that need to be resolved are:

- Equivalent levels of harm (i.e. dosage corresponding to injury or fatality) for CO_2 exposures need to be established. This is discussed in Chapter 5.
- The similarities and differences between CO_2 and natural gas pipelines need to be better understood. These are reviewed in Chapter 6.
- Information is needed to establish credible ‘source terms’ for different release scenarios. These are reviewed in Chapter 7.
- Dispersion modelling tools are required at each stage of the safety management study process. The different types of models that are available are reviewed in Chapter 8 with guidance provided on specific models that may be regarded as ‘fit for purpose’.
- International best practice guidelines on additional risk mitigation methods specific to CO_2 pipelines are reviewed in Chapter 9.

In some circumstances, a quantitative risk assessment (QRA) approach may be required to meet regulatory requirements for land-use planning. Recent international research efforts have focussed on developing improved tools for QRA specifically for CO_2 pipelines. The resulting guidance has been published (McGillivray et al. 2014) and may be regarded as the state of the art.

The main emphasis of the remainder of this report, therefore, will be on providing guidance to assist with the design of CO_2 pipelines in accordance with the qualitative risk matrix methodology specified in AS 2885.1.

5 CO_2 HEALTH AND ENVIRONMENTAL EFFECTS

5.1 Summary

CO_2 is a normal product of metabolism in humans and plays a role in control of the body's major vital processes. Elevated concentrations of CO_2 in the air can cause the concentration of CO_2 in the bloodstream to rise, increasing the acidity of the blood and triggering adverse effects on the respiratory, cardiovascular and central nervous systems. This effect is called CO_2 intoxication and, depending on the level of exposure, can produce symptoms ranging from headaches through to death.

The health hazards of CO_2 are well understood, resulting in well defined occupational exposure limits. In Australia, the Short Term Exposure Limit (STEL) in the workplace is 3 vol% CO_2 for 15 minutes over the course of an 8 hour day.

Emergency response criteria, which would be most appropriate for an accidental release from a CO_2 pipeline, are not so well defined. In the United States, Protective Action Criteria (PAC) have been defined, which provide guidelines for emergency planning. In Australia, the only equivalent guidance appears to be the 'Protection Action Decision Guide for Emergency Services in Victoria'. Unlike the PAC, which defines three levels of emergency response, the Australian 'Protective Action Decision Guide' specifies only one conservative level of response, at 3 vol% CO_2 for 15 minutes.

Use of the risk matrix in AS 2885.1 requires a determination of the potential for a release from a pipeline to reach a populated area and cause injury or fatality. The risk matrix requires assigning risks to different 'severity classes', which creates the need for to define CO_2 exposure criteria that define the 'threshold of injury' and 'threshold of fatality'.

AS 2885.1 defines these criteria for methane pipelines in terms of harm resulting from different levels of thermal radiation from a fireball. No equivalent criteria are provided for CO_2 pipelines. To date, there have been no published reports that equate the effects of CO_2 intoxication to the AS 2885.1 severity classes.

It is suggested that the US PAC emergency response criteria, particularly the Temporary Emergency Exposure Limit (TEEL) definitions, can provide useful guidance in this regard.

It is recommended that for AS 2885.1 safety management studies of CO_2 pipelines:

- 'Severe' = threshold of injury = 3 vol% CO_2 (30,000 ppm or 54,000 mg/m^3) for 60 minutes (TEEL-2)
- 'Major' = threshold of fatality = 5 vol % CO_2 (50,000 ppm or 90,000 mg/m^3) for 60 minutes (TEEL-3)
- 'Catastrophic' = 7 vol% CO_2 (70,000 ppm or 126,000 mg/m^3) for 60 minutes

There is currently insufficient data to allow definition of the AS 2885.1 severity classes for CO_2 exposure times of less than 60 minutes. In the context of AS 2885.1, a conservative a CO_2 pipeline design should not consider exposure time, and should instead place limits on exposure concentration.

If land use planning regulations in Australia require the use of QRA for proposed new CO_2 pipelines, it is recommended that the Specified Level of Toxicity (SLOT) and Significant Likelihood of Death (SLOD) values, and the Health and Safety Laboratory (HSL) probit equation (McGillivray and Wilday 2009) be used.

There is currently no reason to expect that the minor level of impurities in a new CO_2 pipeline in Australia will have any significant health implications.

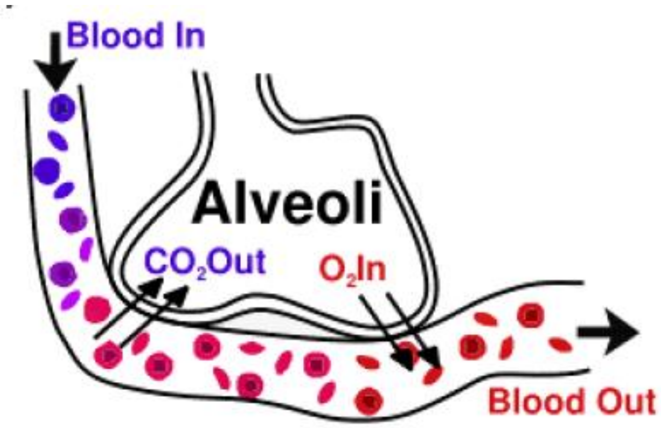
The environmental effects of a CO_2 release have been determined to impact animals in similar ways to humans (DNV 2013), and have small and short term effects on plant life (Lake et al. 2012).

5.2 Health hazards of CO_2

CO_2 is naturally present in air at a concentration of approximately 0.04% by volume (NOAA 2014). It is a normal product of metabolism in human beings and plays a role in control of the human body's major vital processes, including control of breathing, vascular dilation or constriction, and blood pH levels (Harper 2011a).

The concentration of CO_2 in the bloodstream is regulated by gas exchange within tiny air sacs in the lungs, called alveoli. Oxygen from the air diffuses across the alveolar membrane into the blood, and CO_2 from the blood enters the alveoli. The CO_2 is eliminated from the body during exhalation. This process is illustrated in Figure 5.1.

Figure 5.1: Gas exchange in the lungs



If the concentration of CO_2 in the ambient air increases, less CO_2 can diffuse out of the blood and into the alveoli. Higher concentrations of CO_2 in the blood can increase its acidity, triggering adverse effects on the respiratory, cardiovascular and central nervous systems. This effect is called CO_2 intoxication (EIGA 2011).

Depending on the CO_2 concentration inhaled and the exposure duration, toxicological symptoms range from headaches, increased respiratory and heart rate, dizziness, muscle twitching, confusion, unconsciousness, coma and death (Harper 2011a). Table 5.1 describes the effect of increasing concentration of CO_2 according to the US Environmental Protection Agency (US EPA).

Table 5.1: Acute health effects of high concentrations of carbon dioxide

CO_2 Concentration (%)	Time	Effects
17 - 30	Within 1 minute	Loss of controlled and purposeful activity, unconsciousness, convulsions, coma, death
>17	<1 minute	Convulsions, coma, death
>10 - 15	1 minute to several minutes	Dizziness, drowsiness, severe muscle twitching, unconsciousness
7 - 10	1.5 minutes to 1 hour	Headache, increased heart rate, shortness of breath, dizziness, sweating, rapid breathing
6	1 – 2 minutes	Hearing and visual disturbances
	≤ 16 minutes	Headache, dyspnea
	Several hours	Tremors
4 - 5	Within a few minutes	Headache, dizziness, increased blood pressure, uncomfortable dyspnea
3	1 hour	Mild headache, sweating, and dyspnea at rest
2	Several hours	Headache, dyspnea upon mild exertion

Sources: (USEPA 2000), (Langford 2005)

The clinical definition of dyspnea is an uncomfortable awareness of one's breathing effort. It is a normal symptom of heavy exertion but becomes pathological if it occurs in unexpected situations (Shiber and Santana 2006).

Inhaled concentrations of >3% CO_2 will produce distress in exposed individuals, with the effects becoming more marked as the concentration increases. However, if affected individuals are removed from the vicinity and treated with 100% oxygen, most casualties then recover quickly. In severe cases, assisted ventilation may be required. Acid-base disturbances usually correct themselves rapidly and treatment is rarely necessary. Fatalities can be expected at concentrations >17% (Langford 2005).

It is important to note, however, that these concentration-related effects are not universal. Individual tolerances can vary widely, depending on the age, fitness and health status of the person, as well as the temperature and humidity of the air (EIGA 2011).

Note also that CO_2 intoxication is entirely independent of the effects of oxygen deficiency (i.e. asphyxiation). For CO_2 to reduce the oxygen concentration in air down to a level that is immediately dangerous to life, the CO_2 concentration would need to be in the order of 50% v/v (Harper 2011a).

A CO_2 concentration of 9.5% would reduce the concentration of oxygen to 19%. This oxygen concentration is only slightly lower than the normal 21% and is not harmful. However, the high CO_2 concentration would certainly be harmful after a few minutes (EIGA 2011).

In addition to the health risks associated with CO_2 intoxication, a cloud of CO_2 will also be very cold. Release of dense phase CO_2 to atmosphere, whether through a leak or vent, will result in a very high velocity, very low temperature jet of gas and potentially dry ice solids. Anyone exposed to this will suffer cryogenic burns and possibly impact injuries. Inhalation of such cold gas would also cause severe internal injuries (Johnson et al. 2009). Any nearby process equipment and other infrastructure would also be rapidly cooled. Depending on the location, an appropriate emergency management plan may also need to consider the implications of this as well (Connolly and Cusco 2007).

5.3 Occupational exposure standards

Working with, or exposure to CO_2 can be dangerous, particularly in poorly ventilated confined areas. Fatalities have occurred in the holds of ships, in the production of silage, in the sewage industry, during cleaning and maintenance of vats in breweries and wineries, and from the sudden release of CO_2 from fire extinguishers or dry ice sublimation (Langford 2005). Australian Standard AS 2865-1995 *Safe Working in Confined Spaces* details precautions which should be observed in such environments.

Various regulatory authorities have defined occupational exposure standards, which limit the concentration of substances to which workers may be exposed. For CO_2, these are presented in Table 5.2, where it can be seen that long term exposure is allowed at concentrations of 0.5%; shorter term exposure is allowed up to 1.5-3%. The threshold for a substance above which respirators must be worn, known as the concentration Immediately Dangerous to Life and Health (IDLH), is also defined. The IDLH for CO_2 is defined by the US National Institute for Occupational Safety and Health (NIOSH) as 4%.

Table 5.2: CO_2 occupational exposure standards and their uses

Carbon Dioxide Concentration (%)	Criterion	Use	Source
4	IDLH (USA/UK)	Immediately Dangerous To Life And Health (respirators must be worn above this concentration) This level is also used as the concentration from which escape is considered possible in 30 minutes without any escape-impairing or irreversible effects.(HSE 2010b)	(NIOSH 1994)
3	STEL (Australia)	Short Term Exposure Limit (Workplace exposure limit for a short term (15 minute) reference period)	(Safe Work Australia 2011)
3	Offshore Survivability Criterion (UK)	The maximum exposure (dose) that may be received with a negligible statistical probability of fatality and without impairment of an individual's ability to escape (15 minute exposure time)	(HSE 2010a)
1.5	STEL (UK)	Short Term Exposure Limit (Workplace exposure limit for a short term (15 minute) reference period)	(UKHPA 2010)
0.5	NIOSH PEL (USA)	Permissible Exposure Limit. Maximum concentration of a substance to which an employee may be exposed, averaged over an 8 hour 'working day'. Used in the USA.	(NIOSH 1994)
0.5	LTEL (UK)	Long Term Exposure Limit (Workplace exposure limit equivalent to the USA PEL)	(UKHPA 2010)

5.4 Emergency response criteria

Emergency response criteria have been set by various organisations for substances in terms of concentration. The purpose of these criteria is to protect people; specifically members of the public, and the concentrations are usually below the IDLH value (worker escape criterion). The criteria are collectively referred to as Protective Action Criteria (PAC) (US-DOE 2012) and comprise, in order of preference by the US Department of Energy (DOE):

- AEGL (Acute Emergency Guideline Level)

Threshold exposure limits for the general public including susceptible individuals. Three levels (AEGL-1, AEGL-2, AEGL-3) are developed for each of five exposure periods (10 minutes, 30 minutes, 1 hour, 4 hours, and 8 hours) and are distinguished by varying degrees of severity of toxic effects from notable discomfort, irritation (not permanent) to life-threatening adverse health effects or death.

- ERPG (Emergency Response Planning Guideline)

The maximum concentration in air below which it is believed nearly all individuals could be exposed for up to one hour without experiencing effects defined for three levels of severity (ERPG1, ERPG2, ERPG3) ranging from mild transient adverse health effects to life-threatening health effects.

- TEEL (Temporary Emergency Exposure Limit)

The airborne concentration (of a substance) above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience effects defined for three levels of severity (TEEL 1, 2, 3)[27]:

  - **TEEL-1** is the concentration above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic, non-sensory effects. However, these effects are not disabling and are transient and reversible upon cessation of exposure.
  - **TEEL-2** is the concentration above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting, adverse health effects or an impaired ability to escape.
  - **TEEL-3** is the concentration above which it is predicted that the general population, including susceptible individuals, could experience life-threatening adverse health effects or death.

AEGLs and ERPGs are not available for CO_2 (US-DOE 2012). TEELs for CO_2 are shown in Table 5.3.

Table 5.3: CO_2 Temporary Emergency Exposure Limits

Material	TEEL-1	TEEL-2	TEEL-3	unit
Carbon dioxide	3	3	5	%

In Australia, the only guidance found is in the Protection Action Decision Guide for Emergency Services in Victoria (MFESBoard 2012), which provides information to emergency planners on Best Practice principles for community protective actions during potential airborne hazards caused by industrial or transport accidents. This document recognises that Occupational Exposure Standards, which were developed to protect workers over an 8 hour day, *do not provide protection for the general public, particularly the sensitive population, including infants, the elderly and people with respiratory diseases.*

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[27] http://www.atlintl.com/doe/teels/teel/teeldef.html

The Protective Action Decision Guide uses a hierarchy-based method for selecting air quality reference values that are appropriate for protecting the public from short-term exposure to chemicals in air. These values follow three exposure levels: the Acute Exposure Guideline Levels (AEGL's), the Emergency Response Planning Guidelines (ERPG), and the Australian Occupational Exposure Standards (Table 5.4).

Table 5.4: Order of selection for short-term community exposure standards[28]

Hierarchy	Air Quality Exposure Standards	Selection Guide
↓	Acute exposure guideline levels (AEGLs)	Use AEGLs first. Values for 227 chemicals currently available
	Emergency response planning guidelines (ERPGs)	Use ERPG if no AEGL. Values for 136 chemicals available
	Australian occupational exposure standards	Use 8 hr TWA or 15 min. STEL if no AEGL or ERPG available

According to the Protective Action Decision Guide, current Best Practice principles suggest that, in the absence of better information, the safe short-term exposure limit for CO_2 should be the 15 min STEL value, i.e. 3%.

This value is consistent with the 60 min TEEL-2 value, which is used in the US PAC as the *concentration above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting, adverse health effects or an impaired ability to escape*'[29].

The Australian Protective Action Decision Guide is therefore more conservative than the US Protective Action Criteria because it limits the exposure to 3% CO_2 to 15 minutes rather than 1 hour.

5.5 Acute toxicity criteria

5.5.1 Concentration threshold

The risk matrix used in the AS 2885.1 safety management study (see Figure 4.1) includes four severity classes that result in injury or the risk of fatality:

- Minor – Injury or illness requiring first aid treatment
- Severe – Injury or illness requiring hospital treatment
- Major – Few fatalities; several people with life-threatening injuries
- Catastrophic – Multiple fatalities result.

For methane pipelines, AS 2885.1 defines levels of thermal radiation equating to 'threshold of injury' and 'threshold of fatality' as:

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[28] MFB 2012

[29] http://www.atlintl.com/doe/teels/teel/teeldef.html

- Threshold of injury = 4.7 kW/m^2
- Threshold of fatality = 12.6 kW/m^2

It is possible to define these thresholds of harmful thermal radiation with some precision, since human sensitivity to heat damage is uniform throughout the population.

In the AS 2885.1 risk matrix, the 'threshold of injury' corresponds to a 'Severe' classification, while the 'threshold of fatality' applies to both the 'Major' and 'Catastrophic' classifications.

In Australia, AS 2885.1 does not specify the 'threshold of injury' or 'threshold of fatality' for CO_2. The definition of such terms is problematic, because the short- and long-term effects of CO_2 intoxication are quite different from those of thermal radiation exposure. Concentrations of more than 3% CO_2 will produce distressing symptoms, with the effects becoming more marked as the concentration increases. However, most individuals will not experience permanent injury, provided that they are quickly removed from the vicinity and treated with 100% oxygen. Fatalities can be expected at concentrations of more than 17%, although susceptible individuals may succumb at lower concentrations.

To date, there have been no published reports that equate the effects of CO_2 intoxication to the AS 2885.1 severity classes.

It is suggested that the US PAC emergency response criteria, particularly the Temporary Emergency Exposure Limit (TEEL) definitions, can provide useful guidance in this regard. To illustrate, the TEEL criteria are compared against the AS 2885.1 severity classes in Table 5.5.

Table 5.5: Comparison of AS 2885.1 Severity Class with TEEL values

AS 2885.1 Severity Class	Temporary Emergency Exposure Limit
Severe *Injury or illness requiring hospital treatment*	TEEL-2 (3 vol% CO_2, 60 min) *The concentration above which the general population could experience irreversible or other serious, long-lasting, adverse health effects or an impaired ability to escape.*
Major *Few fatalities; several people with life-threatening injuries*	TEEL-3 (5 vol% CO_2, 60 min) *The concentration above which the general population could experience life-threatening adverse health effects or death.*
Catastrophic *Multiple fatalities result*	Not defined

This comparison suggests that the 'threshold of injury', corresponding to the AS 2885.1 'Severe' risk classification, can be equated to the TEEL-2 value, i.e. exposure to 3 vol% CO_2 (30,000 ppm or 54,000 mg/m^3) for 60 minutes.

Similarly, the 'threshold of fatality', corresponding to the AS 2885.1 'Major' risk classification, can be equated to the TEEL-3 value, i.e. exposure to 5 vol% CO_2 (50,000 ppm or 90,000 mg/m^3) for 60 minutes.

A comparison with the health effects of CO_2 shown in Table 1 will show that the TEEL values are quite conservative. This reflects the fact that individual responses to CO_2 intoxication can vary widely.

Note that a TEEL value corresponding to the AS 2885.1 'Catastrophic' classification has not been defined for CO_2. Based on the data shown in Table 5.1, and conservative nature of TEEL values, it is suggested that exposure to 7 vol% CO_2 for 60 minutes is an appropriate definition of 'Catastrophic'.

Therefore, it is recommended that for AS 2885.1 safety management studies of CO_2 pipelines:

- 'Severe' = threshold of injury = 3 vol% CO_2 (30,000 ppm or 54,000 mg/m^3) for 60 minutes (TEEL-2)
- 'Major' = threshold of fatality = 5 vol% CO_2 (50,000 ppm or 90,000 mg/m^3) for 60 minutes (TEEL-3)
- 'Catastrophic' = 7 vol% CO_2 (70,000 ppm or 126,000 mg/m^3) for 60 minutes

There is currently insufficient data to allow definition of the AS 2885.1 severity classes for CO_2 exposure times of less than 60 minutes. In the context of AS 2885.1, a conservative a CO_2 pipeline design should not consider exposure time, and should instead place limits on exposure concentration.

5.5.2 Dosage of CO_2

When undertaking a QRA, it is necessary to consider both the exposure time and concentration to determine a dose threshold. For example, this technique may be used for the case where a large quantity of CO_2 released over a short duration resulting in a CO_2 'cloud' passing over terrain.

The Health and Safety Executive (HSE) in Great Britain requires duty holders to base assessments on the SLOT and SLOD. For land use planning the SLOT is defined as causing (McGillivray and Wilday 2009):

- severe distress to almost everyone in the area
- substantial fraction of exposed population requiring medical attention
- some people seriously injured, requiring prolonged treatment
- highly susceptible people possibly being killed, likely to cause 1-5% lethality rate from a single exposure to a certain concentration over a known amount of time.

SLOD is defined as causing 50% lethality from a single exposure over a known amount of time. The SLOT and SLOD for CO_2 are based on a probability unit or probit. Probit equations take the form:

$$Pr = A + B\,ln(c^n t)$$

where:

c concentration (ppm)

t time (min)

These can then be converted to a probability of fatality using the error function transform:

$$\text{Probability} = 0.5\left[1 + \text{erf}\left(\frac{\text{Pr} - 5}{\sqrt{2}}\right)\right]$$

The Toxic Load (TL) is calculated as:

$$\text{TL} = \text{c}^{\text{n}}\text{t}$$

There are probits published for many common industrial toxic materials (TNO 2005b). In the case of CO_2, the Health and Safety Laboratory (HSL) has used the following constants for the probit equation (McGillivray and Wilday 2009):

A = -90.8 B = 1.01 n = 8

This equation indicates that the health effects of CO_2 are strongly non-linear with concentration, with the toxic load increasing as c^8.t. That is, exposure to a high concentration for a short time is many times worse than exposure to half that concentration for twice as long.

The HSL probit function was based upon extrapolation from non-lethal CO_2 concentrations and does not accurately quantify the lethal toxicity, as required by the probit relationship. There are also several other probit functions for CO_2 reported in the literature, but none of them is based on extensive experimental work (Knoope et al. 2014). An acute toxicity study in rats was recently undertaken to address this shortcoming, but it was found that a single probit function did not fit the experimental data. Separate equations were needed for the 40-45% and 44-52% concentration ranges, and the variability in the data did not allow the derivation of a meaningful value of 'n' (Muijser et al. 2014).

According to the Dutch National Institute for Public Health and the Environment (RIVM), there is currently insufficient data for a reliable probit function for CO_2. At this stage, RIVM recommends the use of the semi-quantitative estimates shown in Table 5.6 as conservative guidelines for human exposure of up to a one hour (ter Burg and Bos 2009).

Table 5.6: Acute health effects of carbon dioxide - Dutch advice

CO_2 (vol% in air)	Consequence
5 - 10	No deaths are expected for exposure times of less than 60 minutes
10 - 15	Serious effects and possible mortality may start to occur for exposure times of less than 60 minutes
20 - 25	a high level of mortality may occur for exposure times of less than 60 minutes

The use of SLOT, SLOD and probit functions rely on accurate quantification of the toxicity of CO_2 to humans. There is insufficient data available to define these values sufficiently well for humans, and acute toxicity studies in mice have not been able to provide better data. This creates a major source of uncertainty for the use of QRA for CO_2 pipelines (Koornneef et al. 2010) (Knoope et al. 2014). The semi-quantitative estimates recommended by RIVM set 'reality limits' for QRA, but do not help to make the probit function more accurate.

In addition, the 'threshold of fatality' that may be inferred from the RIVM recommendation is 10% CO_2, which is double the TEEL-3 value. It is likely that the RIVM value is derived from experimental data with healthy volunteers and does not take into account the presence of susceptible individuals in the population.

For the time being, the knowledge gaps relating to the toxicity of CO_2 mean that the QRA approach does not offer a higher degree of confidence than the qualitative risk assessment specified by AS 2885.1.

If land use planning regulations in Australia require the use of QRA for proposed new CO_2 pipelines, it is recommended that the SLOT and SLOD values, and the HSL probit equation (McGillivray and Wilday 2009) be used, despite the acknowledged uncertainties. They have also been adopted in the 'Recommended Practice for Design and Operation of CO_2 Pipelines' (DNV 2010), and used in 'Technical Guidance on Hazard Analysis for Onshore Carbon Capture Installations and Onshore Pipelines' (Energy Institute 2010b).

5.6 Environmental hazards of CO_2

The acute environmental impact of a catastrophic release of CO_2 whilst being transported by pipeline have been considered in a report by DNV (DNV 2013). Animals exposed to high CO_2 concentrations are affected in similar ways to humans, (i.e. respiratory distress, narcosis and mortality), with the effect dependant on behaviour and body size.

Long-term, subsurface releases of CO_2 will cause die-off of local vegetation. CO_2 will increase the pH of groundwater and displace oxygen from the soil, and can harm plant growth through altered nutrient availability and root anoxia. CO_2

concentrations above 5 vol% may be dangerous to vegetation and phytotoxic at around 20 vol% (DNV 2013).

However (Lake et al. 2012) conducted an experiment to determine the impact of a pipeline rupture on plants, simulating CO_2 pooling on the ground for 8 hours. In two separate experiments, the mean CO_2 concentrations were 42.4% (mean minimum 12.2% CO_2, mean maximum 58.0% CO_2) and 35.1% (mean minimum 11.8% CO_2, mean maximum 48.2% CO_2). No significant impacts on plant biochemistry were observed, and plant growth was not affected 3 months later. It was concluded that the effects on plants of an 8 hour catastrophic leak of CO_2 are likely to be small and short term. On the other hand, the effects on local fauna may be severe and may have longer-term ecological implications.

5.7 Health Implications of Impurities in CO_2

In principle, the impurities in the CO_2 stream may pose a health risk through exposure to toxic compounds in the event of short-term, sudden leakages. The specific impurities present will depend on the source of the CO_2, but may include sulphur oxides (SO_x), nitrogen oxides (NO_x), CH_4, H_2S, solvent residues, etc. However, the level of such impurities in any new CO_2 pipeline in Australia is likely to be very low, consistent with the forthcoming ISO standard.

The Cooperative Research Centre for Greenhouse Gas Technologies (CO_2CRC) conducted a QRA analysis of the potential health impacts of the impurities in a supercritical CO_2 pipeline, using composition data similar to that shown in Table 3.4. It was found that the any health impacts of a release to atmosphere would be due to the CO_2 itself, while the impact of minor impurities is likely to be insignificant (Hooper et al. 2005).

Thus, there is currently no reason to expect that the minor level of impurities in a new CO_2 pipeline in Australia will have any significant health implications.

6 COMPARISON WITH METHANE (NATURAL GAS) PIPELINES

6.1 Summary

The general public is familiar with the presence of natural gas (methane) transmission pipelines, whereas carbon dioxide transmission pipelines are comparatively rare. This Chapter reviews the factors that can contribute toward community acceptance of a new CO_2 pipeline and the technical issues that need to be addressed in order to ensure that the associated risks are acceptable.

It is important to actively engage the local community in the process from an early stage, so they have ample opportunity to understand the rationale for the project and the likely risks and benefits to all concerned.

In the UK, community members appreciated being educated about the properties of CO_2 and learning that, unlike methane, CO_2 is not explosive and that its high density results in a very different dispersion pattern.

The community would also benefit from learning about the CO_2-specific factors that must be addressed to achieve the level of reliability associated with natural gas pipelines. Issues such as corrosion control and ductile fracture control present particular challenges for CO_2 pipelines, but recent research has provided the tools needed for the task.

A significant difference between natural gas and CO_2 pipelines is the *mechanism for harm* in the event of an accidental rupture. A natural gas pipeline rupture can create an initial fireball that is extremely dangerous to people and property, with potential effects distances of several hundred metres. The effects distances associated with rupture of a CO_2 pipeline, on the other hand, would be influenced by wind speed, direction and terrain effects, which would potentially result in a smaller affected area.

It is important for the community to be aware of the differences, and that suitable dispersion modelling tools are available to ensure that the risks are managed appropriately.

6.2 Community perception

The general public is familiar with the presence of methane transmission pipelines, whereas carbon dioxide transmission pipelines are comparatively rare. In the USA there is 514,000 km of methane pipelines and only about 5,600 km of CO_2 pipelines. In comparison, Australia has 33,000 km of methane pipelines and less than 20 km of CO_2 pipelines.

The CO_2 pipelines in the USA are all located in sparsely populated regions and are predominantly associated with enhanced oil recovery operations. The local communities understand the economic benefits associated with the CO_2 pipelines and are prepared to tolerate any associated risks. In contrast, any new CO_2

transmission pipeline in Australia will be an unknown quantity to the local community, which will have concerns about possible health and environmental risks.

Public concern can become a serious threat to a project if not handled in time and in a careful manner. It is important to gain acceptance from the community at the planning stage for pipelines that may pass close to populations. Actions and strategies should be tailored to the needs of the local community, based on lessons learned from previous projects (IEAGHG 2013).

In the UK, the COOLTRANS project has undertaken a study of public perceptions of CO_2 and its transportation by pipeline. The COOLTRANS study involved two focus groups, in which members of the lay public were guided through detailed discussions relating to CO_2 and its transport by pipeline (O'Keefe et al. 2013).

The study found that the participants were familiar with CO_2 but not with details of its sources or properties. Participants responded positively to being presented with information about the properties of CO_2, which allowed a better understanding of some of the consequences of potential exposure to CO_2.They were reassured to learn that, unlike methane, CO_2 is not explosive and that its high density results in a very different dispersion pattern.

Focus group participants were told about the risk assessment process and shown the proposed route of the CO_2 pipeline. Participants were reassured to learn of the wide variety of issues that had to be considered during the development of a pipeline. However, their concerns extended beyond the immediate physical risks prioritised in the risk assessment, and included the physical disruption and impact on the landscape and a sense of bearing the burden of energy supply infrastructure in the region. The participants were able to rationalise the need to balance these risks against the wider benefits to climate change mitigation and the potential benefits to the local economy.

This study found that trust in the companies responsible for the pipeline is crucial. At the proposal stage, it is important that the relative benefits of a project are perceived to be distributed fairly between the developer and the local community. Once a decision has been made to build the pipeline, the local community must trust the developer to minimise risks during the selection of the route and during the subsequent construction, operation and maintenance of the pipeline.

The COOLTRANS study found that members of the public respond positively to being given detailed information about the motivations and processes behind the proposed pipeline development, and that they appreciate the opportunity to have their questions answered. It was concluded that the type and level of engagement has to be tailored to suit different audiences, and that opportunities for the community to engage should be provided in a variety of ways (O'Keefe et al. 2013).

Ecofys, a consultancy group in the UK, interviewed the proponents of actual of proposed CO_2 pipelines in the UK, Europe, the USA and Canada to understand the key drivers of public concern (IEAGHG 2013). Public anxiety was found to be a major concern, associated with not being able to understand risks and consequences, and dissatisfaction with the quality of information provided by project proponents.

Feedback from respondents reinforced the need for project staff to communicate simply and clearly and address the concerns of local residents. Most projects used websites, public meetings and telephone helplines as a means of communication.

Interestingly, it was found that the CO_2 pipeline is usually not the focal point of public opposition. Most concerns relate to either the capture (especially the building of a new power plant or production plant) or the storage part of the project (IEAGHG 2013).

The results of the COOLTRANS and Ecofys studies are directly applicable to Australia, where CO_2 pipelines represent a largely unknown quantity. The main lesson is that the local community needs to be actively engaged in the process from an early stage, and given ample opportunity to understand the rationale for the project and the likely risks and benefits to all concerned.

6.3 Hazard comparison

In one sense, transmission of methane is potentially much more dangerous than CO_2. Methane is lighter than air and highly flammable, so any leak from a pipeline is likely to ignite, causing gas burn injuries or fatalities and major damage to the pipeline. In contrast, CO_2 is heavier than air and not flammable. Exposure to CO_2 at 3-10 vol% causes CO_2 intoxication, which can be distressing and potentially debilitating, but is reversible by treatment with 100% oxygen. Exposure to CO_2 at more than 17 vol% is fatal.

Both methane and CO_2 are colourless and odourless, and can cause death by asphyxiation (suffocation) in enclosed spaces. Methane accumulates near the top of enclosed spaces, while CO_2 settles to the bottom[30].

Leaks of CO_2 to the atmosphere are not dispersed as quickly as methane, and may collect in depressions in the land, in tanks and basements and in other low-lying areas near the pipeline route. Any such accumulation of CO_2 is difficult to detect without specialised equipment, and can quickly asphyxiate a person entering that space.

A comparison of other characteristics of CO_2 and natural gas pipelines is provided in Table 6.1, reproduced from (IEAGHG 2013).

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[30] http://www.cdc.gov/niosh/docs/90-103/

Table 6.1: Comparison of characteristics of CO_2 and natural gas

Characteristic	Natural Gas at typical pipeline conditions	CO_2 at typical pipeline conditions
Flammability (Explosions)	Yes. Imperative to avoid explosive mixtures of natural gas and air in the pipeline at all times. Influences start-up procedures.	No. Confined mixtures of air and CO_2 pose no explosion issues.
Flammability (Fires)	Releases of natural gas can result in large fireballs.	Not combustible. No combustion issues with releases of CO_2, intentional or otherwise.
Corrosivity in the presence of water	Not a serious problem for corrosion as no compounds are formed. Common use of corrosion inhibitors.	CO_2 plus water = Carbonic Acid. Extremely corrosive, especially in the presence of water. Requires measures to keep the gas extremely dry or stainless steel pipe and equipment. Influences commissioning and start-up procedures.
Depressuring characteristics (Joule Thompson effect)	Like any gas, natural gas cools as it depressures, but not unusually so in the range of pressures and temperatures usually experienced in natural gas pipeline systems.	CO_2 cools greatly as it depressures in pipeline conditions, creating extremely low temperatures that threaten to cause brittle failure of steel pipe. Influences start-up and shutdown procedures.
Depressuring characteristics (rate of depressurisation)	A longitudinal rupture of a pipeline will be self-limiting, as the release of the gas through the initial failure quickly depressures the line to the point where the crack cannot propagate.	A longitudinal rupture of a pipeline could propagate for long distances because the CO_2 depressures slowly. Pipeline must be designed with periodic crack arrestors to stop crack propagation.
Presence of more than one phase at pipeline conditions	No multiphase issues (but see Hydrates, below). Natural gas is a gas at all expected pipeline conditions. The absence of issues with multi phases gives the natural gas pipeline designer a much wider range of acceptable design conditions to work with.	Yes. CO_2 can be a liquid or a gas at common pipeline conditions. Typical response is to operate the entire pipeline at supercritical pressures, which avoids the possibility of liquid CO_2 forming. The need to maintain CO_2 pipeline pressures above the critical point results in a much smaller range of acceptable design conditions, at pressures that are higher than for typical Natural Gas pipelines.
Hydrate formation (solid material composed of gas and water)	Possible. Necessary to maintain low water contents or face addition of hydrate inhibiting chemicals.	Possible. Meeting the water content specification to avoid corrosion issues should also avoid hydrate formation.

As noted in Table 6.1, one of the significant differences is that methane is transported in the gas phase while CO_2 is transported as a supercritical fluid. Greater control of operating pressure is required for CO_2 pipelines to prevent the formation of gas or solid phases. Despite this, methane and CO_2 pipelines are of similar diameter (100-900 mm) and operate at similar pressures (8-20 MPa).

Since CO_2 and methane pipelines are similar in diameter and operating pressure, it is commonly assumed that the associated risks are similar (Koornneef et al. 2010). The accident statistics tend to confirm the view that CO_2 pipelines are no more hazardous than methane pipelines. For example, during the period from 1986 to 2001, there were 1,287 accidental release incidents reported for methane pipelines in the USA. Of these, 217 resulted in injury and 58 resulted in fatalities. During the same period, there were only 10 incidents reported for CO_2 pipelines, with no injuries or fatalities (Gale and Davison 2004).

However, such statistics should not be used to imply that CO_2 pipelines are no more hazardous than methane pipelines, because of the very small sample size available for CO_2 incidents.

6.3.1 Structural factors to minimise risk differences

It has been suggested that the failure rate associated with CO_2 and methane pipelines would only be comparable if the rates of internal corrosion and the modes of failure are also similar (Wang and Duncan 2014).

The CO_2-specific factors that must be addressed to ensure satisfactory pipeline integrity, and to minimise differences in pipeline materials behaviour, are discussed below.

6.3.1.1 CO_2-specific factors affecting pipeline integrity

Pipelines should be designed for the temperatures, pressures and materials that they transport. Dry CO_2 is inert to most common industrial materials but will react with water to form carbonic acid, which is highly corrosive to carbon steels. In addition, at high pressures, CO_2 may combine with water and other impurities to form hydrates that can form plugs and damage the pipeline or associated equipment. These problems are well understood in the oil and gas industries, and can be resolved by drying the gas using conventional technologies. To date, there have been no reported CO_2 pipeline losses of containment caused by internal corrosion (DNV 2010).

An acceptable level of water in the CO_2 stream should be specified during the design phase and actively monitored during pipeline operations. Remedial actions must be taken if the water content rises above the specified level.

Transporting CO_2 under supercritical conditions requires that the temperature and pressure must be carefully controlled to prevent phase changes, under both steady-state and transient conditions. A suitable thermodynamic-hydraulic model should be established during the design phase to facilitate pipeline design and simulation of release scenarios (DNV 2010).

The (DNV 2010) guidance note suggests that ‘tuning of the Equation of State models may be required to obtain stable solution when applied to near pure CO_2, particularly close to the critical point’. The available models that may be considered fit for purpose in this application are reviewed in Section 8.11.

In addition, protective measures must be employed to guard against corrosion and damage to CO_2 pipelines. No internal corrosion protection is required for Carbon-Manganese steel pipes in the absence of free water. In pipeline sections where free water may be present, internal polyethylene (PE) liners may be used (DNV 2010). Supercritical CO_2 can damage some elastomer sealing materials. Viton valve seats and Flexitallic, nitrile and EPDM gaskets are often used in the USA for CO_2 pipelines (Gale and Davison 2004). Dry CO_2 has poor lubricating properties but can deteriorate many of the greases used in valves, pumps, etc. This is a particular concern for safety critical valves (e.g. block valves, check valves and pressure relief valves) where poor lubrication may compromise operation in an emergency situation (DNV 2010). Further guidance on suitable materials of construction are provided in (Oosterkamp and Ramsen 2008) and on pipeline construction in (Energy Institute 2010a).

6.3.1.2 Ductile fracture control

Pipelines transporting CO_2 must comply with the fracture control requirements of AS 2885.1, Section 4.8. In particular, it is essential to prevent catastrophic ductile running fractures, which involve the rapid tearing of the pipeline and release of massive volumes in a very short space of time. Such fractures can initiate from defects caused by mechanical damage, soil movement, corrosion, etc., and will propagate if the stress acting on the defect is greater than the fracture toughness of the pipe. Propagation of the fracture will stop if the pipeline depressurises faster than the fracture propagation speed (DNV 2010).

In comparison with methane, CO_2 has an unusually high saturation pressure, making CO_2 pipelines potentially more susceptible to fracture propagation (Mahgerefteh et al. 2012). In addition, the decompression behaviour of CO_2 is significantly different from that of methane because of the phase changes that occur as the fluid decompresses. The decompression velocity varies as a complex function of temperature and pressure, and is also affected by the presence of impurities in the pipeline.

Propagating fractures are described as either brittle or ductile, although brittle fracture propagation is not an issue in modern pipeline steel (Cosham and Eiber 2008a). A ductile fracture will not propagate if there is insufficient energy in the system to overcome the resistance to propagation. The driving force for a running fracture is the internal pressure. The saturation pressure is key to determining the toughness required to arrest a propagating ductile fracture. Factors that increase the saturation pressure will increase the required arrest toughness (Cosham and Eiber 2008a).

Appendix BB of AS 2885.1 provides guidance on estimating the required fracture toughness of CO_2 pipelines and development of a suitable fracture control plan. This guidance was based on (Cosham and Eiber 2007), and needs to be updated in light of subsequent developments. (Cosham and Eiber 2008a, b) and (Cosham 2012) identified that, for CO_2 pipelines:

- Increasing the initial temperature will increase the arrest toughness.
- Decreasing the initial pressure will increase the arrest toughness.
- The addition of other components such as hydrogen, oxygen, nitrogen or methane will increase the arrest toughness.

These findings were subsequently verified experimentally during a series of shock tube tests undertaken by National Grid in the UK (Cosham et al. 2012).

Two full-scale fracture propagation tests were subsequently conducted using dense phase CO_2-rich mixtures as part of the COOLTRANS research programme. It was found that the standard method used to predict the toughness required to arrest a running ductile fracture in natural gas pipelines was inadequate to account for the experimental data. The predicted toughness would need to be increased by a factor of 1.5 to 2.4 would be required to conservatively predict all of the ‘arrest’ data points. It was concluded that the toughness prediction method used for natural gas pipelines is not (currently) applicable to a pipeline transporting dense phase CO_2, because the driving force is higher than predicted. *Therefore the operator is faced with the difficult and pragmatic choice of either conducting a full-scale fracture propagation test to validate the design of a pipeline, or installing mechanical crack arrestors* (Cosham et al. 2014).

The issue of the effect of small concentrations of impurities on the required arrest toughness was addressed by the EU-funded CO_2PipeHaz project, which developed and validated a Dynamic Boundary Fracture Model (DBFM) to calculate CO_2 pipeline decompression and fracture propagation velocity. The DBFM accounts for all the important fluid/structure interactions taking place during fracture propagation, including unsteady real fluid flow, heat transfer, friction, and progressive variation of the crack tip pressure loading. The Modified Peng-Robinson equation of state is used, which can account for the presence of fluid impurities (Mahgerefteh et al. 2012).

Simulation studies with DBFM suggest that, for pure CO_2, the fracture length is very short in the temperature range 0-20^{o}C, but becomes very long at 30^{o}C. Similarly, the presence of the impurities expected from an oxy-fuel CO_2 capture system resulted in long running fractures (Mahgerefteh et al. 2012). The DBFM has been incorporated into the commercial software package PIPETECH. However, the DBFM has been validated only against experimental release data for natural gas containing impurities, but not CO_2 containing impurities. Therefore the utility of

PIPETECH to estimate the required fracture toughness of CO_2 pipelines remains unclear.

Further work on the effect of impurities on ductile fracture propagation is continuing in the current CO_2Quest project. One of the objectives of CO_2Quest is to:

> *Develop and validate fluid/structure fracture models for ductile and brittle fracture propagation in* CO_2 *pipelines. Apply these models, based on various candidate pipeline steels, to identify the type of impurities and operating conditions that have the most adverse impact on a pipeline's resistance to withstanding long running fractures*.[31]

The fact that long-distance, high-pressure CO_2 pipelines have been designed, constructed and operated successfully for many years indicates that the design issues can be successfully addressed (Cosham and Eiber 2008a). Mechanical crack arrestors are used on the CO_2 pipelines built in North America during the 1970s and 1980s, when modern high-toughness piping was not available. The 329 km Dakota Gasification pipeline, constructed in 2000, does not use mechanical crack arrestors (Cosham 2012).

The CO_2 transported in the Dakota Gasification pipeline is a by-product of lignite gasification. The CO_2 is recovered using a cold methanol wash and flashed off under vacuum (Rectisol process). The resulting CO_2 stream is 96.8% pure, containing 1.1% H_2S, 1.0% ethane, 0.3% methane and 0.8% 'other' as impurities (Perry and Eliason 2004).

Similarly, the Vattenfall 30 MW lignite oxyfuel pilot plant at Schwarze Pumpe produced food grade CO_2 with a purity of >99.7 vol% (Martens et al. 2015). The SaskPower Boundary Dam lignite power station is reported to produce food grade CO_2 at 99.999% purity using the Cansolv amine adsorption process[32].

Thus it is definitely possible to produce CO_2 at a quality that is safe for pipeline transportation, but removal of impurities adds significantly to the cost of CCS. A better understanding of the effect of impurities on CO_2 properties will eventually allow more economical pipeline designs to be developed.

A suitable fracture control plan may also include the use crack arrestors to provide extra strength to withstand the stress of cracking and limit the extent of rupture. Crack arrestors may be comprised of a thickened region of metal ('sleeves') or of a laminated or woven material ('ClockSpring'). In North America, the typical spacing between each arrestor is 300-500 m.

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[31] http://www.co2quest.eu/ano.htm

[32] M. Monea, Presentation on the Boundary Dam CCS project, The University of Melbourne, 19 May 2015

7 CREDIBLE RELEASE SCENARIOS

7.1 Summary

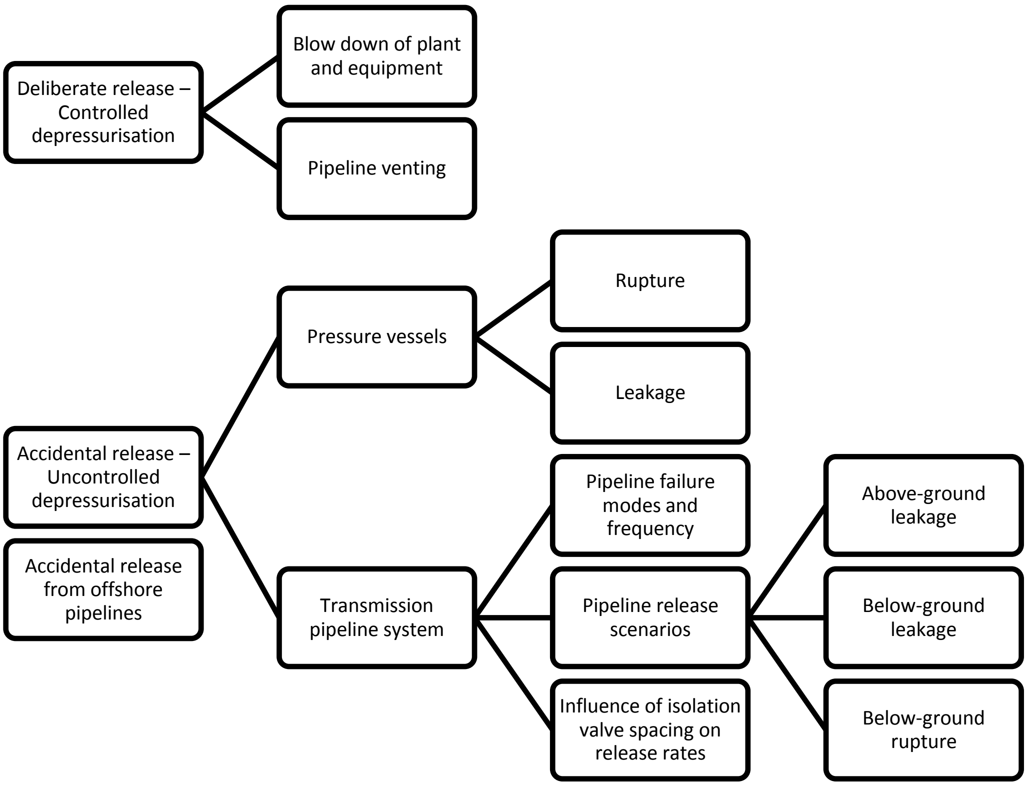
A safety management study undertaken according to AS 2885.1 must identify any high consequence events that impose major risks to the project, community and environment. In order to do this, it is necessary to characterise the nature of the CO_2 release that may be expected, so that appropriate source terms for dispersion modelling may be correctly defined.

A range of different release scenarios is possible, depending on whether the release is deliberate or accidental, major or minor, from a storage tank, pipeline or valve, or from below or above ground.

This Chapter reviews the information available on each of these scenarios, with the aim of providing guidance on appropriate source terms for the dense gas dispersion models discussed in Chapter 8.

In summary, the various release scenarios considered are as follows Figure 7.1.

Figure 7.1: Release scenarios



In each case, guidance is provided based on a review of the current state of the art.

7.2 CO_2 release source terms

CCS infrastructure comprises a range of facilities for capture, transport and storage of CO_2. A useful overview of the variety of technologies encountered in CCS systems is provided in (Energy Institute 2010a). The 'capture' infrastructure would comprise process equipment, and thus release scenarios would depend on the exact equipment type, pressure and temperature. The 'transport' infrastructure would comprise transmission pipelines, with associated valves, vents, pressure booster stations and scraper launchers/ receivers, culminating in an entry point to the ‘storage’ location; usually a sub-surface geological formation.

Potential releases of CO_2 to atmosphere at any point in the CCS system may be either deliberate or accidental. The resulting sudden pressure drop as the CO_2 enters the atmosphere will cause a transition from the supercritical state to the gas and/or solid state. This will be accompanied by a substantial drop in temperature and possible change of state within the pipeline itself, creating potential for damage to the pipeline infrastructure.

The health risks associated with a loss of containment will depend on the nature of the release. Consequence analysis of any identified threat to the pipeline will require an assessment of the potential likelihood of the occurrence and the physical situation that is likely to result. The release scenario starts with a loss of containment, and then may be described by an event tree (McGillivray et al. 2014).

Modelling the source characteristics is perhaps the most critical step in the accurate estimation of downwind air concentrations following a deliberate or accidental release of CO_2. The emission calculations may involve two- or three-phase releases, emission rates that vary dramatically over time, and the release of very dense, cold gas. For modelling purposes, the emissions characteristics are known as the ‘source term’. Characterisation of the source term involves considerations such as whether the CO_2 release should be regarded as ‘instantaneous’ or ‘continuous’, the orientation of the release, whether it is a jet or a pool, and whether it is single or multi-phase (Hanna et al. 1996).

Determination of the source emission rate involves for basic sequential steps (Hanna et al. 1996):

(1) Determine the time dependence of the CO_2 release;

(2) Select the most applicable source term model for the situation;

(3) Gather specific input data and physical properties necessary for the source term model; and

(4) Calculate the source emission rate.

A range of different scenarios is possible, depending on whether the release is deliberate or accidental, major or minor, from a storage tank, pipeline or valve, or below or above ground.

This Chapter reviews the information available on each of these scenarios, with the aim of providing guidance on appropriate source terms for the dense gas dispersion models discussed in Chapter 8.

7.3 Potential release scenarios

7.3.1 Deliberate release – Controlled depressurisation

7.3.1.1 Blowdown of plant and equipment

Deliberate release of CO_2 from CCS equipment will be essential from time to time, to allow for plant maintenance. Pressure vessels and associated pipework are distinct from pipelines in that they fall under separate regulation and separate Australian standards. For example, AS 2885 does not apply to pressure vessels, but these are covered by AS 1210. Similarly, pipelines are generally regulated under separate legislation (e.g. Pipeline Act 2005 in Victoria) from storage and processing facilities, which are covered by the Work Health and Safety Act and regulations in most states in Australia.

There are other differences, e.g. pressure vessels and associated equipment are generally above ground, but inside a site with a boundary fence, rather than buried underground with no physical separation (apart from ground cover) from populated areas. In addition, it would be usual to determine the acceptability of siting an industrial development through a development application which would require, in many circumstances, a site-specific quantitative risk assessment. This being the case, a very detailed analysis of all equipment at the specific site would be required. It would therefore be normal to analyse several parts of the capture system to cover representative pressure, temperature, phase and location combinations. This is in contrast to a new pipeline which may be more amenable to a generic approach, as per AS 2885.

The design of blowdown equipment must take into consideration the fact that CO_2 has a large liquid to gas expansion factor. For example, care must be taken in selection of isolation valves, to avoid the risk of catastrophic failure. Special cryogenic valves with 'cavity pressure relief holes' are required. Engineers should be aware of the proven engineering practices that have been developed for liquid natural gas, which also has a large liquid to gas expansion factor (Energy Institute 2010a).

Blowdown of equipment must be done slowly, to prevent the formation of 'dry ice' within the system. There is also a danger that the blowdown pipe can become blocked with solid, giving the impression that the vessel has been emptied. Subsequent warming of the pipe would cause it to unblock, leading to an uncontrolled discharge of CO_2 with potential safety consequences for nearby personnel (Energy Institute 2010a). Useful guidance on safe drainage and blowdown of CO_2 plant and equipment is provided in (Connolly and Cusco 2007) and the European Industrial Gases Association (EIGA) newsletter 70/99/E on ‘CO_2 ice plugs’[33].

The mass emission rate at the hole or aperture is strongly determined by whether the pressurized liquefied gas flashes before, at, or after the hole. If the CO_2 does not flash until after the hole, the mass emission rate is a maximum, calculated by the Bernoulli formula for a liquid. If the CO_2 flashes before the hole, such as it would for a significant length of pipe attached to the vessel, then the mass emission rate can be as much as a factor of 5 to 10 less than the '100% liquid' Bernoulli rate.

For CO_2 and other chemicals with a very low boiling rate, any aerosol formed during the flashing process is likely to quickly evaporate. This is even more likely for an intentional routine venting process, where the emission rate will be minimized. Thus any subsequent downwind dispersion assumes a cloud consisting of 100% gas.

7.3.1.2 Pipeline venting

A venting station is required at each of the isolation valves along the length of the pipeline. For maintenance or repair the section concerned can be isolated and depressurised without the whole line being emptied (Energy Institute 2010a). Depressurizing CO_2 from pipeline-injection pressures to atmospheric pressure is noisy and cold, with auto-refrigeration temperatures down to -90°C. Blowdowns must be controlled over significantly longer times than in normal methane pipelines, to prevent excessively low temperature gradients, dry ice formation and pipe embrittlement.

Typically, 6-8 hours are required to blow down a 32 km section of pipeline (Mohitpour et al. 2008). A 50 km long section of 600 mm pipeline containing 9,300 tonnes of supercritical CO_2 took 10.3 hours to depressurize from 8 MPa to atmospheric pressure (Clausen et al. 2012). Dry ice can be seen during blow down (Oosterkamp and Ramsen 2008).

Noise generation, dry ice formation and the plume dispersion behaviour are all strongly related to the transient behaviour of the CO_2 inside the pipeline during depressurization. This means that in order to calculate valid safety zones around a CO_2 vent stack, it is crucial to be able to predict the transient behaviour of CO_2 during depressurization using properly validated pipeline simulations tools (Clausen et al. 2012). The simulation tools that are available for this task are discussed in Section 8.7.7.1.

Atmospheric conditions can influence the CO_2 plume dispersion during blowdown. The CO_2 tends to collect at ground level on overcast, rainy days without wind. No such problems occur during sunny, windy conditions (Oosterkamp and Ramsen 2008).

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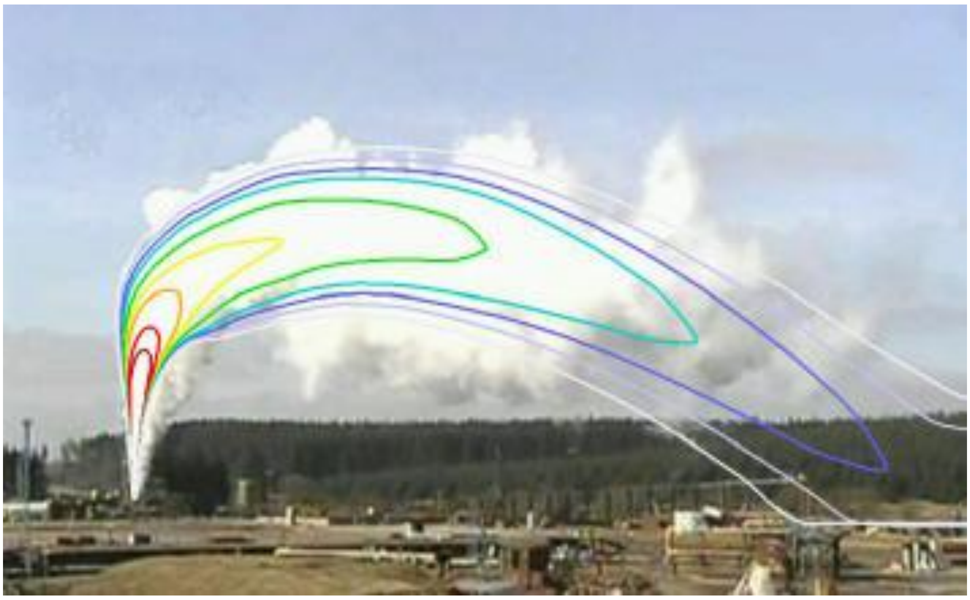
[33] https://www.eiga.eu

For modelling purposes, the source conditions during venting should be relatively well defined, such as vent height and diameter, nearby buildings and terrain contours, and plume fluid- and thermodynamic conditions (Britter et al. 2011).

It is very important to be able to accurately characterise the flow and physical properties of the emerging fluid jet. When blowdown is initiated, the pressure in the pipeline will fall from the initial operating pressure of the pipeline to the saturation pressure. The dense-phase CO_2 will then start to boil, producing a vapour dome on top of the liquid. The liquid layer within the pipeline will gradually fall. Close to the end of the release, a two-phase mixture of vapour and entrained liquid droplets will be released, with the liquid droplets turning into solid CO_2 particles as the pressure falls below the triple point pressure (Gebbeken and Eggers 1996). Recent work to characterise the composition of the vapour jet is discussed in Section 8.7.1.3.

Figure 7.2 shows an experimental release from a 25 mm diameter vent in a 914 mm diameter pipeline containing dense phase CO_2, conducted as part of the COOLTRANS project (Allason et al. 2014).

Figure 7.2: CO_2 plume release from a vent



This illustration shows a comparison between the observed CO_2 plume emanating from the vent and the gas concentration profiles calculated using an integral model described in (Cleaver et al. 2003). The calculations show the gas plume slumping toward the ground, even though this is not clear to the eye. This highlights the need for CO_2 dispersion modelling during the design of venting stations to prevent any acute impact to personnel.

(DNV 2010) provides guidelines for the design of vent stations, which require the use of dispersion simulations and a suitable model for pipeline decompression.

7.3.2 Accidental release – Uncontrolled depressurisation

7.3.2.1 Rupture of pressure vessels

Rupture of a vessel containing pressurised, liquefied CO_2 may be regarded as a Boiling Liquid Expanding Vapour Explosion (BLEVE), the entire CO_2 mass in the vessel is released instantaneously (Zhang et al. 2013). A catastrophic vessel failure would be expected to not just release a large quantity of CO_2 for subsequent dispersion, but also release overpressure and vessel fragments that may cause injury or fatalities.

There are three incidents on record where CO_2 storage vessels have ruptured due to accidental overpressurisation, as described in (Energy Institute 2010b). Such incidents can have a number of consequences (Clayton and Griffin 1995):

- The cold liquid released can freeze personnel.
- Fragments can be thrown with tremendous force.
- Part of the vessel with CO_2 still expanding can act like a rocket.
- The rapid transition from supercritical to atmospheric pressure can create shock waves that cause damage, fatalities, and injuries.

Localised overpressure and vessel fragmentation effects may be considered using standard equations in the TNO Yellow Book (TNO 2005d), or (CCPS 2010); however, the effects distances from these phenomena may not be adequately addressed by the toxic dispersion modelling. In other words, the distance to a fatal concentration of CO_2 generated by the toxic dispersion may be larger than the more localised overpressure effects and the ejection of relatively few, large fragments.

In terms of dispersion modelling for a vessel catastrophic failure, it is important to know the size of the cloud that instantaneously forms. Although this is a difficult scientific topic with much uncertainty, a widely used rule of thumb is that there is an initial 'factor of ten' dilution of the pure gas/aerosol volume with ambient air (Britter and McQuaid 1988). More accurate estimates may be possible using the models developed for vapour cloud explosions, as discussed in (OGP 2010), (Heudier et al. 2013) and (Coldrick 2014).

Experimental work has been done to characterise the BLEVE blast wave resulting from the controlled rupture of 40 litre liquid CO_2 bottles (Van der Voort et al. 2012) (van der Voort et al. 2013). It was found that the experimental data could be adequately simulated using an existing inertia-limited BLEVE model. The results showed that below the homogeneous nucleation temperature, the BLEVE blast does not disappear abruptly, but instead follows a gradual decay. Predictions with the numerical BLEVE blast model were found to overestimate the observed blast peak overpressure and impulse, but qualitatively showed a similar behaviour. The discrepancy was attributed to the energy lost by the acceleration of the cylinder parts. It was suggested that the blast-reducing effects of the tank shell would disappear with commercial-scale storage vessels.

Specific information on failure rates of CO_2 process equipment has not been identified in the public domain. A possible analogous case is that of Liquefied Petroleum Gas (LPG) pressure vessels, which are reported to have a catastrophic failure rate of $2x10^{-6}$ per vessel year (HSE 2012).

7.3.2.2 *Leakage from process vessels*

The TNO 'Purple Book' provides examples of typical accidental release scenarios for process equipment, largely comprised of historical data from the onshore chemical industry (TNO 2005b). Examples relevant to CCS infrastructure are shown in Table 7.1.

Table 7.1: Scenarios for loss of containment from various equipment types

Equipment	Scenario
Pressure Vessels	Instantaneous release of the complete inventory
	Continuous release of the complete inventory in 10 min at a constant rate of release
	Continuous release from a hole with an effective diameter of 10 mm
Pipework	Full bore rupture
	Leak outflow is from a leak with an effective diameter of 10% of the nominal diameter, a maximum of 50 mm
Pumps	Catastrophic failure - full bore rupture of the largest connecting pipe
	Leak outflow is from a leak with an effective diameter of 10% of the nominal diameter, a maximum of 50 mm.

The HSE has compiled statistics for failure rate and event data for use in Land Use Planning cases, providing hole size frequency and failure rates for a wide range of process industry equipment (HSE 2012). Although there is no data provided specifically for CO_2 equipment, the information provided may serve as a useful basis for a QRA analysis, e.g. as illustrated in (Harper 2011b).

7.3.2.3 *Transmission pipeline system*

7.3.2.3.1 Pipeline failure modes and frequency

A review of loss of containment events for CO_2 pipelines used for EOR in the United States was undertaken by (Duncan et al. 2009). It was found that the main cause of pipeline incidents was component failure, rather than corrosion or human errors. This was regarded as the result of successful implementation of anti-corrosion measures.

Both (Gale and Davison 2004) and (Johnson et al. 2009) have reviewed the statistics relating to CO_2 pipeline incidents from the Office of Pipeline Safety of the US Department of Transportation, for the period 1986 to 2001. They found that, of the 10 incidents during that time, 4 were due to relief valve failure, 3 were due to weld/gasket/valve packing failure, 2 were due to corrosion and 1 was caused by third party damage. Two of these incidents resulted in injury. There was a separate incident in which a fatality occurred, but this was associated with welding work and not as a direct consequence of pipeline operation (Johnson et al. 2009). During the period 2002-2008 there were 18 incidents reported, with no injuries or fatalities (Johnson et al. 2009).

For the entire period from 1986 to 2008, the causes of pipeline failure were found to be (Johnson et al. 2009):

- Corrosion – 45%
- Equipment failure – 17%
- Material and/or weld failure – 17%
- Other (e.g. excavation damage/ incorrect operation) – 21%

The Energy Institute has compiled international pipeline failure rate data from the following sources:

- European Gas Pipeline Incident Data Group (EGIG)
- UK Pipeline Operators Association (UKOPA)
- Conservation of Clean Air and Water in Europe (CONCAWE)
- Pipeline and Hazardous Material Safety Administration in the US (PHMSA)

The overall failure rate data was summarised as shown in Table 7.2 (Energy Institute 2010a).

Table 7.2: Summary of pipeline failure data (incidents per 1000 km/year)

	EGIG	**UKOPA**	**CONCAWE**	**PHMSA**
Overall	0.37	0.25	0.56	0.33
Latest five-year rolling average	0.14	0.028	0.34	NA

(Duncan and Wang 2014) provide a review of the complex issues involved in deriving failure rate frequency data for CO_2 pipelines based on natural gas transmission pipelines. They point out that the use of incident statistics from the PHMSA is misleading, because most recorded incidents in the data set are pinhole leaks and other minor incidents. The frequency of minor accidents provides no basis for predicting rates of serious incidents. Through a careful analysis of the available data, (Duncan and Wang 2014) found that there has been systemic overestimation of the risks associated with CO_2 pipelines in the past, suggesting that previous QRA assessments of components of CCS may be orders of magnitude too high. They concluded that the likelihood of significant (potentially lethal) releases of CO_2 from pipelines is most likely to range from 10^{-6} to 10^{-7}, which would be regarded as an acceptable to negligible range of risk.

(Wang and Duncan 2014) analysed the failure rate data for natural gas transmission pipelines in the PHMSA database. For pipelines up to 508 mm diameter, leakage accounted for 42.6% and rupture 28.0% of the total. For pipelines greater than 508 mm diameter, leakage accounted for 39.4% of the total and rupture 44.5%. In each case, the remaining incidents included weld, joint and valve failure.

For leakages in pipelines larger than 508 mm, 61% were related to pinholes, 17% to connection failures and 22% to punctures. Most punctures were less than 76 mm diameter (Wang and Duncan 2014).

Similarly:

- Data for UK gas pipelines for the period 1992—2007 show that pinholes occurred at approximately twice the frequency of punctures and an order of magnitude more frequent than ruptures (Hopkins et al. 2009).
- EGIG data for 1970—2010 shows that pinholes (diameter of defect equal to or less than 20 mm) account for approximately 50% of all incidents, holes (diameter of defect more than 20 mm and equal to or less than the diameter of the pipeline) approximately 40% and ruptures approximately 10%. About half the incidents were due to external interference (EGIG 2011).
- Data from UKOPA for onshore Major Accident Hazard Pipelines in the UK, covering operating experience up to the end of 2011, provided frequency rates for a wider range of holes sizes, as reproduced in Table 7.3 (McConnell and Haswell 2012).

Table 7.3: Leak frequency vs hole size - UKOPA data

Equivalent hole size class$^{(b)}$	Number of incidents	Frequency (incidents per 1000km-yr)
Full Bore$^{(a)}$ and Above	7	0.009
110mm – Full Bore$^{(a)}$	3	0.004
40mm – 110mm	7	0.009
20mm – 40mm	23	0.028
6mm – 20mm	31	0.038
0 – 6mm	114	0.140
(a) Full Bore is equivalent to the diameter of pipeline (b) Equivalent hole size quoted in this report is the circular hole diameter in mm with an area equivalent to the observed (usually non-circular) hole size.		

It will be observed that the available pipeline failure data is not entirely consistent. If a QRA analysis is required for a CO_2 pipeline in Australia, the data provided in Table 7.4 is recommended as a conservative estimate.

Table 7.4: Leak frequency vs hole size - suggested values

Category	Hole range, mm	Representative hole equivalent diameter, mm	Frequency (events per 1000 km-yrs)	
			Lower	Upper
Pinhole	> 0 <=20mm	20	0.160$^{(a)}$	0.178 $^{(b)}$
Puncture	20mm < pipe diameter	50	0.037$^{(b)}$	0.142$^{(a)}$
Rupture	Pipe diameter or greater	Line diameter$^{(c)}$	0.013$^{(b)}$	0.05$^{(a)}$
Total (based on methane pipelines)			0.21	0.37
Total for comparison (CO_2 pipeline data)			0.33	
(a) EGIG (b) UKOPA (c) This is consistent with the AS 2885 definition for rupture, i.e. 'failure of the pipe such that the cylinder has opened to a size equivalent to its diameter'.				

7.3.2.3.2 Pipeline release scenarios

A CO_2 transmission pipeline will be composed of both above- and below-ground components. The vast majority of the pipeline will be buried for protection, but isolation valves will have to be accessible for maintenance and vent stations will require above-ground valves and pipework. This creates a range of possible scenarios for accidental CO_2 release, i.e.:

- Above-ground leakage
- Below-ground leakage
- Below-ground rupture

Each of these scenarios is considered below.

Leakage from above-ground pipeline infrastructure

The analysis in Section 7.3.2.3.1 suggests that the most likely form of leakage will be in the form of a pinhole of less than 20 mm diameter, and more likely less than 6 mm diameter.

Small leaks above ground will be easy to detect. They will be noisy and will be visible as a white jet of frozen water vapour. The main health hazard associated with such leaks is the risk of CO_2 accumulating in enclosed spaces in the vicinity of the pipeline infrastructure, which can lead to death by asphyxiation for personnel entering that space. If the enclosed space is large enough, or atmospheric conditions are calm enough, the CO_2 may flow at ground level and flow down through drains or to lower working levels, and may eventually accumulate at low points some distance from the pipeline itself.

There is a risk that maintenance personnel may be attracted to the location of a leak by the noise it is making, and may inadvertently enter areas full of accumulated CO_2. Appropriate safety protocols and monitoring systems should be established for work in areas of exposed pipework and infrastructure.

Larger leaks will be very obvious, and will be so loud that personnel may be unable to approach the area until the pipework section has been isolated and vented. In this case, the health hazard will be to people at some distance from the pipeline, in the path of the dispersing gas cloud.

For a pipeline section above ground, the release may be modelled as a jet. For consequence analysis, the most conservative approach is usually to assume that the release is horizontal (Hanna et al. 1996) (see Section 7.4.2.2

Leakage from buried pipelines

A pinhole leak in a buried pipeline will be very difficult to detect. The escaping CO_2 will follow the path of least resistance, which will usually be by diffusion through the soil. Under calm atmospheric conditions the CO_2 may accumulate at ground level, especially if the leak occurs under a local depression (Chow et al. 2009). Long term leaks of this nature may eventually acidify the soil and lower the soil oxygen level, causing localised death of affected vegetation (Lake et al. 2012).

Larger punctures and ruptures of a buried CO_2 pipeline will be easy to detect because they are noisy and produce a plume of gas made visible by condensing water vapour. There is currently no clear consensus on the most suitable approach to modelling the release of CO_2 from a buried pipeline. The COOLTRANS research programme in the UK included 8 full-scale puncture tests which were designed to produce data to better understand the likely consequences. Dense phase CO_2 was released from a 914 mm pipeline buried at a depth of 1.2 m, through holes of either 25 mm or 50 mm diameter (Allason et al. 2012).

The flow pattern that resulted was strongly dependent on the nature of the surrounding soil. In clay soil, release from the smaller puncture *'lifted and broke the soil surface but was not sufficient to blow the soil away completely. It appeared that an underground ‘cavern’ was created around the release and this was connected to the surface via a number of distinct flow paths or ‘tracking routes’, each with a diameter of typically 100 mm.'* The exit velocity from these flow paths was estimated to be about 40 m/s (Allason et al. 2012).

It was found that a distinct crater formed in the sandy soils and for some of the clay soil experiments. 'The craters had steep sides and the flow emerged from them in an upward direction, with a distinct component of vertical velocity' of between 40 m/s and 60 m/s. Typically, a 25 mm puncture at 150 bar produced a 3 m diameter crater in sandy soil, while craters in clay soil were about half as large.

The vertical exit velocity was found to depend on both the orientation of the puncture and the nature of the soil. Velocities varied between about 60 m/s and 20 m/s, with the lowest velocities associated with punctures located on the bottom of the buried pipeline (Allason et al. 2014).

Based on experience with buried natural gas pipelines, it may be expected that, under certain circumstances, a hole in a high pressure CO_2 pipeline may propagate to a full bore rupture, resulting in two open pipe sections with a crater in between.

(McGillivray and Wilday 2009) reviewed the crater dimensions recorded from historical gas pipeline ruptures in the UK. Craters ranged in length from 3.3 m to 152 m, and in width from 1.7 m to 33 m. While the pipelines were typically buried 1-4 m deep, the crater depth ranged from 1.7 m to 7.6 m.

As well as experiments with punctured pipelines, the COOLTRANS programme also included full-scale ruptures of buried CO_2 pipeline sections (Allason et al. 2012). The available information suggests that a full bore rupture of a commercial CO_2 pipeline would create a large crater and a substantially vertical initial plume.

The full-scale release data created by the COOLTRANS programme has been used to develop a CFD model for simulation of the flow patterns created by CO_2 release from punctured or ruptured pipelines (Wareing et al. 2015). The release data and the CFD model have been used by DNV-GL to develop a series of correlations to describe the flow emerging from the crater of a buried CO_2 pipeline. A relationship was developed between the source Richardson number and the wind speed, to determine whether or not a source 'blanket' will form. Models were developed to define the initial conditions of a ground level source. Separate models were developed to predict the size of the crater that forms, the flow out of the crater, and an equivalent ground level dispersion source (Cleaver et al. 2015).

The correlations developed through the COOLTRANS work have been incorporated into FROST, a risk assessment package developed by DNV-GL[34].

7.3.3 Accidental release from offshore pipelines

Experience from modelling releases from subsea methane pipelines should be directly relevant to CO_2 pipelines as well. Releases from shallow water subsea pipelines may be expected to blow away the water cover, effectively behaving like a vertical release from an above-ground pipeline (Engebø et al. 2013).

Releases at greater depth will result in a plume of gas rising to the surface. The diameter of the plume at the sea surface can be taken to be 20% of the depth to the release point, regardless of the flow rate. The gas velocity at the surface is consequently reduced in proportion to the increase in area (Engebø et al. 2013).

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[34] P. Cleaver, email communication, 5 June 2015

Useful guidance can also be gained from experience with offshore natural gas pipelines (Rew et al. 1995).

7.4 Time dependence of the release

Estimation of the time dependence of the CO_2 release rate depends on characterising the time-dependent pressure within the process vessel or pipeline, as well as the flow of the resulting CO_2 stream.

7.4.1 Transient pipeline depressurisation

Release of CO_2 from a pipeline, whether deliberate or accidental, will cause the pressure in the pipeline to fall. As the pressure falls, the CO_2 remaining in the pipeline will transition from being a supercritical fluid phase, to a two-phase liquid and ultimately to a gas phase. This transition will alter the flow conditions within the pipeline, the driving force at the point of discharge, and the properties of the escaping fluid.

Experimental and modelling work undertaken by the CO_2PipeHaz project has shown that, for pipeline sections of tens of kilometres length, the composition of the venting fluid will change from liquid-vapour to solid-vapour when the system pressure drops to 518 kPa abs (5.18 bar abs) (Martynov et al. 2014). Dry ice particles can then contribute to the escaping jet, increasing the size and density of the CO_2 plume. Subsequent decompression may result in solid CO_2 forming in the pipeline. If this occurs, both the inventory release rate and CO_2 plume dispersion behaviour will be affected. For a 20 km pipeline section, simulations suggest that about 90% of the inventory remains in the pipeline after the pressure drops to 518 kPa, so emergency response planning requires a detailed understanding of the latter stages of decompression (Martynov et al. 2014).

Accurate calculation of the CO_2 cloud dispersal behaviour depends upon being able to correctly simulate the transient flowrate and properties of the CO_2 stream for the duration of the release, especially the complex fluid dynamics associated with the transition from single to two-phase flow. (Aursand et al. 2013) provide a review of the modelling issues involved.

There are currently eight commercially available pipeline simulation tools that may be applicable for CO_2 pipelines:

- PIPEBREAK
- MORROW
- OLGA
- LEDAFLOW
- PIPEPHASE
- TACITE/PIPEPHASE

- PIPETECH
- gCCS

The capabilities of the models are summarised in the following paragraphs.

7.4.1.1 *PIPEBREAK*

The DNV-GL consequence model PHAST incorporates two, time-varying models for long pipelines; GASPIPE for vapour releases and PIPEBREAK for liquid releases (Witlox et al. 2011). PIPEBREAK is an integral two-phase flow model which can simulate both choked and unchoked flow conditions, and is therefore suitable for fluids that boil at temperatures significantly below ambient (Webber et al. 1999).

7.4.1.2 *MORROW*

The TNO consequence model EFFECTS incorporates two transient depressurisation models. The Wilson model is specifically for gas releases from long pipelines (Yellow Book third edition 1997, section 2.5.2.5), while the Morrow model was developed for releases of liquefied gas from long pipelines (Yellow Book third edition 1997 section 2.5.3.6) The Morrow model was originally developed to estimate the time-dependent flow rate of LPG from a damaged pipeline (Morrow et al. 1983).

7.4.1.3 *OLGA*

OLGA is widely used in the oil industry and is available from Slumberger[35]. The single-component two-phase module of OLGA, which uses the Span-Wagner equation of state, is regarded as the most suitable for CO_2 transport although it is unable to account for the presence of impurities (Aursand et al. 2013).

The performance of OLGA was evaluated during the depressurisation of a 50km long, 24 inches diameter CO_2 pipeline, where it was found that the presence of small amounts of impurities caused the model simulations to differ significantly from the measured data (Clausen et al. 2012).

(Munkejord et al. 2013) provide some useful examples of the application of OLGA in the design of CO_2 pipelines.

(Esfahanizadeh and Dabir 2013) used the commercial package PVTsim (by Calsep – version 18), to predict the transient phase state and thermodynamic properties in a pipeline containing a mixture of CO_2, methane and water. PVTism uses the Soave-Redlich-Kwong equation of state, which is more accurate than the Span-Wagner EOS. PVTism was used to generate a fluid file as an input to OLGA, which was then used to model a full-bore rupture of a CO_2 pipeline. The calculated fluid release rate, velocity, temperature and solid CO_2 fraction were then used as an input to PHAST, which was used to model the dispersion behaviour of the resulting CO_2 plume.

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[35] www.software.slb.com/products/foundation/Pages/olga.aspx

7.4.1.4 LEDAFLOW

LEDAFLOW is a transient multiphase flow simulation tool available from Kongsberg[36]. It was mainly developed for three-phase oil-gas-water mixtures, and in its current form has not been validated for CO_2 transport simulations.

7.4.1.5 PIPEPHASE

PIPEPHASE is a hazard and risk assessment package that was developed to estimate the failure mode and frequency, the gas outflow rate, crater formation, dispersion, ignition and thermal effects for natural gas pipelines, and is available from DNV-GL[37]. It has not yet been validated for CO_2 transport simulations.

7.4.1.6 TACITE/PIPEPHASE

TACITE is a transient multiphase flow simulation tool that is currently licensed as an add-on module to PIPEPHASE[38]. The models of TACITE have been developed and validated for methane transport, and have not yet been validated for CO_2 transport (Aursand et al. 2013).

7.4.1.7 PIPETECH

PIPETECH is a transient multi-component simulation tool developed by Professor Haroun Mahgerefteh at Interglobe Limited, London. PIPETECH has a thermodynamics modules which can account for both CO_2 and impurities, uses the Homogeneous Equilibrium Model for two-phase flashing flow, and it has the ability to model the evolution of pipeline cracks via a coupled fluid-fracture model (Aursand et al. 2013).

PIPETECH is used by the HSE in the UK in determining advice to local land authorities on control of land use in the vicinity of major accident hazard pipelines. A study by HSL found that PIPETECH was able to produce satisfactory simulations of historical large-scale accidental LPG releases and provided a good comparison with measurements from a ruptured pipeline carrying natural gas (Webber et al. 2010).

The CO_2PipeHaz project found that PIPETECH was able to provide reasonably good simulations of experimental CO_2 release data, with a discrepancy of generally less than 10%. The model accounted for formation of solid CO_2 particles and predicted the experimentally observed pressure stabilisation near the triple point pressure. (Brown et al. 2014). The outflow code was subsequently integrated with CFD models to simulate releases from CO_2 pipelines in complex terrain (Woolley et al. 2014b).

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[36] http://www.kongsberg.com/en/kogt/products%20and%20services/flow%20assurance/flow%20assurance%20software/

[37] http://www.gl-group.com/pdf/Hazard_and_Risk_Management_DS.pdf

[38] http://iom.invensys.com/AP/Pages/SimSci_ProcessEngSuite_UpstreamOptimizationSuite.aspx

Access to PIPETECH is available through the coordinator of the CO_2PipeHaz project, Prof Haroun Mahgerefteh, University College London[39].

7.4.1.8 *gCCS*

gCCS is a part of the gPROMS suite of process modelling tools, available from Process Systems Enterprise Ltd[40]. It has been developed for design of all the major components of a CCS system, containing steady-state and dynamic models for power generation, through capture, compression, transmission to injection. The pipeline simulation model uses gSAFT to calculate the thermodynamic properties of the fluid. gSAFT is based on the SAFT-VR equation of state, which is suitable for use with CO_2.

In addition to these commercial models, many academic models have also been developed. In the Australian context, the Energy Pipelines CRC has developed a FLUENT model which accounts for the presence of impurities in the CO_2 stream. The model incorporates the GERG-2008 equation of state to simulate fluid decompression characteristics following a CO_2 pipeline rupture (Elshahomi et al. 2015).

7.4.2 Release characteristics

The ‘source term’ represents the physical and chemical properties of the escaping CO_2 stream. This includes a number of different aspects to consider, including whether the release should be regarded as ‘instantaneous’ or ‘continuous’, the orientation of the release, whether it is a jet or a pool, and whether it is single or multi-phase. Each of these is discussed below.

7.4.2.1 *Instantaneous or continuous release*

Actual accidental releases are nearly always time varying. Many transport and dispersion models can accept inputs of time-varying source terms (e.g. mass-emission rate, volume flux, temperature and density, aerosol content, etc.). However, several of the older and/or simpler models require specification of whether the release is instantaneous or continuous (over a finite duration t_d).

The standard definitions are based on the view of the cloud at the release point. An instantaneous release is one that only occurs over a relatively limited period of time (a few seconds at most) and 'looks like' a puff, whereas a continuous release has an extended duration and the emission rate is nearly continuous in time. From the point of view of the concentration time series seen at a specific receptor at a distance X, a source that is continuous over a time period t_d will produce a puff-like time series at that location if $t_d << X/u$, where u is the wind speed (Britter and McQuaid 1988). The distinction between a puff-like or plume-like cloud shape and concentration time series at a given location thus depends on t_d, X, and u.

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[39] http://www.ucl.ac.uk/chemeng/people/magherefteh/profile

[40] http://www.psenterprise.com/gproms.html

The time required for the released CO_2 to reach a downwind distance, X/u, is compared to the actual emission duration t_d. If the emission duration is longer than the time it takes for the CO_2 to reach a downwind distance of interest, the release may be considered continuous (Britter and McQuaid 1988). Otherwise, the release should be modelled as being instantaneous (Hanna et al. 2012).

7.4.2.2 *Orientation of the release*

It is also important in the near-field (X < about 100 m) to characterise the orientation of the release aperture. A horizontal release at ground level will have different dispersion characteristics in the near-field than a vertical release, and a semi-stagnant release in a bunded area or crater may behave differently again, depending on the cloud's locally defined Richardson number (Ri*), (refer to section 8.3.2.4).

The momentum of the CO_2 release is also an important factor to consider. A high velocity jet will entrain ambient air more rapidly and thus may lead to different dispersion behaviour than a slow release from a shallow depression. However, as stated above, if the release is of finite duration and the receptor of interest is sufficiently far downwind, the nature of the release is less significant than the total quantity emitted (Hanna et al. 2012).

7.4.2.3 *Phase composition of the release*

If the CO_2 emerges from the rupture initially in liquid form, and has a sufficiently large superheat, it will rapidly flash into a two- or three-phase mixture, comprising gaseous CO_2, aerosol droplets of liquid CO_2, and possibly finely-dispersed particles of solid CO_2. The two (or three) phase mixture will have an effective density larger than that of pure CO_2 gas alone. When aerosols are present, the density can be as high as 20 to 30 times that of ambient air.

The pressure in the initial momentum jet may not decrease to ambient pressures until several metres from the hole. The worst-case (i.e. maximum downwind concentrations) would assume that the CO_2 is all in the liquid phase as it passes through the hole, and the Bernoulli formula for mass emissions of a pressurized liquid will apply. If flashing occurs at or before the hole, the emission rate might be 5-10 times less than the worst-case Bernoulli mass emission rate.

The tools for modelling dense phase CO_2 releases have improved significantly in recent years. (Gant et al. 2014) provide a comprehensive overview of these developments.

(Energy Institute 2010b) recommended the use of two-phase flashing flow models, ignoring any solid formation. In such applications, (Britter et al. 2011) recommend that the (Leung 1995, 1990) Omega model for flashing jets be used. Other models for flashing jets exist but most give similar results (within a factor of two or three) because they have all been developed and/or tuned to the same field and laboratory tests.

(Webber 2011) presented a strategy for extending existing two-phase homogeneous integral models to the three-phase case.

DNV-GL has modified its PHAST software package to account for the effects of solid CO_2, with new formulas for flashing, source emissions rate, and solid particle size distributions (Witlox et al. 2009; Witlox et al. 2011). The revised PHAST version 6.6 was validated against near-field experimental release data (Witlox et al. 2013a).

Researchers at TNO have developed a semi-empirical model for solid CO_2 particle size in CO_2 jets. Simulation of large-scale CO_2 releases indicated that the final solid particle size would only be of the order of a few microns (Hulsbosch-Dam et al. 2012). This source term model will be included in the new EFFECTS version 10 simulation package, due for release in the coming months[41].

As part of the COOLTRANS programme, researchers at the University of Leeds developed a model for three-phase sonic jets of CO_2 (Wareing et al. 2013), which was validated against experimental data for dense gas pipeline release (Wareing et al. 2014).

The recent experimental trials of full-scale dense phase CO_2 pipeline ruptures have led to significantly improved models for dense phase CO_2 jet release. At the outset of this work there was a concern that a large pipeline rupture would lead to the formation of solid CO_2 'dry ice' particles, which could 'snow out' to form a solid deposit that would subsequently slowly sublimate (Molag and Dam 2011). In such an event, there was concern that the slowly-subliming bank of dry ice snow would create a longer-lasting health hazard. In such a scenario, the source term would have to include a separate ‘pool area’ source.

‘Snow out’ of dry ice was not observed in any of the recent COOLTRANS large-scale dense phase CO_2 release experiments (Allason et al. 2012). At this stage there is no way to estimate the likelihood of extensive ‘snow out’ following a catastrophic CO_2 pipeline failure, involving larger volumes and longer times of release, as such an event has never occurred.

7.4.2.4 *Conservative release characteristics*

For consequence assessment purposes, it is often sufficient to consider the most conservative set of release characteristics, i.e. the ‘worst case scenario’. It may not be considered necessary to evaluate the discharge rate as a function of time, but only the maximum discharge rate.

For dense-phase CO_2 pipelines, the maximum discharge rate will occur in the first minutes after release. For example, when a 50 km long, 600 mm diameter pipeline carrying supercritical CO_2 was vented through a 200 mm valve, the maximum discharge rate was reached within the first minute. By 5 minutes the rate had fallen below 50% of the maximum, and to 25% by 30 minutes (Clausen et al. 2012).

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[41] van Swinderen J (2014) TNO Urban Environment & Safety, email communication, 7 July

The current recommended guidance for CO_2 pipelines

> *is to approximate (in a suitable modelling software package) the time-varying flowrate from the long pipeline with the average release rate over 20 seconds. This gives what is believed to be a conservative set of results. Where more accurate and less conservative results are required, and there is a rapid variation in the release rate of carbon dioxide, then the more rigorous time varying along-wind-diffusion method should be used.* (Energy Institute 2010b).

For methane pipelines, AS 2885.1[42] requires that the energy release rate or radiation contour be established by

> *calculation of the quasi-steady state volumetric flow 30 seconds after the initiating event, determined by a suitable unsteady state hydraulic analysis model, and the relevant equivalent hole size. The calculation shall assume the pipeline is at maximum allowable operating pressure (MAOP) at the time of gas release*.

For consequence analysis of CO_2 pipelines in accordance with AS 2885.1, the choice of whether to use a release rate averaged over the first 20 or 30 seconds of release is somewhat arbitrary. There is likely to be little practical difference between the two values, so either method would seem to be appropriate.

In most instances, it is conservative to assume that the CO_2 release is horizontal at ground level, and that the terrain is flat. This scenario would minimise the dispersion of the CO_2 cloud before it reaches a downwind receptor.

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[42] AS 2885.1 – 2012 Section 4.10

8 CO_2 DISPERSION MODELLING

8.1 Summary

This Chapter considers the criteria that must be considered for a dense gas dispersion model to be considered ‘fit for purpose’ in the design of a CO_2 pipeline in Australia. It reviews the different types of models that have been developed, their validation, their limitations, their suitability for different stages of the design process, and their availability. It discusses the ability of different models to calculate the ‘source terms’ specific to a CO_2 release, and their ability to account for complex terrain and variable atmospheric conditions. This section also discusses the uncertainties associated with the predictions of dense gas dispersion models, and how these can be taken into account during consequence analysis. Finally, this section reviews the regulatory status of dense gas dispersion models, both overseas and in Australia, and provides examples of the previous use of specific models in the design of commercial CO_2 pipelines. This overview allows a recommendation of models that may be considered ‘fit for purpose’ for CO_2 pipeline design in Australia.

8.2 What is meant by ‘fit for purpose’

To date, only two CO_2 pipelines have been built in Australia. Both of these (totalling about 15 km) are in Western Australia, and were permitted under the Petroleum Pipelines Act 1969 (WA) with no requirement for dense gas dispersion modelling.

The Air Pollution Model (TAPM) has been evaluated for monitoring of CO_2 leakage from geosequestration at the CO_2CRC Otway project in Victoria (Etheridge et al. 2011), but this model does not include dense gas dispersion capabilities. At the concentrations measured in this application, CO_2 can validly be simulated using a Gaussian dispersion model such as TAPM.

Consequently, most regulatory agencies in Australia have little to no experience with dense gas dispersion modelling. In Victoria, the Environmental Protection Agency specifies the use of AERMOD as its standard air pollution dispersion regulatory model (Vic-EPA 2013). However, AERMOD is a Gaussian dispersion model, and is not suitable for modelling dense gas dispersion.

In order for an AS 2885.1 safety management study to be undertaken for a new CO_2 pipeline in Australia, it will be necessary for design engineers and regulators to agree on the dispersion models that are suited to this task. Only models that are regarded as ‘fit for purpose’ will be acceptable.

There are several evaluation criteria to consider when conducting a ‘fit for purpose’ analysis, depending on the questions that the models under review will be used to answer. In this document, the goal is to understand whether available models can reliably simulate the release and dispersion of CO_2 from a pipeline, either as the result of an accidental release or the deliberate use of venting systems. The use of a ‘fit for purpose’ model during pipeline design would allow for better decision-making with regard to pipeline design and safety. Similarly, ‘fit for purpose’ models could also be used to prepare for and respond to any accidents involving the pipeline. To determine if a given dense gas dispersion model is ‘fit for purpose,’ this section evaluates the following criteria:

- Availability, ease of use, technical support – Is the model readily available for free download or purchase? Is extensive training required to run the model? Does use of the model require command-line data entry or is a graphical user interface available?
- Validation history – Have model results been compared to observations from actual release scenarios? Did such validation work confirm the general accuracy and precision of model results? Has model validation been conducted for CO_2 releases specifically, or only for other dense gas releases? Were validation scenarios similar to potential pipeline release scenarios?
- Ability to calculate appropriate source terms – Does the model simulate finite duration time-variable releases? Can the model simulate dispersion from different source types (e.g. horizontal and vertical jets, ground-level or elevated releases)? Does the model have the internal capability to calculate release rates and source jet thermodynamic conditions, or must release rates and other initial conditions be calculated separately and provided as a model input? Does use of the model require detailed, complex inputs and are they easily acquired?
- Ability to account for complex terrain and variable atmospheric conditions. Is the model able to simulate site-specific terrain and meteorological conditions?
- Applicability to different stages of the design process. Is the model fit for use in initial pipeline planning? Is the model fit for use in an emergency response situation? Is the model fit for use in the reconstruction of specific accidents?
- Acceptability to regulators – Have regulatory agencies in the United States, Europe and Australia previously endorsed specific models for CO_2 release modelling? Have particular models been used in previous CO_2 pipeline design efforts?

These criteria are described in more detail below, and each factor is evaluated for select models to determine their fitness for purpose in simulating a release from a CO_2 pipeline. Specific model limitations and possible measures to account for these limitations are also discussed, as relevant.

8.3 Dense gas dispersion phenomena

8.3.1 Characteristics of a dense gas release

In a dense gas release with small upwards-directed momentum and a sufficiently large cloud Richardson Number, the plume slumps to the ground and then diffuses horizontally.

The cloud Richardson number Ri* for a ground-based slumping cloud can be defined (Hanna and Chang 2001b) as:

$$Ri^* = \left(g\frac{(\rho_c - \rho_a)}{\rho_a}\right) h / _{u^{*2}}$$

where g is the acceleration of gravity, h is the local cloud depth, ρ_c is local cloud density, ρ_a is ambient density, and u* is the ambient friction velocity (equal to about 5% to 10% of the wind speed at a height of 10 m) (Hanna et al. 1996). Later paragraphs on Ri* use slightly different definitions for the cloud length scale and the ambient atmosphere velocity scale, but all are based on the same fundamental scientific rationale.

Even if the release is a vertical upward jet, if the Ri* (modified so the length scale is plume width rather than h) is large enough, the plume will stop moving upward and turn downward as it moves downwind. When the cloud slumps to the ground, the momentum of the fall may cause the centre of the cloud to dip while the edges bulge.

If Ri* is large enough, the interior of the dense gas cloud may be characterised by a lower degree of vertical turbulent mixing than in a neutrally buoyant gas cloud, which may tend to stabilise the cloud and allow it to flow over the ground surface. Depending on wind speed, the pancake-shaped cloud may elongate and spread as the wind moves it along, but may linger in the vicinity of the source region for extended periods of time (e.g., an hour or more) or follow the downhill slope and can pool temporarily in valleys and low spots (Koopman and Ermak 2007) and (Hanna et al. 2012).

If Ri* is large, this dense gas slumping cannot be adequately modelled using the standard Gaussian models used to characterise the atmospheric dispersion of most industrial pollutants, which have neutral or positive buoyancy. Moreover, complete characterisation of the dispersion of CO_2 released from a pipeline under supercritical conditions requires a detailed understanding of a range of interrelated phenomena, including:

- The pressure in the pipeline as it progressively empties during venting;
- Whether the release is ‘instantaneous’ or ‘continuous’ or 'transient';
- Whether the release has high or low momentum, and the height and direction of release;
- The near-source (downwind distance (X) < about 100 m) nature of the release, e.g. its composition and flowrate, and whether it contains liquid drops or solid particles;
- The impaction of the dense two-phase jet on surfaces (e.g. ground, terrain slopes, buildings, tanks, pipes, vehicles, vegetation);

- The rate of entrainment of air with the gas stream, and the resulting intensity of turbulence within the gas cloud;
- The longer-range dispersion of the gas cloud under the influence of weather conditions and local terrain;
- The closer-range dispersion in the presence of buildings or other obstacles; and
- The effects of turbulence-induced concentration fluctuations on the harm impact at specific sites downwind.

Each of these aspects is discussed in greater detail in the following sections. Note that the standard reference text covering this material is (Hanna et al. 1996), which should be regarded as a first point of reference for the new reader. The material that follows is intended to serve as a primer in dense gas dispersion modelling, and to provide an update on relevant recent developments in the field.

8.3.2 Aspects to be modelled

8.3.2.1 Source term

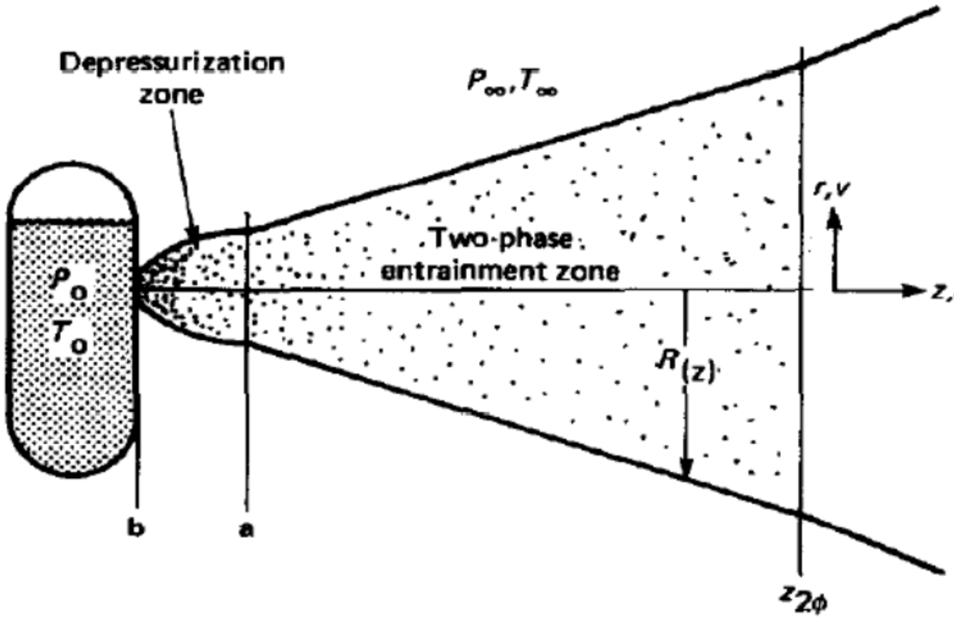
The ‘source term’ describes the characteristics of the CO_2 emission at the point of release. The issues involved in selecting and quantifying an appropriate source term were described in Chapter 7.

Ideally, a suitable model would include the ability to account for any source term of interest. Otherwise, it may be necessary to input the source term conditions manually, or couple the dispersion model with a suitable source term model.

8.3.2.2 Entrainment zone

A short distance downstream of the point of release, air will be entrained into the CO_2 stream because of the large velocity difference between the jet and the ambient air. This will increase the volume and reduce the velocity of the gaseous stream. The resulting ‘entrainment zone’ is shown in Figure 8.1.

Figure 8.1: Entrainment zone between release jet and dense cloud



Most current models do not assume entrainment into the jet while flashing is underway and start to parameterize entrainment after flashing ceases and the jet pressure has decreased close to ambient.

A jet of CO_2 will contain both vapour and solid CO_2 particles at the sublimation temperature of -78^{o}C. In the entrainment zone, the CO_2 vapour is diluted with air, reducing the vapour pressure and causing the solid CO_2 particles to sublime. As a result, the temperature in the jet can fall to as low as -100 ^{o}C. The temperature follows the saturation curve for solid-vapour equilibrium in the (vapour) pressure-temperature phase diagram as the distance from the orifice increases. This process continues up to the point where all of the solid CO_2 has been sublimated. Further entrainment into the jet beyond this point causes the temperature to increase, as the cold CO_2-air stream mixes with warmer ambient air (Dixon et al. 2012).

Generally, the thermodynamic effects associated with jet expansion and reduction to atmospheric pressure are important only in the first few metres near the source, and have negligible effect on ground level concentrations at downwind distances of 100 m or more (Hanna et al. 1996). Based on the large-scale release data to date, it is expected that any solid CO_2 particles will sublimate relatively quickly due to the low boiling point of CO_2, similar to the evaporation of aerosol droplets in Cl_2 and NH_3 releases. At distances beyond about 100 m it is likely that all of the mass is in the gas phase, eg (Witlox et al. 2011).

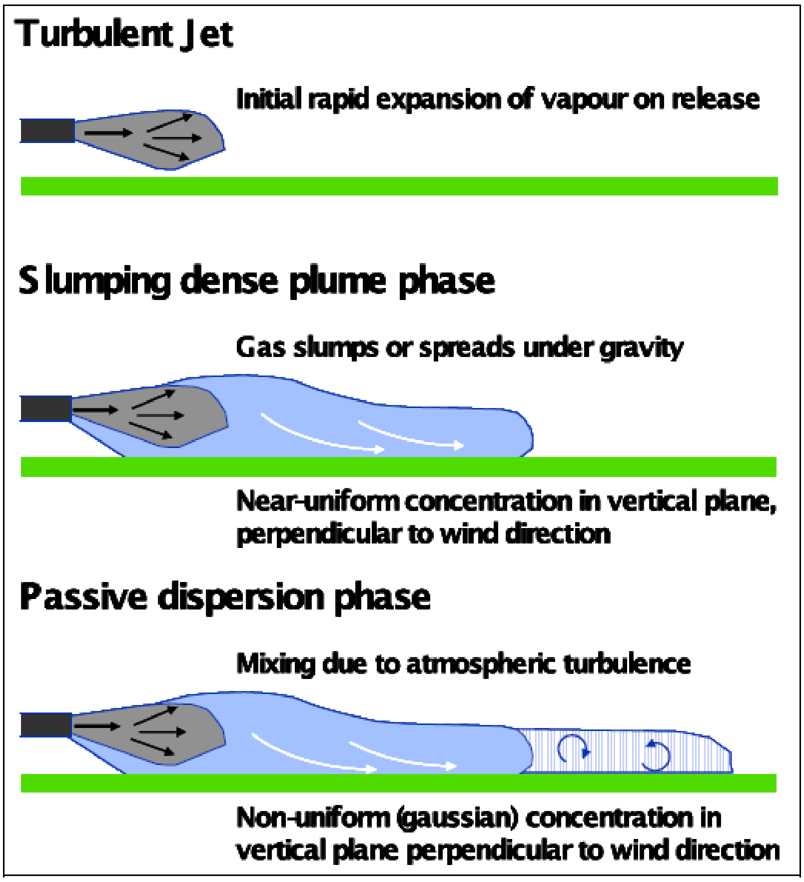
8.3.2.3 *Dense gas dispersion*

According to (Hunt et al. 1984), in general, dispersion of a dense gas may be expected to pass through four phases:

- In the initial phase, the motion of the cloud is predominantly determined by the inertia of the cloud and the mean atmospheric flow.
- In the gravity spreading phase, both buoyancy and the external mean flow are the dominant forces.
- In the nearly-passive phase, external ambient turbulence also becomes a significant force.
- In the passive phase, the motion of the cloud is entirely controlled by the external ambient turbulence and the external mean flow.

Such 'typical' behaviour for a horizontal, ground-level release is illustrated in Figure 8.2.

Figure 8.2: Generalised development of a dense gas cloud



However, it is possible that the dense two-phase cloud may be so large (i.e. very large Ri*) that it is not quickly entrained into the passing ambient air flow. Instead, when ambient winds are low, it may form a dense, shallow, nearly-stationary cloud that stays around the source area for many minutes (Hanna et al. 2012).

This phenomenon was observed during the COOLTRANS experimental programme, where it was found that the dispersion behaviour of the CO_2 cloud depended the size and direction of the release, as well as the wind speed. It was observed that the CO_2 plume could either blow away and slump to the ground some distance away, or else form a ground level ‘blanket’ surrounding the source, as shown in Figure 8.3. The ‘blankets’ tended to be produced by lower momentum releases in lower wind speeds (Allason et al. 2014).

Figure 8.3: Vertical discharge versus ‘blanket’ formation

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These observations are consistent with established dense gas dispersion theory. In in a vertical jet release of a dense gas, the velocity and concentration of the rising gas cloud are strongly affected by dilution with entrained ambient air, which is a function of both the jet velocity and the wind speed (Ooms and Duijm 1984).

8.3.2.4 Neutral gas dispersion

Because the CO_2 cloud is continuously being diluted by entrained ambient air, the dense gas regime will eventually be followed by a regime in which ambient turbulence dominates the dispersion. The distance from the source at which this occurs will depend upon the size of the release and the wind speed. It is appropriate to apply dense gas models if the initial potential energy of the CO_2 cloud is significant when compared with the kinetic energy of the ambient air. The ratio of these two energies is characterised as the initial Richardson number, Ri_o (Hanna et al. 1996).

The following specific definitions of Ri_o can be given in terms of known initial parameters:

Continuous plumes at ground level: $$Ri_o = \frac{g(\rho_{po} - \rho_a)}{\rho_a} \frac{V_{co}}{D_o u_*^3}$$

Instantaneous cloud at ground level: $$Ri_o = \frac{g(\rho_{po} - \rho_a)}{\rho_a} \frac{V_{io}}{D_o^2 u_*^2}$$

where $(\rho_{po} - \rho_a)$ is the difference between the initial plume density and the ambient density, V_{co} is the initial volume flow rate for continuous plumes, V_{io} is the initial volume of an instantaneous cloud, D_o is the initial cloud width, and u* is the friction velocity (Hanna et al. 1996).

Ri can also be defined locally (as Ri*) using the values of the parameters (e.g. ρ_p and D) at any downwind distance.

The transition from dense gas behaviour to neutral gas behaviour at the source location or at any downwind distance is typically assumed to occur at a critical value of Ri_o or Ri* of about 50. From that point, it is appropriate to model the gas cloud dispersion using a standard Gaussian atmospheric dispersion model.

8.3.3 The significance of density

Just because a release is dense at the point that it enters the atmosphere, it does not follow that a dense gas model has to be used. For small releases and/or small concentrations, it is adequate to use a passive (neutral) gas model (Britter and McQuaid 1988). This is why SF_6 can be used as a passive tracer in the atmosphere. Since it can be detected at tiny concentrations and the background is usually very low, only a small amount of tracer must be released. Within a metre from the source, the concentration drops to 1% or less and the excess density effects are insignificant.

(Hanna et al. 1982) review the formulations in passive (neutral) gas dispersion models, which are much more numerous and more thoroughly evaluated than dense gas dispersion models. The most widely used passive gas dispersion model in the U.S. for industrial sources is the EPA's publically-available AERMOD (Cimorelli et al. 2005; Perry et al. 2005). These models do include buoyant plume algorithms to treat the rise of the heated stack plume. TAPM has a similar role in Australia (Hurley 2008), and has recently been used for calculating dispersion of slow seepage of CO_2 gas from area sources above sequestration sites (Etheridge et al. 2011). The emission rate of CO_2 was sufficiently small that it behaved as a passive gas.

The effective density of CO_2 could be as much as ten or twenty times that of ambient air. But is it necessary to account for this increased density when modelling the CO_2 plume? The effective density of the released CO_2 is due to three effects: larger molecular weight, two-phase release with imbedded tiny aerosols, and cold temperature. Due just to the molecular weight effect, CO_2 gas is about 50 % denser than air at ambient temperatures and pressures, and when the pressurized liquefied CO_2 is released, it will flash to a mixture of gas and solid particles, causing evaporative cooling and causing the presence of imbedded solid particles. If CO_2 gas is at its boiling point, the density difference with respect to ambient air increases by another 10 to 20 %.

As mentioned earlier, the initial Richardson number Ri_o of the cloud must exceed a critical value, Ri_c, of about 50 before it is necessary to account for the increased density. If $Ri_o < Ri_c$, then the scenario can be modelled with a passive (neutral) gas dispersion model. If $Ri_o > Ri_c$, then a dense gas model should be used until downwind distances are reached where the local $Ri^* < Ri_c$.

Most dispersion models employ arbitrary assumptions marking the transition point between the dense gas and passive gas algorithms. The most commonly used transition assumption is that dense gas effects cease when the density perturbation $(\rho_{po} - \rho_a)/\rho_a$ drops below some limit (e.g., 0.01 or 0.001) (Hanna et al. 1996).

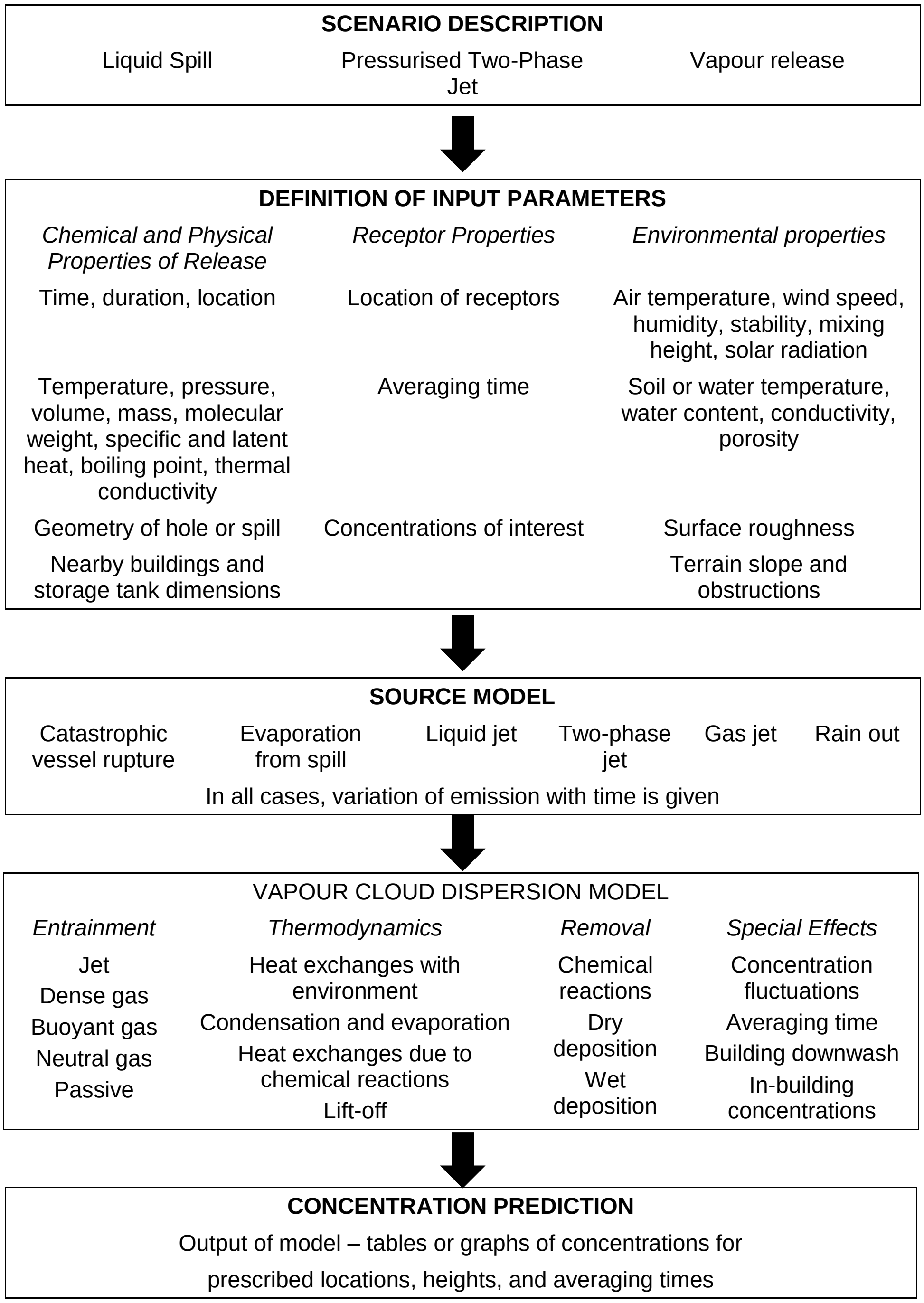
A value of 0.01 is consistent with recent results obtained within the COOLTRANS programme. HSL performed a sensitivity analysis using PHAST for horizontal jet releases of dense-phase CO_2. The results showed that the wind speed only started to have a significant effect on the dispersion behaviour once the CO_2 concentrations had fallen below 1 vol% CO_2 (Gant et al. 2013).

Therefore, it may be assumed for consequence analysis purposes that CO_2 will behave as a dense gas at all concentrations of importance to human health.

8.4 Overview of modelling sequence

Implementation of a model simulation of the dispersion of a dense gas requires a sequence of individual calculations, as summarised in Figure 8.4.

Figure 8.4: Summary of modelling sequence



SCENARIO DESCRIPTION

Liquid Spill	Pressurised Two-Phase Jet	Vapour release

DEFINITION OF INPUT PARAMETERS

Chemical and Physical Properties of Release	*Receptor Properties*	*Environmental properties*
Time, duration, location	Location of receptors	Air temperature, wind speed, humidity, stability, mixing height, solar radiation
Temperature, pressure, volume, mass, molecular weight, specific and latent heat, boiling point, thermal conductivity	Averaging time	Soil or water temperature, water content, conductivity, porosity
Geometry of hole or spill	Concentrations of interest	Surface roughness
Nearby buildings and storage tank dimensions		Terrain slope and obstructions

SOURCE MODEL

Catastrophic vessel rupture	Evaporation from spill	Liquid jet	Two-phase jet	Gas jet	Rain out

In all cases, variation of emission with time is given

VAPOUR CLOUD DISPERSION MODEL

Entrainment	*Thermodynamics*	*Removal*	*Special Effects*
Jet Dense gas Buoyant gas Neutral gas Passive	Heat exchanges with environment Condensation and evaporation Heat exchanges due to chemical reactions Lift-off	Chemical reactions Dry deposition Wet deposition	Concentration fluctuations Averaging time Building downwash In-building concentrations

CONCENTRATION PREDICTION

Output of model – tables or graphs of concentrations for prescribed locations, heights, and averaging times

8.5 Types of dense gas dispersion models

There is a wide range of dense gas dispersion models that have been developed since the 1970s, by academics, industrial researchers, consultancies, the military and regulatory agencies. (Markiewicz 2012) provides a good overview that illustrates the diversity of models that have been developed over the years.

It is not the intention of this section to provide a comprehensive survey of all the dense gas dispersion models ever developed. Instead, this section focuses on several models that are currently available and may be potential candidates for this ’fit for purpose’ analysis.

These models fall into four categories:

- Empirical correlations
- Integral models & shallow layers
- Lagrangian puff and particle dispersion models
- CFD models.

Table 8.1 shows the models that were considered.

Table 8.1: Summary of models

Model Category	Model Name	
Empirical correlations	‘Workbook on the dispersion of dense gases’ is the main reference.	
Integral	HGSYSTEM	SAFER/TRACE
	SLAB	GASTAR
	DEGADIS	PHAST
	ALOHA	EFFECTS
Lagrangian	QUIC	ArRisk
	SCIPUFF	CHARM
CFD	FLUENT OpenFOAM PANACHE	FLACS ANSYS-CFX

8.5.1 Empirical correlations

This type of model seeks to relate several quantities by an empirical relation, assuming that the experimentally-derived relationship is applicable under other conditions. For example, these models provide a correlation between the centreline concentration and downwind distance for either instantaneous or continuous dense gas releases.

The empirical relations should be based on fundamental science principles (for example, dimensional analysis).

The best known example is the equations and nomograms in the ‘Workbook on the dispersion of dense gases’ (Britter and McQuaid 1988). Experimental data from many laboratory and field studies were plotted in dimensionless form, and are intended to provide guidance that incorporates the primary physical principles.

These correlations do not account for variables such as surface roughness length, averaging time or atmospheric stability conditions, and the effects of the initial source are assumed to be unimportant at the downwind distances of interest (Hanna et al. 1996). Nevertheless, in the (Hanna et al. 1993a) evaluation of several dense gas models with data from several field experiments, the Britter and McQuaid formulations provided just as good agreement with observations as the other more complicated models.

The Workbook correlations are regarded as a useful tool, and provide a convenient method to estimate the behaviour of dense gas clouds. The nomograms correlate well with the available large-scale experimental data, and are suitable for use within the range of data covered by the field observations. The Workbook correlations are only recommended for use as a benchmark screening model, and should not be applied to scenarios that are not very closely related to the original observations (Hanna et al. 1996). This means that they may not be suitable for use in modelling large-scale releases of CO_2, which fall well outside the bounds of the experimental data used in the Workbook. The fundamental dimensionless relations are probably still valid, although the scaling 'constants' and power law coefficients may be different.

8.5.2 Integral models

Integral models assume that the gas cloud has a dense central core, with Gaussian edges to the sides and vertically (Colenbrander 1980) and (te Riele 1977). They use ordinary differential equations (as opposed to partial differential equations) to describe the bulk properties (or integral properties) of a dense gas cloud, including the radius of the gas plume, the plume’s velocity, and centre line concentrations within the gas plume. Dense gas dispersion is typically modelled from a point just downstream of the source to a point where the density of the cloud becomes ‘neutral’. After this point the cloud can be modelled using standard Gaussian atmospheric dispersion models. Integral models may have the capability to calculate release rates, but often the strength of the source and release rates over time must be calculated separately using a separate source term model.

Shallow Layer models are based on equations developed for shallow water scenarios. They use depth-averaged variables to describe the flow behaviour using equations originally developed to model the flow of bodies of water. However, the basic approach is similar to the integral models for dense gas dispersion in air.

The integral models considered herein are: HGSYSTEM, SLAB, DEGADIS, ALOHA, SAFER TRACE, GASTAR, PHAST and EFFECTS. The shallow layer models considered herein are SLAM, DISPLAY, TWODEE, DENS20. An overview of each model is provided below.

8.5.2.1 *HGSYSTEM*

HGSYSTEM is a suite of programs designed by Shell Research Ltd and select industry groups to assess the release of gases, liquids, and two-phase mixtures from a variety of sources and the subsequent dispersion of heavier-than-air and neutrally buoyant gases (Shell 1994). The suite of HGSYSTEM model components may be used separately or consecutively to describe a release from a source, near-field dispersion, and far-field dispersion (Fthenakis 1999). This system utilizes the HEGADAS program, which was the first integral model code developed for heavy gas dispersion. The code was originally developed to treat dispersion of LNG vapor evaporated from the surface of a spilled pool (i.e., an areas source). Further development of HEGADAS is described by (Witlox 1988). HGSYSTEM also includes models for initial two-phase jet releases and for instantaneous puff releases. Details on HGSYSTEM are available at www.hgsystem.com, where the code can be downloaded for free. The HGSYSTEM does not have an inbuilt Graphical User Interface (GUI) and must be run using a command prompt window and a text editor to modify the input files. The modular nature of HGSYSTEM, the versatility of the system, and the lack of a GUI increase model complexity, requiring more substantial training in the model.

Shell uses the Fire Release Explosion Dispersion (FRED) software that incorporates HGSYSTEM, and it used to be sold as a commercial package. However, since 2012 FRED continues to be used by Shell but is no longer commercially available.

8.5.2.2 *SLAB*

The SLAB model was developed by the Lawrence Livermore National Laboratory of the United States to simulate the atmospheric transport and dispersion of dense gases (Ermak 1990). The code for SLAB is freely available for download from the US EPA website (US-EPA 2012) and may be run using a DOS prompt window. The US EPA used SLAB to develop the tables in its RMP (Risk Management Plan) Guidelines. A GUI for SLAB, called SLAB View, can be purchased from Lakes Environmental (Lakes Environmental 2014). SLAB (with a GUI) is also available in the following commercial packages:

- BREEZE (Breeze 2014).
- EFFECTS (TNO 2014)
- CANARY (Johnson and Cornwell 2007) (Quest 2014)

SLAB is generally considered to contain excellent science, and is relatively easy to use, particularly with a GUI, though specific training in the model design and input-output parameters is required.

8.5.2.3 *DEGADIS*

The Dense Gas Dispersion (DEGADIS) model was originally developed for the United States Coast Guard and the Gas Research Institute to simulate the atmospheric dispersion of dense gases following LNG spills (Havens and Spicer 1988). Algorithms for simulating two-phase jet releases were added in the 1990s. The code for DEGADIS is freely available for download from the US EPA website (US-EPA 2012) and may be run in a DOS prompt window. A simplified version of DEGADIS is used as the dense gas model in ALOHA. DEGADIS (with a GUI) is also available as an option in the BREEZE Incident Analyst software package (Breeze 2014). DEGADIS is considered to be relatively difficult to use, particularly. Substantial training in model design and input-output parameters is required.

8.5.2.4 *ALOHA*

ALOHA (Areal Locations of Hazardous Atmospheres) was developed by the United States Environmental Protection Agency and National Oceanic and Atmospheric Administration to simulate airborne releases of hazardous chemicals (Reynolds 1992). Most fire departments in the US have CAMEO/ALOHA. The United States National Safety Council distributes ALOHA and provides technical support. ALOHA can be used to model the release and dispersion of both neutrally buoyant and dense gases. Dense gas dispersion within ALOHA is based on the DEGADIS model, though the DEGADIS variant included within ALOHA has been simplified. ALOHA users may choose between several specified release options, including a gas leak from a ruptured pipe. Based on the selected scenario, the program will calculate the release rate as a function of time. The user may also specify a release rate using the direct source option (US-EPA 2007). ALOHA is freely available as part of the CAMEO (Computer-Aided Management of Emergency Systems) suite of software applications (US-EPA 2014). This suite includes a freely available GUI that is easy to use and is used by many fire departments and emergency responders in the United States. The model includes a database of chemical parameters for a number of chemicals, including CO_2 and default options for source emissions. The ALOHA GUI has been specifically designed for simplicity of use in the emergency response environment.

8.5.2.5 *SAFER TRACE*

The SAFER Systems TRACE (Toxic Release Analysis of Chemical Emissions) module is a dispersion modelling tool that can simulate a wide range of accidental toxic gas releases, including those associated with dense gas releases. The program is menu driven, and contains several separate modules to estimate the release and dispersion of chemicals. SAFER TRACE is a commercially-available set of consequence assessment tools and is available for purchase (Safer Systems 2014). SAFER TRACE is designed for speed and ease of use, though specific training in the model design and input-output parameters is required.

SAFER/TRACE is often purchased along with a comprehensive system that includes an on-site meteorological tower, on-site computers, and automatic communications to plant managers and emergency responders. It was once a fully-owned subsidiary of Dupont, who installed the system at many of their plants, but has been an independent company for the past 10 years.

TRACE scientists have contributed model outputs to several model comparison studies such as (Hanna et al. 1993b; Hanna et al. 2008), and are currently active members of the modelling group for the Jack Rabbit II chlorine field experiment.

8.5.2.6 GASTAR

GASTAR is a dense gas dispersion model developed by Cambridge Environmental Research Consultants (CERC 2009) in association with the HSE. Rex Britter was the primary developer of GASTAR and original author of the technical documentation. GASTAR can model dispersion of dense gases from a number of accident and emergency response scenarios. However, GASTAR is unable to calculate the source terms for all these scenarios, so they must be provided by the user.

GASTAR can be purchased from CERC (CERC 2014). The application has a Windows friendly GUI, simplifying input data entry and providing flexible examination of output. Although GASTAR is also supplied with a database of material properties for common toxic and flammable substances, CO_2 is not included in the database and the physical properties of CO_2 must be added by the user. GASTAR is designed to be as straightforward as possible, though specific training in the model design and input-output parameters is required.

8.5.2.7 PHAST

Process Hazard Analysis Screening Tool (PHAST) is a consequence analysis program for modelling accidental releases of hazardous materials (Witlox and Holt 1999). PHAST is available commercially from DNV-GL[43], a non-governmental organization that establishes and maintains technical standards, and supports this activity by undertaking in-house and sponsored research. The PHAST software is capable of assessing release rates from accidents and modelling subsequent dense gas dispersion. The PHAST GUI allows for a wide range of tabular and graphical output. PHAST is designed to be quick to setup and run and to require relatively limited training. PHAST has recently been enhanced to include results from CO_2 field experiments involving jets. The model has been widely evaluated against a comprehensive set of field observations and the results reported in the peer-reviewed literature.

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[43] http://www.dnv.com/services/software/products/phast_safeti/phast

8.5.2.8 EFFECTS

EFFECTS is a consequence analysis program for modelling hazards from accidental releases of hazardous materials. EFFECTS is available commercially from Netherlands Organisation for Applied Scientific Research (TNO 2014), which is an independent a non-profit organization. EFFECTS incorporates the SLAB dense gas dispersion model (Bakkum and Duijm 2005). EFFECTS is capable of assessing release rates from accidents and modelling subsequent dense gas dispersion, with the methods and calculations published in the 'coloured books' (TNO 2005a, b, d, c). The GUI allows for a wide range of tabular and graphical output.

8.5.2.9 Shallow layer models with methodology transferred from water modelling studies

Shallow Layer models are based on equations developed for shallow water scenarios. They use depth-averaged variables to describe the flow behaviour using equations originally developed to model the flow of bodies of water. However, the basic approach is similar to the integral models for dense gas dispersion in air. Complex terrain can be accounted for by including the downslope buoyancy force, while entrainment is included using empirical formulae (Hankin 2003).

A number of shallow layer models have been developed for dense gas dispersion, including SLAM (Shallow LAyer Model), DISPLAY (DISPersion using shallow LAYer modelling), TWODEE (TWO Dimensional shallow layer model) and DENS20. Both TWODEE and DENS20 have been used to simulate dense gas dispersion over complex terrain. DENS20 was used to simulate the Porton Downs Freon-air controlled release experiment (Lee and Meroney 1988), and TWODEE has been used to model the dispersion of natural CO_2 releases (Chiodini et al. 2010)

The use of shallow layer models has largely been superseded by CFD modelling techniques, so most are no longer available. A FORTRAN 90 version of TWODEE is available for download from Osservatorio Vesuviano (Datasim 2009), but this is not user friendly. The FORTRAN version was originally developed by HSE to support research into dense gas dispersion, but was not intended to be used as a risk assessment decision tool. A new version of the model, TWODEE-2, was recently evaluated as a possible alternative to CFD modelling, but was not recommended for practical use (Lisbona et al. 2014).

There are no shallow layer models that are available in user-friendly form for CO_2 dispersion studies, so this type of model will not be considered further in this report.

8.5.3 Lagrangian particle and plume dispersion models

Lagrangian particle and plume dispersion models have been developed to address the problem of characterising the dispersion of toxic gases in the presence of wind fields that are variable in time and space. The term Lagrangian in this case means 'following the flow field'. The transport and dispersion of either particles or puffs are simulated by Lagrangian models, and they can be applied to any type of terrain (flat, hilly, urban, forest canopy, etc). For example, (Kaplan and Dinar 1996) describe a Lagrangian particle model applied to built-up urban areas, which are characterised by complex flow phenomena in the wake of buildings and flow channelling in the streets.

In general, Lagrangian modelling involves tracing the trajectories of fluid markers (particles or puffs) in a turbulent flow field, using a coordinate system that follows the fluid flow. The flow field is typically modelled by combining an initial wind field with a number of empirical correlations describing the turbulence structure. In urban applications, additional empirical correlations are provided for wakes formed on the upwind, lee-side and far-wake regions associated with buildings. The velocity and acceleration of a fluid particle are characterised in terms of the Lagrangian turbulent velocity and the Lagrangian time scale (Kaplan and Dinar 1996).

Lagrangian models are very well suited to simulating passive dispersion, where the flow field (i.e. wind) is essentially fixed and the particles or puffs follow the flow. However, for dense-gas dispersion, the flow field is itself modified by the flow of dense gas. It is inherently a more coupled problem than passive dispersion. The benefits of using Lagrangian models to simulate dense-gas dispersion are therefore less clear.

However, simulations using Lagrangian dispersion models can be run relatively quickly, making this a useful method for use in emergency response situations.

The Lagrangian models considered herein are: QUIC, SCIPUFF and MicroSPRAY. An overview of each model is provided below.

8.5.3.1 QUIC

The Quick Urban & Industrial Complex (QUIC) dispersion modelling system was developed at the Los Alamos National Laboratory (LANL) in the USA to predict the 3-dimensional flow of pollutants around buildings and other obstacles. It is comprised of QUIC-URB, a model that computes a 3D mass-consistent wind field for flows around buildings, QUIC-PLUME, a model that describes dispersion near buildings, and a graphical user interface QUIC-GUI. The QUIC-PLUME model includes the ability to model the dispersion of heavier-than-air gases (Williams et al. 2005).

QUIC is currently available from LANL for non-profit research purposes only, but commercial licensing is currently under consideration. More than 200 research licences have been granted for QUIC, in applications ranging from urban micro-scale air quality, to dense gas dispersion for accidental releases, to homeland security applications[44]. Further details about QUIC are available from the LANL

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[44] M. Brown, personal communication, 2014

website[45]. As it is not commercially available, this model will not be considered in detail in this report.

8.5.3.2 *SCIPUFF*

The SCIPUFF (Second-order Closure Integrated Puff) transport and dispersion model uses a Gaussian puff methodology to provide a three-dimensional, time-dependent Lagrangian solution to the turbulent diffusion equations (Sykes et al. 1999). It solves the Navier-Stokes conservation equations to give a reasonable representation of buoyant jets and dense gas slumping effects. It can also represent flashing jets, evaporating droplets and the associated thermodynamics effects (Sykes 2010). The dense gas capabilities have been thoroughly evaluated with all available dense gas field experiments, and it was used in the (Hanna et al. 2008) comparison of several models to chlorine railcar accidents. It was recently updated to include the (Witlox et al. 2007) recommendations for estimating aerosol drop size distributions, and that version is currently being used as the primary model to plan the Jack Rabbit II chlorine field experiments.

SCIPUFF was originally developed in the 1980s for application to power plant stack plumes (Sykes et al. 1989), and the data archive from the Kincaid power plant field experiment was used for model development and testing at that time. SCIPUFF has subsequently been used by several US government agencies and industrial associations as a basis for their development of a number of different modelling platforms for various atmospheric dispersion problem scenarios. A few examples are listed below:

a) SCICHEM

The Electric Power Research Institute (EPRI), which sponsored the initial development of SCIPUFF in the 1980s, used the model as a basis for the development over the past 15 years of SCICHEM (SCIPUFF with CHEMistry), which represents detailed chemical interactions between pollutants in the plume and entrained ambient air. The main concern is fossil power plant plumes, where the chemical reaction system involves ozone, nitrogen oxides, and reactive hydrocarbons. SCICHEM is described by (Chowdhury et al. 2012) and SCICHEM 3.0 can be ordered through the EPRI website[46].

The version of SCIPUFF used in SCICHEM can simulate dense gas dispersion on a uniform slope. The model parameters have been adjusted to provide an acceptable fit against field-scale dense gas release data (Sykes et al. 1999). However, although SCICHEM can handle momentum jets and dense gas effects, it is almost exclusively

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[45] www.lanl.gov/projects/quic

[46] http://www.epri.com/abstracts/Pages/ProductAbstract.aspx?ProductId=000000000001025625

used for stack plume applications. It is not clear whether the momentum jet/dense gas algorithms in SCICHEM can easily be implemented through the model’s GUI[47].

The publicly-available SCIPUFF (recommended by the US EPA) has been widely distributed. The dense gas capability has been recently included, but must be requested specifically from the Sage developers.

b) CMAQ

SCICHEM has been incorporated as the so-called 'plume-in-grid' module in the US EPA’s Community Multi-scale Air Quality Model (CMAQ), a modular, open-source air quality management tool. This implementation has not included the dense gas module. CMAQ is an Eulerian grid model that typically runs on a regional domain with a horizontal grid size of 12 km (sometimes 36 km for much larger (continental) scales, and sometimes smaller (4 km) for urban scales), and thus cannot resolve any plumes with sizes less than the grid size. CMAQ is focussed on regional pollutants such as ozone and PM. To more accurately simulate plumes from large point sources, a model such as SCICHEM is used to simulate the plume transport and dispersion to distances where its size is larger than the grid size, after which it is 'absorbed' into the CMAQ grid. Because it slows down CMAQ to run the plume module, only the largest sources are usually modelled with SCICHEM. CMAQ can be downloaded via the US EPA website[48]. However, the developers did not have small-scale hazardous dense gas releases in mind.

Thus, it is concluded that, if SCICHEM is being considered for application to CO_2 pipeline releases, testing is required to assure that the GUI will support that type of application.

c) HPAC/SCIPUFF

The US Department of Defense (DOD) sponsored the development of the Hazard Prediction and Assessment Capability (HPAC) as a tool for predicting the effects of hazardous materials release into the atmosphere and its impact on civilian and military populations. HPAC includes the SCIPUFF atmospheric transport and dispersion model, with dense gas modelling capabilities. In complex urban environments, MicroSwiftSpray (MSS) or the Urban Dispersion Model (UDM) are used to calculate detailed flow and dispersion around individual buildings (DTRA 2008). The (Witlox et al. 2007) model for drop size distributions has been added in recent DOD applications for calculating releases of chlorine from railcars.

Chapter 14 of the SCIPUFF 2.2 technical document (Sykes et al. 2004), describes pool evaporation, momentum jet, and dense gas modules having been satisfactorily evaluated with many field data sets, including those in the widely-used Modelers Data Archive (MDA). The MDA includes the Burro (LNG), Coyote (LNG), Thorney

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[47] I. Sykes, personal communication, 2015

[48] http://www.epa.gov/amad/Research/RIA/cmaq.html

Island (Freon), Maplin Sands (LNG), Desert Tortoise (anhydrous ammonia), Goldfish (HF), and Kit Fox (CO_2). This information was published in (Sykes et al. 1999).

Besides SCIPUFF, the comprehensive HPAC model system also includes extensive databases for chemical and biological and radiological releases, and for various munitions. Terrain files are accessible and the model can obtain gridded time dependent meteorological data at any time from a special weather server maintained by the DOD. HPAC also includes exposure and health effects modules.

HPAC is available by license from the Defense Threat Reduction Agency to the US government, government contractors and educational institutions for non-commercial research[49]. SCIPUFF has been used as part of HPAC to investigate the consequences of large-scale accidental releases of chlorine (Hanna et al. 2008; Buckley et al. 2012). It is currently being used to simulate 10 ton releases of pressurized liquefied chlorine as part of planning for the Jack Rabbit II field experiments, planned for 2015 and 2016.

d) PC-SCIPUFF

In 2000 a public domain version of SCIPUFF was released, in which all defence-related sources (e.g. munitions characteristics) were removed. This version, known as PC-SCIPUFF, is available for download from Sage Management[50]. The original version (SCIPUFF 1.3) did not have any dense gas capabilities. However, a newer version, SCIPUFF 2.2 (Sykes et al. 2004), which does include flashing momentum jets and dense gas slumping, is also available on request by Sage Management. That version does not have an on-line Help document[51].

8.5.3.3 *MicroSPRAY*

SPRAY is a three-dimensional Lagrangian particle dispersion model developed by Arianet S.r.I. in collaboration with Aria Technologies SA. SPRAY is designed to simulate the atmospheric dispersion of pollutants at both ‘local’ scale (about 10x10 km^2 to 100x100 km^2) and ‘micro’ scale (about 1x1 km^2 domains with grid cells of the order of metres). The microscale option is known as MicroSPRAY, and is the appropriate version of SPRAY for use in consequence modelling. MicroSPRAY is available commercially as part of the Micro-SWIFT-SPRAY (MSS) package, distributed by AriaNet in Italy[52] and Aria in France[53]. SWIFT is a fast 3-D meteorological processor, which generates a mass-consistent wind field and turbulence patterns from supplied meteorological, topographical and building array

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[49] http://www.govexec.com/defense/2002/11/pentagon-distributes-software-for-modeling-effects-of-attacks/13014/

[50] http://www.sage-mgt.net/services-and-solutions/modeling-and-simulation/scipuff-dispersion-model

[51] I. Sykes, personal communication, 2015

[52] www.aria-net.it

[53] www.aria.fr

data. In addition to its use in the MSS package, SPRAY can also be coupled with other meteorological processors such as CFD (MERCURE/SATURNE) or mesoscale (RAMS/WRF) meteorological models.

MicroSPRAY can simulate continuous or instantaneous releases, time varying sources, elevated and ground level emissions, cloud spread at ground due to gravity, bouncing against obstacles as well as deposition on the ground. It is able to deal with two-phase (vapour-liquid) releases, aerosol evaporation and latent heat processes in the dispersing plume. It takes into account plumes without initial momentum and with arbitrarily orientation (horizontal, vertical or oblique in any direction), as well as pool evaporation. The present version of MicroSPRAY does not account for flashing of the liquid, as a separate source emission model is required (Mortarini et al. 2012). MicroSPRAY has recently been modified to simulate the dispersion of dense gases in complex terrain, and successfully validated against experimental field release data (Anfossi et al. 2010) (Mortarini et al. 2014).

A feature of SPRAY is that, like SCIPUFF, it predicts the variance of concentration fluctuations as a scalar quantity carried along by each particle (Tinarelli et al. 2010). In addition to calculating the ensemble mean concentration at any point downwind, SPRAY can also estimate the probability of the concentration exceeding the ‘threshold of harm’ at that point[54].

The MSS package can run on either Windows or Unix environments, and requires training in its use, particularly in coupling the program with the output of suitable emission models.

MSS is currently included as an option in the DOD HPAC/SCIPUFF modelling system. Its capabilities are similar to those of QUIC.

In addition, a user-friendly interfaced version, called ArRisk, is available from AriaNet, which includes the SPRAY code. ArRisk was developed in partnership with the Italian Institute for Occupational Safety and Injury Prevention, and was designed safety analysis, emergency planning and real-time emergency management. ArRisk includes a database of thermodynamic and risk parameters for more than 400 chemicals, including carbon dioxide. It can simulate two-phase discharge from punctured tanks or pipes and integrating the results with SPRAY. The GUI of ArRisk allows easy input of meteorological and topographical data (including buildings), and visualisation of the results using an embedded graphic system.

8.5.3.4 CHARM

CHARM (Complex Hazardous Air Release Model) is a commercial Lagrangian puff model available from CharmModel.com. Two versions of CHARM are available:

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[54] G. Tinarelli, personal communication, 2014

- The flat terrain version simulates a continuous release as a series of discrete puffs, which is a computationally quick approach, making this version of CHARM suitable for use in preliminary screening and emergency response scenarios.
- The complex terrain version uses a 3D grid to perform the simulation, which is slower but useful for more detailed simulations.

CHARM operates in the Microsoft Windows environment, with an intuitive GUI and familiar menus and dialogue boxes. It is documented and comes with an on-line help system.

CHARM calculates the radiation footprint, overpressure footprint, or concentration of a chemical plume, and predicts the dispersion of the release. Simulation results are presented as tables as well as 2D and 3D graphics.

CHARM makes use of a 3D mass-consistent diagnostic wind model, similar to what is done in SCIPUFF, MSS, and QUIC.

Lagrangian particle dispersion models may represent a ‘next generation’ dense gas modelling approach, as they have the potential to allow modelling of dense gas dispersion in complex terrain and urban environments.

8.5.4 Computational Fluid Dynamics models

Three-Dimensional (3D) Eulerian grid CFD models use a set of advection-reaction-diffusion partial differential equations to describe the atmospheric dispersion of chemical species. The equations that are being solved include the Navier Stokes equations of motion, the equation of state, and several thermodynamic and chemical equations. Unlike Integral models, which use ordinary differential equations to describe the bulk properties of a dense gas cloud, the Eulerian approach is to calculate the specific cloud properties at each individual node of a 3D grid.

Numerical Weather Prediction (NWP) models used for weather forecasting can be considered Computational Fluid Dynamics (CFD) models, although their typical horizontal grid size is about 10 km. For dense gas applications, CFD models have horizontal grid sizes of 1 to 10 m.

The main advantage of CFD models applied to dense gas scenarios over the integral models and Lagrangian puff and particle models discussed above is that they allow for the explicit representation of complex terrain and space and time variable meteorological conditions and their effects on gas flow and dispersion.

The main disadvantage of CFD modelling is that it is generally substantially more expensive and time-consuming than the use of the integral models, though modern commercial CFD models are somewhat more user friendly and faster than historical systems. Use of CFD modelling requires significant specialised expertise.

While CFD models produce a more precise answer that is variable in time and space, it has not been demonstrated that they are any more accurate than simpler models when compared with field experiment observations.

This report evaluates five specific CFD models: FLUENT, OpenFOAM, PANACHE, FLACS and ANSYS-CFX.

8.5.4.1 FLUENT

FLUENT is a general-purpose CFD platform that can simulate the physics of dense gas releases and dispersion, as well as a wide variety of other physical phenomena. The model is not explicitly set up to simulate releases of dense gases. To simulate such a release requires extensive modeller effort and expertise to prepare the scenario. The modeller must set up the parameters of the source itself and set up an atmospheric parameterization scheme using user-defined-functions. The modeller must build the 3D domain using computer aided design (CAD) software and mesh the modelling domain into a grid of discrete fluid cells. The modeller must also make a set of decisions regarding the use of physical models, numerical solver schemes, and solver convergence criteria. The sophistication of the simulation is scalable depending on the purposes of the modelling – at its most basic level, the software can simulate the dispersion of a dense gas tracer through a steady-state, neutral atmosphere. With a more complex setup, the software has the capability of handling complex source configurations, chemistry, and phase-change physics, heat transfer, and transient atmospheric flows using Large Eddy Simulation. FLUENT CFD software is distributed by ANSYS[55]. The model is typically licensed under an annual contract with a fee that is scaled to the computational capabilities of the licensee's computer platform. FLUENT is currently integrated into the ANSYS Workbench Platform GUI, which provides integration of CFD meshing and solving capabilities with a sophisticated CAD interface. Versions of the software are available for Windows and Linux environments. ANSYS offers an extensive set of training courses and resources for the user. The 'introduction to ANSYS FLUENT' is a 5-day workshop that is recommended for new users of the software. Additional courses are provided to help users gain expertise in meshing and various applications.

A FLUENT model has been used to simulate the dispersion of dense gases in urban environments (Meroney 2010) and over irregular terrain (Meroney 2012). However, the accuracy of this model has not been validated against field-scale dense gas release data.

In Australia, the Energy Pipelines Cooperative Research Centre (EPCRC) has developed a FLUENT model to simulate the release and near-field dispersion of a supercritical CO_2 jet release (Liu et al. 2014; Elshahomi et al. 2015).

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[55] ANSYS Inc (2014) Fluid Dynamics: ANSYS Fluent. http://www.ansys.com/Products/Simulation+Technology/Fluid+Dynamics/Fluid+Dynamics+Products/ANSYS+Fluent.

8.5.4.2 OpenFOAM

OpenFOAM is an open source CFD toolbox that contains an extensive set of modules to solve complex fluid flow problems. Since OpenFOAM is a general-purpose CFD model, it is not pre-configured to simulate the atmospheric transport and dispersion of dense gases. However, an experienced modeller can adapt OpenFOAM to simulate the release and dispersion of dense gases, as modules are available to simulate chemical reactions, complex turbulence, heat and radiation transfer, and other complex phenomena. The toolbox does not contain a GUI or convenient set of tools for developing the complex geometry and meshing often required for simulation of dense gas releases in the atmosphere. OpenFOAM does contain meshing tools, but they may be limited in capability and may require extensive modeller programming to use properly. Users typically employ 3rd-party CAD software to build the modelling domain and cell mesh, which can be converted for use in OpenFOAM.

OpenFOAM is a command-line driven set of tools, operated through a set of scripts. Model setup is conducted through user configuration of scripts and input files. The user must compile the CFD solver from the set of individual physics modules available. Therefore, OpenFOAM is highly complex and difficult to use, and requires extensive modeller training, skill, and experience to operate. To conduct atmospheric dispersion modelling of a dense gas, the user must build a modelling platform essentially 'from scratch,' combining the required physics modules. The modeller must build and prescribe the boundary condition modules and select a proper set of numerical schemes for the simulation. With the appropriate modeller, OpenFOAM is very flexible and can simulate a huge range of scenarios.

OpenFOAM is currently maintained and distributed by the OpenFOAM Foundation and OpenCFD Ltd. It can be freely downloaded at www.openfoam.org. The model is configured to work in a Linux environment, but several commercial companies have developed GUIs for use of the software in Windows, including CFD Support and blueCFD-Cored by blueCAPE[56]. OpenFOAM training is provided by OpenCFD Ltd comprising an introductory 'foundation' class, and an advanced class for general-purpose use of the software.

OpenFOAM has been used to simulate dense gas dispersion and validated against wind tunnel data for both high and low turbulence conditions (Mack and Spruijt 2013). (Dixon et al. 2012) developed an OpenFOAM model for CO_2 dispersion, assuming homogeneous equilibrium between solid particles and the surrounding vapour. The model was able to adequately simulate small-scale CO_2 release experiments conducted at GL Spadeadam.

An OpenFOAM model of far-field CO_2 dispersion was developed as part of the COOLTRANS project. The model incorporated the homogeneous equilibrium

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[56] http://www.cfdsupport.com/index.html

method for fully compressible two-phase flow, treatment of the transient atmospheric boundary conditions and time-varying inlet source conditions. The model was validated against several experimental releases and the predictions showed 'promising' agreement with the available experimental data. In the majority of cases, the predicted peak CO_2 concentrations were higher than the measured values (Wen et al. 2013).

8.5.4.3 PANACHE

Fluidyn-PANACHE is a commercial package of software modules for modelling atmospheric flows, developed by Fluidyn/Transoft in collaboration with the French Ministry and Environmental Agency. It is a self-contained, fully 3D CFD software package designed to simulate atmospheric flow and pollutant dispersion in complex environments, i.e. with topography, buildings, land covers and usages. Fluidyn-PANACHE has been designed for use by environmental or industrial safety engineers with limited knowledge in CFD simulation. It is claimed to be easy to use even if the topography is very complex, with a user-friendly GUI (Fluidyn 2014).

Fluidyn-PANACHE has been used to model the dispersion of CO_2 releases and was evaluated against the Prairie Grass and Kit Fox field experiments (Mazzoldi et al. 2008). It found that the default κ-ε turbulence model led to an under-prediction of the maximum arc-wise concentrations by up to a factor of five. They therefore used a one-equation (k-l) turbulence model for the Kit Fox tests and the Prairie Grass tests in stable atmospheric conditions. Use of this model was demonstrated in simulated releases from a CO_2 pipeline, for both punctures (Mazzoldi et al. 2011) and full-bore rupture (Mazzoldi et al. 2013), although these more recent works did not include any further validation of Fluidyn-PANACHE.

8.5.4.4 FLACS

The FLACS (FLame ACceleration Simulator) is a commercial CFD model, available from GexCon in Norway. FLACS was developed to simulate the dispersion of gas leaks and subsequent explosions in offshore oil and gas platforms. FLACS uses a distributed porosity approach for parameterising buildings and other obstacles, which serves to significantly (by factors of 10 to 100) reduce the run time needed for the code (Hjertager 1985).

GexCon recommends that new users of FLACS attend a 3-day introductory training course. Additional courses for experienced users are conducted from time to time.

FLACS has been used to model the dispersion of dense gases. It was found to achieve acceptable results in simulation of field release experiments (neutral and slightly dense gases) involving obstacle arrays (Hanna et al. 2004). It has been satisfactorily evaluated with the CO_2 observations from the Kit Fox field experiment. It has also been used to simulate the dispersion of chlorine at industrial locations and the Chicago urban area (Hanna et al. 2011).

GexCon was a partner in the CO_2PipeHaz project, where FLACS dispersion model predictions were compared to data from CO_2 experiments conducted by INERIS (Gant et al. 2014).

8.5.4.5 ANSYS-CFX

ANSYS-CFX software is a general purpose commercial fluid dynamics program that has been applied to solve wide-ranging fluid flow problems for over 20 years. The software is claimed to include 'an abundant choice of physical models to capture virtually any type of phenomena related to fluid flow'. The flow solver and associated physical models are integrated with a user-friendly GUI, with extensive capabilities for customization and automation.

(Dixon et al. 2012) developed a model for dispersion of CO_2 using a Lagrangian particle-tracking model in ANSYS-CFX. The model included solid particles in the CO_2 jet source, with an initial diameter of 5 µm, a temperature of -78^oC and a velocity equal to the surrounding CO_2 gas. The model allowed for slip between the gas and solid phases. The simulation provided reasonable agreement with small-scale experimental releases undertaken at GL Spadeadam, although the simulated plume was narrower than expected. This was thought to be due to the use of the standard κ-ε turbulence model.

An improved version of this model, incorporating the three-phase sonic jet CFD model developed at the University of Leeds (Wareing et al. 2013), was developed by HSL. The performance of the model was evaluated using experimental data produced in the CO_2PipeHaz project, and was found to provide reasonable agreement with the measurements. It was concluded that more and better experimental data is needed to properly evaluate the merits of the CFD modelling approach (Gant et al. 2014).

8.5.5 Preliminary comments on ‘fitness for purpose’

This section has provided an overview of the types of dense gas dispersion models that are currently available, including integral models, Lagrangian particle and plume dispersion models and CFD models. This selection spans a wide range of capabilities, from the simulation of simplified scenarios to the recreation of complex situations. With the advancement in model capabilities typically comes the need for more experienced modellers, additional time, and increased budget.

Integral models represent the ‘standard’ approach to dense gas dispersion modelling. They use simplifying assumptions that allow for short computation time, and have proven to represent a reasonable compromise. Langrangian particle and plume models are a potential ‘next generation’ approach, allowing modelling of dense gas dispersion in complex terrain and urban environments with only modest computational resources. CFD models have the potential to handle complex situations in fine detail, but at a high computational cost.

One of the biggest factors that differentiate the various models is their ability to handle CO_2-specific source terms. Dense-phase CO_2 will flash to a gas-solid particle mixture rather than a gas-liquid aerosol mixture. However, most models with source emissions modules can only simulate releases (and evaporation/sublimation) of CO_2 using the same formulations as for other pressurized liquefied gases. Models such as SLAB, DEGADIS, and HGSYSTEM can simulate the two-phase jet by defining an initial 'equivalent gas density' which is the g/m^3 of all CO_2 (gas or solid) in the cloud.

Dense-gas models with no functionality to account for the sublimation of solid CO_2 into gas will not be as accurate as those that do. Both PHAST and EFFECTS have been upgraded to reflect observations made during recent large-scale CO_2 release experiments. For example, PHAST can account for the depressurisation/flashing, sublimation of CO_2 solids in the jet and dense-gas dispersion, transitioning to passive dispersion further downstream. Such models therefore seem better suited to modelling CO_2 releases than other models that simply simulate dense-gas dispersion.

Models that do not include functionality for the complex physics could however be used in conjunction with an appropriate source/near-field dispersion model that properly accounts for the behaviour in the first 100-200 m of the release.

CFD models have been the focus of recent development work. While such models show great promise, their potential is limited by the level of expertise required in their formulation and the large computational resources needed for their execution.

Lagrangian particle dispersion models have the potential to become a ‘next generation’ dense gas modelling approach, allowing modelling of dense gas dispersion in complex terrain and urban environments with faster computation times than CFD models.

The following sections extend the considerations of ‘fitness for purpose’ to cover the ability of selected models to calculate appropriate source terms, and their validation against large-scale experimental data.

8.6 Calculation of appropriate source terms

In order for a model to accurately simulate CO_2 releases from a pipeline and dispersion of the released CO_2, it should be able to consider both the transient (non-steady-state) nature of the release and the properties of the CO_2 source. For each of the models considered, the physical and chemical properties of the escaping CO_2 are specified by a set of ‘source terms’.

8.6.1 Transient pipeline depressurisation

Accurate modelling of the discharge of CO_2 from pipelines requires the ability to accurately model the pipeline decompression process. There are a number of commercial pipeline simulation tools that can potentially be used for this purpose, which were reviewed in Section 7.4.1.

OLGA, a standard simulation tool used in the oil industry, is useful for pure CO_2, but cannot account for the influence of impurities on the fluid properties. It has been suggested that the commercial package PVTism, which uses the Soave-Redlich-Kwong equation of state, is more suitable for handling impure CO_2 streams, in conjunction with OLGA (Esfahanizadeh and Dabir 2013).

The CO_2PipeHaz project developed and validated an improved version of PIPETECH, which was used in conjunction with CFD modelling for CO_2 releases in complex terrain. CO_2PipeHaz recommended that this methodology should be used for any parts of the pipeline which are identified as having critical hazard ranges and/or risk. It was recommended that simpler methods, which are much faster to run, should be used to identify potentially critical parts and to carry out sensitivity analysis (Wilday and Saw 2013).

The gCCS modelling tool is suitable for use in the design of CO_2 pipelines. Although the current version of the SAFT equation of state is not as sophisticated as that incorporated into PIPETECH, it is likely to be updated in the future.

Of the dense gas dispersion modelling tools considered in this chapter, only two contain integrated algorithms to simulate pipeline decompression:

- The DNV-GL consequence model PHAST incorporates PIPEBREAK for time-varying liquid releases.
- The TNO consequence model EFFECTS incorporates the MORROW model for releases of liquefied gas from long pipelines.

While both DNV-GL and TNO have been involved in the recent experimental CO_2 release trials, it is unclear whether either of the pipeline depressurisation algorithms have subsequently been fine-tuned specifically for CO_2.

From a user perspective, the advantage of employing either PHAST or EFFECTS is that it is not necessary to couple the output from one proprietary software package to the input of another. Pipeline depressurisation is handled seamlessly in both of these models.

8.6.2 CO_2 release source term components

Again, from a user perspective it would be convenient for a selected dense gas dispersion model to include the ability to simulate a range of different source terms, e.g.:

- Ability to model release rates from breaches in pressurized pipelines and blowdown vents, among other sources.

- Ability to model dispersion of transient releases, during which the emissions rate will change over time.
- Ability to model dispersion from both elevated and ground-level sources.
- Ability to model dispersion from multiple source types (e.g. pool, jet) with varying orientations (e.g. vertical, horizontal).
- Ability to model dispersion of multiphase releases and transitions between phases (e.g. gases and solids).

As shown in Table 8.2, the selected models vary in their ability to calculate emission rates, handle multiple source types and orientations, and simulate multi-phase (i.e. liquid, gas, or solid) emissions.

Table 8.2: Summary of source term capabilities

Model Category	Model Name	Emission Rates	Available Release Profiles(c)	Available Source Types	Multiphase Release
Integral	SLAB	User input	C, I, T	Ground-level area (liquid pool evaporation); ground-level and elevated, horizontal and vertical jets; volume (instantaneous only)	Limited[(a)]
	DEGADIS	User input	C, I, T	Ground-level area and vertical jets[(b)]	Limited[(a)]
	HGSYSTEM	Calculated for certain release scenarios (e.g. pool evaporation, pressurised reservoirs)	C, T	Area, ground-level and elevated jet in any direction including horizontal and vertical	Yes
	ALOHA	Calculated for certain release scenarios (e.g. pool evaporation, storage tank releases and gas releases from pipelines)	C, I, T	Ground-level area, ground-level jet (no initial momentum for jet releases, which may result in errors near the release point)[(b)]	Limited[(a)]
	SAFER/ TRACE	Calculated for certain release scenarios (e.g. pool evaporation, pressurised reservoirs)	C, I, T	Area and jet, ground-level and elevated	Yes
	GASTAR	Calculated for certain release scenarios (e.g. pool evaporation)	C, I, T	Area, ground-level and elevated jet in any direction including horizontal and vertical	Yes
	PHAST	Calculated for certain release scenarios. Jet release calculation has been validated against pressurised CO_2 releases (Witlox et al. 2013a)	C, I, T	Area; ground-level and elevated jets in multiple directions including horizontal and vertical	Yes
	EFFECTS	Calculated for certain release scenarios (e.g. pool evaporation, pressurised reservoirs)	C, I, T	Ground-level area (liquid pool evaporation); ground-level and elevated, horizontal and vertical jets; volume (instantaneous only)	Yes v10
Lagrangian	CHARM	Calculated for certain release scenarios (e.g. pool evaporation, storage tank releases and supercritical gas releases from pipelines)	C, I, T	Area, ground-level and elevated jet in any direction including horizontal and vertical	Yes
	QUIC	all scenarios	C, I, T	Area, ground-level and elevated jet in any direction including horizontal and vertical	No

Model Category	Model Name	Emission Rates	Available Release Profiles(c)	Available Source Types	Multiphase Release
	SCIPUFF	all scenarios	C, I, T	Area, ground-level and elevated jet in any direction including horizontal and vertical	Yes
	SPRAY/ ArRisk	Calculated for certain release scenarios (e.g. pool evaporation, storage tank releases and supercritical gas releases from pipelines)	C, I, T	SPRAY: User 'builds' the source; Model capable of representing any built source configuration ArRisk: Area; ground-level and elevated jets in multiple directions including horizontal and vertical	Yes
CFD	FLUENT, OpenFOAM, PANACHE, FLACS, ANSYS-CFX	User input	C, I, T	User 'builds' the source; Model capable of representing any built source configuration	Yes

Sources: (US-EPA 2007; CERC 2009; Spicer and Havens 1989; Ermak 1990; Safer Systems 2014; OpenFOAM 2014; ANSYS 2013)

(a) SLAB, DEGADIS, and ALOHA have a limited capability to evaluate multiphase releases. These models simulate a two-phase jet by defining an initial 'equivalent gas density' of all CO_2 (gas or solid) in the cloud.

(b) Experiments by Donat and Shatzmann showed that release angle had a large influence on jet dispersion, which is important since accidents often have non-vertical jet flow (Donat and Schatzmann 1999). Horizontal flow is now often considered for accident modelling as it can serve as a worst case scenario for dense gas accumulation. The inability of DEGADIS and ALOHA (which is based on a simplified version of DEGADIS) to consider horizontal jet releases could be a significant limitation in many pipeline-related scenarios.

(c) C= Continuous, I=Instantaneous, T=Transient

8.6.3 Comments on ‘fitness for purpose’ for calculating source terms

For accurate calculation of the source term, it is necessary to correctly characterise the initial CO_2 stream as single- or multi-phase, continuous, time-variable or instantaneous, at constant or falling pressure. A suitable model for transient pipeline depressurisation is required, to provide the correct input to the selected dispersion model.

As shown in Table 8.3, the dispersion models differ in their ability to handle a variety of source release configurations.

The publicly-available ALOHA model has simplified source emissions formulas with certain specifications 'hard-wired' so as to prevent users from defining unrealistic combinations of inputs. This limits the user’s ability to adapt ALOHA to certain release scenarios. ALOHA is unable to handle elevated jets or jets oriented in the horizontal direction. In particular, the inability to handle a horizontal jet release could be problematic as it is generally regarded as the release scenario that may result in the highest impacts.

The ArRisk tool was developed as a compromise solution for convenient use in safety analysis, emergency planning and real-time emergency management. It can simulate two-phase discharge of CO_2 from punctured tanks or pipes and integrate the results with the Lagrangian particle dispersion model SPRAY.

The more complex CFD models can potentially handle a wide variety of source configurations, because the user can create a 3D representation of the source within the modelling domain. However, at this stage, each of the CFD models evaluated has been constructed to treat a specific scenario. There is currently no such thing as a ‘general purpose’ CFD model.

All of the selected models are capable of considering multiphase (e.g. gas, liquid) releases to some extent; however, the models differ in their ability to realistically represent all of the chemical and physical processes that may occur in the event of a pipeline depressurization.

For example, integral models such as SLAB, DEGADIS, HGSYSTEM, TRACE and GASTAR simulate a two-phase jet by defining an initial 'equivalent gas density' which is the g/m^3 of all CO_2 (gas or solid) in the cloud. However, these models are unable to account for sublimation of solid CO_2 particles into vapour, which will affect the density and temperature of the cloud.

The developers of both PHAST and EFFECTS have been involved in recent large-scale experimental releases of CO_2, and have used the data to create modified algorithms to account for the formation of solid CO_2 particles. From version 6.6, PHAST has incorporated new formulae for flashing, source emissions rate, and solid particle size distributions. However, the current version of EFFECTS does not include the latest information in the models; updated models will be included in

EFFECTS 10, which is apparently scheduled for release in the near future. As such, PHAST is currently the only integral model that specifically incorporates the latest understanding of CO_2 behaviour.

The jet model formulation in SCIPUFF (Sykes et al. 2008; DTRA 2008) (Chowdhury et al. 2012), which treats both positive and negative buoyancy, has the widest range of source and dispersion modelling options of any publicly-available dense gas model. However, it does not include the ability to account for solid CO_2 formation.

As part of the COOLTRANS programme, the University of Leeds has developed a CFD model for jet releases of CO_2 which accounts for solid particle formation (Wareing et al. 2013). This model has been used to develop a series of correlations to predict the velocity and dilution of the flow emerging from the crater resulting from a puncture or rupture of a buried CO_2 pipeline (Cleaver and Halford 2015). Both the CFD model and the numerical correlations are suitable for use as source terms for other models.

Similarly, the Energy Pipelines CRC in Australia has developed a FLUENT CFD model for simulation of CO_2 release source terms (Liu et al. 2014).

Selection of a ‘fit for purpose’ model will depend on the intended application. Models with limited options, such as ALOHA, are widely used in emergency response planning because they are quick and easy to use. CFD models require a high level of skill to create, and are usually developed for specific scenarios, but can then be interfaced with simpler models to produce a powerful package.

Currently, PHAST 6.6 or later and the forthcoming EFFECTS 10 represent the only two commercial packages that include the ability to account for both a wide range of source terms and the formation of solid CO_2 particles. Other modelling approaches can certainly be used to achieve a similar outcome, but would require greater effort to assemble and interface the various model components.

8.7 Validation of dense gas dispersion models

The following section goes into some detail to describe the validation procedure for dense gas dispersion models. The topics that are reviewed are as follows:

- experimental systems
- scaling issues
- dense gas experimental data sets
- evaluation of models against experimental data
- model acceptance criteria
- validation of models
- model evaluations with CO_2 field study observations

- evaluation of fitness for purpose
- uncertainties in model simulations.

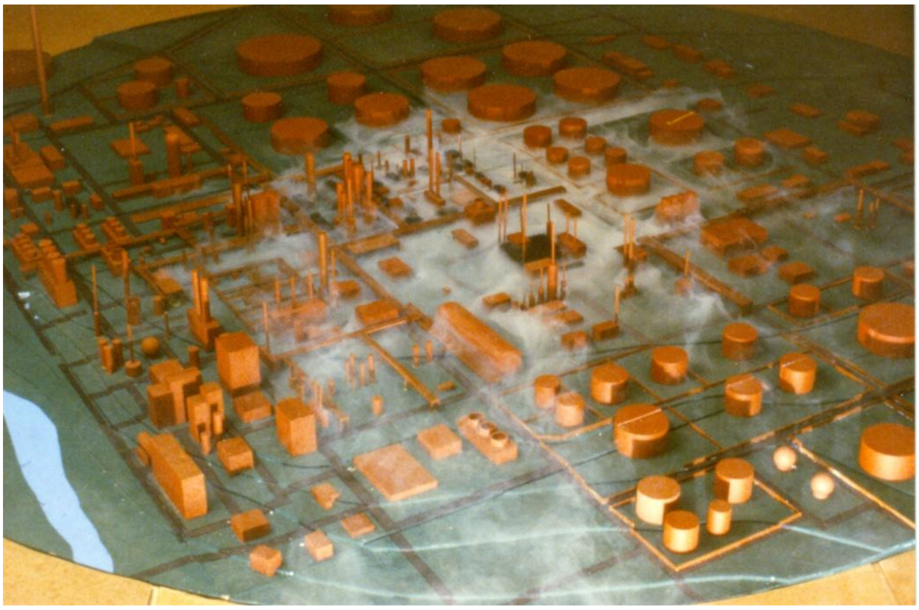
Unfortunately, this is a highly technical and specialised area, and may not be of direct interest for many readers. However, in the absence of any recent reviews of this area (the standard is still (Hanna et al. 1996)), it is necessary for this section to cover a lot of ground.

8.7.1 Experimental systems which provide observations used for model evaluation

8.7.1.1 Scaled physical modelling

Scaled down physical models of a specific release scenario can be powerful tools for characterising gas releases. Both water channels and wind tunnels may be employed, using model liquid systems and appropriate measurement instruments. These models are effectively analogue computers that embody the full complexity of the system without any simplifying assumptions. They have been used to develop some of the fundamental design correlations used in analytical dense gas models, to plan field experiments, and for validation of numerical code. Physical modelling is most useful for near source dispersion estimates where mechanically induced turbulence is present from structures such as buildings and tanks, and where mathematical modelling involves a high level of uncertainty (Petersen 2011). Figure 8.5 shows a wind tunnel simulation of a dense gas release in an industrial site, showing the dense gas persisting as a relatively shallow cloud over the entire area.

Figure 8.5: Wind tunnel modelling of gas dispersion in a complex environment



(Meroney 1982) provides a good general review of the theory and application of wind tunnel experiments for characterising dense gas dispersion. (Meroney 1987) demonstrated that physical modelling can successfully simulate the results achieved in field scale dense gas experiments. (Britter and McQuaid 1988) use several sets of data from physical modelling to develop and test their empirical correlations.

A limitation of wind tunnel studies is that, for low wind speeds, the cloud motion may become laminarised with dispersion governed by the molecular diffusivity. (Briggs et al. 2001) describe these issues related to wind tunnel modelling of the Kit Fox CO_2 modelling scenarios.

8.7.1.2 *Experimental field releases - Dense gas dispersion studies*

Large-scale experimental releases of dense gases have been undertaken by the US and UK governments to help quantify the potential hazards associated with accidental releases and to provide the data necessary for the development of suitable mathematical models. Several series of dense gas experiments were conducted during the 1980s, including the following four that are often used in model evaluation:

- The Burro/Coyote series of LNG releases at China Lake, California, sponsored by the US Department of Energy (Koopman et al. 1982).
- The Maplin Sands series of LPG releases on water, conducted by the Shell Company in the UK (Puttock et al. 1984).
- The Thorney Island Freon releases (McQuaid 1985) (Brighton et al. 1994) sponsored by the UK Health and Safety Executive.
- The Desert Tortoise anhydrous ammonia (Goldwire et al. 1985) and the Goldfish HF releases (Blewitt et al. 1987) conducted by the US Department of Energy.

An overview of these experiments was provided by (Havens 1992). Data from these experiments have been used in the development and evaluation of most dense gas models. It could be said that most models have been calibrated or tuned to these data sets (Hanna et al. 1991). The field data sets are publicly available in the Modelers Data Archive (MDA) distributed freely by Chang and Hanna.

In the past ten years, there have been additional field studies in the US, such as the Jack Rabbit experiments at the Dugway Proving Ground in Nevada, involving releases of pressurized liquefied chlorine and anhydrous ammonia. With wind speeds less than about 2 m/s, the Jack Rabbit release formed dense two phase clouds that stayed around the source location for 30 to 60 minutes after the tank storage tank emptied (Hanna et al. 2012). Figure 8.6 shows the appearance of a cloud of chlorine, 22 seconds after the release began. The tank contained one ton and the release valve is pointed down.

Figure 8.6: Jack Rabbit trial 2-PC chlorine cloud

The Wild Stallions chlorine field experiments also took place at Dugway Proving Ground, and investigated the behaviour of the one-ton cylinder and the chlorine cloud after a fast rupture of a pipe or a medium sized hole or a complete rupture (Babarsky 2009). After the initial cloud formation by the momentum jet, the chlorine cloud slumped to the ground.

The Jack Rabbit II field experiment is currently being planned. In the summer of 2015 and 2016, several releases of 10 tons of pressurized liquefied chlorine will take place. About half of the releases will be in open flat terrain and about half will be in a ‘mock urban’ area. Concentrations will be measured on arcs out to a distance of 11 km.

One of the first comprehensive field studies involving CO_2 was the so-called EPA I study carried out at the Nevada Test Site, Nevada, US in the early 1990s. The CO_2 gas was released from a 2.25 m^2 area source at ground level and the ground surface was a flat desert. Reports by (Coulombe 1995a, b) and by (Egami et al. 1996) describe the experiments and list the data. (Briggs 1995, 1996) was the chief scientist from the EPA and published two analyses as conference papers. His solution was similar to the dense gas theory by (Van Ulden 1984) and (Colenbrander 1980).

Shortly after the EPA I experiment, the larger Petroleum Environmental Research Forum (PERF) study was initiated, and was carried out under an industry-EPA-DOE cooperative agreement in the US. (Hanna and Steinberg 2001). The PERF study included experiments with a dense gas (CO_2) released from a line source at three wind tunnels (Briggs et al. 2001). The PERF study also included CO_2 releases at the

Nevada Test Site, using a release set-up similar to that used for EPA I (Hanna and Chang 2001a). This field study was named Kit Fox. There were three different Equivalent Roughness Patterns (ERP), with many 2.4 m square billboard-type plywood panels; Uniform Roughness Array (URA), with many 0.2 m by 0.8 m panels, and flat desert (also called EPA-II). The ERP and URA panels were intended to represent an approximate 1/10-scale chemical processing facility.

(Hanna and Chang 2001a) carried out extensive analysis and model evaluations with the ERP and URA, and this Kit Fox data has consequently been used in several papers (e.g. (Mazzoldi et al. 2008)). To date, however, the flat desert EPA II data have not been adequately analysed.

8.7.1.3 *Experimental field releases - Jet characterisation studies*

The AIChE/CCPS sponsored a set of field experiments addressing droplet formation and rainout in two-phase jets formed from releases of pressurized liquefied gases. (Quest 1992) and (Johnson and Woodward 1999) describe the data set, which was used to develop the RELEASE model (Woodward 1995; Johnson and Woodward 1999). (Britter et al. 2011) use the RELEASE droplet data to further test the RELEASE model and the (Witlox et al. 2007) revised model for estimating droplet sizes (similar performance was found).

Many laboratory and field experiments have been used by (Leung 1995, 1990) to develop the Omega method for estimating the mass emission rate in flashing jets, which depends on the hole geometry, vessel wall thickness, and pipe length. The Omega method is utilised in the widely-used Homogeneous Equilibrium Model for two-phase flashing discharge.

A series of field experiments have taken place in Europe over the past ten years to investigate various details of jets formed after release of pressurized liquefied gas. The INERIS FLIE experiments, performed in France during 2004, involved 94 flashing releases of propane and butane (Ichard et al. 2009). Witlox and colleagues have been part of a series of Joint Industry Programs (JIPs), which led to improved parameterizations of droplet formation and understanding of jet thermodynamics (Witlox et al. 2007; Witlox et al. 2011) and (Cleary et al. 2007).

In Europe, DNV has led a Joint Industry Program (JIP) involving releases of pressurized liquefied CO_2. Most interest is in near-field scientific issues (i.e. source emissions, jet structure, solid particle formation and possible deposition, re-evaporation, transition of jet to dense gas slumping model). The first experimental program (JIP1) involved collection of release and dispersion data from liquid and supercritical CO_2 releases through holes with diameters up to 25mm, and the second program (JIP2) collected data from long pipe depressurisation experiments. (Witlox et al. 2011; Witlox et al. 2009) describe the results from these trials, which delivered data on CO_2 solid particle size distributions and jet thermodynamics. The data themselves are made available through project reports (e.g. (Advantica 2007;

DNV 2012a, b). The result of a third experimental program (JIP3) have recently been made available. These trials involved the release of liquid phase CO_2, at initial pressures up to around 10 MPa, through holes ranging in diameter from 25mm to 150 mm. The data is available for download from the DNV-GL website[57].

Other CO_2 jet experiments have been carried out and are discussed in the literature. For example, vertically-pointing CO_2 jets were released and studied by (Kuijper 2008) and analysed by (Mazzoldi et al. 2011).

The thermohydraulics of CO_2 discharge was studied in a series of high pressure vessel blowdown studies as part of the CATO2 project[58] (Ahmad et al. 2013b; Ahmad et al. 2013a).

The National Grid COOLTRANS project involved a comprehensive series of experiments at Spadeadam, from which the University of Leeds developed a three-phase sonic CFD model for near-field dispersion (Wareing et al. 2013), (Wareing et al. 2014).

8.7.2 Scaling issues

For many hazardous chemicals it is not safe to carry out a field experiment where the mass released is as large as the amount involved in a real full-scale 'worst-case' scenario. For example, a railcar of pressurized liquefied chlorine contains 60 to 90 tons. Or, a full rupture of a 1 m diameter CO_2 pipeline, with shut-off valves every 30 km, might release over 1000 tons of CO_2, which government authorities would not allow.

Consequently, it is often assumed that the basic physics and chemistry principles apply across scales, and can be satisfactorily interpreted as long as relevant dimensionless numbers, such as Richardson or Froude number, are used. Thus the Kit Fox experiment, with CO_2 released at a rate of about 1 to 4 kg/s from a 2.25 m^2 area source at ground level in the midst of many 2.4 m tall billboards, was regarded as a 1/10 scale simulation of HF releases in chemical processing plants (Hanna and Steinberg 2001). In Kit Fox, CO_2 was a surrogate for a two-phase HF cloud.

Wind tunnels and water channels use the same scaling rationale, with typical distance scaling of 1/100 or 1/200, and surrogate chemicals to represent the proper density of the actual chemical of interest (Meroney 1987; Briggs et al. 2001). If HF or chlorine were released at high concentrations in a wind tunnel, severe corrosion of the wind tunnel and fan would occur, and samplers might be destroyed. As described in (Britter and McQuaid 1988), a series of wind tunnel tests using CO_2 as a tracer was conducted by McQuaid.

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[57] www.dnvgl.com/ccus

[58] http://www.co2-cato.org

Unfortunately, some phenomena do not scale well, such as the size and behaviour of liquid or solid aerosols formed during the flashing process. The size of chlorine liquid drops or CO_2 solid particles is mainly determined by the chemical properties and the degree of superheat, and will be about the same (i.e. median diameters of about 20 or 30 μm for chlorine and 3 to 5 μm for CO_2) for a small scale release as a very large scale release. In such cases, flashing experiments are done using small-to-medium releases that can be controlled and confined, assuming that the resulting scientific relations and parameterizations will also apply to a realistic large scale release.

Another scenario that does not scale well is the formation of the large persistent initial dense two-phase cloud around the source region during light winds. This persistent cloud becomes much more likely as the mass of emissions increases, and a much larger wind speed is required to disperse the initial dense cloud. Because of the high concentrations (> 10 %) in that cloud, concentration samplers can become saturated and not provide good data.

One of the few available full-size field experiments is the planned (for 2015 and 2016) Jack Rabbit II chlorine release of 10 to 20 tons of pressurized liquefied gas in each of about 20 trials. A typical railcar in the US carries about 90 tons of chlorine.

It is important to note that field and laboratory experiments can also be limited in scope and their applicability to the scenario being modelled. For example, field experiments to simulate dense gas releases from a buried pipeline have been limited. The COOLTRANS project represents the first effort to validate dense gas models on data from full-scale tests simulating buried pipeline releases (Gant 2012). When using a model with limited field study validation, it is important to consider the specifics of the modelled scenario and whether these specifics may impact model interpretation. For example, the differences between a buried pipeline release and releases that have been better studied in the field are expected to be most significant near the point of release. Therefore, the uncertainty arising from a lack of field study data may only be significant near the point of release (Hanna et al. 2012) (Hanna et al. 1993b).

8.7.3 Dense gas experimental data sets

Over the past 20 years, Dr. Joseph Chang and Dr. Steven Hanna have compiled the Modelers Data Archive (MDA), a set of about 50 data sets from 30 field experiments that cover a wide range of conditions, eg, different plume densities (dense, buoyant, and neutral), spatial scales ranging from 0.1 to 1,000 km, flat vs. complex terrain, daytime vs. night time conditions, surface vs. elevated release, point vs. line source, rural vs. urban land use, and episodic vs. routine releases.

These data sets are freely available to the scientific community, and have been widely used in research on dense gas model development and evaluation. In some cases, MDA has become the only known source of certain data sets. The MDA contains electronic versions of the data reports as well as the observations themselves and 'read-me' files defining all variables and assumptions. Model evaluations can be quickly conducted since the observed concentrations are set up to be easily used as model inputs.

The MDA includes the Burro, Maplin Sands, Thorney Island, Desert Tortoise, Goldfish and Kit Fox dense gas data sets. Other data bases, such as EPA I and II and JIP CO_2 phase 2 are also available but are not yet in the MDA format. The CO_2 jet experiments by (Kuijper 2008) and (Wareing et al. 2014) have not yet been made available to the MDA.

A Model Evaluation Protocol (MEP) was also developed by HSL for the National Fire Protection Association, which is used to approve dispersion models for use in siting studies for LNG facilities in the USA. (Ivings et al. 2007) describes the MEP, (Coldrick et al. 2009), provides a validation database of processed experimental data of dense-gas dispersion experiments, and (Webber et al. 2009) report on appropriate source term models. FLACS, PHAST, DEGADIS, FDS and the integral model used by HSE (DRIFT) have been compared to this validation database.

HSL has developed the framework for a MEP for CO_2 discharge and dispersion models as part of the COOLTRANS programme (Gant 2012). It is expected that the outcome will be a review of the capabilities and limitations of various pipeline discharge and dispersion models, and an independent assessment of their performance. Work on the CO_2 MEP is ongoing, and the final outcome has not yet been published.

8.7.4 Evaluation of models against experimental data

There are several sets of dispersion model evaluation methodologies and software available. A scientific peer review and assessment of fitness-for-purpose should be included. A quantitative statistical assessment of model performance is a major component. Similar statistical performance measures are used by several groups, due to the fact that they have all participated in the same workshops over the years. A widely used quantitative method for dispersion model evaluation is called the European Union Harmonization of Air Quality Models for Regulatory Purposes 'Model Validation Kit' (MVK)[59]. The MVK contains model evaluation software as well as field data archives, refer to (Olesen and Chang 2010).

The BOOT model evaluation software is a central part of the MVK and is also available separately from Joseph Chang or Steven Hanna[60]. It was developed in the late 1980s and has been steadily improved over the past 25 years. The original journal article describing the method is (Hanna 1989), which presents the model performance measures and then describes how to estimate confidence intervals on

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[59] http://www.harmo.org/kit/

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the performance measures. Examples of applications of the BOOT software and general model evaluation concepts are found in (Hanna et al. 1993a; Hanna et al. 1997; Hanna and Davis 2002) and (Chang and Hanna 2004).

The published quantitative statistical evaluations of dispersion models have several common themes. The comparisons always use visual tools such as scatter plots, as well as quantitative performance measures. The primary performance measures in BOOT are defined below, where the symbol C represents concentration, subscripts p and o refer to predicted and observed, and the overbar represents an average.

Fractional Mean Bias

$$FB = 2(\overline{C_o - C_p})/(\overline{C_o} + \overline{C_p}) \qquad (1)$$

Normalized Mean Square Error

$$NMSE = \overline{((C_o - C_p)^2)}/(\overline{C_o} * \overline{C_p}) \qquad (2)$$

Geometric Mean

$$MG = \exp((\overline{\ln C_o}) - (\overline{\ln C_p})) \qquad (3)$$

Geometric Variance

$$VG = \exp\,\overline{((\ln C_o - \ln C_p)^2)} \qquad (4)$$

Fraction of C_p within a factor of two of C_o

FAC2 (fraction where $0.5 < C_p/C_o < 2$) (5)

Normalized Absolute Difference

$$NAD = \overline{|C_o - C_p|}/(\overline{C_o} + \overline{C_p}) \qquad (6)$$

In addition, the median, average, and maximum of C_o and C_p are often listed in summary tables. Note that the above equations are generic and apply to any kinds of data pairings, including arc-maximum and paired-in-space comparisons; and any kinds of variables, including concentration normalized by the emission rate, Q. (Hanna and Chang 2001a) also included evaluations of the model’s estimates of dense cloud width and depth.

In addition to calculating the above performance measures, the BOOT software determines whether 1) the mean bias measures (FB and MG) for a single model, or 2) the difference in performance measures between two models are significantly different from zero with 95 % confidence. The model uses either the Bootstrap or the Jackknife re-sampling methods to calculate the statistical significance.

8.7.5 Model acceptance criteria

One method of establishing the validity of a model is to determine whether it meets a set of model acceptance criteria (Chang and Hanna 2004). These criteria provide quantitative guidelines for comparing model outputs with field experiments. The model acceptance criteria should include scientific credibility and ability to replicate field experiments. In addition, no major technical problems should be identifiable during a peer review of the model technical documentation.

Based on their experience in evaluating dispersion models with field experiment observations, (Chang and Hanna 2004) and (Hanna and Chang 2012) have suggested quantitative 'acceptance criteria' based on the fractional bias FB, the Normalized Mean Square Error (NMSE), the fraction within a factor of two (FAC2), and the Normalized Absolute Difference, NAD.

(Chang and Hanna 2004) reviewed many rural evaluation exercises, involving many models and many types of observations, and suggested some preliminary acceptance criteria based on results from five rural field experiments concerned with dispersion. The proposed rural acceptance criteria are:

RURAL

$|FB| < \sim 0.30$	i.e. the relative mean bias < about 0.3
NMSE < ~3	i.e. the random scatter < ~1.7 times the mean
FAC2 > ~0.50	i.e. the fraction of C_p within a factor of two of C_o exceeds 0.50
NAD < ~0.30	i.e. the fractional area for errors < ~0.30

FB, NMSE, and FAC2 are based on arc-maximum concentrations; while NAD is based on threshold-based paired-in-space comparisons.

The rural acceptance criteria were defined using a common sense justification that the criteria should not be so stringent that they are not met by most widely-used models, and should not be so easy that they are met by all models. Thus these criteria should be met, on average, by the available widely-used and tested models in the literature. It was also recognized that often a model will do very well at one field site and not so well at another field site. Therefore an overall criterion was that the above individual criteria should be met over half the time, on average, at all field experiments tested.

Model performance for urban and other complicated applications is not expected to be as good as that for rural applications due to variability introduced by, for example, buildings and differing land use. Based on experiences with urban model evaluations and review of the literature, (Hanna and Chang 2012) recommended that the model acceptance criteria for urban applications be relaxed by roughly a factor of 2 from those for rural cases.

URBAN

$\lvert FB \rvert < \sim 0.67$	i.e. the relative mean bias < a factor of ~2
NMSE < ~6	i.e. the random scatter < ~2.4 times the mean
FAC2 > ~0.30	i.e. the fraction of C_p within a factor of two of C_o exceeds 0.30
NAD < ~0.50	i.e. the fractional area for errors < ~0.50

Again, FB, NMSE, and FAC2 are based on arc-maximum comparisons; and NAD is based on threshold-based paired-in-space comparisons.

The same comprehensive acceptance criterion applies as for rural comparisons, where at least half of the performance measure criteria should be met for at least half of the field experiments considered.

Note that the acceptance criteria are based for the most part on research-grade field experiments over relatively flat terrain. Departures from these conditions should require increases in the acceptance criteria.

8.7.6 Validation of models

A number of laboratory and field experiment datasets are available for dense gas model validation. These datasets include results from many dense gas release experiments that have been conducted over the last decades, including releases of different gases (e.g. ammonia, hydrogen fluoride, chlorine) and simulations of different source configurations (e.g. area emissions, vertical jets, horizontal jets, angled jets).

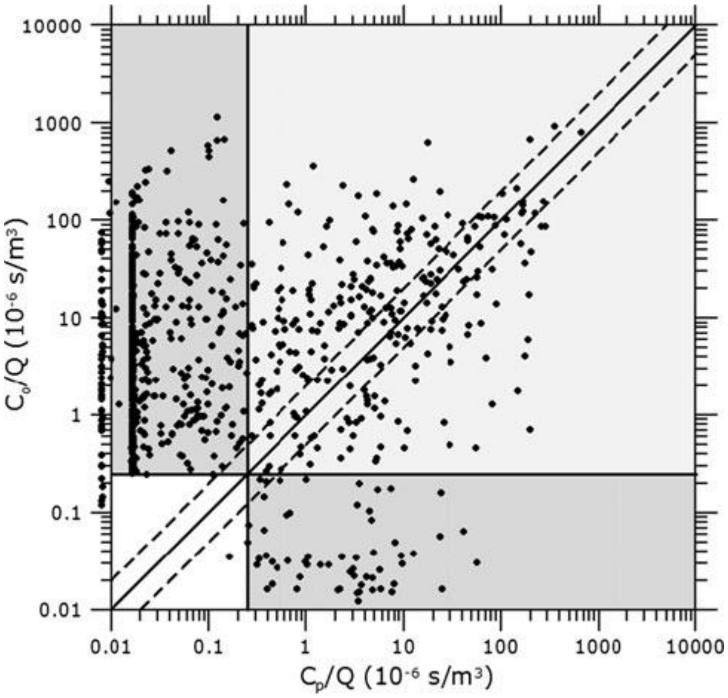
The performance measures in equations (1) to (5) were used in the (Hanna et al. 1993a) evaluation of 15 dense gas models with data from eight field studies. It was concluded that most of the models' predictions of arc maximum concentration agreed with the predictions fairly well, with a magnitude of FB less than about 0.3 and an NMSE less than about 1 (i.e. the relative mean bias is less that about plus and minus 30 % and the typical scatter is about equal to the mean).

There is a major distinction between comparing the arc maximum concentrations and the 'all sampler' paired in time and space concentrations. The arc maximum occurs at a single sampler along an arc of several samplers at a certain downwind distance. The predicted arc maximum might be at a sampler near one edge of the arc and the observed arc maximum might be at a sampler near the other edge. This removes the complications of uncertainties in wind direction. When 'paired in space and time' concentrations are compared, the scatter is inevitably larger. This can be seen in Figure 8.7 and Figure 8.8, where scatter plots are shown first for paired in time and space data, and second for arc maxima.

There is much more scatter for the paired in time and space data, where there were many samplers with false positives and false negatives. In Figure 8.8 (for arc maxima), about half of the points are 'within a factor of two'.

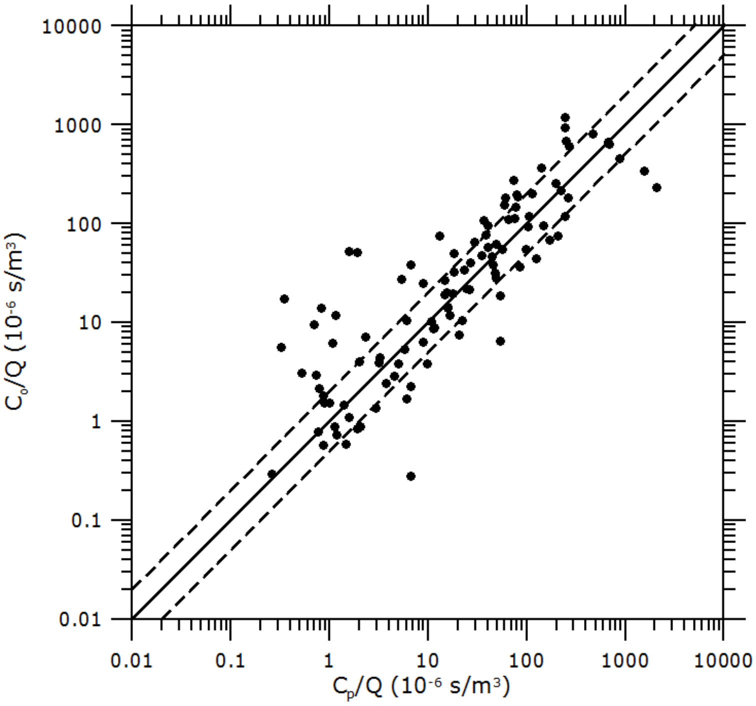
As discussed in (Hanna et al. 1996), the chemical processing industries are primarily interested in the arc maximum concentrations and how they vary with downwind distances. They recognize that the wind direction is variable and it is difficult to model the exact cloud trajectory (path).

Figure 8.7: Example of a scatter plot of observed versus predicted concentrations when the data are paired in time and space



(The solid diagonal line is perfect agreement, and the dashed lines represent plus and minus factor of two agreement.)

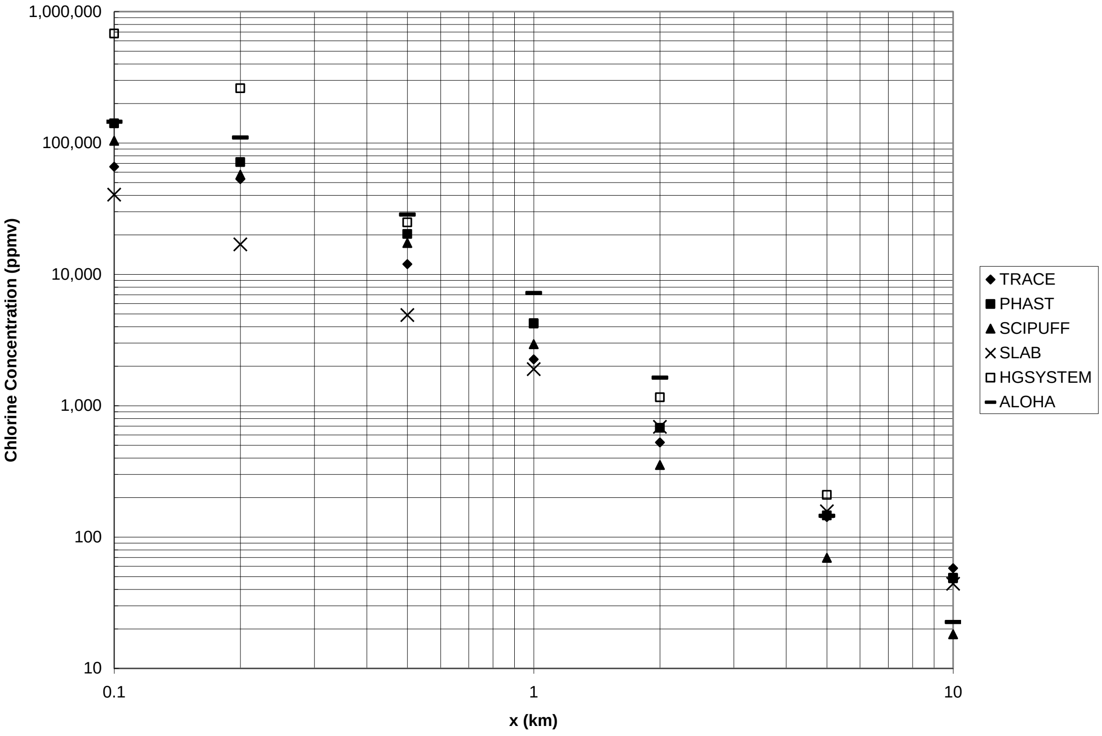
Figure 8.8: Scatter plot of observed versus predicted concentrations for arc maxima concentrations



(The solid diagonal line is perfect agreement, and the dashed lines represent plus and minus factor of two agreement.)

(Hanna et al. 2009) compared the predictions of six dense gas models (TRACE, PHAST, SCIPUFF, SLAB, HGSYSTEM, and ALOHA/DEGADIS) for the release conditions associated with three major chlorine railcar accidents (Festus, Macdona, and Graniteville). There were no chlorine concentration data taken while the chlorine cloud was present, since the cloud cleared out of the area within one hour. Figure 8.9 presents the predicted arc-maximum concentrations for Graniteville. All six models were provided with the same mass emission rate. At any given downwind distance, the range of concentration predictions of the six models covers about one order of magnitude (factor of ten). The relative positions of the six models switch from one distance to the next. For example, SCIPUFF is at the low end of the range at distance of 1 km and less, and is near the high end by a distance of 10 km.

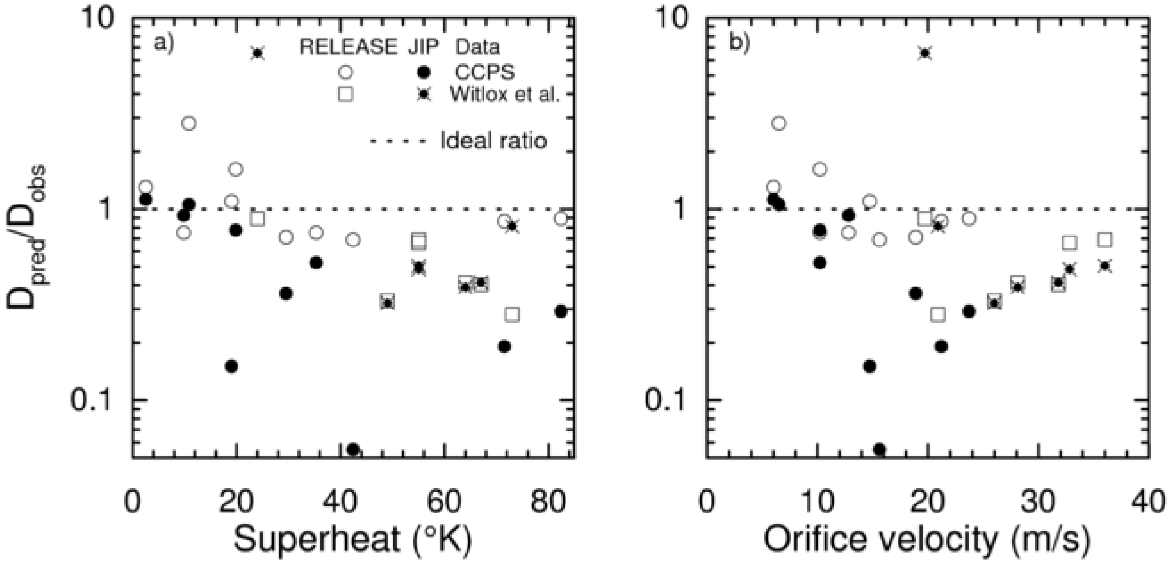
Figure 8.9: Plot of maximum 10 min average concentration (ppm of chlorine) on plume centreline versus downwind distance, x



Examples of additional evaluations of dense gas dispersion models with 'non CO_2' data sets are given by (Meroney 1987; Britter and McQuaid 1988), (Brighton et al. 1994), (Duijm and Carissimo 2001), and (CERC 2002).

Another category of dense gas field data includes dense two phase jets from releases of pressurized liquefied gases. As an example of evaluations of the ability of models to predict drop sizes, Figure 8.10 shows the (Britter et al. 2011) tests of the RELEASE and (Witlox et al. 2007) models for prediction of drop sizes observed during two field campaigns. The field data used for evaluation are from AIChE/CCPS (Quest 1992) and (Witlox et al. 2007).

Figure 8.10: Predicted-to-observed droplet diameter ratio, D_{pred}/D_{obs}, as a function of liquid superheat and orifice velocity



It is seen that the two models have roughly equivalent accuracy. The RELEASE authors include several evaluations of their model with their field data (Woodward 1995; Johnson and Woodward 1999; Ramsdale and Tickle 2000) carried out an independent evaluation. The evaluations show that factor of two scatter is typical.

The (Witlox et al. 2007) model was recently selected over the RELEASE model for inclusion in the HPAC/SCIPUFF dense gas dispersion modelling system. It was concluded that RELEASE contained several empirical correlations while the (Witlox et al. 2007) model was based on more fundamental science and on more recent field experiments.

However, due to the expense of conducting field trials, it is difficult to obtain experimental data for a statistically-significant number of experiments for many different scenarios (Davies 1987). Therefore, although many of the selected models have been validated against the available data sets, there are still a number of scenarios that have not been tested or have been tested only minimally. Also, it is worth noting that developers of the models have often been involved in the validation process (i.e. the evaluations are not independent) or have tweaked their models to calibrate or 'tune' to the available experimental data. Therefore, there may be limitations in applying the models to new scenarios or types of releases not well characterized by the existing datasets.

Table 8.3 provides a brief history of dense gas validation for selected models. This table is not intended to include every validation study that has been conducted for these models, but instead to reflect the general extent of these studies. An attempt is made to emphasize independent validation studies, and it is pointed out that most model technical documents contain results of validation studies carried out by the developers.

Table 8.3: Model validation history with dense gas field experiments

Model Category	Model	Description of Validation History
Integral	HGSYSTEM	This model was evaluated (along with others) using data from a series of field experiment releases of LNG, ammonia, Freon, and hydrogen fluoride. HGSYSTEM was among the evaluated models that produced the most consistent predictions of plume centreline concentrations (Hanna et al. 1993a). (Hanna and Chang 2001a) used the Kit Fox CO_2 field data to improve the HGSYSTEM entrainment formulations. The updated model produced little mean bias when evaluated with the full Kit Fox data set. When used to simulate a series of major chlorine railcar incidents, the evaluated models (including HGSYSTEM) performed within about one order of magnitude of each other, but no observed data were available to verify the estimates (Hanna et al. 2008).
	SLAB	This model was evaluated (along with others) using data from a series of field experiment releases of liquefied natural gas (LNG), ammonia, Freon, and hydrogen fluoride. SLAB was among the models that produced the most consistent predictions of plume centreline concentrations (Hanna et al. 1993a). When used to simulate a series of major chlorine railcar incidents, the evaluated models (including SLAB) performed within about one order of magnitude of each other, but no observed data were available to verify the estimates (Hanna et al. 2008). An evaluation was conducted using two trials from the Jack Rabbit experiments, which included releases of 1 to 2 tons of chlorine gas. SLAB was the only model run. The modelled data comparison showed 'fair results' but merited additional study (Hanna et al. 2012).
	DEGADIS	An evaluation was performed using a variety of dense gas field experiments on flat terrain conducted in the 1980s, including releases of LNG, liquefied petroleum gas, ammonia, Freon-nitrogen mixtures, nitrogen tetroxide, and hydrogen fluoride. The DEGADIS predictions were found to be consistent with the observations from the tests, which 'suggests that the point of diminishing returns has been reached in the development of models for this (limited) application' (Havens 1992). The model was evaluated (along with others) using data from a series of field experiment releases of ammonia and hydrogen fluoride using horizontal jet releases. This model was listed as having 'reasonable performance' when it was corrected for initial dilution, but otherwise had prediction uncertainties that were greater than the mean value (Hanna et al. 1991). Further evaluations (Hanna et al. 1993b) added field experiment releases of liquefied natural gas (LNG) and Freon, with the result that DEGADIS was among the group of well-performing models. When used to simulate a series of major chlorine railcar incidents, the evaluated models (including DEGADIS) performed within about one order of magnitude of each other, but no observed data were available to verify the estimates (Hanna et al. 2008). The US PHMSA evaluated DEGADIS against wind tunnel data and field data from the Maplin Sands, Burro, Coyote and Thorney Island trials. DEGADIS was found to be generally over-predictive for maximum arc-wise concentrations often by a factor of 2 or more. It was recommended that a safety factor of 2 be applied to maximum arc-wise concentrations. Alternatively, a distance safety factor of 2 may be used (FERC 2011).

Model Category	Model	Description of Validation History
	ALOHA	This model was evaluated (along with others) using data from a series of field experiment releases of ammonia and hydrogen fluoride using horizontal jet releases. ALOHA had uncertainties equal to about two times the mean observed value, which was documented as 'relatively poor performance' compared to the other models (Hanna et al. 1991). When used to simulate a series of major chlorine railcar incidents, the evaluated models (including ALOHA) performed within about one order of magnitude of each other but no observed data were available to verify the estimates (Hanna et al. 2008)
	SAFER/ TRACE	This model was evaluated (along with others) using data from a series of field experiment releases of ammonia and hydrogen fluoride using horizontal jet releases. This model was listed as having 'reasonable performance,' but data were not available to differentiate SAFER/TRACE from other models with reasonable performance (Hanna et al. 1991). This model was evaluated (along with others) using data from a series of field experiment releases of LNG, ammonia, Freon, and hydrogen fluoride. SAFER/TRACE was among the evaluated models that produced the most consistent predictions of plume centreline concentrations (Hanna et al. 1993a). When used to simulate a series of major chlorine railcar incidents, the evaluated models (including TRACE) performed within about one order of magnitude of each other but no observed data were available to verify the estimates (Hanna et al. 2008).
	GASTAR	This model was evaluated (along with others) using data from a series of field experiment releases of LNG, ammonia, Freon, and hydrogen fluoride. GASTAR was among the evaluated models that produced the most consistent predictions of plume centreline concentrations (Hanna et al. 1993a).
	PHAST	This model was evaluated (along with others) using data from a series of field experiment releases of ammonia and hydrogen fluoride using horizontal jet releases. PHAST was listed as having 'reasonable performance,' but data were not available to differentiate PHAST from other models with reasonable performance (Hanna et al. 1991). The model was evaluated (along with others) using data from a series of field experiment releases of LNG, ammonia, Freon, and hydrogen fluoride. PHAST was among the evaluated models that produced the most consistent predictions of plume centreline concentrations (Hanna et al. 1993a). Extensive model evaluation was done during the EU-funded SMEDIS (Scientific Model Evaluation of Dense Gas Dispersion Models) project (CERC 2002). Model outputs were compared for a series of major chlorine railcar incidents. The models (including PHAST) performed within about one order of magnitude of each other but no observed data were available to verify the estimates (Hanna et al. 2008). PHMSA has evaluated PHAST against the MEP and approved the use of this model for LNG siting in the USA (Witlox et al. 2013b).
	EFFECTS	Refer to SLAB, which is the dense gas dispersion model included in EFFECTS.
Lagrangian	QUIC	The performance of this model for simulating dispersion of tracer gases in an urban environment was evaluated against Joint Urban 2003 field experiment, with satisfactory results (Hanna et al. 2011). Validation against dense gas field releases has not yet been undertaken.

Model Category	Model	Description of Validation History
	SCIPUFF	This model was evaluated by comparing predicted maximum centreline concentrations with dense gas field experimental data in the Model Data Archive (MDA). SCIPUFF produced a good fit to the trial data, with a geometric mean of 1.098 and geometric variance of 1.355 (Sykes 2010). Model outputs were compared for a series of major chlorine railcar incidents. The models (including SCIPUFF) performed within about one order of magnitude of each other but no observed data were available to verify the estimates (Hanna et al. 2008). SCIPUFF is currently the model of choice for DOD and DHS use, however, the version with a dense gas module that is publically available is an earlier version.
	ArRisk (a)	(Anfossi et al. 2010) reports on work done to evaluate the models ability to simulate the dispersion of heavy gases. Comparisons were made against two field experiments (Thorney Island and Kit Fox) and a chlorine railway accident (Macdona). In addition, comparison against several experiments of the MDA was carried out. It was concluded that the model was fit for purpose, according to the (Chang and Hanna 2004) criteria.
	CHARM	An early flat terrain version of this model was evaluated (along with others) using data from a series of field experiment releases of LNG, ammonia, Freon, and hydrogen fluoride. CHARM was among the evaluated models that produced the most consistent predictions of plume centreline concentrations (Hanna et al. 1993a). CHARM was independently confirmed to perform well against some of the same field data (Touma et al. 1995).
CFD	FLUENT OpenFOAM PANACHE FLACS ANSYS-CFX	CFD models have also been validated against dense gas field experiment results. In general, their accuracy has been found to be similar to that of integral models (Carissmo et al. 2001), (Mack and Spruijt 2013) (Hanna et al. 2004).
(a) includes MicroSWIFT-SPRAY		

A comparison of the validation history indicates that most of the selected integral models do not show a statistically significant difference in performance when evaluated against a suite of dense gas field experiments. Also, published scientific reviews of the integral models show few major differences, which is not unexpected since they are all based on the same fundamental physical concepts and have been calibrated with the generally the same field experiments.

The development and application of the Lagrangian dispersion model SCIPUFF has been strongly supported by the US Government and other countries (UK, Canada, Australia, New Zealand). It is currently used in the CMAQ air quality model and the HPAC hazard assessment tool, both of which are regarded as state of the art. Similarly, the Lagrangian particle dispersion model MicroSPRAY is also used in HPAC to simulate dispersion around buildings. However, CMAQ and HPAC are not available for commercial use in Australia and there is not much information on model validation within the publicly available literature. Nevertheless, both SCIPUFF and MicroSPRAY may be regarded as suitable for simulation of dense gas dispersion in complex terrain, assuming that a high-resolution meteorological model is available to provide suitable wind, turbulence, and temperature fields.

CFD models have also been validated against dense gas field experiment results. In general, their accuracy has been found to be similar to that of integral models (Carissmo et al. 2001),(Mack and Spruijt 2013), (Hanna et al. 2004). However, the accuracy of CFD model results is dependent on the configuration and methodology used to perform the simulation and can vary significantly depending on the model inputs selected.

The main interest in CFD models is that they can model very low wind speed dispersion and account for terrain and obstacles. Many of the dense-gas validation experiments consider unobstructed flat terrain data therefore it may be unsurprising that CFD and integral models perform equally well there. However, integral models perform much less well in very low wind speeds, or with obstructions/complex terrain (Gant and Atkinson 2011).

There are significant issues that still need to be overcome with CFD models, which have been demonstrated to produce significantly different results for the same scenario in inter-model comparison exercises. The French Working Group on atmospheric dispersion modelling has done some recent work on this (Lacome and Truchot 2013). CFD models are slower to run than integral or Lagrangian models, which means they are unsuitable to be used routinely for risk assessment. However, CFD models are very useful for investigating certain complex situations (e.g. very low wind speeds/terrain). They can also be very helpful in developing more accurate source terms for use in simpler integral models, e.g. (Wareing et al. 2013), (Cleaver and Halford 2015).

8.7.7 Model evaluations with CO_2 field study observations

There have been only a small number of field scale CO_2 release experiments that can be used to validate far-field dense gas dispersion models. The most widely-used for model evaluations is the Kit Fox field experiment, in which a ground level release of a CO_2 area source was conducted at the Nevada Test Site across a set of panels erected to approximate the buildings and other obstacles at a chemical processing facility (Hanna and Steinberg 2001). (Hanna and Chang 2001a) compared HGSYSTEM/HEGADAS predictions with the Kit Fox CO_2 arc-maximum data. Mean relative bias is less than about 50 %. However, the field data were used to tune or calibrate the model entrainment constants, so the evaluation is not independent. (Mazzoldi et al. 2008) and (Hanna et al. 2004) evaluated CFD model performance with the Kit Fox data.

The McQuaid wind tunnel tests (Britter and McQuaid 1988) using CO_2 as a dense gas were carried out in three locations as part of the same study in which the Kit Fox field experiment was conducted. Those data have been used by (Briggs et al. 2001) to improve the vertical entrainment formulation used in many dense gas models (e.g. HEGADAS and DEGADIS).

The EPA I and II tests were performed in a flat desert setting using a ground-level, area source, but were used only for preliminary evaluations by EPA scientists (Hanna and Chang 2001a). (Briggs 1995, 1996) fit the 'constants' in some simple existing dense gas dispersion physical relations to the EPA I CO_2 experiment data. Since then, to our knowledge, no one has used those data. The full EPA I data archive has recently been obtained, as well as the EPA II data archive, from the group at Desert Research Institute who carried out the experiment.

The Kit Fox, EPA I and II, and McQuaid experiments all involved line or area sources, and are not directly relevant to near-field modelling of two-phase jet releases associated with CO_2 pipeline ruptures. The CO_2PipeTrans, CO_2PipeHaz and COOLTRANS projects have produced experimental data for CO_2 jets containing vapour-liquid and vapour-solid mixtures. This data can be used to validate near-field models, which can then be used as source terms for dense gas dispersion models. Near-field models were discussed in Section 8.6, so their validation is not considered here.

Table 8.4 provides a summary of model validation studies that have been performed with the selected models using CO_2 data. This table is not intended to include every validation study that has been conducted for these models, but instead to reflect the general extent of these studies.

Table 8.4: Model validation history with CO_2 field and laboratory experiments

Model Category	Model	Description of Validation History
Integral	HGSYSTEM	Used to 'satisfactorily simulate the observed concentrations' of Kit Fox, but the model should not be considered to have been independently validated because the Kit Fox data were used to calibrate the model (Hanna and Chang 2001a). HEGADAS, the dense gas dispersion module of HGSYSTEM, has been validated using the McQuaid wind tunnel data (Witlox and Holt 1999). HEGADAS was incorporated into a model (FRED), developed by Shell, that has been evaluated successfully against COOLTRANS data. It was concluded that FRED 'performs adequately for the purpose for which it is intended, which is providing hazard distances from free releases'(Dixon et al. 2012).
	SLAB	Validated with Kit Fox data (Hanna and Steinberg 2001).
	DEGADIS	Validated with Kit Fox data (Hanna and Steinberg 2001).
	ALOHA	Compared to Kit Fox data as part of the validation of a separate CFD model. Despite limitations due to necessary simplifications, the model results were 'well within the range for model acceptability' (Mazzoldi et al. 2008).
	SAFER/ TRACE	Validated with Kit Fox data (Hanna and Steinberg 2001).
	GASTAR	No validation information against CO_2 found.
	PHAST	This model has received the most extensive evaluation with CO_2 experimental data as a result of DNV's involvement with the ongoing JIP projects. The model has predicted concentrations accurately ('well within a factor of two') in experiments that included pressurized, liquid CO_2 releases from a vessel in both steady-state and time-varying conditions (Witlox et al. 2013a). Additional research has included efforts to incorporate and investigate the model's sensitivity to gas-to-solid phase transitions (Witlox et al. 2009), (Witlox et al. 2011; Witlox et al. 2013a). Also evaluated using the Kit Fox and McQuaid experimental datasets (Wilcox et al. 2014) and the INERIS test releases as part of the CO_2PipeHaz project (Gant et al. 2014). A protocol for investigating the sensitivity of model predictions of CO_2 concentrations has been demonstrated using PHAST (Gant et al. 2013).
	EFFECTS	Refer to SLAB, which is the dense gas dispersion model included in EFFECTS.
Lagrangian	QUIC	No validation information against CO_2 found.
	SCIPUFF	No validation information against CO_2 found.
	ArRisk MicroSPRAY	Satisfactorily simulated the results of the Kit Fox CO_2 field release experiment (Anfossi et al. 2010).

Model Category	Model	Description of Validation History
	CHARM (flat terrain)	No validation information against CO_2 found.
	CHARM (complex terrain)	No validation information found.
CFD	FLUENT	Evaluated against Kit Fox (Hanna et al. 2004).
	OpenFOAM	No validation information found.
	PANACHE	PANACHE has been used to model the dispersion of CO_2 releases and was evaluated favourably against the Prairie Grass and Kit Fox field experiments (Mazzoldi et al. 2008). This comparison is questionable because of the ad-hoc use of k-epsilon or k-l turbulence models to achieve good agreement with the data.
	FLACS	Evaluated against Kit Fox (Hanna et al. 2004).
	ANSYS-CFX	No validation information against CO_2 found.

8.7.7.1 *Pipeline blowdown*

The behaviour of a dense gas leaving a vertical stack was theoretically modelled by (Ooms and Duijm 1984). The theories they developed were later validated in a series of experimental verifications, including tests that were conducted using gas mixtures containing CO_2 (Li et al. 1986; Cleaver and Edwards 1990; Schatzmann et al. 1993; Donat and Schatzmann 1999).

The DEGADIS and SLAB models have each been tested against a scenario involving a vertical butane gas jet release, although observed data were not available for comparison (Hanna et al. 1996). One base run and three sensitivity runs were conducted for each model, including changes to stack height, source diameter, and averaging time. When the models were applied to this scenario, they showed 'a similar level of skill (as measured by mean bias and scatter)' when compared to field experiment data (Hanna et al. 1996). Both models predicated that the plume would rise initially and then sink to the ground, where the models would treat the subsequent dispersion as a ground-based area source (Hanna et al. 1996).

As part of the COOLTRANS programme, a test release of CO_2 was conducted through a 50 mm vent at a height of 3 m. Up to 40 sensors were located at distances of up to 200 m away from the release point to monitor CO_2 concentrations. The resulting white visible plume consisted mostly of condensed water vapour, resulting from the very low CO_2 plume temperature. It was observed that the visible plume extended significantly beyond the region in which the plume would be harmful (Wen et al. 2013). The experiment was simulated using the University of Leeds sonic jet CFD model as the source term (Wareing et al. 2013) and an OpenFOAM model for dense gas dispersion (CO_2FOAM) developed at Kingston University (Wen et al. 2013).

8.7.7.2 Release from offshore pipelines

Based on a review of the literature, experimental validation of the selected models for a scenario with an offshore pipeline release has not been conducted. However, one study (Engebø et al. 2013) did attempt to model such a scenario, noting that 'releases of gas in greater water depth will result in a plume of gas rising to the sea surface' (Engebø et al. 2013). Estimates were made of the impact of release depth on the plume diameter, and the authors suggested that a subsea release could be modelled by assuming a reduction of release velocity proportional to the increased release area at the water surface (Engebø et al. 2013).

8.7.8 Comments on 'fitness for purpose' with respect to validation

Most of the validation work on dense gas models has been done using far-field data (i.e. past the immediate influence of the source term) for a range of gases, with relatively little done specifically with CO_2.

A comparison of the validation history shows that most of the selected integral models do not show a statistically significant difference in performance. Also, published scientific reviews of the integral models show few major differences, which is not unexpected since they are all based on the same fundamental physical concepts and have been calibrated with the generally the same field experiments.

Based mainly on their use by government agencies in the US, both SCIPUFF and MicroSPRAY may be regarded as suitable for simulation of dense gas dispersion in complex terrain. However, this assumes that an accompanying high-resolution meteorological model is available to provide suitable wind, turbulence, and temperature fields.

CFD models have also been validated against dense gas field experiment results. In general, their accuracy has been found to be similar to that of integral models. However, this is not to say that all CFD models are equally good. The accuracy of CFD model results is dependent on the configuration and methodology used to perform the simulation and can vary significantly depending on the model inputs selected.

There is very little far-field CO_2 dispersion data available for model comparison. The available information is consistent with the behaviour of other dense gases, so these trials to not affect the conclusions drawn from other dense gas experiments.

Based on the model performance and validation history, all of the selected models have been validated against multiple dense gas datasets, but no single model has clearly out-performed the others.

8.7.9 Natural or inherent uncertainties in model simulations

8.7.9.1 Sources of model uncertainty

There is a fundamental uncertainty in all dispersion model estimates because the atmosphere has much natural variability. The general topic has been discussed in a number of papers and workshop reports, e.g. (Hanna 1978, 1988, 1993, 2007; Irwin and Hanna 2005; Hanna and Yang 2001)

One major reason for dispersion model uncertainties is the uncertainty in the mass emission rate. Even with in-stack samplers, the uncertainty is plus and minus about 20 or 30 %. In the absence of local sampling, Toxic Industrial Chemicals (TIC) source emissions models can be used for industrial stacks, tanks, valves, and pipes where the source opening and direction and location are known. It is assumed that thermodynamic variables (e.g., pressure, temperature) and state variables (e.g., chemical composition and phase) are also known. In this case the uncertainty is at least a factor of two.

Another major contributor to the total model uncertainty is wind direction uncertainty or variability, which is largest at small mean wind speeds. For example, at a wind speed of 2 m/s, there is about a plus and minus 30 degree uncertainty in wind direction, and hence plume direction. Thus the plume may meander back and forth over a sampler location near the plume mean centreline, with a period on the order of one to ten minutes. For sampler locations close to the mean plume edge, the meandering may cause single short term periods of high concentration when the plume swings over that sampler for a few seconds or minutes. As a cloud of dense gas diffuses away from the source under the influence of the prevailing wind, in-plume turbulent fluctuations will cause the concentration to fluctuate at any given point downwind. Integral dense gas dispersion models do not directly calculate these concentration fluctuations, and mainly provide predictions of the ‘ensemble mean maximum concentration’ as a function of distance downwind of the release. Some integral models parameterize the turbulent fluctuations by prescribing a probability distribution function (PDF) and variance for the fluctuating concentrations (exponential and clipped normal PDFs are most frequently assumed).

The ‘ensemble mean maximum’ refers to the average maximum concentration that would result from a large number of releases made under similar conditions (Wilson 1995). Validation of dense gas models is often done on the basis of their being able to predict the ensemble mean maximum concentration, assuming that a large number of field trials could have been performed.

Due to the difficulty of controlling all the variables in a large scale field trial, especially weather conditions, it is expected that the actual concentration measurements at a particular location will not be the same as the ‘ensemble mean’ for that point. Thus, it is unrealistic to expect that a model prediction will match the observations made in any given field trial experiment. The predicted maximum concentration at any point downwind is an estimate of the mean of maxima from a large number of hypothetical experiments.

The above considerations of the causes of uncertainty are the basis for the ‘factor of two’ fitness for purpose criterion proposed by (Chang and Hanna 2004) for rural field experiments. That is, if a model can predict a concentration that is within a factor of 2 of the observed data for reasonably well-defined research-grade field experiments, it may be regarded as fit for purpose.

8.7.9.2 *Safety implications of model uncertainty*

The ‘factor of two’ rule of thumb for comparison of model predictions with field experiment observations also implies that any dense gas model prediction will have a corresponding ‘factor of two’ margin of error. This assumes that the source emissions are reasonably well known. Thus, a model simulation showing a concentration profile of CO_2 equivalent to a 3 vol% TEEL value may be underestimating or overestimating by a factor of 2.

For a conservative hazard analysis, it would therefore more appropriate to use a CO_2 concentration of 1.5 vol% as the safety threshold.

A similar conservative approach is already used in safety analysis of natural gas facilities. Natural gas can be ignited by a spark at concentrations higher than 5 vol%, the lower flammability limit (LFL). Nevertheless, the US Federal Safety Standard of Liquefied Natural Gas facilities requires a safety ‘factor of two’ and specifies that, for risk assessment purposes, the critical value of LFL should be calculated as 2.5 vol% (Ohba et al. 2004). This approach is also recommended by the HSE in the UK (Webber 2007).

8.7.9.3 *Effect of model uncertainty on hazard distance*

It should not be assumed that the ‘factor of two’ rule of thumb also applies to the model-calculated hazard distance corresponding to a particular concentration, say 3 vol% $CO_{2.}$ This assumption would result in an unnecessarily large hazard distance. It can be shown using basic dispersion theory and observations during field experiments that the corresponding rule of thumb for uncertainty of modelled hazard distances is a range of about plus and minus 40 to 60%.

For example, (Gant and Kelsey 2012) have recently explored the potential impact of concentration fluctuations on the hazard distance associated with a CO_2 release. They assumed that 'the concentration fluctuates by a factor of two with a prescribed square-wave variation over time', i.e. that the concentration was twice the mean for half of the time, and zero for the remaining time. This probability function was combined with a simple dispersion model and probit functions for SLOT and SLOD for a QRA analysis. They found that the distance from the jet source to the SLOT or SLOD was approximately 50% higher when the factor-of-two parameterized model is adopted, compared to the approach where concentration fluctuations are ignored.

Large-scale field experiments have shown that, for an instantaneous release of a dense gas, there is a power law relationship between concentration and distance from the source, i.e.

$$\frac{C_i}{C_{io}} = \frac{V_i}{V_{io}} = \left(\frac{x}{V_{io}^{1/3}}\right)^{-n}$$

where V_{io} is the initial cloud volume, and V_i is the volume at a distance, x, from the source (Hanna et al. 1996). A similar relationship was derived from analysis of three large accidental Chlorine releases (Hanna et al. 2008). The available data suggests that the power law exponent, n, has a value of between 1.5 and 2.0.

This means that the distances, x_1 and x_2, between two concentrations, C_1 and C_2, in a dense gas cloud may be expressed as:

$$\frac{x_2}{x_1} = \left(\frac{C_1}{C_2}\right)^{1/n}$$

If C_2 is half C_1, and n is between 1.5 and 2.0, then x_2/x_1 will be between $(2)^{1/2}$ and $(2)^{1/1.5}$, i.e. 1.41 and 1.59. Thus, a ‘factor of two’ safety margin of error would lead to a 40% - 60% increase in the estimated hazard distance. This result, derived from experimental data, is consistent with the theoretical result of (Gant and Kelsey 2012).

The simple Gaussian plume model also leads to the above result. For a ground level continuous release, C is proportional to $1/\sigma_y\sigma_z$, and the plume dispersion parameters σ_y and σ_z are proportional to x^p, with p about 1 for lateral dispersion and between 0.5 and 1.0 for vertical dispersion. This also leads to a plus and minus 40% to 60% uncertainty range in hazard distance.

Therefore, for the purposes of hazard consequence assessment, it is recommended that a conservative hazard distance be calculated either by:

- Using a concentration end point equivalent to half the TEEL value; or
- Using the TEEL concentration to calculate a hazard distance, and then increasing this distance by 50%.

8.8 Dealing with complex terrain & variable atmospheric conditions

8.8.1 Complications arising from complex terrain

When modelling the transport and dispersion of hazardous gases, chemical processing industries and regulating agencies throughout the world often accept the assumption of flat terrain, instead of attempting to define the path that a dense cloud may take over or around complex terrain. It is argued that flat-terrain models are adequate (fit-for-purpose) because they tend to define the worst case at any downwind distance. Other reasons for this assumption are 1) the lack of field experiment data for dense gases in complex terrain, and 2) the lack of validated model algorithms that can handle a variety of complex terrain, especially small scale features such as roadside ditches where dense gas clouds can pool and flow downstream.

Although flat terrain is a conservative assumption in most circumstances, flat-terrain models will not necessarily be conservative in all terrain settings. Particularly when wind speeds are low, the plume may tend to ‘flow downhill’ towards population centres (de Nevers 1984) or become temporarily 'trapped' in trenches, behind hills, etc. (Chow et al. 2009). Detailed wind-tunnel studies of such phenomena were conducted using physical models by (McBride et al. 2001), who observed:

- channelling of dense gas clouds along valley floors or cuttings
- diversion of gas clouds by tall buildings or hills
- preferential flow of dense gas clouds down slopes (including upwind flow)
- entrapment of dense gas clouds within the wake zones formed in the lee of hills
- lateral spreading of dense gases at the foot of upslopes
- deviations of the direction of travel of dense gas clouds due to features upwind of the release location (affecting local wind patterns)
- enhanced dispersion of dense gases released on ridges or hill tops as a result of local acceleration of the wind.

As discussed earlier, the dense gas cloud will not exhibit behaviour different from that of a neutrally-buoyant cloud unless the excess density and the cloud dimensions are large enough and the wind speed small enough that the critical Richardson number criterion is exceeded.

8.8.1.1 Modelling the effects of structures on dense gas dispersion

The research on dense gas dispersion in this area has tended to model topographical features as either simple geometric shapes (e.g. slopes, fences, boxes) or as increased surface roughness. The practical focus has tended to be on the dispersion behaviour of dense gases in complex industrial or urban environments, and on strategies to mitigate the hazards of a dense gas release, rather than on characterising flow patterns in response to local topography. However, there are useful lessons to be drawn from the available literature, which are directly relevant to the design of a CO_2 pipeline in Australia.

A very good summary of the literature in this area as of about 1995 is provided in (Schulman et al. 1996). The effect of surface structure on dense gas dispersion was categorised under four headings: (1) isolated structures, (2) clusters of structures, (3) confining structures and (4) sheltering structures. A brief summary of the impact of these structures is provided in Table 8.5.

Table 8.5: Modelling the effects of structures on dense gas dispersion

Scenario		Guidance
Isolated structures	Release well upwind of the structure	The concentration of a dense gas cloud at a surface position downwind of the structure will be equal to or less than the estimated concentration in the absence of the structure. The dense gas plume may bifurcate around the structure with relatively little effect on the concentration, or it may be somewhat diluted by turbulence generated in the lee of the structure.
	Release just upwind of the structure	The concentration of a dense gas cloud may be substantially reduced by the increased entrainment of air into the downstream wake of a structure close to the source. At distances further downstream, however, plume concentrations will be very close to those anticipated without the structure.
	Release downwind of the structure	A dense gas released in the lee of an upwind structure will disperse in the windward direction as usual, but there may be some stratification of the gas in the recirculating wake at ground-level near the structure.
Clusters of structures		Arrays of structures (e.g. industrial sites) can, with appropriate care, be modelled as an equivalent uniform surface roughness, as long as the dense gas cloud size is deeper than the obstacle heights and is broader than several structures.
Sheltering structures		This refers to situations in which the mean air velocity is reduced, causing the influence of the negative buoyancy of the cloud to become more apparent. This can occur at the base of a slope or immediately downwind of a structure. Integral models cannot account for the possible increased localised concentration in such situations. This category also includes the release of dense gas in a complex of street canyons, which are actually partially sheltering <u>and</u> confining. It has been shown that, for a release within the street canyon, high ground-level gas concentrations can be maintained over substantially increased distances in that street canyon.
Confining structures		This includes structures such as bunds and fences, which can mitigate the effect of the release by limiting the escape of gas and enhancing dilution of the gas as it escapes over or around the barrier. This can result in reductions in plume concentrations downwind, although there is a possibility of high concentrations encountered inside the confined area. This category also includes porous barriers (e.g. pipe racks, dense shrubs, perimeter trees), which can increase the dilution due to turbulence and lead to smaller concentrations downfield. Confinement can also lead to higher dense gas concentrations inside the barrier, such as when the spread of the plume is constrained by a confining fence on one or more sides. The extreme situation is when the gas is completely enclosed by a surrounding barrier, in which case the rate of release is governed by detrainment into the air passing overhead. (Schulman et al. 1996) concluded that, in the majority of the above scenarios, the effects of obstructions on dense gas concentration are minor in comparison with the factor-of-two uncertainty of integral models. However, factor of five increases have been observed in street canyon scenarios and much larger increases may be expected as the degree of confinement or sheltering increases. Detrainment of dense gas from an enclosure or a depression may sometimes be accounted for in simple integral models. An equation for the rate of detrainment of a dense gas from a depression was proposed by (Briggs et al. 1990), and was later found to be consistent with data from the Jack Rabbit chlorine release experiments (Hanna et al. 2012). The SLAB, HEGADAS and DEGADIS models make use of the source blanket concept, which parameterizes the same effects suggested by (Briggs et al. 1990).

8.8.1.2 The effect of topographical scale on dense gas dispersion

A complementary approach to incorporating terrain into dispersion modelling scenarios was suggested by (Britter and McQuaid 1988), in which different strategies are applied depending on whether a topographical feature is significantly larger or smaller than the size of the release. Following this approach:

(a) When the topographic feature is small compared to the scale of the release, it can be regarded as an isolated structure or cluster of structures, as discussed in Table 8.5.

(b) When the topographic feature is large compared to the scale of the release, the terrain can be regarded as a simple slope, a sheltering structure or a confining structure, as discussed in Table 8.6.

Table 8.6: Modelling the effects of topographical scale on dense gas dispersion

<table>
<tr><th>Scenario</th><th>General Guidance</th><th>Detailed Guidance</th></tr>
<tr>
<td>Simple slope</td>
<td><p>For ‘instantaneous’ releases, the dispersion of a dense gas moving on a slope may be affected by the direction of the prevailing wind:</p>

When the wind and slope are opposed, the plume/cloud widens and its dilution is enhanced. In strong winds the cloud becomes sufficiently dilute to be carried uphill.
When the wind is down the slope, the plume/cloud is narrower and there is less dilution, so the concentration will be higher at downwind plume locations.

<p>For hazard assessment purposes, therefore, the usual practice is to ignore any short-range slope effects and assume flat terrain as the worst case scenario.</p></td>
<td><p>Wind-tunnel studies have suggested that, under some conditions, the angle of a sloping surface may have a relatively insignificant effect on the hazard zone expected for a dense gas such as CO_2. The relative velocity of a dense gas cloud (compared to the velocity of the ambient atmosphere) will increase as the slope is increased, but this increases the rate of entrainment of ambient air, which has a decelerating effect. Overall, the distance downstream to a particular centreline concentration is not much affected (Ross et al. 2002) (Britter and Linden 1980).</p>
<p>It was concluded that '<i>the bulk motion of the current is controlled by the front of a current, as for an axisymmetric current on a horizontal surface. Any integral model which predicts this part of the flow reasonably accurately will give a fair prediction for the bulk motion of the current</i>' (Ross et al. 2002).</p>
<p>The slope of the terrain will only be able to influence the flow of CO_2, if at all, while the cloud remains significantly dense (i.e. $Ri > Ri_c$).</p>

For small scale releases, of the order of 5 to 10 tonnes releases of dense gases will be influenced by terrain only in the near field (< 100 m).
For medium-sized releases, of the order of 100 tonnes, terrain will have an influence over distances of <300 or 400 m
For huge releases such as major ruptures of a large CO_2 pipeline the distance may extend to several kilometres.

<p>It is not a simple matter to model the topography at scales of several hundred metres, since topographical mapping may not be available at such resolution. As discussed above, surface features usually have a dispersive effect, causing enhanced vertical and lateral mixing, and a reduction in the hazard distance. The greatest hazard effect would result from an unimpeded direct cloud travelling over a flat surface.</p></td>
</tr>
<tr>
<td>Sheltering or confining structures</td>
<td colspan="2"><p>In some situations, topographical features such as valleys, hillsides and depressions can effectively be regarded as sheltering or confining structures, as discussed in Table 8.5. For example:</p>

A valley with sides higher than the plume, and assuming the cloud is spread across the width of the valley, is equivalent to a street canyon, and will allow the plume to travel significantly further at high concentration. Modelling of this scenario is problematic, because there have been no large-scale experimental studies to produce data for model validation.
A hill may divert the flow of the plume, in the same manner as a fence.

<p>A depression may trap a dense gas cloud, particularly during calm conditions, acting as a confining enclosure.</p></td>
</tr>
</table>

8.8.2 Complications arising from variable atmospheric conditions

Wind speed is always one of the key inputs to dispersion models, with consequence assessments based on a range of wind speeds and atmospheric stabilities. Under light wind conditions, an ‘instantaneous’ release will spread out widely near the source, and will become diluted before moving very far downwind. With moderate wind speeds, however, the cloud has less lateral spread and can travel further downwind before dispersing. Thus, moderate wind speeds may sometimes represent the worst case for instantaneous releases (Hanna et al. 1996).

In calm conditions, with very low wind speeds, of the order 0.5–1 m/s, the dispersion of the cloud will be reduced, and it will travel further along the ground due to gravity slumping. Under these conditions, topographical features can direct the flow of the gas, and stable pooling can occur in local depressions. Depending on the size of the depression and other conditions, the cloud may only disperse downwind when the wind speed increases or the ground becomes warmer.

The wind direction is also an important variable. For example, it is possible for the direction of flow of a dense gas cloud to be reversed in the presence of a strong opposing wind, even on steeply sloping ground (Hankin 2004).

8.8.3 Modelling of complex terrain and weather

The selected models differ substantially in their ability to consider the impact of complex meteorological conditions, terrain, and other obstructions (e.g. buildings) on dense gas dispersion. As these factors may be important under certain circumstances, compares each model’s treatment of terrain, obstruction, and meteorology.

As summarized in Table 8.7, the integral models generally do not account for terrain and assume a flat surface. The simplified similarity or box models and the slab models (HEGADAS, DEGADIS, SLAB, SCIPUFF, and GASTAR) treat the forces acting on the dense cloud at any downwind distance as bulk properties. As a result, these models do not account for the effects of ditches and ridges and other local terrain. GASTAR can treat a constant slope, but this model feature has not been adequately validated.

Additionally, very few of the integral models account for flow and dispersion disturbances caused by nearby buildings or other obstacles.

The CFD model FLACS has been shown to provide useful simulations for releases in industrial areas with complex terrain (Dharmavaram et al. 2005). FLACS was also used by the CO_2PipeHaz project to simulate CO_2 releases in complex terrain (Woolley et al. 2014b).

An intermediate approach, between simpler integral models and CFD models, is to use a diagnostic mass-consistent wind model to account for flow variations in and around terrain and buildings, and to use a Lagrangian particle model to simulate dense gas dispersion. The widely-used SCIPUFF (Sykes 2010) and Micro-Spray (Anfossi et al. 2010; Mortarini et al. 2013) models are in the latter category. The Lagrangian models, whilst not able to model the complexity of terrain to the same degree as CFD models, allow for relatively straightforward import of terrain data from publicly available sources and have faster run times. However, there is no suitable large-scale experimental data available for validation of the performance of these models.

It was stated earlier that the chemical industries and regulatory agencies generally accept 'flat-terrain' simulation as representing the ‘worst case’ scenario. Except in the near field (right around the source), the topography tends to be dispersive, causing enhanced vertical and lateral mixing.

Similarly, very few of the dense gas models account for flow and dispersion disturbances caused by nearby buildings or other obstacles because, in general, such flow disturbances tend to be dispersive. Therefore it is regarded as conservative to ignore the buildings.

The various models also differ in their ability to capture complex meteorological conditions. For example, ALOHA uses a single wind speed and atmospheric stability class to represent meteorological conditions over an entire simulation, whereas SAFER/TRACE and GASTAR can account for spatially varying wind fields. Models such as CAMEO/ALOHA account for the uncertainty in wind direction (i.e. plume path) by defining pie-shaped sectors in which the maximum centreline concentration might occur (e.g. 45° is a rough rule of thumb).

Both SCIPUFF and MicroSPRAY/ArRisk accept detailed meteorological input files to account for changes in wind speed and direction at any point in the computational grid. These models use wind field calculation methods (mass-consistent diagnostic wind models) that have been well accepted in passive gas regulatory models.

CFD models could theoretically use Large-Eddy-Simulation to account for time-variable small-scale, complex meteorological conditions across the modelling domain. However, CFD models do not contain built-in atmospheric simulation systems, so the wind field must be calculated from fundamental equations. Such simulations cannot easily be verified, so their accuracy is uncertain. It would require significant time, effort, and modeller expertise to use CFD methods effectively.

As part of the CO_2PipeHaz project, two different CFD models were developed for far-field CO_2 dispersion, one using ANSYS-CFX and the other using FLACS. Realistic terrain data was obtained from the UK Ordnance Survey. This preliminary work highlighted the need for two-way coupling between the near- and far-field dispersion models, especially under low wind conditions. While this should be possible to achieve, it would not be a trivial matter (Woolley et al. 2014b).

Lagrangian models can account for complex atmospheric conditions by using numerical approximation methods. SCIPUFF and MicroSPRAY/ArRisk have gained acceptance for use in modelling complex scenarios. They are appropriate for use as an adjunct to the simpler integral models, particularly in high consequence locations.

Table 8.7: Treatment of terrain and weather conditions

Model Category	Model Name	Accounts for Complex Terrain	Accounts for Obstructions (e.g. buildings)	Accounts for wind variability in space?	Meteorological Considerations
Integral	SLAB	No	No	No	Uses P-G or M
	DEGADIS	No	No	No	Uses P-G
	HGSYSTEM	No	Limited (building canyon only)	No	Uses P-G
	ALOHA	No	No	No	Uses P-G
	SAFER/ TRACE	No	No	Limited	User may enter wind speed and P-G
	GASTAR	No (constant slope only)	Yes	Limited	User may enter wind speed and P-G or M for each specified slope.
	PHAST	No	No	No	Uses P-G
	EFFECTS	No	No	No	Uses P-G or M
Lagrangian	SCIPUFF	Yes	Parameterized	Yes	Allows NWP or diagnostic wind inputs, wide variety of observations
	MicroSWIFT/ ArRisk	Yes	Yes	Yes	Mass-consistent diagnostic wind model; Wind variability in space can be coupled with 3D terrain maps.
CFD	FLUENT, OpenFOAM, PANACHE, FLACS, ANSYS-CFX	Yes	Yes	Capable	Atmospheric simulation based on solution of Navier-Stokes equations of motion, state, and thermodynamics.
Notes: P = Pasquill-Gifford Stability Class, M = Monin-Obukhov length QUIC, referred to in Section 8.5.3.1 has similar capabilities to MicroSWIFT. Sources: (US-EPA 2007; CERC 2009; Spicer and Havens 1989; Ermak 1990; HGSYSTEM 2014; Safer Systems 2014; ANSYS 2013; OpenFOAM 2014; TNO 2014)					

8.8.4 Comments on ‘fitness for purpose’ for dealing with complex terrain

As noted in Section 4.6.1, Appendix BB of AS 2885.1 recommends that *the measurement length shall be extended locally wherever the landform suggests that spread of the gas cloud in a particular direction may be promoted by gravity drainage.* However, it has been shown here that the slope of the terrain will only be able to influence the flow of CO_2, if at all, while the cloud remains significantly dense (i.e. $Ri > Ri_c$).

- For small scale releases, of the order of 5 to 10 tonnes releases of dense gases will be influenced by terrain only in the near field (< 100 m).
- For medium-sized releases, of the order of 100 tonnes, terrain will have an influence over distances of <300 or 400 m.
- For huge releases such as major ruptures of a large CO_2 pipeline the distance may extend to several kilometres.

This is especially the case under low wind speed conditions, which increases the value of Ri. In calm conditions, with very low wind speeds, the dispersion of the cloud will be reduced, and it will travel further along the ground due to gravity slumping. Under these conditions, topographical features can direct the flow of the gas, and stable pooling can occur in local depressions.

At higher wind speeds, the value of Ri is decreased and topographical features tend to have a dispersive effect, causing enhanced vertical and lateral mixing, and a reduction in the hazard distance.

For this reason, it is usually argued that flat-terrain models are fit-for-purpose because they tend to define the worst case at any downwind distance. The greatest hazard would result from a dense cloud travelling unimpeded over a flat surface.

Thus, the recommendation in Appendix BB of AS 2885.1 is specific for very calm conditions. Under windy conditions it will generally not apply, especially for small to medium-sized releases. For very large releases, the plume will be large in comparison to local topographical features, and will travel unimpeded even under windy conditions.

Consequence assessment studies will usually be concerned with the effects of large potential CO_2 releases, for which the plume may be expected to travel unimpeded over the surface. In this application, integral models may be regarded as fit for purpose in most circumstances.

Integral models may not be appropriate in situations where the local terrain has the potential to be significantly larger than the size of the gas plume. For example, a steep hillside may block the path of the plume and divert it in another direction. Where such conditions are a possibility, common sense should be applied to determine the applicability of any modelling approach.

If simulation of dense gas dispersion in complex terrain or atmospheric conditions is essential, either Lagrangian models or CFD models may be considered. However, caution is necessary in applying such models, as there is currently no large-scale experimental data available to validate such models on anything but flat terrain.

8.9 Applicability at different stages of pipeline design

8.9.1 Prior use of dispersion modelling in CO_2 pipeline design

Dense gas dispersion models can play an important role at various stages in the lifecycle of a CO_2 pipeline, including preliminary pipeline design, threat consequence analysis; during emergency response activities; and during accident reconstruction.

Public information on the use of dispersion models in the design of commercial CO_2 pipelines is limited because such work is usually of a commercial nature.

SLAB (as part of CANARY) was used in the environmental impact assessment for the FutureGen 2.0 project in Illinois (US Department of Energy 2007). CANARY has been used in risk analysis studies for CO_2 pipelines in the USA and Spain[61].

In addition, in the United Kingdom, the Health and Safety Laboratory has developed a risk assessment methodology for high pressure CO_2 pipelines using integral dispersion models, which was demonstrated using PHAST (McGillivray et al. 2014). PHAST was also used to perform a risk analysis of a generic CO_2 pipeline in the UK for the Department of Trade and Industry (Vendrig et al. 2003).

8.9.2 Review of pipeline stages requiring dispersion modelling

The attributes required of a dense gas dispersion model may vary at different stages during the lifetime of a CO_2 pipeline. As mentioned in Section 4.5, AS 2885.1 specifies that a safety management study must be employed at various stages throughout the entire life of the pipeline. As a minimum, during the preliminary design and approval stage, the detailed design stage, the pre-construction review and the pre-commissioning review.

8.9.2.1 Preliminary design stage

AS 2885.1 has provides graphical design tools, developed with the use of validated software models, that allow an engineer to develop a preliminary design for a natural gas pipeline without the need for additional detailed modelling. This level of detail is sufficient to specify the measurement length based on the proposed pipeline operating conditions, and to allocate individual location classes along the proposed route. According to the ALARP principle, it is preferable to route the pipeline to avoid any high consequence locations, but if this is not possible then appropriate strategies have to be proposed to mitigate the associated risk. For natural gas pipelines, this level of detail should be sufficient to gain regulatory approval to proceed to the detailed design stage.

In Section 4.6.1, it was shown that the AS 2885.1 definition of measurement length is not directly applicable to CO_2 pipelines. However, the currently available evidence is that the distances to equivalent levels of risk are roughly comparable between CO_2 and natural gas for the same pressure, temperature and puncture size.

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[61] J. Cornwell, communication via email, 1 July 2014

Accordingly, the evidence supports the current recommendation in Appendix BB of AS 2885.1 that, for CO_2 pipelines, *the measurement length for definition of the location class limits shall be estimated on the basis that the pipeline is transporting natural gas*.

Thus, the design tools that are provided in AS 2885.1 may be regarded as applicable to the preliminary design stage of a new CO_2 pipeline in Australia. It should be possible to gain regulatory approval to proceed to the detailed design stage without the need for additional detailed modelling.

8.9.2.2 Detailed design through to construction

During the detailed design stage, it will be necessary to undertake consequence analysis to assist in the selection of isolation valve locations and vent stations along the length of the pipeline, as well as the maximum allowable discharge rate in high consequence locations.

In these applications, the design tools provided in AS 2885.1 are not adequate, so a model such as those discussed in this report will be required. At this stage of design it is generally accepted that the assumption of flat terrain will usually provide conservative design data, although the designer must apply common sense and be aware of possible implications of significant topographical features along the pipeline route.

8.9.2.3 Pipeline operation

AS 2885.1 specifies that the safety management study process must continue throughout the working life of the pipeline. It would be appropriate to continue to use the same modelling approach adopted during detailed pipeline design, so that achievement of ALARP can be documented.

AS 2885.1 requires that CO_2 pipeline operators will develop an emergency response plan, to ensure an effective response in the event of any unplanned release of CO_2. This may involve desktop simulations of potential incidents and response planning. Since the emergency response plan can be developed over an extended period, it would be appropriate to use the same simulation modelling tools as during the detailed design stage.

It may also be desirable, although not mandatory, to develop software tools for use during emergency incident response. In this application, the modelling software would need to be user-friendly and provide quick answers. In emergency situations, it may be acceptable to use a more streamlined model with reduced functionality but increased speed. Emergency response modelling could require running a model with minimal training in a short time frame so that, for example, evacuation of an impacted area could be advised, if necessary.

During accident reconstruction, use of a more complex model that can more accurately reflect the specific conditions at an accident location may be justified, particularly since longer modelling times would be offset by the limited number of scenarios to be modelled.

8.9.3 Comments on ‘fitness for purpose’ relative to stages of operation

At the preliminary design phase, it is not necessary to employ specialist dispersion modelling tools. The graphical design tools in AS 2885.1, which were developed for the design of natural gas pipelines, are also suitable for use with CO_2 pipelines.

At the detailed design stage, and subsequent stages including pipeline operation, integral models such as SLAB, DEGADIS, HGSYSTEM, GASTAR, SAFER TRACE, EFFECTS or PHAST may be applicable. Each model has its strengths and weaknesses, which need to be understood when making a selection. Specifically in relation to CO_2 pipeline design, PHAST version 6.6 or later and EFFECTS version 10 (when it is released) would have to be considered as prime candidates, as they have both include pipeline depressurisation algorithms and have both been revised to reflect the outcome of recent large-scale CO_2 release experiments.

Other integral models may also be applicable, provided that due consideration is given to ensuring that the source term input is as accurate as possible. This may involve coupling together two or more separate models, to adequately treat the pipeline depressurisation, jet release and dense gas dispersion aspects. There is no inherent reason that CFD modelling could not be used for one or more of these applications, provided that the model had been satisfactorily validated.

If complex terrain is a particular issue in a high consequence location, then it may be necessary to consider Lagrangian or CFD modelling tools. However, these are only useful tools if they can be properly validated for complex terrain. Such terrain validation studies have not been done for any of the models considered in this report. Further work is needed to develop useful design tools from Lagrangian or CFD models. For the time being, dealing with complex terrain issues requires a dose of common sense.

For emergency response activities, models such as ALOHA, SAFER TRACE and ArRisk may be appropriate. The limitations of each model need to be understood, to ensure that a likely emergency scenario can be adequately simulated. More comprehensive models with streamlined user interfaces, such as PHAST or EFFECTS, may also be considered.

During accident reconstruction, the same model used during the design phase is likely to be used in the first instance. In complex urban or industrial environments, however, construction of a detailed CFD model of the specific layout may be the only way to adequately simulate the finer details of CO_2 dispersion.

8.10 Regulatory status of dense gas dispersion models

8.10.1 Regulatory status in the United States of America

In the United States, interstate CO_2 pipelines are regulated by the Pipeline and Hazardous Materials Safety Administration (PHMSA), which is a part of the Department of Transportation (PHMSA 2014). Recent CO_2 transportation experience (outside of CCS) in the United States has also resulted in standards and best practice guidance documents for CO_2 pipeline design, construction, and operation. These include the ASME B31.4 Pipeline Transportation Systems for Liquids and Slurries (2012) (ASME 2012).

In practice, government agencies in the United States use various models for evaluation of dense gas releases:

- The United States National Oceanic and Atmospheric Administration (NOAA) originally developed the ALOHA model, which incorporates DEGADIS.
- The US Environmental Protection Agency (EPA) uses and recommends only publicly-available models (e.g. DEGADIS, HGSYSTEM, SLAB, ALOHA).
- The PHMSA has approved the use of DEGADIS, FEM3A, FLACS AND PHAST for dispersion of dense gas resulting from LNG spills.
- PHAST has been purchased by several chemical industries (e.g. DuPont, Air Products). They generally use PHAST together with other models (e.g. TRACE, SLAB) to bracket issues under evaluation.
- SCIPUFF is presently the most widely-used model in DOD and DHS studies of all types of toxic industrial chemicals, and is the core NARAC model.

As noted above, specific to CO_2 releases, the DOE conducted a risk assessment using SLAB for the FutureGen 2.0 project in Illinois (US Department of Energy 2007).

8.10.2 Regulatory status in Europe

European agencies have established a number of standards applicable to pipelines transporting CO_2, although none directly address transport in the context of Carbon Capture Storage or as a highly pressurized fluid in a pipeline (Global CCS Institute 2014).

Similar to the United States, some governmental organizations in Europe have also used dense gas models specifically for risk assessments of CO_2 pipeline releases. As mentioned above, PHAST was used for risk assessment in the United Kingdom by the Health and Safety Laboratory and in a project for the Department of Trade and Industry (McGillivray et al. 2014; Vendrig et al. 2003). PHAST is well known and recommended by the French Administration, and is the default model used in the

Netherlands (within SAFETI-NL). Alternative models can still be used in the Netherlands, but need to be justified on a case-by-case basis to RIVM.

8.10.3 Regulatory status and comments on ‘fitness for purpose’ in Australia

Most regulatory agencies in Australia have little to no experience with dense gas dispersion modelling. In Victoria, the Environmental Protection Agency specifies the use of AERMOD as its standard air pollution dispersion regulatory model (Vic-EPA 2013). However, AERMOD is a Gaussian dispersion model, and is not suitable for modelling dense gas dispersion.

In order for an AS 2885.1 safety management study to be undertaken for a new CO_2 pipeline in Australia, it will be necessary for design engineers and regulators to agree on the dispersion models that are suited to this task. Only models that are regarded as ‘fit for purpose’ will be acceptable.

Based on the experience in the United States and Europe, it may be expected that DEGADIS, HGSYSTEM, SLAB (including EFFECTS), ALOHA, PHAST and SCIPUFF may be acceptable to Australian regulators. In principle, a case could be made for other models considered in this report, depending on the specific requirements of the project.

Arguably, SLAB (including EFFECTS) and PHAST may be most ‘fit for purpose’ because they have been successfully utilized in previous CO_2 transport design projects. Of these, PHAST version 6.6 or later and the forthcoming EFFECTS version 10 have been subject to the greatest refinement using recent large-scale CO_2 release data.

8.11 Overall conclusions on ‘fitness for purpose’

Table 8.8 summarizes the fit for purposes review of the selected models. Each model has strengths and weaknesses, and the ‘best’ choice will depend on a number of different factors.

Cost is obviously an important consideration. Commercial models such as PHAST and EFFECTS have been updated in line with recent research results, so they may be regarded as ‘state of the art’.

SLAB is also available as part of commercial packages from Quest Consultants (CANARY) and Breeze (Incident Analyst[62]). DEGADIS is also available as part of the Incident Analyst package. These packages may also be regarded as fit for purpose.

ALOHA and SAFER/TRACE may also be regarded as fit for purpose for specific applications, provided that their limitations are understood.

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[62] http://www.breeze-software.com/IncidentAnalyst/

Acceptability to regulators is also another important consideration. Regulatory bodies in Australia have generally tended to follow the lead of US regulators, and thus would be expected to favour models such as SLAB (including EFFECTS), PHAST and ALOHA. In the end, regulators will consider any potential model on its merits, so any of the models mentioned above could be candidates.

The more complex Lagrangian models cannot be recommended as primary design tools. Their lack of field trial validation is a significant limitation.

CFD models have been developed as useful design tools during the CO_2PipeTrans, CO_2PipeHaz and COOLTRANS projects. A CFD model for multi-phase CO_2 jets has been used to develop design correlations that can be utilised as source terms for integral models. Like other models, CFD models need to be properly validated and their limitations understood. Their sensitivity to user-selected input conditions is an issue that has yet to be adequately resolved. However, their ability to model complex physical situations and low wind conditions means that they are likely to play an increasing role in the future. At this stage, without further validation, it is difficult to recommend CFD models for far-field dense gas dispersion as completely fit for purpose.

Table 8.8: Summary of evaluation criteria for selected models

Model Category	Model Name	Free?	Availability of Graphical User Interface	Complexity of Inputs	Validated against dense gas experiments	Validated against CO_2 experiments	Able to represent a range of source configurations	Ability to account for complex terrain and obstructions	Ability to account for complex meteorology
Integral	SLAB	Yes	Purchase	Medium	Yes	Low	Medium	None	Low
	DEGADIS	Yes	Purchase	Medium to High	Yes	Medium	Low	None	Low
	HGSYSTEM	Yes	No	Medium to High	Yes	Medium	High	Low	Low
	ALOHA	Yes	Free	Low	Yes	Low	Low	None	Low
	EFFECTS (v10)	No	Purchase	Medium	Yes	High	High	None	Low
	SAFER/TRACE	No	Purchase	Medium	Yes	Low	High	None	Low
	GASTAR	No	Purchase	Medium	Yes	Low	High	Medium	Medium
	PHAST	No	Purchase	Medium	Yes	High	High	None	Low
Lagrangian	*QUIC*(b)	*Yes*	*Free*	*Medium*	*Yes*	*Low*	*High*	*High*	*High*
	SCIPUFF	Yes	Free	High	Yes	Low	High	Medium	Medium
	ArRisk(a)	No	Purchase	Medium	Yes	Low	High	High	High
	CHARM (flat terrain)	No	Purchase	Medium	Yes	Low	High	None	Medium
	CHARM (complex terrain)	No	Purchase	Medium	No	Low	High	High	Medium
FD	FLUENT, PANACHE, FLACS, ANSYS-CFX	No	Purchase	High	Yes	Low	High	High	High
	OpenFOAM	Yes	Purchase	High	Yes	Low	High	High	High

(a) Includes MicroSWIFT-SPRAY

(b) Currently only available for non-profit research purposes.

9 ADDITIONAL RISK MITIGATION MEASURES

9.1 Summary

The main focus of this report has been the application of dense gas dispersion modelling to hazard consequence analysis for design of new CO_2 transportation pipelines in Australia. Chapter 5 summarised the approaches specified in AS 2885.1 to reduce the risk of harm caused by either a controlled or accidental discharge from a CO_2 pipeline, with particular reference to dense gas dispersion modelling.

Section 4.8.2 briefly described the different measures that are specified in AS 2885.1 to mitigate the risk of pipeline damage and improve operational safety. In addition to these generic measures, there is a range of additional risk reduction methods for CO_2 pipelines that have been developed as international best practice.

This Chapter provides a brief summary of the reference documents that provide guidance on best practice for CO_2 pipelines, covering everything from design issues, materials of construction, fabrication techniques, corrosion control, pipeline monitoring and control, pigging, venting, integrity assessment and operational safety.

This Chapter also considers the potential for adding mercaptans to the CO_2 to make a leak easier to detect, as is done with natural gas. However, it is concluded that this is not currently done and further research is needed to understand the full practical ramifications of doing so.

9.2 International best practice

The literature described in Table 9.1 should be consulted for specific technical information on the safe operation of CO_2 pipelines.

Table 9.1: International best practice - literature

Document	Description
'State-of-the-art overview of CO_2 pipeline transport with relevance to offshore pipelines' (Oosterkamp and Ramsen 2008)	Discusses materials of construction, process measurement and control, operational issues and experiences at CO_2 pipelines in the United States.
'Good plant design and operation for onshore carbon capture installations and onshore pipelines' (Energy Institute 2010a)	Provides guidance on design and operational issues, materials selection, construction techniques, leak detection and operational safety.
'Design and operation of CO_2 pipelines' (DNV 2010)	Provides specific guidance for CO_2 pipelines, covering design, construction, corrosion control, operation, monitoring and integrity assessment considerations.

Document	Description
'Guidance on CCS CO_2 safety and environment – Major accident hazard risk management' (DNV 2013)	Section 3.4.1 of Level 4 of CO_2RISKMAN provides guidance on maximising the inherent safety of a CO_2 pipeline system. Examples of some relevant design measures include: • Minimise need for hands-on system operation or interactions • Minimise start/stop and non-steady state operating • Increase the separation distance between the pipeline and populated areas • Avoid environmentally sensitive areas • Location and protection of escape routes • Location and protection of muster areas • Route the pipeline at a lower topographical elevation than adjacent populations, and increase the separation distance when the elevation must be higher • Avoid having valve pits or other below-ground access points • Create earth banks or other manmade physical features to direct/move a CO_2 release away from people or other safety critical areas • Avoid hazardous concentrations of other substances (e.g. H_2S) in the CO_2 stream Section 3.4.2 of Level 4 of CO_2RISKMAN provides guidance on specific preventative measures to reduce the likelihood of a range of failure mechanisms. This provides a valuable resource for CO_2 pipeline designers and should be consulted.
' CO_2 pipelines good practice guidelines' (Wilday and Saw 2013)	This is a useful reference compendium that includes reviews of the following: Existing international guidelines for pipelines in general Existing guidelines that are specific to CO_2 pipelines Contributions made by the CO_2PipeHaz project to good practice for decision support Methodology for decision support for CO_2 pipelines.

9.3 Odourants

CO_2 presents a hazard because it is a colourless and odourless asphyxiant that can accumulate in enclosed spaces. People entering such spaces may be quickly overwhelmed and killed. With methane, where pockets of accumulated gas may present an explosion risk, it is standard practice to add strongly-smelling mercaptans to the gas so that it may be readily detected. It has been suggested that mercaptans could also be added to CO_2 intended for transportation by pipeline (Gale and Davison 2004).

At the present time, the only CO_2 pipeline containing mercaptans is the Weyburn pipeline from the Dakota Gasification Company, which carries CO_2 extracted from synthesis gas produced from lignite. The mercaptan in the CO_2 was not added deliberately, but arises from contaminants present in the lignite. The presence of this natural odourant in the pipeline has helped in the identification and remediation of CO_2 leakages (Gale and Davison 2004).

It is currently not standard practice to deliberately add mercaptans to CO_2 pipelines. There is insufficient knowledge about the interactions between CO_2 and trace components at supercritical pressures. There is a risk that the mercaptans would react with other gas components or the pipeline materials and lose potency (Crippen et al. 2013), or that such interactions would adversely affect the pipeline integrity. Further research is needed to understand the potential impact of trace levels of mercaptans on CO_2 pipeline performance.

10 CONCLUSIONS

10.1 Overview

The investigation addressed two key topics:

- a critical review of current pipeline design standards.
- identification of a fit-for-purpose CO_2 dispersion model.

10.2 Critical review of current pipeline design standards

AS2885 is the applicable standard for design, construction and management of pipelines in Australia.

The investigation made the following conclusions in relation to the applicability of AS 2885 for safe design and operation of CO_2 pipelines (refer to Section 8.9.2):

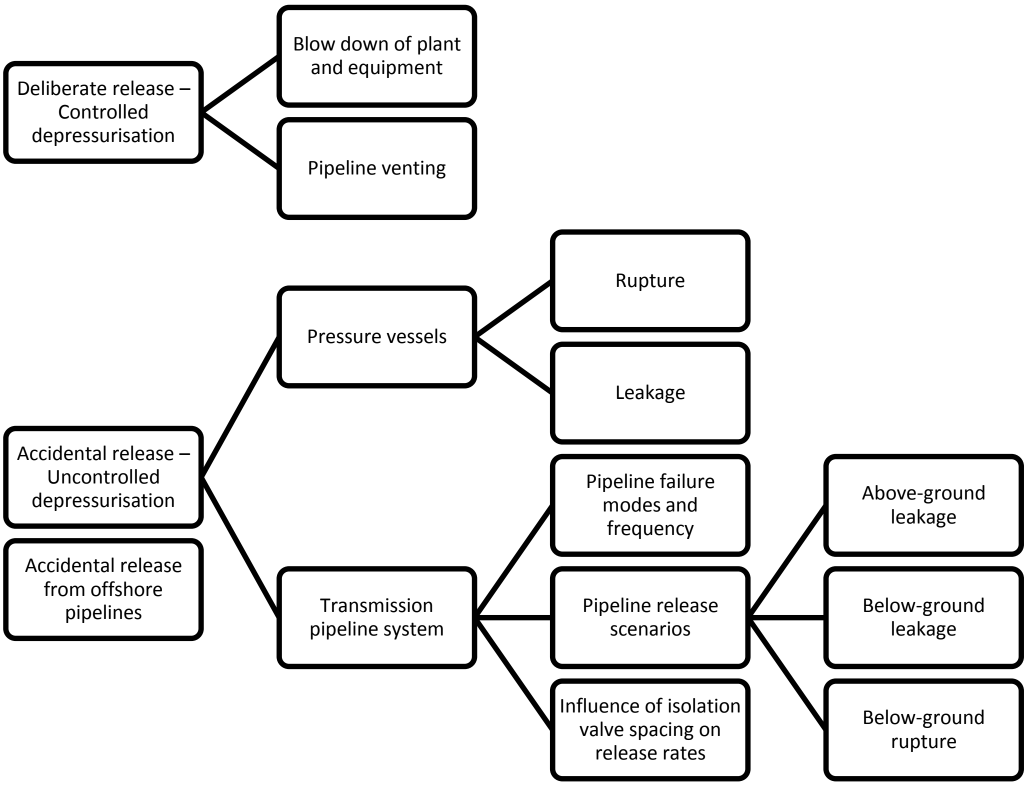
- For the **preliminary design stage** of a new CO_2 pipeline in Australia, the design tools provided in AS 2885.1 are applicable. It should be possible to gain regulatory approval to proceed to the detailed design stage without the need for additional detailed modelling. In particular, this report supports the current recommendation in Appendix BB of AS 2885.1 that, for CO_2 pipelines, ‘the measurement length for definition of the location class limits shall be estimated on the basis that the pipeline is transporting natural gas’.
- For the subsequent **detailed design stage**, consequence analysis will be necessary to help identify the measurement length, to select locations for isolation valves and vent stations along the length of the pipeline, and to determine the maximum allowable discharge rate in high consequence locations.
- During the **working life of the pipeline**, AS 2885.1 also specifies that the safety management study process must continue, and that an appropriate emergency response plan be developed.

For both the detailed design phase and pipeline working life, the design tools provided in AS 2885.1 are not adequate. Modelling tools suitable for simulating the dispersion characteristics of dense, cold clouds of CO_2 gas must be used. This finding leads into the second key topic of the investigation – identifying a fit-for-purpose model.

10.3 Identification of a 'fit for purpose' CO_2 dispersion model

A range of different release scenarios are possible from CO_2 transportation infrastructure, depending on whether the release is deliberate or accidental, major or minor, from a storage tank, pipeline or valve, or from below or above ground. For each of these scenarios, it is necessary to quantify the appropriate ‘source term’ as an input to a dense gas dispersion model. In this report the modelling issues for each of the release scenarios shown in Figure 10.1 were reviewed.

Figure 10.1: Release scenarios



Guidance is provided for each of these cases, based on a review of the current 'state of the art'.

A significant difference between natural gas and CO_2 pipelines is the *mechanism for harm* in the event of an accidental rupture. A natural gas pipeline rupture can create an initial fireball that is extremely dangerous to people and property, with potential effects distances of several hundred metres. The effects distances associated with rupture of a CO_2 pipeline, on the other hand, would be influenced by wind speed, direction and terrain effects, which would potentially result in a smaller affected area.

It is important for the community to be aware of the differences, and that suitable dispersion modelling tools are available to ensure that the risks are managed appropriately.

This report provides guidance on the dispersion modelling techniques that may be regarded as ‘fit for purpose’ for use in CO_2 pipeline design and safety management studies according to AS 2885.1. Most regulatory agencies in Australia have little experience with dense gas dispersion modelling. In Victoria, the Environmental Protection Agency specifies the use of AERMOD as its standard air pollution dispersion regulatory model. However, AERMOD is a Gaussian dispersion model, and is not suitable for modelling dense gas dispersion.

In order for an AS 2885.1 safety management study to be undertaken for a new CO_2 pipeline in Australia, it will be necessary for design engineers and regulators to agree on the dispersion models that are suited to this task. Only models that are regarded as ‘fit for purpose’ will be acceptable. The assessment was based on a number of criteria:

- Availability, ease of use, access to technical support
- Ability to calculate appropriate source terms for different CO_2 release scenarios
- Validation history, particularly with CO_2
- Ability to account for complex terrain and variable atmospheric conditions
- Applicability to different stages of the design process
- Acceptability to Australian regulators.

In addition, modelling of a release of dense phase CO_2 from a pipeline requires consideration of a number of different aspects, including transient pipeline depressurisation, multi-phase jet release, and dispersion of both dense and neutral gas. Ideally, a single software package should be able to account for all these factors, but this is not always the case.

Modelling of a release of dense phase CO_2 from a pipeline requires consideration of a number of aspects, including transient pipeline depressurisation, multi-phase jet release, and dispersion of both dense and neutral gas.

A range of dense gas dispersion models were investigated, including empirical correlations, integral models, Lagrangian particle and plume dispersion models and computational fluid dynamics (CFD) models. Selected models were reviewed and evaluated against the various criteria to determine if they could be considered ‘fit for purpose’. Table 10.1 shows the models that were considered.

Table 10.1: Summary of models

Model Category	Model Name	
Empirical correlations	‘Workbook on the dispersion of dense gases’ is the main reference.	
Integral	HGSYSTEM	SAFER/TRACE
	SLAB	GASTAR
	DEGADIS	PHAST
	ALOHA	EFFECTS
Lagrangian	QUIC	ArRisk
	SCIPUFF	CHARM
CFD	FLUENT OpenFOAM PANACHE	FLACS ANSYS-CFX

Only two dense gas dispersion models include the ability to simulate pipeline depressurisation: the DNV-GL model PHAST and the TNO model EFFECTS. All other models would require input from a separate modelling tool to perform this simulation. Additionally, both DNV-GL and TNO have participated in recent major research projects (CO_2PipeTrans, CO_2PipeHaz and COOLTRANS), all of which aim to improve understanding of the phenomena that occur when dense phase CO_2 is released to atmospheric conditions.

PHAST version 6.6 and later and the forthcoming EFFECTS 10 are the only two commercial packages that can account for both a wide range of source terms and the formation of solid CO_2 particles. While other modelling approaches can be used to achieve a similar outcome, they would require greater effort to assemble and interface the various model components.

From a regulatory perspective, based on the experience in the United States and Europe, the models DEGADIS, HGSYSTEM, SLAB (including EFFECTS), ALOHA, PHAST and SCIPUFF may all be acceptable to Australian regulators. Of these, PHAST version 6.6 and later and the forthcoming EFFECTS 10 have been subject to the greatest refinement using CO_2 release data. This does not preclude a case being made, in principle, for other models considered in this report, depending on the specific requirements of the project.

PHAST and EFFECTS are both types of integral models, which are generally designed to simulate dense gas dispersion over flat terrain. Conversely, Lagrangian and CFD models have the added ability to incorporate complex terrain effects. However, a review of the issues involved found that terrain effects can usually be ignored, as they generally tend to increase dispersion of the dense gas cloud, and therefore reduce the hazard distance. For this reason, flat terrain models can generally be considered fit-for-purpose because they tend to define the worst case at any downwind distance.

The more complex Lagrangian models cannot be recommended as primary design tools. Their lack of field trial validation presents a significant limitation.

CFD models need to be properly validated and their limitations understood. Their sensitivity to user-selected input conditions is an issue that has yet to be adequately resolved. However, their ability to model complex physical situations and low wind conditions means that they are likely to play an increasing role in the future.

Integral models may be regarded as fit for purpose in most circumstances. However, integral models may not be appropriate in situations where the local terrain has the potential to be significantly larger than the size of the gas plume. Where such conditions are a possibility, common sense should be used to determine the applicability of any modelling approach.

This study has found that, for most stages of pipeline design and operation, integral models such as SLAB, DEGADIS, HGSYSTEM, GASTAR, SAFER TRACE, EFFECTS or PHAST may be applicable. Each model has its strengths and weaknesses, which need to be understood when making a selection. PHAST from version 6.6 and EFFECTS 10 (when it is released) would have to be considered as prime candidates.

One of the main issues identified during this analysis was that predictions from acceptable dense gas models had a ‘factor of two’ margin of error. This has implications for the hazard distance calculated using the models. To account for this margin of error, this report recommends that a conservative hazard distance be calculated, either by:

- using a concentration profile equivalent to half the ‘threshold of injury (or fatality)’ value; or
- using the ‘threshold of injury (or fatality)’ value to calculate a hazard distance, and then increasing this distance by 50%.

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