MOOSE's PorousFlow module

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Abstract

This document describes the physics captured by MOOSE's PorousFlow module, as well as describing various numerical aspects and tips to ensure good convergence.

Each nontrivial test in the test suite *has its own separate documentation* and these should help users understand more clearly how to build a PorousFlow input file.

Within this document, black text indicates functionality that has been implemented and tested and red text indicates functionality that should be implemented by December 2017.

Contents

Chapter 1

Physical equations

The equations for heat flow, fluid flow, solid mechanics, and chemical reactions are defined here. Notation is introduced throughout, but summarised in Section 1.1. The Lagrangian coordinate system is used since it co-moves with the mesh.

1.1 Notation

Symbol	Units	Physical description
A^κ	kg.kg^{-1}	Mass of absorbed species κ per mass of rock grain material.
$\mathcal{A}^i_\beta$	symbolic	Chemical species i in phase β
A_m	m^2.L^{-1}	specific reactive surface area for mineral m
$\alpha_{\beta,L}$	m	Longitudinal dispersivity of phase β.
$\alpha_{\beta,T}$	m	Transverse dispersivity of phase β.
α_B	dimensionless	Biot coefficient. I believe we can treat this as a constant Material parameter.
α_f	K^{-1}	Volumetric coefficient of thermal expansion of the fluid.
α_T	K^{-1}	Volumetric coefficient of thermal expansion of the drained porous skeleton (ie, the porous rock without fluid, or which a fluid that is free to move in and out of the rock).
$\mathbf{b}$	m.s^{-2}	External force density acting on the porous solid. This could be gravitational acceleration, or a load-density from a platten.
β	dimensionless	Index representing phase. For example, β might parameterise liquid ($\beta = 0$), gas ($\beta = 1$) and NAPL ($\beta = 2$).
C_R	J.kg^{-1}.K^{-1}	Specific heat capacity of rock grains.
C_{ijkl}	Pa	Drained compliance tensor of the porous solid (ie, inverse of E_{ijkl}).
C^i_β	moles per litre	concentration of species i

Symbol	Units	Physical description
C_v	J.kg^{-1}.K^{-1}	Fluid specific heat capacity at constant volume.
C_p	J.kg^{-1}.K^{-1}	Fluid specific heat capacity at constant pressure.
χ_β^κ	kg.kg^{-1}	Mass fraction of component κ present in phase β.
$\mathcal{D}_\beta^\kappa$	m^2.s^{-1}	Fluid dispersion tensor for species κ in phase β.
$D_{\beta,L}^\kappa$	m^2.s^{-1}	Longitudional dispersion coefficient for species κ in phase β.
$D_{\beta,T}^\kappa$	m^2.s^{-1}	Transverse dispersion coefficient for species κ in phase β.
d_β^κ	m^2.s^{-1}	Molecular diffusion coefficient for component κ in phase β.
$\delta_{l\beta}$	dimenionless	Kronecker delta, unity if $\beta = l$, else zero.
$\mathcal{E}$	J.m^{-3}	Energy density of the rock-fluid system.
$\mathcal{E}_\beta$	J.kg^{-1}	Internal energy of fluid phase β. In the simplest case this is just $c_\beta T$, where c_β is the fluid's specific heat capacity.
ϵ_{ij}	dimensionless	Strain tensor of the porous solid $((\nabla_k u_l + \nabla_l u_k)/2)$.
$\epsilon_{ij}^{\text{elastic}}$	dimensionless	Elastic strain tensor of the porous solid. The total strain $\epsilon = \epsilon^{\text{elastic}} + \epsilon^{\text{plastic}}$.
$\epsilon_{ij}^{\text{plastic}}$	dimensionless	Plastic strain tensor of the porous solid. The total strain $\epsilon = \epsilon^{\text{elastic}} + \epsilon^{\text{plastic}}$.
η	dimensionless	exponent in rate expression
E_{ijkl}	Pa	"Drained" elasticity tensor of the porous skeleton (ie, this enters the stress-strain relation when fluid is allowed to freely drain from the skeleton, or when the skeleton is dry).
ϕ	dimensionless	Porosity of the solid.
ϕ_m	dimensionless	volume fraction of mineral in solid
$\mathbf{F}$	kg.s^{-1}.m^{-2}	Fluid flux. This is a sum of the advective (Darcy) flux, and a diffusive-and-dispersive flux.
$\mathbf{F}^T$	J.s^{-1}.m^{-2}	Heat flux. This is a sum of heat conduction through the rock-fluid system, and convection with the fluid.
$\mathbf{g}$	m.s^{-2}	Acceleration due to gravity. It is a vector pointing downwards (eg $(0, 0, -10)$).
γ_β^i	dimensionless	activity coefficient of species i in phase β
h_β	J.kg^{-1}	Specific enthalpy of fluid phase β. In the simplest case this is just $c_\beta T$ where c_β is the fluid's specific heat capacity.
H_κ	Pa	Henry coefficient for species κ which describes the solubility of the species in the aqueous phase.
I_m	mol.L^{-1}.s^{-1}	mineral reaction rate

Symbol	Units	Physical description
κ	dimensionless	Index representing species. For example, κ might parameterise water ($\kappa = 0$), air ($\kappa = 1$), and H_2 ($\kappa = 2$). It parameterises things that cannot be dcomposed into other species, but can change phase. For instance, sometimes it might be appropriate to consider air as a single species, while at other times it might be appropriate to consider it to be a mixture of nitrogen and oxygen ($\kappa = 0$ and $\kappa = 1$, say).
k	m^2	Permeability tensor of rock.
$k_{r,\beta}$	dimensionless	Relative permeability of phase β. This is a nonlinear function of the independent variables. Often it is just a function of the phase's saturation, but with Klinkenberg effects it will be a function of the gas pressure too. In the single-phase, fully-saturated case it is unity.
K	Pa	Bulk modulus of the drained porous skeleton. I think in the anisotropic situation $1/K == \delta_{ij}\delta_{kl}C_{ijkl}$.
K_β^i	depends on reaction	equilibrium constant for secondary species i in phase β
K_f	Pa	Bulk modulus of the fluid.
k_m	$mol.m^{-2}.s^{-1}$	mineral rate constant
Λ	s^{-1}	Radioactive decay rate of a fluid species
λ	$J.s^{-1}.m^{-1}.K^{-1}$	Thermal conductivity of the rock-fluid system ($J.s^{-1}.m^{-1}.K^{-1} = kg.m.s^{-3}.K^{-1}$). It is a tensorial quantity to allow modelling of anisotropic situations, and is a function of the rock and fluid-phase's thermal conductivities
λ_{dry}	$J.s^{-1}.m^{-1}.K^{-1}$	Thermal conductivity of the rock-fluid system when aqueous phase saturation is zero.
λ_{wet}	$J.s^{-1}.m^{-1}.K^{-1}$	Thermal conductivity of the rock-fluid system when aqueous phase saturation is unity.
λ_R	$J.s^{-1}.m^{-1}.K^{-1}$	Thermal conductivity of the rock grains.
λ_f	$J.s^{-1}.m^{-1}.K^{-1}$	Thermal conductivity of the fluid phase (single phase case).
M	$kg.m^{-3}$	Mass density
μ	Pa.s	Dynamic viscosity measured in Pa.s or $kg.m^{-1}.s^{-1}$. This is a nonlinear function of the independent variables.
ν	dimensionless	Fraction of plastic-deformation energy that becomes heat energy. Probably $\nu = 1$ is correct.
ν_β^{ij}	dimensionless	stoichiometric coeffcient of basis species j in equilibrium reaction for secondary species j
∇	m^{-1}	Spatial differential operator
Ω_m	dimensionless	mineral saturation ratio
P	Pa	Fluid porepressure
P_f	Pa	Measure of porepressure used in the effective stress. Often this is chosen to be $\sum_\beta S_\beta P_\beta$.
P_L	Pa	Langmuir pressure

Symbol	Units	Physical description
Φ_β^j	moles per litre	Total concentration of basis species j in phase β
q	kg.m^{-3}.s^{-1}	Fluid source
q^j	mol.L^{-1}.s^{-1}	source of chemical species
q^T	J.m^{-3}.s^{-1}	Heat source.
ρ	kg.m^{-3}	Fluid density
ρ_R	kg.m^{-3}	Density of rock grains (so that $(1-\phi)\rho_R$ is the density of the dry porous rock).
ρ_{mat}	kg.m^{-3}	The mass-density of the fluid-filled porous solid $\rho_{\text{mat}} = (1-\phi)\rho_R + \phi\sum_\beta S_\beta\rho_\beta$.
ρ_L	kg.m^{-3}	Langmuir density
S	dimensionless	Saturation
S_l	dimensionless	saturation of aqueous phase
σ_{ij}^{tot}	Pa	Total stress. An externally applied mechanical force will create a nonzero σ^{tot}, and conversely, resolving σ^{tot} into forces yields the forces on nodes in the finite-element mesh.
σ_{ij}^{eff}	Pa	Effective stress.
t	s	Time
T	K	Temperature.
$\tau_0\tau_\beta$	dimensionless	The phase tortuosity, which includes a porous-medium dependent factor τ_0 and a coefficient $\tau_\beta = \tau_\beta(S_\beta)$.
τ_L	s	Langmuir desorption time constant
θ	dimensionless	exponent in rate expression
$\mathbf{u}$	m.s^{-1}	Deformation vector of the porous solid.
$\mathbf{v}$	m.s^{-1}	Darcy velocity (volume flux)
$\mathbf{v}_s$	m.s^{-1}	Velocity of the solid $= \partial\mathbf{u}/\partial t$, where $\mathbf{u}$ is the solid mechanical displacement vector of the porous solid.
$\overline{V}_m$	L.mol^{-1}	molar volume

Table 1.1: Notation introduced throughout Section 1.

1.2 Fluid flow

Mass conservation for fluid species κ is described by the continuity equation

$$0 = \frac{\partial M^\kappa}{\partial t} + M^\kappa\nabla\cdot\mathbf{v}_s + \nabla\cdot\mathbf{F}^\kappa + \Lambda M^\kappa - q^\kappa \; . \tag{1.1}$$

Here M is the mass of fluid per volume of rock (measured in kg.m^{-3}), $\mathbf{v}_s$ is the velocity of the porous solid skeleton (measured in m.s^{-1}), $\mathbf{F}$ is the flux (a vector, measured kg.s^{-1}.m^{-2}), Λ is a radioactive decay rate, and q is a source (measured in kg.m^{-3}.s^{-1}).

The coupling to the solid mechanics is via the $M\nabla\cdot\mathbf{v}_s$ term, as well as via changes in porosity and permeability described in Section 3.14 and Section 3.13. Coupling to heat flow and chemical

reactions is via the equations of state used within the terms of Eqn (1.1), as well as the source term q^κ.

The species are parameterised by $\kappa = 1, \dots$. For example, κ might parameterise water, air, H_2, a solute, and so on. κ parameterises things which cannot be decomposed into other species, but can change phase. For instance, sometimes it might be appropriate to consider air as a single species (say $\kappa = 1$), while other times it might be apropriate to consider it to be a mixture of nitrogen and oxygen ($\kappa = 1$ and $\kappa = 2$). To model chemical precipitation, a solid phase, which is distinct from the porous skeleton, may also be used (its relative permeability will be zero: see below).

1.2.1 Mass density: M

The mass of species κ per volume of rock is written as a sum over all phases present in the system:

$$M^\kappa = \phi \sum_\beta S_\beta \rho_\beta \chi_\beta^\kappa + (1 - \phi) C^\kappa \tag{1.2}$$

The solid's porosity is ϕ. S_β is the saturation of phase β (solid, liquid, gas, NAPL). ρ_β is the density of phase β. χ_β^κ is the mass fraction of component κ present in phase β. The final term represents fluid absorption into the porous-rock skeleton: C^κ is the mass of absorbed species per volume of solid rock-grain material, and its dynamics is specified in Section 1.5.1.

The density ρ_β is a function of pressure, mass fraction, and so on, as described by the equation of state used (Chapter 3).

The saturation and mass fractions must obey

$$\sum_\beta S_\beta = 1 , \tag{1.3}$$

$$\sum_\kappa \chi_\beta^\kappa = 1 \quad \forall \beta . \tag{1.4}$$

1.2.2 Flux: F

The flux is a sum of advective flux and diffusive-and-dispersive flux:

$$\mathbf{F}^\kappa = \sum_\beta \chi_\beta^\kappa \mathbf{F}_\beta^{\text{advective}} + \mathbf{F}_{\text{diffusion+dispersion}}^\kappa . \tag{1.5}$$

Advection

Advective flux is governed by Darcy's law. Each phase is assumed to obey Darcy's law. Each phase has its own density, ρ_β, relative permeability $k_{r,\beta}$, viscosity μ_β, and pressure P_β. These

may all be nonlinear functions of the independent variables. With them, we can form the advective Darcy flux:

$$\mathbf{F}_\beta^{\text{advective}} = \rho_\beta \mathbf{v}_\beta = -\rho_\beta \frac{k\, k_{\text{r},\beta}}{\mu_\beta} (\nabla P_\beta - \rho_\beta \mathbf{g}) \tag{1.6}$$

In this equation $\mathbf{v}_\beta$ is the Darcy velocity (volume flux, measured in m.s^{-1}) in phase β. It is used below in the diffusive-and-dispersion flux too.

The absolute permeability is denoted by k and it is a tensor. The relative permeability[1] of phase β is denoted by $k_{\text{r},\beta}$. It is always a function of the saturation(s), but with Klinkenberg effects, it may also be a function of the gas pressure. Relative permeability can also be hysteretic, so that it depends on the history of saturation.

In some cirumstances $K_{ij}\nabla_j T$ is added to the above Darcy flux to model thermo-osmosis (with some K_{ij} tensor parameterising its strength), i.e. a gradient of temperature induces fluid flow.

Also note:

- The pressure in phase β is

$$P_\beta = P + P_{c,\beta} \tag{1.7}$$

  where P is the reference pressure (usually taken to be the gas phase), and $P_{c,\beta}$ is the capillary pressure (nonpositive if the reference phase is the gas phase). The capillary pressure is often a function of saturation, and various forms have been coded into the PorousFlow module: see Section 3.8. **The capillary pressure relationship used in a model can have a great bearing on both the speed of convergence and the results obtained.**

  The capillary pressure relationship can also be hysteretic, in that it can depend on the history of the saturation.

  The pressure in a gas phase is the sum of the gas partial pressures: $P_{\text{gas}} = \sum_\kappa P_{\text{gas}}^\kappa$. (The partial pressure of a gaseous species is $P_{\text{gas}}^\kappa = P_{\text{gas}} N^\kappa / N$ where N is the number of molecules. This is Dalton's law.) The partial pressure concept is reasonable for dilute gases, but is less useful for dense gases.

- The mass-fraction of a species in the aqueous phase is often computed using Henry's law:

$$\chi_{\text{aqueous}}^\kappa = P_{\text{gas}}^\kappa / H_\kappa \ , \tag{1.8}$$

  where H_κ is the Henry coefficient[2]. Occasionally this law is not accurate enough, and there are more complicated alternatives. Chapter 3 discusses various equations of state that include computations of Henry's coefficients.

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[1] In reality relative permeability is actually a tensor (for example it's usually different in lateral and vertical directions) but is most often treated as a scalar, since it's hard to get parameters for the tensorial case. In the PorousFlow module it is treated as a scalar.

[2] Unforuntately, the Henry coefficient has multiple definitions which makes looking up numerical values complicated.

- When a liquid and a gaseous phase exist, the simplest equation for vapour pressure is

$$P_{\text{vapour}} = P_{\text{sat}}(T) , \tag{1.9}$$

which is just the saturated vapour pressure of the liquid phase. This can set the temperature T from the gaseous pressure, or vice-versa, depending on the choice of independent variables. A more complicated alternative is the Kelvin equation for vapour pressure that takes into account vapour pressure lowering due to capillarity and phase adsorption affects

$$P_{\text{vapour}} = \exp\left(\frac{M_w P_{c,l}(S_l)}{\rho_l R(T + 273.15)}\right) P_{sat}(T) . \tag{1.10}$$

Here M_w is the molecular weight of water; $P_{c,l} = P_{c,l}(S_l) \leq 0$ is the capillary pressure — the difference between aqueous (liquid water) and gas phase pressures — a function of S_l; ρ_l is the aqueous (liquid water) density; R is the universal gas constant; T is the temperature; P_{sat} is the saturated vapour pressure of the bulk aqueous (liquid water) phase.

Diffusion and hydrodynamic dispersion

Diffusion and dispersion are proportional to the gradient of χ_β^κ. The TOUGH2 manual[3], in Appendix D, contains a nice discussion of diffusion-dispersion. Here we use the common expression

$$\mathbf{F}_{\text{diffusion+dispersion}}^\kappa = -\sum_\beta \rho_\beta \mathcal{D}_\beta^\kappa \nabla \chi_\beta^\kappa \tag{1.11}$$

Note $\mathbf{F}$ is a vector, $\mathcal{D}$ is a 2-tensor and ∇ a vector. The hydrodynamic dispersion tensor is

$$\mathcal{D}_\beta^\kappa = D_{\beta,T}^\kappa \mathcal{I} + \frac{D_{\beta,L}^\kappa - D_{\beta,T}^\kappa}{\mathbf{v}_\beta^2} \mathbf{v}_\beta \mathbf{v}_\beta , \tag{1.12}$$

where

$$D_{\beta,L}^\kappa = \phi \tau_0 \tau_\beta d_\beta^\kappa + \alpha_{\beta,L} |\mathbf{v}|_\beta , \tag{1.13}$$
$$D_{\beta,T}^\kappa = \phi \tau_0 \tau_\beta d_\beta^\kappa + \alpha_{\beta,T} |\mathbf{v}|_\beta . \tag{1.14}$$

These are called the longitudinal and transverse dispersion coefficients. d_β^κ is the molecular diffusion coefficient for component κ in phase β. $\tau_0 \tau_\beta$ is the tortuosity which includes a porous medium dependent factor τ_0 and a coefficient $\tau_\beta = \tau_\beta(S_\beta)$, and α_L and α_T are the longitudinal and transverse dispersivities. It is common to set the hydrodynamic dispersion to zero by setting $\alpha_{\beta,T} = 0 = \alpha_{\beta,L}$.

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[3]TOUGH2 Users's Guide, Version 2. Karsten Pruess, Curt Oldenburg, George Moridis. Earth Sciences Division, LBNL, Univ California, Berkeley. November 1999, revised August 2011. LBNL-43134 (revised).

1.3 Heat flow

Energy conservation for heat is described by the continuity equation

$$0 = \frac{\partial \mathcal{E}}{\partial t} + \mathcal{E}\nabla \cdot \mathbf{v}_s + \nabla \cdot \mathbf{F}^T - \nu(1-\phi)\sigma_{ij}^{\text{eff}}\frac{\partial}{\partial t}\epsilon_{ij}^{\text{plastic}} - q^T \tag{1.15}$$

Here $\mathcal{E}$ is the energy per unit volume in the rock-fluid system, $\mathbf{v}_s$ is velocity of the porous solid skeleton, $\mathbf{F}^T$ is the heat flux, ν describes the ratio of plastic-deformation energy that gets transferred to heat energy, σ_{ij}^{eff} is the effective stress (see Eqn (1.25)), $\epsilon_{ij}^{\text{plastic}}$ is the plastic strain, and q^T is a heat source.

The coupling to the solid mechanics is via the $\mathcal{E}\nabla \cdot \mathbf{v}_s$ term, the $\nu(1-\phi)\sigma_{ij}^{\text{eff}}\frac{\partial}{\partial t}\epsilon_{ij}^{\text{plastic}}$ term, as well as via changes in porosity and permeability described in Section 3.14 and Section 3.13 Coupling to the fluid flow and chemical reactions is via the equations of state used within the terms of Eqn (1.15), as well as the source term q^T. Joule-Thompson effects[4] may be included via the fluid properties (Chapter 3).

Here it is assumed the liquids and solid are in local thermal equilibrium i.e. there is a single local temperature in all phases. If this doesn't hold, one is also normally in the high-flow regime where the flow is non-Darcy as well.

Sometimes a term is added that captures the thermal power due to volumetric expansion of the fluid, $K\beta T\nabla \cdot \mathbf{v}$, where K is the bulk modulus of the fluid or solid, β is the thermal expansion coefficient, and $\mathbf{v}$ is the Darcy velocity. This is not included in the Porous Flow module currently.

1.3.1 Energy density: $\mathcal{E}$

The energy per unit volume is

$$\mathcal{E} = (1-\phi)\rho_R C_R T + \phi\sum_\beta S_\beta \rho_\beta \mathcal{E}_\beta + \sum_\kappa (1-\phi)\rho^R \mathcal{E}_{\text{abs}\,\kappa} A^\kappa \tag{1.16}$$

The notation is: porosity ϕ; grain density ρ_R; specific heat capacity of rock C_R; temperature T; saturation of phase S_β (solid, liquid, gas, NAPL); density of phase ρ_β; internal energy in phase $\mathcal{E}_\beta$; internal energy of absorbed species $\mathcal{E}_{\text{abs}\,\kappa}$.

1.3.2 Heat flux: $\mathbf{F}^T$

The heat flux is a sum of heat conduction and convection with the fluid:

$$\mathbf{F}^T = -\lambda\nabla T + \sum_\beta h_\beta \mathbf{F}_\beta \ . \tag{1.17}$$

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[4]See for instance Eqn (1) of SA Mathias et al. "Analytical solution for Joule-Thomson cooling during CO_2 geo-sequestration in depleted oil and gas reservoirs" http://www.osti.gov/scitech/servlets/purl/985333

Here λ is the tensorial thermal conductivity of the rock-fluid system, which is a function of the thermal conductivities of rock and fluid phases. Usually λ will be diagonal but in anisotropic porous materials it may not be. The specificy enthalpy of phase β is denoted by h_β, and $\mathbf{F}_\beta$ is the advective Darcy flux.

1.3.3   A simple example

Consider just the fluid terms of the heat-flow Eqn (1.15). For notational simplicity, consider just one fully-saturated phase so that $\mathcal{E} = \phi \rho_\beta \mathcal{E}_\beta$. Here $\mathcal{E}_\beta$ has SI units J.kg^{-1}. Also consider the fluid flux with no conduction so that $\mathbf{F}^T = h_\beta \rho_\beta \mathbf{v}_\beta$. Integrating Eqn (1.15) over an arbitrary volume Ω, and employing integration by parts yields

$$0 = \frac{\partial}{\partial t} \int_\Omega \phi \rho_\beta \mathcal{E}_\beta + \int_{\partial \Omega} h_\beta \rho_\beta \mathbf{n} \cdot \mathbf{v}_\beta \ . \tag{1.18}$$

The first term on the RHS is the heat energy of the fluid in the fixed volume Ω. Since the volume is fixed, it is appropriate to use the specific heat at constant volume, C_v^β, in the expression for the fluid energy-per-mass:

$$\mathcal{E}_\beta = C_v^\beta T \ . \tag{1.19}$$

The second term on the RHS describes the change in heat energy due to fluid entering or leaving the volume with velocity $\mathbf{v}_\beta$. This change in heat energy can be decomposed into two parts in the following way. Imagine that fluid is entering the volume Ω. Firstly, imagine a new, slightly bigger volume Ω' that contains all the fluid that will enter Ω during the small time dt. The heat energy contained in the fluid within the small volume $\Omega' - \Omega$ is the extra heat energy added during fluid flow. This is simply

$$\int_{\partial \Omega} C_v T \rho \mathbf{n} \cdot \mathbf{v} \mathrm{d}t \ . \tag{1.20}$$

We now know the total heat energy within the new volume, Ω'. The second step must be to squash this new volume back to the original Ω. This costs energy, which is just calculated using force$\times$distance. The force must be equal to the fluid pressure (multiplied by the infinitesimal area element), and the distance is exactly $\mathbf{n} \cdot \mathbf{v} \mathrm{d}t$, meaning the second contribution is

$$\int_{\partial \Omega} P \mathbf{n} \cdot \mathbf{v} \mathrm{d}t \ . \tag{1.21}$$

Collecting these ideas together Eqn (1.15) reads, in this simple example

$$0 = \frac{\partial}{\partial t} \phi \rho C_v T + \nabla \cdot \left(C_v T + \frac{P}{\rho} \right) \rho \mathbf{v} \ . \tag{1.22}$$

The superscript β denoting the phase number has been omitted.

Finally, two small observations might be useful.

1. Given the above discussion, it is clear that the enthalpy can be written as

$$h_\beta = \mathcal{E}_\beta + P_\beta/\rho_\beta \ . \tag{1.23}$$

2. For an ideal gas, $P/\rho = RT$, so the enthalpy,

$$h_\beta = C_\mathrm{v} T + \frac{P}{\rho} = C_{\beta,\mathrm{v}} T + RT = C_{\beta,\mathrm{p}} T \ , \tag{1.24}$$

where $C_{\beta,\mathrm{p}}$ is the specific heat capacity at constant pressure of the ideal gas phase.

1.4   Solid mechanics

Most of the solid mechanics used by the Porous Flow module is handled by the Tensor Mechanics module. This section provides a brief overview, concentrating on the aspects that differ from pure solid mechanics.

Denote the total stress tensor by σ^tot. An externally applied mechanical force will create a nonzero σ^tot, and conversely, resolving σ^tot into forces yields the forces on nodes in the finite-element mesh.

Denote the effective stress tensor by σ^eff. It is defined by

$$\sigma_{ij}^\mathrm{eff} = \sigma_{ij}^\mathrm{tot} + \alpha_B \delta_{ij} P_f \ . \tag{1.25}$$

The notation is as follows.

- P_f is a measure of porepressure. In single-phase, fully-saturated situations it is traditional to use $P_f = P_\beta$. However, for multi-phase situations $P_f = \sum_\beta S_\beta P_\beta$ is also used. Yet other expressions involve Bishop's parameter.

- α_B is the "Biot coefficient". This obeys $0 \le \alpha_B \le 1$. For a multi-phase system, the Biot coefficient is often chosen to be $\alpha_B = 1$. The Biot coefficient is interpreted physically by the following. If, by pumping fluid into a porous material, the P_f porepressure is increased by ΔP_f, and at the same time a mechanical external force applies an incremental pressure equaling $\alpha_B \Delta P_f$, then the volume of the porous solid remains static. (During this process, the porevolume and porosity will change, however, as quantified in Section 3.14.)

It is assumed that the elastic constitutive law reads

$$\sigma_{ij}^\mathrm{eff} = E_{ijkl}(\epsilon_{kl}^\mathrm{elastic} - \delta_{kl}\alpha_T T) \ , \tag{1.26}$$

with α_T being the thermal expansion coefficient of the drained porous skeleton, and $\epsilon_{kl} = (\nabla_k u_l + \nabla_l u_k)/2$ being the usual total strain tensor (u is the deformation of the porous solid),

which can be split into the elastic and plastic parts, $\epsilon = \epsilon^{\text{elastic}} + \epsilon^{\text{plastic}}$, and E_{ijkl} being the elasticity tensor (the so-called "drained" version). The generalisation to large strain is obvious. The inverse of the consistutive law is

$$\epsilon_{ij}^{\text{elastic}} - \delta_{kl}\alpha_T T = C_{ijkl}\sigma_{ij}^{\text{eff}} \ , \tag{1.27}$$

with C being the compliance tensor.

It is assumed that the conservation of momentum is

$$\rho_{\text{mat}}\frac{\partial v_s^j}{\partial t} = \nabla_i \sigma_{ij}^{\text{tot}} + \rho_{\text{mat}} b_j = \nabla_i \sigma_{ij}^{\text{eff}} - \alpha_B \nabla_j P_f + \rho_{\text{mat}} b_j \ , \tag{1.28}$$

where $\mathbf{v}_s = \partial\mathbf{u}/\partial t$ is the velocity of the solid skeleton, ρ_{mat} is the mass-density of the material (this is the "undrained" density: $\rho_{\text{mat}} = (1-\phi)\rho^R + \phi\sum_\beta S_\beta\rho_\beta$), and b_j are the components of the external force density (for example, the gravitational acceleration). Here any terms of $O(v^2)$ have been explicitly ignored , and it's been assumed that to this order the velocity of each phase is identical to the velocity of the solid skeleton (otherwise there are terms involving $\partial\mathbf{F}/\partial t$ on the left-hand side).

It is assumed that the *effective stress not the total stress* enters into the consitutive law (as above), and the plasticity, and the insitu stresses, and almost everywhere else. One exception is specifying Neumann boundary conditions for the displacements where the total stresses are being specified, as can be seen from Eqn (1.28). Therefore, MOOSE will use effective stress, and not total stress, internally. If one needs to input or output total stress, one must subtract $\alpha_B\nabla_j P_f$ from MOOSE's stress.

1.5   Chemical reactions

1.5.1   Adsorption and desorption

The fluid mass Eqn 1.2 contains contributions from adsorped species: C'^κ is the mass of absorped species per volume of solid rock-grain material. Its dynamics involves no advective flux terms, as PorousFlow assumes that the adsorped species are trapped in the solid matrix. The governing equation is

$$0 = \frac{\partial}{\partial t}(1-\phi)C^\kappa + (1-\phi)C^\kappa\nabla\cdot\mathbf{v}_s + L^\kappa \ . \tag{1.29}$$

The $(1-\phi)$ terms account for the porosity of the solid skeleton (so $(1-\phi)C'^\kappa$ is the mass of adsorped species per volume of porous skeleton), the coupling to the solid mechanics is via the second term, and L^κ governs the adsorption-desorption process.

Currently, PorousFlow assumes that C'^κ is a primary MOOSE variable (that is, defined in the [Variables] block of the MOOSE input file). This is in contrast to the remainder of PorousFlow where the primary variables can be arbitrary (so that variable switching and persistent variables can be used in difficult problems). Usually C'^κ will have `family=MONOMIAL` and `order=CONSTANT`.

PorousFlow assumes that L follows the Langmuir form:

$$L = \frac{1}{\tau_L}\left(C - \frac{\rho_L P}{P_L + P}\right) \tag{1.30}$$

Here L is the mass-density rate (kg.m^{-3}.s^{-1}) of material moving from the adsorbed state to the porespace. The notation is as follows.

- ρ_L is the so-called Langmuir density, which is adsorbed-gas-mass per volume of solid rock-grain material (kg.m^{-3}). In terms of the often used Langmuir volume, V_L, it is $\rho_L = V_L \times$ (gas density at STP).

- P_L is the Langmuir pressure (Pa)

- P is the relevant phase pressure (which will be the pressure of the gas phase). Currently, PorousFlow assumes that P is a primary MOOSE variable (that is, defined in the [Variables] block of the MOOSE input file). This is in contrast to the remainder of PorousFlow where the primary variables can be arbitrary.

- τ_L is the time constant. Two time constants may be defined: one for desorption, and one for adsorption, so

$$\tau_L = \begin{cases} \tau_{L,\text{ desorption}} & \text{if } C > \frac{\rho_L P}{P_L + P} \\ \tau_{L,\text{ adsorption}} & \text{otherwise} \end{cases} \tag{1.31}$$

A mollifier may also be defined to mollify the step-change between desorption and adsorption.

1.5.2 General geochemistry

The first step in defining the chemistry is to choose a set of basis species in the liquid phase, such that every other chemical species, including minerals (now all referred to as secondary species) can be expressed via combinations of these basis species.

Let j index the basis species in the liquid phase, denoted by $\mathcal{A}_l^j$, and i index the secondary species, $\mathcal{A}_\beta^i$. Then the reactions that connect these are given by

$$\mathcal{A}_\beta^i \rightleftharpoons \sum_j \nu_\beta^{ji} \mathcal{A}_l^j \tag{1.32}$$

where the ν_β^{ji} are the stoichiometric coefficients.

Now define the total concentration of basis species j in fluid phase β, denoted Ψ_β^j, by

$$\Psi_\beta^j = \delta_{l\beta} C_l^j + \sum_i \nu_\beta^{ji} C_\beta^i \tag{1.33}$$

where the C_β^i is the concentration of secondary species i in phase β, C_l^j is the concentration of basis species j in the liquid phase, and $\delta_{l\beta}$ is the Kronecker delta ($= 1$ if $\beta = l$, else $= 0$).

The concentrations of the secondary species C_β^i are obtained from the basis species concentrations by mass action equations of the form

$$C_\beta^i = \frac{K_\beta^i}{\gamma_\beta^i} \prod_j (\gamma_l^j C_l^j)^{\nu_\beta^{ji}} \tag{1.34}$$

where K_β^i is the equilibrium constant and γ_β^i is the activity coefficient of species i in phase β. There are various possible relationships for computing activity coefficients that depend both on properties of that species (e.g. valence and ionic radius) and the total ionic strength (which depends on all the ion concentrations).

In all these, the concentration units are moles per litre.

Now define the total concentration accumulation of basis species j by M^j, which is given by

$$M^j = \phi \sum_\beta S_\beta \Psi_\beta^j \tag{1.35}$$

where the sum in Eqn (1.35) is over the fluid phases only, and as before ϕ is the porosity and S_β is the phase saturation.

The continuity equation is then

$$0 = \frac{\partial M^j}{\partial t} + M^j \nabla \cdot \mathbf{v}_s + \nabla \cdot \mathbf{F}^j - q^j . \tag{1.36}$$

Here $\mathbf{F}$ is the flux (a vector, measured mol.s^{-1}.L^{-1}), and q^j is a source (measured in mol.L^{-1}.s^{-1}).

For minerals indexed by m one has

$$\frac{\partial \phi_m}{\partial t} = \overline{V}_m I_m \tag{1.37}$$

where ϕ_m is the volume fraction of that mineral, $\overline{V}_m$ is the molar volume, and I_m is the mineral reaction rate. The porosity is related to the mineral volume fractions by

$$\phi = 1 - \sum_m \phi_m \tag{1.38}$$

The total flux $\mathbf{F}^j$ in Eqn (1.36) is given by

$$\mathbf{F}^j = \sum_\beta (\mathbf{v}_\beta - \phi S_\beta \mathcal{D}_\beta^j \nabla) \Psi_\beta^j \tag{1.39}$$

which incorporates the advective and diffusive transport of chemical species in the sum over the fluid phases. $\mathcal{D}_\beta^j$ is the hydrodynamic dispersion tensor in phase β of species j, including

effects of tortuosity, dispersion etc, as in Eqn (1.12). It's common to assume the this tensor is the same for all species in that phase.

First define the mineral saturation ratio Ω_m by

$$\Omega_m = K_m^{-1} \prod_j (C^j)^{\nu_{mj}} (\gamma^j)^{\nu_{mj}} \tag{1.40}$$

where K_m is the equilibrium constant for the reaction. There are a variety of possible rate expressions. One of the simplest is to write

$$I_m = \pm k_m A_m |1 - \Omega_m^\theta|^\eta \tag{1.41}$$

where the rate I_m is positive for dissolution and negative for precipitation, A_m is the specific reactive surface area per litre for mineral m, and the exponents θ and η are specific to each mineral reaction, but are often both taken to be unity. The rate constant k_m (mole/(m^2 s)) is a function of temperature.

1.6   Example use case: Single-phase single-component fully-saturated fluid

Since the number of phases and components is unity, the subscripts β and κ may be dropped. Since $\chi = 1$ there is no diffusion nor dispersion. Assume that the relative permeability is unity. Mass conservation of the fluid (Eqns (1.1), (1.2), (1.5), (1.6), (1.11), (1.12), (1.13) and (1.14)) reads

$$0 = \frac{\partial}{\partial t} \phi \rho + \nabla \cdot (\phi \rho \mathbf{v}_s) - \nabla_i \cdot \left(\frac{\rho k_{ij}}{\mu} (\nabla_j P - \rho g_j) \right) - q^{\text{fluid}} , \tag{1.42}$$

where P is the porepressure of the fluid and will be one of MOOSE's variables in this case.

Make the following assumptions:

- the fluid's internal energy is $\mathcal{E} = cT$, where c is the fluid's specific heat capacity;

- the fluid's specific enthalpy is $h = cT$;

- the rock-fluid thermal conductivity is a weighted sum of the rock-grain and fluid thermal conductivities: $\lambda = (1 - \phi)\lambda^R + \phi \lambda^f$

The heat-energy conservation equation (Eqn (1.15), (1.16) and (1.17)) is

$$\begin{aligned} 0 = & \frac{\partial}{\partial t} \left((1 - \phi) \rho_R C_R T + \phi \rho c T \right) + \nabla \cdot \left(((1 - \phi) \rho_R C_R T + \phi \rho c T) \mathbf{v}_s \right) \\ & - \nabla \cdot \left(((1 - \phi) \lambda^R + \phi \lambda^f) \nabla T \right) - \nabla \cdot \left(cT \frac{\rho k_{ij}}{\mu} (\nabla_j P - \rho g_j) \right) - q^{\text{T}} , \end{aligned} \tag{1.43}$$

where T is the temperature of the fluid-rock system and will be one of MOOSE's variables in this case. Under the additional assumptions that the following parameters are constant (or very nearly so): ϕ, ρ_R, C_R, c, λ^R, λ^f, this equations reads

$$0 = C\frac{\partial T}{\partial t} + C\nabla \cdot (T\mathbf{v}_s) - \lambda\nabla^2 T - \nabla \cdot \left(\rho c T \frac{k_{ij}}{\mu}(\nabla_j P - \rho g_j)\right) - q^{\mathrm{T}} , \qquad (1.44)$$

with $C = (1 - \phi)\rho_R C_R + \phi\rho c$ being the macroscopic heat capacity.

Eqns (1.42) and (1.44) with $\mathbf{v}_s = 0$ are the equations of FALCON. Using the assumption $\rho = \rho_0 \exp(P/K_f - \alpha_T^f T)$, where K_f is the constant bulk modulus of the fluid, and α_T^f is its constant thermal expansion coefficient, these two equations are those of FLAC's THM.[5]

The effective stress is given in Eqn (1.25), with $P_f = P$. The elastic constitutive equation is Eqn (1.26). Conservation of momentum is given in Eqn (1.28), with $\rho_{\mathrm{mat}} = (1 - \phi)\rho_R + \phi\rho$. The variables are the 3 displacements (in 3 dimensional problems), u_i.

The evolution of porosity is given in Eqn (3.18). In many situations of interest, the change in porosity is very small.

In summary, the variables for this case can be the porepressure P, the temperature T, and the three displacements u_i.

The following parameters depend, in principle, on the porepressure, temperature and (derivatives of) the displacements: porous-rock insitu permeability tensor k_{ij}; rock-grain density ρ_R; rock-grain specific heat capacity C_R; rock-grain thermal conductivity λ^R; fluid density ρ; fluid viscosity μ; fluid thermal conductivity λ^f; fluid specific heat capacity c. All these can be coded into a suite of Materials, as described in Chapter 3.

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[5]There is one possible inconsistency: FLAC's Eqn(12) of FLAC7.0 "Thermal Analysis (2011) writes $\beta = n\beta_f + (1 - n)\beta_g$, whereas the formulation here would give $\beta = n\beta_f + (\alpha_B - n)\beta_g$. FLAC has a habit of sneakily putting $\alpha_B = 1$ without saying, because some of their formulation is only correct to $\alpha_B = 1$, so I'm not sure whether this is FLAC's error/assumption, or an error in the porosity evolution equation Eqn (3.18) here.

Chapter 2

Boundaries and line-sinks

2.1 Boundaries

MOOSE's Dirichlet and Neumann boundary conditions enable simulation of simple scenarios. The Porous Flow module includes a very flexible boundary condition that allows many different scenarios to be modelled. The boundary condition is built by adding various options to a basic sink in the following way.

The basic sink is

$$s = f(t, x) \, , \tag{2.1}$$

where f is a MOOSE Function of time and position on the boundary. If $f > 0$ then the boundary condition will act as a sink, while if $f < 0$ the boundary condition acts as a source. If applied to a fluid-component equation, the function f has units kg.m^{-2}.s^{-1}. If applied to the heat equation, the function f has units J.m^{-2}.s^{-1}. These units are potentially modified if the extra building blocks enumerated below are used.

The basic sink may be multiplied by a MOOSE Functions of the pressure of a fluid phase *or* the temperature:

$$s = f(t, x) \times g(P^{\beta}) \quad \text{or} \quad s = f(t, x) \times g(T) \, . \tag{2.2}$$

Here the units of $f \times g$ are kg.m^{-2}.s^{-1} (for fluids) or J.m^{-1}.s^{-1} (for heat). Some commonly use forms have been hard-coded into the Porous Flow module for ease of use in simulations:

- a piecewise linear function (for simulating fluid or heat exchange with an external environment via a conductivity term, for instance);

- a half-gaussian (for simulating evapotranspiration, for instance)

- a half-cubic (for simulating evapotranspiration).

In addition, the sink may be multiplied by any or all of the following quantities

- Fluid relative permeability

- Fluid mobility ($k_{ij}n_in_jk_r\rho/\nu$, where n is the normal vector to the boundary)

- Fluid mass fraction

- Fluid enthalpy

- Fluid internal energy

- Thermal conductivity

It is likely that multiplication by generalised concentrations will also be needed.

2.1.1 Example: fixing fluid porepressures using the PorousFlowSink

Frequently in PorousFlow simulations fixing fluid porepressures using Dirichlet conditions is inappropriate.

1. Physically a Dirichlet condition corresponds to an environment outside a model providing a limitless source (or sink) of fluid and that does not happen in reality.

2. The Variables used may not be porepressure, so a straightforward translation to "fixing porepressure" is not easy.

3. The Dirichlet condition can lead to extremely poor convergence as it forces areas near the boundary close to unphysical or unlikely regions in parameter space.

It is advantageous to think of what the boundary condition is physically trying to represent before using Dirichlet conditions, and often a PorousFlowSink is more appropriate to use. For instance, at the top of a groundwater-gas model, gas can freely enter the model from the atmosphere, and escape the model to the atmosphere, which may be modelled using a PorousFlowSink. Water can exit the model if the water porepressure increases above atmospheric pressure, but the recharge if porepressure is lowered may be zero. Again this may be modelled using a PorousFlowSink.

When fixing porepressures (or temperatures) using a PorousFlowSink, what should the "conductance" be? Consider an imaginary environment that sits at distance L from the model. The imaginary environment provides a limitless source or sink of fluid, but that fluid must travel through the distance L between the model and the imaginary environment. The flux of fluid from the model to this environment is (approximately)

$$f = \frac{\rho k_{nn}k_{\mathrm{r}}}{\mu}\frac{P - P_{\mathrm{e}}}{L} \ . \tag{2.3}$$

A similar equation holds for temperature (but in PorousFlow simulations the heat is sometimes supplied by the fluid, in which case the appropriate equation to use for the heat may be the

above equation multiplied by the enthalpy). Here k_{nn} is the permeability of the region between the model and the imaginary environment, k_{r} is the relative permeability in this region, ρ and μ are the fluid density and viscosity. The environment porepressure is P_{e} and the boundary porepressure is P.

If $L \sim 0$ this effectively fixes the porepressure to $P \sim P_{\mathrm{e}}$, since f is very large otherwise (physically: fluid is rapidly removed or added to the system by the environment to ensure $P = P_{\mathrm{e}}$). If $L \sim \infty$ the boundary flux is almost zero and does nothing.

Eqn (2.3) may be implemented in a number of ways. A `PorousFlowPiecewiseLinearSink` may be constructed that models
$$f = C(P - P_{\mathrm{e}}) \, , \tag{2.4}$$
that is, with `pt_vals = '-1E9+`P_{e}` `P_{e}` 1E9+`P_{e}`'` and `multipliers = '-C`$\times$`1E9 0 C`$\times$`1E9'` (the `1E9` is just an example: the point is that it should be much greater than any expected porepressure). The numerical value of the conductance, C, is $\rho k_{nn} k_{\mathrm{r}} / \mu / L$, must be set at an appropriate value for the model.

Alternately, a `PorousFlowPiecewiseLinearSink` may be constructed that has `use_mobility = true` and `use_relperm = true`, and then $C = 1/L$. This has three advantages: (1) the MOOSE input file is simpler; (2) MOOSE automatically chooses the correct mobility and relative permeability to use; (3) these parameters are appropriate to the model so it reduces the potential for difficult numerical situations occuring.

Finally, if P_{e} is varying over the boundary, the flux should be split
$$f = CP - CP_{\mathrm{e}} \, . \tag{2.5}$$

Two PorousFlowSinks may be used. The first term is a `PorousFlowPiecewiseLinearSink` as just described (with $P_{\mathrm{e}} = 0$). The second term is a plain `PorousFlowSink` with a `flux_function` that is exactly equal to P_{e}.

2.1.2   Example: injection of fluid at a fixed temperature

A boundary condition corresponding to injection of fluid at a constant rate at a fixed temperature could involve: (1) using a Dirichlet condition for temperature; (2) using $f = -1$ without any multiplicative factors. More complicated examples with heat and fluid injection and production are detailed in the test suite documentation `newton_cooling` and `sinks`.

2.1.3   Fluids that both enter and exit the boundary

Commonly, if fluid or heat is exiting the porous material, multiplication by relative permeaility, mobility, mass fraction, enthalpy or thermal conductivity is necessary, while if fluid or heat is entering the porous material this multiplication is not necessary. Two sinks can be constructed

in a MOOSE input file: one involving "production" which is only active for $P > P_\mathrm{e}$ using a Piecewise-linear sink (here P_e is the environmental pressure); and one involving "injection", which is only active for $P < P_\mathrm{e}$ using a piecewise-linear sink multiplied by the appropriate factors.

2.2   Line sinks

Polyline sinks and sources are modelled as sequences of discrete points:

$$\text{polyline} \sim \{x_0, \ x_1, \ x_2, \ldots, x_N\} \ . \tag{2.6}$$

The sink is

$$s = \sum_i f(P_i) w_i \delta(x - x_i) \ . \tag{2.7}$$

Here s is a volume source, measured in kg.m^{-3}.s^{-1} (or J.m^{-3}.s^{-1} for heat flow), which when integrated over the finite element yields just the sink "strength", f, which has units kg.s^{-1} for fluid flow, or J.s^{-1} for heat flow. The strength, f, is a function of porepressure or temperature, and may involve other quantities, as enumerated below. The convention followed is:

- A sink has $s > 0$. This removes fluid or heat from the simulation domain.

- A source has $s < 0$. This adds fluid or heat to the simulation domain.

The input parameters for each PorousFlow line sink involve a plaintext file whose lines are space-separated quantities:

$$\texttt{w_i x_i y_i z_i} \tag{2.8}$$

The weighting terms, w_i, are for user convenience, but for the Peaceman borehole case they are the borehole radius at point x_i.

The basic sink may be multiplied by any or all of the following quantities

- Fluid relative permeability

- Fluid mobility $(k_r \rho / \nu)$

- Fluid mass fraction

- Fluid enthalpy

- Fluid internal energy

That is, f in Eqn (2.7) may be replaced by $f k_r$, $f \times$mobility, etc. (The units of $f k_r$, $f \times$mobility, etc, are kg.s^{-1} for fluid flow, or J.s^{-1} for heat flow.) All these additional multiplicative factors are evaluated at the nodal positions, not at point x_i, to ensure superior numerical convergence (see Sec 4.2). For instance, a fluid sink may extract fluid at a given rate, and therefore in a simulation that includes, the same sink multiplied by fluid enthalpy should be applied to the temperature variable.

2.2.1 Poly-line sinks as functions of porepressure or temperature

`PorousFlowPolyLineSinks` are a special case of the general line sink. The function, f in Eqn (2.7) is assumed to be a piecewise linear function of porepressure or temperature. In addition, a multiplication by the line-length associated to x_i is also performed. Specifically:

$$f(P_i) = \tfrac{1}{2} \left(|x_i - x_{i-1}| + |x_i - x_{i+1}| \right) L(P_i) \ , \tag{2.9}$$

where L is a piecewise-linear function, specified by the user in the MOOSE input file.

These types of sinks are useful in describing groundwater—surface water interactions via streams and swamps. Often a riverbed conductance, measured in kg.Pa^{-1}.s^{-1} is defined, which is

$$C = \frac{k_{zz}\rho}{L\mu} L_{\text{seg}} W_{\text{seg}} \ . \tag{2.10}$$

Here k_{zz} is the vertical component of the permeability tensor, ρ is the fluid density, μ is the fluid viscosity, and L is a distance variable related to the riverbed thickness. The other parameters are L_{seg} and W_{seg}, which are, respectively, the length and width of the segment of river that the point x_i is representing. The multiplication by L_{seg} is already handled by Eqn (2.9), and the other terms of C will enter into the piecewise linear function, L. Three standard types of L are used in groundwater models.

- A perennial stream, where fluid can seep from the porespace to the stream, and vice versa. Then $L \propto (P - P_{\text{atm}})$, where the proportionality constant involves the terms in C, and P_{atm} involves the river stage height.

- An ephemral stream, where fluid can only seep from the porespace to the stream, but not viceversa has $L \propto (P - P_{\text{atm}})$ if $P > P_{\text{atm}}$, and zero otherwise. This is a pure sink since $s > 0$ always.

- A rate-limited stream, where fluid can exchange between the groundwater and stream, but the rate is limited. This can be modelled by using a piecewise linear L that does not exceed given limits.

2.2.2 Peaceman Boreholes

Wellbores are implemented using the method first described by Peaceman[1] Here f is a special function (measured in kg.s^{-1} in standard units) defined in terms of the pressure at a point at the wall of the wellbore (which is an input parameter)

$$P_{\text{wellbore}}(x_i) = P_{\text{bot}} + \gamma \cdot (x_i - x_i^{\text{bot}}) \ . \tag{2.11}$$

The form of f is

$$f(P_i, x_i) = W \left| C(P_i - P_{\text{wellbore}}) \right| \frac{k_{\text{r}}\rho}{\mu} (P_i - P_{\text{wellbore}}) \tag{2.12}$$

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[1]DW Peaceman "Interpretation of well-block pressures in numerical reservoir simulation with nonsquare grid blocks and anisotropic permeability" Society of Petroleum Engineers of AIME, June 1983, pp 531–543

For boreholes that involve heat only, the P in the above expressions should be replaced by the temperature.

There are a number of parameters in these expressions:

- P_{bot} is an input parameter. It is the pressure at the bottom of the wellbore.

- x_i^{bot} is the position of the bottom of the wellbore.

- γ is a weight vector pointing downwards (product of fluid density and gravity). This means that $P_{\text{wellbore}}(x_i)$ will be the pressure at point x_i in the wellbore, due to gravitational head. If these gravitational effects are undesirable, the user may simply specify $\gamma = (0, 0, 0)$.

- k_{r}, ρ, and μ are the fluid relative permeability, density and viscosity. Hence the term $k_{\text{r}}\rho/\mu$ is the mobility, so users should choose to multiply by the mobility when using `PorousFlowPeacemanBorehole`. Recall that all the multiplicative factors, including mobility, are evaluated at the nodal positions, not the position x_i. This ensures superior numerical convergence.

- In the PorousFlow implementation C is called the "character" of the wellbore. There are two standard choices (note that f depends only on the absolute value $|C|$):

    - $C = 1$ for $P > P_{\text{wellbore}}$, and zero otherwise. In this case the wellbore is called a "production" wellbore, and it acts as a sink, removing fluid from the porespace.

    - $C = -1$ for $P < P_{\text{wellbore}}$, and zero otherwise. In this case the wellbore is called an "injection" wellbore, and it acts as a source, adding fluid to the porespace.

    Generalising, C may be chosen so that $|C| \neq 1$, which is useful for time-varying borehole strengths. The above two choices are generalised to: if $C > 0$ the wellbore is active only for $P > P_{\text{wellbore}}$ (and has zero strength otherwise); if $C < 0$ the wellbore is active only for $P < P_{\text{wellbore}}$.

- The function W is called the well-constant of the wellbore, and is measured in units of length^3.

Peaceman described the form of W by performing 2D analytical and numerical calculations to obtain the following formulae

$$W = 2\pi\sqrt{\kappa_{xx}\kappa_{yy}}L_z/\ln(r_e/r_{\text{bh}}) \,, \tag{2.13}$$

In this formula: the borehole is oriented along the z direction; κ_{xx} and κ_{yy} are the diagonal components of the permeability tensor in the (x, y) plane; L_z is the length of the borehole, r_{bh} is the borehole radius (an input parameter, which is encoded in the plaintext file of points: see Eqn (2.8)); and, r_e is the effective borehole radius. For a cell-centred finite-difference approach, Peaceman found that

$$r_e = 0.28 \frac{\sqrt{\sqrt{\kappa_{xx}/\kappa_{yy}}L_x^2 + \sqrt{\kappa_{yy}/\kappa_{xx}}L_y^2}}{(\kappa_{xx}/\kappa_{yy})^{1/4} + (\kappa_{yy}/\kappa_{xx})^{1/4}} = 0.2 \frac{\sqrt{\frac{1}{2}\sqrt{\kappa_{xx}/\kappa_{yy}}L_x^2 + \frac{1}{2}\sqrt{\kappa_{yy}/\kappa_{xx}}L_y^2}}{\frac{1}{2}(\kappa_{xx}/\kappa_{yy})^{1/4} + \frac{1}{2}(\kappa_{yy}/\kappa_{xx})^{1/4}} \,. \tag{2.14}$$

Here L_x and L_y are the finite-difference spatial sizes. Other authors have generalised Peaceman's approach to writing W for different geometrical situations. Some of these are contained in the article by, Chen and Zhang[2], where they show that for a finite element situation with square elements of size L, the borehole at a nodal position, and isotropic permeability

$$r_e = 0.113L \ . \tag{2.15}$$

Note that the 0.113 is substantially different to Peaceman's 0.2, demonstrating that this method of introducing wellbores dependent on the geometry. The user may specify this quantity via the `re_constant` input parameter (which defaults to Peaceman's 0.28).

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[2]Z Chen and Y Zhang "Well flow models for various numerical methods" International Journal of Numerical Analysis and Modelling 6 (2009) 375–388

Chapter 3

Equations of state and other functions

This chapter briefly outlines the Porous Flow Materials.

3.1 Brine

A high-precision equation of state for brine can be used to obtain the following quantities:

1. density
2. viscosity
3. internal energy
4. enthalpy

3.2 CO_2

A high-precision equation of state for CO_2 can be used to obtain the following quantities:

1. density
2. viscosity
3. internal energy
4. enthalpy

3.3   Water and steam

A high-precision equation of state for water and steam can be used to obtain the following quantities:

1. density

2. viscosity

3. internal energy

4. enthalpy

3.4   An ideal gas

The following quantities can be obtained for an ideal gas

1. density

2. viscosity

3. internal energy

4. enthalpy

3.5   Methane

A high-precision equation of state for methane can be used to obtain the following quantities:

1. density

2. viscosity

3. internal energy

4. enthalpy

3.6 A simplified fluid

Simplified fluid properties:

1. density $\rho = \rho_0 \exp(P/K_f - \alpha_f T)$, where K_f (the bulk modulus) and α_f (the thermal expansion coefficient) are constant.

2. viscosity is constant

3. internal energy $\mathcal{E} = C_v T$, where C_v (the specific heat capacity at constant volume) is constant.

4. enthalpy $h = C_p T$, where C_p (the specific heat capacity at constant pressure) is constant.

5. Constant thermal conductivity

3.7 CO$_2$ and brine

3.8 Capillary pressure relationships

3.8.1 Van Genuchten

van Genuchten's capillary-pressure relationship[1] is

$$S_{\text{eff}} = \begin{cases} 1 & \text{if } P \geq 0 \text{ ,} \\ (1 + (-\alpha P)^{1/(1-m)})^{-m} & \text{if } P < 0 \text{ .} \end{cases} \tag{3.1}$$

or

$$P_c = \begin{cases} 0 & \text{if } S_{\text{eff}} >= 1.0 \text{ ,} \\ \frac{1}{\alpha}(S_{\text{eff}}^{-1/m} - 1)^{1-m} & \text{if } S_{\text{eff}} < 1 \end{cases} \tag{3.2}$$

The effective saturation has been denoted by S_{eff} and P is the porepressure, which is the *negative* of the capillary pressure: $P = -P_c$. Here α and m are user-defined parameters. The parameter m must satisfy

$$0 < m < 1 \text{ .} \tag{3.3}$$

Sometimes the van Genuchten function is defined in terms of the parameter

$$n = \frac{1}{1-m} > 1 \text{ .} \tag{3.4}$$

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[1]van Genuchten, M. Th., "A closed for equation for predicting the hydraulic conductivity of unsaturated soils" Soil Sci. Soc., 44, 892-898 (1980)

In van Genuchten's paper, he finds good fits with experimental data for various soils and rock when the parameter m ranges between about 0.5 and 0.9 (meaning $2 < n < 10$, roughly), and α is beween $4 \times 10^{-5}\,\mathrm{Pa}^{-1}$ and $2 \times 10^{-4}\,\mathrm{Pa}^{-1}$. Figure 3.1 shows the shape of the van Genuchten suction, P_c, as a function of S_{eff}.

Numerically there are three important features of Eqn (3.1).

1. S_{eff} is a monotonically decreasing function of P_c, which is necessary for a unique solution.

2. $P_c \to \infty$ as $S_{\mathrm{eff}} \to 0$. As mentioned above, this is not justifiable physically, but numerically it is extremely advantageous over $P_c \to P_c^0 < \infty$, as this latter version often causes algorithms to "get stuck" around $S_{\mathrm{eff}} = 0$. As also mentioned above, because of the low relative permeability around S_{eff}, physically realistic problems rarely explore the $S_{\mathrm{eff}} \sim 0$ region.

3. $S_{\mathrm{eff}} \to 1$ and $\mathrm{d}S_{\mathrm{eff}}/\mathrm{d}P_c \to 0^+$ as $P_c \to 0$, for all m. This ensures that there is continuity in the porepressure, P, and the derivative $\mathrm{d}S/\mathrm{d}P$ around full saturation (remember that by definition $S_{\mathrm{eff}} = 1$ for $P_c < 0$). Also $\mathrm{d}^2 S_{\mathrm{eff}}/\mathrm{d}P_c^2 \to 0$ as $P_c \to 0^+$ if $m > 0.5$.

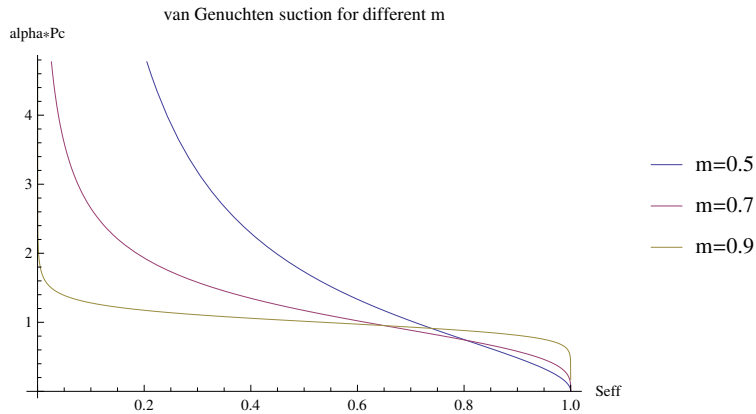I encourage users to set $m > 0.5$.

Figure 3.1: αP_c as a function of S_{eff} as given by van Genuchten's expression Eqn (3.1). Three values of m are shown: 0.5, 0.7 and 0.9 (the $m = 0.5$ case has largest P_c around $S_{\mathrm{eff}} \sim 0$).

A modification of Eqn (3.1) is available where S_{eff} is replaced by $S_{\mathrm{eff}}r$ and P_c by $P_c - P_c(r)$. Here $0 < r \leq 1$ is a scale factor. This means the derivative $\mathrm{d}S_{\mathrm{eff}}/\mathrm{d}P_c \neq 0$ as $S_{\mathrm{eff}} \to 1$. Occasionally setting $r < 1$ is advantageous in fully-saturated 2-phase simulations that have the two porepressures as their independent nonlinear variables.

3.8.2 Broadbridge-White

The Broadbridge-White[2] capillarity relationship valid for small K_n is

$$S_{\text{eff}} = S_n + (S_s - S_n)\frac{c}{1 + L(x)} \ . \tag{3.5}$$

where

$$x = (c-1)e^{c-1-cP/\lambda} \ , \tag{3.6}$$

and $L(x)$ is the Lambert W-function that satisfies $L(z)e^{L(z)} = z$. This is of limited use in real simulations, and is only used in the Porous Flow module for comparison with the analytical solutions of Broadbridge and White, and Warrick, Lomen and Islas[3] for multi-phase infiltration and drainage problems.

3.8.3 Rogers-Stallybrass-Clements

The Rogers-Stallybrass-Clements capillary relationship[4] is

$$S_{\text{eff}} = \frac{1}{\sqrt{1 + \exp((P_c - A)/B)}} \ , \tag{3.7}$$

when the oil viscosity is exactly twice the water viscosity. This is of limited use in real simulations, and is only used in the Porous Flow module for comparison with the analytical solutions offered by the authors for multi-phase infiltration and drainage problems.

3.9 Density

For simple calculations with water, the fluid bulk modulus, B, may be taken to be constant, so that the fluid density is

$$\rho = \rho_0 e^{P/B} \ , \tag{3.8}$$

where P is the fluid pressure. It is common to use $\rho_0 = 1000\,\text{kg.m}^{-3}$ and $B = 2\,\text{GPa}$.

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[2]P Broadbridge, I White "Constant rate rainfall infiltration: A versatile nonlinear model, 1 Analytical solution". Water Resources Research 24 (1988) 145–154.

[3]AW Warrick, DO Lomen and A Islas, "An analytical solution to Richards' Equation for a Draining Soil Profile", Water Resources Research 26 (1990) 253–258.

[4]C Rogers, MP Stallybrass and DL Clements "On two phase filtration under gravity and with boundary infiltration: application of a Backlund transformation" Nonlinear Analysis, Theory, Methods and Applications 7 (1983) 785–799

3.10 Tortuosity and diffusion coefficients

The tortuosity may be constant, or it may follow the Millington-Quirk[5] form

$$\tau_\beta = \phi^{1/3} S_\beta^{10/3}$$

(3.9)

The molecular diffusion coefficients, d_β^κ, are assumed to be constant.

3.11 Effective fluid pressure

The effective fluid pressure used in the definition of the fluid effective stress Eqn (1.25) is

$$P = \sum_\beta S_\beta P_\beta .$$

(3.10)

3.12 Enthalpy and energy-density

The specific enthalpy h_β, for a phase β, may be defined using one of the high-precision equation of states (eg see Section 3.3), or the relationship

$$h_\beta = \mathcal{E}_\beta + aP_\beta/\rho_\beta .$$

(3.11)

It is usually appropriate to use $a = 1$, however for comparison with other codes it may be useful to use $a = 0$.

The internal energy density $\mathcal{E}_\beta$ for a phase may be defined using one of the high-precision equation of states, or the relationship

$$\mathcal{E}_\beta = C_v T .$$

(3.12)

may be used.

3.13 Permeability

The porous-material's insitu permeability tensor can be constant, or it can take one of the following forms in which k_{ij}^0 is the i, j component of a user-defined tensor:

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[5]Millington and Quirk, Permeability of Porous Solids, Trans. Faraday Soc., 57, 1200- 1207, 1961

3.13.1 Tensor multiplied by scalar variable

$$k_{ij} = k_{ij}^0 k_0 \; , \tag{3.13}$$

where k_0 is a scalar variable that could be a function of depth, for example.

3.13.2 Exponential

$$k_{ij} = k_{ij}^0 e^{a\phi} \; , \tag{3.14}$$

where ϕ is the porosity, and a is a user-defined constant.

3.13.3 Kozeny-Carman

Using the Kozeny-Carman relationship[6]

$$k_{ij} = k_{ij}^0 \frac{\phi^n}{(1-\phi)^m} \; . \tag{3.15}$$

Here n and m are user-defined constants.

3.13.4 Permeability with a solid phase

A solid phase (from chemical precipitation, for instance) can be included in the framework described herein simply by setting its relative permeability to zero. However, in this case, the absolute permeability of the porous material should be

$$k = k^{\text{without solid phase}}(1 - S_{\text{s}})^2 \; , \tag{3.16}$$

where S_{s} is the solid-phase saturation.

3.14 Porosity

Porosity may be fixed at a constant value, or it may be a function of the effective porepressure, the volumetric strain and/or the temperature, as discussed below.

The evolution of the porosity[7] is governed by

$$\frac{\partial \phi}{\partial t} = (\alpha_B - \phi)\frac{\partial}{\partial t}\left(\epsilon_{ii}^{\text{total}} - \alpha_T T\right) + \frac{(1-\alpha_B)(\alpha_B - \phi)}{K}\frac{\partial P_f}{\partial t} \; . \tag{3.17}$$

---

[6]Oelkers 1996: Reviews in Mineralogy v. 34, p. 131-192

[7]This is a generalisation of Eqn(18) in Y Chen, C Zhou and L Jing "Modeling coupled THM processes of geological porous media with multiphase flow: Theory and vlidation against laboratory and field scale experiments" Computers and Geotechnics 36 (2009) 1308-1329

Here K is the bulk modulus of the drained porous skeleton: $1/K = \delta_{ij}\delta_{kl}C_{ijkl}$. This has solution

$$\phi = \alpha_B + (\phi_0 - \alpha_B) \times \exp\left(\frac{\alpha_B - 1}{K}(P_f - P_f^{\mathrm{ref}}) - \epsilon_{ii}^{\mathrm{total}} + \alpha_T(T - T^{\mathrm{ref}})\right) , \tag{3.18}$$

where ϕ_0 is the porosity at reference porepressure, zero elastic strain and reference temperature. Note this porosity can become negative, and an option for ensuring positivity is detailed below.

The evolution of porosity is motivated further in the appendix Chapter C.

Without porepressure effects, the correct expression for porosity as a function of volumetric strain and temperature is

$$\phi = 1 + (\phi_0 - 1) \times \exp\left(-\epsilon_{ii}^{\mathrm{total}} + \alpha_T(T - T^{\mathrm{ref}})\right) . \tag{3.19}$$

These expressions may be modified to include the effects of plasticity.

The exponential expressions Eqn (3.18) and Eqn (3.19) can yield negative porosity values, which are unphysical. To ensure positivity of ϕ, PorousFlow offers the following option. First write both equations in the form

$$\phi = A + (B - A)\exp(x) . \tag{3.20}$$

In deriving specific forms for A, B and x, above, it has been assumed that x is small. Since physically $1 \geq A > B > 0$, for $x < 0$ the porosity will be physically meaningful, but for $x \gg 0$, ϕ can become negative. For example, for positive volumetric strain ($x < 0$) the porosity is always physically meaningful. However, when the porous material is squashed with negative and large volumetric strain ($x \gg 0$) the porosity can become negative.

Define

$$C = \log(A/(A - B)) . \tag{3.21}$$

Then, for $x > 0$, the above expression for ϕ is replaced by

$$\phi = A + (B - A)\exp\left(C(1 - \exp(-x/C))\right) \geq 0 . \tag{3.22}$$

At first glance this expression may appear rather obscure. It has been constructed to satisfy the following requirements:

1. As $x \to 0$, $\phi \to B$, which is necessary for continuity at $x = 0$.

2. As $x \to \infty$, $\phi \to 0$, which is physically desireable.

3. The expression is monotonically decreasing, which is both physically desirable and computationally desirable (otherwise there may be non-unique solutions in a PorousFlow simulation).

4. Finally, at $x = 0$, its derivative is $\phi' = B - A$, as desired from continuity of the derivative at $x = 0$.

3.15 Relative permeability relationships

The relative permeability of a phase is a function of its effective saturation:

$$S_{\text{eff}}(S) = \frac{S - S_{\text{res}}^{\beta}}{1 - \sum_{\beta'} S_{\text{res}}^{\beta'}} \tag{3.23}$$

In this equation S_{res}^{β} is the residual saturation for phase β. If $S_{\text{eff}} < 0$ then the relative permeability is zero, while if $S_{\text{eff}} > 1$ then the relative permeability is unity. Otherwise, the relative permeability is given by the expressions below.

3.15.1 Constant

$$k_{\text{r}} = C \ . \tag{3.24}$$

This is not recommended because there is nothing to discourage phase disappearance, which manifests itself in poor convergence. Usually $k_{\text{r}}(S) \to 0$ as $S \to 0$ is a much better choice.

3.15.2 Corey

$$k_{\text{r}} = S_{\text{eff}}^{n} \ . \tag{3.25}$$

where n is a user-defined quantity.

3.15.3 Broadbridge-White

$$k_{\text{r}} = K_n + \frac{K_s - K_n}{(c - 1)(c - S_{\text{eff}})} S_{\text{eff}}^2 \ . \tag{3.26}$$

3.15.4 van Genuchten and cut van Genuchten

$$k_{\text{r}} = \sqrt{S_{\text{eff}}} \left(1 - (1 - S_{\text{eff}}^{1/m})^m \right)^2 \ . \tag{3.27}$$

This has the numerical disadvantage that its derivative as $S_{\text{eff}} \to 1$ is crappy. This means that simulations where the saturation oscillates around $S_{\text{eff}} = 1$ do not converge well. Therefore, a "cut" version of the van-Genuchten expression is also offered, which is almost definitely indistinguishable experimentally from the original expression:

$$k_{\text{r}} = \begin{cases} \text{van Genuchten} & \text{for } S_{\text{eff}} < S_c \\ \text{cubic} & \text{for } S_{\text{eff}} \geq S_c \ . \end{cases} \tag{3.28}$$

Here the cubic is chosen so that its value and derivative match the van Genuchten expression at $S = S_c$, and so that it is unity at $S_{\text{eff}} = 1$.

3.15.5 FLAC

$$k_{\mathrm{r}} = (n+1)S_{\mathrm{eff}}^{n} - nS_{\mathrm{eff}}^{n+1} \; . \tag{3.29}$$

This has the distinct advantage over the Corey formulation that its derivative is continuous at $S_{\mathrm{eff}} = 1$.

3.16 Thermal conductivity

Currently the Porous Flow module implements two simple approaches to the functional dependence of thermal conductivity on the rock and fluid-phase conductivities.

3.16.1 Ideal

A "wet" thermal conductivity, λ_{wet}, and a "dry" thermal conductivity λ_{dry}, are defined (both of which are tensors), and

$$\lambda = \lambda_{\mathrm{dry}} + S_{\mathrm{aqueous}}^{n}(\lambda_{\mathrm{wet}} - \lambda_{\mathrm{dry}}) \tag{3.30}$$

where S_{aqueous} is the aqueous phase saturation, and n is a user-defined exponent.

3.16.2 Linear variation with porosity

For the single phase, fully saturated case, a linear variation of thermal conductivity with porosity is defined:

$$\lambda = \lambda_R(1 - \phi) + \lambda_f \phi \tag{3.31}$$

where λ_R is the thermal conductivity of the rock grains and λ_f is the thermal conductivity of the fluid phase.

The dependence of fluid thermal conductivity on temperature may be handled within the fluid property modules (to accommodate the kind of large changes that can occur when water flashes to steam). The solid thermal conductivities also have a slight dependence on pressure, but it is sometimes difficult to obtain reliable data for these dependencies.

3.17   Porous medium density

The density ρ_{mat} of the rock-fluid system appears in the inertial and body force terms of the conservation of momentum Eqn (1.28), thus it is required for dynamic mechanical simulations, and for mechanical simulations involving gravity for example. Currently the Porous Flow module implements a simple relationship with porosity and fluid density for the single phase, fully saturated case:

$$\rho_{\mathrm{mat}} = \rho_R(1 - \phi) + \rho\phi \qquad (3.32)$$

Alternatively ρ_{mat} can be specified as a constant.

3.18   Viscosity

Viscosity may be taken as constant, or the high-precision equations of state may be used to define it.

Chapter 4

Implementation details and numerical issues

4.1 Independent (nonlinear) variables

The Porous Flow module was designed from the ground up to be able to employ variable switching, or persistent variables, instead of the more common pressure-temperature-displacement set of variables. Most simulations in the test-suite use these common set of variables, but it is up to the user to specify which variables are independent, and which variables are dependent (usually the dependent variables will be MOOSE AuxVariables). A good choice of variables can lead to much improved convergence.

4.2 Lumping and upwinding

The Porous Flow module employs fluid-mass and heat-energy lumping to the nodes, as well as full upwinding of the advective flow terms. This ensures far superior numerical convergence, especially in situations where mass-fractions of phases are close to disappearing.

4.2.1 Lumping

Consider here just the fluid-flow equation, as the heat-energy equation is analogous. The time-derivative term in Eqn (1.1) is discretised as

$$\psi \frac{M^\kappa - M^\kappa_{\mathrm{old}}}{\mathrm{d}t} \ . \tag{4.1}$$

Here ψ is the test function that we are integrating against. An alternative discretisation would be $\psi\phi(S\rho)'\dot{P}$ (in the single-phase situation), but Eqn (4.1) conserves mass more effectively than

other alternatives.

In the standard finite-element scheme, M^κ and its individual parts (porosity, saturation, etc) are evaluated at each quadrature point. However, in PorousFlow, everything in the time derivative is evaluated at the nodes. Specifically, M^κ at a node depends only on the independent variables at that node. It has been shown in many papers that this lumping is advantageous for mass conservation and reduces spurious oscillations of the pressure around sharp fronts[1]

The cause of oscillations around sharp fronts, and how mass lumping removes the oscillations, can be illustrated through a simple example.
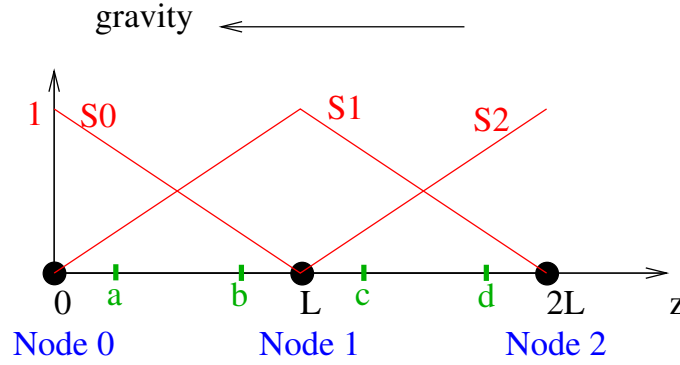

Figure 4.1: Two elements of length L. Linear Lagrange shape/test functions for each node are shown in red (S_0 for node 0, S_1 for node 1, and S_2 for node 2). Gravity acts in the direction $-z$. Gauss points are shown in green.

Consider the situation in Figure 4.1, and suppose that Node 2 has high potential, and that nodes 0 and 1 are at residual saturation where the relative permeability is zero. Then fluid will flow from node 2 to node 1 (and then to node 0 in the next time step). For simplicity, imagine that the fluid mass, M, is a linear function of the potential. Then, up to constants, the discretised mass-conservation equation without mass lumping reads

$$\begin{pmatrix} 2 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 2 \end{pmatrix} \begin{pmatrix} \dot{M}_0 \\ \dot{M}_1 \\ \dot{M}_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} \tag{4.2}$$

The matrix on the LHS comes from performing the numerical integration of M over the two elements. Note that it is not diagonal because the integration over an element depends on the mass at both of its two nodes. The RHS encodes that no fluid is flowing between nodes 0 and 1, but fluid is flowing from node 2 to node 1.

The important point is the solution of these sets of equations is

$$\dot{M}_0 < 0 . \tag{4.3}$$

This means the finite element solution of the mass-conservation equation will be oscillatory around fronts.

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[1]MA Celia, ET Bouloutas and RL Zabra "A general mass-conservative numerical solution for the unsaturated flow equation" Water Resources Research 26 (1990) 1483–1496.

However, with mass lumping, the matrix in the above equation becomes diagonal, and the solution is $\dot{M}_0 = 0$. Explicitly, the contribution to the residual at node a is

$$\sum_{\text{qp}} \psi_a^{\text{qp}} \frac{M_a^\kappa - M_{a,\ \text{old}}^\kappa}{\mathrm{d}t} \ . \tag{4.4}$$

where M is evaluated at node a using the independent (Nonlinear) variables evaluated at that node, and qp are the quadpoints.

There is one small complication. Porosity may be dependent on volumetric strain, which is dependent on the gradients of the displacement variables, which are evaluated at the quadpoints, not the nodes. In this case, the porosity at node a is assumed to be dependent on the volumetric strain evaluated at the closest quadpoint to the node.

4.2.2   Upwinding

Upwinding is necessary[2] in scenarios with nonlinear advection, such as the physics modelled by PorousFlow. For multi-phase situations many upwinding schemes can lead to disaster as the algorithm attempts to withdraw fluid from a node where there is no fluid. I believe that for situations where one phase disappears, or almost disappears, full upwinding is advisable, and hence PorousFlow always employs full upwinding. It has the numerical disadvantage that it is not smooth (in contrast to the SUPG upwinding scheme[3], for instance), so that close to steady-state where the fluxes are zero, the upwind direction can oscillate, leading to nonconvergence, however this is dealt with by placing a cutoff on the upwinding in PorousFlow. The remainder of this section describes full upwinding for the single-phase unsaturated situation. The multi-phase, multi-component scenario, and the advective term in the heat-flow equation are analogous.

The weak form of the Darcy flux of Eqn (1.6) for a single element is

$$R_a = \int_{\text{element}} \nabla_i \psi_a \frac{\rho k_{ij}\, k_{\text{r}}}{\mu} (\nabla_j P - \rho g_j) \ . \tag{4.5}$$

Here ψ_a is the test function that we are integrating against, and R_a is the contribution to the residual for this test function. Define

$$m = \frac{\rho k_{\text{r}}}{\mu} \ , \tag{4.6}$$

---

[2]Eg, see PS Huyakorn and GF Pinder "A new finite element technique for the solution of two-phase flow through porous media" Advances in Water Resources 1 (1978) 285–298. See also V Dalen "Simplified finite-element models for reservoir flow problems" SPEJ (Oct 1979) 333–343. See also R Helmig and R Huber "Comparison of Galerkin-type discretization techniques for two-phase flow in heterogeneous porous media" Advances in Water Resources 21 (1998) 697–711.

[3]AN Brooks and TJR Hughes "Streamline upwind/Petrov-Galerkin formulations for convection dominated flows with particular emphasis on the incompressible Navier-Stokes equations" Computer Methods in Aplied Mechanics and Engineering 32 (1982) 199–259. TJR Hughes and M Mallet "A new finite element formulation for computational fluid dynamics: III. The generalized streamline operator for multidimensional advective-diffusive systems" Computer Methods in Applied Mechanics and Engineering 58 (1986) 305–328. TJR Hughes, M Mallet and A Mizukami "A new finite element formulation for computational fluid dynamics: II. Beyond SUPG" Computer Methods in Applied Mechanics and Engineering 54 (1986) 341–355

which is traditionally called the mobility.

Upwinding is all a matter of choosing where in the element to evaluate m in the above integral. The sophisticated SUPG approach was designed to weight m on the upstream side of the element. Consider for a moment taking m outside the integral:

$$\tilde{R}_a = m \int_{\text{element}} \nabla_i \psi_a \kappa_{ij} (\nabla_j P - \rho g_j) = m I_a \ . \tag{4.7}$$

$\tilde{R}$ is not exactly R, but note:

- the original R_a is the mass flux flowing out of node a;

- so I_a is thereby intepreted as a measure of fluid flow out of node a.

This leads to the following definition of upwinding:

$$R_a \equiv m_a I_a \quad \text{if} \quad I_a \geq 0 \ . \tag{4.8}$$

The nodes for which $I_a \geq 0$ are called "upwind nodes", since fluid is flowing from them to the "downwind nodes". I think this approach was first introduced by Dalen[4] in 1979.

The residual at the downwind nodes is determined by conserving mass. Specifically, let

$$I_{\text{up}} = \sum_{I_a \geq 0} I_a \quad \text{and} \quad I_{\text{down}} = -\sum_{I_a < 0} I_a \ . \tag{4.9}$$

Then

$$R_a = I_a \frac{I_{\text{up}}}{I_{\text{down}}} \quad \text{for} \quad I_a < 0 \ . \tag{4.10}$$

Then $\sum_a R_a = 0$ as required by mass conservation within the element (which originates from $\sum_a \psi_a = 1$).

The fully-upwind method is extremely advantageous to use if fluid saturations ever approach residual saturation (where $\kappa_{\text{rel}} = 0$) or zero density, for then the mobility is zero and it becomes impossible to withdraw fluid from such a node (in practice this may still happen due to precision loss or other related nasty artifacts that I will not describe here).

Prescribed sinks, either from the boundary or from internal objects such as wellbores, are also fully-upwinded in PorousFlow since they also potentially suffer from phase-disappearence problems.

4.3   Preconditioners and linear solvers

MOOSE allows users to utilise the full power of the PETSc preconditioners and linear solvers. The following choices have been found to be effective for various types of PorousFlow simulations.

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[4]V Dalen "Simplified finite-element models for reservoir flow problems" SPEJ (Oct 1979) 333–343

- `pc_type = bjacobi, ksp_type = bcgs`.

- `pc_type = bjacobi, ksp_type = gmres`.

- `pc_type = asm, pc_asm_overlap = 2, sub_pc_type = lu, sub_pc_factor_shift_type = NONZERO, ksp_type = gmres`.

- `pc_type = asm, pc_asm_overlap = 2, sub_pc_type = lu, sub_pc_factor_shift_type = NONZERO, ksp_type = gmres` along with the following options `-ksp_diagonal_scale -ksp_diagonal_scale_fix -ksp_gmres_modifiedgramschmidt`.

4.4 Setting the global convergence criterion, and scaling the variables

It is very important to set the global convergence criterion appropriately. This is the `nl_abs_tol`, or equivalently, PETSc's $-$`snes_atol`. Of course the arguments below will also inform the setting of the relative tolerance `nl_rel_tol` (or PETSc's $-$`snes_rtol`). If set too small, then MOOSE will appear not to converge and will need very small timesteps in order to "do anything". If set too large, then MOOSE will converge to the "wrong" result. Here are some tips to estimate the global convergence criterion.

4.4.1 Fluids

1. Determine an appopriate tolerance on what you mean by "steadystate". For instance, in a single-phase simulation with reasonably large constant fluid bulk modulus, and gravity acting in the $-z$ direction, the steadystate solution is $P = -\rho_0 g z$ (up to a constant). In the case of water, this reads $P = -10000z$ (approximately).

   Instead of this, suppose you would be happy to say the model is at steadystate if $P = -(\rho_0 g + \epsilon)z$. Here ϵ needn't be constant: it may switch in sign, but its magnitude $|\epsilon|$ is roughly the same over the domain of interest. For instance, for water, an error of $|\epsilon| = 1\,\mathrm{Pa.m}^{-1}$ might be suitable in your problem.

   Then recall that the residual is just

   $$R = \left| \int \nabla_i \left(\frac{\kappa_{ij} \kappa_{\mathrm{rel}} \rho}{\mu} (\nabla_j P + \rho g_j) \right) \right| \tag{4.11}$$

   Evaluate this for your "almost-steadystate" solution.

   For instance, in the case of water just quoted, $\nabla P + \rho g \sim |\epsilon|$, and the $\rho \sim \rho_0$, and the integral just becomes V, the volume of the region of interest, so

   $$R \approx V |\kappa| \rho_0 / \mu \epsilon . \tag{4.12}$$

   For water, this gives $R \approx V |\kappa| \times 10^6 \epsilon$, using standard values for ρ_0 and μ.

2. In the previous step, an appropriate tolernace on the residual was given as $V|\kappa|\rho_0\epsilon/\mu$. Now the volume of interest, V, must be specified. Often this is not the entire mesh, but a small region where most of the interesting dynamics occurs, and the remainder of the mesh exists just to provide reasonable boundary conditions for this "interesting" region. The residual in the "boring" region can be thought of as virtually zero, while the residual in the "interesting" region is $V_{\text{interesting}}|\kappa|\rho_0\epsilon/\mu$. This is the absolute nonlinear residual that you should aim for.

3. In the previous steps, I've implicitly assumed κ is constant, ρ is virtually constant at ρ_0, only a single-phase situation, etc. In many cases these assumptions are not valid, so the integral of Eqn (4.11) cannot be done as trivially as in the previous steps. In these cases, I simply suggest to build a model with initial conditions like $P = -(\rho_0 g + \epsilon)z$, and just see what the initial residual is. That will give you an idea of how big a reasonable residual tolerance should be.

4.4.2 Heat

A similar method can be used to estimate the convergence criterion for heat-flow problems. Suppose there is both heat conduction, and fluid advection. Suppose that ϵ_{fluid} is the acceptable error in the fluid equations (as in the previous section). Suppose that $\nabla T \approx \epsilon_{\text{heat}}$ is an acceptable error for the temperature. For instance being incorrect by $\epsilon = 10^{-3}\,\text{K.m}^{-1}$ might be appropriate for your problem.

Then the residual is approximately

$$R \approx V(\lambda\epsilon_{\text{heat}} + h|\kappa|\rho_0\epsilon_{\text{fluid}}/\mu) \;, \tag{4.13}$$

The last term is just the fluid enthalpy, h, multiplied by the fluid residual.

4.4.3 Mechanics

Very similar methods can be used in simulations where mechanical deformations are active. Roughly speaking, MOOSE is attempting to set $\nabla\sigma^{\text{tot}} = 0$. Determine the error in $\nabla\sigma$ that you are willing to accept, and label it $|\epsilon|$. For instance $\epsilon = 1\,\text{Pa.m}^{-1}$ might be appropriate for your problem. You may determine ϵ from consideration of stresses directly, or you may wish to consider what the accpetable error in strains or displacements would be, and then use the elasticity tensor to find ϵ.

The nonlinear residual will be

$$R \approx V|\epsilon| \;, \tag{4.14}$$

where V is the volume of interest.

4.4.4 Scaling the variables

Often it is appropriate to scale the variables in order to weight their contributions to the overall nonlinear residual appropriately. For instance, suppose the previous arguments provided

$$
\begin{aligned}
R_{\text{fluid}} &\sim 10^{-9}V \ , \\
R_{\text{heat}} &\sim (10^{-3} + 10^{6} \times 10^{-9})V \ , \\
R_{\text{mech}} &\sim V \ ,
\end{aligned}
\tag{4.15}
$$

(with the same V in each case). Then, a scaling of around 10^9 on the porepressure variable (or whatever MOOSE variable is associated to the fluid equation) would be appropriate. Similarly, a scaling of around 10^3 on the temperature variable would be appropriate.

4.5 Fully saturated formulations

In fully-saturated, single-phase simulations the upwinding described in Section 4.2.2 is typically unnecessary. Moreover, the standard PorousFlow Kernels are somewhat inefficient in the fully-saturated case since Material Properties such as relative permeabilities and saturations actually do not need to be computed. PorousFlow offers some Kernels that may be used in this situation, as described below. They also have some minor disadvantages that are described below.

In fully-saturated, single-phase, single-component simulations, the mass lumping described in Section 4.2.1 is typically unncessary. More importantly, in many real-life situations, the time derivative of the fluid mass may be linearised, which leads to improved convergence. Porous-Flow offers a Kernel that may be used in this situation, as described below. It too has some disadvantages and other unique features.

4.5.1 Non-upwinded flux Kernels for fully-saturated, single-phase simulations

The following Kernels are available.

1. `PorousFlowFullySaturatedDarcyBase` models $\nabla_i \left((\rho)k_{ij}(\nabla_j P - \rho g_j) \right)/\mu$. This is fully-saturated, single-phase, single-component fluid flow. No upwinding is performed. The initial multiplication by ρ is optional (indicated by the parenthases): the reason for this is described in Section 4.5.2.

2. `PorousFlowFullySaturatedDarcyFlow` models $\nabla_i \left(\chi^\kappa \rho k_{ij}(\nabla_j P - \rho g_j) \right)/\mu$. This is fully-saturated, single-phase, multi-component fluid flow, for fluid component κ. No upwinding is performed.

3. `PorousFlowFullySaturatedHeatAdvection` models $\nabla_i (h\rho k_{ij}(\nabla_j P - \rho g_j)/\mu$. This is heat advection via fully-saturated, single-phase, multi-component fluid flow. No upwinding is performed.

Note that no Kernel includes the relative permeability, for it is always unity. This means that a RelativePermeability Material is not needed, which saves in computation time. Similarly, the saturation does not need to be computed, and various Nodal Materials (such as the density evaluated at the nodes) do not need to be computed. This makes input files smaller, and saves on computation time. In a full-scale simulation, we have recorded computational saving of about 4%.

Possibly the greatest advantage in using these Kernels is the reduced diffusion of fronts of temperature and fluid species. The full upwinding used in the remainder of PorousFlow adds diffusion compared with the non upwinded case. These effects are quantified by example in the documentation for the heat advection tests, and the documentation for sinks where the transport of a fluid component is explored. An example is shown in Figure 4.2.
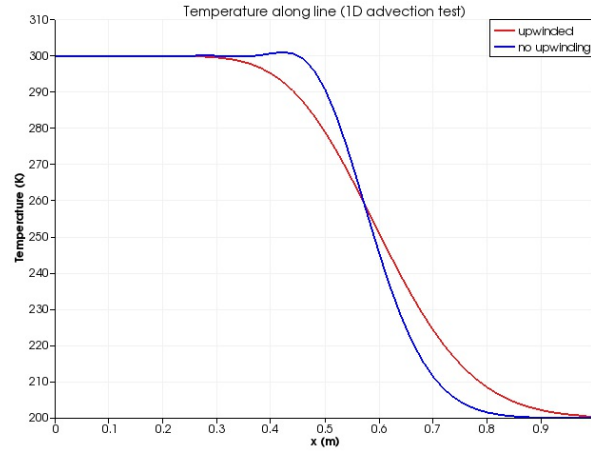

Figure 4.2: Heat advection via a fluid in 1D. The fluid flows with a constant velocity from the left to the right. The initial temperature distribution is a uniform 200 K everywhere. Then the left-hand side is raised to 300 K and fixed at that temperature. This causes a front of 300 K to move right. Without any diffusion a sharp front would advect from left to right. The upwinding adds diffusion, while no upwinding adds less diffusion.

The disadvantage of using the FullySaturated Kernels is that the physics is no longer completely controlled. The whole point of full upwinding is to ensure that no unphysical behaviour manifests itself, such as negative saturations or negative mass fractions. It is clear from Figure 4.2 that the temperature has risen slightly above 300 K ahead of the front, which is unphysical.

46

4.5.2 Non-lumped time derivative of fluid mass for fully-saturated, single-phase, single-component simulations

Consider a fully-saturated, single-phase, single-component fluid in a THM simulation. The time-derivatve terms from Eqn (1.1) are

$$\frac{\partial}{\partial t}\phi\rho + \phi\rho\dot{\epsilon}_v \ , \tag{4.16}$$

where $\dot{\epsilon}_v = \nabla \cdot \mathbf{v}_s$. Using the THM evolution of porosity given by Eqn (3.17), along with the assumption that the fluid bulk modulus, K_f, and its volumetric thermal expansion coefficient, α_f, are constant with fluid density given by

$$\rho = \rho_0 \exp(P/K_f - \alpha_f T) \ , \tag{4.17}$$

the time derivative terms may be written as

$$\rho\left(\frac{1}{M}\dot{P} + \alpha_B\dot{\epsilon}_v - A\dot{T}\right) \ . \tag{4.18}$$

Here M is the so-called Biot Modulus:

$$\frac{1}{M} = \frac{\phi}{K_f} + \frac{(1 - \alpha_B)(\alpha_B - \phi)}{K} \ , \tag{4.19}$$

and A is an effective volumetric thermal expansion coefficient:

$$A = (\alpha_B - \phi)\alpha_T + \phi\alpha_f \ . \tag{4.20}$$

Notice that disregarding the premultiplication by ρ, the above time-derivative terms would be linear in the variables P, displacement, and T, if M and A were constant.

In standard poro-mechanics it is usual to calculate M and A at the initial stage of simulation, and keep them fixed forever afterwards. Of course this is an approximation since M and A were derived using the explicit assumption of a porosity that depended on P, ϵ_v, and T, but it makes finding analytical solutions much easier. Therefore, PorousFlow offers the following Materials and Kernels. Using these Materials and Kernel allows immediate and precise comparison with analytical and numerical solutions of poro-mechanics.

1. `PorousFlowConstantBiotModulus` Material, which computes M given by Eqn (4.19) during the initial stage of simulation, and keeps it fixed thereafter. It requires a Porosity Material, but that Material's Property is only used during the initial computation.

2. `PorousFlowConstantThermalExpansionCoefficient` Material, which computes A given by Eqn (4.20) during the the initial stage of simulation, and keeps it fixed thereafter. It requires a Porosity Material, but that Material's Property is only used during the initial computation.

3. `PorousFlowFullySaturatedMassTimeDerivative` Kernel, which computes one of the following contributions, depending upon a user-defined flag:

   (a) $(\rho)\dot{P}/M$ for fluid-flow-only problems;

(b) $(\rho)(\dot{P}/M - A\dot{T})$ for TH problems;

(c) $(\rho)(\dot{P}/M + \alpha_B \dot{\epsilon}_v)$ for HM problems;

(d) $(\rho)(\dot{P}/M + \alpha_B \dot{\epsilon}_v - A\dot{T})$ for THM problems.

None of these employ lumping, which is largely unecessary in this single-phase, single-component situation. This means only "quad-point" Materials are needed. In fact, when using the FullySaturated flow Kernels described in Sec 4.5.1, *only* standard Materials evaluated at the quadpoints are needed, which saves on computation time and input-file length.

In each case, the initial pre-multiplication by ρ is optional (indicated by the parenthases around ρ) as described in the next paragraph.

When the Kernel is pre-multiplied by ρ, which is the default, it is computing the time derivative of fluid mass. This allows the Kernel to be easily used with the remainder of PorousFlow: the BCs, the Postprocessors, the AuxKernels, and the DiracKernels are all based on mass.

When the pre-multiplication is not performed, they are computing the time derivative of fluid volume. This has two great advantages:

1. the time-derivatives are linearised, resulting in excellent nonlinear convergence;

2. comparing with results from poro-mechanics theory is straightforward.

However, this means additional care must be taken.

1. The flow Kernel `PorousFlowFullySaturatedDarcyBase` should also not pre-multiply by density.

2. The BCs, Postprocessors, AuxKernels, and DiracKernels must be written in such a way to operate in the fluid-volume scenario rather than the default fluid-mass scenario.

3. The flag `consistent_with_displaced_mesh` should be set to `false` in the `PorousFlowVolumetricStrain` Material.

Chapter 5

Actions

The Material system used by PorousFlow is highly modularised and flexible. However, typical input files require numerous Materials, many of them depending on other Materials, and it is not clear why some Materials are even needed (for instance all the "Joiner" Materials). PorousFlow therefore offers some Actions, which aim to help users build minimal input files easily.

The PorousFlow Actions attempt to add only a minimal number of Materials and Kernels that are needed to solve a particular type of problem. It is therefore very likely that you will have to add extra Materials if you add extra Kernels, AuxKernels or Postprocessors into your input file.

The remainder of this Chapter describes the Actions that are currently available.

5.1   PorousFlowUnsaturated

This Action adds Kernels and Materials necessary to solve single-phase, multi-component, saturated-unsaturated physics. (A single fluid component may also be modelled.) The physics may be optionally coupled to heat and mechanics, in which case Kernels and Materials for those physics are also added. Auxillary Variables for saturation, effective stress and Darcy velocity are also optionally added.

This Action employs the standard mass lumping and full upwinding described elsewhere in this document. The saturation is computed using van Genuchten's expression.

No Kernels for diffusion and dispersion of fluid components are added. To run a simulation, you will also need to provide other Materials for each mesh block, depending on your simulation type, viz: permeability; porosity, elasticity tensor, strain calculator, stress calculator, matrix internal energy, thermal conductivity and diffusivity.

5.2   PorousFlowFullySaturated

This Action adds Kernels and Materials necessary to solve single-phase, multi-component, saturated physics. (A single fluid component may also be modelled.) The physics may be optionally coupled to heat and mechanics, in which case Kernels and Materials for those physics are also added. Auxillary Variables for effective stress and Darcy velocity are also optionally added.

This Action employs mass lumping, but no upwinding of fluid flow is performed. As described in Section 4.5, this means that the results will be slightly different from using the Porous-FlowUnsaturated Action.

No Kernels for diffusion and dispersion of fluid components are added. To run a simulation, you will also need to provide other Materials for each mesh block, depending on your simulation type, viz: permeability; porosity, elasticity tensor, strain calculator, stress calculator, matrix internal energy, thermal conductivity and diffusivity.

5.3   PorousFlowBasicTHM

This Action adds Kernels and Materials necessary to solve single-phase, single-component, saturated physics. The physics may be optionally coupled to heat and mechanics, in which case Kernels and Materials for those physics are also added. Auxillary Variables for effective stress and Darcy velocity are also optionally added.

This Action employs no mass lumping, and does no upwinding of fluid flow. As described in Section 4.5, this means that the results will be slightly different from using the PorousFlowUn-saturated Action. The Action also allows optional multiplication of the fluid equation by the fluid density. Without the multiplication the fluid equations are usually essentially linear (depending on the fluid properties) but care must be taken when using other PorousFlow objects that assume the multiplication has occured.

To run a simulation, you will also need to provide other Materials for each mesh block, depending on your simulation type, viz: permeability; porosity, elasticity tensor, strain calculator, stress calculator, matrix internal energy, cthermal conductivity, diffusivity, constant Biot Modulus, constant thermal expansion coefficient.

Appendix A

The continuity equation

The derivation of the continuity equation is fundamental to the fluid and heat flow DEs, and is included in this section. The notation in this appendix is different from that in the main report.

A.1 Eulerian coordinates

Introduce the notion of the "spatial coordinate frame". It is the coordinate frame of a stationary observer who is looking at the deforming porous solid from the outside. Denote its coordinates by $\mathbf{x}$, and the derivatives with respect those coordinates by ∇.

Let Ω be a volume that is attached to particles of the porous-solid skeleton. As the porous solid deforms, so too will Ω. Denote the velocity of the porous solid is $\mathbf{v}_s$, measured in the spatial coordinate frame: $\mathbf{v}_s = \mathbf{v}_s(x,t)$. Then the change of a small volume element $\mathrm{d}\Omega$ is computed by calculating the Jacobian, and it is

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathrm{d}\Omega) = \nabla \cdot \mathbf{v}_s \mathrm{d}\Omega \ . \tag{A.1}$$

Remember the derivative ∇ is differentiating with respect to the coordinates of the spatial coordinate frame. This formula is easy to motivate because $\nabla \cdot \mathbf{v}_s = \dot{\epsilon}_{ii}$ which is the time derivative of the volumetric strain.

Let M represent a quantity that is attached to the porous-solid skeleton, for instance the mass density of the solid. Express M in the spatial coordinate frame: $M = M(x,t)$. As the porous solid deforms

$$\frac{\mathrm{d}}{\mathrm{d}t}M = \frac{\partial}{\partial t}M + \mathbf{v}_s \cdot \nabla M \ . \tag{A.2}$$

The second term is easy to motivate if you consider a constant velocity with the spatially-dependent but temporally-constant M.

The continuity equation is

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega M \mathrm{d}\Omega + \int_{\partial\Omega} \mathbf{F} \cdot \mathbf{n}\, \mathrm{d}A = 0 \;, \tag{A.3}$$

where $\mathbf{F}$ is the flux of M out of Ω, n is the outward unit normal, and $\mathrm{d}A$ is the area element on $\partial\Omega$ (which is the surface of Ω). Using the above expressions, and the divergence theorem, the continuity equation reads

$$\int_\Omega \left(\frac{\partial}{\partial t} M + \nabla \cdot (M\mathbf{v}_s) + \nabla \cdot \mathbf{F} \right) \mathrm{d}\Omega = 0 \;. \tag{A.4}$$

Specialising M and $\mathbf{F}$ to fluids and heat gives the equations mentioned in the main text.

A.2 Lagrangian coordinates

Introduce the notion of the "material coordinate frame". It is the coordinate frame of an observer who is fixed to a certain point in the porous solid (eg, a particular finite-element node). Denote the coordinates in this frame by X. This is the frame used throughout this report. Fluid properties (pressures, mass fractions), the temperature, etc, are all stored at the finite-element nodes or the quadpoints, and move with the mesh. At the very least, an Eulerian description would be inconvenient when visualising with paraview.

Introduce the material derivative $\mathrm{D}/\mathrm{D}t$. If M is any property that is expressed in terms of the "spatial coordinate frame" (Eulerian coordinates): $M = \tilde{M}(x,t)$, then the material derivative is

$$\frac{\mathrm{D}}{\mathrm{D}t} \tilde{M}(x,t) = \frac{\partial}{\partial t} \tilde{M}(x,t) + \mathbf{v}_s \cdot \nabla \tilde{M}(x,t) \;. \tag{A.5}$$

The continuity Eqn (A.4) can be re-written as

$$0 = \frac{\mathrm{D}}{\mathrm{D}t} M + M \nabla \cdot \mathrm{v}_s \;. \tag{A.6}$$

However, if M is expressed in terms of the Lagrangian coordinates:

$$M = M(X,t) \;, \tag{A.7}$$

(generally $M(X,t)$ will have a different functional form than $\tilde{M}(x,t)$, thus the tilde to emphasise the difference) then the material derivative is expressed by

$$\frac{\mathrm{D}}{\mathrm{D}t} M(X,t) = \frac{\partial}{\partial t} M(X,t) \;, \tag{A.8}$$

but the continuity equation has the identical form:

$$0 = \frac{\mathrm{D}}{\mathrm{D}t} M + M \nabla \cdot \mathrm{v}_s \;. \tag{A.9}$$

Appendix B

Benchmark studies to perform

B.1 Use case: Two-component, two-phase, nonisothermal

This solution will benchmark the two-phase immiscible flow and thermal equations in of the code against the semi-analytical solutions in LaForce et al (AWR, 73 (2014a) $227-241$). (Note: These will have to be written because they are copy/pasted from manuscript)

The analytical solutions assume that pressure changes in the reservoir are small, so that fluid volume, density, and viscosity are all constant. Fluids and the solid are treated as incompressible. It is also assumed that changes in temperature do not impact any of the solid or fluid properties. With these assumptions the thermal and saturation equations become

$$[S_1 + \beta] \frac{\partial T_{D1}}{\partial t_D} + [f_1 + \alpha] \frac{\partial D1}{\partial r_D} = k_{Tt} \gamma_j \frac{\partial^2 D1}{\partial z_D^2} \tag{B.1}$$

$$\frac{\partial S_1}{\partial t_D} + \frac{\partial f_1}{\partial r_D} = 0 \tag{B.2}$$

$$\alpha = \frac{\rho_2 C_2}{(\rho_1 C_1 - \rho_2 C_2)} \tag{B.3}$$

$$\beta = \frac{\rho_2 C_2 + \frac{1-\phi_r}{\phi_r} \rho_s C_s}{(\rho_1 C_1 - \rho_2 C_2)} \tag{B.4}$$

where S_1 is the saturation of the water phase, f_1 is the fractional flow of the water (resident) phase, T_{D1} is temperature and r_D is radial distance. The C_j are the mass-based heat capacity of fluid 1, 2, or the formation rock. The parameters α and β in Eqns B.3—(B.4) are constant throughout the displacement. Dimensionless variables are defined in LaForce et al (2014a).

The relative permeability of the phases are from one of the TOUGH2 models

$$
\begin{aligned}
k_{r1} &= \hat{S}^4 \\
k_{r2} &= \left(1 - \hat{S}\right)^2 \left(1 - \hat{S}^2\right) \\
\hat{S} &= \frac{S_1 - S_{1r}}{1 - S_{1r} - S_{2r}}
\end{aligned}
\tag{B.5}
$$

In the analytical model, heat loss from the reservoir to the over/under burden is handled via a heat sink term that approximates the diffusive process.

$$
k_{Tt} \frac{\partial^2 T_D}{\partial z^2} \rightarrow -U T_D.
\tag{B.6}
$$

Note: It may be useful to solve these equations with $U = 0$ initially.

In this formulation the thermal properties of the reservoir and the adjacent formations may be different, but the over- and under-burden must have the same thermal properties for vertical symmetry. It will be interesting to test the simulator on the full Eqn (B.1) with vertical heat diffusion vs a simulated solution with the heat sink.

B.2 Two-component, two-phase, nonisothermal, forward coupled stress

This solution will benchmark the code against the semi-analytical solutions in LaForce et al (AWR, 73 (2014) $242 - 253$), which takes the saturation and temperature solution from above and also calculates pressure and stress in the reservoir. The semi-analytical solutions are strictly forward-coupled, so that pressure does not impact the saturation or temperature profiles, and stress has no impact on pressure, saturation or temperature. In that work, pressure and stress are calculated at a given snapshot in time, t_D^*. This gives pressure and stress equations with no time dependence:

$$
\frac{\partial P}{\partial r_D} = \frac{q}{4\pi h k r_D} \frac{1}{M}
\tag{B.7}
$$

where M is the mobility of the overall fluid composition at r_D.

The displacement u, of the porous medium at a fixed time is given by **Note: Notation may not be consistent with the above!!**:

$$\frac{d}{d\xi}\left(\frac{1}{\xi}\frac{d}{d\xi}(\xi u_D)\right) = \frac{\partial T_{D2}}{\partial \xi} + \frac{(1-2\nu)}{(1-\nu)}\frac{\partial P_D}{\partial \xi} \tag{B.8}$$

where $\xi = \frac{r}{r_w}$ for well radius r_w, and ν is the drained Poisson ratio. All other dimensionless groups given in LaForce et al (2014b).

In these equations stresses are defined as positive if they are tensile and negative if they are compressive. The stress at the wall of the well will have equal magnitude as the fluid pressure, but opposite sign so that at the wellbore the effective radial stress is always zero. These equations can be solved analytically on a finite reservoir domain for either zero stress or zero displacement outer boundary conditions.

Appendix C

Evolution of porosity for an isothermal situation

The evolution of porosity is fundamental to the coupling between flow and solid mechanics. Consider the isothermal situation with no plasticity.

Denote the change of a quantity, q, by Δq. Recall that the porosity is defined by $\phi = V_\mathrm{f}/V$, where V is an arbitrary volume of the porous material, and V_f is the porevolume within that volume. Also, by definition of the effective stress,

$$\Delta \epsilon_{ij} = C_{ijkl}(\Delta\sigma_{ij}^\mathrm{tot} + \alpha_B \delta_{ij}\Delta P_\mathrm{f}) \ . \tag{C.1}$$

Taking the trace of this equation, and using $V^{-1}\Delta V = \Delta\epsilon_{ii}$ yields

$$\frac{\Delta V}{V} = \delta_{ij}C_{ijkl}(\Delta\sigma_{ij}^\mathrm{tot} + \alpha_B\delta_{ij}\Delta P_\mathrm{f}) \ . \tag{C.2}$$

In most instances it is appropriate to write this equation as

$$\frac{\Delta V}{V} = -\frac{1}{K}(P_\mathrm{mech} - \alpha_B\delta_{ij}\Delta P_\mathrm{f}) \ . \tag{C.3}$$

where the total mechanical pressure is

$$P_\mathrm{mech} = -\mathrm{Tr}\sigma/3 \ . \tag{C.4}$$

and K is the so-called "drained" bulk modulus $K = \delta_{ij}C_{ijkl}\delta_{kl}$. To find the evolution equation for porosity, a similar equation for $\Delta V_\mathrm{f}/V_\mathrm{f}$ must be derived.

Assuming linearity

$$\frac{\Delta V_\mathrm{f}}{V_\mathrm{f}} = A_{ij}(\Delta\sigma_{ij}^\mathrm{tot} + B\delta_{ij}\Delta P_\mathrm{f}) \ . \tag{C.5}$$

The Betti-Maxwell reciprocal theorem yields A_{ij} and B, as is now shown.

The work increment is

$$\mathrm{d}W = -P_\mathrm{mech}\mathrm{d}V + P_\mathrm{f}\mathrm{d}V_\mathrm{f} \ , \tag{C.6}$$

So during some deformation that takes P_{mech} from P^i_{mech} to P^f_{mech}, and P_{f} from P^i_{f} to P^f_{f}, the total work is

$$
\begin{aligned}
W &= -\int P_{\text{mech}} \mathrm{d}V + \int P_{\text{f}} \mathrm{d}V_{\text{f}} , \\
&= \frac{V}{K} \int_{P^i_{\text{mech}}}^{P^f_{\text{mech}}} P_{\text{mech}} \mathrm{d}P_{\text{mech}} - \frac{V\alpha_B}{K} \int_{P^i_{\text{f}}}^{P^f_{\text{f}}} P_{\text{mech}} \mathrm{d}P_{\text{f}} + V_{\text{f}} A_{ii} \int_{P^i_{\text{mech}}}^{P^f_{\text{mech}}} P_{\text{f}} \mathrm{d}P_{\text{mech}} + V_{\text{f}} A_{ii} B \int_{P^i_{\text{f}}}^{P^f_{\text{f}}} P_{\text{f}} \mathrm{d}P_{\text{f}} \quad \text{(C.7)}
\end{aligned}
$$

Now consider two experiments:

1. First take P_{mech} from 0 to P_{mech} with P_{f} fixed at 0. Then, leaving P_{mech} fixed, take P_{f} from 0 to P_{f}. The first takes work $V P^2_{\text{mech}}/(2K)$, while the second takes work $-\alpha_B V P_{\text{mech}} P_{\text{f}}/K + V_{\text{f}} A_{ii} B P^2_{\text{f}}/2$.

2. First take P_{f} from 0 to P_{f} with P_{mech} fixed at 0. Then, leaving P_{f} fixed, take P_{mech} from 0 to P_{mech}. The first takes work $V_{\text{f}} A_{ii} B P^2_{\text{f}}/2$, and the second takes work $V P^2_{\text{mech}}/(2K) + V_{\text{f}} P_{\text{mech}} A_{ii} P_{\text{f}}$.

The two experiments must give the same work done (this is called the Betti-Maxwell reciprocal theorem), which yields

$$
A_{ij} = \alpha_B C_{ijkl} \delta_{kl}/\phi . \tag{C.8}
$$

Now to identify B. Consider a so-called "ideal porous material", which is characterised by a fully-connected pore space and a homogeneous and isotropic matrix material. In this case, applying a uniform porepressure, P_f, and an equal mechanical pressure, $P_{\text{mech}} = P_f$, the solid material will experience a uniform pressure throughout its skeleton. This means it will deform uniformly without any shape change, and

$$
\frac{\Delta V_{\text{f}}}{V_{\text{f}}} = \frac{\Delta V}{V} . \tag{C.9}
$$

Substituting this equation, this specific pressure condition, and Eqn (C.8) into Eqns (C.3) and (C.5), yields

$$
B = 1 + \phi - \phi/\alpha_B . \tag{C.10}
$$

Now that A_{ij} and B have been identified, they may be substituted into Eqn (C.5). Rearranging yields

$$
\frac{\Delta V_{\text{f}}}{V_{\text{f}}} = \frac{\alpha_B}{\phi} \delta_{ij} C_{ijkl} \left[\Delta\sigma^{\text{tot}}_{kl} + \alpha_B \delta_{kl} \Delta P_{\text{f}} \right] + \frac{\delta_{ij}\delta_{kl}C_{ijkl}}{\phi}(1 - \alpha_B)(\alpha_B - \phi)\Delta P_f \tag{C.11}
$$

Using the expression for $\Delta V/V$ yields

$$
\Delta V_{\text{f}} = V\alpha_B \Delta\epsilon_{ii} + V\delta_{ij}\delta_{kl}C_{ijkl}(1 - \alpha_B)(\alpha_B - \phi)\Delta P_f \tag{C.12}
$$

Now $\Delta\phi = V^{-1}\Delta V_{\text{f}} - V_{\text{f}}V^{-2}\Delta V$, so using the definition of K yields

$$
\frac{\partial\phi}{\partial t} = (\alpha_B - \phi)\frac{\partial\epsilon_{ii}}{\partial t} + \frac{(1 - \alpha_B)(\alpha_B - \phi)}{K}\frac{\partial P_{\text{f}}}{\partial t} , \tag{C.13}
$$

as written in Eqn (3.17).