

EOS3nn:
An iTOUGH2 Module for
Non-Newtonian Liquid and Gas Flow

Documentation and User's Guide
Version 1.0

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ABSTRACT

This report documents the iTOUGH2 module EOS3nn, developed for modeling two-phase isothermal flow of a non-Newtonian liquid and a non-condensable gas in multidimensional, porous and fractured geologic media. This document supplements the TOUGH2 and iTOUGH2 user's guides and is therefore not a self-contained manual. It presents information on the physical processes modeled and the mathematical and numerical methods used. Also included are two sample problems for code testing and benchmarking. Modeling scenarios and approaches are discussed to illustrate problem setup and usage of the EOS3nn module.

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1. Introduction

EOS3nn was developed as a module of the iTOUGH2 simulator (Pruess et al., 1999; Finsterle, 2002a,b,c) for modeling two-phase flow of a non-Newtonian liquid and gas in an isothermal porous medium system. EOS3nn is derived from the EOS3 module as implemented into iTOUGH2. Note that iTOUGH2 can be executed in forward mode for standard predictive modeling. EOS3nn preserves most of the features and capabilities of the EOS3 module with the addition of non-Newtonian flow behavior. The main difference is that EOS3nn is a non-compositional model, i.e., there is no phase partitioning of the two components: The gas phase consists of a non-condensable gas (default: air), and the liquid phase consists of a non-Newtonian fluid. Note, however, that EOS3nn is able to handle single-phase liquid, two-phase gas-liquid, and single-phase gas conditions. Unlike EOS3, EOS3nn is restricted to isothermal conditions.

The EOS3nn module takes into account simultaneous flow of two fluids through porous and fractured media. The first fluid phase is a non-Newtonian liquid, and the second is an ideal, non-condensable gas, which is treated as a Newtonian fluid. Fluid flow in the two phases occurs under pressure, viscous, and gravity forces according to the generalized Darcy law. The interference between the phases during flow through porous media is described by means of relative permeability and capillary pressure functions. The governing partial differential equations for mass balances of the two phases are spatially discretized using the integral finite difference (IFD) numerical method (Narasimhan and Witherspoon, 1976; Pruess, 1991). Time is discretized using first-order finite differences. The discrete nonlinear equations are solved fully implicitly using a Newton-Raphson iteration scheme.

Flow and displacement of non-Newtonian fluids through porous media occurs in many subsurface systems, related to underground natural resource recovery and storage projects, as well as environmental remediation schemes. The different flow regimes involved in multiphase subsurface flow have been largely ignored in groundwater modeling practice. Previous modeling studies and groundwater models can handle only

Newtonian fluids, while EOS3nn has incorporated a power-law/Bingham rheological model for treatment of non-Newtonian flow behavior in a two-phase system.

EOS3nn module is available as a FORTRAN77 source code. It can be installed on many different platforms (Unix, Linux, PC, mainframes). The test cases discussed in Section 5 were run under Linux using an executable created by the Portland Group Fortran compiler. Slight differences in results obtained on other platforms are expected due to the different implementation of floating-point operations and optimization options. The code structure of the EOS3nn module is identical to that of the EOS3 of the iTOUGH2 code (Pruess et al., 1999; Finsterle, 2002a,b,c). In particular, input/output formats and most user features are identical. In addition to the standard TOUGH2 and iTOUGH2 input, the user needs to supply properties of the non-Newtonian fluid through the SELEC data block (see Section 3).

2. Physical Processes, Mathematical Model, and Numerical Implementation

In the EOS3nn formulation, the multiphase system is assumed to be composed of only two mass components: a non-condensable gas and a non-Newtonian liquid. Although each of the two phases may consist of multiple components, they are here treated as a single “pseudo-component” fluid with averaged properties of the phase. The two fluid components, non-condensable gas and non-Newtonian liquid are assumed to be present only in their associated phases, i.e., mass transfer between phases for the components by phase partitioning has been neglected. Therefore, EOS3nn is a non-compositional model, which is the main difference to the EOS3 module. The liquid phase consists of the non-Newtonian fluid, and the gas phase consists of the non-condensable gas. Consequently, the two components non-condensable gas and non-Newtonian fluid are strictly related to the two phases gas and liquid, respectively.

Each phase flows in response to pressures, gravitational and capillary forces according to the multiphase extension of Darcy's law, which includes the effects of relative permeability and capillary pressures. Transport of the two mass components occurs by advection only, i.e., carried by flow of the associated fluid phase. Effects of molecular diffusion or hydrodynamic dispersion are ignored in both phases. In addition, the system is assumed to be isothermal, i.e., heat transfer and its effects on fluid properties are not included.

The liquid phase is regarded as a non-Newtonian fluid, described by a generalized power-law/Bingham rheological model, as discussed below. The gas phase is always treated as a Newtonian fluid. Gas phase density is considered to be a function of temperature and pressure, and is described using the ideal gas law. Like a Newtonian fluid, a non-Newtonian fluid flows in porous media according to the generalized Darcy law. However, the apparent viscosity for the non-Newtonian fluid depends on the shear rate or pore velocity (Savins, 1969).

2.1 Governing Equations

As discussed above, the multiphase system is assumed to be isothermal and composed of two mass components or two phases, gas and the non-Newtonian liquid. The two components are assumed to be present only in their associated phases, gas and liquid, respectively. For an isothermal system containing two mass components, two mass balance equations are needed to fully describe the thermodynamic state of the system. The balance equations for component or phase β ($\beta=nn$ for the non-Newtonian fluid, and $\beta=g$ for the Newtonian non-condensable gas) are written as follows:

$$\frac{\partial}{\partial t}(\phi S_{\beta} \rho_{\beta}) = -\nabla \cdot (\rho_{\beta} \vec{V}_{\beta}) + q_{\beta} \quad (1a)$$

where the Darcy velocity of phase β is defined as:

$$\vec{V}_\beta = -\frac{k k_{r\beta}}{\mu_\beta} (\nabla P_\beta - \rho_\beta g \nabla D) \quad (1b)$$

where:

ρ_β : density of phase β

ϕ : effective porosity

μ_β : viscosity of phase β

S_β : saturation of phase β

P_β : pressure of phase β

q_β : sink/source term of phase β per unit volume of formation

g : gravitational acceleration

$k_{r\beta}$: relative permeability to phase β

k : absolute (intrinsic) permeability

D : depth

2.2 Constitutive Relations

The governing equations (1) of mass conservation for two phases need to be supplemented with constitutive equations, which express all the (secondary) parameters as functions of a set of (primary) thermodynamic variables. The following relationships are used to complete the mathematical description of two-phase flow of Newtonian and non-Newtonian fluids through porous media.

2.2.1 Saturation Constraint

In addition to the governing equations (1), there is a supplementary equation given by:

$$S_{nn} + S_g = 1 \quad (2)$$

2.2.2 Capillary Pressure Functions

The pressures between the two phases are related by:

$$P_{nn} = P_g - P_c(S_{nn}) \quad (3)$$

where P_c is the gas-water capillary pressure of the two-phase system and is assumed to be a function of water saturation only, i.e., effect of non-Newtonian behavior on capillary forces is ignored.

iTOUGH2 offers a number of capillary pressure models, which are functions of model-specific parameters.

2.2.3 Relative Permeability Functions

The relative permeabilities are also assumed to be functions of fluid saturations only and not to be affected by non-Newtonian behavior when simulating non-Newtonian liquid flow. The relative permeability to the non-Newtonian phase is

$$k_{rnn} = k_{rnn}(S_{nn}) \quad (4)$$

and for gas phase,

$$k_{rg} = k_{rg}(S_{nn}) \quad (5)$$

iTOUGH2 offers a number of relative permeability models, which are functions of model-specific parameters. It should be mentioned that even though any relative permeability/capillary pressure functions of the TOUGH2 code can be used with the EOS3nn module, it is assumed that the residual liquid saturation is provided through variable RP(2) (see block RPCAP . 1 or ROCKS . 1 . 2).

2.2.4 Fluid Densities

The densities of the Newtonian and non-Newtonian fluids are treated as functions of phase pressures:

$$\rho_{\beta} = \rho_{\beta}(P_{\beta}) \quad (6)$$

For liquid, the following linear form is used:

$$\rho_{nn} = \rho_{nn}^o (1 + C_{nn} (P_{nn} - P^o)) \quad (7)$$

here, ρ_{nn}^o is the density of the non-Newtonian liquid at reference pressure P^o ; and C_{nn} is the compressibility of phase nn. The gas density is calculated using the ideal gas law:

$$\rho_g = \frac{P_g M}{RT} \quad (8)$$

where M is the molecular weight of the non-condensable gas, R is the universal gas constant, and T is the reference temperature of the formation.

2.2.5 Treatment of Non-Newtonian Behavior

For the non-Newtonian liquid, an apparent viscosity is needed for calculating Darcy flow using Equation (2). The apparent viscosity may be expressed in general as a function of saturation and flow potential gradient (Wu and Pruess, 1996):

$$\mu_{nn} = \mu_{nn}(S_{nn}, \nabla \Phi_{nn}) \quad (9)$$

where the flow potential gradient is defined as

$$\nabla\Phi_{nn} = \nabla P_{nn} - \rho_{nn} g \nabla D \quad (10)$$

Multiple apparent viscosity functions, or rheological correlations, for non-Newtonian fluids in porous media have been proposed, expressing the viscosity as a function of the pore velocity or the potential gradient (Savins, 1969). The power-law model (Christopher and Middleman, 1965) is the most widely used rheological correlation for non-Newtonian fluids. It describes the rheological property of shear-thinning fluids, such as polymer and foam solutions, in porous medium flow. Another common non-Newtonian class of fluids is the Bingham fluid (Wu et al., 1992). The numerical treatment of porous medium flow of power-law and Bingham plastic fluids is discussed in detail in Wu and Pruess (1998).

EOS3nn uses a new rheological correlation for a generalized non-Newtonian fluid, combining the power-law model with that for Bingham fluids. The apparent viscosity for the power-law/Bingham fluid flow is the given by:

$$\mu_{nn} = \mu_{eff} \left(\frac{k k_{rnn}}{\mu_{eff}} \left(|\nabla\Phi_e| \right) \right)^{\frac{n-1}{n}} \quad (11)$$

where n is the power-law index; $\nabla\Phi_e$ is the effective potential gradient, whose scalar component in the flow direction X is defined as

$$(\nabla\Phi_e)_x = (\nabla\Phi)_x - G \quad \text{for } (\nabla\Phi)_x > G \quad (12a)$$

$$(\nabla\Phi_e)_x = (\nabla\Phi)_x + G \quad \text{for } (\nabla\Phi)_x < -G \quad (12b)$$

$$(\nabla\Phi_e)_x = 0 \quad \text{for } -G \leq (\nabla\Phi)_x \leq G \quad (12c)$$

where G is the minimum potential gradient required to make a Bingham fluid flow.

In Equation (11), μ_{eff} is defined as:

$$\mu_{\text{eff}} = \frac{H}{12} \left(9 + \frac{3}{n} \right)^n \left\{ 150 k k_{rnn} \phi (S_{nn} - S_{nnir}) \right\}^{(1-n)/2} \quad (13)$$

where H is a consistence parameter, and S_{nnir} is the irreducible or residual saturation of the non-Newtonian fluid.

The two power-law parameters, n and H, as well as the Bingham parameter, G, are normally obtained from laboratory measurement and data fitting. The power-law index, n, ranges between 0 and 1 for a shear-thinning fluid. Note that the viscosity from Equation (11) becomes infinite as the flow potential gradient tends to zero for a shear-thinning fluid. Therefore, direct use of (11) in numerical calculations will cause numerical difficulties. Instead, a linear interpolation scheme is used if the potential gradient becomes very small. The viscosity for a small value of potential gradient is calculated by the following interpolation:

$$\mu_{nn} = \mu_1 + \frac{\mu_1 - \mu_2}{\delta_1 - \delta_2} (|\nabla \Phi_e| - \delta_1) \quad (14)$$

for $|\nabla \Phi_e| < \delta_1$, where the two interpolation parameters are δ_1 (~ 10 Pa/m) and δ_2 [$(\delta_1 - \delta_2) = 10^{-7}$ Pa/m], and μ_1 and μ_2 are estimated as:

$$\mu_j = \mu_{\text{eff}} \left(\frac{k k_{rnn}}{\mu_{\text{eff}}} \delta_j \right)^{\frac{n-1}{n}} \quad (j=1, 2) \quad (15)$$

On the other hand, when potential gradients become very large, the apparent viscosity tends to zero. To avoid the numerical problems associated with zero viscosity, a minimum or threshold viscosity value is introduced.

Table 1 summarizes the EOS3nn module in terms of mass components, phases, parameter options, and primary variables.

Table 1. Summary Description of the EOS3nn Module

Components	#1: Non-Newtonian fluid component #2: Non-condensable gas (default: air)
Phases	#1: Gas #2: Non-Newtonian liquid phase
Parameter choices, block MULTI (NK, NEQ, NPH, NB)	(2, 2, 2, 6)
Primary Variables ^{&}	(P_g , S_{nn}): (Gas pressure, liquid saturation)
^{&} Primary variables apply to single-phase liquid, two-phase gas-liquid, and single-phase gas conditions; no parameter switching required.	

3. Input Data

The input data formats for EOS3nn are identical to those used by the EOS3 module (Pruess, 1991). However, EOS3nn requires additional input describing the properties of the gas and non-Newtonian liquid, which are supplied using the SELEC data block:

SELECtion keyword to introduce data describing gas and liquid properties.

Record SELEC.1

Format (I5)
IE(1)

IE(1) Set equal to 2 indicating that two additional records are read. The records contain reference gas-phase properties and properties of the non-Newtonian liquid.

Record SELEC.2

Format (8E10.4)

FE(I), I=1,2,..., 8

- FE(1) FE(1) = ρ_g^o [kg/m³]: density of the gas phase at reference pressure and reference temperature. If FE(1) is set equal to 0 (default), the gas density will be calculated internally for air under the reference conditions.
- FE(2) FE(2) = μ_g [Pa·s]: dynamic viscosity of the gas phase at reference pressure and reference temperature. If FE(1) is set equal to 0 (default), gas viscosity will be calculated internally for air under the reference conditions.
- FE(3) FE(3) = ρ_{nn}^o [kg/m³]: density of the non-Newtonian liquid at reference pressure and reference temperature. If FE(3) is set equal to 0 (default), the liquid density will be calculated internally for water under reference conditions.
- FE(4) FE(4) = μ_w [Pa·s]: dynamic viscosity of the non-Newtonian fluid at reference pressure and reference temperature. If FE(3) is set equal to 0 (default), the viscosity will be calculated internally for water under reference conditions.
- FE(5) FE(5) = C_{nn} [1/Pa]: compressibility of the non-Newtonian liquid at reference pressure and reference temperature. If FE(3) is set equal to 0 (default), the compressibility will be calculated internally for water under reference conditions.
- FE(6) FE(6) = T^0 [°C]: reference temperature. If FE(6) is set equal to 0 (default), the reference temperature is set to 15 °C.
- FE(7) FE(7) = P^0 [Pa]: reference pressure. If FE(6) is set equal to 0 (default), the reference pressure is set to 1.013E5 Pa.
- FE(8) FE(8) = H [Pa·sⁿ]: power-law consistence coefficient.

Record SELEC.3

Format (3E10.4)

FE(I), I=9, 10, 11

- FE(9) FE(9) = n : power-law exponential index.
- FE(10) FE(10) = G [Pa/m]: minimum potential gradient of Bingham fluid. If zero, the liquid becomes a power-law non-Newtonian fluid.
- FE(11) FE(11) = μ_{min} [Pa·s]: minimum non-Newtonian liquid viscosity. If FE(11) is set equal to 0 (default), μ_{min} is set to 10⁻⁵ (Pa·s).

Note that all the parameters listed here can be subjected to estimation by inverse modeling using the iTOUGH2 command >> SELEC (see Finsterle, 2002b).

4. Code Installation

Users of the EOS3nn module receive the iTOUGH2 FORTRAN source code. It can be compiled on various platforms (specifically Unix workstations, Linux boxes, and PCs). The distribution contains instructions and support files for compilation of iTOUGH2 on a number of different platforms. In general, iTOUGH2/EOS3nn consists of the following source files, which need to be compiled and linked using appropriate compiler and linker options specific to the compiler and operating environment:

```
it2main.f
it2input.f
it2xxxx.f
it2user.f
mdep$(platform).f
t2cg22.f
t2solv.f
eos3nn.f
t2f.f
meshm.f
ma28.f
ifsdummy.f
pvmdummy.f
gslibdum.f
```

In addition to the files listed above, there is a number of include-files that need to be present in the installation directory. One of those include-files, file `maxsize.inc`, contains parameter statements that define the size of major arrays and thus the maximum problem size that can be handled. Error messages in the iTOUGH2 output file alert the user if array sizes are insufficient, and which parameter in file `maxsize.inc` needs to be increased.

Before compiling iTOUGH2/EOS3nn, subroutine `MULTI` in file `t2f.f` must be renamed (e.g., to `MULTIx`) to avoid multiply defined subroutine names. File `mdep$(platform).f` contains system calls specific to the platform `$(platform)`. For specific applications, files `ifsdummy.f`, `pvmdummy.f` and `gslibdummy.f` must be replaced with files `ifs.f`, `pvm.f`, and `gslib.f`, respectively.

Follow the instructions for installation, compilation, linking, and execution that are provided along with the iTOUGH2 distribution (see files read.me, it2install, it2make, Makefile or other documentation).

The sample problems discussed in Section 5 can be found in a subdirectory sampleNN.

5. Sample Problems

Two sample problems are provided in this section for testing the implementation of non-Newtonian fluid flow into iTOUGH2 and for demonstration of the EOS3nn module usage. The two problems are also intended to show input data and output formats. The two sample problems were run on a Linux platform; slight differences to the solutions obtained on other platforms using different compilers are expected. The two sample problems can be described as follows:

- (1) One-dimensional, two-phase displacement of a Newtonian gas by a power-law non-Newtonian liquid; comparison with the numerical solution obtained with the MSFLOW multiphase flow simulator (Wu, 1998).
- (2) One-dimensional, two-phase displacement of a Newtonian gas by a power-law/Bingham non-Newtonian liquid; comparison with the numerical solution obtained with the MSFLOW multiphase flow simulator (Wu, 1998).

A detailed description of the two test problems is provided in the following subsections, including values of the physical parameters, grids, and model conditions used in the simulation. The numerical results and comparisons to the MSFLOW simulator are presented.

Because no analytical solutions are available for non-Newtonian liquid and gas displacement problems, EOS3nn is tested through comparison with another numerical multiphase flow simulator (MSFLOW, Wu, 1998). MSFLOW is a three-phase flow simulator for oil, water, and gas. Its capability to model non-Newtonian flow has been verified using analytical solutions for single-phase liquid and liquid-liquid displacements.

5.1 Sample Problem 1: Displacement of Air by a Power-Law Non-Newtonian Liquid

Sample Problem 1 considers one-dimensional immiscible displacement of air by a non-Newtonian, power-law liquid. The displacement occurs in a uniform, homogeneous, horizontal, one-dimensional rock column, which is initially saturated with 80% gas and 20% liquid. A power-law fluid is injected at the inlet at a constant injection rate, displacing the *in-situ* mobile gas. The 1-D horizontal column is 104 m long and discretized into 300 elements with a uniform grid spacing of $\Delta x = 0.02$ m for the first 200 elements and $\Delta x = 1$ m for the remaining 100 elements.

Rock and fluid properties are given in Table 2 and in Figure 1, which shows an excerpt from the input file. As shown in Table 2 and Figure 1, default gas properties (air) are invoked by setting FE(1) and FE(2) to zero. Reference density and viscosity are internally calculated based on the reference temperature and pressure given in FE(6) and FE(7), respectively, assuming the non-condensable gas is air. Setting FE(10) = G = 0 makes the liquid a power-law non-Newtonian fluid. The van Genuchten (1980) relative permeability and capillary pressure relations are used with the parameters shown in Table 2.

Type “itough2 sam1NN 3nn” to execute the first sample problem (the input file and the reference output file are provided in a subdirectory sampleNN). Figure 2 shows an excerpt from the output file with the simulation results after 1,000 days of displacement. A comparison of the saturation profiles calculated with iTOUGH2/EOS3nn and MSFLOW after 100 and 1,000 days of power-law fluid injection is shown in Figure 3; the numerical results from the two simulators are in agreement.

Table 2. Parameters for Sample Problems

Parameter	Value	Unit
Porosity	$\phi = 0.20$	-
Reference liquid density	$\rho_{nm}^0 = 1,000$	kg m^{-3}
Water phase viscosity	$\mu_w = 1 \times 10^{-3}$	$\text{Pa}\cdot\text{s}$
Power-law index	$n = 0.5$	-
Power-law coefficient	$H = 0.01$	$\text{Pa}\cdot\text{s}^{0.5}$
Minimum pressure gradient Sample Problem 1 Sample Problem 2	$G = 0$ $G = 10^4$	Pa/m Pa/m
Permeability	$k = 10^{-12}$	m^2
Injection rate	$q = 10^{-4}$	kg s^{-1}
Injection time	$t = 1,000$	day
Irreducible liquid saturation	$S_{nmir} = 0.2$	
Reference temperature	$T^0 = 20$	$^{\circ}\text{C}$
Reference pressure	$P^0 = 1.013 \times 10^5$	Pa
van Genuchten parameters	$m = 0.3$ $\alpha = 10^{-6}$	- Pa^{-1}

```

samNN1: gas displacement by power-law non-Newtonian liquid
ROCKS-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
soil1      2 2.500      0.2000      0.1000E-11 .1000E-11 .1000E-11 1.000      1000.
           1.0000
           7      0.3000      0.2000      1.000      1.000
           7      0.3000      0.2000      0.1000E-05 .1000E+08 1.000

PARAM-----1-----*-----123456789012345678901234-----*-----5-----*-----6-----*-----7-----*-----8
4 25000      500010000000000000000030 03400 0.00e-05      00000
0.00000E00 8.6400E07 1.000E+02      9.80665      3.0
1.0000e-3
1.000000000000000E+05      .20

TIMES-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
3      1
3.6000E05 3.6000E06 8.6400E06

SELEC-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
2
0.0      0.0      1000.      0.001 1.00e-10      20.00 1.013e5 0.01000
0.5      0.0      1.0e-5

GENER-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
All 1      COM1 1.00000e-4

ELEM-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
All 1      soil10.2000E-010.4000E-01      0.1000E-010.5000E+00-.5000E+00
All 2      soil10.2000E-010.4000E-01      0.3000E-010.5000E+00-.5000E+00
All 3      soil10.2000E-010.4000E-01      0.5000E-010.5000E+00-.5000E+00
... ..
Z1198      soil10.1000E+010.2000E+01      0.9750E+020.5000E+00-.5000E+00
Z1199      soil10.1000E+010.2000E+01      0.9850E+020.5000E+00-.5000E+00
Y11 1      soil10.1000E+520.2000E+01      0.9950E+020.5000E+00-.5000E+00

CONNE-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
All 1A11 2      10.1000E-010.1000E-010.1000E+01
All 2A11 3      10.1000E-010.1000E-010.1000E+01
All 3A11 4      10.1000E-010.1000E-010.1000E+01
... ..
Z1197Z1198      10.5000E+000.5000E+000.1000E+01
Z1198Z1199      10.5000E+000.5000E+000.1000E+01
Z1199Y11 1      10.5000E+000.5000E+000.1000E+01

START-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
INCON-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8
All 1      1.0000e05      0.20000      0.20000      20.

ENDCY-----1-----*-----2-----*-----3-----*-----4-----*-----5-----*-----6-----*-----7-----*-----8

```

Figure 1. Excerpt from iTOUGH2/EOS3nn input file samNN1 for displacement of gas by power-law non-Newtonian liquid.

 ARRAY DIMENSIONS (SEE FILE maxsize.inc)

MAXEL	=	5000	Maximum number of elements
MAXCON	=	20000	Maximum number of connections
MAXK	=	2	Maximum number of components
MAXEQ	=	3	Maximum number of equations
MAXPH	=	2	Maximum number of phases
MAXB	=	6	Maximum number of phase-dependent secondary variables
MAXSS	=	100	Maximum number of sinks/sources
MAVTAB	=	100	Maximum average number of table entries per sink/source
MAXROC	=	100	Maximum number of rock types
MAXTSP	=	5	Maximum number of specified time steps, divided by eight
MAXLAY	=	10	Maximum number of reservoir layers for wells on deliverability
MXRPCP	=	7	Maximum number of parameters for relative permeability and capillary pressure functions
MXPCTB	=	30	Maximum number of points in table for ECM capillary pressure
MXTBC	=	5	Maximum number of elements with time vs. boundary condition
MXTBCT	=	4000	Maximum number of time vs. pressure data
MAXTIM	=	600	Maximum number of calibration times
MAXN	=	20	Maximum number of parameters to be estimated
MAXO	=	100	Maximum number of datasets
MAXM	=	1400	Maximum number of calibration points
MAXPD	=	1000	Maximum number of paired data
MAXR	=	300	Maximum number of elements or indices of each parameter or observation
MAXBRK	=	20	Maximum number of points in time at which SAVE file is written for restart
MAXEBRK	=	20	Maximum number of elements with new initial conditions after restart
MAXCOEFF	=	5	Maximum number of coefficients for data modeling functions
MAXMCS	=	100	Maximum number of Monte Carlo simulations
MAXCURVE	=	100	Maximum number of curves to be plotted
MAXXGR	=	3	Dimension of third index of array XGUESSR
MTYPE	=	17	Number of observation types
MPFMT	=	6	Number of plot file formats

PROGRAM	VERSION	DATE	COMMENT
---------	---------	------	---------

iTOUGH2		Current version	iTOUGH2 V5.1 (AUGUST, 2002)
iTOUGH	1.0	1 AUGUST 1992	ITOUGH User's Guide, Version 1.0, Report NIB 92-99
iTOUGH2	2.2	1 FEBRUARY 1994	iTOUGH2 User's Guide, Version 2.2, Report LBL-34581
iTOUGH2	3.0	12 JULY 1996	YMP Software qualification, Report LBNL-39489
iTOUGH2	3.1	1 APRIL 1997	iTOUGH2 Command Reference, Version 3.1, Report LBNL-40041
iTOUGH2	3.2	30 JUNE 1998	YMP Software Qualification, Report LBNL-42002
iTOUGH2	3.3	1 OCTOBER 1998	Parallelization using PVM, Report LBNL-42261
iTOUGH2	4.0	19 JANUARY 1999	Released by Energy Science and Technology Software Center
iTOUGH2	5.0	31 JULY 2002	Qualified for use within Yucca Mountain Project

Figure 2 (cont.). Excerpt from iTOUGH2/EOS3nn output file samNN1.out

WHATCOM	1.0	10	AUGUST	1993	#35: Q: WHAT COMPUTER IS USED? A: LINUX	
CALLSIG	1.0	5	DECEMBER	1995	#112: SIGNAL HANDLER	
CPUSEC	1.0	10	AUGUST	1993	#--: RETURNS CPU-TIME (VERSION LINUX)	
OPENFILE	4.0	19	JANUARY	1999	#31: OPENS MOST OF THE FILES	
LENOS	1.0	1	MARCH	1992	#28: RETURNS LENGTH OF LINE	
PREC	1.0	1	AUGUST	1992	#86: CALCULATE MACHINE DEPENDENT CONSTANTS	
ITHEADER	3.2	27	MAY	1998	#29: PRINTS iTOUGH2 HEADER	
DAYTIM	1.0	10	AUGUST	1993	#32: RETURNS DATE AND TIME (VERSION SUN)	
THEADER	5.0	12	JULY	2002	#30: PRINTS TOUGH2 HEADER	
SOLVTYPE	1.0	1	OCTOBER	1999	INITIALIZE PARAMETERS FOR THE SOLVER PACKAGE	
INPUT	5.0	12	JULY	2002	READ ALL DATA PROVIDED THROUGH FILE INPUT	
CHECKMAX	5.0	12	JULY	2002	#41: CHECK KEY DIMENSIONS	
FLOPP	1.0	11	APRIL	1991	CALCULATE NUMBER OF SIGNIFICANT DIGITS FOR FLOATING POINT ARITHMETIC	
RFILE	5.0	12	JULY	2002	INITIALIZE DATA FROM FILES MESH OR MINC, GENER, AND INCON	
ITINPUT	1.0	1	AUGUST	1992	# 2: READS COMMANDS OF COMMAND LEVEL 1	
READCOMM	2.5	14	JUNE	1996	#24: READS A COMMAND	
FINDKEY	4.2	22	FEBRUARY	2000	#25: READS A KEYWORD	
LTU	1.0	1	AUGUST	1992	#26: CONVERTS LOWER TO UPPER CASE	
GETINDEX	3.3	17	JULY	1998	#45: GETS INDEX OF ELEMENTS, CONNECTIONS, AND SOURCES	
INIGUESS	5.0	12	JULY	2002	#38: INITIAL GUESS OF PARAMETERS (XGUESS)	
IXLBXUB	2.1	21	SEPTEMBER	1993	#43: INITIALIZES ARRAY XLB AND XUB	
SETWSCAL	4.3	18	SEPTEMBER	2000	#39: INITIALIZES ARRAY WSCALE	
OBSMEAN	1.0	1	AUGUST	1992	#40: CALCULATES MEAN OF OBSERVATIONS	
SETXSCAL	1.0	1	AUGUST	1992	#42: INITIALIZES ARRAY XSCALE	
IN_OUT	5.0	12	JULY	2002	#35: PRINTS A SUMMARY OF INPUT DATA	
TIMEWIND	5.0	12	JULY	2002	#53: SETS TIME WINDOW	
PRSTATUS	3.1	20	FEBRUARY	1997	#91: PRINTS STATUS MESSAGES	
ERRORMSG	2.5	21	MARCH	1996	#34: PRINTS ERROR MESSAGES	
FCNLEV	5.0	12	JULY	2002	#50: RETURNS WEIGHTED RESIDUAL VECTOR	
UPDATE	5.0	12	JULY	2002	#37: UPDATES PARAMETERS	
PRIORINF	2.1	21	SEPTEMBER	1993	#48: PRIOR INFORMATION	
OBSERVAT	5.0	12	JULY	2002	#62: COMPARES MEASURED AND CALCULATED QUANTITIES	
GETMESH	3.2	20	JUNE	1998	#47: READS FILE MESH, MINC, GENER, AND INCON	
GETINCON	5.0	12	JULY	2002	#46: READS FILE INCON	
INITTOUG	5.0	12	JULY	2002	#54: INITIALIZES TOUGH2 RUN (REPLACES CYCIT)	
EOS3nn	1.0	10	JUNE	2002	EOS3nn ... EOS MODULE FOR Non-Newtonian-WATER/AIR	
WGPROP	1.0	12	JUNE	2002	DEFAULT PROPERTIES MODULE FOR WATER/GAS(AIR)	
SAT	4.2	MOS	16	JULY	1999	STEAM TABLE EQUATION: SATURATION PRESSURE AS FUNCTION OF TEMPERATURE
COWAT	4.2	MOS	16	JULY	1999	LIQUID WATER DENSITY AND INT. ENERGY AS FUNCTION OF TEMPERATURE AND PRESSURE
SUPST	4.2	MOS	16	JULY	1999	VAPOR DENSITY AND INTERNAL ENERGY AS FUNCTION OF TEMPERATURE AND PRESSURE

Figure 2 (cont.). Excerpt from iTOUGH2/EOS3nn output file samNN1.out

VISW	1.0		22 JANUARY	1990	VISCOSITY OF LIQUID WATER AS FUNCTION OF TEMPERATURE AND PRESSURE
VISCO	1.0		1 FEBRUARY	1990	CALCULATE VISCOSITY OF VAPOR-AIR MIXTURES
COVIS	1.0		1 FEBRUARY	1990	COEFFICIENT FOR GAS PHASE VISCOSITY CALCULATION
VISS	1.0		22 JANUARY	1990	VISCOSITY OF VAPOR AS FUNCTION OF TEMPERATURE
PCAP	5.1		1 AUGUST	2002	CAPILLARY PRESSURE FUNCTIONS
RELP	4.4		9 FEBRUARY	2001	RELATIVE PERMEABILITIES
BALLA	3.3		17 JULY	1998	PERFORM SUMMARY BALANCES FOR VOLUME, MASS, AND ENERGY
CALLTOUG	5.0		12 JULY	2002	#55: CALLS TOUGH2 FOR ONE TIME STEP
TSTEP	3.1		27 MARCH	1997	ADJUST TIME STEPS TO COINCIDE WITH USER-DEFINED TARGET TIMES
MULTI	5.1	NN	6 AUGUST	2002	ASSEMBLE ALL ACCUMULATION AND FLOW TERMS, NON-NEWTONIAN FLUIDS
QU	5.0		12 JULY	2002	ASSEMBLE ALL SOURCE AND SINK TERMS
					"RIGOROUS" STEP RATE CAPABILITY FOR MOP(12) = 2
LINEQ	2.0		4 OCTOBER	1999	INTERFACE FOR LINEAR EQUATION SOLVERS T2CG2
					CAN CALL A DIRECT SOLVER OR A PACKAGE OF CONJUGATE GRADIENT SOLVERS
VISNN	5.1	NN	6 AUGUST	2002	NON-NEWTONIAN FLUID VISCOSITY
VISNNO	5.1	NN	6 AUGUST	2002	INITIAL NON-NEWTONIAN FLUID VISCOSITY
CONVER	5.0		12 JULY	2002	UPDATE PRIMARY VARIABLES AFTER CONVERGENCE IS ACHIEVED
OUT	5.0		12 MARCH	2001	PRINT RESULTS FOR ELEMENTS, CONNECTIONS, AND SINKS/SOURCES
SATW	5.0		12 JULY	2002	STEAM TABLE EQUATION: SATURATION PRESSURE AS FUNCTION OF TEMPERATURE, PSAT(SL->0) ->
TERMINAT	5.0		12 JULY	2002	61: PERFORM ERROR ANALYSIS AND TERMINATE iTOUGH2
PLOTFILE	4.0		19 JANUARY	1999	#58: WRITES PLOTFILE IN PLOPO-FORMAT
WRIFI	5.0		12 JULY	2002	AT THE COMPLETION OF A TOUGH2 RUN, WRITE PRIMARY VARIABLES ON FILE SAVE
QNORMAL	2.5		13 JANUARY	1996	#87: RETURNS QUANTILE OF NORMAL DISTRIBUTION
MOMENT	3.3		28 OCTOBER	1998	#90: MOMENTS OF DISTRIBUTION
PLOTIF	1.0		15 FEBRUARY	1993	#96: PLOT INTERFACE
REFORMAT	4.0		19 JANUARY	1999	#97: REFORMATS PLOT FILES
QUOTES	1.0		15 FEBRUARY	1993	#98: RETURNS TEXT BETWEEN QUOTES
WRITEPAR	4.2		27 JULY	1999	#56: WRITE BEST FIT PARAMETER SET AND BLOCK ROCKS

=====
--- 403rd iTOUGH2 simulation job completed: 7-Aug-02 10:59 --- CPU time used = 89.44 sec.

Figure 2 (cont.). Excerpt from iTOUGH2/EOS3nn output file samNN1.out

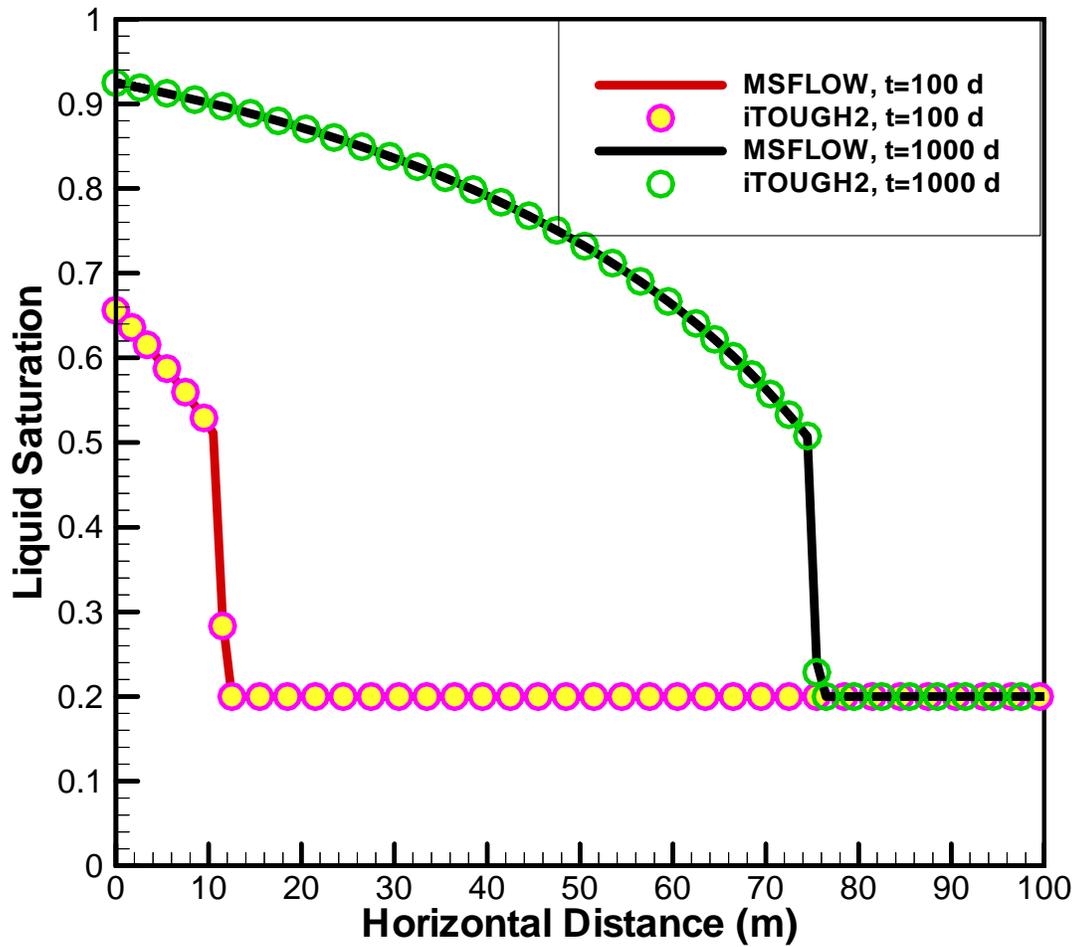


Figure 3. Comparison of the liquid saturation profiles calculated with iTOUGH2/EOS3nn (circles) and MSFLOW (lines) at $t = 100$ and 1,000 days of power-law fluid displacement.

5.2 Sample Problem 2: Displacement of Air by a Power-Law/Bingham Non-Newtonian Liquid

Sample Problem 2 is a slightly modified version of the previous one-dimensional immiscible displacement problem described in Section 5.1. The same model grid, rock and fluid properties are used as summarized in Table 2 and Figure 1 above, with the exception that the parameter FE(10) is set to $G = 10,000$ Pa/m. The parameter G represents the minimum pressure gradient for flow of Bingham non-Newtonian fluids.

Type “itough2 sam2NN 3nn” to execute the first sample problem (the input file and the reference output file are provided in a subdirectory sampleNN).

A comparison of the saturation profiles calculated from iTOUGH2/EOS3nn and MSFLOW after 100 and 1,000 days of power-law/Bingham fluid displacement is shown in Figure 4. The numerical results from the two simulators are in very good agreement at the early time of 100 days. There are, however, slight differences between the two solutions at the late time of 1,000 days. A further check of the simulation results revealed that the small differences are a result of the different time stepping scheme implemented in the two codes, leading to different times discretization errors, with iTOUGH2/EOS3nn taking smaller times steps than MSFLOW. This explains why the saturation profiles obtained with EOS3nn are somewhat steeper than those obtained with MSFLOW.

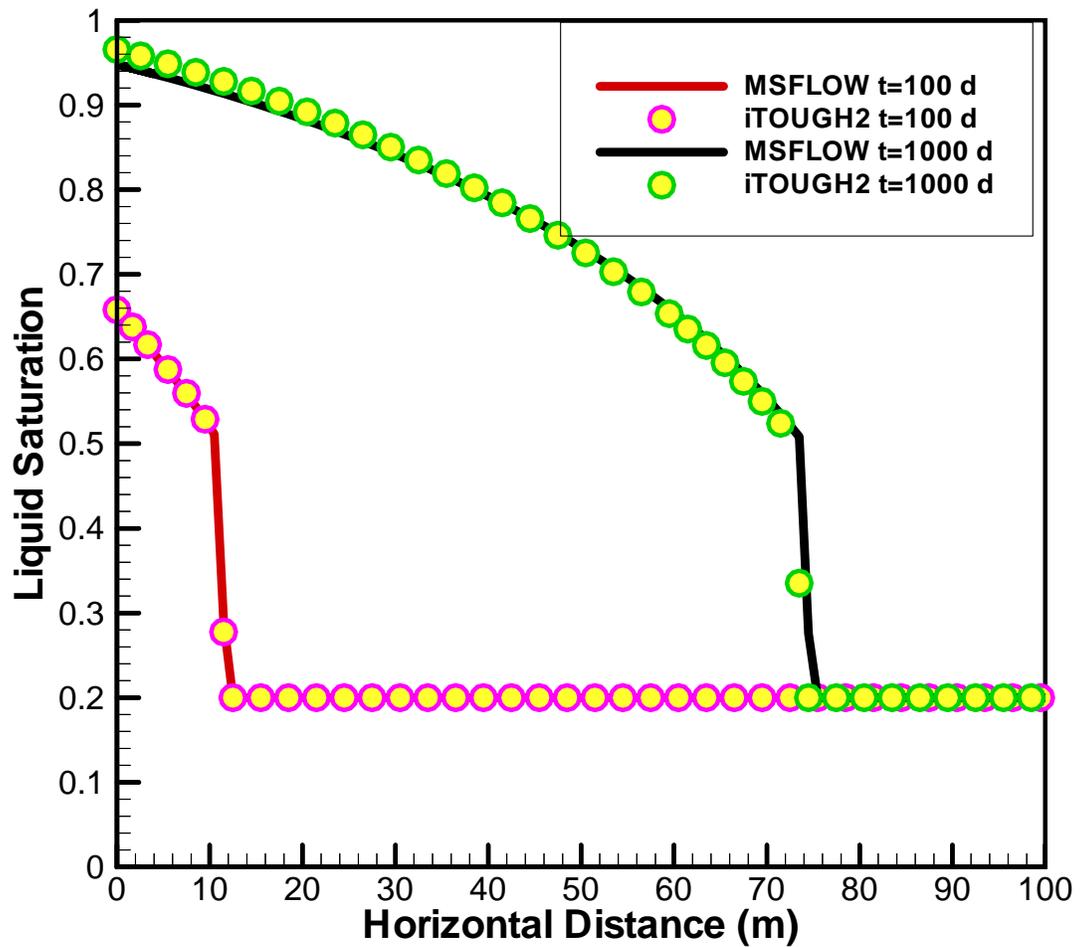


Figure 4. Comparison of the liquid saturation profiles obtained with iTOUGH2/EOS3nn (circles) and MSFLOW (lines) at $t = 100$ and 1,000 days of power-law/Bingham fluid displacement.

Acknowledgment

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