

Chemical Reaction Modeling in GPRS

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1 Introduction

Chemical reactions are generally divided into two groups, specifically, equilibrium reactions and kinetic reactions. Equilibrium reactions refer to the reactions that proceed quickly over the time step of the calculation. We assume that these reactions remain in equilibrium at all times. A chemical reaction should be considered as an equilibrium reaction only if it is reversible and sufficiently fast (compared to the simulation time step). Kinetic reactions, by contrast, do not necessarily remain in equilibrium over the time step of interest. Reaction kinetics must be taken into account for all chemical reactions that are not equilibrium reactions.

GPRS has been extended to simulate both kinetic and equilibrium reactions separately. The formulation and implementation of chemical reaction modeling have been documented in detail in Fan (2010). We now describe the specific keywords used in modeling chemical reactions. Besides reaction modeling, the simulation samples included with this document include a number of extensions to the rock modeling and aqueous phase modeling, which will also be included here.

2 New Keywords

2.1 Rock Data

HEATERS

Specify the number of heaters. This keyword is followed by $n_h + 1$ integers, where n_h is the number of blocks designated as “heaters”. The first integer is the number of heater wells ($=n_h$). The remaining n_h integers specify the locations of heater blocks. The heater position should be given in the sequence of active blocks only; i.e, if there are n_{ab} active blocks, the value should not exceed $n_{ab} - 1$.

The heater temperature control scheme is required. At present, all of the heaters are assumed to have the same heating scheme. The heating scheme is described by a table which specifies the temperature of the heaters at given date. The following input section shows an example of heater input.

```
HEATERS # number of Heaters
2
# Heater Positions(active blocks only, starts from 0)
0 11

# Date(day) HeaterTemp (R)
NUM_OF_TABLE_ENTRIES 2
0 1109.67
1e-8 1109.67
```

NMINERALS n_m

The number of minerals. This keyword is followed by an integer. Following the number of minerals, without additional keywords, the user defines names for each mineral. Mineral names should be separated by space(s). Following the

mineral names, without additional keywords, the user specifies molar weight for each mineral.

INIT_MINERAL_ i

The user specifies initial concentration for i th mineral at each block. The unit for this keyword is [lb mol]/ft³. The keyword is followed by n_b values, where n_b is the number of blocks. If only one value is specified, the initial concentration is constant at every block. If more than one minerals exist, repeat this keyword. For example,

NMINERALS 2

#Mineral Names

Kerogen_A Kerogen_B

#Molar Weight

14.7 29.4

#Initial Concentrations

INIT_MINERAL_1

0.7

INIT_MINERAL_2

0.2

END

SPECIFIC_AREA

This is an optional keyword that reads the specific area (in [m²]/[m³]) for each mineral. The keyword is followed by n_m real numbers, each representing the specific area for each of the minerals. The specific area is defined as the surface (reactive) area per unit volume.

2.2 Aqueous Component Data

A number of keywords are required to specify ions in the aqueous phase. At present, the aqueous phase is simulated as the “oil” phase in the GPRS’s compositional mode. We note that the modeling of aqueous ions in black-oil models are yet to be implemented. In addition, when aqueous phase is modeled as “oil” phase, there will not be water phase in the model. When aqueous components are added to the compositional modeling, the phase-component relationship needs to be updated. A common error of modeling aqueous components is that the content of PHASE_COMP_RELATION_DATA is not updated properly after specifying aqueous components.

AQUCOMP_PHASE OIL

This keywords specifies which phase (gas, oil, water) in GPRS is modeled as the aqueous phase. In current simulations, because we treat aqueous components (i.e., ions) in equivalent to hydrocarbon components, OIL should always be selected. *If three-phase simulations are of interest, then WATER should be selected, in which case the phases to model are gas, oil, and aqueous phases.*

NAQUCOMPONENTS n_a

This keyword specifies the number of aqueous components (ions) n_a . The hydrocarbon components and H₂O are not included. Followed the number of ions are the ion names, delimited by space(s). Molar weights are specified by n_a real numbers in [g]/[mol]. Then n_a real numbers are required to specify the ion charges of each aqueous component, followed by n_a real numbers that specify the electrolyte sizes in Angstrom. Initial ion molalities (in [mol]/[kg]) are given for each ion (assuming homogeneous ion distribution in all blocks).

AQU_XIJ_UPSCALE

This is an optional keyword that determines if the molar fractions of aqueous components are calculated in their scaled space. Because the ion molality may be many orders of magnitude lower than molar fractions of hydrocarbon components, proper scaling of molalities can improve the stability of modeling. The user may or may not use this keyword, though scaling is recommended for the cases with very small ion concentrations.

2.3 Chemical Data

In addition to existing GPRS input, the user should prepare the input file following the format specified in this section. The chemistry option is activated by the keyword CHEM_DATA after the fluid data section and rock-fluid data section. The chemistry input section begins with CHEM_DATA and ends with END_CHEM. Within the chemistry section, there are a number of new keywords to be specified in the following order.

NELEMENTS n_e

The number of elements involved in all components (hydrocarbons, aqueous and mineral components).

NREACTIONS n_r

The number of chemical reactions. If the same reaction occurs in different phases, define the reaction in each phase as a separate reaction. Element balance in each reaction is advised.

CONSERVE_EQS COMPONENT | ELEMENT

This keyword specifies the type of conservation equations. The user chooses between COMPONENT and ELEMENT, which represents component balance equations and element balance equations. In general, if all of the reactions are kinetic reactions, COMPONENT is used. If there are one or more equilibrium reactions, ELEMENT must be used.

CONCENTR_MODLE ON | OFF

This keyword specifies if the concentration module is activated or not. The user chooses between ON or OFF. If the reaction laws involve any type of concentrations, the concentration module should be ON. If the reaction laws only involve activities, the concentration module should be OFF. Note that turning concentration module ON will incur additional computation in linearization step.

ACTIVITY_MODLE ON | OFF

This keyword specifies if the activity module is activated or not. The user chooses between ON or OFF. If the reaction laws involve any type of activities, the activity module should be ON. If the reaction laws only involve concentrations, the activity module should be OFF. Note that turning activity module ON will incur additional computation in linearization step.

KINETICR_CUTOFF

This keyword is followed by $n_{tot,c}$ real numbers, where $n_{tot,c}$ is the total number of components (the total number of components is equal to the sum of the numbers of hydrocarbon components, aqueous components and mineral components). Each real number specifies the lowest activity or concentration at which kinetic reaction rates can be calculated. If the concentration (or activity) of any component in a reaction law falls below the cut-off value, the reaction rate is set to zero. Specifying zero under this keyword means the kinetic rates will always be calculated, regardless of the value of component activity or concentration.

Element Names

The user specifies name for each element.

Element Molar Weight

The user input molecular weight of each element.

Stoichiometric Number

This keyword defines the chemical formula for each component. The user provides a table of $n_e \times n_{tot,c}$ values, specifying the number of elements in each component. We recall that n_e is the number of elements, and $n_{tot,c}$ is the total number of components.

Reaction Laws

The user defines each reaction and the parameters of each reaction. There are a number of pre-defined reactions.

- RATE.ELEM or RATE. This keyword indicates the reaction is an elementary kinetic reaction. The keyword is followed by two values k_r and E_{act} , where k_r is the kinetic rate in field unit (e.g. [lbmol]/[ft]³/[day]) and E_{act} is the activation energy in standard unit (i.e., [kJ]/[mol]).
- RATE.ELEM.REV. This keyword indicates the reaction is a reversible elementary kinetic reaction. The keyword is followed by four values. The first two values are forward reaction rate constant and activation energy (refer to RATE.ELEM). The third and fourth values are backward reaction rate constant and activation energy. The units are the same as those specified in RATE.ELEM.
- RATE.MIN. This keyword indicates the reaction is a reversible mineral dissolution and precipitation reaction determined by a generalized mineral dissolution law. The keyword is followed by four values. The first value is an integer which gives the index of the principle mineral involved in this reaction (there is only one principle mineral in each reaction in the generalized dissolution law). The second value is the dimensionless equilibrium constant $\log_{10} K_{eq}$. The third value is reaction rate constant in [mol]/[m]/[m]/[s]. The fourth value is activation energy in [kJ]/[mol]. Refer to equation (2.44) in Fan (2010) for detailed description.
- RATE.MIN.IR. This keyword indicates that the reaction is an irreversible reaction for mineral dissolution or precipitation. The values required for this keyword are the same as those for RATE.MIN.
- EQL. This keyword indicates the reaction is an equilibrium reaction. The keyword is followed by a dimensionless equilibrium constant $\log_{10} K_{eq}$, where K_{eq} is determined in terms of component *concentrations*.
- EQL.AQU. This keyword indicates the reaction is an equilibrium reaction. The keyword is followed by a dimensionless equilibrium constant $\log_{10} K_{eq}$, where K_{eq} is determined in terms of component *activities*.
- RATE.ECBM. This keyword indicates the reaction is an ECBM adsorption process that follows Langmuir isotherm. This keyword is followed by $5+n_{hc}$ values, where n_{hc} is the number of hydrocarbon components. The first value is the adsorbent bulk density ρ_s in [kg/m³]. The second value is the saturation capacity per unit mass adsorbent q_i in [mol]/[g]. The third value is the mass transfer coefficient k_{mi} in 1/[s]. The fourth value is the component index of the component involved in this reaction. The fifth value is an integer that specifies the number of hydrocarbon components ($=n_{hc}$) involved in the Langmuir equation. The sixth to $(5+n_{hc})$ values specifies each Langmuir constant for each hydrocarbon component. *We now describe the equations involved in this reaction. The mass transfer rate of component i from gas phase to adsorbed phase is given by $r_i = k_{mi}(n_i^* - n_i)$, where r_i is the mass transfer rate, k_{mi} is the mass transfer coefficient, n_i^* is the equilibrium phase concentration of component i determined by Langmuir equation, and n_i is the actual concentration of component i . The Langmuir equation for calculating n_i^* is given by*

$$n_i^* = \frac{\rho_s q_i b_i p_g x_{ig}}{1 + p_g \sum_j^{n_{hc}} b_j x_{jg}}, \quad (1)$$

where ρ_s is bulk density, q_i is saturation capacity per unit mass adsorbent, b_i is the Langmuir constant of component i , p_g is gas phase pressure and x_{ig} is molar fraction of component i in gas phase.

Stoichiometric Coefficients

This keyword defines the chemical reaction by specifying stoichiometric coefficients for each reaction. The user provides a table of $n_r \times (2n_{hc} + n_a + n_m)$ values, where n_r is the number of reactions, n_{hc} is the number of hydrocarbon components, n_a is the number of aqueous components, and n_m is the number of mineral components. Because the chemical reaction is implemented in a generalized form; therefore, two coefficients are required for each hydrocarbon component, one for gas phase and the other for oil phase.

3 Samples

3.1 In-situ Upgrading

To illustrate the capabilities of chemical kinetics in GPRS, an in-situ upgrading case has been designed to simulate the thermal-chemical process consisting of kerogen decomposition and oil cracking. The sample shown in this report is 1-D case for simplicity. Two-dimensional and three-dimensional cases are documented in Fan (2010).

Description of Example Case

An oil shale reservoir is considered to be the source rock of hydrocarbons. The reservoir parameters have been listed in Table 1. The 1-D reservoir consists of 11 blocks. One producer is located at the center block. Two heaters are placed at the two ends of the blocks. The heaters are operated at constant temperature.

Table 1: Parameters used in example case

Parameter	Sample Case
grid	$11 \times 1 \times 1$
block size	$2 \times 1 \times 55.77 \text{ ft}^3$
tops	68.89 ft
porosity	0.05
permeability $k_x=k_y=3k_z$	300 md
initial temperature	70 °F
heater temperature	700 °F
initial pressure	40.61 psi
initial kerogen concentration	0.7 lbmol/ft ³
rock compressibility	$3 \times 10^{-6}/\text{psi}$
thermal conductivity	7 Btu/ft/day/°F
residual oil saturation	0.05

In this compositional simulation, a total of 5 components are considered. The properties of each component are listed in Table 2. The pore space of oil shale formation is assumed to be initially saturated with nitrogen and carbon dioxide. Upon heating, the kerogens decompose to a number of hydrocarbon components, ranging from light oil components to heavy oil components. The initial in-situ gases (N₂ and CO₂) are produced from the central producer at early time. Eventually, the hydrocarbon products resulted from either kerogen decomposition or oil cracking are produced.

The reactions included in the model were determined based on the data of Wellington et al. (2005). These reactions were modified slightly to account for the components defined in the Green River oil shale. We use two components, IC₃₇ and IC₁₃, to represent the ‘heavy oil’ and ‘light oil’ in Wellington et al. (2005). The adapted chemical reactions and kinetic data are listed in Table 3.

Example Case Results

The oil and gas production rates are shown in Figure 1. We note that the initial production of gas is mostly in-situ N₂ or CO₂. The hydrocarbon gases are produced mainly after 100 days.

Table 2: Compositions and properties – Green River shale pyrolysis and lumped components

(a) Pyrolysis components from Green River oil shale (from Braun and Burnham 1990)					(b) Lumped components (IC represents lumped pseudo-component)				
Species Name	Molar Weight (g/mol)	Crit. Pressure (psi)	Crit. Temp (R)	Accentric Factor	Species Name	Molar Weight (g/mol)	Crit. Pressure (psi)	Crit. Temp (R)	Accentric Factor
CO ₂	44.01	1070.40	547.53	0.239	CO ₂	44.01	1070.40	547.53	0.239
N ₂	28.01	491.68	227.13	0.039	N ₂	28.01	491.68	227.13	0.039
CH ₄	16.04	667.18	342.33	0.011	IC ₂	30.07	668.48	519.74	0.008
CH _x	44.10	616.42	666.33	0.153	–	–	–	–	–
Oil-1	86	493.14	979.53	0.227	IC ₁₃	169.52	348.82	1287.65	0.365
Oil-2	114	426.42	1103.73	0.300	–	–	–	–	–
Oil-3	142	374.20	1218.93	0.307	–	–	–	–	–
Oil-4	177	333.59	1323.33	0.379	–	–	–	–	–
Oil-5	212	292.98	1413.33	0.426	–	–	–	–	–
Oil-6	261	253.82	1506.93	0.511	–	–	–	–	–
Oil-7	317	213.21	1595.13	0.594	IC ₃₇	465.83	135.69	1732.11	0.818
Oil-8	380	174.05	1674.33	0.664	–	–	–	–	–
Oil-9	464	133.44	1751.73	0.762	–	–	–	–	–
Oil-10	562	92.82	1793.13	0.941	–	–	–	–	–
Oil-11	703	92.82	1830.93	1.31	–	–	–	–	–

Table 3: Kinetic reactions in MDP-S case (adapted from Wellington et al., 2005)

No.	Reactions	Freq. Factor	Act. Energy (kJ/mol)
1	KER(s)→0.0096 IC ₃₇ +0.0178 IC ₁₃ +0.04475 IC ₂ +0.00541 CO ₂	3.74×10 ¹²	161.600
2	IC ₃₇ (g)→1.853 IC ₁₃ + 0.045 IC ₂	2.65×10 ²⁰	206.034
3	IC ₃₇ (o)→0.2063 IC ₉ + 2.365 IC ₂	6.25×10 ¹⁶	206.034
4	IC ₁₃ (g)→5.73 IC ₂	3.82×10 ²⁰	219.328
5	IC ₁₃ (o)→0.573 IC ₂	9.85×10 ¹⁶	219.328

The other simulation results are shown in Figure 2. We observe that the temperature of the reservoir increases because of heating at the two heaters at two ends. Initially, there is no oil in the reservoir. Upon heating, the kerogens decomposes to hydrocarbons and oil starts to form. The oil saturation first increases and then decreases, and so is the pressure. This is because the remaining of kerogen is ever decreasing.

Time Step Control

With the introduction of chemistry in the compositional simulation, the parameters used for time step control are of much difference than the traditional compositional simulation. The user may experience some time-step cut or small time steps. These situations are normal because the physics become much more complicated due to component appearing and disappearing.

Nevertheless, there are two ways to make smooth runs. One way is to tune the parameters of the time-step control. We know that the new time step is controlled by the changes in the unknowns over the previous time step using the equation

$$\Delta t^{n+1} = \Delta t^n \min \left[\frac{(1 + \omega)\eta_c}{\delta_c + \omega\eta_c} \right], \quad (2)$$

where Δt^{n+1} is the next time step, Δt^n is the current time step, ω is a tuning factor, δ_c is a parameter for each

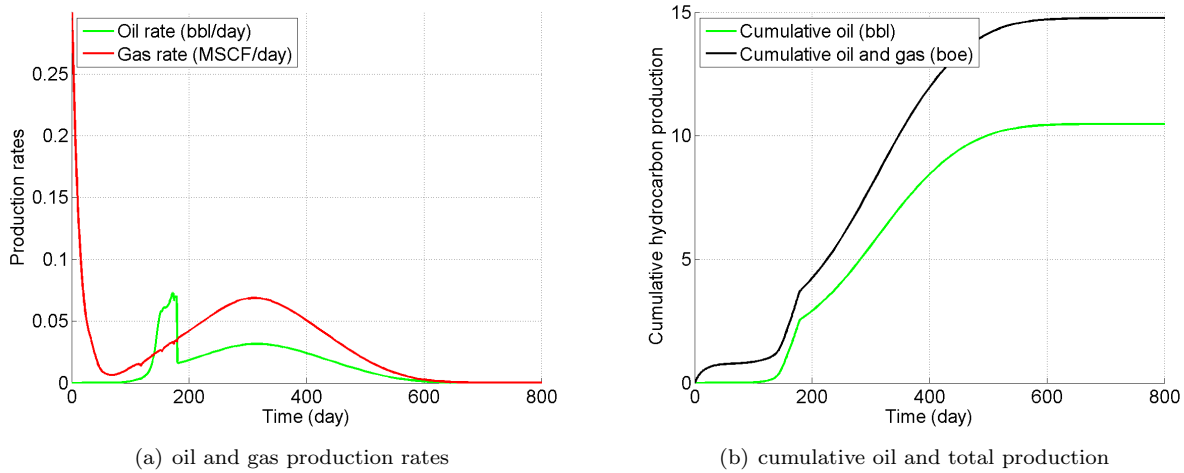


Figure 1: Oil and gas production results from example case

variable, η_c is the desired change for each variable, and the minimum is over all grid blocks (Cao, 2002). The key parameter affecting the convergence stability is the parameter η_c . Our numerical experiments show that the desired variable change when chemical reactions are present should be specified to be much smaller than in compositional simulations without reactions. Suggested parameter values for the in-situ upgrading simulations are listed in Table 4. The parameter of ω normally is tuned between 0 and 1. An alternative way to improve the GPRS performance in

Table 4: Example of time step control parameters used in GPRS

Parameters	Value (no reactions)	Value (with kinetics)
δ_c	0	0
ω	0.5	1
η for p	200 psi	10 psi
η for S_j	0.02	0.01
η for X_{ij}	0.02	0.001

terms of time step control is to use multi-time time step control. The usage of multi-time control has been documented previously. Our numerical experiments on this example case show that the user has to obtain good knowledge of the time step sizes in order to obtain good performance.

3.2 CO₂ Mineralization

A verification case was carried out to compare the results from GPRS with GEM-GHG Computer Modelling Group (2008), a commercial simulator. This comparison case is designed to verify the various modules implemented in GPRS, including the B-dot activity model, chemical equilibrium calculations, mineral kinetic laws, and the numerical solution algorithm. We note that GEM-GHG uses a formulation equivalent to the component-based formulation, while we apply the element-based formulation in this case.

Description of Reservoir

We consider a one-dimensional horizontal reservoir extending 306 m in the x direction and 3 m in both the y and z directions. The reservoir is discretized uniformly into 102 blocks. Initially, the reservoir is saturated with brine. We inject a pure CO₂ stream from the left-most block at constant bottomhole pressure (BHP). A producer under BHP

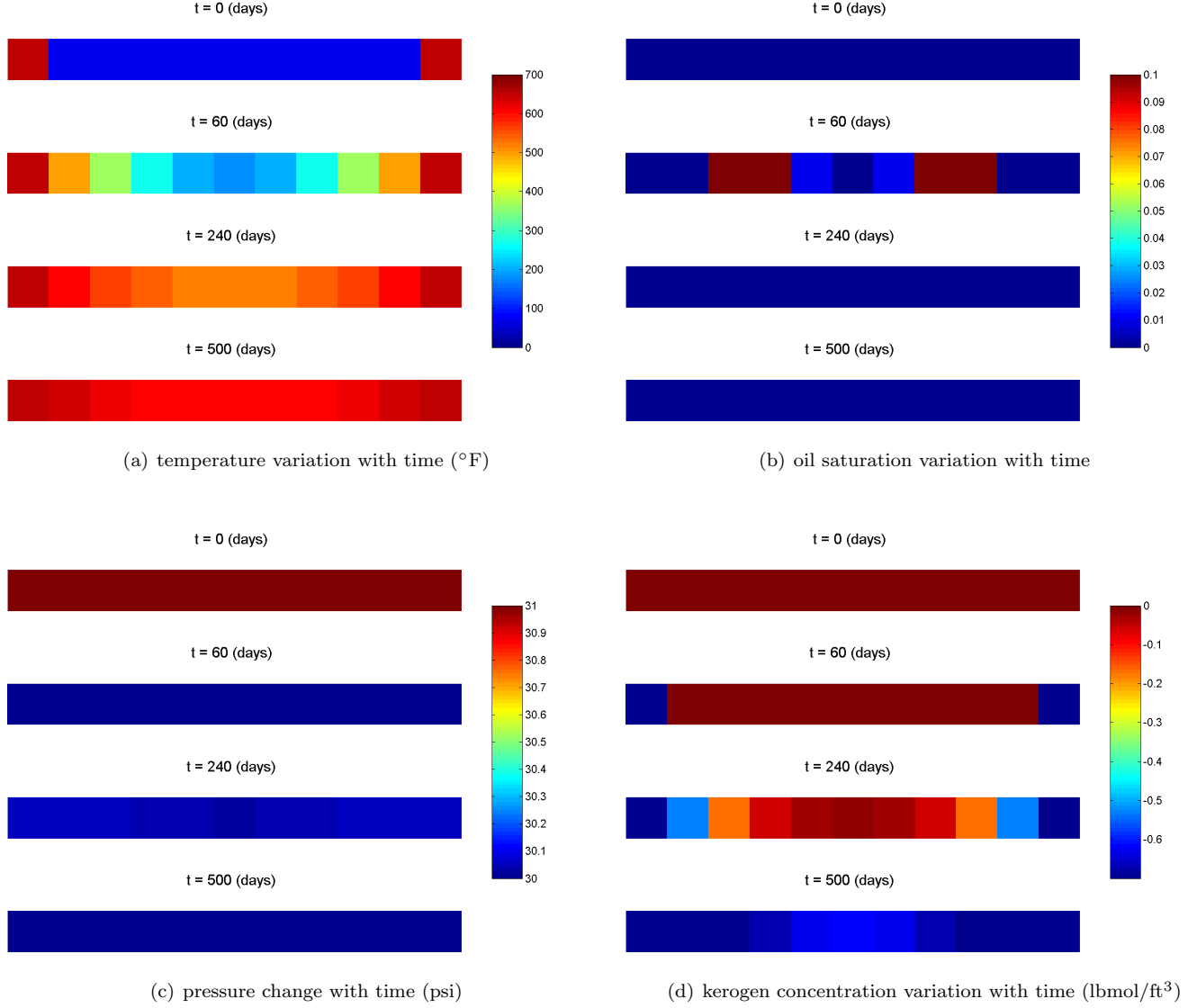


Figure 2: Top view of simulation results in base case

control is located at the right-most block to maintain injectivity. The relevant parameters for this problem are given in Table 5.

Mineral and Aqueous Reactions

This case involves eight minerals and 12 chemical reactions. The parameters associated with the ions are listed in Table 6. The initial molalities of the ions are obtained by simulating a batch system (one grid block) for 5,000 years to ensure that chemical equilibrium is honored at initial conditions. The chemical reactions and mineral kinetic data were specified in in Tables 7 and 8.

Simulation Results

Figures 3 and 4 present the ion molalities and mineral net changes after 50 days of injection. The symbols represent the results from GPRS and the lines represent the results from GEM-GHG. It is evident that the results from these

Table 5: Summary of input parameters for the verification case

Parameter	Value
grid (n_x, n_y, n_z)	(102, 1, 1)
grid block size	3 m \times 3 m \times 3 m
reservoir temperature	50 °C
initial pressure	3.46 MPa (502 psi)
porosity	0.10
permeability	$k_x=k_y=k_z=9.869 \times 10^{-14}$ m ² (100 md)
injector location	(1,1,1)
injector BHP	4.14 MPa (600 psi)
producer location	(102,1,1)
producer BHP	0.69 MPa (100 psi)

Table 6: Input parameters for each ion for the verification case

Ion symbol	charge	size (Å)	initial molality (mol/kg)
H ⁺	1	9	5.71E-07
Al ⁺⁺⁺	3	9	3.13E-12
Fe ⁺⁺	2	6	2.73E-04
SiO ₂ (aq)	0	3	4.73E-04
K ⁺	1	3	9.89E-03
Ca ⁺⁺	2	6	2.52E-02
Mg ⁺⁺	2	8	2.62E-03
HCO ₃ ⁻	-1	4.5	2.14E-03
CO ₃ ⁻⁻	-2	4.5	4.23E-07
OH ⁻	-1	3.5	4.49E-08
Al(OH) ₂ ⁺	1	5	1.28E-09

Table 7: Chemical reactions for CO₂ mineralization

No.	Reaction
(1)	CO ₂ (aq) + H ₂ O = H ⁺ + HCO ₃ ⁻
(2)	CO ₃ ⁻⁻ + H ⁺ = HCO ₃ ⁻
(3)	OH ⁻ + H ⁺ = H ₂ O
(4)	Al(OH) ₂ ⁺ + 2 H ⁺ = Al ⁺⁺⁺ + 2 H ₂ O
(5)	Annite + 10 H ⁺ = 3 Fe ⁺⁺ + 3 SiO ₂ (aq) + Al ⁺⁺⁺ + 6 H ₂ O + K ⁺
(6)	Anorthite + 8 H ⁺ = 4 H ₂ O + Ca ⁺⁺ + 2 Al ⁺⁺⁺ + 2 SiO ₂ (aq)
(7)	Calcite + H ⁺ = Ca ⁺⁺ + HCO ₃ ⁻
(8)	Chalcedony = SiO ₂ (aq)
(9)	Dolomite + 2 H ⁺ = Ca ⁺⁺ + Mg ⁺⁺ + 2 HCO ₃ ⁻
(10)	Illite + 8 H ⁺ = 5 H ₂ O + 0.6K ⁺ + 0.25Mg ⁺⁺ + 2.3Al ⁺⁺⁺ + 3.5SiO ₂ (aq)
(11)	Kaolinite + 6 H ⁺ = 5 H ₂ O + 2 Al ⁺⁺⁺ + 2 SiO ₂ (aq)
(12)	Siderite + H ⁺ = HCO ₃ ⁻ + Fe ⁺⁺

Table 8: Mineral formula, precipitation and dissolution parameters

Mineral	Formula	$\log_{10}(K)$ (mol/m ² /s)	Surf. Area (m ² /m ³)	$\log_{10}(K_{eq})$
Annite	AlKFe ₃ Si ₃ O ₁₀ (OH) ₂	-14.0	4400	28.61
Anorthite	CaAl ₂ Si ₂ O ₈	-12.0	88	25.82
Calcite	CaCO ₃	-8.80	88	1.60
Chalcedony	SiO ₂	-13.9	7128	-3.62
Dolomite	CaMg(CO ₃) ₂	-9.22	88	2.25
Illite	Mg _{0.25} K _{0.6} Al _{2.3} Si _{3.5} O ₁₂ H ₂	-14.0	26400	9.07
Kaolinite	Al ₂ Si ₂ O ₅ (OH) ₄	-13.0	17600	6.82
Siderite	FeCO ₃	-9.22	88	-0.37

two simulators are in very close agreement. We note that at 50 days, the injected CO₂ has flooded approximately 65% of the reservoir. The chemical system ahead of the CO₂ front is essentially not affected. This case provides a degree of verification of CO₂ mineralization modeling capabilities implemented in GPRS.

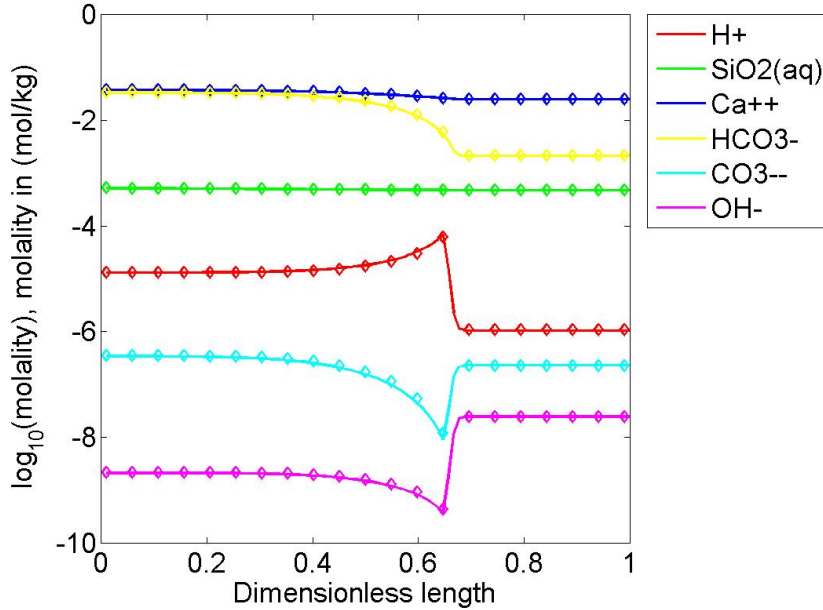


Figure 3: Comparison of ion molalities (mol/kg) from GPRS and GEM-GHG for 1-D case at 50 days. Symbols represent GPRS results, lines represent GEM-GHG results.

3.3 Preliminary Modeling of ECBM

The modeling of enhanced coal-bed methane can be achieved with the extensions of multi-component rock modeling and chemical reaction modeling, both of which are described in this document earlier. We now present a 1-D case model and its preliminary simulation results. We note that application of ECBM modeling with GPRS to 2-D and 3-D cases are yet to be explored.

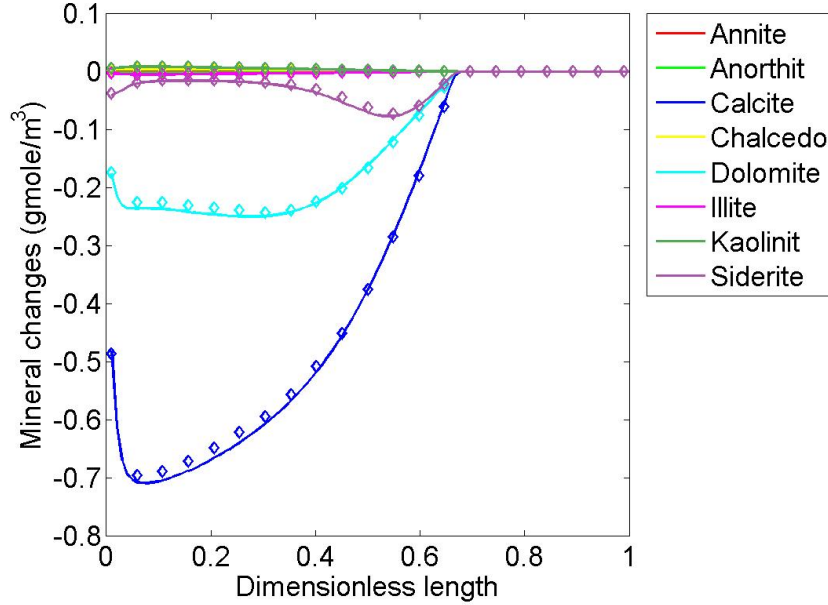


Figure 4: Comparison of mineral changes (mol/m^3) from GPRS and GEM-GHG for 1-D case at 50 days. Symbols represent GPRS results, lines represent GEM-GHG results.

Model Description

The 1-D reservoir is 100 m in x direction, 1 m in y direction and 1 m in z direction. There are 100 simulation blocks, each representing one cubic meter. The permeability is 10 md in all directions and the porosity is 0.2 in all blocks. There are three hydrocarbon components considered in the model; specifically, they are carbon dioxide, nitrogen and methane. The initial reservoir pore space is saturated with methane.

Adsorption

Adsorption and desorption are modeled as one reversible reaction. Initially, because there is only methane in the pore space, equilibrium is assumed between the free methane and adsorbed methane. In the simulation, we inject carbon dioxide from one end of reservoir and produce a mixture of gases from the other end. Both the injector and producer are modeled with constant BHP control. The reaction we used is $M(g) \leftrightarrow M(s)$, where M represents CO_2 , N_2 or CH_4 , and 'g' indicates the gaseous state and 's' indicates adsorbed state.

Simulation Results

Figure 5 shows the evolutions of gas phase compositions and concentrations of adsorbed components. The case clearly shows that carbon dioxide replaces methane in the gas phase and adsorbed (solid) phase. Meanwhile, the carbon dioxide in the adsorbed phase propagates with $\text{CO}_2(g)$ movement. Because the adsorption of CO_2 is a kinetic process, we observe that equilibrium between gaseous $\text{CO}_2(g)$ and adsorbed $\text{CO}_2(s)$ has not been reached at 50 days, though the pore space has filled with carbon dioxide at 50 days.

4 Conclusions and Future Work

The chemical modeling framework has been incorporated in GPRS. The chemical kinetics and equilibria have been implemented fully implicitly. Since the chemical reaction term has been discretized at the same time with the flow terms, the current chemical reaction modeling is fully-coupled with both fluid flow and phase equilibria.

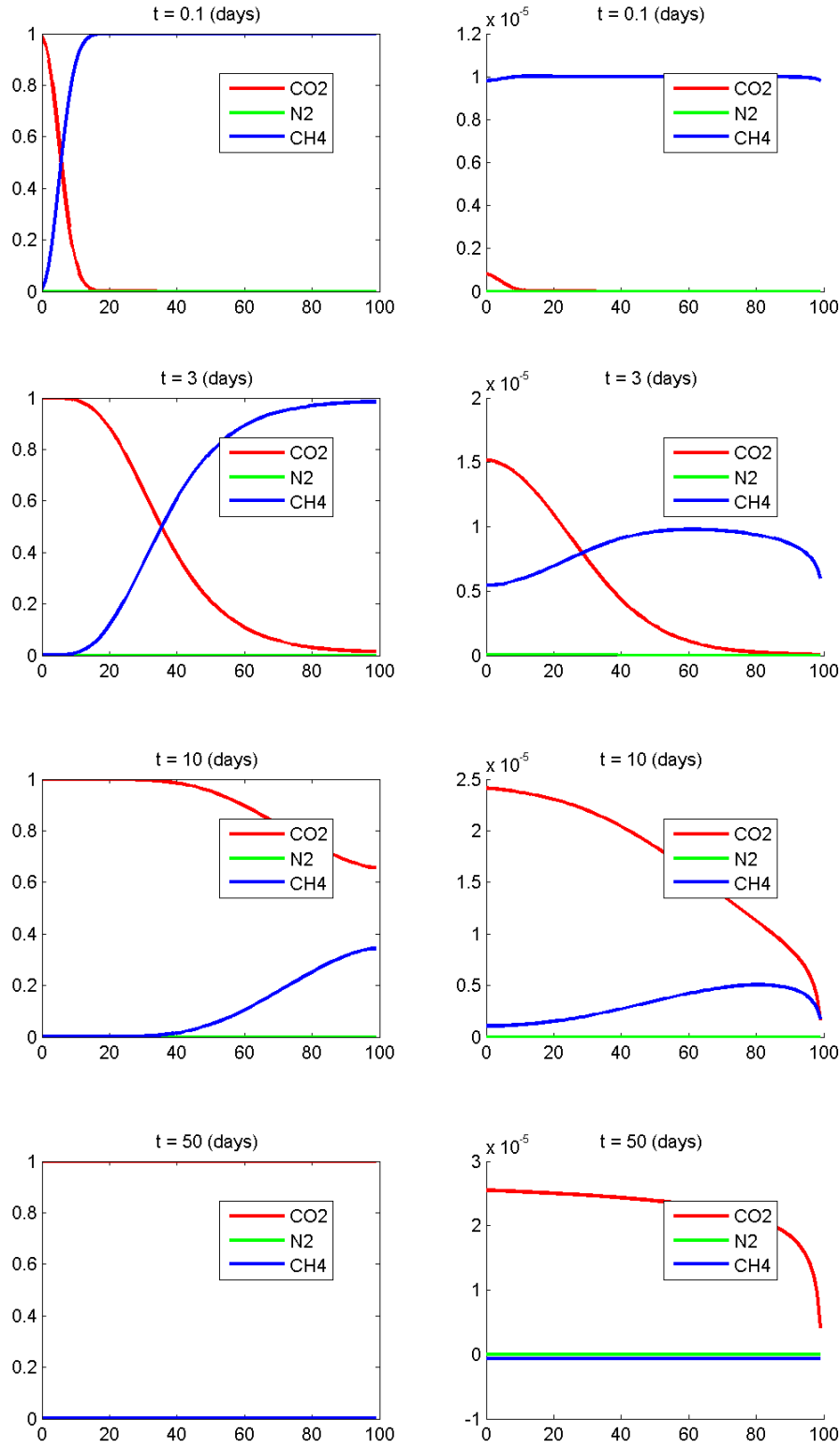


Figure 5: Component molar fractions (left) and adsorbed component concentrations (right) changes with time

The examples in this report demonstrate the GPRS's capability to simulate very complicated thermal-chemical compositional models. Aqueous-phase modeling and multi-component rock-phase modeling are also new to GPRS. If the problem involves both reactions and ions in aqueous phase (or minerals in rock phase), it is recommended to test the aqueous (or rock modeling) without reactions first. Once the model setup in GPRS can comfortably handle the phases (gas, oil, aqueous, and/or rock) correctly, the chemical reaction module is added to achieve multicomponent reactive transport simulations. We note that advanced thermal wells are required in the future to model realistic in-situ conversion problems. In addition, further investigation will be required to advance the performance of GPRS for chemical reaction cases.

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