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Review

Risks and Safety of CO_2 Transport via Pipeline: A Review of Risk Analysis and Modeling Approaches for Accidental Releases

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Abstract: Carbon capture and storage is considered an effective mitigation strategy to reduce the most challenging emissions from heavy industries and gas processing. The safe transport of carbon dioxide via pipelines is an important aspect for developing large-scale Carbon Capture and Storage projects. Dispersion modeling for heavy gas such as carbon dioxide is considerably different from natural gas. The set up for modeling simulations is more challenging than conventional natural gas pipeline for several reasons, such as the differences in thermodynamics that must be considered. Moreover, when the carbon dioxide is transported in dense or liquid phase, the rapid phase changing, and possible consequent formation of solids should be considered. Finally, the equation of state required for accurate prediction of parameters is generally different than the ones applicable for natural gas. The main scope of this comprehensive review is to identify the most important parameters, critical events, suitable models, and identification of dispersion modeling issues. An extensive literature review of experiments conducted in the last ten years has been developed, experimental data, integral and simplified model, as well as CFD modeling issues has been identified and reported in the work proposed to highlight the advances and the gaps that could need further research activities.

Keywords: carbon dioxide; CO_2 transport; CO_2 pipeline; accidental release; experimental modeling; dispersion modeling

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1. Introduction

Climate change is presently a recognized and well-established problem that must be managed globally. The level of greenhouse gases, including CO_2, increased dramatically in recent decades. The level of CO_2 in the atmosphere has overtaken 416 ppm in 2021. Strong climate targets and investments have been planned among all the strategic energy sectors, from building efficiency to the decarbonization of steel and coal plants. According to the International Energy Agency, many strategies have been included to reach net-zero in 2050; according to the International Energy Agency, carbon capture use and storage (CCUS) can contribute up to 9% on a global scenario [1]. Due to its wide range of applications, carbon capture and storage is considered an effective mitigation strategy to reduce the most challenging emission from heavy industries and gas processing. CCUS is deemed a solution for the most challenging emissions, which accounts for 20% of the planet's global emission of CO_2 of the earth. The steel industry, cement, aluminum, and chemical plants are included in these so-called "hard to abate" emissions [2,3]. Since CCUS can be retrofitted to existing technologies, it can present a solution to coal power plants recently constructed to abate the capital expenditure by limiting the emission in the atmosphere. More than 2000 GW of coal-fired capacity are in operation worldwide in 2021, and 167 GW are under construction [2]. The market of hydrogen production is expanding in recent years; in 2021 producing hydrogen from gas and coal-based plants with CCUS is generally less expensive than using renewable energy for water electrolysis. The "blue hydrogen", produced from non-renewable as gas or coal with CO_2 sequestration, is considered a viable strategy during the transition to a green hydrogen-based economy [2,4]. Since the captured CO_2 must be stored in saline aquifers or depleted hydrocarbon reservoirs, there is the necessity to transport it from the capture source to a storage site. In the literature, many studies address the techno-economic aspects [5–11] as well as the safety aspects associated with CO_2 transport [12–18]. In the U.S., CO_2 is transported since the 80s, and there are more than 8000 km of CO_2 pipelines currently in operations, mainly related to the enhanced oil recovery activities [19]. The safe transport of carbon dioxide via pipelines is an important aspect for developing large-scale CCUS projects. CO_2 is usually transported in dense phase or liquid state, in high-pressure pipelines for economic reasons [7,20–24]. Even if tons of CO_2 are transported every day in the U.S., most of the pipelines are located in not densely populated areas [25]. In the near future, CCUS projects, in Europe and other countries, might be developed to cross densely populated areas; an accurate risk assessment is therefore required. Since CO_2 is toxic at certain concentrations, the accidental release of large inventories can pose an asphyxiation risk to human and other biologic life forms that needs to be assessed and prevented or mitigated (i.e., Lake Nyos disaster in 1986 [26,27]). A detailed risk analysis can be required to develop and route a CO_2 pipeline [28,29]. Vianello et al. [30] performed a risk assessment of a CO_2 pipeline network case study in the UK, an heavy gas integral model have been used in the work. The results noted that in proximity of the pipeline network the population can be exposed at serious injuries; however, the authors identified some gaps in the consequence analysis. An accidental release study should be included to determine the safety distances from the pipeline [29]. Mazzoldi et al. [31] investigated with integral models and CFD the safety distances related to CCS projects, the authors highlights that the over estimation provided by Gaussian models can potentially compromise entire project development. Since CO_2 is considerably different from natural gas (i.e., CO_2 density is higher than air density), the most used simplified dispersion models could be not suitable for the correct simulation of the release. To obtain an accurate prediction of CO_2 dispersion behavior, a computational fluid dynamics (CFD) approach could be required for the most challenging scenarios when the topography is complex, and hills are presents. The main scope of the review is to evaluate which tools are suitable for the accurate simulations of CO_2 release; simplified models and CFD models available in the literature and commercially have been considered. A complete review of the main aspects related to release modeling for CO_2 from a pipeline rupture scenario has been analyzed and discussed in this work. Furthermore, to highlights the advances and the gaps that could need further research work, experimental data, integral and simplified model, as well as CFD modeling issues has been identified and reported in the comprehensive review proposed.

2. Risk Analysis for CO_2 Pipelines

The risk management strategy should be based on relevant industry good practice which focuses on inherent safety and the prevention of incidents with the potential to endanger people, the environment, or properties. Compared to natural gas, there are less companies with relevant experience in full-scale CCS projects development and few projects has been completed so far [2]. Thus, great care should be taken during hazard identification and management when dealing with CCS projects. According to DNV-GL [32], carbon dioxide pipelines should be designed with acceptable risk. The growing interests from energy companies in CCS will lead to the development of new generation CO_2 pipeline systems that will require thorough risk assessments and to be design within acceptable risk levels as required by DNV-GL [32]. Since the fluid is usually transported in dense phase, there is the potential for large inventories of CO_2 being released in the atmosphere which could reach populated areas with hazardous concentrations. According to ISO 13623 [33] and DNV-GL-RP-F104 [32], CO_2 is categorized as a category C fluid. However, there is a guidance note stating that it is recommended that CO2 is categorized by category E unless long operational experience exists. This requires higher safety factors in the design.

To properly assess the risk of an installation, it is necessary to evaluate the potential consequence of an accidental release. The complex thermodynamic of the phenomena and the limited experience in handling CO_2 are points of concern that need further investigation for a proper assessment.

In this work, the focus is dedicated to the review of the experimental studies carried out to better understand the behavior of CO_2 and of the possible consequence modeling strategies.

3. Experimental Release Tests for CO_2-Rich Mixtures

3.1. Joint Industry Projects and Research Projects

Experimental release tests can be very expensive and usually are not affordable for small-medium laboratories, especially for large-scale scenarios. Several experimental works have been reported in the literature; these can be classified in large-scale and small scale experiments. Furthermore, the aim of the studies can be considered to be an additional parameter for the categorization. Most of the experimental work analyzed can be divided between far-field and near-field modeling. Studying the behavior and thermodynamics evolution in the near field is typically carried out in small scale set up or laboratory scale. During a release, the monitoring of far-field evolution has been developed in large-scale or full-scale outdoor experiments. Since the costs and infrastructure necessary for a large-scale set up are not easily sustainable by a single research center or university, several Joint Industry Projects (JIP) and Research Projects (RP) have been developed over the years. The most important JIPs and RPs are reported in Table 1 with the associated period, scale, and objectives.

Table 1. Relevant CO_2 pipeline related JIPs and RPs programs during the years.

JIP/RP Name	Years/Period	Scale	Objectives and Scope
CO2SAFEARREST	2016–2019	Full-scale	Burst tests research program. Two full-scale tests with buried pipeline (CO_2-N_2 mixture), 24 inches.
COSHER	2011–2015	Large-Scale	Obtain data to support the development of models to determine safety zones/consequence distances.
CO2PIPETRANS	2009–2015	Medium-Scale Large-Scale	Fill the knowledge gap identified in the DNV-RP-J202. Results of the project were included in DNVGL-RP-F104 (2017).
COOLTRANS	2011–2015	Large-Scale	Identify and propose solutions to key issues relating to the safe routing, design, construction and operation of onshore CO_2 pipelines in the UK.
CO2PIPEHAZ	2009–2013	Small Scale Large-Scale	Improve the understanding of the hazards represented by CO_2 releases.
CO2QUEST	2013–2016	Small Scale Medium-Scale	Study the impact of the quality of CO_2 on storage and transport.
CATO	2004–2008 2010–2014 2015-ongoing	N/A	A national program, which includes complete studies in all aspects of CCS.
CO2EUROPIPE	2009–2011	N/A	Outline guidance to elements of the European plan to develop large-scale EU CO_2 infrastructure.
CO2RISKMAN	2010–2013	N/A	Development of industry guideline to assist the designer and projects on the emerging CCS industry. Potential hazards associated with handling CCS CO_2 streams are discussed.

CO2SAFEARREST was a full-scale burst tests research program for carbon dioxide pipelines. The project involved two full-scale burst tests of 24 inches, X65 buried line pipes using a mixture of carbon dioxide and nitrogen. The COSHER project included large-scale experiments to provide release and dispersion data from the full-bore rupture of a CO_2 dense phase underground pipeline. A total of 13 partners were involved. The project's main objective was to obtain data to support the development of models for the determination of safety zones/consequence distances. A series of release test from high-pressure CO_2 pipelines were performed in 2013. In particular, the areas of specific interest were CO_2 behavior after release from high-pressure pipelines, the atmospheric dispersion of the CO_2 and the cooling on the pipeline wall due to depressurization. The project CO2PIPETRANS was divided into two phases. Several significant knowledge gaps were identified in phase 1, which resulted in the publication of DNV-RP-J202. Phase 2 of the project aimed at filling these knowledge gaps through experimental research; the results have been included in DNVGL-RP-F104 (2017). Fourteen partners in total participated in the project. The data collected during the two programs of medium-scale CO_2 release experiments previously managed by BP and Shell were made publicly available by the JIP.

COOLTRANS was a research and development project which aimed at identifying, addressing and resolving key issues related to onshore pipelines transporting dense phase CO_2 in the United Kingdom (UK). Main aspects from secure routing to construction have been addressed. A series of large-scale pipeline accidental release experiments and modeling have been included in the research program. Several experiments to evaluate the ecological impact of CO_2 emissions from pipelines, development of a new risk assessment framework and public consultation have been included. A total of 11 partners were involved in this project, the small scale experimental tests were conducted by Nottingham University and Leeds University, while large-scale tests were performed by GL Noble Denton (now DNV).

CO2PIPEHAZ was a European Program involving experts from the UK, China, and European countries to develop and test mathematical models to establish the safety of CO_2 pipelines. Small- and large-scale experiments to validate the models were carried out to improve the understanding of the hazards represented by CO_2 releases. A total of seven partners were involved; the experimental tests were conducted by INERIS (FR) and University College London (UK), and Dalian University of Technology (China).

The CO2QUEST project was coordinated by the University College of London and involved the participation of 12 partners. The main objective was to study the impact of the quality of CO_2 on storage and transport. Small and medium-scale experiments were performed by INERIS (FR) from high-pressure pipelines with a range of impurities. Large-scale controlled experiments were developed by Dalian University of Technology (DUT), in China.

The CATO program is the research program ongoing in the Netherlands. The acronym stands for CO_2 capture, transport and storage in Dutch. The third phase of CATO started at the end of 2014. The publications are included in several planned CCUS projects in the Port of Rotterdam, including the Porthos project [2].

The project CO2EUROPIPE was a European project with the objective to outline recommended practice in order to develop a large-scale European CO_2 infrastructure. In particular, the description of the infrastructure required for large-scale transport of CO_2, including injection facilities and the possibility to re-use of available infrastructure for the transport of natural gas.

Finally, the CO2RISKMAN project, initiated and led by DNV, aims to develop an industry guidance that provides useful references to assist the CCUS industry. The most common issues management as well as potential hazards associated with handling CO_2 streams are discussed. A total of 17 partners contribute to the development of the guidelines. The guidance is composed of four documents with a bottom-up simplification structure where the most detailed document is located at the bottom, while the executive summary is on top. The project did not include experimental activities; thus, considerations on risks and safety management are relevant to the overall accidental release testing and mitigation.

3.2. Experimental Testing

A literature review of the most important experimental studies related to CO_2 release and dispersion is reported. Particular attention has been paid to large-scale tests for accuracy and readiness to develop validation and comparison studies by reducing the scale-up errors compared to operating pipelines. To highlight the main aspects related to a CO_2 release, a schematic diagram has been reported in Figure 1. The release can be divided in near-field (phase change, expansion, air-mixing and solid formation) and far-field zone, where the atmospheric dispersion of the heavy CO_2 cloud continues at large distances start.

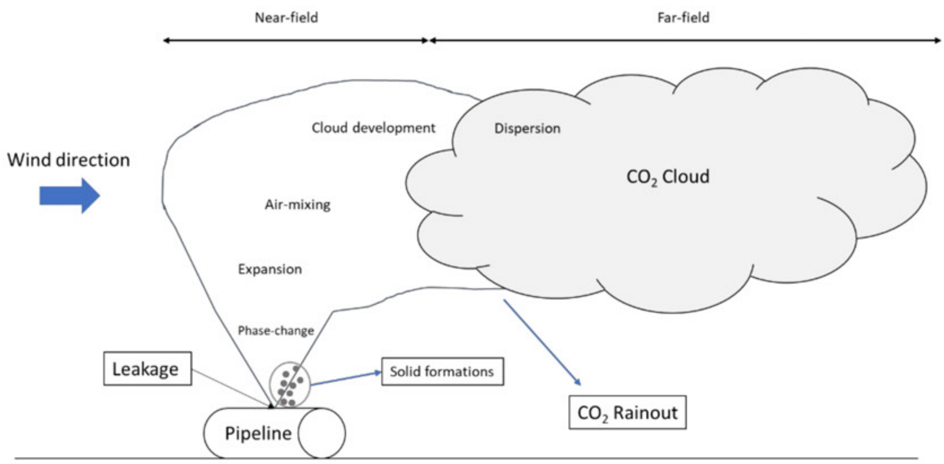

Figure 1. Schematization of a CO_2 release from an onshore pipeline.

The analysis focused first on near-field experiments that highlighted important release aspects. Since near-field modeling can strongly impact the far-field modeling and the definition of safety distances, particular attention should be reserved to these aspects. Pursell [34] presented some results from laboratory scale release tests performed in Health and Safety Laboratory (UK). The experiments were performed both for liquid and gas phase of CO_2 from release orifices of 2 and 4 mm (diameter), the set up was connected to a pressurized vessel containing CO_2 at pressure from 40 to 55 barg. The rapid expansion of the fluid downstream the orifice occurs approx. following an isenthalpic expansion to atmospheric pressure, then the CO_2 jet continues to expand as it entrains and mixes with the surrounding air. A schematization of the expansion zone downstream of the orifice is reported in Figure 2.

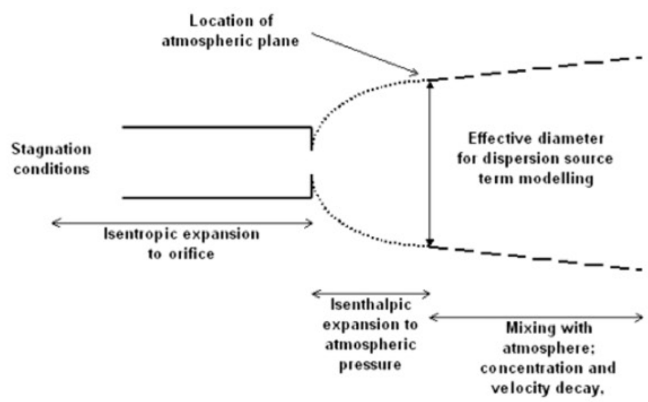

Figure 2. Schematic diagram of the expansion zone (Reproduced from Pursell [34]).

Useful data were obtained by analyzing the images, such as the length of the expansion zone and the effective diameter of the jet at the point where it reaches atmospheric pressure. Since it is not easy to define the location of the shock front in liquid releases, the effective diameter could be useful for dispersion calculations (assuming a gas phase equivalent diameter) since it is often used to define the size of the pseudo-source. Results showed that liquid releases led to an effective diameter up to 30% larger than the corresponding gas phase in the diameter of the analyzed orifice. Guo et al. [35] studied the near-field characteristics and dispersion behaviour of supercritical [36], gaseous, and dense-phase CO_2 experimentally. A large-scale pipeline set up with an internal diameter of 233 mm and a total length of 258 m was constructed during the CO2QUEST project. Six tests have been performed, and several orifice diameters have been tested from 15 mm to full-bore rupture. The near-field behavior and the under-expanded jet flow structure have been analyzed; solid phase formation was observed. The sublimation of solid CO_2 removes heat from the gas phase with a consequent temperature reduction. The formation of solid CO_2 can impact the properties and the shape of the cloud. Based on the experimental data performed by Guo et al. [35], the development of the visible cloud can be divided into three stages: a "rapid expansion", a "metastable stage", and a "slow attenuation *stage*". The distance of the 50,000 ppm concentration contour for three orifice diameters was determined in all the experiments. The maximum safety distance of 160 m has been measured for the full-bore rupture at the initial condition of 9.1 Mpa at 21.6 °C (dense phase). Safety distances measured for dense phase were consistently greater than gas phase tests.

An experimental study of supercritical CO_2 leakage has been reported by Fan et al. [37]. The pressure and temperature conditions analyzed varied from 81 to 110 bar and 34.9 °C to 100.9 °C. The authors noted how the mass flow rate decreases with the increase of upstream temperature and length-diameter ratio and increases with the increase of upstream pressure. However, the effect of upstream temperature variation (at approx. 100 bar) on the jet structure was not so evident in the range between 37.6 °C and 40.1 °C.

An experiment with various measurement methods was developed by Teng et al. [38] to carry out controllable CO_2 release from a high-pressure vessel. Pure liquid CO_2 has been used for the experiments, orifice diameter of 1 and 2 mm. Initial pressure varies from 80 bar to 100 bar, while temperature from 301 K to 313 K. The lowest temperatures measured were −41.9 °C (1 mm diameter) and −45 °C (2 mm diameter). The maximum velocity along the jet centreline was 250 m/s. The results suggest that for a supercritical CO_2 leakage, dry ice particles with size between 1 and 3 µm can be formed. The initial temperature shows limited impact on the size of dry ice particles, while a wider size distribution can be addressed to a higher initial pressure. Li et al. [39] developed a reduced scale facility with dry super-critical CO_2 to analyse the jet plume's early stage flow characteristics in the near-field. Initial pressure was set up to 8.02 Mpa; the velocity in the centreline of jet plume was measured from different leakage sizes (0.5, 1, 3, 5 mm), showing a correlation with the depressurization process during the leakage.

Ahmad [40] reported the results based on COSHER JIP; a large-scale rupture test was conducted on a loop test built in Spadeadam (UK). A 219 mm diameter pipeline buried underground filled with dense phase CO_2 has been used. Temperature, pressure, concentration distribution and dispersion cloud have been considered with low wind conditions 1.9 m/s. Approximately 136 ton of CO_2 were released in 204 s. The maximum height of the plume was registered at 60 m from the ground while the maximum horizontal extension at 400 m, the minimum temperature registered during the release was −78 °C. The test has been conducted at approx. 150 bar and the average temperature of the fluid in the reservoir was around 13 °C. In Figure 3 the visible cloud formed after the rupture is reported at subsequent times; images have been captured from a video.

Figure 3. The visible cloud behavior after the rupture; from left to right, at 10, 30 and 120 s from the break (This figures were published from *International Journal of Greenhouse Gas Control*, Ahmad et al. [40], Copyright Elsevier, 2015).

In 2017, other tests were carried out in Spadeadam (UK); two full-scale burst tests were performed during CO2SafeArrest JIP to evaluate the fracture propagation and arrest characteristics and CO_2 dispersion in the atmosphere [41,42]. The outer diameter of the test section was a steel pipe 610 mm, 85 m long, connected to approx. 120 m long reservoirs at both ends. A mixture of 91% CO_2 and N_2 pressurized to about 15 MPa was adopted. The pipeline rupture was induced by initiating the crack with explosives; several sensors (temperature, pressure, oxygen cells) have been positioned over a pattern terrain in the vicinity of the crack. Two burst tests have been conducted; for the first test, all the pipe test section was buried under a 1 m deep soil cover, while in the second test, only half the length of the pipe test section was buried. The resulting crack propagated in both directions as the pipe wall was torn open sideways. The CO_2 cloud reached an altitude peak of 250 m, as well as the debris thrown out of the crater formed. As reported in the schematization of Figure 4, the crater extension measured approx. 45 m in the horizontal (pipe direction) while the perpendicular extension varied between 5.8 m and 9 m. The average width of the crater is about 7.4 m, which is 12 times of the outer pipe diameter.

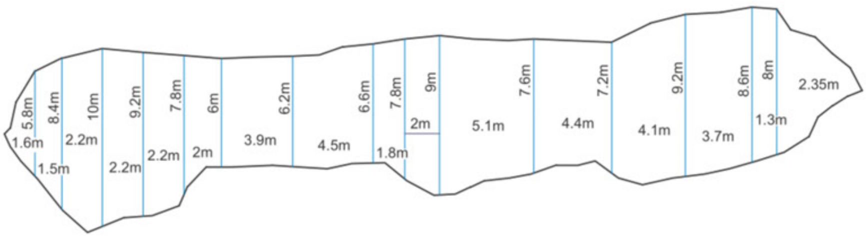

Figure 4. Crater outline and length measured after the rupture test (This figure was published from *Applied Energy*, Liu et al. [42], Copyright: Elsevier, 2019).

In the work of Allason et al. [43], the COOLTRANS experimental campaign has been described and some considerations are reported. During the program, vertical pipe venting and puncture tests have been performed.

In the venting experiments no rain out of solid CO_2 was observed and the plume dispersed upward and reached the ground some distance away downstream of the release but a low concentration. The pressure along the pipeline was observed to be relatively constant and there is an indication that some solid CO_2 could form during vent operations. The experimental set up for the puncture experiments consisted of 914 mm outer diameter pipeline buried 1.2 m below ground and supplied with dense phase CO_2. The puncture experiments have shown that the nature of the surrounding soil can impact the nature of the flow into the atmosphere. The flow from the punctures was observed to stall in the atmosphere above the source and, in low wind speed conditions, a 'blanket' was observed to form around and over the source. Moreover, the results from the puncture tests show that the random variations in wind direction and turbulent fluctuations within the plume, combined with the high toxicity index for CO_2, lead to differences in the calculated integrated dose.

Guo et al. [44] studied experimentally the dispersion of CO_2 during vertical leakage (15 mm diameter orifice). Gas phase, dense phase and supercritical have been considered in the study. A large-scale pipeline with internal diameter and length were 233 mm and 258 m, was constructed. The instantaneous pressure reduction at rupture was accompanied by a sharp temperature drop provoking a phase change. Test 2 (9 Mpa-19.9 °C) show the formation of dry ice particles at the bottom of the pipeline. In Test 3 (8.4 Mpa-35.7 °C), the supercritical CO_2 transformed into the gas-liquid phase when the pressure dropped to critical pressure. During the vertical release, three phases have been identified: rapid expansion, sedimentation, and slow attenuation stages. The fluid transformed rapidly into a gas-liquid mixture and then to gas-liquid-solid phases for the dense phase test depressurization as the pressure fell below triple point pressure. Moreover, in the dense phase test, CO_2 more easily formed a high concentration cloud at ground level.

The experimental testing campaign review clearly highlights the differences between the management of a natural gas release and a dense phase CO_2 release. The high CO_2 density and the dry ice formation are two of the main points that should be analyzed carefully and can become challenging in the modeling phase. The rapid depressurization and the phase changing from liquid to gas is also a point of concern that will require a dedicated modeling approach that is substantially different from natural gas. As with natural gas the crater formation and the height reached from the CO_2 cloud can impact the safety distance required, thus should be modeled accurately.

4. Modeling CO_2 Accidental Releases

Modeling a release of a CO_2 pipeline requires the assessment of some important aspects, such as transient conditions, multi-phase jet, as well as the dispersion behavior. A rapid pressure drop will follow the release of CO2 from a pipeline; the pressure and temperature reduction a phase transition from liquid-vapor is expected. Moreover, for lower temperature the formation of solids is also a possibility. The phase transition can impact the flow conditions within the pipeline and the properties of the fluid. The precise simulation of transient depressurization, with regards of flow rate and thermodynamic properties of CO_2 during the release, will impact the accuracy of the cloud dispersion prediction. Specific focus must be reserved to phase transition and density prediction of the CO_2 during transient operations in order to better predict solid formations. Release and dispersion studies are required for risk evaluations. Three main steps can be identified in dispersion modeling:

- Outflow calculations
- Expansion to atmospheric pressure (near-field)
- Far-field dispersion

Some specific difficulties for modeling CO_2 releases can be highlighted, which may constitute a limitation in developing accurate simulations, in particular: the selection of an Equation of State for an accurate description of the thermodynamic properties throughout the release process, the modeling of phase changing (from dense phase to gaseous), prediction of solid phase formation, the validity of homogeneous equilibrium (HEM) assumption. Another aspect to be considered is the very limited experience in CO_2 pipeline modeling; for this reason, most codes and simplified models need to be assessed and validated with experimental tests data. Two main approaches are available to model an accidental release:

- Simplified models
- CFD models

The simplified models usually require very low CPU usage compared to CFD models; hence they are faster and optimized for risk analysis. However, a simplified model, such as an integral model, is based on several assumptions and simplifications to the physics of the phenomena; for these reasons they need to be extensively validated with real case data, experimental tests. CFD models can provide a very detailed description of the physics and the behavior of a CO_2 release; this kind of approach is required when a complex topography, specific environment conditions or presence of buildings or other obstructions in the nearby area. These models require high experience and specific knowledge from the user to be set up and executed, compared to simplified integral models. Moreover, the uncertainties specific to CO_2 related to limited experience and optimization often require custom-made inputs and user-defined functions to be implemented in commercial CFD software. The flowchart reported in Figure 5 represents a modeling strategy based on the one proposed by Woolley et al. [45] about the needs to create a link between the near-field and the far-field modeling. Moreover, the thermodynamic modeling of the main properties from the flow models needs to be inputted correctly during the near-field model.

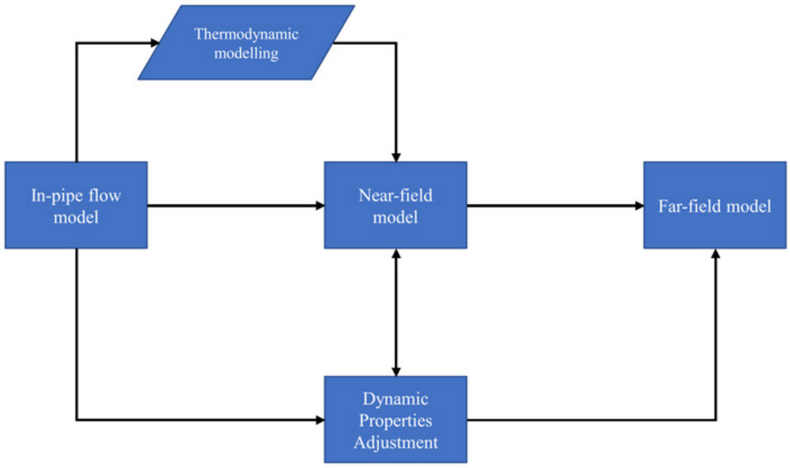

Figure 5. Integrated thermo-physical modeling strategy.

4.1. Simplified Models

The most commonly available simplified models are the integral models implemented in existing commercially available software. The most relevant studies related to CO_2 modeling through integral models have been reported. Since most risks in the oil and gas industry come from flammable liquids or gases, none of them was originally designed to take into account inert gas such as CO_2. The main models identified during the literature review are:

- FRED
- PHAST
- ALOHA
- EFFECTS

FRED is an integral model developed from Shell, it adopts a semi-empirical jet model for the first part of the release and a similarity model for the dense gas dispersion. FRED assumes the homogeneous equilibrium model (HEM) between the CO_2 phases. The dispersion of CO_2 is calculated through the model AEROPLUME, the model HEGADAS can be then invoked for develop the simulation starting from AEROPLUME results. It should be noted that AEROPLUME is intended to predict the near-source behavior. Then, far from the source, the dispersion is better modeled by a far-field model. For this purpose, either HEGADAS or another model PGPLUME are invoked to finish the calculations. Indeed, Shell program HEGADAS is a dense gas model specifically developed to account for the restricted mixing of dense gas clouds [46–48].

PHAST (by DNV) is a hazard assessment software package for modeling atmospheric releases of flammable or toxic chemicals. The Unified Dispersion Model (UDM) included in PHAST, can simulate unpressurized and pressurized releases, time-dependent releases, complex thermodynamic behavior and different atmospheric conditions. The HEM is used for the two-phase flow jet. Finally, solid particles deposition on the ground is not considered in version 6.7 [49].

The Gaussian model ALOHA can handle several hazardous scenarios such as toxic gas dispersion, fires, and explosions. The aerial dispersion model included in ALOHA can estimate the movement and dispersion of chemical gas clouds; both the Gaussian and heavy gas model are also available. The Gaussian model is used for the dispersion prediction for gases which buoyancy is close to air, namely the gases that have the same density as air [50]. The heavy gas dispersion calculations implemented in ALOHA are based on those used in the DEGADIS model [51].

The simplified model EFFECTS contains a series of models from the Yellow Book [52] that allows detailed modeling and quantitative assessment of gas releases, liquid or pressurized liquefied gas, two-phase, and spray release. The model applied for the gas release from a long pipeline (Wilson model) is suitable for total rupture of a long gas pipeline. Heavy gas dispersion models are available for rapid gas release, pool evaporation, horizontal or vertical jet. Liquefied gas from long pipeline is modeled with the "Morrow model". The model can be used to calculate the behavior of expanding pressurized liquid in a pipeline after a rupture [53].

To investigate the capability of the simplified models reported, identify the weakness and the most suitable models for carbon dioxide modeling, importance has been reserved to validation and comparison studies. Several studies related to CO_2 accidental release modeling have been conducted. Comparison between experimental data and integral models is considered more relevant; however, the comparison with CFD models has also been considered.

Dixon et al. [46] compared the integral model FRED with two CFD models (OpenFOAM and ANSYS-CFX) and experimental data. The horizontal releases tests conducted by Shell at Spadeadam (UK) test facility were considered (orifice diameter up to 25.4 mm). The thermodynamics library employed by FRED usually cannot account for solid CO_2, the liquid-vapor saturation line was instead derived to atm. pressure. The concentration and plume width predicted from the FRED model produced slightly better agreement with the data than both CFD models. Despite the prediction of solid particles, the FRED model overall reproduced well the hazard distances. Mazzoldi et al. [54] performed a comparison against experimental data reported by Hanna et al. [55] with the Gaussian model ALOHA and presented an evaluation of the atmospheric dispersion CFD tool Fluidyn-PANACHE. The author noted that for CO_2, the application of threat zones modeled with Gaussian methods to population densities were over-conservative.

Hazards identification resulting from releases of high-pressure CO_2 was also part of the review performed from HSL [56]. According to the authors, to overcome the high computational costs, a practical alternative could be the creation of a statistical model of the results based on many consequence model calculations results. A hundred PHAST simulations performed with PHAST have been used to run a sensitivity analysis with a Gaussian emulator. The releases consisted of above ground, steady-state horizontal, diameter from 12.7 to 50.8 mm of dense phase CO_2 (100–150 bar, approx. at ambient temperature). A Bayesian analysis has been performed rapidly using PHAST outputs. In the analysis of Gant et al. [49] developed with PHAST, seven model inputs have been considered to highlight the most sensitive parameter during the modeling scenario for CO_2 releases. These scenarios were mainly relevant, in scale, to leaks from large diameter onshore vessels or non-buried pipes. The main factor that have been varied for the sensitivity analysis were the temperature and pressure, the wind speed, the outer diameter and humidity. In the range evaluated (pressure range within 100 and 150 bar), the greatest influence on the dispersion distance can be addressed to release point height and orifice diameter.

Simulation results from an integral model and two different CFD models have been compared to data experiments conducted by INERIS [57]. The integral model PHAST adopted produced similar results to the ANSYS-CFX model, particularly the centerline temperatures were under-predicted by up to 20 °C, while an over-prediction of the centerline concentrations by up to 8% v/v has been registered. Witlox et al. [58] performed a validation of the experimental data from CO2PIPETRANS with the consequence-modelling package included in PHAST 6.7. The results from the tests performed by BP and Shell during the JIP between 2006 and 2010 have been considered for high-pressure releases. A total of nine tests from BP and eight tests from Shell have been considered for the validation procedure. Several orifice diameters from 6.3 mm to 25.62 mm are reported for the validation; the minimum release duration of 40 s was registered for the biggest orifice, namely 25.62 mm, while a maximum release duration >700 s for the 6.3 mm orifice diameter. Two different models available in PHAST have been used for the simulation of steady-state liquid release (DISK model) and time-varying releases (TVDI model). The metastable assumption was not implemented first, but flashing was allowed in correspondence to the orifice; to have more precise concentrations prediction, conservation of momentum was considered for the expansion from orifice. The global accuracy of PHAST in the near-field was not affected by wind direction deviation, while the far-field accuracy has been impacted. Compared to British Petrol (BP) data, in the near field, the averaged concentration output from PHAST seems to match with good accuracy. A larger effect of averaging was observed downstream (at 20 m and 40 m) with more deviation compared to experimental data. Generally, the estimation provided by PHAST resulted conservative in terms of averaged concentrations. Shell experiments results were generally under-predicted by PHAST. However, a better accuracy for the steady-state has been registered if compared with BP experimental data. For time-varying releases, the Peng-Robinson EOS produces the most accurate results, especially for the flow rate predictions since the equation provides accurate density values.

According to the results, the PHAST discharge and dispersion models predicted the release rates and concentrations accurately. The EFFECTS model was used in some works [15,59] to estimate the dispersion from a CO_2 pipeline. EFFECTS models are sensitive to initial pressure, temperature, composition and orifice size [52]. Due to the different models included, such model seems well suited to modeling CO_2 releases. However, no publicly available detailed validation with CO_2 release experimental tests has been found in this literature review.

4.2. CFD Models

The most relevant studies related to CO_2 modeling with CFD have been reported. Specific attention has been reserved to commercially available software and their capability to handle CO_2 releases. The main CFD codes identified during the literature review are:

- ANSYS FLUENT
- ANSYS-CFX
- FLACS
- OpenFOAM
- FLUIDYN PANACHE

To have an understanding of the main weaknesses and identify the most suitable models, great attention has been given to validation and comparison studies. Validation against experimental data are considered fundamental; however, comparison with other CFD models has been taken into account too. Considering that due to computational costs it is not feasible to model the entire phenomenon (from outflow to far-field dispersion) in a single simulation, each study focused either on the outflow and near field or on the far field; some publications presented an integrated approach in subsequent steps. The integration of near-field and far-field models is complex and time consuming, thus it is considered feasible only for specific situations. The work of Fiates et al. [60] focused on the customization of a computational tool for handling gas dispersion of heavy gases, such as LNG and CO_2. The hybrid switch model (HSM) addresses the deficiencies of the HEM approach when applied to CO_2 releases and considers equilibrium, non-equilibrium, solid formation and phase change. The model has been implemented in OpenFOAM. Experimental tests of British Petroleum and Shell reported by Witlox et al. [61] were used to validate the HSM to estimate the discharge leak rate and properties. A comparison with HEM and frozen model shows the better results of the new model.

During CO2SafeArrest JIP, full-scale burst tests of CO_2 pipeline were performed in 2017–2018. Godbole et al. [41] described the numerical and experimental investigation of the dispersion of CO_2 in the atmosphere following its release in the burst tests. The maximum CO_2 concentration was reasonably well predicted in the simulations done with CFX. The time of arrival of the CO_2 cloud was overestimated compared to measurements, especially at more distant locations. This could be due to the impact of average wind speed assumed in the simulations.

More recently, Liu et al. [42] performed numerical simulations of CO_2 release from a full-scale pipeline. ANSYS Fluent was used for CFD simulation of the release, the species transport model was employed to predict the fraction of each species and the turbulence was modeled with the k-ω SST model. The authors highlight that the wind direction as well as the pipe orientation, can affect the calculated consequence distance especially for high speed wind conditions. The major consequence distance (more than 1500 m) calculated for 50,000 ppm envelope was reached from an 800 mm (ID) at wind speed of 10 km/h. In general, it was observed that the consequence distance increases with the wind speed; however, for large releases, even at lower wind speed it can reach long distances. Another experiment (Wen et al. [62]) was used to compare the dispersion process. The analysis indicates good agreement with experimental data. However, the author recommended further investigating the influence of the atmospheric boundary layer.

Mack et al. [63] presented CFD calculation of heavy gas dispersion based on experimental results and extrapolated them to a representative full-bore rupture scenario of a CO_2 pipeline. Several full-scale CO_2 pipeline release scenarios have been simulated, including a representative terrain topology. The OpenFOAM software, 7×10^5 nodes, k-ε turbulence model has been used to simulate a pipeline rupture scenario in a representative terrain of 2.4×2.4 km. From the results presented, it is clear how terrain plays a significant role at lower wind speeds. According to author, large CFD modeling becomes fundamental especially in the vicinity of depression because it can overcome the limitations of simple models.

Liu B. et al. [64] performed several simulations with ANSYS FLUENT to investigate the effect of CO_2 dispersion over two different topographies: a flat terrain with an axisymmetric hill and a simplified model of an urban area with buildings. The approach has been validated through an experimental scaled model in a partially enclosed box-shaped space. According to the results, the CFD model slightly underestimated the CO_2 concentration in the near-field region close to the source. In the hilly terrain case, CO_2 tends to disperse around the hill, while in the urban scenario, most of the CO_2 was trapped in the street downwind of the source with less significant lateral spread.

The work presented by Gant et al. [57] tested the ANSYS-CFX and FLACS codes to model far-field CO_2 dispersion employing the same source conditions for the CO_2 jet. A Lagrangian particle-tracking model was used in CFX code, heat transfer between the gaseous phase and dry ice was simulated using the Ranze-Marshall correlation, while the k-ω SST turbulence model has been selected. In FLACS, a two-phase RANS with Lagrangian method has been used, the standard k-ε model for turbulence and a cartesian grid was adopted. The CFX code was sensitive to the source condition, while FLACS was sensitive to solid CO_2 particle size. Liu et al. [65] presented a CFD model to predict the atmospheric dispersion of CO_2 over complex terrains. ANSYS Fluent was used to carry out the simulations. Based on the RANS approach, turbulence was modeled using the k-ε model. The wind velocity profile was described through an atmospheric boundary layer (ABL) using a power-law correlation. Mazzoldi et al. [66] performed dispersion simulations with the CFD code Fluidyn-PANACHE, the Peng-Robinson EOS has been used together with a k-ε approach for the turbulence. The author noted how the version of the software (4.0724) could not account for the presence of a solid phase within a gas flow. Liu et al. [67] presented a two-stage CFD model using real gas EOS developed in ANSYS FLUENT. A standard RANS approach while a User-Defined Real Gas Model for CO_2 properties has been created following Peng-Robinson EOS. Both k-ε and k-ω SST models for turbulence have been evaluated and compared with acceptable results; the k-ω SST model was employed in the work.

A more complex approach is the integrated approach described by Woolley et al. [45] that couples the near-field modeling with the far field. As described in Figure 5, this approach can be adopted in order to obtain a higher level of accuracy if compared with conventional modeling strategies. The integration of output from the near-field model as input for the far field model will also require some adjustment of the most relevant thermodynamic properties. The disadvantages of this approach are the CPU requirements as well as the complexity of the thermodynamic calculations involved. Few examples are available in the literature of successful applications of this modeling strategy.

The near-field multi-phase modeling of a CO_2 release has been reported by Woolley et al. [68]. A second-order accurate upwind finite volume solution scheme and the k-ε model for turbulence were employed while the properties have been derived from a composite EOS. The gas phase properties were calculated with the Peng–Robinson EOS, while the dense phase and saturation pressure were derived from tabular data generated with the Span and Wagner EOS. An adaptive finite volume grid algorithm has been applied with 3D rectangular mesh and the homogeneous relaxation model (HRM) has been implemented to consider the delay in vaporization during the decompression process. Far-field dispersion modeling was undertaken using two different CFD codes, namely FLACS and ANSYS-CFX, in both cases the Eularian-Lagrangian formulation was used. The input for the far-field calculation is derived from the near-field simulation. In CFX, heat transfer between gas and solid phases was modeled using the Ranz–Marshall correlation while turbulence effects were simulated with the k-ω SST formulation. In FLACS, two-phase CO_2 dispersion are modeled using an Euler–Lagrangian method; a RANS approach was employed, while turbulence is modeled using a standard k-ε model. Particle deposition and interaction with obstacles was modeled, while collisions, breakup and coalescence between particles have been neglected. A two-phase gas-solid CO_2 stream was considered at the crater outlet. FLACS and ANSYS-CFX have been applied also for dispersion calculations in realistic terrain. A domain size of 10 km × 5 km with a height of 1 km has been considered in the FLACS simulation, accounting 2.7 million nodes thanks to multi-block Cartesian mesh. Same terrain modeling required more than three million nodes in CFX for a very smaller area even with an unstructured mesh. All the particles sublimated in the air in the simulations performed with CFX due to smaller size of particles assumed (20 µm), on the other hand the larger particles diameter adopted in the FLACS (300 µm) simulations led to some solid CO_2 rain out to the terrain. The results suggest that banks of solid could formed with particle size in the order of 300 µm or larger. Near-field and far-field models have been coupled with the thermophysical property with an integrate approach. The resources required were found to be significant (weeks) in terms of computing time.

5. Discussion

In the previous sections, the most common and commercially available simplified models and CFD models have been analyzed. Comparison based on a literature review of experimental and numerical works has been included. The most relevant and detailed data were referred to the validation performed with PHAST and FRED packages. Some works reported using the Gaussian model ALOHA; however, this is deemed unsuitable due to the considerable over-prediction. Some work addressed the use of EFFECTS, but no validation data have been reported so far. Based on the literature analyzed, the commercial software available that include the possibility to account for solid CO_2 formation and several source terms are PHAST and FRED.

Moreover, PHAST and FRED have been compared with large-scale CO_2 release experiments (Shell and BP data included in CO2PIPETRANS). According to recent research and development reports, good performance for both FRED and PHAST have been reported. The results presented a good agreement in concentration prediction and temperature over distances, for both PHAST and FRED, compared with experimental tests. Thus, these integral models are suggested when the topography does not present significant complexity or great variations.

During the review of CFD models, specific importance has been given to the works that included a validation between experimental tests and simulations. A total of five commercially available codes have been reviewed as described in the previous sections. The overall CFD codes review for CO_2 modeling was divided between the near-field analysis and the far-field dispersion. In most works, a RANS approach with an Eulerian-Lagrangian formulation was adopted, with the k-ε turbulence model. In some cases, the k-ω SST has been preferred. Particle-tracking methods to account for solid phase formation were proposed by some authors with considerable computational efforts. Good results have been obtained for the three-phase simulation, even if this strategy is not easy to implement and manage for standard users. The particles size of CO_2 is an important input; a comparative study reported a complete sublimation of the particles in the air in the simulations performed with CFX (20 μm), while the larger particles diameter adopted in the FLACS simulations (300 μm) led to some solid CO_2 rain out.

6. Conclusions

This review underlined the need to approach the near-field modeling and the far-field modeling in two separate ways. The near-field modeling of a CO_2 release requires specific knowledge of the gas-dynamic phenomena in sonic and supersonic transitions, namely Mach number, wave motion, and sonic speed. The CFD code that performed better when compared to experimental tests was ANSYS-CFX. The importance of customizable input properties, such as implementing a specific equation of state or a lookup table, should not be underestimated to capture the near-field phenomenon correctly. Better results have been reported when the fluid data were supplied to the CFD code from a stable and acknowledged EOS. Thus, the CFX code performed better than the FLUENT package, both included in the ANSYS Workbench suite since it can easily accept real gas properties (RGP) tables as input data compared to FLUENT.

The far-field modeling should be treated as a separate problem, starting from the results of a near-field simulation or experimental tests at the desired conditions. Even though simulating the entire phase transition is theoretically feasible, in practice, it is hard to simulate with a single CFD code, with issues mainly related to time steps and grid refinement. Every code reported in the literature can potentially be adopted to model the far-field dispersion; however, some differences can be outlined. The unstructured hexahedrons mesh available by default in the ANSYS packages seems more suitable for specific cases when obstacles and hilly terrain need to be modeled. On the other hand, a Cartesian mesh, as the one available in FLACS, considerably reduces the number of cells required for far-field dispersion simulations, hence should be preferred when the details of the behavior near surfaces are not needed as an output.

Finally, the terrain effects can be dominant for CO_2 dispersion; for this reason, CFD modeling, especially in the vicinity of depression or large differences in terrain heights close to a CO_2 pipeline route, can overcome the limitations of simple models such as integral models.

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