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Facing Emerging Risks in Carbon Sequestration Networks. A Comprehensive Source Modelling Approach

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Tackling risks in emerging infrastructures is a key point in making them acceptable and safer. Carbon Sequestration pipeline networks, as part of the Carbon Capture and Storage chains, are linked to the handling of large amounts of CO_2 and may be subjected to failures and ruptures. This results in large pressurized and multiphase releases of CO_2 that behaves as a denser-than-air and asphyxiant gas. The lack of a comprehensive modelling approach in this sense makes employed risk safety procedures often unreliable and lacking.

In this work, a comprehensive modelling approach, based on self-collected experimental data, is proposed with the aim of filling existing gaps. Results well match experimental data and the modelling procedure allows for the estimation of characteristic parameters linked to heat transfer phenomena and the incidence of geometry and operative conditions on the release evolution.

The occurrence of the solid phase and the applicability of the isothermal hypothesis is discussed showing that specific geometric and operative conditions are required.

1. Introduction

The Carbon Sequestration chain is experiencing large investigations and pilot projects to make it feasible as a medium to long term solution to govern the Global Warming (IEA, 2010; IEAGHG, 2013). It is implemented as a vast pipeline network infrastructure able to handle large amounts of liquid and supercritical CO_2, captured from large stationary sources. Besides technical operative aspects dealing with this innovative technique, safety-related issues emerge given the asphyxiant and denser-than-air behaviour of the CO_2 (Webber, 2011). In addition, the complexity of such large infrastructures linked to unavoidable failures leads to possible ruptures that result in a CO_2 pressurized release (Turner, 2006).

The rapid depressurization of the CO_2 from a pressurized domain is characterized by peculiar aspects mainly related to its thermodynamic behaviour (Mocellin et al., 2016a):

- the stored CO_2 may undergo bi-phase or even a three-phase release once the mixture involves the solid-vapor existence domain;
- the release takes place with relevant heat transfer phenomena, deviating from ideal transformations;
- the domain geometry as well as the initial amount play a key role in determining the release evolution;
- abovementioned aspects are quite always neglected in actual employed QRA procedures (Mocellin et al., 2016c).

It is clear how applied procedures lack the core of any CO_2 release phenomenon and inaccuracies arise as suggested by some authors (Martynov et al., 2014). In addition, simplified and truncated approaches are proposed to fulfil timing in response to an emergency.

Considering this, the present work illustrates a comprehensive modelling approach that embodies all discussed gaps. Specific results are collected and discussed to focus on main CO_2 release features applied to the Carbon Sequestration infrastructures' operations.

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2. Model equations, assumptions and solving procedure

The modelling approach deals with the establishment of a pressurized release of CO_2 following the pipeline rupture. The occurring transient phenomenon evolves from the Carbon Sequestration operative conditions (P_0, T_0) to the final state according to the non-stationary balance equations illustrated hereafter. A schematic domain is represented in Figure 1.

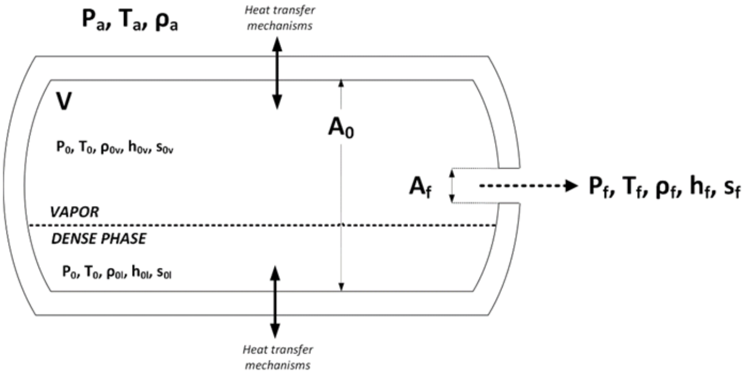

Figure 1: Schematic representation of the modelled domain. A multiphase approach is adopted along with the description of phase change and heat transfer mechanisms.

Coupled mass and energy balances apply to the domain as of eq. (1)-(2):

$$\frac{d}{dt}(\rho_0 V) = -\dot{m}_0 = -\gamma_d \rho_1 A_1 \left[-2\left(\int_0^1 \rho^{-1} dP + \frac{1}{2}\langle u_1 \rangle^2 \sum_i \varphi_i\right)\right]^{1/2} \left[1 - \left(\frac{\rho_1 A_1}{\rho_0 A_0}\right)^2\right]^{1/2} \tag{1}$$

$$\frac{d}{dt}(\rho_0 V \widetilde{u_0}) = V\left[\rho_0 \frac{d\widetilde{u_0}}{dt} + \widetilde{u_0}\frac{d\rho_0}{dt}\right] = -\dot{m}_0\left(\widetilde{u_0} + \frac{P_0}{\rho_0}\right) + \dot{q_v} A_{int} \tag{2}$$

Eq. (1)-(2) are supplemented with the interphase mass balances that accounts for all mass fluxes linked to phase change mechanisms:

$$\frac{dm_i}{dt} = \sum_j \dot{m_{j \to i}} - \sum_j \dot{m_{i \to j}} - \dot{m_{i,out}} \tag{3}$$

Interphase mass balances apply for the solid, liquid and vapor phase together with the equations related to heat transfer phenomena occurring because of phase change processes and heat exchanges with surroundings.

Eq. (1)-(2) apply to bulk conditions (subscript *0*) and the path to orifice conditions (subscript *1*) is based on a specific thermodynamic path that requires modelling. The expansion evolution considers the heat transfer as well as friction phenomena that alter the CO_2 energetic content through a reversibility parameter χ:

$$\frac{d(Pv)}{dt} = \frac{P_0(t) - P_0(t - \Delta t)}{\rho_{CO_2,0}(t)}\chi \tag{4}$$

The parameter χ invokes all main contributions to the transformation irreversibility namely heat transfer, shock wave formation and frictions phenomena and ranges from 0 (completely irreversible transformation) to 1 (fully reversible transformation, ideally isentropic). Heat transfer mechanisms are based on the occurrence of natural and forced convection, conduction across the vessel walls and phase change-related thermal fluxes. In this sense, the occurrence of different phases is invoked by additional specific mass balances and descriptive correlations of main phase change mechanisms that are considered: boiling, condensation, solidification and sublimation. The detailed modelling approach is given in (Mocellin et al., 2018).

The model, consisting of mass and energy balances (global and for each expected phase) and correlations for friction and heat transfer is supplemented by the Yokozeki equation of state (Mocellin et al., 2016b), descriptive of the CO_2 thermodynamic behaviour.

The entire model structure is numerically solved by means of coupled 4th-order Runge-Kutta schemes. An explicit time integration is employed in an iterative procedure in which the occurrence of choked-flow states is also checked (Figure 2). As of Figure 2, the main model outputs concern the time profiles of the most important variables in the QRA consequence estimation procedure (mass flow rate, pressure, temperature profiles in time both at bulk and orifice conditions; total discharge time and instantaneous mixture quality). Additional data on heat transfer mechanisms and phase change processes are obtained.

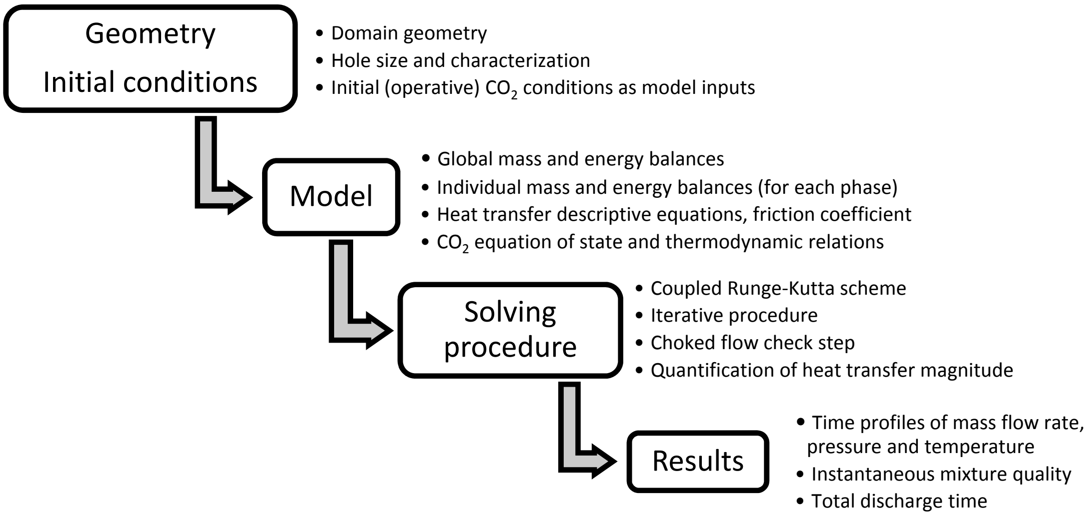

Figure 2: Basic flow chart of the proposed modelling approach.

3. Results and discussion

3.1 Model performance compared to laboratory scale experimental data

Self-made experimental data on rapid CO_2 depressurizations from a vessel were used to assess the model performances (Mocellin et al., 2018). The model positively matches the experimental trials even under different initial charging conditions and aggregation states. The results goodness was finally assessed against the total discharge time, intended as a robust indicator of the performance, being linked to the whole dynamics and the instantaneous CO_2 aggregation state. Results are collected in Figure 3a.

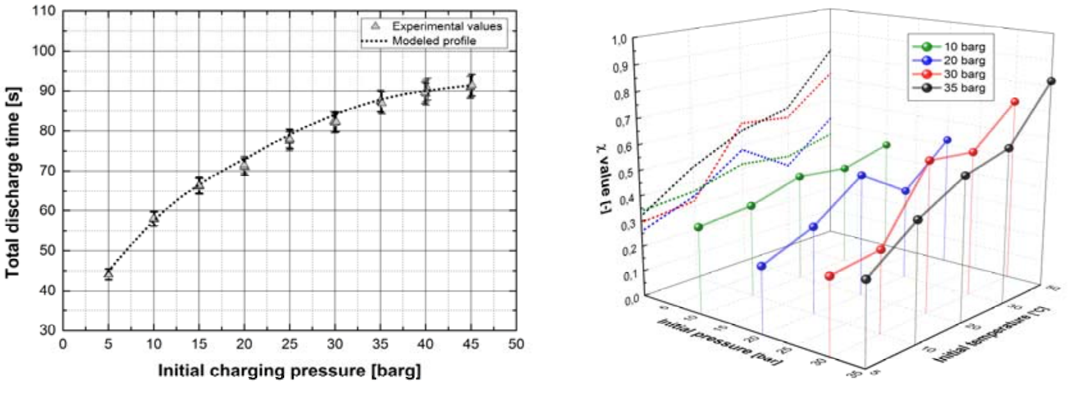

Figure 3. a- Experimental and predicted total discharge time. b- quantified χ values for different initial conditions.

The positive match with the total discharge time is linked to a robust prediction of the time evolution of the mixture density. This parameter is resulting from complex interactions between the instantaneous thermal gradients and the heat transfer phenomena as well as the frictional flow to orifice conditions. In this sense, results show that relevant variations in the reversibility parameter occur (Figure 3b). The maximum observed value is always below 0.85 with a major contribution played by heat transfer related-equivalent work (see eq. (4)). A certain degree of irreversibility is thus expected and the occurrence of heat transfer with surroundings discard the adiabatic evolution that is usually invoked in QRA procedures applied to carbon sequestration.

The overall coefficient of heat transfer experiences large variations in the initial steps of the release where pressure gradients are widest. The maximum observed value almost matches the condition of minimum bulk CO_2 temperature with a progressive decrease once the solid walls balance the thermal induced gradients.
At a laboratory scale, heat transfer mechanisms play a key role in determining the release evolution that can not therefore be neglected. Once the scale is enhanced, for example in large real-scale operations, the heat transfer processes magnitude is very sensitive to the domain size and the operative conditions.

3.2 Model extension to real-scale large operations

Large scale Carbon Sequestration operations are performed in dedicated pipelines with specifications listed in Table 1 (IEAGHG, 2013).

Table 1. Carbon sequestration infrastructure specifications.

Length, km	External diameter, mm	Thickness, mm	Min pressure, barg	Max pressure, barg
1.9-808	152-921	5.2-27	3-151	21-200

Results of the model application show that the release evolution, in large scale domains, is mainly governed by the following parameters:

- geometry: pipeline length L and internal diameter D expressed in terms of L/D parameter;
- orifice size diameter d expressed in terms of d/D parameter;
- operative conditions: pressure and temperature, or equivalently CO_2 density.

In this sense, all listed parameters influence the bulk thermal dynamic inducing variations in the temperature time profile, minimum expected temperature and in the (P,T) evolution path. The total amount of CO_2 initially subjected to the release determines the relative importance of heat transfer mechanisms with respect to the heat capacity given by the solid walls. The bulk of very long pipelines carrying liquid CO_2 subjected to a release may evolve isothermally for most of the accident with global temperature variations limited to 2-5 °C. This scenario does not apply with gaseous charges (EOR operations) being the heat capacity minimal compared to the solid walls. The isothermal hypothesis can be safely invoked if $d/D < 0.20$, independently on the operative conditions. Thermal profiles are always coupled with peculiar pressure and mass flow rate trends that exhibit slope variations corresponding to the onset of a multiphase mixture. Some distinct steps in the mass flow rate profiles are observed in the case of the CO_2, respectively linked to the liquid-vapor and the solid-vapor domain (Figure 4a).

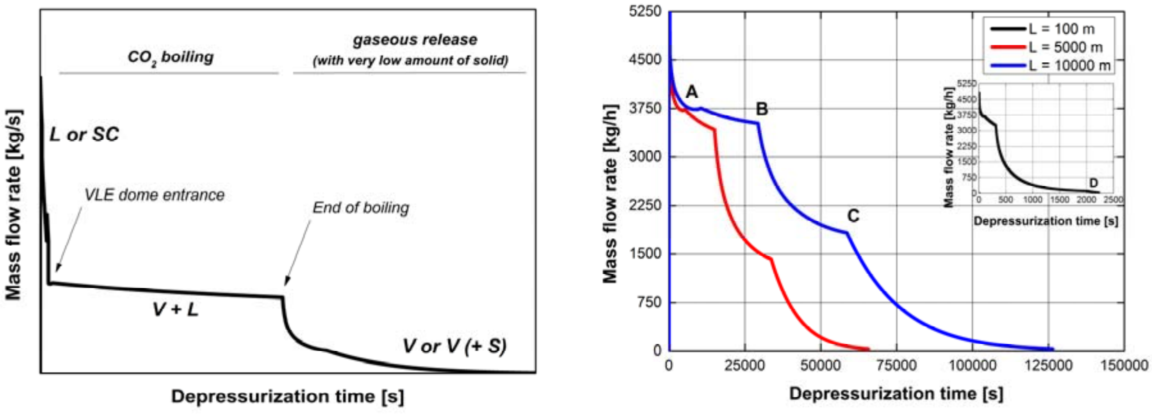

Figure 4. a- Release evolution: characteristic CO_2 mass flow rate time trend. b- CO_2 mass flow rate trends as a result of a release from a pipeline operated at 60 bar and 20 °C.

As of Figure 4b, this trend is preserved independently on the length of the pipeline (i.e. the total amount of CO_2 being discharged) even if the key points are shifted in time. In the A-B segment the CO_2 mass flow rate is almost constant matching the persistence of the liquid phase in the pipeline bulk. A subsequent decreasing trend (B-C) is observed due to the gaseous CO_2 being formed and lowering the mixture density. In the case of very short pipelines, an additional step D is observed matching the establishment of a solid-vapor mixture. The solid phase appearance (in the final release steps) is expected once $L < 1500$ m and $d/D > 0.30$. In any case, larger release orifices enhance the thermal effects and the CO_2 solid content, that cannot be thus neglected in an exhaustive QRA modelling. Variated operative conditions (pipeline pressure and external temperature) alter the following release parameters:

- overall degree of reversibility χ;
- amount of solid phase discharged;
- average mixture mass flow rate discharged during the onset of boiling mechanisms (A-C segment);
- time to complete depletion of bulk boiling processes.

Altered parameters as a result of a variation in the operative pressure are reported in Table 2.

Table 2. Release parameters' alterations due to a varied operative pressure and orifice size.

Op. pressure, bar	d/D, adim	Time to saturated conditions, min	Time to complete boiling, min	Averaged mass flow rate during boiling, kg s^{-1}
150	0.1	19.0	675.0	11.9
60		2.6	530.0	13.1
150	0.4	2.5	57.5	187.5
60		0.9	41.5	215.0

3.3 Model application to real existing CCS and EOR projects

Model performances were tested against existing CCS and EOR infrastructures, especially with respect to the total discharge time, the occurrence of the solid phase and the average degree of reversibility χ.

The analysis was applied to the Cortez Pipeline (Kinder Morgan, TX, USA) and the Snøhvit infrastructure (Statoil, Norway) whose operative conditions are listed in Table 3.

Table 3. Pipeline specs (IEAGHG, 2013).

Name	Capacity, Mton yr^{-1}	Length, km	Diameter, mm	Pressure, bar
Cortez pipeline	19.3	803	726	186
Snøhvit pipeline	0.7	153	200	100

Different scenarios were simulated, namely a small ($d/D = 0.10$) and large ($d/D = 0.40$) rupture on 1.0 and 5.0 km- pipeline segments. Results are collected in Table 4-5.

Table 4. Simulation results with $d/D = 0.10$, small rupture.

Name	Segment length, km	Total discharge time, h	Solid phase	Mean χ
Cortez pipeline	1.0	3.70	-	0.76
	5.0	17.60	-	0.77
Snøhvit pipeline	1.0	3.50	-	0.71
	5.0	17.40	-	0.77

Table 5. Simulation results with $d/D = 0.40$, large rupture.

Name	Segment length, km	Total discharge time, h	Solid phase	Mean χ
Cortez pipeline	1.0	0.34	after 0.23 h both in the bulk and orifice	0.83
	5.0	1.50	-	0.81
Snøhvit pipeline	1.0	0.30	After 0.22 h both in the bulk and orifice	0.86
	5.0	1.46	-	0.82

The model application showed that, as reported in Table 4, no solid phase appearance is expected in the case of a small rupture where lower degrees of reversibility are observed. In this sense, a modelling approach oriented to the solid phase description is not required in the QRA procedure. On the contrary, a large rupture scenario determines the occurrence of solid CO_2 because of the induced cooling mechanisms. This is expected both in the bulk and at the orifice conditions with the establishment of a solid-vapor process leading to solid contents up to 20 % m/m. In this case, the solid phase description can not be ignored since both the mixture properties and its behavior at choked conditions are sensitive to the solid CO_2 (Raimondi, 2016; Luberti et al., 2016).

Once the pipeline segment length subjected to release is increased, this occurrence vanishes matching the fact that the solid appearance is more likely in short pipeline tranches subjected to large ruptures (par. 3.2).

It was observed that ignoring the appearance of solid CO_2 results in:

- the overestimation of the total discharge time up to 35 %;
- the estimation of a misleading temperature in the pipeline bulk that is reflected in an erroneous density assessment;
- the omission of all hazards related to the formation of a sublimating bank near the release point resulting from the dry-ice deposition.

4. Conclusions

A comprehensive modelling approach for CO_2 pressurized releases from carbon sequestration infrastructures was proposed. The model fully agrees with the experimental data and estimated parameters well explain collected results. The holistic approach is promising in the description of all main expected processes during a rapid release of CO_2 including the establishment of multiphase releases, the occurrence of solid CO_2 and heat transfer processes unavoidably related to irreversible mechanisms.

Results show that whatever a CO_2 release occurs, ideal assumptions usually employed in actual QRA procedures are never met. A parameter, expression of the main sources of thermodynamic irreversibility (frictions, heat transfer, …), is employed and shows that the expansion path to atmospheric conditions is not approaching an ideal reversible transformation with a degree of reversibility never higher than 0.85.

The release evolution is sensitive to two main groups of parameters: the geometry (expressed in terms of L, L/D and d/D) and the operative conditions (pipeline pressure and temperature, i.e. CO_2 density). Specific combinations allow for the bulk isothermal hypothesis ($d/D < 0.20$, independently on the operative conditions) and the solid phase occurrence ($L < 1500$ m and $d/D > 0.30$), especially in the pipeline bulk. Heat transfer processes with the surrounding pipeline walls are responsible for the release evolution and are mainly governed by the total amount of CO_2 initially confined in the pipeline, through the listed parameters. Heat phenomena play a key role in determining the instantaneous bulk CO_2 density which in turn outlines a characteristic mass flow rate profile. Different steps are observed, matching the main phase change mechanisms that are taking place during the release. In addition, the operative conditions have a strong effect on some parameter linked to the phase change processes (χ parameter, time to saturated conditions and to complete boiling, average discharged mass flow rate during boiling).

The application to some real scale existing CCS and EOR projects shows that the solid phase occurrence is expected. Once a non-exhaustive QRA study that ignores this aspect is invoked, results are characterized by a certain degree of inaccuracy that lacks a specific scenario related to carbon sequestration operations like the formation of a sublimating bank.

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