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A New Straightforward Darcy-Scale Compositional Solver in OpenFOAM for CO_2/Water Mutual Solubility in CO_2 Storage Processes in Aquifers

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Abstract: Advancing the modeling of evaporation and salt precipitation is essential in CO_2 storage processes in aquifers. OpenFOAM provides a platform for computational fluid dynamics (CFD) modeling with its open-source C++ object-oriented architecture that can especially be used in the development of fluid flow models in porous media. Some OpenFOAM packages have been developed in this area, and their codes are available for use. Despite this, the existing OpenFOAM literature does not include a model that incorporates multicomponent interactions in multi-phase flow systems, referred to as compositional modeling, at the Darcy scale. This existing gap is addressed in this paper, where a new simple model in OpenFOAM is introduced that aims to model the interaction of CO_2 and H_2O components in CO_2 storage processes in aquifers at the Darcy scale. The model, named compositionalIGFoam, incorporates a compositional solver by extending the impesFoam solver of the porousMultiphaseFoam package, while assuming some simplifications, to account for CO_2/water mutual dissolution, relevant to carbon capture and storage (CCS) processes in aquifers. The functionality of the compositionalIGFoam solver was assessed by showcasing its ability to reproduce the outcomes of existing examples. In addition to that, the process of gas injection into a water-saturated core sample was simulated using the developed model to mimic CO_2 injection into aquifers. The CMG-GEM commercial compositional simulator was used to compare its results with the coreflood model of this study. Phenomenal agreement was achieved with the GEM model, showing only 1.8% and 0.4% error for both components. This confirms the accuracy and reliability of the developed model. In conclusion, this study enhances the state of the art in porous media modeling using OpenFOAM 10, providing a valuable tool for examining fluid interactions in subsurface environments, especially within the context of CCS processes.

Keywords: OpenFOAM; CO_2 storage; CO_2 dissolution; water evaporation; compositional solver

Citation: Papi, A.; Jahanbakhsh, A.; Maroto-Valer, M.M. A New Straightforward Darcy-Scale Compositional Solver in OpenFOAM for CO_2/Water Mutual Solubility in CO_2 Storage Processes in Aquifers. *Energies* **2024**, *17*, 3401. https://doi.org/10.3390/en17143401

Academic Editors: Adam Smoliński and Alberto Pettinau

Received: 20 May 2024
Revised: 16 June 2024
Accepted: 9 July 2024
Published: 11 July 2024

1. Introduction

This paper is an extension of the conference paper in [1]. More developments of the existing tools and models for evaporation and salt precipitation in carbon capture and storage (CCS) processes in porous media are necessary [2,3]. OpenFOAM [4] is an open-source computational fluid dynamics (CFD) platform that leverages its C++ object-oriented architecture to provide a flexible environment for modeling complex fluid flow phenomena [5,6]. A model that accurately represents the multicomponent interaction of multi-phase flow systems at the Darcy scale, such as the interaction of CO_2 and H_2O components between liquid and gas phases in CO_2 storage processes in aquifers, is lacking in the current OpenFOAM literature. Meanwhile, for pore-scale and free-flow systems, the advancements are satisfactory [7,8].

There are various available packages that have been developed to model fluid flow in porous media with OpenFOAM [8,9]. A summary comparison of these packages is given in Table 1. Although these packages are available to use, the advancements in this area still remain relatively under-developed. More research efforts are needed to push the boundaries in this field by developing and refining current models. The packages within OpenFOAM that include porous medium models, such as porousSimpleFoam (single-phase) [10,11] or porousInterFoam (multi-phase) [4], only deal with fluid flow. A source term is added into the Navier–Stokes momentum equations of these models to account for the porous medium contribution in the form of a Darcy–Forchheimer equation that may include a Darcy (D) and a Forchheimer (F) term as the porous structure's resistance forces [10]. The porousInterIsoFoam package by Missios et al. (2023) [12], which is a developed version of porousInterFoam with a different interface advection scheme, also works the same way. The porousMedia4Foam package by Soulaine et al. (2021) [13] consists of three main solvers that solve for a fully Darcy model, a hybrid multi-continuum Navier–Stokes/Darcy scale model, and a constant-velocity passive scalar species transport model in the single phase. The package allows coupling with geochemical models such as PHREEQC for aqueous species reactive transport modeling [14]. The hybridPorousInterFoam package by Carrillo et al. (2020) [7] is an integrated two-phase hybrid solver that switches between a fully Navier–Stokes flow and a pure Darcy flow, depending on the geometry. The current version of the porousMultiphaseFoam (PMF) package by Horgue et al. (2022) [9] has a number of solvers including impesFoam [15]. The impesFoam module solves for the IMPES solution of incompressible two-phase fluid flow in porous media [16]. The upstreamFoam package by Lange et al. (2023) [17] is a development of the impesFoam solver for compressible fluids. None of these packages, however, consider species transport of multi-phase flow systems within a porous space, so they are not appropriate for modeling compositional phenomena such as water evaporation in CO_2 storage processes. PMF has other porous media solvers that mainly have applications in groundwater modeling, such as water flow in soil, the passive scalar transport of species in soil or the species transport of soil contaminants in the two-phase flow of a water/air system using Richard's equation [9]. Hence, they need to be modified for direct applications in CO_2/H_2 storage, oil and gas or geothermal energy topics. The GeoChemFoam package by Maes and Menke (2021) [8] solves for a variety of models in the pore scale, including single-phase passive scalar transport, multi-phase fluid flow with or without species transport and reaction, etc. [18,19].

Table 1. A comparison between porous media packages in OpenFOAM.

Package	Developer	Darcy Flow	Free Flow	Multi-Phase	Transport	Reactive Transport	Compressible
porousSimpleFoam	OpenFOAM [4]	✓	✓	×	×	×	×
porousInterFoam	OpenFOAM [4]	✓	✓	✓	×	×	✓
porousInterIsoFoam	Missios et al. (2023) [12]	✓	✓	✓	×	×	✓
porousMedia4Foam	Soulaine et al. (2021) [13]	✓	✓	×	✓	✓	✓
hybridPorousInterFoam	Carrillo et al. (2020) [7]	✓	✓	✓	×	×	✓
porousMultiphaseFoam	Horgue et al. (2022) [9]	✓	×	✓	✓	×	✓
impesFoam	Horgue et al. (2015) [15]	✓	×	✓	×	×	×
upstreamFoam	Lange et al. (2023) [17]	✓	×	✓	×	×	✓
GeoChemFoam	Maes and Menke (2021) [8]	×	✓	✓	✓	✓	×

In this study, the impesFoam solver of the PMF package which solves a two-phase incompressible fluid flow model in porous media was chosen as a base code and its code was modified to accommodate a compositional solver.

The model developed in this study is the first of its kind in OpenFOAM to address multi-phase, mutual CO_2/water interactions at the Darcy scale in a one-dimensional (1D) framework. It can specifically be used to model the 1D coreflood injection of CO_2 into brine-filled samples that can mimic CO_2 injection into aquifers. Moreover, it is expandable to include salt precipitation phenomena, thereby offering a versatile toolset for studying complex fluid–rock interactions in subsurface environments.

2. Numerical Method

In impesFoam, which is a Black Oil model (i.e., where the phases are treated as constant-composition pseudo-components [20]), the pressure and saturation equations are solved concurrently while treating the fluid phases as two distinct interfaces. IMPES is an acronym for Implicit Pressure Explicit Saturation. In this method, an implicit approach is adopted to solve the pressure equation with current timestep values, while an explicit approach is used to solve the saturation equation with previous timestep values to address the coupling of these two parameters [16]. The saturation and pressure equations for incompressible two-phase fluids in impesFoam are written as follows:

$$\varphi \frac{\partial S_i}{\partial t} + \nabla . \boldsymbol{U_i} = q_{i,inj}\, i \;=\; l \text{ or } g \tag{1}$$

$$\nabla . \left(-\frac{K k_{rg}}{\mu_g} (\nabla p_g - \rho_g \boldsymbol{g}) \right) + \nabla . \left(-\frac{K k_{rl}}{\mu_l} (\nabla p_g - \rho_g \boldsymbol{g} - \nabla \mathrm{p}_c) \right) = q_{l,inj} + q_{g,inj} \tag{2}$$

$$\boldsymbol{U_i} = -\frac{K k_{ri}}{\mu_i} (\nabla p_i - \rho_i \boldsymbol{g}) \text{ i } = \text{ l or g} \tag{3}$$

where $\boldsymbol{g}$ is the gravitational acceleration and p_i, S_i, $\boldsymbol{U_i}$, ρ_i, k_{ri}, μ_i and $q_{i,inj}$ are the gas or liquid's pressure, saturation, Darcy velocity [21,22], density, relative permeability, viscosity and injection rate (saturation is defined as the ratio of the fluid's volume to the rock's void space [23]). K and φ are the rock's porosity and permeability and p_c is the capillary pressure. For more information on the details of the model, please refer to Ref. [15].

In the compositional model, mass transfer occurs by the interaction of gas and liquid phases. This study focuses on compositionally solving for a two-phase (gas–liquid) binary-component (CO_2–H_2O) system. This implies that two additional species transport equations must be incorporated into the impesFoam solver for both the gas and liquid phases and subsequently solved. Solving for one component would be sufficient as the other component can be derived from it. Additionally, the gas and liquid components are in equilibrium. If the liquid is assumed a dilute solution, this can be reflected in the form of Henry's law for the CO_2 component [24].

In the following, x_{CO2} and y_{CO2} refer to the CO_2 component in the liquid and gas phase, respectively. The mass balance equation for the CO_2 component in the liquid phase (xCO_2) is as follows [3]:

$$\varphi \frac{\partial (x_{CO2} S_w)}{\partial t} + \nabla . (x_{CO2} \boldsymbol{U_w}) - \varphi\, D_{CO2,w}\, \nabla . (S_w \nabla x_{CO2}) = q_{CO2,inj} \tag{4}$$

And Henry's law for the mole fraction of CO_2 in the gas phase (yCO_2) states the following [24]:

$$\mathrm{y}CO_2 = \frac{H_{CO2}}{P_g} \times \mathrm{x}CO_2 \tag{5}$$

where $D_{CO2,w}$ and H_{CO2} are the CO_2 diffusion coefficient in water and Henry's law constant. On the other hand, if an ideal behavior is considered, the gas pressure can be calculated

using the summation of the partial pressure of each component. Based on Henry's and Rault's laws [25], it can be written as follows:

$$P_g = P^g_{CO2} + P^g_{H2O} = H_{CO2} \times xCO_2 + P^{sat} \times yCO_2 = H \times xCO_2 + P^{sat} \times (1 - xCO_2) \quad (6)$$

where P^{sat} is the water pure component saturation pressure. In other words, the CO_2 component in the liquid phase can be calculated from gas pressure as follows:

$$xCO_2 = \frac{P_g - P^{sat}}{H - P^{sat}} \quad (7)$$

We applied these changes to the compositions in the impesFoam solver to come up with a compositional solver, named compositionalIGFoam. The algorithm is shown in Figure 1 and is in two parts: in the first part, the IMPES method solves for the saturation and pressure equations, respectively, using Equations (1) and (2). In the second part, the compositional solver solves for the aqueous and gaseous compositions of carbon dioxide using Equations (7) and (5), respectively. The other two components are calculated by subtracting their respective phase components from 1. These calculations start from time zero, are conducted at each time-step and proceed to the next time-step.

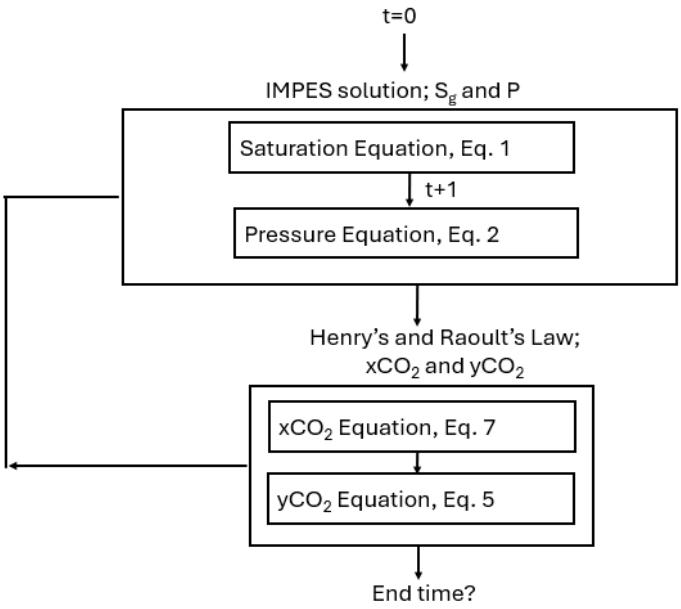


Figure 1. The numerical algorithm.

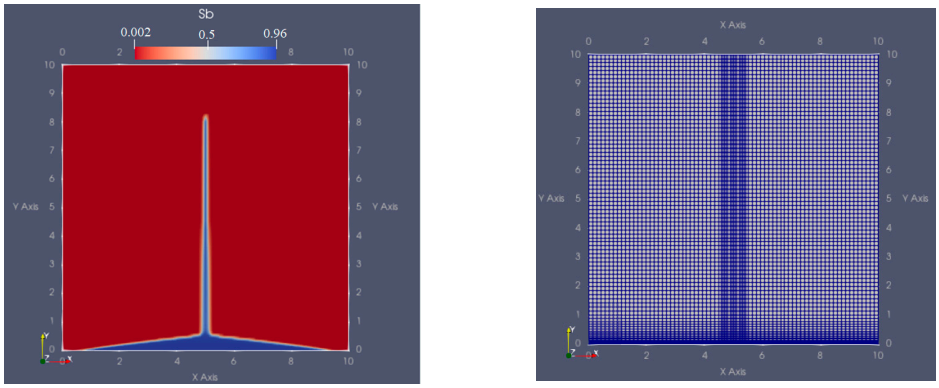
Input variables that are taken as scalar fields include the initial conditions for pressure, saturation, velocities and all the compositions. Constant parameters include gravitational acceleration and the permeability file. Phases' density and viscosity, porosity, relative permeability and capillary pressure models are given to the model through transport properties. The constants, such as Henry's constant or saturation pressure, are included in the thermophysical properties file. This study addresses H_2O-CO_2 interactions. If a different system such as H_2O-CH_4 was to be used, the input parameters would need to be modified accordingly (e.g., Henry's constant).

3. Results

Models: Water Injection and Gas Injection

The developed compositional solver was initially used to replicate the results of a water injection case example in the porousMultiphaseFoam package (impesFoam tutorials—the injection case [26]) to assess its functionality. The model works well in reproducing the results. In this case example, water is being injected from the middle into a bounded porous

medium filled with gas which is open at a constant pressure from the top face. The water saturation profile is shown in Figure 2a. Water flows down from the injection point due to gravity and spreads over the bottom side of the porous model. For better illustrations, using OpenFOAM's *blockmesh* meshing utilities, we also improved the solution quality by refining the model's mesh towards the center and bottom face of the model where most changes to flow occur (Figure 2b). By doing so, a sharp phase interphase is captured, and saturation smearing of the original model is removed.



(**a**) (**b**)

Figure 2. (**a**) Water saturation distribution using our developed model, along with (**b**) the new mesh resolution.

The code was then modified to consider the case of injecting gas into a liquid enclosure, as is the case in the CCS processes in aquifers. By repeating the previous tutorial for the case of injecting a gas into a liquid-filled porous medium using this solver, the solution becomes that shown in Figure 3, where the gas flows upward and leaves the enclosure at the constant pressure of the top face of the medium, as was expected due to buoyancy. This code is compiled as a new module named compositionalIGFoam in the porousMultiphaseFoam package and is put forward for the simulation of CCS processes in aquifers.

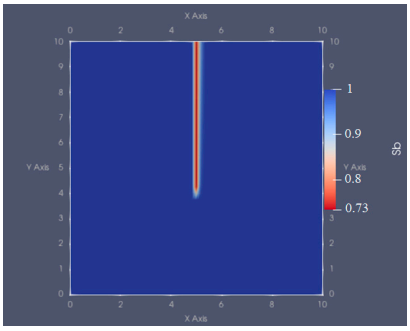


Figure 3. Gas saturation distribution of the case of gas injection into a porous enclosure.

4. Validation

The Water-Saturated Coreflood Model

To further evaluate compositionalIGFoam, we aimed to simulate the CO_2 coreflood experiments of water. By doing so, the model's ability to simulate a gas–liquid fluid flow and water/CO_2 mutual solubility in a CCS process in an aquifer is demonstrated. In order to simulate this process, a water-saturated core sample of dimensions 8 cm in length and 3.5 cm in diameter with a meshing of $100 \times 1 \times 1$ was considered, as shown in Figure 4. The flow model is assumed to be 1D to resemble a coreflood experiment. CO_2 is injected at the left-hand side with an injection rate of 30 cc/min and the model is kept at a constant pressure of 10^7 Pa at the right-hand side.

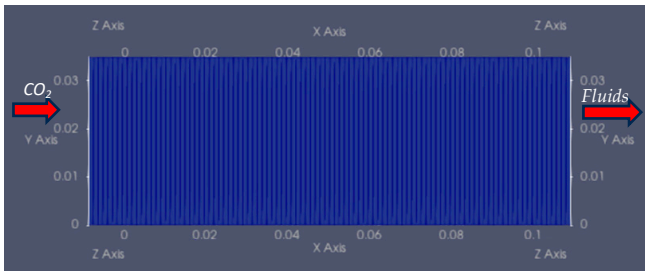


Figure 4. The coreflood model.

A Brooks–Corey relative permeability and capillary pressure model have been used with the parameters given in Table 2, which also includes other numerical parameters.

Table 2. The numerical parameters.

Rock and Fluid Parameters		Brooks–Corey k_r/P_c Model Parameters	
T	65 °C	$k_{rw,max}$	1
K	100 md	$k_{rg,max}$	1
P	10^7 Pa	S_{wr}	0.001
φ	0.5	$S_{g,crit}$	0.999
H_{CO2}	2.9×10^8 Pa	P_{c0}	5 Pa
P^{sat}	2×10^4 Pa	n	4
μ_w	10^{-3} kg/m.s	α	0.2
μ_{CO2}	1.76×10^{-5} kg/m.s		
ρ_w	1000 kg/m^3		
ρ_{CO2}	1 kg/m^3		

To benchmark the solution of compositionalIGFoam solver, an equivalent model was created in CMG-GEM compositional simulator [27], and the solution results, i.e., the final compositional distributions of CO_2 and water, were compared.

After CO_2 is injected into the fully water-saturated core sample, it pushes the water out of the model. A moving saturation front will be formed and the CO_2 saturation inside the model starts to increase. Water saturation can reduce down to its residual water saturation value. The mutual solubility of CO_2/water is occurred, i.e., CO_2 molecules are dissolved into the liquid phase and water molecules are transferred into the gas phase. The species distributions at the breakthrough point for both the solvers are shown in Figure 5. An equilibrium approach is assumed in this study, meaning that the values of CO_2 in the liquid and gas phase will always be in equilibrium. The same holds for water molecules in the liquid and gas phase. After the first touch of fluids with each other at the inlet, both fluids become saturated to their equilibrium value. Therefore, after CO_2 is flooded all over the core model, a uniform water composition in the liquid phase (xH_2O) and CO_2 composition in the gas phase (yCO_2) ensues. As can be seen from Figure 5a,c, the value of xH_2O from the compositionalIGFoam solver (the model of this study) and the CMG-GEM solver is estimated at 0.9656 and 0.9832, respectively, i.e., an error of 1.8%, which is a great match. The respective yCO_2 values (CO_2 composition in the gas phase) at this point are calculated at 0.9981 and 0.9938, i.e., an error of 0.4%, which shows they are in a phenomenal agreement (Figure 5b,d).

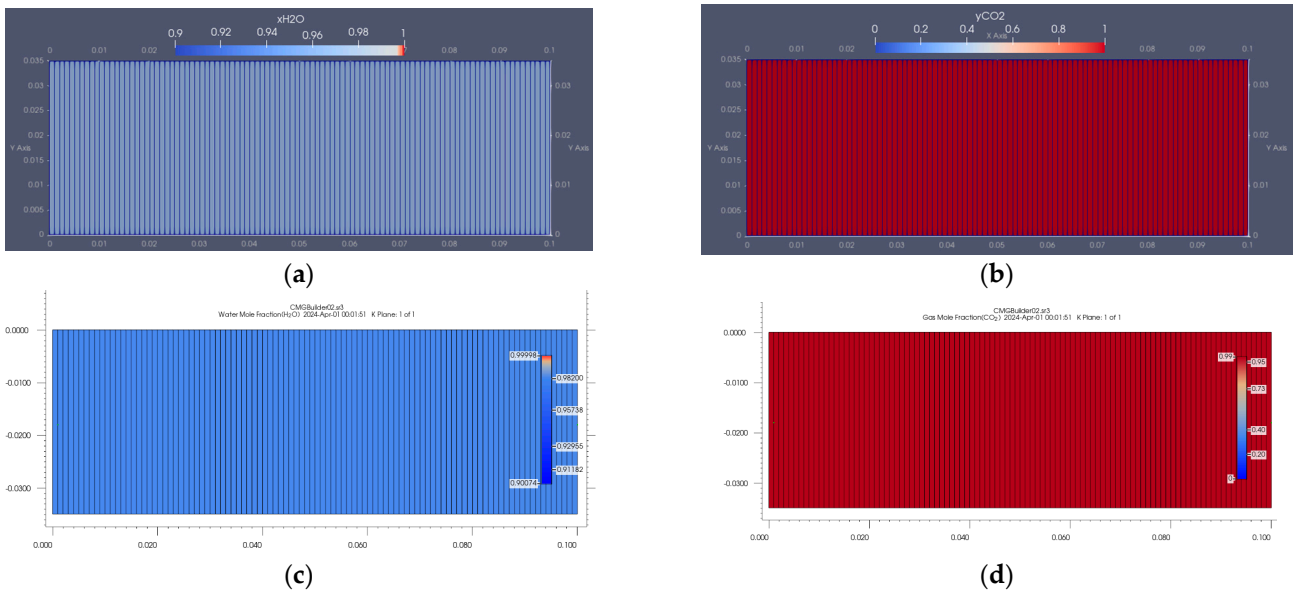


Figure 5. The water composition in the liquid phase (xH_2O) and CO_2 composition in the gas phase (yCO_2) of (**a**,**c**) compositionalIGFoam (this study) and (**b**,**d**) CMG-GEM simulator.

The values of CO_2 in the liquid and H_2O in the gas phase (xCO_2 and yH_2O, respectively) can be calculated from their phase composition counterparts at the breakthrough time and are summarized in Table 3.

Table 3. Comparison of the binary composition of the coreflood model in CMG-GEM and our study.

Component / Model	xH_2O	xCO_2	yH_2O	yCO_2
CMG-GEM	0.9832	0.0168	0.0062	0.9938
compositionalIGFoam (this work)	0.9656	0.0344	0.0019	0.9981

Previous compositional models of porous media in OpenFOAM were in the pore-scale and free flow systems [7,8]. This work, however, presents such a model in the Darcy scale in OpenFOAM. Compared to other compositional models in the area, such as CMG-GEM, this model addresses CO_2/water interactions with a straightforward and reliable approach by assuming ideal gas and dilute solution behaviors that do not require solving complicated species transport equations, thus making it a readily available candidate for fast initial evaluations of CO_2/water interactions. Also, as it is based on the OpenFOAM platform, it provides open-source access features that helps the community for future developments.

5. Conclusions

An OpenFOAM solver was developed in this study. The compositionalIGFoam solver simulates fluid flow and multicomponent interphase interactions in porous media, such as CO_2/water dissolution in CO_2 storage processes in aquifers. This fills the gap in this field where a Darcy-scale solver was lacking in the OpenFoam platform. The validation of the model against the CMG-GEM commercial compositional simulator with less than 2% compositional error demonstrates the reliability of this solver. The model's capability of handling gas–liquid interactions, including species transport and phase equilibrium, provides applications in CCS and H_2 storage processes, oil and gas reservoir engineering and geothermal energies. By providing an open-source and versatile platform, this study contributes to the ongoing efforts to address critical challenges in energy and environment.

Moving forward, the developed model offers opportunities for further improvements such as refining the numerical methods, incorporating additional geochemical reactions, and extending the model to simulate more complex subsurface processes. Additionally, the

model's expandability to include evaporation and salt precipitation phenomena opens up possibilities for studying broader aspects of fluid–rock interactions in saline aquifers.

In this regard, in the next stages, the numerical method will be improved by coupling incompressible fluid flow and transport equations to come up with a model that can incorporate evaporation. The evaporative model is further developed to include two more aqueous components, i.e., chlorine and sodium ions. By doing so, it can be extended to a salt precipitation model where a third solid phase can appear in the system, i.e., a three-phase flow system. Moreover, the reaction of the aqueous components with each other and with the rock (dissolution/precipitation) can also be considered. Experiments and, to some extent, some of the current numerical tools can come to play for validating such a model.

In summary, compositionalIGFoam creates a basis to develop the cutting-edge technology in porous media to model gas–liquid/fluid–rock interactions, water evaporation and salt precipitation, species transport and phase equilibria with OpenFOAM that provides an invaluable tool for scrutinizing the underground phenomena. Salt precipitation is an issue that not only emerges in CO_2 storage applications but also in H_2 storage processes. Apart from CCS and H_2 storage, a wider implication of this work is in the petroleum industry where Enhanced Oil Recovery (EOR) techniques with CO_2 are used for boosting the production. Another application is in the geothermal energies where CO_2 Plume Geothermal (CPG) systems are used for the Carbon Capture, Utilization and Storage (CCUS) purposes where the unique specifications of CO_2 come into play to increase geothermal energy recovery while this greenhouse gas agent is sequestered underground.

Author Contributions: Conceptualization, A.P. and A.J.; data curation, A.P.; formal analysis, A.P. and A.J.; funding acquisition, M.M.M.-V.; investigation, A.P. and A.J.; methodology, A.P., A.J. and M.M.M.-V.; project administration, M.M.M.-V.; resources, M.M.M.-V.; software, A.P. and A.J.; supervision, A.J. and M.M.M.-V.; validation, A.P.; visualization, A.P.; writing—original draft, A.P.; writing—review and editing, A.J. and M.M.M.-V. All authors have read and agreed to the published version of the manuscript.

Funding: This work acknowledges the support received from the UKRI Industrial Challenge Fund (ISCF) within the UK Industrial Decarbonisation Research and Innovation Centre (IDRIC) award number: EP/V027050/1. Amir Jahanbakhsh and M. Mercedes Maroto-Valer would like to thank the European Research Council (ERC) for funding the MILEPOST project (Grant agreement no.: 695070) under the European Union's Horizon 2020 research and innovation program. The ERC is not responsible for the views presented in this work, and they are only the views of authors. The use made from the information contained here will not pose any responsibility on the ERC. The authors also would like to express appreciation for the CMG team for license provision and their support during this study.

Data Availability Statement: The data presented in this study are openly available on GitHub (https://github.com/Ali-Papi, accessed on 1 July 2024).

Conflicts of Interest: The authors declare no conflicts of interest.

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