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Modelling of Carbon Dioxide Venting in Carbon Capture and Storage Studies: Design and Safety Implications

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Abstract

The reduction of the impact of carbon dioxide on the environment is a key driver of the energy transition, which will progressively reduce the use of fossil fuels and will promote the development of viable technologies. This process will be based on renewable energy sources to reduce, to any possible extent, the production and the release of carbon dioxide into the atmosphere. CCS (Carbon Capture and Storage) projects are more and more an ineludible stage of this process. In the last decade, a significant segment of chemical engineering research has been devoted to the management of carbon dioxide release scenarios, which can result both from an accidental loss of containment or from an emergency venting of carbon dioxide streams. This gas is asphyxiating and toxic, depending on concentration levels. Consequently, acquiring familiarity with its dispersion modelling is a key task for process and process safety engineers. On the other hand, carbon dioxide presents a very peculiar behaviour, as it is a dense gas and, below the triple point, its release can produce solid formation. The article presents a relatively simple multi-stage validated model, covering the release scenario from the source, as a heavy gas, up to the neutral Gaussian dispersion, considering also the very low temperatures possibly resulting from the JT (Joule Thomson) effect. Two case studies, carried out through the *Megaris Platform*, illustrate the application of the methodology. It can be useful in the design phase and in the QRA studies, to properly size and locate the venting stack and to minimize any health upsets for the operators

Paper type: Research paper

Keywords: Carbon capture and storage, Carbon dioxide, dispersion, Dense gas, Probit function.

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Introduction

Carbon Capture and Storage (CCS) is a relatively new process of chemical engineering. Its adoption is dictated by the necessity to create a barrier to the migration of carbon dioxide to the atmosphere. Consequently, process segments consisting of significantly high concentrations of this gas have been introduced, with the result that accidental or emergency releases may cause the formation of toxic clouds at ground level. In this respect, the knowledge of the behaviour of the gas is of paramount importance. The adoption of validated software is generally effective in providing the outcome of the release scenarios, but some specific evidence is required to carry out a more comprehensive analysis, to completely define the risks mapping. Carbon dioxide behaves as a dense gas, both because of its molecular weight, which is much greater than that of air, and because frequently it is released at a temperature much lower than atmospheric temperature. **Figure 1** shows the release of a mixture of carbon monoxide and carbon dioxide, through a hole, showing that CO is dispersed as neutral gas (density as air), whereas carbon dioxide drops down. This is the typical scenario of a syngas.

Single models provide the result of single events, whereas in this case, the following multi-stage cloud evolution is expected:

- momentum-dominated release from a stack or from a hole
- slump-down of the cloud to the ground level
- dense gas horizontal migration until the bulk-density (air+CO_2 mixture) approaches the density of air
- neutral dispersion

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Moving from the release to the passive dispersion, the concentration behaviour following the gas impingement with the ground is not described by any validated model, as the well-known Britter McQuaid method describes the dense gas flow just below a certain concentration threshold. The available software, unless it is specifically calibrated, does not cover the whole scenario, with the result that the final outcome of the dispersion can be uncertain. However, the process safety engineer must make sure that the toxic effects are fully identified and properly managed. This article shows how can this scenario be modelled using simple validated equations, and, above all, it describes the behaviour of the cloud dispersion throughout its entire evolution, introducing some novelty in the methodology. Two different case studies illustrate the application of the multi-stage approach.

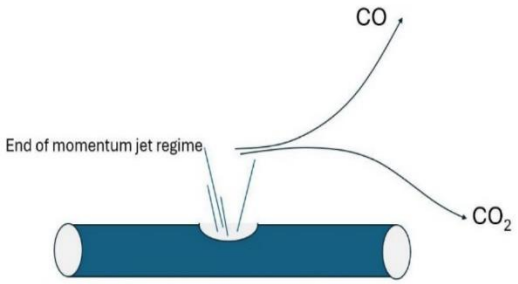

Fig. 1 Dispersion of CO and CO2.

1.1 Harmful effects of carbon dioxide

The toxicity of carbon dioxide is currently quantified through the SLOT and SLOD parameters provided by the British HSE. Notably, the probit functions for this gas can be determined based on the definition of the two parameters.

- SLOT: probability of death for 1% of people
- SLOD: probability of death 50% of people

Furthermore, the form of the probit function is:

$$Pr=a+b\ln(C^n \cdot t) \quad (1)$$

where:

Pr is the Probit function, which is related to probability, C is the substance concentration, expressed as ppm, t is the exposure time, minutes, a and b are unitless coefficients, and n is an exponent defined for the specific substance. HSE data for carbon dioxide are shown in **Table 1**. a and b for any substances can be calculated by writing down the probit function values corresponding to 1% and 50% probabilities of death from the following table.

Table 1 - SLOT and SLOD for CO_2.

Substance	n	SLOT ($ppm^n \times min$)	SLOD ($ppm^n \times min$)
Carbon Dioxide	8	1.50×10^{40}	1.50×10^{41}

Table 2 Probit functions versus probabilities correlations.

%	0	1	2	3	4	5	6	7	8	9
0	-	2.67	2.95	3.12	3.25	3.36	3.45	3.52	3.59	3.66
10	3.72	3.77	3.82	3.87	3.92	3.96	4.01	4.05	4.08	4.12
20	4.16	4.19	4.23	4.26	4.29	4.33	4.36	4.39	4.42	4.12
30	4.48	4.5	4.53	4.56	4.59	4.61	4.64	4.67	4.69	4.72
40	4.75	4.77	4.80	4.82	4.85	4.87	4.90	4.92	4.95	4.97
50	5.00	5.03	5.05	5.08	5.10	5.13	5.15	5.18	5.20	5.50
60	5.25	5.28	5.31	5.33	5.36	5.39	5.41	5.44	5.47	5.50
70	5.52	5.55	5.58	5.61	5.64	5.67	5.71	5.74	5.77	5.81
80	5.84	5.88	5.92	5.95	5.99	6.04	6.08	6.13	6.17	6.23
90	6.28	6.34	6.41	6.48	6.55	6.64	6.75	6.88	7.05	7.33
	0.00	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90
99	7.33	7.37	7.41	7.46	7.51	7.58	7.65	7.75	7.88	8.09

Specifically:

$$2.67=a+b\ln(C^n t) \quad (2)$$

$$5.00=a+b\ln(C^n t) \quad (3)$$

Being $C^n\ t$ the SLOT and the SLOD values (toxic loads), respectively. Solving the equation system, it results:

Table 3 Probit function coefficients for CO_2.

Substance	*n*	*a*	*b*	SLOT (ppm^n×min)	SLOD (ppm^n×min)
Carbon Dioxide	8	-90.94	1.01	1.5×10^{40}	1.50×10^{41}

So, the Probit function for CO_2 is:

$$Pr=-90.4+1.01\ln(C^8\ t) \quad (4)$$

Equation 4, through Table 2, will provide the probability of death for CO_2 inhalation. Other important parameters are the TLV-TWA and the STEL, which are provided by HSE (2020) and are 5000 ppm and 15000 ppm, respectively.

1 Materials and Methods

1.1 Models

The dispersion scenario for a vertically released stream of carbon dioxide has been depicted in **Figure 2**. The gas leaves a stack of height h_s, with a mass flow rate W_{CO2} at temperature T_o. A momentum-driven initial rise Δh is experienced, after which the flow slumps to the ground, due to its molecular weight that is significantly greater than that of air, and, eventually, due to its temperature, which, following a depressurisation expansion, might result in lower than ambient temperature.

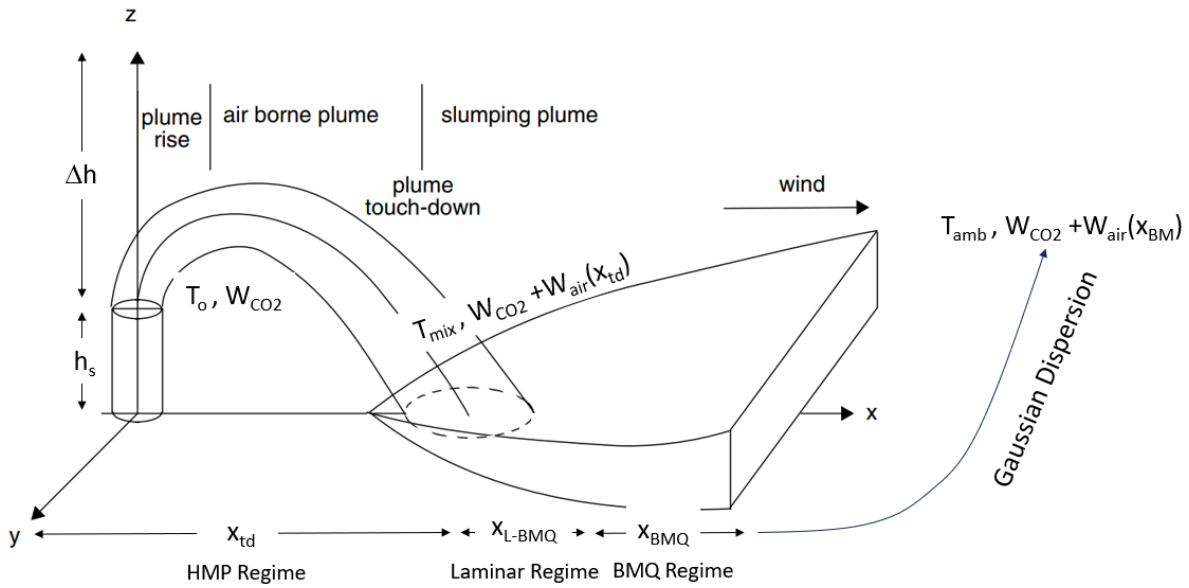

Fig. 2 Dispersion Scenario.

Four sequential fluid dynamic stages are identified. Notably:

1. a dense gas stage, leading the emitted gas to move down, eventually touching the ground at a given concentration; this is identified as HMP regime
2. a laminar stage, wherein the fluid moves for a certain distance according to a pure laminar regime
3. a dense gas stage consisting of the gas travel at ground level, referred to as BMQ regime
4. the final neutral (Gaussian) dispersion stage

The first three stages have been approached, according to the sequential adoption of validated models and referenced equations, as detailed in the following sections.

2 Results and Discussion

2.1 HMP Regime

This regime is described according to the dense gas model presented by Hoot, Meroney and Peterka (1973) and recommended by CCPS (1996). It applies to upward-pointing releases but provides results also for horizontal releases. Notably, regarding Figure 2, the following resolutive equations are provided. The model has been adopted to assess the outcome of important dense gas dispersion scenarios, such as the Jack Rabbit II trial 8 chlorine field experiment (Hanna *et al*., 2021).
The maximum initial rise can be calculated according to the following relationship:

$$\frac{\Delta h}{2 \cdot R_o} = 1.32 \cdot \left(\frac{w_o}{u}\right)^{\frac{1}{3}} \cdot \left(\frac{\rho_o}{\rho_a}\right)^{\frac{1}{3}} \cdot \left[\frac{{w_o}^2 \cdot \rho_o}{2 \cdot R_o \cdot g \cdot (\rho_o - \rho_a)}\right]^{\frac{1}{3}} \quad (5)$$

where: ΔH is the maximum initial rise, m, R_o is the stack/hole radius, m, w_o is the gas velocity at the outlet, m/s, u is wind velocity, m/s, ρ_o is the gas density at the outlet conditions, kg/m^3, ρ_a is the ambient density, kg/m^3, g is the acceleration of gravity, m/s^2.

The touch-down distance x_{td}, at which the centreline of the dense plume strikes the ground, is given by the analytical relation:

$$\frac{x_{td}}{2 \cdot R_o} = \frac{w_o \cdot u \cdot \rho_o}{2 \cdot R_o \cdot g \cdot (\rho_o - \rho_a)} + 0.56 \cdot \left\{\left(\frac{\Delta h}{2 \cdot R_o}\right)^3 \cdot \left[\left(2 + \frac{h_s}{\Delta h}\right)^3 - 1\right] \cdot \frac{u^2 \cdot \rho_a}{2 \cdot R_o \cdot g \cdot (\rho_o - \rho_a)}\right\}^{\frac{1}{2}} \quad (6)$$

where all terms are known, except h_s, that is the hole or stack height above ground.

Finally, the ratio of the maximum concentration at x_{td} to the initial concentration C_o is:

$$\frac{C(x_{td})}{C_o} = 2.43 \cdot \left(\frac{w_o}{u}\right) \cdot \left(\frac{h_s + 2 \cdot \Delta h}{2 \cdot R_o}\right)^{-1.95} \quad (7)$$

2.2 Laminar Regime

After impinging the ground, the cloud is assumed to be driven by its true and/or apparent (i.e. cryogenic) density, travelling along grade for a given distance, so a dense gas model must be applied. Unfortunately, the most credited model, i.e. Britter McQuaid method, is applicable for a concentration range, which falls within the 0.1 and 0.002 fractions of a virtual 100% CO_2 initial concentration (virtual means that, even if it is the mixture with air, just the CO_2 part of the flow is considered). Unfortunately, from x_{td} (100% of the virtual CO_2 molar concentration) to 10% of CO_2, validated simplified models are not available, so the concentration profile along this segment is unknown. However, Benintendi (2011), based on the laminar flow of jet flames has adapted the original model developed by Aalburg *et al*. (2005) to the case of laminar flow. This equation can be written as:

$$x_L = \frac{3 \cdot C_f \cdot R_E \cdot Sc}{32 \cdot c_L(x_L)} \quad (8)$$

Where x_L is the generic distance from the x_{td}, $c_L(x_L)$ is the fraction of $c(x_{td})$ at x_L, the value of which falls between 1 (touch down distance) and 0.1 (beginning of BMQ regime), C_f is a coefficient is an empirical coefficient ≈1, R_E is the Reynolds number, S_c is Schmidt number. It is worth noting that, in equation 8, all terms are substantially constant, so it describes a hyperbolic function, which can be simplified as:

$$x_L = \frac{K}{c_L(x_L)} \quad (9)$$

where K is therefore constant and must be identified.

This function has defined boundary limits, i.e.: $c_L(0)$=1, $c_L(x_{L\text{-}BMQ})$=0.1, where $x_{L\text{-}BMQ}$ is the distance from x_{td} where the BMQ regime starts. This distance can be calculated by applying the Britter McQuaid method, then, backwards, *K* is defined in equation 9, so that the concentration profile along the laminar regime is fully defined.

2.3 Britter McQuaid Regime

As stated, the BMQ model (1988) identifies concentrations of heavy gas on the ground against distances from the release, starting from 0.1 fraction of the initial concentration up to 0.002 fraction of the same initial concentration. It has also been highlighted that the definition of the distance from the release at 0.1 allows one to obtain backwards the profile of the laminar regime. **Figure 3**. shows the nomogram provided by the authors of the model for continuous releases, with the definition of the following terms:
$g'_o=g(\rho_o-\rho_a)/\rho_a$, m/s^2, being ρ_o *and* ρ_a initial plume density and air density respectively, *Uref* is wind velocity, m/s, q_o is the initial volumetric flow, m^3/s, c_m is the concentration at distance x, c_o is the initial concentration

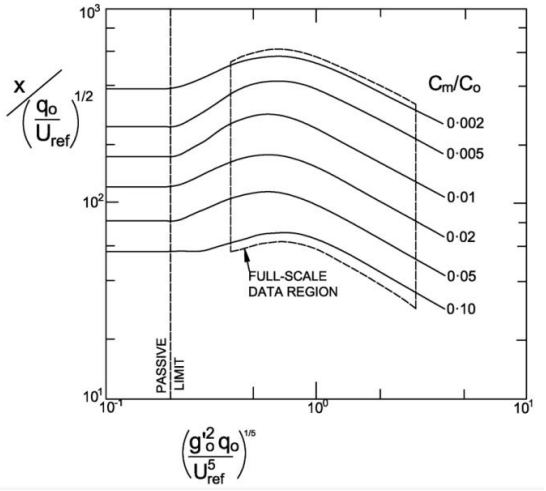

Fig. 3 Britter McQuaid nomogram for continuous release.

Megaris Platform has implemented the mathematical functions describing the curves included in the nomogram, both for instantaneous and continuous releases. Once the gas has attained the 0.002 fraction of the initial concentration, the mixture may likely be considered to evolve according to passive dispersion and the cloud will not present any toxic hazard, as the maximum possible concentration would be 2000 ppm for a pure CO_2 flow.

2.4 Case Studies

Two case studies have been analysed, the former being an upward release, and the latter a horizontal release.

2.4.1 Case Study 1-Upward Release

Including this concentration in equation 4, results from Pr<0, so it is not necessary to proceed further, as no toxic conditions exist, based on the probability of death obtainable from Table 2, which is equal to zero.
However, the touchdown concentration can imply some occupational issues. This circumstance should drive the correct localisation of plant sections, where peoples are expected to stand for long periods of time.
The values of the touchdown concentration and distance are consistent with those obtained through the most reputable commercial software.

Table 4 Inputs and outputs for case study 1.

HMP Dispersion Model	symbol	Unit	Value
Stack height	h_s	m	8
Outlet Temperature	T_o	K	223.16
Outlet radius	R_o	m	0.3
Outlet velocity	w_o	m/s	15
Wind speed	u	m/s	1.5
Ambient Temperature:	T_a	K	288.16
Molecular Weight	MW	g/mol	44.01
Outlet concentration	C_o	v/v	1
Release direction	-	-	Vertical
Flow rate	Q_w	kg/s	4.241
Air Density	ρ_a	kg/m^3	1.226
Outlet density	ρ_o	kg/m^3	2.403
Jet rise	Δh	m	9.1
Touchdown distance	x_{td}	m	47.2
Touchdown concentration	c_{td}	ppm	15334

2.4.2 Case Study 2 - Horizontal Release

The horizontal release has been resolved, showing a significant concentration c_{td}, 62720, at the touchdown distance x_{td}, 77.2 m, from the release point. This value is greater than the IDLH, which is 40000 ppm, according to NIOSH. Consequently, a further analysis of the following regimes is required. Input data and findings are shown on Table 5 and in Figure 4.

Table 5 Inputs and Outputs for Case Study 2.

HMP – Laminar – BMQ Dispersion Model					
HMP Regime					
Item	symbol	Unit	Value	Remarks	
Stack height	h_s	m	8		
Outlet Temperature:	T_o	K	252.72		
Outlet radius	R_o	m	0.05		
Outlet velocity	w_o	m/s	200		
Wind speed	u	m/s	1.5		
Ambient Temperature	T_a	K	288.16		
Molecular Weight	MW	g/mol	44.01		
Starting concentration	C_o	v/v	1		
Release direction	-	-	horizontal		
Mass Flow rate	Q_w	kg/s	1.571		
Air Density	ρ_a	kg/m3	1.226		
Outlet density	ρ_o	kg/m3	2.403		
Jet rise	ΔH	m	0.01		
Touchdown distance	x_{td}	m	77.2		
Touchdown concentration	c_{td}	ppm	62720		
Laminar Regime					
Length of Laminar Regime	$x_{L\text{-}BMQ}$	m	49.4	Calculated from BMQ	
Constant of Aalburg Equation	K	m	6272		
Temperature	T_o	K	285.71	Heat balance (CO_2 + Air)	
Duration	-	-	-	Continuous Plume	
CO_2 mass flow rate	G	kg/s	1.571		
Windspeed at 10 m	u	m/s	1.5		
Ambient Temperature:	T_a	K	288.16		
Concentration at the laminar regime start	C_{td}	ppm	62720	From HMP	
Concentration at a distance from TD	m	0	62720	ppm	HMP
Concentration at a distance from TD	m	9.88	31360	ppm	Laminar regime
Concentration at a distance from TD	m	19.76	15680	ppm	Laminar regime
Concentration at a distance from TD	m	29.64	10453	ppm	Laminar regime
Concentration at a distance from TD	m	39.52	7840	ppm	Laminar regime
Concentration at a distance from TD	m	49.4	6272	ppm	Laminar regime
BMQ Regime					
Concentration at a distance from TD	m	49.4	6272	ppm	Britter McQuaid
Concentration at a distance from TD	m	50	6132	ppm	Britter McQuaid
Concentration at a distance from TD	m	75	2378	ppm	Britter McQuaid
Concentration at a distance from TD	m	100	1257	ppm	Britter McQuaid
Concentration at a distance from TD	m	150	652	ppm	Britter McQuaid
Concentration at a distance from TD	m	300	211	ppm	Britter McQuaid

The findings of the two case studies confirm the adequacy of the methodology to represent the behaviour of a dense gas along its evolution from release to the start of the Gaussian dispersion. In the scientific literature, the various regimes are always presented with stand-alone methods, so it is not immediate to predict the outcome of a release, and, in turn, to identify the toxic effects of the resulting cloud. The HMP method is shown to work very well both for vertical and horizontal release. Moreover, the limits of the BMQ, which is valid only for concentrations starting from the 0.1 fraction threshold onward, have been overcome through the introduction of a laminar regime equation, which allows one to follow the cloud within the more critical concentration bad, as shown in **Figure 4**. The approach is deemed to represent an innovative method for risk assessment of dense gases.

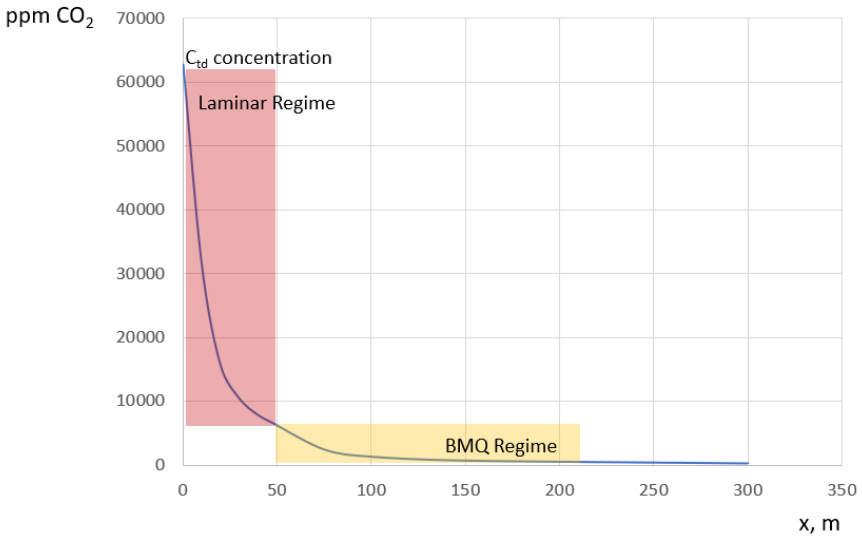

Fig. 4 Profile of CO_2 concentration for Case Study 2.

Conclusions

CCS is a fundamental process to reduce the impact of carbon dioxide on climate change. The article has presented a very simple but comprehensive method, which can support the process safety engineers in CCS studies. The method encompasses more regimes, which is infrequent in the normal analysis of the releases and has introduced a new unpublished calculation segment, named *Laminar Regime*, to cover the gap of the concentration profile before the start of the BMQ regime. The calculations have been carried out by means of *Megaris Platform*, a powerful system including data from up to ten thousand chemicals and dozens of calculation models.
The methodology presented is a valuable tool, even because has the potential to develop the sensitivity capabilities of safety engineers, increasing their attitude to govern the analysis scenarios.

Nomenclature

a and b	=unitless coefficients	[-]
BMQ	=Britter McQuaid	[-]
C	=the substance concentration	[ppm]
C_o	=initial concentration	[ppm]
c_o	=the initial concentration	[ppm]
CCPS	=Centre for Chemical Process Safety	[-]
C_f	=a coefficient is an empirical coefficient ≈1,	[-]
c_m	=the concentration at distance x	[ppm]
Δh	=plume rise	[m]
ΔH	=the maximum initial rise	[m]
DTL	=Dangerous Toxic Load	[-]
g	=the acceleration of gravity	[m/s^2]
HMP	=Hoot Meroney Peterka	[-]
h_s,	=stack or hole height	[m]
HSE	=Health and Safety Executive	[-]
IDLH	=Immediately Dangerous to Life and Health	[-]
JT	=Joule Thomson	[-]
K	=constant of Aarburg equation	[m]
LOC	=Loss Of Containment	[-]
NIOSH	=National Institute for Occupational Safety and Health	[-]
q_o	=the initial volumetric flow	[m^3/s]
QRA	=Quantitative Risk Assessment	[-]
R_o	=the stack/hole radius	[m]
R_E	=Reynolds number	[-]
ρ_o	=the gas density at the outlet conditions	[kg/m^3]
ρ_a	=the ambient density	[kg/m^3]
S_c	=Schmidt number	[-]
SLOD	=Significant Likelihood of Death	[-]

SLOT	=Specified Level of Toxicity	[-]
STEL	=Short-Term Exposure Limit	[-]
T_o.	=initial Tempertaure of CO_2 flow	[K]
t	=the exposure time	[min]
TD	=TouchDown	[-]
TLV	=Threshold Limit Value	[-]
TWA	=Time-Weighted Average	[-]
u	=wind velocity	[m/s]
$Uref$	=wind velocity	[m/s]
W_{CO2}	=CO_2 Mass Flow	[kg/s]
w_o	=the gas velocity at the outlet	[m/s]
x_{td}	=touch down distance	[m]
x_L	=generic distance from x_{td}	[m]

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