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Fast Estimation of Dense Gas Dispersion from Multiple Continuous CO<sub>2</sub>

Surface Leakage Sources for Risk Assessment

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## **Abstract**

Surface leakage of CO<sub>2</sub>, and associated potential impacts on health, safety, and the environment (HSE) are considered hazards of geologic carbon sequestration (GCS). There are two challenges associated with impact assessment of CO<sub>2</sub> surface dispersion. First, the fact that CO<sub>2</sub> is a dense gas makes its dispersion in air a complex process. Rigorous numerical solutions for modeling concentration distributions are relatively time-consuming. Second, impact assessment requires consideration of uncertainty, e.g., quantification of how much uncertainty is propagated through input parameters to model outputs by carrying out large numbers of model runs. In order to assess the potential consequences of surface leakage of CO<sub>2</sub>, it is useful to have a model that executes very quickly for repeated model calculations (e.g., in Monte Carlo mode) of the atmospheric dispersion of CO<sub>2</sub> (concentrations as a function of space and time). In addition, the model should be able to handle multiple surface leakage sources. In this study, we have extended the nomograph approach of Britter and McQuaid (2008) for estimating dense gas plume length from single leakage source to multiple leakage sources. The method is very fast and therefore amenable to general system-level GCS risk assessment including uncertainty quantification within the framework of the National Risk Assessment Partnership (NRAP) Integrated Assessment Model (IAM). The method is conservative in that it assumes the wind could be from any direction, and it handles multiple sources by a simple superposition approach. The method produces results in reasonable agreement with a sophisticated computational fluid dynamics (CFD) code, but runs in a small fraction of the time.

## Introduction

Geologic carbon sequestration (GCS) is widely viewed as necessary to meet greenhouse gas emissions targets set by government agencies around the world. At the same time, it is recognized that GCS carries with it well-known hazards, among which are leakage of CO<sub>2</sub> to potable groundwater and to the atmosphere. Whether leakage out of the ground is by rapid or incipient transport through natural pathways (e.g., coarse or cracked soil, faults, or fractures), or by flow through leaking wellbores (within the tubing or outside of casing in the annular region), the result is emission of a dense gas into the atmosphere (Oldenburg and Unger, 2003; 2004). As the place where plants, humans, and other animals reside, the near-surface region is susceptible to environmental health and safety (EH&S) impacts of leaking CO<sub>2</sub>.

The National Risk Assessment Partnership (NRAP) has developed an integrated assessment model for geologic carbon sequestration risk assessment (NRAP- IAM-CS), hereafter referred to as IAM. Risks considered include containment failure, and related EH&S risks. The IAM model is implemented in GoldSim and comprises integrated reservoir, aquifer, wellbore, and fault models for modeling CO<sub>2</sub> leakage upward from the reservoir and associated impacts to groundwater, and emission to the atmosphere through wellbores. The IAM is designed to handle uncertainty through Monte Carlo simulations using varying uncertain parameters and therefore requires very efficient and rapid simulation models. Several reduced order models (ROMs) have been developed for the IAM for fast execution (e.g., Pau et al., 2013; Jordan et al., 2015).

In order to include in the IAM the EH&S impacts arising from the wellbore leakage of CO<sub>2</sub>, a dense gas, to the atmosphere, we have adapted single-source empirical correlations, developed by Britter and McQuaid (1988), into a multiple-source CO<sub>2</sub> leakage ROM that we refer to as the MSLR (multiple source leakage ROM). The empirical correlations were represented in a

nomograph for predicting plume extent and concentration of dense gases such as liquefied natural gas during potential single-point pipeline and tank failure releases. The original Britter and McQuaid method was developed for single source releases of dense gas that could be either continuous or instantaneous. We assume that CO<sub>2</sub> leakage typically lasts at least for several hours before measures can be taken, therefore the release can be assumed continuous (see the Approach section for details about this). In order to handle multiple leakage sources, we developed a simple conservative superposition approach that combines proximal sources to form representative discrete sources. The inputs to the MSLR are leakage rate(s) from leaky well(s), location(s) of leaky well(s) and wind speed. The MSLR is developed as both a built-in model in the IAM and as a standalone module.

The goal of IAM is to provide a stochastic framework at the system level to explore complex interactions among the uncertain variables, within or between sub-models. The final evaluation is presented in a probabilistic manner based on Monte Carlo simulations. The application of the MSLR for modeling atmospheric dispersion in the IAM is not meant to obtain an accurate estimate of CO<sub>2</sub> concentration for a specific scenario, e.g., for regulators to make decisions for specific land-use planning. Rather, the tool will be mainly used to perform scoping studies. As such, we define a number of general *receptors*, for example, home or business locations where people are present, as well as a *critical concentration*, a threshold concentration limit above which CO<sub>2</sub> becomes hazardous. We are interested in the probability that the receptors are located within the radius of dense gas concentration that is above the critical concentration. These radii are referred to *critical radii*. In addition, to make a probabilistic evaluation possible for such a complex large system (from deep underground to atmosphere), it is important to be able to have

very fast execution of each sub-model. For these reasons we consider it reasonable to use a simple model like the MSLR rather than a more complicated model.

Two types of CO<sub>2</sub> well leakage to the atmosphere are considered in the NRAP IAM. One type of leakage results in a large CO<sub>2</sub> release rate (e.g., on the order of 10 kg/s or more) when the open well option is chosen. This leakage rate is comparable to the leakage rates listed as examples of CO<sub>2</sub> blow out by Aines et. al. (2009), which ranges from 0.2 kg/s (Leroy Gas Storage Facility, WY) ~ 120 kg/s (Sheep Mt., CO). Another well option is to specify the permeability of leaky wells based on different types of existing well-permeability distributions. When the permeability options are used, the leakage rate is much smaller (i.e., CO<sub>2</sub> release rate is on the order of  $\sim 10^{-7}$   $\sim 10^{-5}$  kg/s). For such a small release rate to form a dense gas release, a very small wind speed (i.e., about 1 m/s at a height of 10 m at 25°C and 1 bar atmospheric pressure, given by Equation 4 below) is needed. Even though low concentrations of CO<sub>2</sub> caused by small releases may cause long-term chronic exposure, they are not the main focus of the MSLR in the IAM. Instead, the MSLR focuses on the catastrophic events caused by the IAM open well option, in which the release of CO<sub>2</sub> forms a dense gas cloud.

The purpose of this paper is to describe the extension of the single-source Britter and McQuaid (1988) approach to multiple sources as implemented in the MSLR, and to present some test problems for demonstrating and justifying the MSLR handling of dense gas dispersion in the IAM risk assessment context.

## **Background**

Leakage of dense gases has been widely recognized as potentially hazardous because of the tendency of dense gases to resist dispersion and flow along the ground surface (Britter, 1989)

increasing inhalation hazard to the public (Hankin and Britter, 1998). A dense gas is defined as any gas whose density at the leakage site is higher than the density of the ambient air through which it is being dispersed. Density differences can arise from both thermal and compositional effects. With molecular weight of 44 g/mole, CO<sub>2</sub> leaking out of the ground will be a dense gas relative to air (molecular weight ~ 28 g/mole):  $\rho_{\text{CO}_2} = 1.8 \text{ kg/m}^3$  vs.  $\rho_{\text{air}} = 1.2 \text{ kg/m}^3$  at ambient surface pressure and temperature ( $P$ ,  $T$ ). Interested readers can calculate the density of gas mixtures of varying composition and  $P$ ,  $T$  using the online tool WebGasEOS (Reagan, 2008). Several field campaigns involving intentional releases of dense gas have been carried out to measure dense gas dispersion dynamics for assessing the consequences of leaking liquefied natural gas (e.g., Havens, 1992; Hanna and Chang, 2001).

The human health impacts arising from inhaling CO<sub>2</sub> include physiological, toxic, anesthetic, and lethal effects depending on concentration and exposure time (Benson et al., 2002; Rice, 2004). Therefore in order to assess consequences of leaking CO<sub>2</sub> under failure scenarios involving leakage of CO<sub>2</sub> from deep underground storage reservoirs to the ground surface and atmosphere, an understanding of leakage-related CO<sub>2</sub> concentrations across the landscape is needed. In the absence of field tests aimed at measuring CO<sub>2</sub> plume migration, or a record of careful monitoring of prior CO<sub>2</sub> surface leakage, modeling and simulation of CO<sub>2</sub> dispersion can be used to predict the transport and mixing-related dilution by air over time.

Several different approaches can be used to model dense gas dispersion and assess the consequences of surface leakage of CO<sub>2</sub>. The first approach is based on computational fluid dynamics (CFD) and involves solution of a set of conservation equations described by partial differential equations (e.g., Mazzoldi et al., 2008; Cortis and Oldenburg, 2009). While this method is potentially very accurate and can be used to assess effects of topography (e.g., Chow

et al., 2009) and vigorous source terms such as high-pressure leakage (Aines et al., 2009; Mazzoldi et al., 2013), CFD is computationally very demanding and requires numerous inputs that may not be available or may be very uncertain. The second method is the box-model approach, whereby average plume features are calculated while neglecting the detailed spatial features (e.g., Kunsch and Webber, 2000). We note there is also a hybrid between the first and second approaches called the shallow-layer approach (Hankin and Britter, 1999; Costa et al., 2008) that simplifies the full CFD equations by averaging the properties of the dense gas over its depth assuming the dense gas occupies the lower portions of the domain. None of these methods is practical for the IAM which requires fast execution times to carry out Monte Carlo simulations. Furthermore, CFD methods may not be practical in the context of risk assessment where conservative estimates of CO<sub>2</sub> concentrations are needed for a range of parameter inputs over space and time. Although it is possible to develop statistical emulators or response surface types of ROMs based on the above two approaches, it requires a significant effort for such an approach. In addition, ROMs are usually site specific (i.e., they work well for the site for which they are developed). The IAM which provides the framework for our work requires a generic approach for more general scoping studies of CO<sub>2</sub> surface leakage hazard.

The third approach develops and applies general correlations from careful measurements of field experiments, an example of which is the Britter and McQuaid (1988) method. The Britter and McQuaid approach consolidates user input into dimensionless groups based on the gas of interest and the fundamental flow equations, and uses dimensional analysis along with results of field experiments to create a nomograph. To use this method for modeling a dense gas release, the user only needs to calculate the corresponding dimensionless groups, and fit the parameters to empirical results of plume extent and dispersion on the nomograph. The method is simple and

does not include time-dependent or dynamic aspects, but it produces results that agree well with data from field tests, as shown by a detailed comparison of model predictions with field test data that came from dense gas release under neutral field conditions (stability class D) and moderate wind speeds (Hanna et al., 1993). The validity of the Britter and McQuaid nomograph stems from its derivation from empirical correlations of field data.

The Britter and McQuaid method (1988) was developed for single-source ground-level releases of dense gas, either instantaneous or continuous. Atmospheric stability was found to have little effect on the empirical results and therefore is not part of the nomograph. Most of the field data used by Britter and McQuaid came from dispersion tests in remote rural areas on flat terrain. Therefore, the method is not directly applicable to urban or hilly or mountainous areas. The original Britter and McQuaid method can be easily implemented within an Excel spreadsheet due to the simplicity of the method for single sources. Our adaptation of the Britter and McQuaid method allows multiple leakage sources and therefore requires additional logic that we coded using Fortran90 for fast execution.

## **MSLR Approach**

The Britter and McQuaid method requires a specification of the initial plume volume or the initial plume volume flux, the duration of the release, the initial plume gas density, the wind speed at a height of 10 m, a target critical concentration level downwind, and the ambient gas density. The model then provides an estimate of the downwind distance to the critical concentration. Here we first describe the Britter and McQuaid approach to model dense gas dispersion for a single source continuous release, and then we describe our MSLR procedure for extension to multiple source releases.

## 1. Calculation for a single gas release point

The first step in the calculation is to calculate the initial relative buoyancy  $g_0$  (length/time<sup>2</sup>)

$$g_0 = \frac{g(\rho_0 - \rho_a)}{\rho_a} \quad (1)$$

where  $g$  is the acceleration due to gravity (length/time<sup>2</sup>),  $\rho_0$  is the initial density of released material (mass/volume), and  $\rho_a$  is the density of ambient air (mass/volume).

A characteristic source dimension  $D_c$  (length) for continuous release is defined as:

$$D_c = \left(\frac{q_0}{u}\right)^{0.5} \quad (2)$$

where  $q_0$  is the initial plume volume flux for dense gas dispersion (volume/time), and  $u$  is the wind speed (length/time) at 10 m height.

The criterion for a continuous (in contrast to an instantaneous) release is:

$$\frac{uR_d}{x} \geq 2.5 \quad (3)$$

where  $R_d$  refers to the release duration and  $x$  is the downwind distance in dimensional space (length). As such, this is a criterion related to both release duration and relative location of source and receptor. Actual CO<sub>2</sub> leakage events may take days or even months for mitigation measures to be implemented if the leak is small and difficult to detect or if relief wells are needed to stop well blowouts. Even for a one-day release of CO<sub>2</sub>, if we consider a relatively large maximum downwind distance of 1 km, and assume a small minimum wind speed of 0.03 at 10 m height, the condition of Eq. 3 is satisfied and the release considered in IAM is continuous. The time step of the IAM is one year, and therefore any leak we consider is assumed to last for at least one year, likely a very conservative assumption. We note that even though currently no

intervention is implemented in the IAM when CO<sub>2</sub> leakage happens, in reality it is unlikely that a large leakage will last for a year.

The criterion for a dense cloud representation from continuous releases is:

$$\left(\frac{g_0 q_0}{D_c u^3}\right)^{1/3} \geq 0.15 \quad (4)$$

If this criterion is satisfied, the downwind distance in dimensional space (length) for a given concentration is calculated based on Figure 2.42 and Table 2.15 of Britter and McQuaid (1988) (see Figure 1). For this paper, the focus is on dense gas dispersion from multiple sources. If however, the criterion is not satisfied, Equation 6.38 from Arya (1999) can be used to calculate the concentration at any location. In the case of multiple sources, a straightforward superposition can also be used.

In summary, for a single source release, one needs to calculate a few dimensionless numbers, check the criteria for a dense cloud representation and a continuous release, define a critical concentration, and then use the nomograph of Figure 1 to calculate the corresponding downwind distance of that concentration.

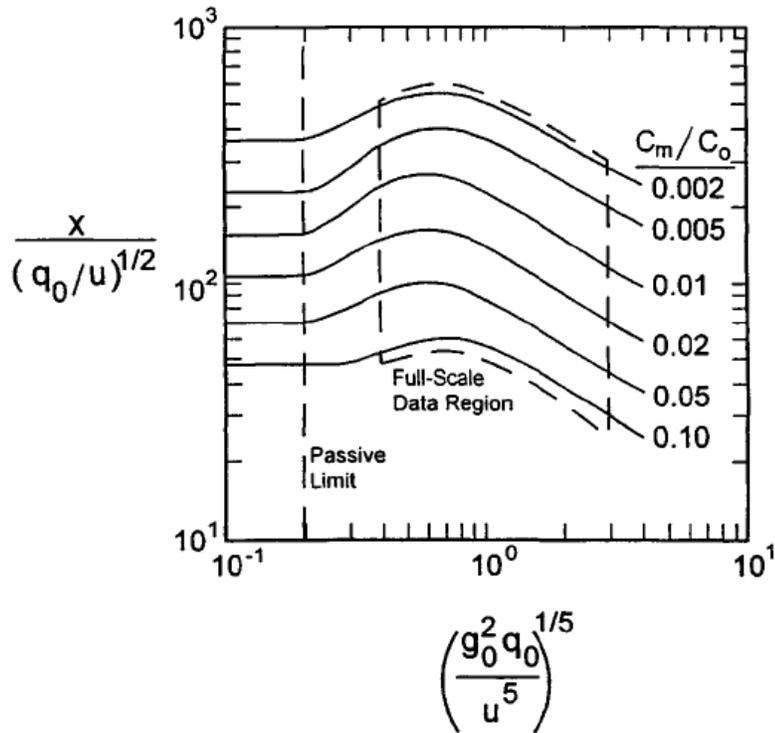


Figure 1. Britter and McQuaid nomograph for estimating plume lengths and concentrations based on dimensionless groups (from Britter and McQuaid, 1988).  $C_m$  is the concentration at receptor location and  $C_0$  is the concentration at the source.

Table 1. Equations used to approximate the curves in Figure 1 (Reproduced from Center for Chemical Process Safety, 1999).

Concentration ratio $C_m/C_0$	Valid range for $\alpha = \frac{1}{5} \log_{10} \left( \frac{g_0^2 q_0}{u^5} \right)$	Equation for $\beta = \log_{10} \left( \frac{x}{(q_0/u)^{0.5}} \right)$
0.1	$\alpha \leq -0.55$	$\beta = 1.75$
0.1	$-0.55 < \alpha \leq -0.14$	$\beta = 0.24\alpha + 1.88$
0.1	$-0.14 < \alpha \leq 1$	$\beta = -0.50\alpha + 1.78$
0.5	$\alpha \leq -0.68$	$\beta = 1.92$
0.5	$-0.68 < \alpha \leq -0.29$	$\beta = 0.36\alpha + 2.16$
0.5	$-0.29 < \alpha \leq -0.18$	$\beta = 2.06$
0.5	$-0.18 < \alpha \leq 1$	$\beta = -0.56\alpha + 1.96$
0.02	$\alpha \leq -0.69$	$\beta = 2.08$
0.02	$-0.69 < \alpha \leq -0.31$	$\beta = 0.45\alpha + 2.39$
0.02	$-0.31 < \alpha \leq -0.16$	$\beta = 2.25$
0.02	$-0.16 < \alpha \leq 1$	$\beta = -0.54\alpha + 2.16$
0.01	$\alpha \leq -0.70$	$\beta = 2.25$
0.01	$-0.70 < \alpha \leq -0.29$	$\beta = 0.49\alpha + 2.59$
0.01	$-0.29 < \alpha \leq -0.20$	$\beta = 2.45$
0.01	$-0.20 < \alpha \leq 1$	$\beta = -0.52\alpha + 2.35$
0.005	$\alpha \leq -0.67$	$\beta = 2.40$
0.005	$-0.67 < \alpha \leq -0.28$	$\beta = 0.59\alpha + 2.80$
0.005	$-0.28 < \alpha \leq -0.15$	$\beta = 2.63$
0.005	$-0.15 < \alpha \leq 1$	$\beta = -0.49\alpha + 2.56$
0.002	$\alpha \leq -0.69$	$\beta = 2.60$
0.002	$-0.69 < \alpha \leq -0.25$	$\beta = 0.39\alpha + 2.87$
0.002	$-0.25 < \alpha \leq -0.13$	$\beta = 2.77$
0.002	$-0.13 < \alpha \leq 1$	$\beta = -0.50\alpha + 2.71$

## 2. Calculation for multiple release points

As discussed above, the IAM considers CO<sub>2</sub> leakage to the atmosphere out of numerous (up to 1000) wells over a large area of the GCS site. In order to use the Britter and McQuaid approach, we adapted the method to be applicable to multiple simultaneous sources. For multiple source releases, we make the following two assumptions:

- The releases of dense gas from all locations last long enough to be considered continuous releases;
- The dense gases emanating from different release locations are all CO<sub>2</sub> and have the same properties, e.g., are at the same pressure, temperature, and initial concentration.
- The wind can be in any direction at different times, but at any one point in time, the wind direction is the same for the entire model domain.

In order to adapt the Britter and McQuaid approach to multiple sources, we apply a superposition approach which is described in the flowchart of Figure 2. Briefly, the algorithm uses the nomograph of Britter and McQuaid to calculate the critical radius of each source. Then the algorithm checks if there is an overlap between the two critical radii for any pair of sources. If both sources are outside of each other's critical radius, the critical radii are used as is. If at least one source is within the critical radius of the other source, the sources are combined and considered to be one source with strength equal to the sum of the two sources. The combined source will be located in between the two locations, with the distance to each source proportional to their strengths. The new set of (possibly combined) sources is then compared in the same way with all of the other sources for a second time. The output of the algorithm includes critical radii of each combined source and flags for each receptor indicating if the CO<sub>2</sub> concentration at that location may be above or below the critical value. This simple approach is very fast to compute

and allows application of the Britter and McQuaid nomograph to estimate the sizes of the critical zones for multiple leakage sources. The MSLR algorithm is coded in Fortran90 and compiled as a dynamic link library (DLL) with the name AtmDisROM.dll in the GoldSim IAM. The algorithm can also be run as a standalone application called by a main program (provided), as described below in the flowchart.

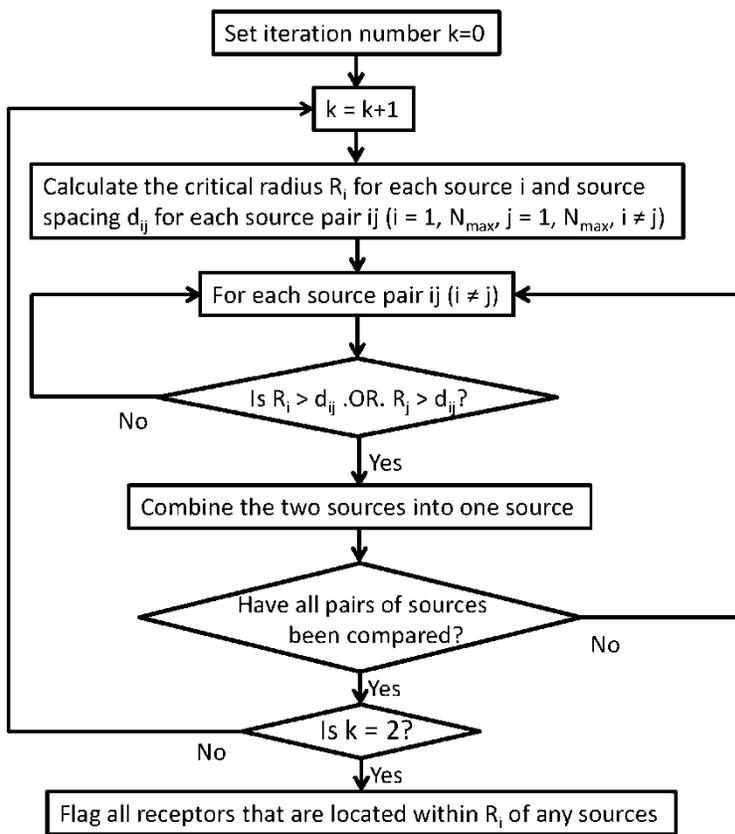


Figure 2. Flowchart showing the logic of the MSLR approach to handle multiple leakage source locations.

### 3. Application in the IAM with Monte Carlo settings

When the MSLR is used within NRAP to evaluate the risk of CO<sub>2</sub> surface leakage, a Monte Carlo simulation is performed reflecting uncertainty in various parts of the IAM model. For

example, the uncertain input parameters of the IAM include CO<sub>2</sub> storage reservoir properties (e.g., permeability, porosity), leakage pathway properties (e.g., open vs closed well, leakage wellbore locations and permeability), and potential leakage into the atmosphere (surface leakage) or shallow aquifer. Even though these parameters are not direct inputs to the MSLR, they all have an impact on the CO<sub>2</sub> surface leakage rates from various wellbore locations. In terms of MSLR, CO<sub>2</sub> surface leakage rates at different locations are the uncertain inputs. Other parameters, for example, wind speed, are deterministic inputs, although they could be uncertain when the MSLR runs independently of the IAM.

The uncertainty around whether a receptor is within or outside of the critical radius is quantified in the MSLR by Monte Carlo simulation in the IAM. Specifically, the number of times that a receptor is within a critical radius divided by the total number of Monte Carlo simulations indicates the probability that this receptor is within a critical radius for the given uncertain inputs.

## **Comparison of MSLR to Fluidyn PANACHE**

One way to increase our confidence in the proposed superposition approach for approximating multiple source releases of CO<sub>2</sub> is to compare our method to a CFD approach. Fluidyn-PANACHE (2010) is a 3-D computational fluid dynamics (CFD) software package for modeling atmospheric flow and transport. In this study the PANACHE model serves as the comparison model. Justification for the use of comparison against PANACHE as a way of establishing the credibility of the superposition and Britter and McQuaid nomograph methods built into the MSLR rests on good agreement between the single-source version of MSLR and PANACHE. In Test Problem 1, we demonstrate that the Britter and McQuaid approach and PANACHE

solutions agree relatively well under certain conditions for single-source releases. In Test Problem 2, we investigate how well the MSLR and PANACHE solutions agree with each other for multiple-source releases under those conditions.

**Test Problem 1: Single source release**

For a single source release, the MSLR method is the same as the Britter and McQuaid (B&M) approach. This comparison is done for both a relatively high wind speed (1A) and low wind speed (1B) situation. The specifics of Test Problem 1A are listed in Table 2. Test problem 1B has only a different wind speed at 10 m height, which is 1 m/s.

Table 2. Input parameters for Test Problem 1A.

Release rate $q$	Wind speed at 10 m height	Ambient temperature	Ambient pressure
10 kg/s	5 m/s	25 °C	0.987 atm

In the MSLR, the density at ambient pressure and temperature of air and CO<sub>2</sub> are 1.21 kg/m<sup>3</sup> and 1.77 kg/m<sup>3</sup>, respectively, and the concentration is normalized by the source concentration (i.e.,  $C/C_0$  is used, where  $C_0$  is the concentration at the source). The numerical value for the left-hand side of Equation 4 is 0.58 and 2.22 for Test Problems 1A and 1B respectively – indicating a dense gas dispersion model is needed.

The 3-D steady-state plume under the same conditions is simulated using PANACHE. We have used a 3D irregular grid with 14,874 elements, 7,595 nodes and 15 layers in the vertical direction (vertical discretization varies from 1 m to 15 m from ground surface upwards and we use the k-eps (2-equation prognostic) turbulence model with log-log weather conditions (log law profile wind speed and temperature). The ground-level plume from PANACHE is used to

compare to the results from the MSLR. The concentration profile from the MSLR is obtained by specifying multiple discrete  $C/C_0$  levels and calculating multiple critical downwind distances  $x$ . Critical downwind distance is calculated for  $C/C_0$  between 0.002 and 0.1 (see Table 1).

In PANACHE, the exit velocity of released mass needs to be provided as an input parameter. This is a parameter related to the density of released  $\text{CO}_2$  and the release area. If we use ambient  $\text{CO}_2$  conditions and assume to reach that ambient condition of  $\text{CO}_2$  density, the release area is about  $100 \text{ m}^2$  and the vertical velocity is about  $0.05 \text{ m/s}$ . As the area is highly uncertain, we performed PANACHE simulations using an exit velocity of both  $1 \text{ m/s}$  and  $1 \text{ cm/s}$ , as shown in Figure 3.

Based on the results from Figure 3, we have three observations: (1) The sensitivity of the PANACHE solutions to exit velocity gets smaller with higher wind speed; (2) MSLR is in better agreement to the PANACHE solution with smaller exit velocity than the one with larger exit velocity; and (3) MSLR is in better agreement to the PANACHE solution when the wind speed is higher. These results are consistent with the fact that the MSLR does not model effects of vertical velocity at the source, so the PANACHE solutions most consistent with MSLR solutions are those with either small vertical exit velocity or large wind speed. It is likely that wind will be highly variable before intervention takes place for  $\text{CO}_2$  leakage, and the largest critical radii over time is the main concern. As a result, predictions of larger rather than smaller critical radii are our interest in order to be conservative.

At  $5 \text{ m/s}$  wind speed, the difference in  $C/C_0$  between the two solutions is in general less than  $0.01$ . We consider this is acceptable for PANACHE to be used to compare solutions with the multiple-source version of MSLR, and  $5 \text{ m/s}$  wind speed is used for Test Problem 2.

In terms of computational cost, it takes a few seconds of CPU time to calculate the MSLR solution, compared to 76 hours of CPU time for the PANACHE solution. Clearly, MSLR method has two advantages over PANACHE solution: First, the simple model is easy to implement and fast to execute; and second, there is no numerical discretization and therefore no boundary effect. The computational savings makes the MSLR method extremely attractive for use in the IAM, and for any risk assessment framework that requires multiple fast simulations.

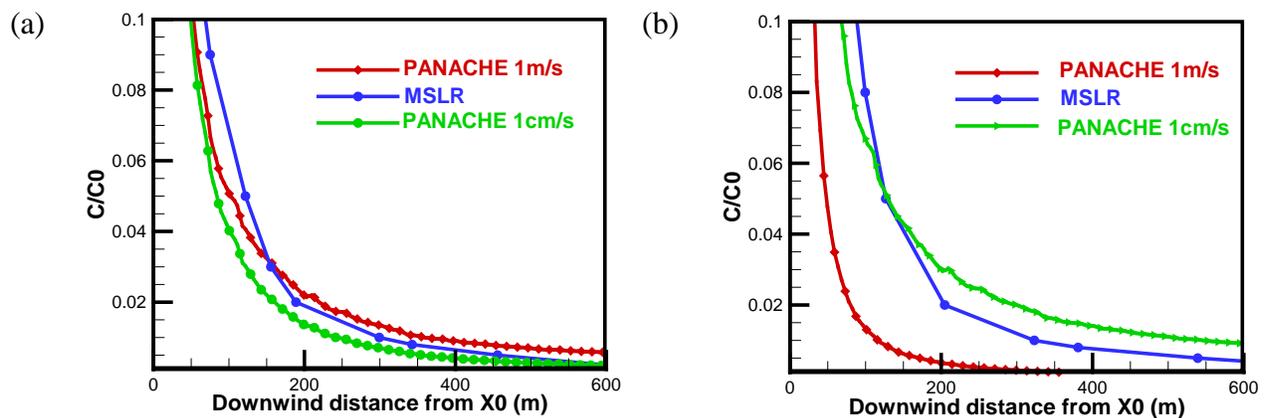


Figure 3. Comparison of the solutions from a single source release problem between MSLR( = B&M because there is only one leakage source) and PANACHE for (a) wind speed  $u = 5$  m/s; and (b)  $u = 1$  m/s PANACHE solutions for vertical exit velocity of 1 m/s and 1 cm/s are shown by the red and green curves, respectively.

**Test Problem 2:** Leakage from two CO<sub>2</sub> sources

In this two-source release example, we investigate MSLR solutions for two possibilities: (1) two CO<sub>2</sub> sources aligned with the wind direction (Test Problem 2A); and (2) two CO<sub>2</sub> sources

aligned at an angle of  $45^\circ$  to the wind direction (Test Problem 2B). The other specifics are the same as in Test Problem 1.

In Test Problem 2A, the locations of the two sources are at  $x_1 = 900$  m,  $y_1 = 1000$  m, and  $x_2 = 950$  m,  $y_2 = 1000$  m, as shown in Figure 4, which is a concentration (mass fraction) contour map from PANACHE. The wind direction is aligned with the two sources, i.e., along the  $x$ -direction. Again, values between 0.002 and 0.1 are considered for  $C/C_0$  in the MSLR method. The critical radii for concentrations in that range are larger than the distance between the two sources (50 m). As a result, MSLR combines the two sources into a single source located at  $x_0 = 925$  m,  $y_0 = 1000$  m. and uses concentration at  $(x_0, y_0)$  for  $C_0$ . The left-hand side of Equation 4 for this case (and same for Test Problem 2A) is 0.65 – indicating the criterion for dense gas dispersion is satisfied. For the PANACHE solution,  $C_0$  should be an average representation of the two source zones, which can be approximated by the upstream source concentration. The comparison of the results from PANACHE and the MSLR is plotted in Figure 5. Again, the two solutions agree well for the concentration range considered, suggesting that combining two sources with overlapping critical radii aligned with the wind direction is a good approximation of two discrete leakage sources.

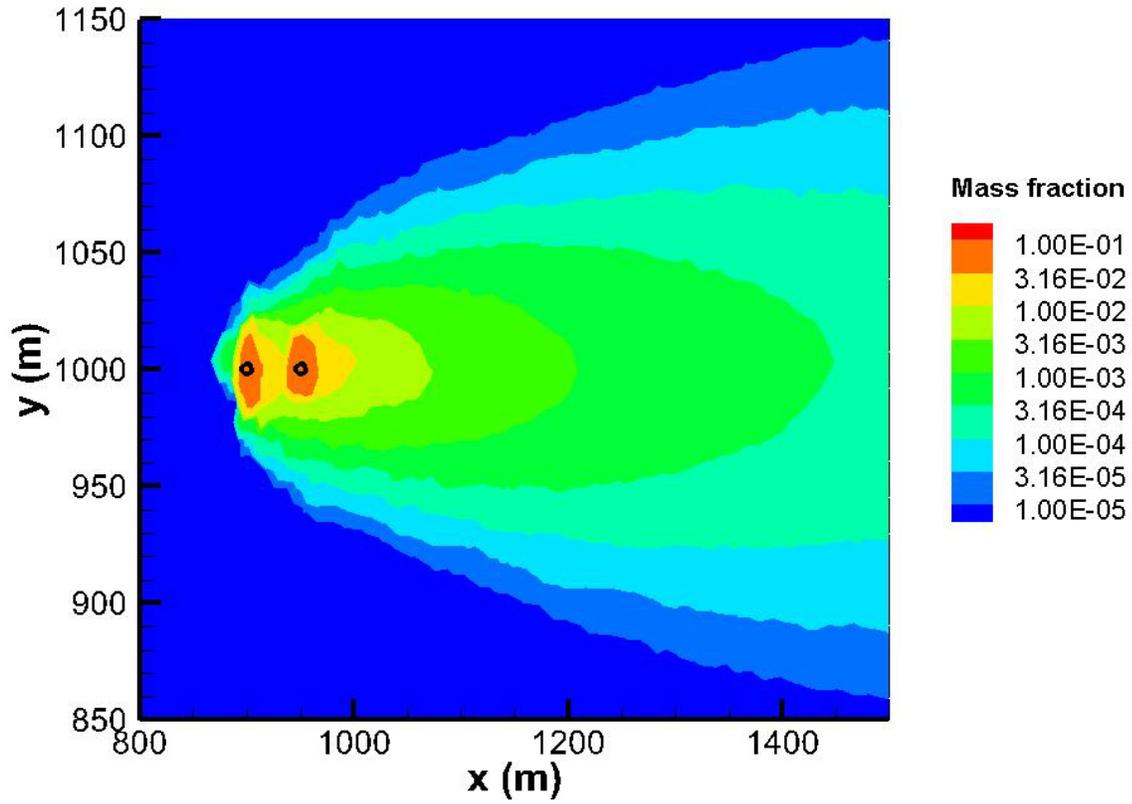


Figure 4. Contours of ground-level concentration from PANACHE for the Test Problem 2A, in which the two CO<sub>2</sub> sources, indicated by the two black circles, are aligned with the wind direction (along the  $x$ -direction).

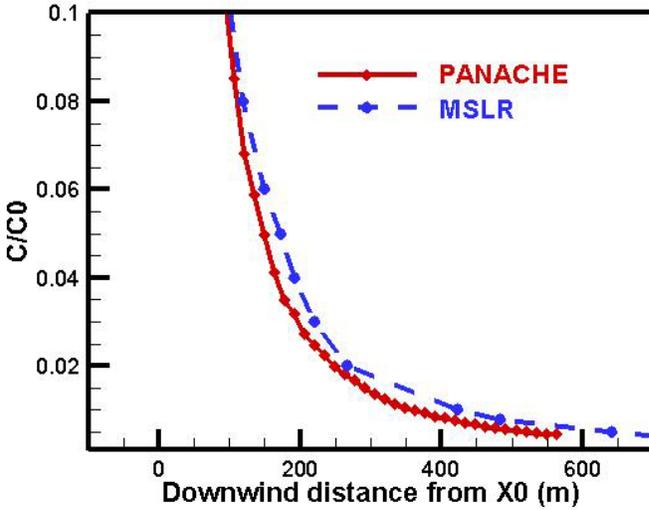


Figure 5.  $C/C_0$  at downwind locations from  $x_0 = 925\text{m}$ ,  $y_0 = 1000\text{m}$  – the combined source location in the MSLR method.

In Test Problem 2B, the two  $\text{CO}_2$  sources are aligned at an angle of  $45^\circ$  to the wind direction and are located at  $x_1 = 900\text{ m}$ ,  $y_1 = 1000\text{ m}$ , and  $x_2 = 935\text{ m}$ ,  $y_2 = 1035\text{ m}$ , with separation distance of  $50\text{ m}$ . Again, values between  $0.002$  and  $0.1$  are considered for  $C/C_0$  and the corresponding critical radii exceed the distance between the sources, so the MSLR again combines the two sources into one new source just as in Test Problem 2A. The high-fidelity solution to Test Problem 2B is shown in Figure 6, by the ground-level contours of the PANACHE solution.

Because the two sources are not aligned in the wind direction, there is more lateral spreading of the  $\text{CO}_2$  than in Test Problem 2A, resulting in slightly lower downwind concentrations. The MSLR approach does not explicitly capture the effective width of sources, but rather adds the sources together and locates them at the midpoint of the line connecting them. In addition, the MSLR does not explicitly model lateral spreading, so the MSLR results for Test Problems 2A

and 2B are nearly identical. On the other hand, PANACHE estimates lower concentrations directly downwind of the sources in Test Problem 2B because there is more lateral dispersion when the sources are aligned at 45 to the wind direction. As a result, the difference between the two solutions is larger than it is in Example 2A, as shown in Figure 7. An extreme case would be one in which the two CO<sub>2</sub> sources are aligned perpendicular to the wind direction, which would lead to even more lateral spreading and greater difference between high-fidelity and MSLR results. The solution given by MSLR is conservative in that it overestimates CO<sub>2</sub> concentration at the downwind end of the plume, or in other words, overestimates the critical radius for typical concentration thresholds, which is appropriate in the risk assessment context for which the MSLR is intended.

To summarize, the MSLR approach provides an approximation of a full 3-D CFD model to simulate surface dispersion of dense gases from multiple release points. The MSLR results match the high-fidelity model results more closely if the release sources are aligned with the wind direction. The results are more conservative if the wind direction is perpendicular to aligned sources. In all cases, the MSLR estimates critical radii around single release points assuming the wind can be in any direction, i.e., the MSLR makes no assumption about wind direction.

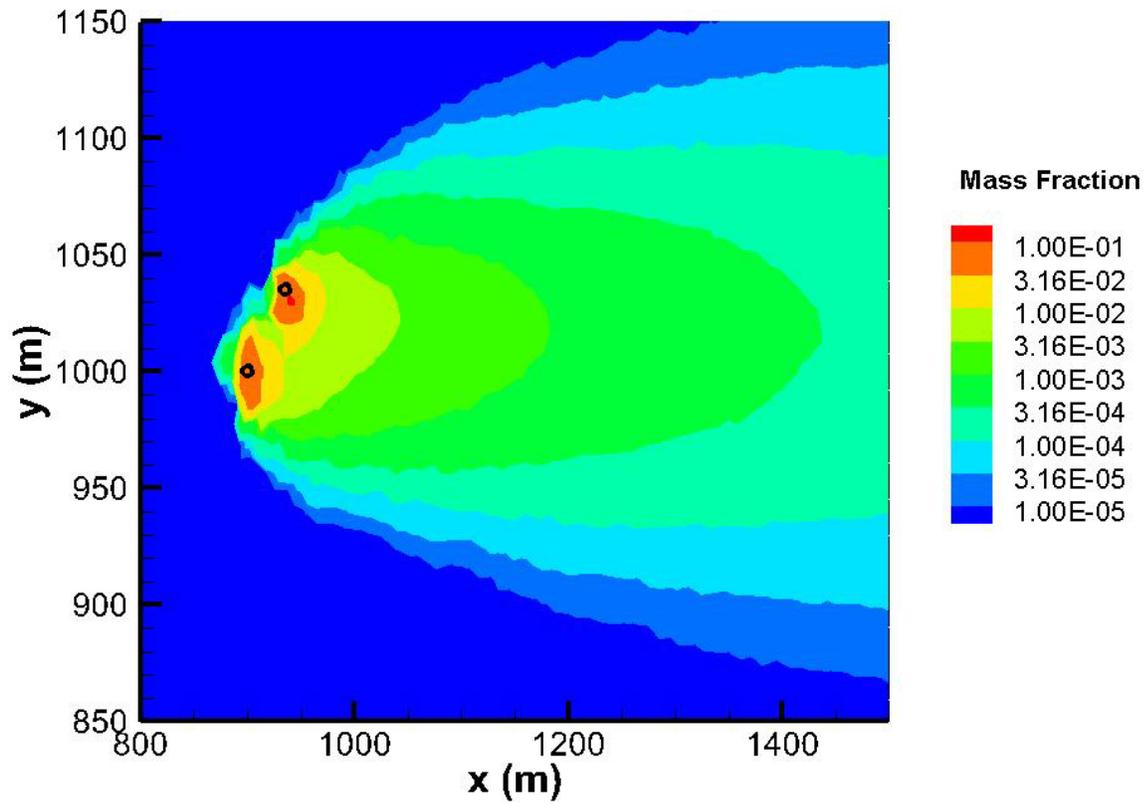


Figure 6. Contour of concentration from PANACHE model for the Test Problem 2B, in which the two CO<sub>2</sub> sources, indicated by the two black circles, are aligned at an angle of 45° (note  $x$ - and  $y$ -direction axes are scaled differently) with the wind direction (along  $x$ -direction).

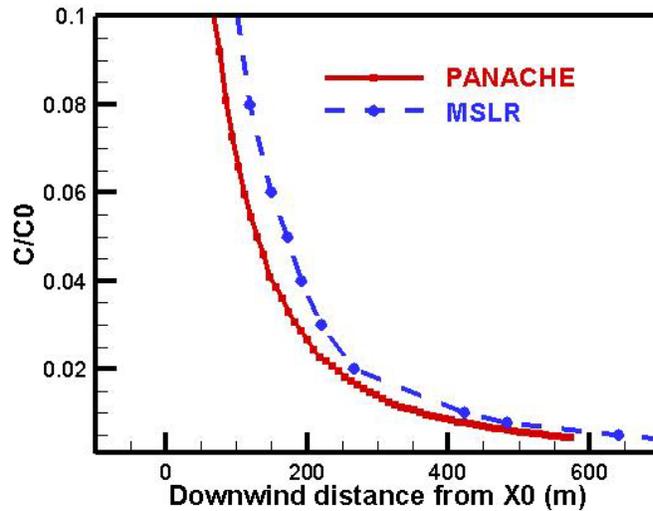


Figure 7.  $C/C_0$  at downwind locations.  $x_0 = 918$  m,  $y_0 = 1018$  m as the center of the plume in the MSLR solution.

## Conclusion

We have developed a very fast method to handle multiple dense gas release sources based on a simple superposition extension to the Britter and McQuaid nomograph. The MSLR calculates critical radii (distances around leakage sources within which the concentration of  $\text{CO}_2$  is above a pre-set value). If one or more receptors are within the critical radius of release source, the IAM flags the receptor(s) as locations with  $\text{CO}_2$  HSE impacts. In addition to the critical radii, the MSLR predicts steady-state downwind concentrations. The MSLR assumes that the wind can be in any direction and does not change over time. Given the variability in the wind direction and one-year time step of the IAM, these assumptions are reasonable. The proposed method has several advantages over CFD approaches for risk assessment: (1) it is simple and easy to implement; (2) it is fast to execute, therefore, a Monte Carlo simulation for uncertainty

propagation study is possible; and (3) there is no boundary effect from a numerical mesh. In conclusion, the MSLR is a fast alternative to a CFD model for dense gas dispersion in the IAM.

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