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Modelling of source term from accidental release of pressurised CO_2

Joyce T. Lopes, Artur Z. Francesconi, Sávio S.V. Vianna*

School of Chemical Engineering, University of Campinas – UNICAMP, Cidade Universitária “Zeferino Vaz” Av. Albert Einstein, 500, CEP 13083-852 Campinas, SP, Brazil

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ABSTRACT

Storage and transportation in carbon capture and sequestration (CCS) technology involve dealing with CO_2 at high pressures, which can lead to accidental releases. To assess and control risks and to calculate the minimum safe distance from tanks and pipelines to populated areas, the source term model of the leakage is extremely important, as it serves as input to model the dispersion of CO_2 into the atmosphere. The modelling of high pressurised CO_2 releases is relatively complex due to its thermofluidynamics particularities. Its triple point pressure is higher than the atmospheric pressure and it has a relatively high Joule–Thomson coefficient depending on the temperature and pressure conditions. Hence, it might lead to a two-phase flow and to solid formation when the depressurisation to atmospheric pressure occurs. Also, the molecular vibration of CO_2 might be important in some leakage scenarios. There are several approaches in the literature which address differently the aspects of the flow, specially regarding thermal and mechanical equilibrium or non-equilibrium. The present work provides an innovative approach for the discharge calculation in accidental high pressure releases. The Homogeneous Non-Equilibrium Model (HNM) is proposed, which accounts for non-equilibrium effects regarding not only metastability but also vibrational relaxation of the molecule. It considers the possible phase transitions and dry ice formation and it is applicable to steady-flow conditions. The model was tested with experimental data from CO2PIPETRANS project, HSE experiments and Cooltrans research programme. It was found that the model works well leading to results which agree with available experimental data. The proposed source model is relatively simple to implement and it does not demand numerical effort. The discussed discharge approach for CO_2 releases emerges as a good alternative to existing models.

1. Introduction

Carbon dioxide is pressurised to be re-injected in reservoirs in order to increase oil recovery (Houston, 2009) and to induce flow in CCS projects (Mazzoldi et al., 2011). The high pressure and large amount of CO_2 in some process plants increase the risk level (Mahgerefteh et al., 1999). A model capable of predicting accurately the leakage is absolutely important to assess and control the risks in many engineering cases. The discharge rate is an important input for modelling the following atmospheric dispersion of the gas and calculate the minimum safe distance from tanks and pipelines to populated areas.

The triple point pressure of carbon dioxide is higher than the atmospheric pressure and its Joule–Thomson coefficient is high at certain conditions. Therefore, considering the expansion from pressurised reservoirs to atmospheric conditions the flow might be biphasic with possible solid formation (dry ice). In addition to that, in some scenarios it could be important to take into consideration the molecular vibration of the CO_2 molecule. Modelling two-phase flow can be challenging because the involved phenomena are not totally understood. Furthermore, CO_2 thermofluidynamics particularities add another level of complexity to the problem.

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* Corresponding author.
E-mail address: savio@feq.unicamp.br (S.S.V. Vianna).

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Nomenclature

Δh_{lv}	specific enthalpy of vaporization
$\Delta \upsilon$	vapor specific volume minus liquid specific volume
γ	specific heat ratio
Φ	ratio of vibrational relaxation time to residence time in the orifice
ρ_l	liquid specific mass
τ_{bubble}	bubble growth time
$\tau_{residence}$	residence time in the orifice
τ_{vib}	vibrational relaxation time
$\tilde{\tau}$	ratio of bubble growth time to residence time in the orifice
υ_l	liquid specific volume
υ_v	vapor specific volume
c_d	discharge coefficient
c_p	specific heat at constant pressure
c_p^{eq}	equilibrium specific heat at constant pressure
c_p^{fr}	frozen or non-equilibrium specific heat at constant pressure
c_{pl}	liquid specific heat at constant pressure
c_{ps}	solid specific heat at constant pressure
d_{ori}	orifice diameter
G	mass flux
G_{AB}	incompressible flow mass flux
G_{BC}	liquid–vapor mass flux
G_{CD}	vapor–solid mass flux
h	specific enthalpy
h_l	liquid specific enthalpy
K_1	experimentally adjusted parameter for CO_2
K_2	experimentally adjusted parameter for CO_2
P_0	stagnation pressure
P_{atm}	atmospheric pressure
P_{tr}	triple point pressure
P_{vap}	vapor pressure
T_0	stagnation temperature
T_f	final temperature
T_{tr}	triple point temperature
U	velocity
U_{AB}	incompressible flow velocity
x	vapor mass fraction

There are a few models in the literature which handle differently the aspects of the flow following high pressure releases, specially regarding equilibrium and non-equilibrium assumptions. Pham and Rusli (2016) provided a robust review of the current models for depressurisation, dispersion and release of CO_2. Two of the most common two-phase flow approaches are HEM (homogeneous equilibrium model) and HRM (homogeneous relaxation model), which were studied and served as bottom line for many authors. Either HEM or HRM assume mechanical equilibrium between constituent phases. The difference between the two models is that the former considers thermal equilibrium while the latter accounts for CO_2 metastability.

HEM was validated by Webber et al. (1999) and Martynov et al. (2013). However, as pointed up by Wallis (1980), it only predicts good results when there is enough time to reach the equilibrium, as in long pipes. Dyer et al. (2007) developed a model that combines incompressible fluid model and HEM in order to account for non-equilibrium. According to the author, the actual mass flow is somewhere between those two approaches based on the fact that if there are not immediately available nucleation spots for bubble initiation, liquids can often depressurize isothermally well below their vapour pressure.

HRM was first proposed by Bilicki and Kestin (1990) and later Angielczyk et al. (2010) provided an expression for vapour quality relaxation time (time vapour quality takes to achieve its equilibrium value). Brown et al. (2013) presented an homogeneous relaxation flow model for predicting the discharge following full bore rupture of dense phase CO_2 pipelines. Benintendi (2014) discusses the non-equilibrium thermodynamic of liquid and supercritical carbon dioxide expansion, illustrating relaxation dynamics through the HRM models and taking into account the singularities of the phase transitions. It presents a case study of CO_2 release, however no comparison to experimental data is provided.

Johnson et al. (2000) have drawn attention to the effects of vibrational relaxation on the discharge coefficient of carbon dioxide. Fiates et al. (2016) presents the Hybrid Switch Model (HSM), that takes those effects into consideration. However, the constant proposed to account for the transition between vibrational equilibrium and non-equilibrium has no physical meaning and it is dependent on experimental data. Additionally, the HSM does not consider CO_2 metastability.

In spite of the great effort made on the subject, there is still a lack of precision in describing the phenomena. The current work aims to provide a new model to calculate CO_2 mass flow rate in the depressurisation region. The Homogeneous Non-Equilibrium Model (HNM) is presented as an innovative approach for the discharge modelling, which takes into consideration not only CO_2 metastability but also the effects of vibrational relaxation. The model accounts for phase transitions and solid formation. It is applicable to steady-flow conditions and initially liquid carbon dioxide. In order to test its performance, the results of the model are compared to experimental data.

2. Modelling

The Homogeneous Non-Equilibrium Model (HNM) calculates the discharge rate considering the stagnation conditions in a pressurised tank. Fig. 1 shows an illustrative scheme of the flow, from the initial stagnation condition in the tank (P_0, T_0) to the final condition in the Mach Disk (P_{atm}, T_f). Mechanical equilibrium will be assumed to model the discharge (i.e. phase slip will not be considered).

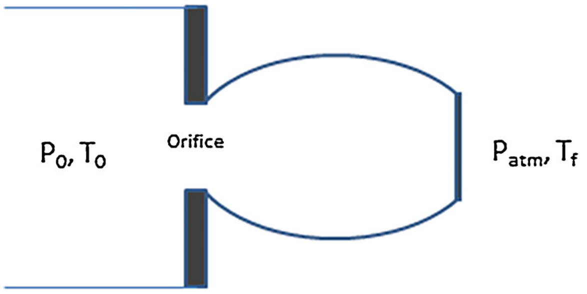

Fig. 1 – Flow illustration from the initial stagnation condition in the tank (P_0, T_0) to the final condition in the Mach Disk (P_{atm}, T_f).