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Overview of TOUGH2, Version 2.0

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Introduction

TOUGH2 is a general-purpose numerical simulation program for multiphase, multicomponent fluid and heat flows in porous and fractured media (Pruess, 1991). Chief application areas are in geothermal reservoir engineering, nuclear waste isolation studies, environmental assessment and remediation, oil and gas production and storage, and flow under variably saturated conditions in the vadose zone (Pruess, 1995).

The governing equations for multiphase fluid and heat flow have the same mathematical form, regardless of the nature and number of fluid phases and components present. This suggests setting up a simulation code with a modular architecture, in which the main flow and transport module can interface with different fluid property modules, allowing for a flexible description of different types of flow systems. Such an architecture was first implemented at Berkeley in a research code known as "MULKOM" in the early 80s and later formed the basis of TOUGH, a more specialized multiphase code for water-air-heat (Pruess, 1987). We now use the term "MULKOM" to denote the general architecture or "blueprint" of the code, while the specific FORTRAN77 implementation is called "TOUGH2."

Since TOUGH2 was first released to the public in 1991, the only change in the "official," publicly available version occurred in 1994, when a set of preconditioned conjugate gradient solvers replaced the previous exclusive reliance on the direct solver MA28 (Moridis and Pruess, 1995). In the intervening years, considerable development of process simulation capabilites and user features has occurred at Berkeley and elsewhere. As had been true for previous versions of the TOUGH/MULKOM codes, work at Berkeley was primarily driven by specific application needs, rather than by a desire for comprehensive process simulation capabilities as such.

Version 2.0 of TOUGH2 includes enhanced versions of the earlier program modules, as well as a selection of newly developed modules for more comprehensive process simulation capabilities. Some of the criteria and objectives used in assembling the new TOUGH2-version were as follows:

- add significant capabilities for simulating flow and transport processes, that will be useful for engineering and geoscience applications;
- add features to improve useability of the code, but avoid encumbering users with "feature creep;"
- keep code changes to the minimum required to achieve desired capabilities;
- remain as much as possible upward compatible with the earlier version;
- stay with FORTRAN77 and publish source code;
- facilitate code maintenance by minimizing the number of independent modules and "minor" variations among them;
- increasingly emphasize solved problems and internal documentation as a way of communicating code features and use.

This paper summarizes the main features and advances of Version 2.0 relative to the earlier release, including (1) several new EOS modules for different fluid mixtures, (2) enhanced capabilities for previously released fluid property modules, (3) description of diffusion and dispersion in multiphase systems, (4) strongly coupled flow and transport processes, (5) coupling between flow in geothermal reservoir and wellbores in two-phase conditions, (6) tracer transport with sorption and radioactive decay, and (7) flow in media with "strong" heterogeneity. In addition, numerous enhancements were made to facilitate applications to more diverse and demanding flow problems.

Full documentation and user instructions for these new modules will be available in a self-contained user's guide (in preparation).

Here we highlight the scope of major enhancements in modeling capabilities for flow and transport of multiphase, multicomponent fluids, and for a coupled treatment of flow in reservoirs and wellbores.

Fluid property modules

The original TOUGH2 released in 1991 provided five different fluid property or "EOS" (equation-of-state) modules. Labeled "EOS1" - "EOS5," these included the main modules for geothermal and nuclear waste applications. The new Version 2.0 release of TOUGH2 includes improved versions of these five EOS modules, as well as several new fluid property modules (Table 1). The subroutines for water properties (COWAT, SUPST, SAT) were replaced with faster routines written by M. O'Sullivan (University of Auckland, New Zealand). In EOS2, an improved correlation for the temperature dependence of CO_2 solubility in water was implemented that remains accurate for temperatures down to 5 °C (see Fig. 1; Battistelli et al., 1997).

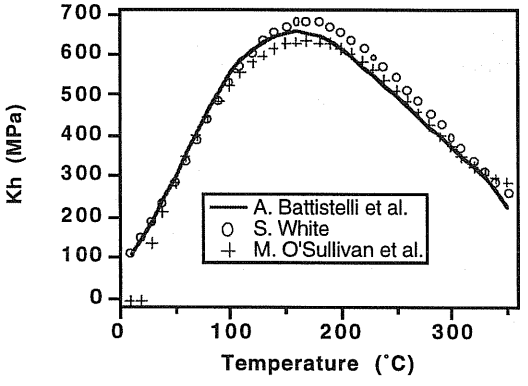

Figure 1. Henry's law coefficient for CO_2 solubility in water. EOS2 initially used a correlation developed by O'Sullivan et al. (1985) for geothermal applications. This was recently replaced with a correlation developed by Battistelli et al. (1997). Another correlation due to S. White (private communication) is also shown for comparison.

EOS4 now has an optional single-component (water only) capability, and initialization of two-phase conditions can be made either by specifying saturation, or relative humidity. We proceed to briefly summarize the new EOS modules.

EOS7

EOS7 is an extension of the EOS3 module. The aqueous phase is described as a mixture of brine (mass fraction X^b) and water (mass fraction $X^w=1-X^b$). Following Reeves et al. (1986) and Herbert et al. (1988), simple mixing models are used for viscosity and density of the aqueous phase. EOS7 does not explicitly describe the solid salt, and does not represent physical constraints on solubility. This type of approach is most suitable for isothermal or moderately non-isothermal flow systems that do not involve strong phase change effects. It is applicable to single-phase and two-phase (water-gas) flow systems with variable salinity, ranging from pure water to saturated NaCl brines.

Table 1. New fluid property modules for TOUGH2

Module	Capabilities
EOS7	water, brine, air
EOS7R	water, brine, air, parent-daughter radionuclides
EOS8	water, "dead" oil, non-condensible gas
EOS9	variably-saturated flow according to Richards' equation
EWASG	water, salt (NaCl), non-condensible gas (includes precipitation and dissolution, with porosity and permeability change)

EOS7R

This is an extension of EOS7 which includes a parent-daughter pair of radionuclide tracers for a total of five mass components. The tracers may partition between aqueous and gas phases, and may sorb on the solid grains. A detailed description is available in a laboratory report (Oldenburg and Pruess, 1995a).

EOS8

This module provides a basic three-phase flow modeling capability for fluid mixtures consisting of water, a non-condensible gas, and a "dead" oil. Most fluid properties are defined through user-supplied parameters. EOS8 contains extensive comments that document the fluid property model and user inputs. This

module is primarily intended as a platform for the development of research applications.

EOS9

EOS9 was designed for applications in vadose zone hydrology. It considers isothermal, saturated-unsaturated flow of water, with air a passive bystander. For these conditions, the general multiphase flow equations solved in TOUGH2 reduce to Richards' (1931) equation (Oldenburg and Pruess, 1993).

EWASG for H_2O-NaCl-CO_2 mixtures

Thermophysical properties

The EWASG fluid property module (Battistelli et al., 1997) features an accurate description of three-phase (aqueous, solid, gas) mixtures of three components (water, sodium chloride, non-condensible gas). The dependence of brine density, enthalpy, viscosity, and vapor pressure on salinity is taken into account, as are effects of salinity on gas solubility ("salting out") and heat of solution. TOUGH2/EWASG includes a capability for modeling precipitation and dissolution of salt, and associated porosity and permeability changes. It also models vapor pressure-lowering effects from suction pressures (capillary and vapor adsorption effects). The thermophysical property correlations used in EWASG are accurate for most conditions of interest in geothermal reservoir studies: temperatures in the range from 100 to 350 °C, fluid pressures up to 80 MPa, CO_2 partial pressures up to 10 MPa, and salt mass fraction up to halite saturation. With the exception of brine enthalpy, thermophysical property correlations are accurate to below 10 °C. Several choices are available for the non-condensible gas (CO_2, air, CH_4, H_2, N_2).

TOUGH2/EWASG considers the rock matrix as inert, except for a single active mineral, NaCl, which may be present in both aqueous solution and as a solid precipitate. Solid precipitated salt is treated in complete analogy to fluid phases (aqueous, gas), except that, being immobile, its relative permeability is identically zero. From mass balances on salt in liquid and solid phases we calculate the volume fraction of precipitated salt in the original pore space ϕ_0, which is termed "solid saturation," and denoted by S_S. A fraction $\phi_0 S_S$ of reservoir volume is occupied by precipitate, while the remaining void space $\phi(S_S) = \phi_0(1-S_S)$ is available for fluid phases. The reduction in pore space reduces the permeability of the medium.

Production from a reservoir with hypersaline brine and CO_2

TOUGH2/EWASG was used to simulate geothermal production from a hypothetical reservoir with high salinity and CO_2. A difficulty in applications is the need to specify the relationship between porosity and permeability change. Laboratory experiments have shown that modest reductions in porosity from chemical precipitation can cause large reductions in permeability (Vaughan, 1987). This is explained by the convergent-divergent nature of natural pore channels, where pore throats can become clogged by precipitation while disconnected void spaces remain in the pore bodies (Verma and Pruess, 1988). The effects depend on pore geometry, and are expected to be quite different for different porous media (Weir and White, 1995). In the simulation presented here, we use a relationship derived by Verma and Pruess (1988) for a tube-in-series pore channel model. We specify a single well that produces at a constant rate of 65 kg/s from an infinite-acting reservoir in 1-D radial flow geometry. Other parameters are given in Table 2.

Table 2. Parameters for production from a saline reservoir with CO_2

Reservoir thickness	500 m
Permeability	50×10^{-15} m^2
Porosity	0.05
Relative permeability Corey curves S_{lr} = S_{gr} =	 0.30 0.05
Rock grain density	2600 kg/m^3
Specific heat	1000 J/kg °C
Thermal conductivity	2.1 W/m °C
Initial conditions	
Temperature	275.55 °C
Gas saturation	0.45
Pressure	60.0 bar
NaCl mass fraction in liquid phase	0.30
CO_2 partial pressure	14.79 bar
Wellblock radius	5 m

Fluid withdrawal causes pressures to drop near the production well. Boiling of reservoir

fluid gives rise to dilution of CO_2 in the gas phase and to increased concentrations of dissolved NaCl, which begins to precipitate when the aqueous solubility limit is reached. As the boiling front recedes from the well, solid precipitate fills approximately 10 % of the original void space (see Fig. 2), causing permeability to decline to approximately 28 % of its original value.

Specifications of this problem (1-D radial geometry, homogeneous medium, uniform initial conditions, constant well rate) were chosen so that a "similarity solution" should be applicable, which should depend on radial distance R and time t only through the similarity variable $x = R^2/t$ (O'Sullivan, 1981). This similarity property should hold even when all complexities of two-phase flow with non-linear relative permeabilities, CO_2 exsolution effects, salt precipitation, and associated porosity and permeability effects are taken into account. Simulated results for two different times ($5x10^5$ and $2x10^6$ seconds) are plotted as a function of the similarity variable in Fig. 2. It is seen that the similarity property holds very accurately for all thermodynamic variables.

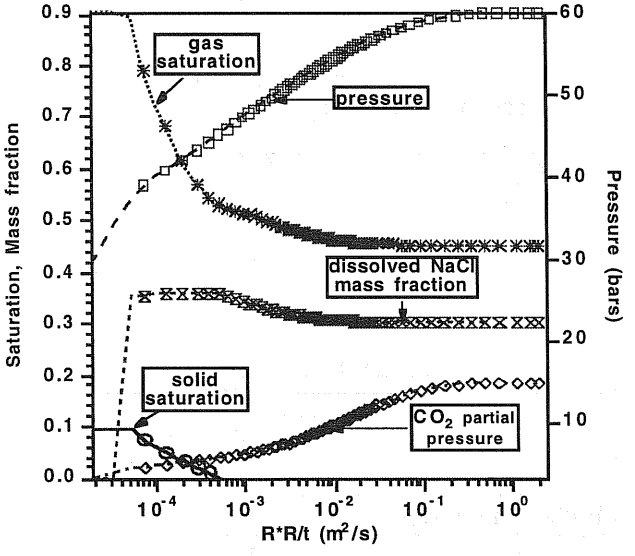

Figure 2. Simulated thermodynamic conditions for 1-D radial flow problem with salinity and non-condensible gas, plotted as a function of the similarity variable $x = R^2/t$. Results at $2x10^6$ seconds are shown as lines, while the data at $t = 5x10^5$ seconds are given as symbols.

Coupled wellbore flow

Geothermal production wells typically operate at (nearly) constant wellhead pressures. As flow rate and flowing enthalpy change with time, wellbore pressure gradients and flowing bottomhole pressures will also change. From a conceptual point of view, the most straightforward way to describe production from geothermal wells is to set up and solve equations for flow in the reservoir and flow in the wellbore in a fully coupled manner. This approach was taken by Hadgu et al. (1995) who coupled the reservoir simulator TOUGH with the wellbore simulator WFSA (Hadgu and Freeston, 1990).

From a practical viewpoint, an alternative approach may be preferable in which the wellbore and reservoir simulations are performed separately. Flowing wellbore pressures may be represented by tables which can be generated through repeated running of a wellbore simulator ahead of the reservoir simulation. As discussed by Murray and Gunn (1993), this offers a number of advantages, including increased robustness and calculational efficiency. It also makes it possible to use different wellbore simulators and two-phase flow correlations without any programming changes in the reservoir simulation code.

We have incorporated a tabular interpolation scheme for dynamic changes of flowing bottomhole pressure into TOUGH2. Flowing enthalpy h at the downhole well feed is known from phase mobilities and enthalpies calculated by the reservoir simulator. The unknown well flow rate q and flowing bottomhole pressure P_{wb} are then obtained by Newton-Raphson iteration on

$$R(q) \equiv q - \left(\sum \frac{k_{r\beta}}{\mu_\beta} \rho_\beta \right) \cdot PI \cdot \left(P - P_{wb}(q,h) \right) = 0 \qquad (1)$$

where $P_{wb}(q,h)$ is interpolated from tables, see Fig. 3. The iterative solution of Eq. (1) was embedded in the "outer" (Newtonian) iteration performed by TOUGH2 on the coupled mass and heat balance equations. Additional computational work in comparison to conventional simulations with constant downhole pressure is insignificant.

Application

As an application example we have considered a reservoir-wellbore system similar to Problem 1 of Hadgu et al. (1995). An exact replication of their test problem is not possible because they did not give complete specifica-

tions in their paper. A well of 0.2 m inside diameter produces from a 500 m thick two-phase reservoir containing water at initial conditions of P = 60 bars, T = $T_{sat}(P)$ = 275.5 °C, S_g = 0.1. Wellhead pressure is 7 bars, and feed zone depth is 1000 m. Fig. 3 shows a contour diagram of flowing bottomhole pressures obtained by running the HOLA wellbore simulator (Aunzo et al., 1991) for a range of flow rates and enthalpies.

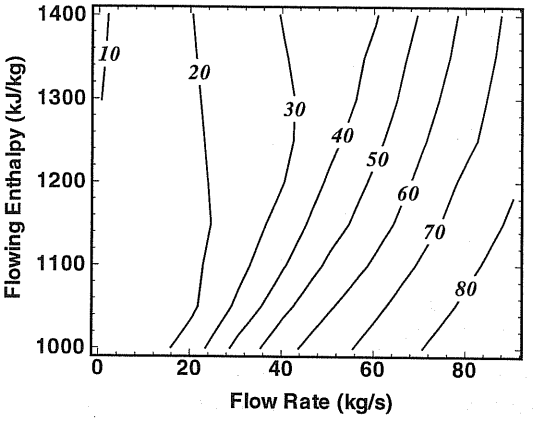

Figure 3. Flowing bottomhole pressures (in bars) at 1000 m feed zone depth for a well of 20 cm (≈ 8 inch) inside diameter, producing at 7 bar wellhead pressure (calculated from HOLA; Aunzo et al., 1991).

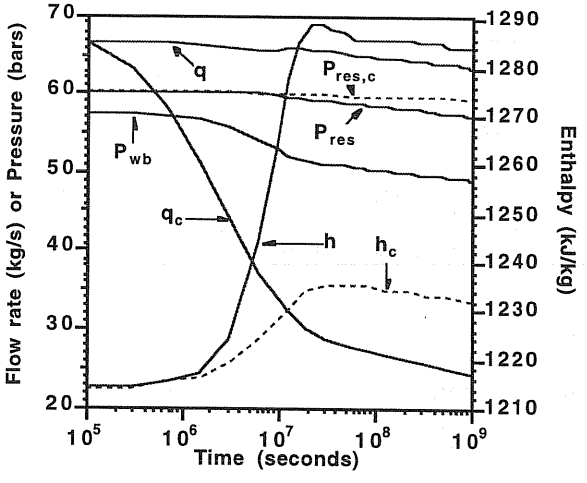

Figure 4. Simulated flow rate (q), flowing enthalpy (h), flowing bottomhole pressure (P_{wb}) and reservoir pressure in well grid block (P_{res}) for a problem adapted from Hadgu et al. (1995). Results obtained for constant bottomhole pressure of P_{wb} = 57.37 bars, labeled q_c, h_c, and $P_{res,c}$, are also shown.

Our coupled reservoir-wellbore flow simulation uses the well pressure data shown in Fig. 3. Results are given in Fig. 4, along with a comparison case in which flowing wellbore pressure was kept constant at the early-time value obtained in the coupled calculation (P_{wb} = 57.37 bars). Our results are similar to those of Hadgu et al. (1995). Flow rates and flowing enthalpies for the coupled model are a few percent higher than those obtained by Hadgu et al., while flowing bottomhole pressures are slightly lower. The simulation with constant bottomhole pressure gives a rapidly declining production rate that agrees well with Hadgu et al. (1995).

Multiphase diffusion and dispersion

Molecular diffusion

All fluid property modules now optionally include diffusive fluxes of all components in all phases. In multiphase conditions, the diffusive flux of mass component κ in phase β is customarily written as

$$\mathbf{f}_\beta^\kappa = -\phi S_\beta \rho_\beta \tau_0 d_\beta^\kappa \nabla X_\beta^\kappa \qquad (2)$$

where ∇X is the mass fraction gradient. The accumulation term in the mass balance equation for component κ includes the same group $\phi S_\beta \rho_\beta$ as appears in Eq. (2), so that the effective diffusion coefficient, $\tau_0 d_\beta^\kappa$, is saturation-independent in this formulation. This does not appear to be realistic.

TOUGH2 offers an alternative, more general expression for multiphase diffusive flux, as follows

$$\mathbf{f}_\beta^\kappa = -\phi \tau_\beta \rho_\beta \tau_0 d_\beta^\kappa \nabla X_\beta^\kappa \qquad (3)$$

$\tau_\beta = \tau_\beta(S_\beta)$ is a saturation-dependent tortuosity which is poorly known at present. In the spirit of conceptual consistency, we currently use the assignment $\tau_\beta(S_\beta) = k_{r\beta}(S_\beta)$.

Hydrodynamic dispersion

Following Scheidegger's seminal paper (1954), the spreading of solute plumes due to "small-scale" randomness of permeable media has traditionally been described in analogy to Fickian diffusion. Much hydrogeological research during the last twenty years has shown this analogy to be of limited validity and usefulness for field problems; yet for

many applications there are no practical alternatives.

We have incorporated a "standard" approach to hydrodynamic dispersion, with appropriate generalization to multiphase flow systems, in a specialized TOUGH2 module known as "T2DM" (Oldenburg and Pruess, 1993, 1995b). Dispersive mass flux is given by

$$\mathbf{F}^{\kappa}\Big|_{dis} = -\sum_{\beta} \rho_{\beta} \overline{\mathbf{D}}_{\beta}^{\kappa} \nabla X_{\beta}^{\kappa} \qquad (4)$$

where

$$\overline{\mathbf{D}}_{\beta}^{\kappa} = D_{\beta,T}^{\kappa} \bar{\mathbf{I}} + \frac{\left(D_{\beta,L}^{\kappa} - D_{\beta,T}^{\kappa}\right)}{u_{\beta}^{2}} \mathbf{u}_{\beta} \mathbf{u}_{\beta} \qquad (5)$$

is the dispersion tensor, with $\mathbf{u}_{\beta}$ the Darcy velocity, and $D_{L,T}$ the longitudinal and transverse dispersion coefficients. Evaluation of dispersive fluxes requires knowledge of the full velocity and concentration gradient vectors at grid block interfaces. These depend not only on conditions in the two grid blocks between which dispersive mass transport occurs, and hence require interpolation using data from several additional grid blocks. T2DM is designed for two-dimensional rectangular grids, which greatly facilitates such interpolation. A fully three-dimensional implementation for general irregular grids is in an earlier stage of development (Wu and Pruess, 1998), and is not included in Version 2.0 of TOUGH2.

Inclusion of dispersive fluxes automatically provides a capability for modeling strongly coupled flow and transport. This is because TOUGH2 fully accounts for all thermophysical property dependencies on primary thermodynamic variables, and all mass and energy balances are solved completely simultaneously. An example where dispersive spreading of salinity has a strong impact on fluid density, and subsequently alters buoyancy effects in advective flow, is given in (Oldenburg and Pruess, 1995b).

Linear equation solvers

Most of the computational work in the numerical simulation of fluid and heat flow arises in the solution of large systems of linear equations. TOUGH2, Version 2.0, features a new solver package "T2SOLV" (Moridis and Pruess, 1998). In addition to the algorithms previously included in T2CG1, T2SOLV includes the BiCGSTAB method (van der Vorst, 1992; Sleijpen and Fokkema, 1993), and a banded direct solver. It also features a choice of different preconditioners for poorly conditioned matrices, such as matrices with mostly zeros in the main diagonal. Test calculations have shown that T2SOLV can handle difficult flow problems for which T2CG1 failed. Full details have been presented in (Moridis and Pruess, 1998).

Miscellaneous code enhancements

We briefly summarize various enhancements made in the new Version 2.0 of TOUGH2. In order to allow for coupled reservoir-wellbore flow simulations, as discussed above, subroutine QU was completely re-written in modular structure. It now features a "rigorous step-rate capability:" for a user-specified table of time-dependent rates, production rate during time stepping can be automatically adjusted in such a manner that the total cumulative mass exchange $\sum q_i (t_{i+1} - t_i)$ is rigorously conserved. An analogous capability is available for flowing enthalpy.

Subroutine MULTI now includes a capability for radiative heat transfer between grid blocks. For strongly heterogeneous media, permeability modifiers ζ can be applied to each grid block, so that $k_n \rightarrow k_n' = \zeta_n \times k_n$. Strength of capillary pressure is scaled consistently with permeability on a grid-block-by-grid-block basis according to $P_{c,n} \rightarrow P_{c,n}' = P_{c,n}/\sqrt{(\zeta_n)}$ (Leverett, 1941). Random permeability modifiers can be internally generated in TOUGH2; for spatially-correlated permeability distributions geostatistical techniques can be used to derive appropriate fields of ζ_n-coefficients (Tompson, 1989; Pruess, 1997).

Discussion and Conclusions

TOUGH2, Version 2.0, consists of a set of program modules that were developed in response to specific types of flow and transport problems. It includes a considerably enhanced set of fluid property modules and additional process simulation capabilities, such as multiphase diffusion and hydrodynamic dispersion, dissolution and precipitation of solids, radiative heat transfer, and coupling between reservoir and wellbore flow. It includes many improvements and new user features, such as generating graphics files, tabulating thermodynamic data, and block-by-block permeability modification for strongly heterogeneous

media. Changes in existing TOUGH2 modules were kept to a minimum, and were only made as needed to achieve the additional functionalities desired. Data inputs are upward compatible with the previous version, so that existing TOUGH2 input files should produce identical results when run with Version 2.0. Additional data inputs are needed to use new, enhanced process simulation capabilities. Coding continues to be in FORTRAN77 for maximum portability.

Even though the Version 2.0 program modules were thoroughly tested individually, their integration into a single program structure is a difficult and potentially "hazardous" task. Many different options can be selected in different program modules. It is not practically possible to exhaustively cross-check the mutual compatibility and proper performance of all options. There is no finite process by which all program bugs that may be present can be identified and corrected. Fixing a bug may cause unanticipated problems elsewhere. Continuing vigilance and application testing are needed. The Version 2.0 program package is currently (April 1998) being readied for "beta-testing" by a small group of experienced users. Public release is expected for early 1999.

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Notation

d_β^κ diffusion coefficient for component κ in phase β, m^2/s.

$\overline{\mathbf{D}}_\beta^\kappa$ dispersion tensor for component κ in phase β, m^2/s.

$D_{\beta,L}^\kappa$ longitudinal dispersions coefficient for component κ in phase β, m^2/s.

$D_{\beta,T}^\kappa$ transverse dispersions coefficient for component κ in phase β, m^2/s.

$\mathbf{f}_\beta^\kappa$ diffusive mass flux of component κ in phase β, kg/s m^2.

$\mathbf{F}^\kappa\big|_{dis}$ diffusive mass flux of component κ in phase β, kg/s m^2.

h specific enthalpy, J/kg.

$\bar{\mathbf{I}}$ identity tensor.

k_n permeability of grid block n, m^2.

$k_{r\beta}$ relative permeability of the β phase.

P pressure, Pa.

$P_{c,n}$ capillary pressure in grid block n, Pa.

PI productivity index, m^3.

P_{wb} wellbore pressure, Pa.

q well flow rate, kg/s.

R residual function for well rate, kg/s.

S_s saturation of solid precipitate.

S_β saturation of phase β.

$\mathbf{u}_\beta$ Darcy velocity, m/s.

X_β^κ component κ mass fraction in phase β.

ζ permeability modification coefficient.

μ_β β phase viscosity, kg/m s.

ρ_β density of phase β, kg/m^3.

τ_0 tortuosity.

τ_β tortuosity factor in phase β.

ϕ porosity.

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