



Integrating a compressible multicomponent two-phase flow into an existing reactive transport simulator



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ABSTRACT

This work aims to incorporate compressible multiphase flow into the conventional reactive transport framework using an operator splitting approach. This new approach would allow us to retain the general paradigm of the flow module independent of the geochemical processes and to model complex multiphase chemical systems, conserving the versatile structure of conventional reactive transport. The phase flow formulation is employed to minimize the number of mass conservation nonlinear equations arising from the flow module. Applying appropriate equations of state facilitated precise descriptions of the compressible multicomponent phases, their thermodynamic properties and relevant fluxes.

The proposed flow coupling method was implemented in the reactive transport software HYTEC. The entire framework preserves its flexibility for further numerical developments. The verification of the coupling was achieved by modeling a problem with a self-similar solution. The simulation of a 2D CO₂-injection problem demonstrates the pertinent physical results and computational efficiency of this method. The coupling method was employed for modeling injection of acid gas mixture in carbonated reservoir.

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1. Introduction

1.1. Background/motivation

Human activity in the subsurface has been expanding and diversifying (waste disposal, mining excavation and high-frequency storage of energy), and the public and regulatory expectations have been increasing. The assessment of each step of underground operations, including environmental impact evaluation, relies on elaborate simulators and leads to an urgent need to develop multiphysics modeling. Reactive transport, a geochemical research and engineering tool, is used in multicomponent systems and sophisticated chemical processes (activity and fugacity correction according to different models, mineral dissolution and precipitation, cation exchange, oxidation and reduction reactions, isotopic fractionation and filtration), in addition to gas evaporation and dissolution (van der Lee et al., 2003; Mayer et al., 2012; Parkhurst and Appelo, 1999; Steefel, 2009; Yeh et al., 2004). Multiphase flow is based on broad experiences in reservoir engineering research, including the thermodynamic modeling of complex phase behavior. In particular, the equations of state were used to simulate

and study interfacial tension, gas, steam and alkaline injection in oil reservoirs and enhanced oil recovery (Delshad et al., 2000; Farajzadeh et al., 2012; Nghiem et al., 2004; Wang et al., 1997).

This work aims to incorporate a compressible multiphase flow module into an existing reactive transport simulator. Our coupling method should therefore meet the following requirements:

1. The new approach should handle the different complex multiphase chemical models and retain the general paradigm of a multiphase flow module independent of the geochemical system and conserve the conventional reactive transport structure;
2. The number of mass conservation nonlinear equations arising from the flow module should be minimized such that the reduced flow system preserves the matrix structure and minimizes the computational intensity;
3. The entire framework should preserve its flexibility for possible non-isothermal, geomechanical and domain decomposition developments in the future.

Reactive transport methods have been extensively investigated over the past two decades (see below). This work focuses on the coupling between multicomponent multiphase flow (MMF¹) and

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¹ The nomenclature is provided in Table 1. The abbreviations are detailed in Table 2.

Table 1
Nomenclature.

| Latin symbols | |
|---------------------|---|
| a_k | activity of potential catalyzing or inhibiting species |
| A_s | specific surface area, [m^2/m^3 solution] or [m^2/kg mineral] |
| $C_{l,k}$ | total liquid mobile concentration of basis species k , [mol/kg w] |
| $C_{s,k}$ | immobile concentration of basis species k , [mol/kg w] |
| $C_{g,m}$ | gas concentration of basis species m , [mol/m^3] |
| C_i | concentration of primary species i in chemical module |
| d | dissolution parameter of transport model |
| dt | time step |
| D_α | molecular diffusion coefficient of phase α , [m^2/s] |
| D_α^e | effective diffusion coefficient of phase α , [m^2/s] |
| \mathbf{D}_α | diffusion-dispersion tensor of fluid phase α |
| e | evaporation parameter of transport model |
| f_i^α | fugacity of species i in phase α |
| \mathbf{F} | residual function |
| \mathbf{g} | gravitational acceleration vector, [m/s^2] |
| \mathbf{J} | Jacobian |
| k | number of iterations in flow coupling |
| k_{kin} | kinetic rate constant in , [$mol/m^2/s$] |
| k_{max}^l | maximum number of iterations in flow coupling |
| k_{max}^r | maximum number of iterations in reactive transport coupling |
| $k_{r\alpha}$ | relative permeability of phase α |
| K | intrinsic permeability, [m^2] |
| \mathbb{K} | intrinsic permeability tensor, [m^2] |
| K_i | K-value/equilibrium ratio |
| K_j | equilibrium constant of reaction j |
| K_s | equilibrium solubility constant of solid phase |
| K_i^h | Henry's law constant |
| M_i | molar mass of species i , [kg/mol] |
| n_α | quantity of matter in phase α |
| \mathbf{n} | normal vector |
| N_c | number of primary species in chemistry module |
| N_f | number of fluid phases α |
| N_g | number of gas species |
| N_{kin} | number of kinetic reactions |
| N_{Nit} | number of Newton iterations |
| N_{Pic} | number of Picard iterations |
| N_p | number of phases |
| N_r | number of independent chemical reactions |
| N_s | number of species in chemistry module |
| p_α | liquid/gas pressure, [Pa] |
| P | pressure, [Pa] |
| \mathbf{P}_c | set of the critical pressures |
| q_α | mass source term of phase α , [kg/s] |
| $q_{\alpha,k}$ | mass source term of species k in phase α , [kg/s] |
| $q_{g,m}$ | source term of basis species m in the gas phase, [mol/m^3] |
| $q_{l,k}$ | source term of basis species k in the liquid phase, [mol/kg w] |
| Q_s | ion activity product |
| $T_{\alpha\beta}$ | reaction term of phases α and β in α transport operator |
| R | gas constant, [$J/K/mol$] |
| R_α | reaction term of phase α , [kg/s] |
| $R_{\alpha,k}$ | reaction term of species k in phase α , [kg/s] |
| $R_{g,m}$ | reaction term of basis species m in the gas phase, [mol/m^3] |
| $R_{l,k}$ | reaction term of basis species k in the liquid phase, [mol/kg w] |
| \mathbf{R} | geochemical reaction operator |
| S_j | concentration of species j in chemical module |
| S_α | saturation of phase α |
| t | calculation time of entire system per time step |
| t_{fl} | calculation time of flow operator per iteration |
| t_{fc} | calculation time of flow coupling per iteration |
| t_{gt} | calculation time of gas transport operator per iteration |
| t_{rtc} | calculation time of reactive transport coupling per iteration |
| T | temperature, °C and K |
| T_i | total concentration in chemistry module |
| \mathbf{T}_c | set of the critical temperatures |
| \mathbf{T}_α | transport operator of phase α |
| \mathbf{u}_α | Darcy's velocity of phase α |
| v | molar volume, [m^3/mol] |
| V_α | volume of porous space occupied by phase α , [m^3] |
| V_{tot} | total volume, [m^3] |
| x_i | mole fraction of basis species i in the liquid phase |
| $X_{\alpha,k}$ | mass fraction of basis species k in phase α |
| \mathbf{x} | vector of primary variables of the flow system |
| y_i | mole fraction of basis species i in the gas phase |

Table 1 (continued)

| Latin symbols | |
|---------------------------------------|---|
| Z | compressibility factor |
| Z_c | set of the critical compressibility factors |
| Greek symbols | |
| $\alpha = \{l, g\}$ | liquid/gas phase |
| α_{ij} | stoichiometric coefficient |
| γ_j | activity coefficient |
| Δ | matrix of binary interaction coefficients of PR EOS |
| ϵ_g | gas quantity tolerance in reactive transport coupling |
| ϵ_{Nf} | residual function tolerance in flow coupling |
| ϵ_{qss} | quasi-stationary state tolerance in flow coupling |
| ϵ_{rt} | tolerance in reactive transport coupling |
| μ_α | viscosity of phase α , [$Pa \cdot s$] |
| ρ_α | mass density of phase α , [kg/m^3] |
| ρ_α^g | density of phase α in the gravity term, [kg/m^3] |
| τ_α | tortuosity of phase α |
| ϕ | porosity |
| ϕ_i^α | fugacity coefficient of species i in phase α |
| ψ_α | volumetric rate of phase α , [m^3/s] |
| Ξ_α | acentric factor set |
| Ω | mathematical transport operator of phase α |
| $\ \cdot \ _\infty$ | infinity norm |
| $\mathbb{1}_{\mathbb{R}_{>0}}(\cdot)$ | indicator function of the set of strictly positive real numbers |

Table 2

Abbreviations.

| | |
|-------|---|
| AIM | adaptive implicit method |
| CFL | Courant-Friedrichs-Lewy number |
| DAE | differential algebraic equations based method |
| DSA | direct substitution approach |
| EOS | equation of state |
| FIM | fully implicit method |
| FVM | finite volume method |
| GIA | global implicit approach |
| IMPEC | implicit pressure/explicit concentration |
| MMF | multiphase multicomponent flow |
| MMRF | multiphase multicomponent reactive flow |
| ODE | ordinary differential equations based method |
| PDE | partial differential equation |
| OSA | operator splitting approach |
| RT | reactive transport |
| SI | saturation index |
| SIA | sequential iterative approach |
| SNIA | sequential non-iterative approach |
| TPFA | two-point flux approximation |

reactive transport (RT) modules and starts by surveying the existing approaches

1.2. A review of multiphase multicomponent flow and reactive transport codes

1.2.1. Operator splitting algorithms between MMF and RT

The strength of the operator-splitting approach (OSA) (sequential iterative (SIA) or sequential non-iterative (SNIA)) arises from the framework flexibility, which allows each model to be developed and verified independently. These are important reasons for selecting the OSA for the coupling between MMF and RT, particularly when extending a hydrogeochemical code from single- to two-phase flow. The following codes apply the OSA: CodeBright (Olivella et al., 1996) (coupling with the reactive transport code RETRASO (Saaltink et al., 2004)), DuMu^X (based on DUNE) (Ahusborde et al., 2015; Vostrikov, 2014), DUNE (Hron et al., 2015), HYDROGEOCHEM (unsaturated) (Yeh et al., 2004, 2012), iCP (Nardi et al., 2014), IPARS (Peszynska and Sun, 2002; Wheeler et al., 2012), MIN3P (the bubble model) (Mayer et al., 2012; Molins and Mayer, 2007), MoReS (Farajzadeh et al., 2012; Wei, 2012), NUFT (Hao et al., 2012), PFLOTRAN (Lichtner et al., 2015; Lu and Lichtner, 2007),

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