Quick Two Phase (Q2P) Manual

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Contents

1 Introduction

Quick Two Phase (Q2P) is a efficient and inflexible specialisation of the Richards' equation. It is designed to be "quick" to write input files, and "quick" to run.

1. Q2P is only valid for 2-phases.
2. The capillary suction is somewhat obscured in Q2P compared with the Richards' formulation. However, this is one of the keys behind Q2P's efficiency. Often the true form of the capillary suction function is unknown in simulations of real-life materials.
3. Q2P is mass-lumped and fully-upwind only, with no options to make it otherwise

2 Theory and MOOSE implementation

2.1 DEs

Call one phase "water", and denote it by the subscript w. Call the other phase "gas", and denote it by the subscript g. The variables of the system are the saturation of water, S_w, and the porepressure of gas P_g. The 2-phase Richards' equations are

$$\begin{aligned} \phi\frac{\partial}{\partial t}(\rho_w S_w) &= \nabla_i\left(\frac{\rho_w\kappa_{ij}\kappa_w^{\rm rel}}{\mu_w}(\nabla_j P_w - \rho_w g_j)\right) + F_w \ , \\ \phi\frac{\partial}{\partial t}(\rho_g S_g) &= \nabla_i\left(\frac{\rho_g\kappa_{ij}\kappa_g^{\rm rel}}{\mu_g}(\nabla_j P_g - \rho_g g_j)\right) + F_w \ . \end{aligned} \tag{2.1}$$

Please see the Richards' Theory Manual for a description of the notation.

By capillarity $P_w = P_g - P_c(S_w)$, and writing in terms of the Q2P variables Eqn (2.1) reads

$$\begin{aligned} \phi\frac{\partial}{\partial t}(\rho_w S_w) - \nabla_i\left(\frac{\rho_w\kappa_{ij}\kappa_w^{\rm rel}}{\mu}(\nabla_j P_g - \rho_w g_j)\right) - \nabla_i\left(\frac{\rho_w\kappa_{ij}D}{\mu_w}\nabla S_w\right) - F_w &= 0 \quad [\text{variable } S_w] \ , \\ \phi\frac{\partial}{\partial t}(\rho_g(1-S_w)) - \nabla_i\left(\frac{\rho_g\kappa_{ij}\kappa_g^{\rm rel}}{\mu}(\nabla_j P_g - \rho_g g_j)\right) - F_g &= 0 \quad [\text{variable } P_g] \end{aligned} \tag{2.2}$$

The main step here has been to define the diffusivity

$$D(S_w) = -\kappa_w(S_w)P_c'(S_w) \geq 0 \ , \tag{2.3}$$

but also it is assumed that

$$\begin{aligned} \rho_w &= \rho_w(P_g) \ , \\ \rho_g &= \rho_g(P_g) \ , \\ \kappa_w^{\rm rel} &= \kappa_w^{\rm rel}(S_w) \ , \\ \kappa_g^{\rm rel} &= \kappa_g^{\rm rel}(S_w) \ . \end{aligned} \tag{2.4}$$

Hence Eqn (2.2) is two equations in two unknowns S_w and P_g.

Often ρ_w is almost constant compared with the range of P_g in the problems, so that the first of Eqn (2.2) looks very similar to a diffusion equation with diffusivity D. While D is in reality a function of S_w, in the Q2P module it is taken to be *constant*. Hence the capillary suction is rather obscured, although D is directly proportional to P_c and has the same units as it. The Q2P module can handle very small D (ie, very small P_c) more efficiently than the full Richards module. However, setting $D = 0$ leads to shocks forming in most problems so it is not recommended.

2.2 Actions

The Q2P action includes all the Q2P Kernels below, as well as, optionally, nodal mass AuxVariables and total fluid mass Postprocessors for mass-balance calculations.

2.3 Kernels

Eqn (2.2) has five terms (along with the source terms) which are encoded in the following kernels.

- Q2PNodalMass encodes both $\phi\rho_w S_w/\mathrm{d}t$ and $\phi\rho_g(1-S_w)/\mathrm{d}t$. It is lumped to the nodes. It is designed to work with the Q2PNegativeNodalMassOld in order to form the time derivative of the fluid masses. This Kernel requires:
  - A Material that defines "porosity".
  - The user to define "fluid_density" which is a RichardsDensity UserObject that defines ρ as a function of P_g.
  - The names of the Variables S_w and P_g.
  - Whether the Variable is porepressure. This latter flag should be false for the water equation, and true for the gas equation.
- Q2PNegativeNodalMassOld encodes the old values of both $-\phi\rho_w S_w/\mathrm{d}t$ and $-\phi\rho_g(1-S_w)/\mathrm{d}t$. It is lumped to the nodes. It is designed to work with the Q2PNodalMass in order to form the time derivative of the fluid masses. This Kernel requires:
  - A Material that defines "porosity".
  - The user to define "fluid_density" which is a RichardsDensity UserObject that defines ρ as a function of P_g.
  - The names of the Variables S_w and P_g.
  - Whether the Variable is porepressure. This latter flag should be false for the water equation, and true for the gas equation.
- Q2PSaturationFlux encodes $-\nabla_i\left(\frac{\rho_w\kappa_{ij}\kappa_w^{\mathrm{rel}}}{\mu}(\nabla_j P_g-\rho_w g_j)\right)$. It is fully upwinded. This Kernel requires:
  - The Variable to be S_w.
  - A Material that defines "gravity" and "permeability".
  - The name of the P_g variable.
  - The fluid dynamic viscosity μ_w.
  - The "fluid_density" which is a RichardsDensity UserObject that defines ρ_w as a function of P_g.
  - The "fluid_relperm" which is a RichardsRelPerm UserObject that defines the fluid relative permeability as a function of the S_w variable. For instance this UserObject could have type RichardsRelPermPower.

- `Q2PPorepressureFlux` encodes $-\nabla_i \left(\frac{\rho_g \kappa_{ij} \kappa_g^{\rm rel}}{\mu} (\nabla_j P_g - \rho_g g_j) \right)$. It is fully upwinded. This Kernel requires:
  - The Variable to be P_g.
  - A Material that defines "gravity" and "permeability".
  - The name of the S_w variable.
  - The fluid dynamic viscosity μ_g.
  - The "fluid_density" which is a RichardsDensity UserObject that defines ρ_g as a function of P_g.
  - The "fluid_relperm" which is a RichardsRelPerm UserObject that defines the fluid relative permeability as a function of the S_w variable. *Note* this could be a Q2PRelPermPowerGas UserObject, and *not* a RichardsRelPermPower UserObject since it must be a function of S_w and not S_g.

- `Q2PSaturationDiffusion` encodes $-\nabla_i \left(\frac{\rho_w \kappa_{ij} D}{\mu_w} \nabla S_w \right)$. It is not upwinded. This Kernel requires:
  - The Variable to be S_w.
  - A Material that defines "permeability".
  - The name of the porepressure variable
  - The "fluid_density" which is a RichardsDensity UserObject that defines ρ_w as a function of P_g.
  - The fluid dynamic viscosity μ_w.
  - The diffusivity D.

2.4 Other classes

2.4.1 Relative permeability

For the water phase, all the "RichardsRelPerm" objects may be used, as they are all functions of S_w. However, for the gas phase, these shouldn't be used. Instead the "Q2PRelPerm" objects should be used. These are:

- `Q2PRelPermPowerGas`. Define $S = S_w/(1-S_{\rm imm})$, where $S_{\rm imm}$ is the immobile saturation of the gas. The relative permeability is

$$\kappa_g^{\rm rel} = \begin{cases} 1 & \text{for } S_w \leq 0 \\ 1-(n+1)S^n + nS^{n+1} & \text{for } 0 < S_w < 1 - S_{\rm imm} \\ 0 & \text{for } S_w \geq 1 - S_{\rm imm} \end{cases} \tag{2.5}$$

2.4.2 Materials

The "Q2PMaterial" is a vastly stripped-down version of "RichardsMaterial". It provides porosity, permeability and gravity only. No mobility, SUPG, etc, calculations are needed, which can enhance compute speed substantially over a similar Richards simulation.

2.4.3 DiracKernels

The “Q2PBorehole” behaves in a similar way to a “RichardsBorehole” but correctly calculates the Jacobian entries in the Q2P setting.

2.4.4 BCs

The “Q2PPiecewiseLinearSink” behaves in a similar way to the “RichardsPiecewiseLinearSink” but correctly calculates the Jacobian entries in the Q2P setting.

2.4.5 Postprocessors

The “Q2PMass” records the water or gas mass. It is not lumped.

3 Tests

The Jacobian of all the Kernels, DiracKernels and BCs are tested.

It is demonstrated that Q2P's steady-state is hydrostatic head as expected.

The flow rates of gas and water into a production borehole are tested and found to be in agreement with expectations as shown in Figure 3.1. At the same time, mass conservation is tested.

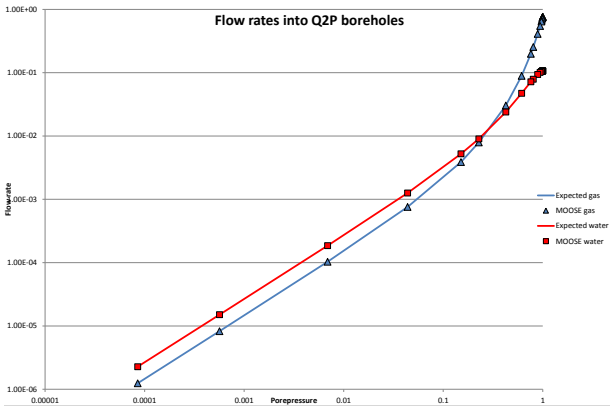

Figure 3.1: Gas and water flow rates into a production borehole. The MOOSE implementation agrees with the expected results.

4 Comments for users

The Richards theory, test and user manual all contain pertinant information for the user on convergence criteria, tips for ensuring and speeding convergence, etc. The following points pertain specifically to the Q2P formulation.

1. Setting the diffusivity can be key to ensuring good convergence. If it is set too small then shocks will form. If you observe this occuring, eg, the saturation varies from 0 to 1 over one element, then D should be increased.

2. I have found the system can exit the physical region $0 \leq S_w \leq 1$ more easily than in the Richards formulation. I'm not sure why this occurs. I have found that setting nonzero immobile saturations prevents this (and nonzero immobile saturations are correct physically anyway).

3. Because two densities treat the gas and water pressures are identical, the water density must be zero at zero pressure. In the Richards formulation this is not the case, as water density can be positive even for negative water pressure. However, in the Q2P situation, if the water pressure is negative then so too is the gas pressure, and in this case the gas density would be undefined. Therefore Q2P requires $P_g \geq 0$. To ensure this, the water density must satisfy $\lim_{P\to 0} \rho_w(P) = 0$. An example is `RichardsDensityConstbulkCut`.