CERC Cambridge Environmental Research Consultants

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PROPOSAL:	P2595: Dispersion modelling of abnormal emissions of CO_2
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SUBMITTED TO:	Anne Aubury, Essar Oil
SUBMITTED BY:	Catheryn Price

Introduction and scope of work

Essar Oil has requested that CERC provides a proposal for dispersion modelling of accidental releases to air of carbon dioxide (CO_2). Additionally, before the modelling assessment is carried out, CERC are required to determine the most appropriate methodology for the dispersion modelling assessment, by means of a review of relevant guidance, and through discussion with specialists at the Environment Agency.

The modelling assessment is required to determine the human health impact of the released CO_2 on the general population, at off-site locations.

The dispersion modelling is required for the 16 scenarios listed in Table 1. Heights for the vents are likely to be 47 m for the Pipelines/AGI, 5 m for the CO2 dehydration and 40 m for the CO2 capture.

CERC experience

CERC was established in 1985 with the aim of making use of new developments in environmental research for practical purposes. The company has 20 high-level technical consultants who are experts in consultancy services and specialist advice. We undertake development and support of CERC's world-leading ADMS and other atmospheric dispersion models, used by industry, consultants, regulators, local authorities and others, in the UK and internationally. We are the developers of GASTAR, a dense gas dispersion model developed in association with the UK Health and Safety Executive (HSE), designed for modelling accident scenarios involving releases of flammable and/or toxic materials. GASTAR is used to model a variety of industrial accidents such as emergency venting, liquid spills, catastrophic tank failure, pipe fractures and multi-phase jets.

CERC has extensive experience expertise in running these models to undertake dispersion assessments, and have carried out many emergency release projects for COMAH assessments and other safety reports involving a wide range of scenarios and materials. These include emergency venting of dense gases; catastrophic failure of cylinders and storage tanks; evaporating pools; warehouse fires; jet releases and chemically reactive source terms. CERC also carries out dispersion modelling for a wide range of industrial sources, including power plants, chemical plants and oil refineries.

Recent clients have included Anglian Water, BP, British Sugar, The Carbon Trust, EDF Energy, Johnson Matthey, Mitsubishi Industries, Rolls-Royce, RWE NPower, Savills and Statoil.

Table 1: List of scenarios to be modelled, as provided by Essar Oil

Plant Area	Case	Heat capacity of gas Cp at 15°C (J/°C/kg)	Average molecular weight (kg/kmol)	Total release rate (kg/s)	Vent exit diameter (inches)	Vent exit temperature (°C)	CO_2 emission rate (kg/s)
Pipelines AGI	PSV-0002_1	834.86	43.982	1.368	4	193	1.367
	PSV-0025_1	834.86	43.982	0.179	2	272	0.179
	BDV-0010_1	835.13	43.966	3.046	6	86.1	3.044
	BDV-0010_2	835.13	43.966	3.794	6	0.7	3.792
	BDV-0010_3	835.13	43.966	3.738	6	-3.8	3.736
	10-AAH-U-001_1	834.86	43.982	0.035	1	0	0.035
	BDV-0001_1	835.13	43.966	20.469	16	86.1	20.455
	BDV-0001_2	835.13	43.966	25.481	16	0.6	25.463
	BDV-0001_3	835.13	43.966	24.720	16	-8.3	24.702
CO_2 Dehydration	10-FAB-U-102_1	1380.29	25.521	0.064	2	90.4	0.026
	10-FAB-U-102_2	834.86	43.982	0.972	2	48.4	0.972
CO_2 Capture Unit	CCU_1	849.15	43.133	20.010	12	35	19.712
	CCU_2	917.61	39.427	4.983	12	116	4.578
	CCU_3	2183.16	14.530	2.114	12	132	1.015
	CCU_4	1039.55	28.011	0.440	12	18	0
	CCU_5	849.15	43.133	8.333	12	35	8.209

Proposed methodology

Choice of model

CO_2 is heavier than air, and those releases involving pure CO_2, as well as those gas mixtures with an average molecular mass value significantly greater than that of air, will tend to fall rapidly towards the ground after being released to air. Despite the fact that the released material is dense, this does not automatically mean that a dense gas model is the best choice to model the release and dispersion. As the recent ADMLC review of dense gas dispersion states, "*Whether the released gas disperses with the characteristics of a dense gas is not simply a matter of whether the released substance has higher density than air.*" [1]

Dense gas models tend to specialise in simulating the slumping and ground-level spreading behaviour of dense gases released at or close to ground level, and are not generally specialised in modelling the initial dispersion of elevated releases from very tall stacks.

CERC's Gaussian plume model, ADMS 5, includes algorithms that monitor the puff/plume behaviour as it disperses, primarily by continuously calculating the Richardson number and using this (along with other metrics) to determine whether the puff/plume is too dense to continue modelling. The plume is 'too dense' when the plume spread is determined by gravity effects instead of atmospheric mixing.

Initial test runs with ADMS 5 suggest that, for most of the release scenarios, the plume would be sufficiently well-mixed with air by the time it has reached ground level to be neutrally-buoyant. In this case, the release will be modelled using ADMS 5, and represented as a point source.

If any of the release scenarios result in plumes that are too dense to model with ADMS 5 (likely to be limited to the heaviest releases from the shortest stacks), the model's own iterative plume rise calculations will determine this, and this will be reported, and the model run will stop. CERC's dense gas model, GASTAR, will then be used for the dispersion modelling for those scenarios.

For all scenarios, tests will be carried out in order to determine the most appropriate model to use in each case.

Dispersion modelling approach

The assessment will be carried out with reference to relevant guidance and other information, primarily the "Air emissions risk assessment for your environmental permit" [2] and "Environmental permitting: air dispersion modelling reports", [3] and supplementary information, such as reports on carbon dioxide dispersion by the UK Health and Safety Executive (HSE).

For those release scenarios where ADMS is suitable for use, meteorological data from the nearest suitable station, Liverpool Airport, will be used in the assessment. Unless otherwise advised, the modelling will be carried out using five recent years of meteorological data, in line with Environment Agency guidance.

[1] Batt, R. Review of dense-gas dispersion for industrial regulation and emergency preparedness and response. Atmospheric Dispersion Modelling Liaison Committee, ADMLC-R13 (2021)
[2] https://www.gov.uk/guidance/air-emissions-risk-assessment-for-your-environmental-permit#detailed-modelling
[3] https://www.gov.uk/guidance/environmental-permitting-air-dispersion-modelling-reports

For any scenarios where GASTAR is used, these will be modelled with a range of meteorological conditions representing stability categories/wind speeds. It is common to model scenarios corresponding to a) typical meteorological conditions in the UK, usually stability category D (neutral) with a wind speed of 5m/s, and b) meteorological conditions that are less typical, but which result in worst-case impacts (to be determined for these scenarios).

Model output

Concentrations will be generated at locations of maximum air quality impacts and at discrete sensitive receptor locations relevant to public exposure.

The results will be provided as tabulated values with some results shown as graphs and/or contour plots, as appropriate.

These output concentrations will be compared against appropriate environmental standards, as discussed in the following section.

A range of averaging times can be considered, if appropriate, depending on the environmental standards assumed and the likely duration of exposure

Environmental Standards

Modelled concentrations of carbon dioxide will be compared with appropriate threshold values for public exposure.

Sources of potential information in relevant thresholds already posited by the Environment Agency include the Public Health England (PHE)/ UK Health Security Agency (UKHSA) Compendium of Chemical Hazards,[4] HSE information on acute carbon dioxide hazards,[5] and the Dangerous Toxic Load (DTL) category of 'specified levels of toxicity' (SLOT). Before commencing the dispersion modelling assessment these, and other sources of information, will be carefully reviewed, and the findings discussed with the Environment Agency, to agree suitable environmental standard for this assessment.

An example of other such sources of information include references relating to indoor air quality. Carbon dioxide exposure and associated threshold values is a key topic in the field of indoor air quality, so information and guidance from this field might be a useful source of information on public exposure. The conclusions of a recent review by the UKHSA,[6] for example, included the suggestion that 1000 ppm CO_2 represents a threshold for 'good or excellent' indoor air quality.

[4] https://www.gov.uk/government/publications/carbon-dioxide-properties-and-incident-management
[5] https://www.hse.gov.uk/carboncapture/carbondioxide.htm

[6] Lowther, S.D., et al. Low Level Carbon Dioxide Indoors—A Pollution Indicator or a Pollutant? A Health-Based Perspective. *Environments* 2021, *8*, 125. https://www.mdpi.com/2076-3298/8/11/125/htm

Reporting

A detailed report will be provided, describing the model input data and assumptions and presenting the results of the modelling.

The report will include a discussion of the meaning and significance of the results.

Data requirements

The information required for the assessment is as follows:

- Detailed site plan with location of all emission points, building locations and heights, and site boundary marked on it
- All vent stack parameters, including height and internal diameter at emission point
- Emissions data for the vent stack, including:
  - Emission rates of CO_2
  - Emission temperature
  - Velocity and volume flow rate of total emission
- Locations of any specific sensitive receptors identified for assessment