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Hazard Analysis of Carbon Sequestration Pipelines. The Effect of Impurities and Insulation Specs on the Release Evolution

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Many emerging risks are related to strategic infrastructures carrying CO_2 for sequestration purposes (CCS and EOR projects). Among these, a pressurized release induced by a rupture is by far the most common hazard scenario that may lead to serious consequences.

A comprehensive source modelling approach should also include the description of effects related to impurities that are commonly included and accepted in captured CO_2 streams. This work suggests a method to assess the influence of impurities with respect to a flow of pure CO_2 and shows that an increasing impurities content alters both the phase change mechanisms and the temperature dynamics inside the pipeline. This effect is very sensitive to the pipeline length subjected to a release and the orifice size.

A detailed analysis of the influence of insulation in the release dynamics shows instead a negligible contribution to the thermal dynamics mainly due to the irrelevant role played by conductive mechanisms with respect to convective and latent-related thermal processes.

1. Introduction: the need of reliable CO_2 source models

The implementation of reliable QRA techniques is essential in making emerging techniques acceptable and safer.

The Carbon Sequestration chain, that consists of three distinct steps (capture, transportation, injection for storage), suffers many hazards mainly related to the handled carbon dioxide that behaves as an asphyxiating and denser-than-air gas. In addition, processed streams are rarely pure being made up of different substances (N_2, CO, CH_4, Ar, NO_x and SO_x).

Among the CCS constituent steps, the transportation phase is critical because it is characterized by extensive infrastructures that handle large amounts of pressurized carbon dioxide streams (Ochoa Bique et al., 2018).

At present, great deal of effort has been paid to the development and the implementation of comprehensive and reliable CO_2 source models able to support the pressurized release characterization (Cao et al., 2018).

In this framework, pressurized releases can be due to (Corsten et al., 2013):

- internal causes (corrosion ruptures, mechanical collapse, over pressure);
- external causes (ground operations, natural events like earthquakes and floods, domino effects).

Once subjected to a failure and thus a sudden release, the CO_2 experiences a set of mechanisms that make it peculiar with respect to usual gaseous and liquid tubed substances and this contingency asks for dedicated source models.

As discussed in Mocellin et al. (Mocellin et al., 2018), peculiarities are mainly linked to the establishment of three-phase releases (solid, liquid and vaporous) and the incidence of phase-change and heat transfer mechanisms in the final outcomes.

In this framework, not only a detailed approach is needed but also a specific thermodynamic approach able to manage three distinct phases and the influence of impurities on the pure CO_2 behaviour.

This work is thus focused on the proposal of a suitable thermodynamic approach and on the investigation of effects related to common expected impurities in the CO_2 flow. Depending on the capture technique (prior to the transportation step), the effect of the O_2, N_2, Ar, NO, H_2O and H_2 is analysed.

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In addition, the contribution of the insulation on the release evolution is inquired through a detailed analysis of its effect on the heat transfer efficiency and the overall release expansion degree of reversibility.

2. Source modelling approach

2.1 Generalities and main mechanisms

The release from a pressurized pipeline is approached by means of mass, momentum and energy balances as reported in Mocellin et al. (Mocellin et al.,2016). The set of nonlinear ODEs is representative of a non-stationary phenomenon that invokes:

- flow rate variations resulting from the non-ideal multiphase flow from the pipeline bulk to orifice conditions;
- temperature fluctuations due to the instantaneous balance between heat fluxes related to convective, latent and conductive processes;
- phase change mechanisms leading to the occurrence of distinct phases contributing to the solid, liquid and vaporous inventory.

The source model is thus descriptive of time-related properties that vary during the release evolution, namely mass and volumetric flow rate, temperature, heat transfer coefficient and multiphase mixture properties.

2.2 Impurities effect modeling and inclusion

Impurities of CO_2 streams are linked to the different technologies adopted in the capture stage that mainly consist in the pre-combustion, post-combustion and oxyfuel techniques (Rackley, 2017). Their presence is linked to the adopted fuel oxidation process (complete or partial), the amount of excess air and process fluids used to purify the carbon dioxide stream.

Pure CO_2 streams can be contaminated by solid traces, liquid and gaseous substances that can experience different aggregation states depending on the operative conditions for transportation. This work deals with liquid and gaseous substances that may affect the CO_2 purity.

On a release modelling perspective, impurities are treated as additional components affecting the stream properties relevant to the depressurization dynamics. The resulting multicomponent mixture is managed with a proper thermodynamic approach that provides a reliable description of pure and mixture properties and solid-vapor-liquid equilibria occurring because of the pressurized release.

Details of the thermodynamic approach are reported in Fig. 1 within the overall release model structure.

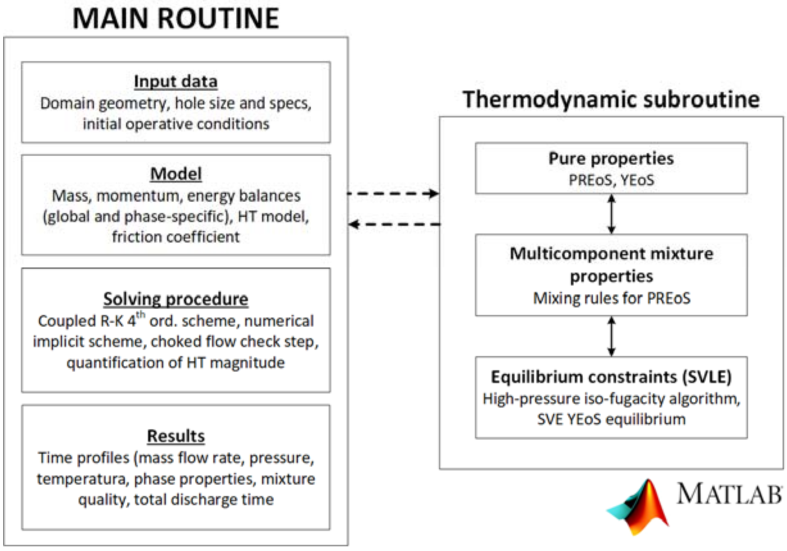


Figure 1: adopted model scheme. Main routine with the release calculation algorithm and the thermodynamic block with relevant pure and mixture property calculator and phase equilibria.

In this work, pure properties are derived according to the reliable Peng-Robinson EoS (PREoS) given the expected behaviour of handled compounds. In addition, the Yokozeki EoS (YEoS) is employed when dealing with the solid phase that is expected because of solidification/sublimation processes of the CO_2.

Vapor-liquid equilibrium calculations are conveniently evaluated by an EoS approach given the high pressure of the system and are based on the general iso-fugacity condition, applied to coexisting phases (solid, liquid, vapor). In this way:

- the pressure effect on the liquid phase properties is included (Poynting correction);
- the vapor phase fugacity is directly found from the EoS;
- a specific approach for the supercritical phase is adopted (unsymmetric normalizing activity);
- the assumption of simple random mixing can be improved with a more sophisticated approach (Huron Vidal mixing rule).

This work deals with the following (most abundant) constituent compounds: CO_2, O_2, N_2, Ar, NO, H_2O and H_2.

2.3 Heat transfer mechanism across the insulation

With respect to model adopted in Mocellin et al. (Mocellin et al., 2018), an additional resistance to heat transfer is introduced. The overall heat transfer mechanism is thus comprehensive of internal convection, conduction across both the steel layer and the insulation thickness and external convection, driven by environmental boundary conditions. Heat transfer is also related to latent exchanges between facing phases that may occur during the release.

Properties of the insulation material are reported in Table 1. Listed properties refer to a commercial PUR/PIR foam insulation material made of rigid polyurethane.

Different thicknesses are used and are expressed with respect to the pipeline steel thickness.

Table 1: Pipeline insulation material.

Thermal conductivity, W m^{-1} K^{-1}	Density, kg m^{-3}	Specific heat capacity, kJ kg^{-1} K^{-1}
0,030	90	1,5

3. Results and discussion

3.1 Effect of impurities on the release evolution

The effect on the release evolution of impurities in the CO_2 flow is evaluated with respect to actual expected stream specs, depending on the capture technique (Table 2). Results are compared with the flow of pure CO_2, in terms of main release parameters (minimum and instantaneous temperature, onset of phase change mechanisms, total release time).

Each simulation is performed on geometric bases reported in Table 3, pipeline specs are preserved with respect to Mocellin et al., 2018.

As a crucial parameter in the determination of the release evolution, the bulk temperature is firstly investigated (Figure 1).

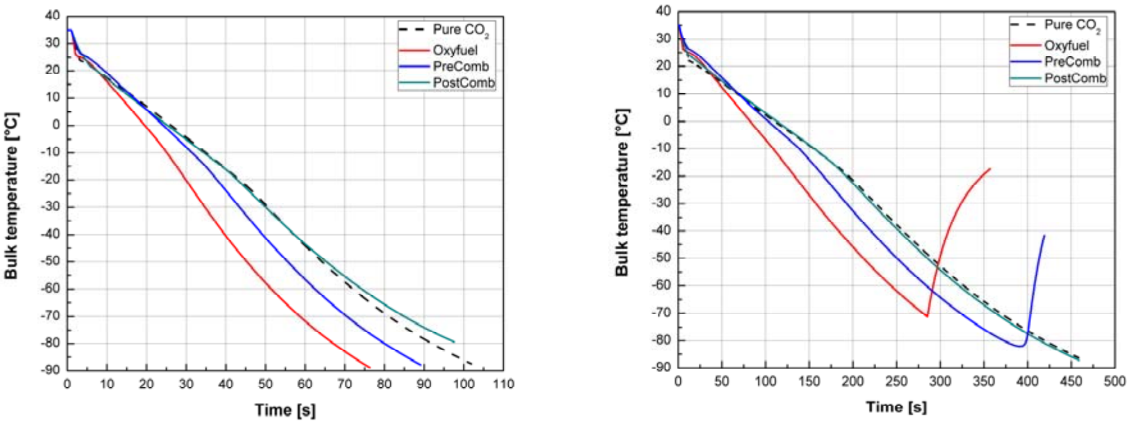
Variations are observed depending on the stream impurity both in terms of temperature dynamics and minimum reached values.

Table 2: CO_2 streams specs (vol. frac) depending on the capture method (Porter et al., 2015).

Component	Pre-combustion	Post-combustion	Oxyfuel
CO_2	0,9802	0,9981	0,9580
O_2	-	0,0003	0,0110
N_2	0,0090	0,0012	0,0200
Ar	0,0001	-	0,0060
NO (mainly NO)	0,0001	0,0001	0,0001
H_2O	0,0005	0,0003	-
H_2	0,0100	-	0,0049

Table 3: Geometric parameters used in the simulation step.

Parameter	Value
Pipeline length L	1000 m 5000 m
Orifice to internal pipeline diameter ratio d/D	0.1 (small puncture) 0.4 (large rupture)



(a)

(b)

Figure 1: Bulk temperature evolution in the rapid depressurization. a- 1000 m pipeline, large rupture; b- 5000 m pipeline, large rupture.

Under large release orifices ($d/D = 0.4$), different behaviours are observed. In small pipelines (Fig. 1a), the dense phase is preserved even with impurities in the CO_2 flow. The overall temperature profile experiences wider variations especially with oxyfuel and pre-combustion derived streams where the amount of impurities is larger. This effect is not only related to varied impurities amount but also to their nature that tends to alter the boiling point of the mixture. Lowest temperature values are observed in the oxyfuel current where the related enhanced mixture density shortens the release duration.

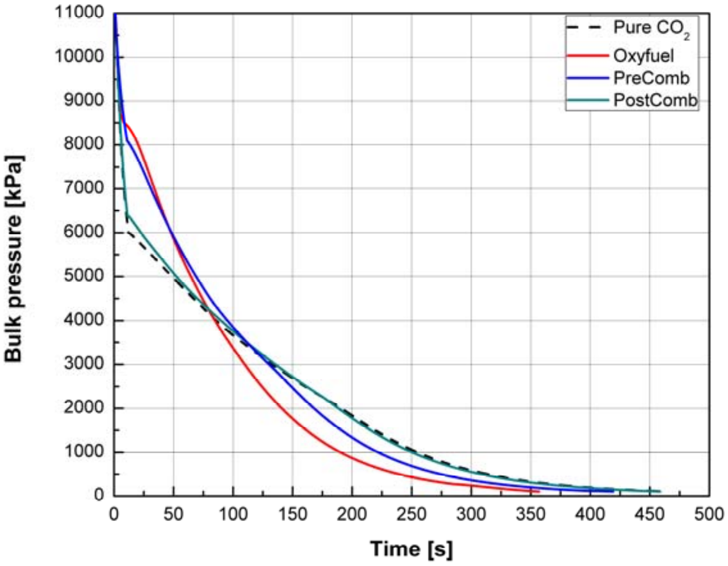


Figure 2: Bulk pipeline pressure evolution. 5000 m pipeline, large rupture.

On the contrary, impurities widely alter the release evolution in longer pipelines. Phase change mechanisms are enhanced with oxyfuel and pre-combustion currents where boiling mechanisms lead to an early depletion of phase change mechanisms in the pipeline bulk (Fig. 2). The final temperature increase is due to a heating mechanism of the gaseous/vaporous phase.

No variations both in a 1000 and 5000 m pipeline sections are observed between the pure CO_2 flow and the outflow process from a post-combustion treatment.

As of Figure 2, impurities alter the onset of boiling mechanisms that are represented by the slope variation in the pressure time profile. Increased amounts of impurities lead to greater onset boiling pressures because of specific interactions between the CO_2 and the other (polar and non-polar) compounds as of the adopted mixing rules in the EoS approach.

Results show that, independently on the impurities amount, the solid-vapor transition (solidification and sublimation) is not affected being very limited quantities involved and that are not highly sensitive to other components.

On a general perspective, modelled time profiles show that the liquid phase enriches in CO_2 with the release evolution up to a molar fraction of 1 that is most of the impurities migrate in the vapor phase because of the vapor-liquid equilibrium.

Main simulations outcomes are listed in Table 4.

Table 4: Impurities effect. Main simulations outcomes.

Parameter	Details
Minimum bulk temperature	Not appreciably affected by impurities.
Temperature evolution	Sensitive to impurities amount. Larger amounts tend to lower the instantaneous pipeline bulk temperature.
Onset of boiling mechanism	Impurities increase the onset pressure and induce steeper pressure decreases.
Solid-vapor transition	Not affected by impurities if limited (applicable to streams from common capture techniques).
Liquid-vapor transition	Liquid phase enrichment in CO_2 till the termination of bulk boiling mechanisms.
Release time	Releases of pure CO_2 are most lasting.

3.2 Effect of the insulation

Insulation with properties listed in Table 1 acts as a modification in the heat transfer process hampering the conductive heat exchange.

Based on the release of pure CO_2, two main distinct simulations are performed under different insulation thickness ($\Psi = 0, \Psi = 2$). Ψ is intended as the ratio between the insulation and the pipeline steel thickness.

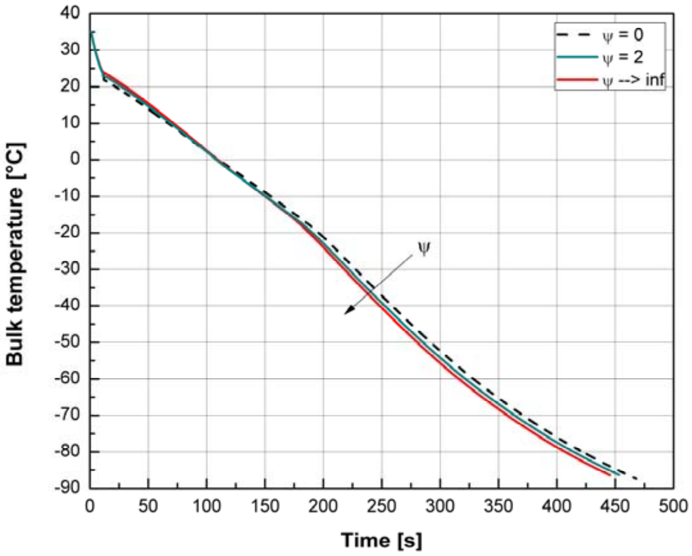


Figure 3: Bulk pipeline temperature evolution. 5000 m pipeline, large rupture. Analysis at different insulation thicknesses (Ψ parameter).

As of Figure 3, an increase in the insulation thickness decrease the instantaneous bulk temperature in the pipeline even if variations are practically irrelevant. The negative variation is due to the enhanced conductive heat transfer resistance induced by a thicker insulation layer. It should be noted that a very large insulation thickness is representative of a limiting condition in the temperature time evolution. This because the conductive resistance in the insulation thickness is minor in determining the total thermal dynamics compared to convective and latent contributions. This is true especially in large releases where the phase change mechanisms are amplified because of larger pressure gradients inside the pipeline.

Under small release holes ($d/D = 0.1$), the influence of the conductive mechanism across the insulation layer is more significant given longer release times and less relevant phase change mechanisms (Mocellin et al., 2018).

In addition, a variation in the conductive resistance to heat flow does not alter the overall degree of reversibility that remains in the range 0.82 (longer pipelines and small orifices) – 0.90 (shorter pipelines and large orifices). The contribution of conductive heat transfer mechanism to the equivalent work is in fact negligible compared to boiling and sublimation mechanisms that are also altered by the presence of impurities (section 3.1).

Main effects of the insulation thickness are summed up in Table 5.

Table 5: Effect of the insulation thickness.

Parameter	Details
Minimum bulk temperature	Not practical variations in minimum bulk temperature. Small holes lengthen the releases evolution and variation within -10 % are observed.
Temperature evolution	No relevant variations in the time dynamics. Phase change mechanisms are mainly governed by pressure gradients rather than heat transfer processes across the insulation.
Onset of boiling mechanism	Unaffected by the insulation thickness.
Release time	No variations are observed given an almost preserved temperature profile.

4. Conclusions

In the perspective of a reliable QRA applied to carbon sequestration infrastructures, a detailed source model was proposed. This work focuses on the effect of impurities in the captured CO_2 streams on main release parameters. The description of their influence was based on reliable thermodynamic models that aim at providing a good description of mutual effects of polar and non-polar compounds on the pure CO_2 release evolution.

The analysis showed that impurities alter many parameters especially linked to the onset and the evolution of boiling mechanisms and the instantaneous temperature profile. In addition, the streams derived from post-combustion capture methods, behave almost comparably to pure CO_2 subjected to a release.

The insulation thickness, instead, has limited effect on the release evolution because the conductive heat resistance is small compared to convective contributions by phase change mechanisms of the CO_2.

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