T2Well/ECO2N Version 1.0:

Multiphase and Non-Isothermal Model for
Coupled Wellbore-Reservoir Flow of
Carbon Dioxide and Variable Salinity Water

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Abstract

At its most basic level, the injection of CO_2 into geologic CO_2 storage sites involves a system comprising the wellbore and the target reservoir. The wellbore is the only conduit available to emplace CO_2 into reservoirs for long-term storage. At the same time, wellbores in general have been identified as the most likely conduit for CO_2 and brine leakage from geologic carbon sequestration (GCS) sites, especially those in sedimentary basins with historical hydrocarbon production. We have developed a coupled wellbore and reservoir model for simulating the dynamics of CO_2 injection and leakage through wellbores. It can be seen as an extension to standard TOUGH2/ECO2N, and can be applied to situations relevant to geologic CO_2 storage involving upward flow (e.g., leakage) and downward flow (injection). The new simulator integrates a wellbore-reservoir system by assigning the wellbore and reservoir to two different sub-domains in which flow is controlled by appropriate physical laws. In the reservoir, we model flow using a standard multiphase Darcy flow approach. In the wellbores, we use the Drift-Flux Model and related conservation equations for describing transient two-phase non-isothermal wellbore flow of CO_2-water mixtures. The mass and thermal energy balance equations are solved numerically by a finite difference scheme with wellbore heat transmission to the surrounding rock handled either semi-analytically or numerically. The momentum balance equation for the flow in the wellbore is solved numerically with a semi-explicit scheme. This manual provides instructions for compilation and use of the new model, and presents some example problems to demonstrate its use.

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1. Introduction

As discrete pathways through geologic formations, boreholes and wells are critical to the success of geologic carbon sequestration (GCS) projects because of the access they provide to storage reservoirs for site characterization, CO_2 injection, monitoring, and fluid withdrawal. On the other hand, boreholes and wells, in particular deep abandoned wells from oil or gas exploration and production activities, are also potential leakage pathways for injected CO_2 and displaced brine. Critical to the efficient and safe implementation of GCS is a detailed understanding of flow and transport processes in boreholes to control CO_2 injection and to model potential leakage up the borehole. In order to facilitate understanding of borehole-flow and transport processes and improve the design of injection operations, we have developed a borehole-flow simulator for CO_2 and variable salinity water that models transient non-isothermal processes involved with the flow of CO_2 in deep boreholes and wells including transitions from supercritical to gaseous phases. The new wellbore flow model is based on the drift-flux model (DFM) approach and is an extension of TOUGH2/ECO2N (Pruess, 2005; Pruess and Spycher, 2007) which can describe single- and two-phase flows of CO_2-water-NaCl mixtures but cannot describe three-phase conditions that would include a situation where both liquid and gaseous CO_2-rich phases coexist. Unlike the coupling approach used in earlier efforts (e.g., Hadgu et al., 1995), the deliverability option in TOUGH2 is not used and the flow in the wellbore is not assumed to be at steady state. Instead, the new software (T2Well/ECO2N) is an integrated simulator of a wellbore-reservoir system of CO_2-brine in which the wellbore and reservoir are two different sub-domains where flow is controlled by different physical laws. In this report, we describe the model equations, provide instructions for using the model, and present several examples. Some of the text and equations related to model development and verification are taken directly from our GHGT-9 Proceedings paper (Pan et al., 2009).

2. Mathematical Formulation

2.1 Introduction

The approach we use for describing wellbore flow is based on the drift-flux model (DFM) (Shi et al., 2005) for one-dimensional (1D) transient two-phase non-isothermal flow of CO_2-water mixtures. Conservation equations for mass, momentum and energy under different flow regimes in the wellbore are solved numerically while heat transmission from the wellbore to the surrounding rock is either handled semi-analytically or numerically. We implement the DFM in TOUGH2 (Pruess et al., 1999) with the ECO2N equation of state module (Pruess, 2005; Pruess and Spycher, 2007). The conventional approach for calculating the mixture velocity in the drift-flux model (DFM) is often based on the steady-state pressure loss equation for wellbore flow (Brill and Mukherjee, 1999). To improve simulation performance in well-bore flow processes involving high fluxes, we have extended the DFM to include the transient terms of the momentum conservation equations in calculating the velocity from the pressure gradient. Only the governing equations and implementations for the wellbore portion are described here whereas the description of the models of flow in the reservoir can be found in the related TOUGH2 documents (Pruess et al., 1999) and will not be repeated here.

2.2 Mass and Energy Conservation

According to mass and energy conservation principles, the generalized conservation equation of mass components and energy in the wellbore can be written as follows:

$$\frac{\partial M^{\kappa}}{\partial t} = q^{\kappa} + F^{\kappa} \tag{1}$$

where superscript κ is the index for the components, $\kappa = 1$ (H_2O), 2 (CO_2), and 3 (energy, taken as internal and kinetic energy here), M^{κ} are the accumulation terms of the components κ; q^{κ} are source/sink terms for mass or energy components; and F^{κ} are the mass or energy transport terms along the borehole due to advective processes. Note that in the description of the mathematical development here, we neglect the NaCl component for brevity as it plays a passive role in the multiphase processes in the wellbore, yet it may be present as a component in ECO2N.

2.3 Accumulation Terms

The accumulation term (M^{κ}) of Eq. 1 for the mass components (H_2O and CO_2) in single- or two-phase system is given by

$$M^{\kappa} = \rho_G S_G X_G^{\kappa} + \rho_L S_L X_L^{\kappa} \quad (\kappa = 1 \text{ and } 2) \tag{2}$$

where X_{β}^{κ} is the mass fraction of component κ in fluid phase β ($\beta = $ G for gas; $\beta = $ L for liquid), ρ_{β} is the density of phase β; and S_{β} is the local saturation of phase β defined as

$$S_G = \frac{A_G}{A} = \frac{A_G}{A_G + A_L} \tag{3}$$

where A is the well cross-sectional area; A_G and A_L denote the cross-sectional areas occupied by gas and liquid over the cross section at a given elevation (or distance along the well). The accumulation term for energy is defined as

$$M^3 = \sum_{\beta} \rho_{\beta} S_{\beta} \left(U_{\beta} + \frac{1}{2} u_{\beta}^2 \right)$$

(4)

where U_{β} is the internal energy of phase β per unit mass and $\frac{1}{2} u_{\beta}^2$ is the kinetic energy per unit mass while u_{β} is the velocity of phase β in the wellbore.

2.4 Flow Terms

Transport along the wellbore is governed in general by processes of advection, diffusion, and dispersion, and is also subject to other processes such as exchanges with the formation at feed or thief zones. The total advective mass transport term for component κ can be written in one-dimension as

$$F^{\kappa} = -\frac{1}{A} \left[\frac{\partial \left(A \rho_G \, X_G^{\kappa} \, S_G \, u_G \right)}{\partial z} + \frac{\partial \left(A \rho_L \, X_L^{\kappa} \, S_L \, u_L \right)}{\partial z} \right]$$

(5)

where u_{β} is the average velocity vector of phase within the wellbore, A is the well cross sectional area, and z is the along-wellbore coordinate (can be vertical, inclined, or horizontal).

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The transport terms for energy in the wellbore include those due to (1) advection, (2) kinetic energy, (3) potential energy, and (4) lateral wellbore heat loss/gain. The overall one-dimensional energy transport term can be written as

$$F^3 = -\lambda \frac{\partial T}{\partial z} - \frac{1}{A}\sum_\beta \frac{\partial}{\partial z}\left(A\,\rho_\beta S_\beta u_\beta \left(h_\beta + \frac{u_\beta^2}{2}\right)\right) - \sum_\beta \left(S_\beta\,\rho_\beta\,u_\beta\,g\cos\theta\right) - q'' \quad (6)$$

where h_β is specific enthalpy of fluid phase β, g is the gravitational acceleration, θ is the incline angle of the wellbore, q'' is the wellbore heat loss/gain per unit length of wellbore (optional if the surrounding formation is not explicitly represented in the numerical grid), and ρ_m is the density of the gas-liquid mixture. λ is the area-averaged thermal conductivity of the wellbore (both phases of the fluids and possible solid portion) and T is the temperature.

Note that the mass or energy exchange terms between a perforated wellbore section and its surrounding formation are omitted from the above equations for simplicity. These terms are calculated as flow through porous media as implemented in normal TOUGH2 except that the nodal distance to the interface on the wellbore side is set to zero in the grid.

2.5 Momentum Conservation Using the Drift-Flux Model (DFM)

In contrast to flow through porous media in which the flux or the velocity can be simply determined from the gradient of pressure and gravity using Darcy's Law, the determination of flow velocity in a wellbore involves solving the appropriate momentum conservation equations. Directly solving the momentum equations of two phase flow is difficult and often not practical as it has to be coupled into a reservoir simulator. Therefore, we invoke the DFM to describe both

single-phase and multiphase flow in wellbores to obtain the advective transport terms (F_β and u_β).

In the following descriptions, the drift-flux model is limited to one dimensional flow though a open pipe or annulus. Therefore, all variables in the development below should be considered as area-averaged or assumed to be constant over the cross-section except for those explicitly noted otherwise.

The drift-flux models were first developed by Zuber and Findlay (1965) and Wallis (1969), among others. Although various nomenclatures and forms of equations were used to describe the drift-flux model in the literature over decades, the basic idea of the drift-flux models is to assume that the gas velocity, u_G, can be related to the volumetric flux of the mixture, j, and the drift velocity of gas, u_d, by the empirical constitutive relationship below:

$$u_G = C_0\, j + u_d \tag{7}$$

Where C_0 is the profile parameter to account for the effect of local gas saturation and velocity profiles over the pipe cross-section. By definition, the volumetric flux j is the volumetrically weighted velocity

$$j = S_G u_G + (1 - S_G) u_L \tag{8}.$$

Therefore, the liquid velocity u_L can be determined as

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$$u_L = \frac{1 - S_G C_0}{1 - S_G} j - \frac{S_G}{1 - S_G} u_d \qquad (9).$$

With the draft-flux model (7)-(9), the momentum equations of two-phase flow in a wellbore can be simplified into a single equation in terms of the mixture velocity u_m and the drift velocity u_d as follows (see Appendix A):

$$\frac{\partial}{\partial t}(\rho_m u_m) + \frac{1}{A}\frac{\partial}{\partial z}\left[A\left(\rho_m u_m^2 + \gamma\right)\right] = -\frac{\partial P}{\partial z} - \frac{\Gamma f \rho_m |u_m| u_m}{2 A} - \rho_m g \cos\theta \qquad (10)$$

where the term $\gamma = \frac{S_G}{1 - S_G} \frac{\rho_G \rho_L \rho_m}{\rho_m^{*2}}\left[(C_0 - 1)u_m + u_d\right]^2$ is caused by slip between the two phases.

The mixture density, ρ_m, and the mixture velocity (velocity of mass center), u_m, are defined as follows:

$$\rho_m = S_G \rho_G + (1 - S_G)\rho_L \qquad (11)$$

and

$$u_m = \frac{S_G \rho_G u_G + (1 - S_G)\rho_L u_L}{\rho_m} \qquad (12)$$

The profile-adjusted average density is defined as follows:

$$\rho_m^* = S_G C_0 \rho_G + (1 - S_G C_0)\rho_L \qquad (13)$$

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Therefore, in the DFM approach, solving the complicated momentum equations of two-phase flow becomes an easier task with two steps. First, we obtain the mixture velocity by solving the simplified momentum Equation (10) and the drift velocity from some empirical relationships. Second, we calculate the gas velocity and the liquid velocity as a function of u_m and u_d as follows:

$$u_G = C_0 \frac{\rho_m}{\rho_m^*} u_m + \frac{\rho_L}{\rho_m^*} u_d$$

$$u_L = \frac{(1 - S_G C_0) \rho_m}{(1 - S_G) \rho_m^*} u_m - \frac{S_G \rho_G}{(1 - S_G) \rho_m^*} u_d$$

(14)

The challenge of the DFM is how to accurately estimate the drift velocity, u_d, and the profile parameter, C_0. In general, two-phase flow occurs in different flow regimes resulting in different interfacial interactions. As a result, both C_0 and u_d could be a function of flow regime and many formulas have been proposed to describe such relationships. Shi et al. (2005) proposed functional forms for the profile parameter and drift velocity with a set of optimized parameters obtained from an extensive set of large-scale pipe flow experiments performed by Oddie et al. (2003) for one-, two-, and three-phase flows at various inclinations, that can be applied continuously for all flow regimes. The following is a summary of the mathematical formulations related to the drift velocity proposed by Shi et al. (2005) that are implemented in T2Well.

First, the drift velocity is calculated as a function of gas saturation and other fluid properties:

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$$u_d = \frac{(1 - C_0 S_G) u_c K(S_G, K_u, C_0) m(\theta)}{C_0 S_G \sqrt{\rho_G / \rho_L} + 1 - C_0 S_G} \qquad (15)$$

where m(θ) describes the inclination (of the wellbore) effect:

$$m(\theta) = m_0 (\cos\theta)^{n_1} (1 + \sin\theta)^{n_2} \qquad (16)$$

where m_0, n_1, and n_2 are all fitted parameters.

K_u is the Kutateladze number, a function of Bond number, N_B (i.e., square of dimensionless wellbore diameter) (Richter, 1981):

$$K_u = \left[\frac{C_{ku}}{\sqrt{N_B}} \left(\sqrt{1 + \frac{N_B}{C_{ku}^2 C_w}} - 1 \right) \right]^{\frac{1}{2}} \qquad (17)$$

Where C_w (assumed to be a constant of 0.008 in the code) is a wall friction factor and the Bond number is defined as:

$$N_B = d^2 \left[\frac{g(\rho_L - \rho_G)}{\sigma_{GL}} \right] \qquad (18)$$

Where d is the wellbore diameter and C_{ku} was 75 in Richter's original formula, which resulted in overestimation of K_u in the range of smaller dimensionless diameter (Richter, 1981), we found that 142 is the better number to fit the experimental data provided in the same paper (Figure 1) and, therefore, is used in T2Well.
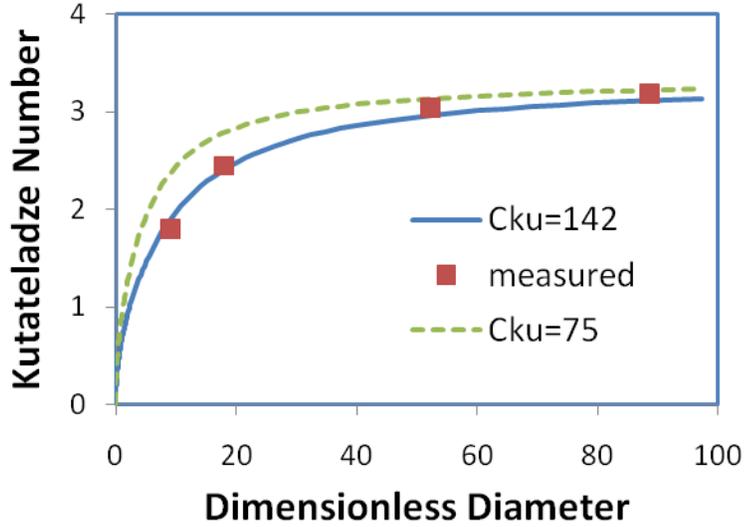
Figure 1. The calculated Kutateladze numbers (Eq. 12) comparing to the measured values as a function of dimensionless diameter (= $\sqrt{N_B}$)

The "characteristic velocity," u_c , is a measure of the velocity of bubble rise in a liquid column, given by

$$u_c = \left[\frac{g\,\sigma_{GL}(\rho_L - \rho_G)}{\rho_L^2} \right]^{1/4} \tag{19}$$

where σ_{GL} is the surface tension between gas and liquid phases.

The function $K(\cdot)$ in (15) is used to make a smooth transition of drift velocity between the bubble rise stage and the film flooding stage. Different from the linear interpolation suggested by Shi et al. (2005), we use the following smooth function:

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$$K = \begin{cases} 1.53 & S_G \le a_1 \\ 1.53 + \dfrac{C_0 K_u - 1.53}{2}\left[1 - \cos\left(\pi\dfrac{S_G - a_1}{a_2 - a_1}\right)\right] & a_1 \le S_G \le a_2 \\ C_0 K_u & S_G \ge a_2 \end{cases} \qquad (20)$$

where a_1 and a_2 are two transition points of gas saturation as suggested by Shi et al. (2005).

Because K is independent of the gas saturation for $S_G \le a_1$ and $S_G \ge a_2$, the function K is

constructed such that $dK/dS_G = 0$ in the neighborhoods of a_1 and a_2, making this derivative

continuous over the entire range of S_G. The fitting parameters, m_0, n_1, n_2, a_1, and a_2 are all

hardwired in the code and the values are obtained from the case of water/gas in Shi et al. (2005)

depending on C_{max} (a user-specified maximum profile parameter between 1.0 and 1.5) as

follows:

Table 1. Empirical parameters of DFM used in T2Well.

Fitting Parameter	Values for $C_{max} = 1.0$	Values for $C_{max} = 1.2$
a_1	0.06	0.06
a_2	0.21	0.12
m_0	1.85	1.27
n_1	0.21	0.24
n_2	0.95	1.08

Source:Shi et al., 2005.

Second, the profile parameter C_0 is calculated using the same formulas suggested by Shi et al.

(2005) as listed below (with different symbols) for completeness:

$$C_0 = \frac{C_{max}}{1 + (C_{max} - 1)\eta^2} \qquad (21)$$

where η is a parameter reflecting the effects of the flow status on the profile parameter and is calculated as follows:

$$\eta = \frac{\beta - B}{1 - B} \qquad \text{subject to the limits } 0 \leq \beta \leq 1 \qquad (22)$$

where B is the threshold parameter above which C_0 starts to drop below C_{max} and β is calculated as follows:

$$\beta = \max\left(S_G, F_V \frac{S_G |u_m|}{u_{sgf}} \right) \qquad (23)$$

Slightly different from Shi et al. (2005), we tied the threshold parameter B as a function of C_{max} :

$$B = \frac{2}{C_{max}} - 1.0667 \qquad (24)$$

Equation (24) provides B = 0.6 for C_{max} = 1.2, which is consistent with the values of a_1 (=0.06) and a_2 (=0.12) (Shi et al., 2005). B varies from 0.9333 (C_{max} = 1.0) to 0.2666 (C_{max} = 1.5). Note that if C_{max} = 1.0 (the optimal value for water/gas system as suggested by Shi et al., 2005), C_0 would be independent of gas saturation or velocity and the profile effect disappears.

Profile flattening can be made more or less sensitive to the gas velocity by adjusting the value of F_v (default =1) in Equation (23) whereas the "flooding" gas superficial velocity, u_{sgf}, is calculated as follows:

$$u_{sgf} = K_u \left(\frac{\rho_L}{\rho_G} \right)^{1/2} u_c \qquad (25)$$

Detailed discussions about the formulas (21)-(25) are described in Shi et al.(2005) and will not be duplicated here.

2.6 Solving the Discretized Equations

In the framework of TOUGH2, the mass and energy flux terms are calculated at each Newtonian iteration from the most recently updated primary variables (usually pressure, mass fractions, and temperature). Within the wellbore at each iteration, we calculate the mixture velocity (Eq. 10) first, then calculate drift velocity (Eq. 15) and finally calculate the gas velocity and the liquid velocity (Eq. 14). As for marching in time, the momentum conservation equation (Eq. 10) is solved semi-explicitly at interfaces of the neighbouring wellbore cells as

$$u_m^{n+1} = \frac{DR^{n+1} + \frac{1}{\Delta t} \rho_m^n u_m^n - \left(\frac{1}{A}\frac{\partial}{\partial z}\left(A \sum_\beta \rho_\beta S_\beta u_\beta^2\right)\right)^n}{\frac{\rho_m^{n+1}}{\Delta t} + \frac{f^n \Gamma \rho_m^{n+1} |u_m^n|}{2A}} \qquad (26)$$

where, the superscripts n and $n+1$ indicate the previous and current time levels, respectively; Δt is the time-step size, and DR is the total driving force given by

$$DR = -\frac{\partial P}{\partial z} - \rho_m \, g \cos\theta \qquad (27).$$

Normally, among the total pressure loss, that caused by elevation change contributes from 80 to 95% and the friction loss represents 5 to 20%, whereas the acceleration loss is normally negligible and can become significant only if a compressible phase exists at relatively low pressures (Brill and Mukhmerjee, 1999) or DR becomes very small (e.g., near hydrostatic state).

Therefore, the approach is more like that of an implicit formulation considering the above normal pressure loss partition. Here, because the spatial acceleration term enters the equation as an explicit term, the original formula of two phase summation (the second term on the left side of Eq. A1) can be used directly instead of involving the mixture velocity and an additional term due to drift velocity. If the change of spatial acceleration over Δt is negligible compared to the driving force, Eq. 26 should provide an accurate solution to Eq. 10. When a system reaches steady state, the solution is an exact numerical solution of Eq. 10 and the accuracy only depends on the grid resolution.

The component mass- and energy-balance equations of Eq. 1 are discretized in space using the conventional integrated finite-difference scheme of TOUGH2 for the wellbore system. Apart from the special treatment of the momentum equation (Eq. 26), time discretization is carried out using a backward, first-order, fully implicit finite-difference scheme. The discrete nonlinear equations for H_2O, CO_2, and energy conservation at node i (well block) can be written in a general form:

$$\left[M_i^{\kappa,n+1} - M_i^{\kappa,n} \right] \frac{V_i}{\Delta t} = F_{i,i+1/2}^{\kappa,n+1} - F_{i,i-1/2}^{\kappa,n+1} + Q_i^{\kappa,n+1} \quad (\kappa = 1, 2, \text{ and } 3) \tag{28}$$

where superscript n denotes the previous time level, with $n+1$ the current time level to be solved; subscript i refers to the index of wellbore grid cell; Δt is time-step size; V_i is the volume of wellbore cell i (wellbore diameter may vary). The flow terms in Eq. 28 are generic and include mass fluxes as well as heat transfer via both phases. The mass flow term is given by

$$F_{ij}^\kappa = A_{ij} \sum_\beta \left(\rho_\beta S_\beta X_\beta^\kappa \right)_{ij+1/2} u_{\beta,ij} \tag{29}$$

The total heat flux along the connection of nodes i and j may be evaluated by

$$F_{ij}^3 = A_{ij} \left\{ -\lambda \frac{\partial T}{\partial z} + \sum_\beta \left[\left(\rho_\beta S_\beta \left(h_\beta + \frac{u_\beta^2}{2} \right) \right)_{ij+1/2} u_{\beta,ij} \right] \right\} \tag{30}$$

where λ is the area-averaged thermal conductivity of the wellbore (both phases of the fluids and possible solid portion).

The heat exchanges between wellbore and the surrounding formation will either be calculated as the "normal" heat flow terms in standard TOUGH2 if the surrounding formation is explicitly represented in the numerical grid or they will be calculated (optionally) semi-analytically if no grid blocks of surrounding formation exist. In the latter case, Q_i^3 including both heat loss/gain by lateral wellbore heat transmission and the potential energy gain (the friction energy loss will convert to heat, and therefore does not affect the overall energy balance) are given by

$$Q_i^3 = -A_{wi} \left(K_{wi} \right) \left[\frac{T_i - T_\infty(z)}{r f(t)} \right] + \sum_\beta \left(\rho_\beta u_\beta \ g \ \cos\theta \right)_i \tag{31}$$

where A_{wi} is the lateral area between wellbore and surrounding formation; K_{wi} is thermal conductivity (or overall heat transfer coefficient) of wellbore/formation; T_i is the temperature in the ith wellbore node, $T_\infty(z)$ is ambient temperature; r is the radium of the wellbore and $f(t)$ is Ramey's well heat loss function (Ramey 1962):

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$$f(t) = \frac{1}{-\ln\left(\frac{r}{2\sqrt{\alpha t}}\right) - 0.29}$$ (32)

where α is the thermal dispersivity of the surrounding formation.

the term u_i is the nodal velocity obtained by averaging the velocities at interfaces. The second term of Eq. 31 reflects net energy gain or loss per unit time due to gravity, calculated as a sum of net potential energy gain rate over both phases for the grid cell i. Again, the prescribed energy source/sink terms or the mass/energy exchange terms between the perforated well section and the surrounding formations are omitted in the above equations for simplicity.

In evaluating the flow terms in Eqs. 29 through 31, subscript $ij + 1/2$ is used to denote a proper averaging or weighting of advective mass transport or heat transfer properties at the interface or along the connection between two blocks or nodes i and j ($j = i - 1$ or $i + 1$). In addition, fully upstream weighting should be used in Eqs. 29 and 30 for numerical stability. In a leaking/feeding zone of the wellbore, the mass or energy inflow/outflow terms are calculated as in standard TOUGH2 (i.e., the flow through porous media).

The standard TOUGH2 fully implicit residual-based method is used to solve the discrete nonlinear equations using Newton iteration. In general, we need to solve for four primary variables in ECO2N (pressure, saturation or mass fractions of H_2O, CO_2, and NaCl in fluids depending on phase conditions, and temperature) per node. The remaining variables such as viscosities, densities, thermal conductivities, etc. are secondary variables which can be calculated from selected primary variables. The Newton iteration process continues until the residuals are reduced below preset convergence levels. The sparse Jacobian matrices arising in Newton's

method are solved by user-selected conjugate gradient provided in TOUGH2. Time-step sizes

tend to be much smaller than typical all-porous media TOUGH2 problems due to the higher flow

rates and sensitivity to time-step size associated with wellbore flow.

Besides the explicit spatial acceleration terms used in solving the momentum equation, all the

velocities used in calculation of kinetic and potential energy in the energy balance equations are

also explicit to avoid unnecessarily slow convergence.

3. Using T2Well/ECO2N

3.1 Compilation

The code was written as a modification to TOUGH2/ECO2N using F90 and compiled and linked under Compaq Visual Fortran 6.6.a on a PC under Windows XP. In particular, the recursive function options shall be selected. For detailed compilation and linking parameters, see Appendix B. A list of the source code files is given below in Table 2:

Table 2. Source code files for T2Well/ECO2N

File name	Description
agra.f	A routine to save liquid and gas volume vs. time to a disk file DOFT and a routine to save a time series of flow rates through user-defined horizons
DFM.f	Wellbore flow model definitions, subroutines, and functions (Module:DriftFluxModel)
mudfv.f	Modified TOUGH2 subroutines CYCIT, MULTI, OUT, etc., wellbore simulation subroutine CalMixtureVelocity
t2cg22x.f	TOUGH2 main program
t2f.f	TOUGH2 subroutines
eco2n_well.f	Equation of state module for water, salt, and CO_2
meshm.f	Meshmaker
t2solv.f	Conjugate gradient linear equation solvers
T2	INCLUDE file with parameters for dimensioning major arrays

3.2 Execution

The executable "Wellbore.exe" was tested in the DOS shell under Windows XP (e.g., Click

Start->Run->cmd to open a DOS shell).

> Command line:
> Wellbore <mainInputFile>mainOutputfile
>
> Note: 1) mainInputfile must exist in the working directory;
> 2) Executable "Wellbore.exe" must be in the working directory or a path must be
> specified for it;
> 3) File "CO2TAB" must be in the working directory too.

3.3 Input files

The formats of input files are the same as those for TOUGH2/ECO2N (Pruess, 2005; Pruess and

Spycher, 2007) except for those noted below.

Main input file – *same as standard input file for TOUGH2/ECO2N, except:*

a) ROCKS data block

The domain (rock) name for the wellbore cells must start with the letter "w" or "x", where "w" indicates normal (open) wellbore cells whereas "x" indicates the special wellbore cells either filled with porous medium or consisting of a bundle of smaller tubes;

In the case of "x" rock, the first permeability (i.e., PER(1) in Record ROCKS.1) will be used as a scaling factor in the calculation of the effective diameter and the friction term (e.g., PER(1) of 100 means that the effective diameter will be 1/100 of the diameter calculated from the cross sectional area); Note that , the permeability of the formation will be used if the fluid flow between wellbore and formation is needed because of zero nodal distance specified in wellbore mesh(see section b below);

A negative value of heat conductivity will turn on the semi-analytical calculation of the thermal exchange between the wellbore cells and the surrounding formation

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via conductive heat flow. The temperature in the surrounding formation ($T_\infty(z)$ in Eq. 31) equals the initial temperature in each wellbore cell. In the case of a re-start run, the ambient temperatures are obtained from the section after "+++" of the INCON block. Note that the surrounding formation cells must not exist in the grid if the semi-analytical calculation is turned on. Otherwise, the thermal exchange between wellbore cells and the surrounding formation would be overestimated because of the heat flow would be calculated by both semi-analytical and normal Fourier Law conduction;

Type 8 capillary function shall be specified for the wellbore domains (i.e., no capillary pressure).

b) **ELEME and CONNE data blocks (or separate MESH file)**

Wellbore cells are identified by their rock name ("w" or "x"). Multiple wellbores or multiple branches of a wellbore are allowed. The first cell of each wellbore must have a cell name starting with the character "*". The wellhead section must always be defined as the first wellbore cell;

The nodal distance of wellbore cells to their interfaces to formation cells (D1 or D2 of well-formation connections) shall be set to zero;

The area of a connection between wellbore cells (multiplied by the average porosity of the adjacent wellbore cells) will be used to calculate the effective diameter d except for the case of annuli (see below);

A negative value of AHT (i.e., the entry after volume) indicates that the wellbore cell represents a section of an annulus and the absolute value of AHT is the outside diameter of the annulus;

The effective perimeter of the cross-section of each wellbore cell, used in calculation of the friction term, is calculated from the areas of the side connections (non w-w connections) if they exist in the mesh. Otherwise, it is calculated from either the cross-section area (the w-w connection) or the provided outside diameter in the case where the "wellbore" region is actually a wellbore annulus (i.e., AHT < 0). Note that in this annulus case, inside walls or tubes must explicitly be represented by grid cells in the grid . However, the lateral connections to the inside tubes or walls must be specified as impermeable (e.g., ISO = 0) to make sure that the flow in both annulus and in the inside tubes(if any) is one dimensional except the heat flow.

c) **SELEC data block**

The parameter at position 9 of the first row IE(9): if = 9, wellbore model turned off, otherwise, wellbore model turned on; all other IEs not used.

If IE(9) is not 9, the following parameters will be used:
    FE(1) –not used.
    FE(2)—Solid fraction (only used if one want to increase thermal stability of wellbore cells by including a "skin" of rock around wellbore or a core of solid inside an annular tunnel in calculation of energy balance but not invoke the usage of the "x" material). This solid fraction would not affect anything else (e.g., the volume of wellbore cell in fluid flow calculation).
    FE(3)—the maximum value of the profile parameter (C_{max})FE(4)--parameter to define special flow types:

(1) homogeneous flow is defined if FE(3) = 1 and FE(4) = 0;
(2) fixed drift velocity is enforced if FE(3) =1 and FE(4) < 0 (the fixed drift velocity is defined as absolute value of FE(4))

    FE(5)—not used
    FE(6)--roughness parameter of the well walls (ε in Eq. A3)
    FE(7) – Fv (= 1 by default), multiplier on the flooding velocity fraction used in Eq. 23.

d) **INCON data block (or separate INCON file for restart)**

For restart runs (those containing "+++" near the end of file INCON), wellbore flow information (velocity, ambient temperature, etc.) must exist (automatically saved to "SAVE" file). In other words, you cannot do a restart wellbore run after a standard TOUGH2 (non-wellbore) run (e.g., IE(9) = 9) .

CO2TAB file

This file contains tabular thermodynamic properties of CO_2 including the definition of the saturation curve (phase transition curve). The default file is provided with the distribution package of the software. The file must be copied to the working directory before running the program. See Pruess (2005) for details on the CO2TAB file.

3.4 Output file

Fixed Name output files:

1) "FStatus" – five status variables of each wellbore cell at every time step and depth: time, distance to wellhead, gas saturation, mass fraction of CO_2 in liquid, pressure, temperature, gas density
2) "Fflow" – five variables of each wellbore connection at every time step and depth: time, distance to wellhead, liquid phase mass flow rate, gas phase mass flow rate, liquid phase velocity, gas phase velocity, mixture velocity
3) "FOFT" – optional (transient output of state variables for user-specified cells in main input file. First two variables are the index and the simulation time, respectively. They are followed by the cell index and five variables at the cell in turn of each cell listed in FOFT section of the main input file. The five variables are pressure, gas saturation, mass fraction of CO_2 in liquid phase, mass fraction of salt in liquid phase, and the temperature, respectively.)
4) "COFT" – optional (transient output of flow rate and velocity for user-specified connections in main input file. Data structure here are very similar to FOFT, except for that here the five variables are gas phase mass flow rate, liquid phase mass flow rate, gas phase velocity, liquid phase velocity, and total CO_2 mass flow rate, respectively, for each connection listed in COFT section in the main input file.)
5) "DOFT" – a time series of total liquid and gas volume (see TOUGH2/ECO2N manual for details)

Main output file *(see TOUGH2/ECO2N manual (Pruess, 2005) for details)*

The formats of this output file are basically the same as that of TOUGH2/ECO2N except a profile of velocities (e.g., the mixture, gas, and liquid phase) in the wellbore is added behind the regular profile output (at user specified output steps).

In addition, some informational outputs regarding wellbore cells, connections, and their geometry features are also included in the front of the main output file.

4. Example Problems

Case 1 Steady-state two-phase flow upward (comparison against analytical solutions)

To verify the wellbore flow solution approach, we simulated a case (Case 1) of steady-state,

isothermal, two-phase (CO_2 as gas and water as liquid) flow through a vertical wellbore of 1000

m length. The details of the problem are described below (Table 3):

Table 3. Parameters of the two-phase wellbore flow problem

Parameter	Value	Note
Length	1000 m	Vertical wellbore
Diameter	0.1 m	Circular
Total (upward) mass flux (G)	50 kg/m^2/s	Gas + Liquid
Gas mass fraction	0.5	$\dfrac{S_G \rho_G u_G}{G}$
Temperature	40 °C	Isothermal
Wellhead Pressure	10^5 Pa	

The specifications of the one-dimensional numerical solution (T2Well/ECO2N) are:
1. 1000 m wellbore with a diameter of 0.1 m

2. Grid resolution 10 m

3. Injection mass rate at bottom: CO_2: 0.19625 kg/s; water: 0.19625 kg/s (Each = 25 kg/m^2/s with a cross sectional area of 7.8500E-03 m^2)

4. Isothermal simulation with a uniform temperature of 40 °C throughout the wellbore

5. Top boundary (outlet) pressure is 10^5 Pa

6. Wall roughness 2.4e-5 m

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The steady state problem is actually solved as a transient problem with adaptive time steps. The ending simulation time is 0.456869E+09 seconds (4100 steps), at which the average pressure loss due to temporal acceleration is about 3.80E-16 (Pa/m). Therefore, the steady state is considered to be reached.

As shown in Figure 2, the numerical solutions are almost identical to the analytical solutions (Pan et al., 2010), thereby verifying the numerical wellbore code (T2Well/EOS3) for this particular problem. Note that the mixing between the CO_2 and the water phases is allowed in the numerical simulation but no mixing is assumed for the analytical solution. However, the almost perfect match between analytical solutions and the numerical solutions implies that the effects of the mixing between the two phases (<2%) on the two phase flow are negligible.
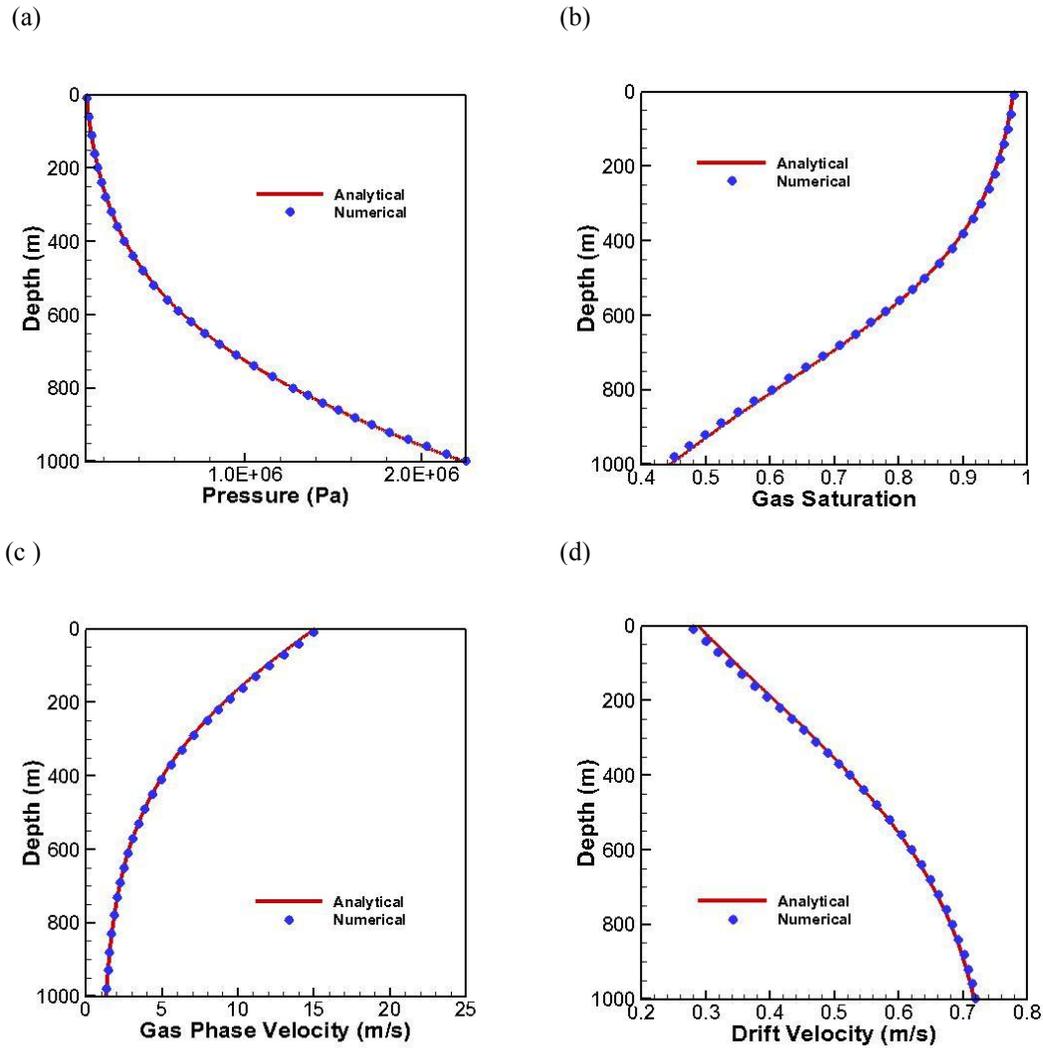
(a)   (b)

(c)   (d)

Figure 2. Case 1: Distribution of pressure, gas saturation, gas-phase velocity, and drift velocity under steady-state, isothermal, two-phase (CO_2/water) flow conditions in a vertical wellbore showing excellent agreement between the two approaches.

In this system, although the mass fraction (CO_2:H_2O) is constant (X =0.5) throughout the wellbore, the gas (CO_2-rich phase) saturation decreases with depth due to pressure increase because of the low density of gas phase at the given pressure range (Figure 2). Meanwhile, the drift velocity (of the gas phase relative to the mean volumetric velocity) increases with depth

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from about 0.28 m/s to 0.72 m/s. However, the gas-phase velocity decreases with depth by about 11 times over 1000 meters (Figure 2).

Case 2 Non-isothermal CO_2 flow through a wellbore initially full of water

This problem is a case of two-phase flow up an open well bore. The scenario envisioned is the tip of a migrating CO_2 plume at 10% gas saturation encountering an open well initially filled with water. The focus here is on flow in the wellbore. The reservoir is assumed to be able to maintain the constant pressure, temperature, and gas saturation during the process. Starting from hydrostatic conditions and a geothermal temperature gradient in the well, an overpressure of 0.1 MPa (1 bar) is applied to the reservoir to mimic an injection-induced overpressure. Wellbore heat transmission to the formation is calculated with the analytical solution. Figure 3 shows part of the input file for Case 2 (with brine in reservoir).

```
*Leakage wellbore DFM* ... 1-D column to 1000 m depth, 10 m vertical grid spacing,0.1 dia
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*---8
wellb   2 2600.e00   1.0000 200.0e-9 200.0e-9 200.0e-9   -2.51    920.
  0.0e-10
    7       .457    .05    1.     .05
    8
wtmos   2 2600.e3    1.0000 200.0e-9 200.0e-9 200.0e-9    2.51   920.e-3
  0.0e-10
    7       .457    .05    1.     .05
    8
botwe   2 2600.e00   0.5000 2.0e-12  2.0e-12  2.0e-12    2.51    920.
  0.0e-10
    7       .457    .01    1.     .01
    8


MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*---8
   3   4   3   6
SELEC...2....3....4....5....6....7....8....9...10...11...12...13...14...15...16
   1                   0   0   0   0   0   0   0   0
    .8     .1    1.2    1.53    0.1 0.046e-3
SOLVR----1----*----2----*----3----*----4----*----5----*----6----*----7----*---8
5 Z1  O0  8.0e-1  1.0e-7
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*---8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*---8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*---8
  28100   1001000300000200  4   3
       3.6e+4   2.e-1   2.0e+1         9.81    2.0
    1.E-4   1.E00
         1.013e5         0.0        1.0          15.
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*---8

… …

ELEME ---
*ta 1      wtmos1.0000E+50           4.0991E-024.0320E-02 1002.000
1Aa 1       wellb7.8500E-020.0000E+00      4.0991E-024.0320E-02  997.000
1Ba 1       wellb7.8500E-020.0000E+00      4.0991E-024.0320E-02  987.000
1Ca 1       wellb7.8500E-020.0000E+00      4.0991E-024.0320E-02  977.000

… …

INCON -- INITIAL CONDITIONS FOR  102 ELEMENTS AT TIME  0.256091E+11

… …

*ta 1       0.90000000E+00
 0.1013253378869E+06 0.0000000000000E-04 1.0000000000000E+00 0.3500000000000E+02
bba 1       0.50000000E+00
 0.9983837982470E+07 1.2000000000000E-01 1.0100000000000E+01 0.6500000000000E+02


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

Figure 3. Input file (portion) of Case 2. Note X2 (mass fraction of NaCl in liquid phase) = 0.12 for the reservoir cell "bba 1", indicating the brine aquifer. For no salt case, this X2 = 0.0.

With reference to Figure 4, we observe in this test problem the early-time upward flow within the well of water at all depths as driven by the 0.1 MPa pressure perturbation at the bottom. The sharp peak of water flow rate through the top at about 200 s is related to the breakthrough of the gas phase (a sudden loss of water cap). Gas flow does not begin until approximately $t = 10$ s when gas is present at the bottom. By $t =$ approximately 200 s, gas flows at the middle and top of the well. The breakthrough through upper portion of the wellbore takes place in very short time period as evidenced by the very small time delay between the gas flow rates at top and middle, a phenomenon of the gas-lift effect. The flow rate of CO_2 reaches approximately 2.33 kg/s in this open well-bore case. The gas phase velocity at the top is much higher than at the middle and bottom, reflecting the acceleration of the gas (CO_2) phase when it transitions from supercritical to gaseous conditions.
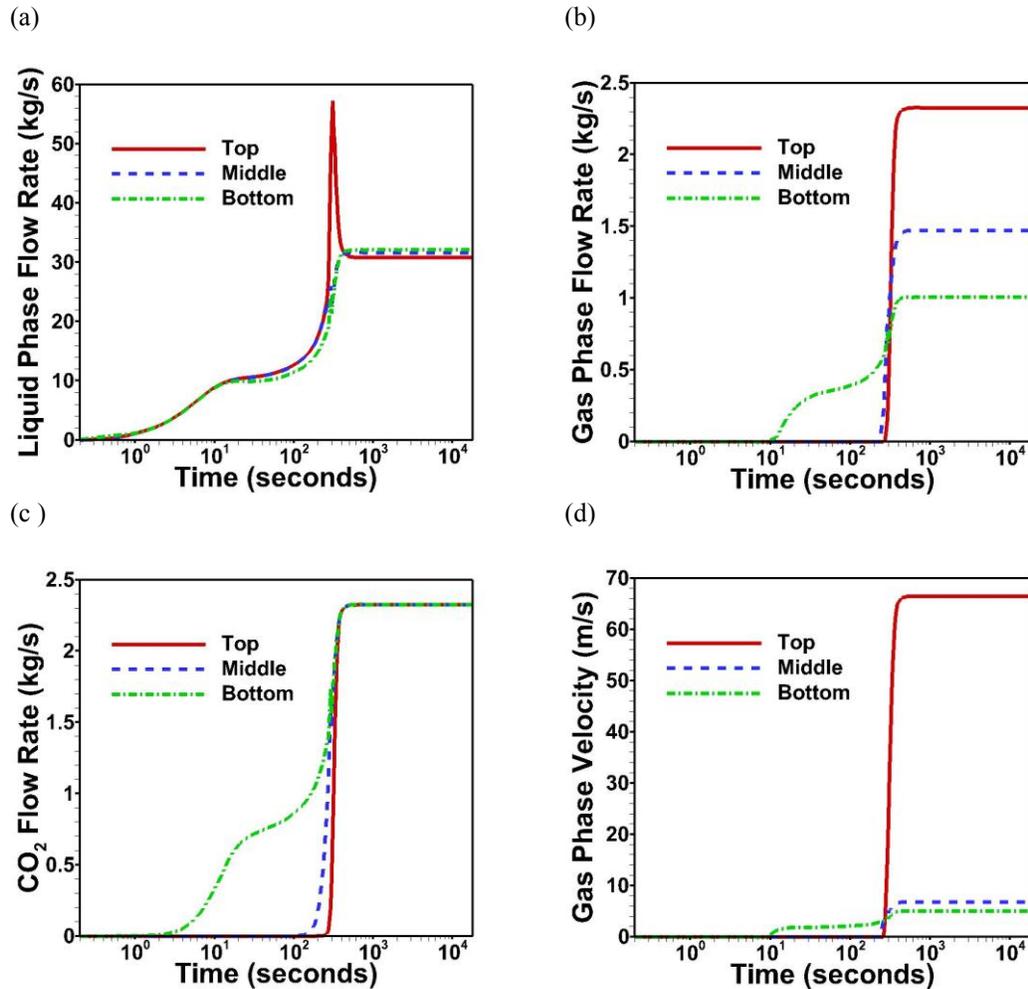
(a)

(b)

(c)

(d)

Figure 4. Case 2: Flow rates and velocities of CO_2 and water at three levels in the well (bottom, middle, and top).

Further insight into the processes modeled can be obtained from Figure 5 which shows gas saturation, gas density, pressure, and temperature throughout the well as a function of time. As shown, the well is initially filled with water and gas enters progressively from the bottom up. After 10 minutes (600 s), gas is fairly evenly distributed throughout the well from 10% at the bottom to nearly all gas at the top. The reason for this increase in gas saturation is the exsolution of gas from the liquid as pressure drops and the large expansion that CO_2 undergoes as it

transitions from supercritical to gaseous conditions. This transition occurs around the critical

pressure (7.4 MPa, or 74 bar) at a depth of approximately 755 m. The gas density plot shows the

sharp decrease in gas density in that region. Temperature also affects CO_2 solubility, but

temperature becomes relatively constant as the steady flow develops resulting in decreasing CO_2

mass fractions being controlled mostly by pressure. The temperature contour shows the

evolution from a conductive profile controlled by the geothermal gradient to an advective profile

controlled by upward fluid flow. In between the initial and steady states, there are some local

maxima arising from the expansion of CO_2 as gas phase rises upwards and transitions to gaseous
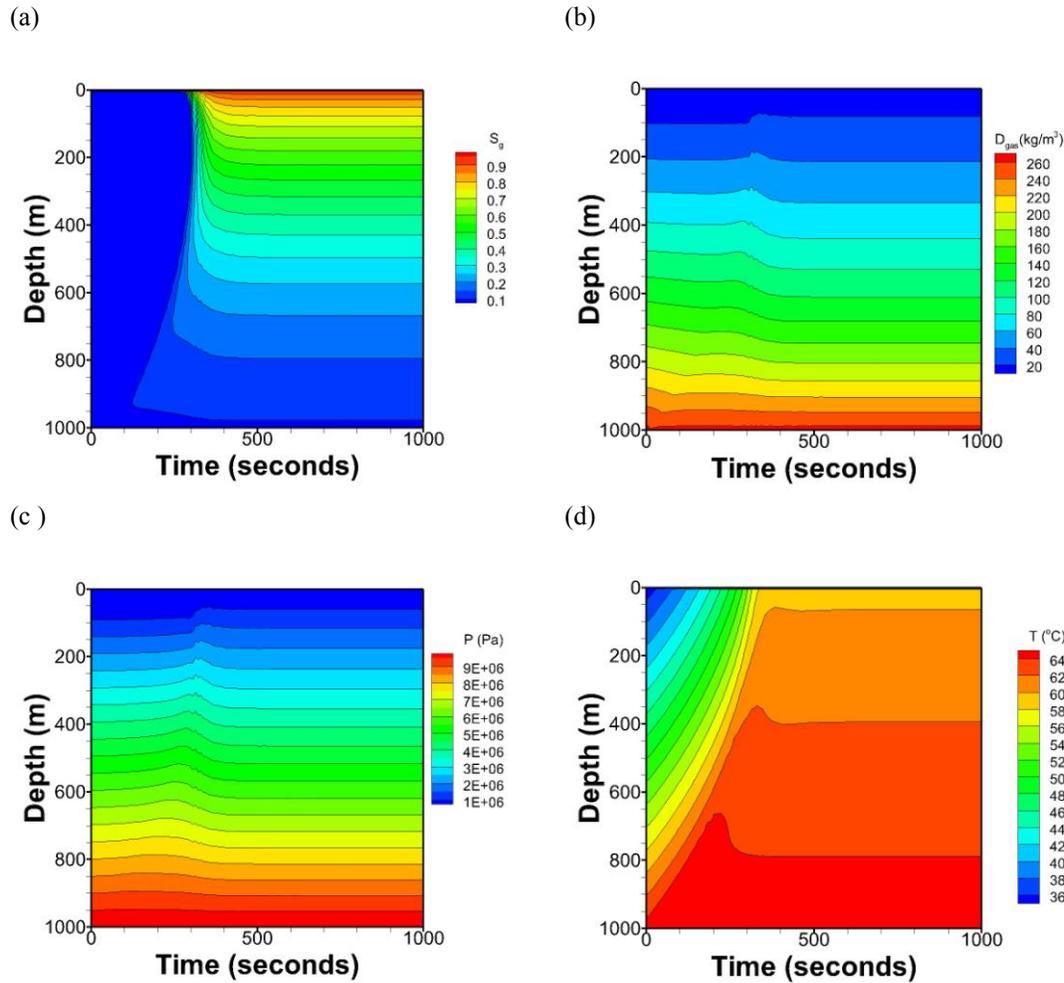
conditions.

(a)

(b)

(c)

(d)

Figure 5. Case 2: Profiles of gas saturation, gas density, pressure, and temperature in the wellbore as a function of time.

Figure 6 shows the CO_2 leakage rates at wellhead from a no-salt aquifer and a brine aquifer under the same conditions. The final flow rate is reduced from 2.33 kg/s of no-salt case to 1.63 kg/s of brine case with slightly delay in the breakthrough of CO_2 too. This is simply because, in this two phase flow situation, heavier brine means more hydrostatic pressure loss so that there is less energy could be used to move CO_2 upward in the brine case than in the no-salt case, for the same injection-induced overpressure.
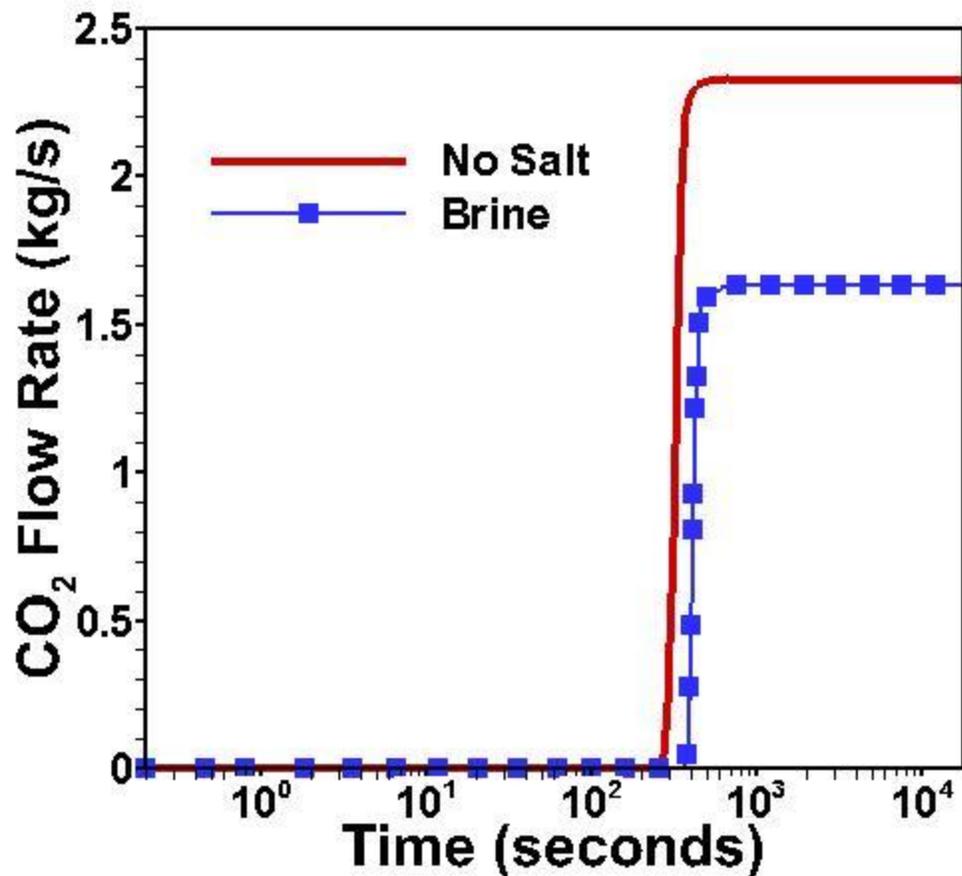
Figure 6. Case 2: The effect of brine on CO_2 leakage rate through wellhead. Mass fraction of salt in the brine is 0.12. All other conditions are the same.

Case 3 Injection of CO_2 into a depleted gas field

This problem is a case of injection of CO_2 into a depleted gas field at a depth of 3000 m below surface, through a wellbore. The focus here is to investigate if the lower pressure in the reservoir could cause a "choke" in wellbore flow due to the down-hole transition to subcritical (gaseous) conditions. The reservoir is assumed to have a thickness of 100 m and an area of 1 km by 1 km. It is fully perforated by a wellbore of 0.18 m in diameter. The initial pore pressure in the reservoir is <= 3.4 MPa. The initial temperature in the reservoir is 90 °C whereas the

temperature in the wellbore gradually reduces to 35 °C as it approaches the surface. An impermeable layer with a constant temperature of 90 ^{o}C is under the reservoir. The formation permeability of the reservoir is 10^{-13} m^2. The injection rate is 100 kg/s at a temperature of 60 ^{o}C. A 2D radially symmetry grid with 416 cells (31 well cells) is used.
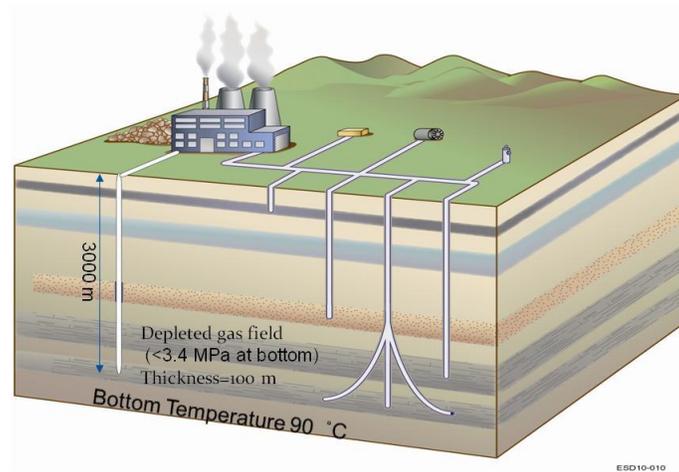

Figure 7. Sketch of injection into a depleted gas field (Case 3).

(a)   (b)

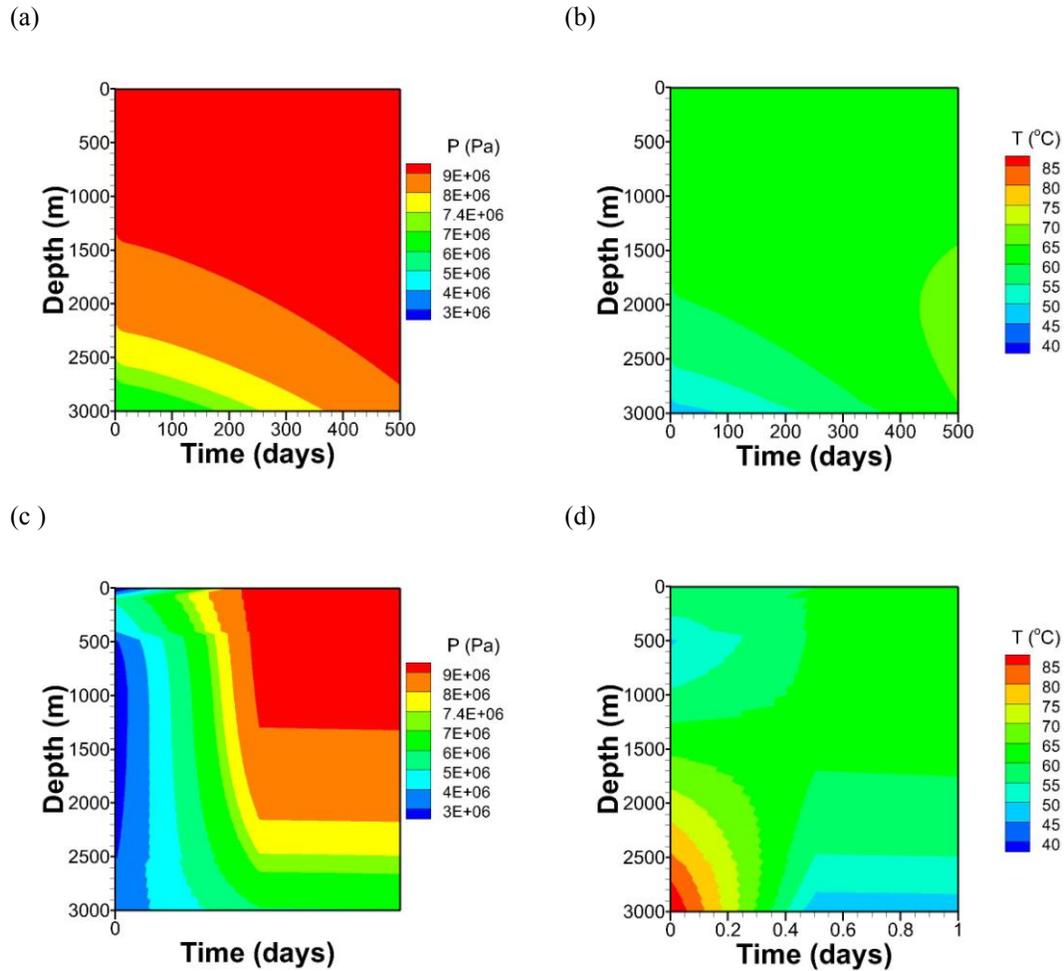(c)   (d)

Figure 8. Case 3: Profiles of pressure and temperature in the injection wellbore as a function of time. (c) and (d) are short time (the first day) plots of (a) and (b), respectively.

As shown in Figure 8, the lower pressure in the wellbore quickly disappears with the injection of

CO_2. Within one day of injection, most of the wellbore reaches the supercritical condition

(Figure 8c) and the entire wellbore is in the supercritical condition after about 240 days of

injection (Figure 8a). Meanwhile, the temperature profile also quickly transforms from a

geothermal gradient dominated one into a convection dominated one within 1 day (Figure 8d)

and then becomes relatively uniform (Figure 8b). The wellhead pressure quickly (within 1 day)

reach above 9 MPa and stay there until the front hits the lateral boundary of the reservoir so that

the pressure in the entire reservoir rises to above the critical pressure (Figure 9). Although the low-pressure at reservoir does keep the lower portion of the wellbore under subcritical condition for a significant period, it does not cause a persistent "choke" in the wellbore. In other words, an extremely high wellhead pressure is not needed to maintain the given injection rate.
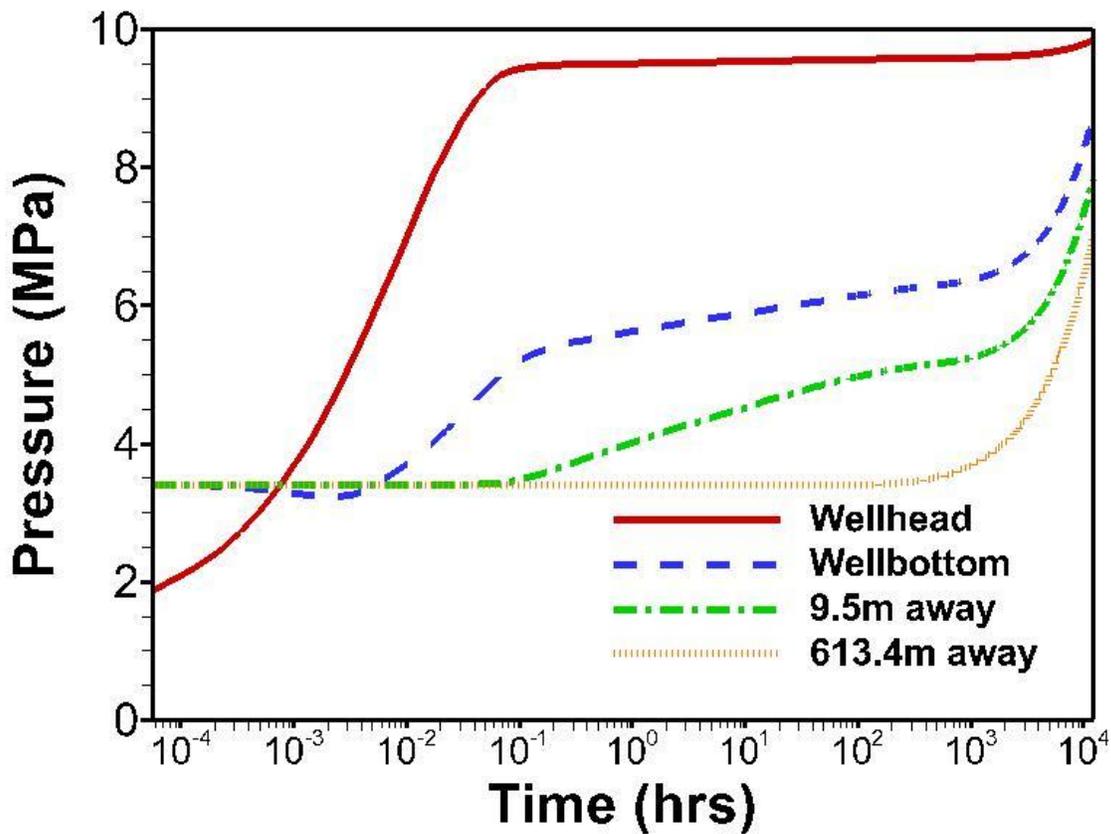

Figure 9. Case 3: Pressure responses to the injection at wellhead, well bottom, and two locations in the reservoir.

5. Conclusions

We have developed a non-isothermal multiphase wellbore simulator for modeling leakage or injection of CO_2 and brine (water and NaCl mixture) in geologic carbon sequestration systems. The wellbore flow model uses the DFM with an enhancement for solving the transient flow equations that makes use of a semi-explicit approach for the momentum equation. The approach allows direct coupling between porous reservoirs and wellbores that is needed to model leakage and injection. Time-step sizes tend to be smaller for T2Well/ECO2N compared to the normal reservoir simulation, but the wellbore is one-dimensional, so overall execution times can be made acceptable by limiting the number of gridblocks in the reservoir region(s). For large-scale reservoir simulations coupled to wellbores, alternative approaches to time-stepping will need to be developed.

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Appendix A. Derivation of the momentum equation

All variables in the development below should be considered as area-averaged or assumed to be constant over the cross-section of a wellbore except for those explicitly noted otherwise.

The combined-phase momentum equation for wellbore (or duct) flow when the axial stress terms are assumed negligible can be written as (Brennen, 2005):

$$\frac{\partial}{\partial t}\left(\sum_{\beta} \rho_{\beta} S_{\beta} u_{\beta} \right) + \frac{1}{A}\frac{\partial}{\partial z}\left(A \sum_{\beta} \rho_{\beta} S_{\beta} u_{\beta}^{2} \right) = -\frac{\partial P}{\partial z} - \frac{\Gamma \tau_{w}}{A} - \rho_{m} g \cos\theta \qquad (A1)$$

where ρ is density, S is saturation, u is velocity, P is the pressure, A is cross-sectional area of the wellbore, Γ, is the perimeter of the cross-section, τ_{w} is the wall shear stress, and θ is the local angle between wellbore section, and the vertical direction. Subscript β indicates phase and m indicates the mixture whereas t is time and z is spatial coordinate along the wellbore. Note that to be consistent with the drift-flux model, the area-averaged variable, P, is defined as the pressure of the mixture regardless of whether the two-phase flow involves a dispersed second phase or a film as the second phase flow because the uniform drift-flux model proposed by Shi et al. (2005) is applied to all flow regimes with the same set of the optimized parameters obtained from fitting to experimental data.

The wall shear stress is the friction force between the fluids and the wellbore wall. Obviously, this term depends on properties and velocities of both the gas and the liquid phases as well as their fractions of the contact area with the wall. Rigorously determining this term would involve

figuring out the detailed two-phase flow structure near the wall, a difficult task that is intended to be avoided by using the drift-flux model. We assume that the stress is proportional to the square of the mixture velocity:

$$\tau_w = \frac{1}{2} f \rho_m |u_m| u_m \tag{A2}$$

where the Fanning friction coefficient (f) is a function of the Reynolds number (Re) (Brill and Mukherjee, 1999, rewritten as Fanning friction coefficient):

$$f = \frac{16}{Re} \qquad \text{for Re} < 2400,$$

$$\text{and} \quad \frac{1}{\sqrt{f}} = -4 \log \left[\frac{2\varepsilon/d}{3.7} - \frac{5.02}{Re} \log \left(\frac{2\varepsilon/d}{3.7} + \frac{13}{Re} \right) \right] \quad \text{for Re} > 2400 \tag{A3}$$

where ε is the roughness of the wellbore and the Reynolds number is defined as $Re = \rho_m u_m d / \mu_m$ where μ_m is the mixture viscosity and d is the wellbore diameter.

Before deriving the momentum conservation equation for the mixture, let us define the mixture density, ρ_m, and the mixture velocity (velocity of mass centre), u_m, as follows:

$$\rho_m = S_G \rho_G + (1 - S_G) \rho_L \tag{A4}$$

$$u_m = \frac{S_G \rho_G u_G + (1 - S_G) \rho_L u_L}{\rho_m} \tag{A5}$$

By inserting (7) and (9) into (A5), we can solve j as a function of u_m and u_d:

$$j = \frac{\rho_m}{\rho_m^*} u_m + \frac{S_G (\rho_L - \rho_G)}{\rho_m^*} u_d \tag{A6}$$

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Where $\rho_m^* = S_G C_0 \rho_G + (1 - S_G C_0)\rho_L$ is the profile-adjusted average density and will reduce to the mixture density if $C_0 = 1$. Note that the mixture velocity and the volumetric flux of the mixture would be equal only if there is no slip between two phases (i.e., $C_0 = 1.0$ and $u_d = 0.0$ or homogeneous flow).

Similarly, the gas velocity and the liquid velocity can also be expressed in terms of u_m and u_d as follows:

$$u_G = C_0 \frac{\rho_m}{\rho_m^*} u_m + \frac{\rho_L}{\rho_m^*} u_d$$

$$u_L = \frac{(1 - S_G C_0)\rho_m}{(1 - S_G)\rho_m^*} u_m - \frac{S_G \rho_G}{(1 - S_G)\rho_m^*} u_d$$

$$(A7)$$

By inserting the stress term (A2) and the phase velocities (A7) into (A1), we can obtain the momentum equation in terms of the mixture velocity u_m and the drift velocity u_d:

$$\frac{\partial}{\partial t}(\rho_m u_m) + \frac{1}{A}\frac{\partial}{\partial z}\left[A\left(\rho_m u_m^2 + \gamma\right)\right] = -\frac{\partial P}{\partial z} - \frac{\Gamma f \rho_m |u_m| u_m}{2A} - \rho_m g \cos\theta \qquad (A8)$$

where the term $\gamma = \frac{S_G}{1 - S_G}\frac{\rho_G \rho_L \rho_m}{\rho_m^{*2}}\left[(C_0 - 1)u_m + u_d\right]^2$ is caused by slip between two phases.

While other terms in (A8) are straightforward, the second term on the left is obtained as below:

$$\sum_\beta \rho_\beta S_\beta u_\beta^2 = S_G \rho_G u_G^2 + (1 - S_G)\rho_L u_L^2$$

$$= S_G \rho_G \left[C_0 \frac{\rho_m}{\rho_m^*} u_m + \frac{\rho_L}{\rho_m^*} u_d \right]^2 + (1 - S_G)\rho_L \left[\frac{(1 - S_G C_0)\rho_m}{(1 - S_G)\rho_m^*} u_m - \frac{S_G \rho_G}{(1 - S_G)\rho_m^*} u_d \right]^2$$

$$= u_m^2 \left(\frac{S_G \rho_G C_0^2 \rho_m^2}{\rho_m^{*2}} + \frac{\rho_L \rho_m^2 (1 - S_G C_0)^2}{(1 - S_G)\rho_m^{*2}} \right) \qquad (A9)$$

$$+ 2 u_m u_d \left(\frac{S_G \rho_G \rho_L \rho_m C_0}{\rho_m^{*2}} - \frac{S_G \rho_G \rho_L \rho_m (1 - S_G C_0)}{(1 - S_G)\rho_m^{*2}} \right)$$

$$+ u_d^2 \left(\frac{S_G \rho_G \rho_L^2}{\rho_m^{*2}} + \frac{\rho_L S_G^2 \rho_G^2}{(1 - S_G)\rho_m^{*2}} \right)$$

In (A9), the u_m^2 term can be reorganized as follows:

$$\rho_m u_m^2 - \rho_m u_m^2 + u_m^2 \left(\frac{S_G \rho_G C_0^2 \rho_m^2}{\rho_m^{*2}} + \frac{\rho_L \rho_m^2 (1 - S_G C_0)^2}{(1 - S_G)\rho_m^{*2}} \right) =$$

$$= \rho_m u_m^2 + \frac{\rho_m u_m^2}{(1 - S_G)\rho_m^{*2}} \left[S_G \rho_G (1 - S_G)\rho_m C_0^2 + \rho_L \rho_m (1 - S_G C_0)^2 - (1 - S_G)\rho_m^{*2} \right] \qquad (A10)$$

By expanding ρ_m^* and recognizing the relationship (A4), the term in [.] of (A10) can be simplified as:

$$S_G \rho_G (1 - S_G)\rho_m C_0^2 + \rho_L \rho_m (1 - S_G C_0)^2 - (1 - S_G)\rho_m^{*2} =$$
$$= S_G \rho_G (1 - S_G)\rho_m C_0^2 + \rho_L \rho_m (1 - S_G C_0)^2 - (1 - S_G)\left[S_G^2 \rho_G^2 C_0^2 + \rho_L^2 (1 - S_G C_0)^2 + 2 S_G \rho_G C_0 \rho_L (1 - S_G C_0) \right] =$$
$$= (1 - S_G) S_G \rho_G C_0^2 (\rho_m - S_G \rho_G) + \rho_L (1 - S_G C_0)^2 (\rho_m - (1 - S_G)\rho_L) - 2 S_G \rho_G C_0 (1 - S_G)\rho_L (1 - S_G C_0) = \qquad (A11)$$
$$= S_G \rho_G \rho_L \left[(1 - S_G)^2 C_0^2 + (1 - S_G C_0)^2 - 2 C_0 (1 - S_G)(1 - S_G C_0) \right] =$$
$$= S_G \rho_G \rho_L [(1 - S_G)C_0 - (1 - S_G C_0)]^2 = S_G \rho_G \rho_L (C_0 - 1)^2$$

Similarly, the $2 u_m u_d$ term in (A9) can be simplified as:

$$2 u_m u_d \left(\frac{S_G \rho_G \rho_L \rho_m C_0}{\rho_m^{*2}} - \frac{S_G \rho_G \rho_L \rho_m (1 - S_G C_0)}{(1 - S_G)\rho_m^{*2}} \right) =$$

$$= \frac{2 u_m u_d S_G \rho_G \rho_L \rho_m}{(1 - S_G)\rho_m^{*2}} [(1 - S_G)C_0 - (1 - S_G C_0)] = \frac{2 u_m u_d S_G \rho_G \rho_L \rho_m}{(1 - S_G)\rho_m^{*2}} (C_0 - 1) \qquad (A12)$$

And the u_d^2 term can be simplified as:

$$u_d^2 \left(\frac{S_G \rho_G \rho_L^2}{\rho_m^{*2}} + \frac{\rho_L S_G^2 \rho_G^2}{(1 - S_G)\rho_m^{*2}} \right) = \frac{S_G \rho_G \rho_L u_d^2}{(1 - S_G)\rho_m^{*2}} [((1 - S_G)\rho_L + S_G \rho_G)] = \frac{S_G \rho_G \rho_L \rho_m u_d^2}{(1 - S_G)\rho_m^{*2}} \qquad (A13)$$

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Putting together (A10) through (A13) into (A9), we obtain:

$$\sum_\beta \rho_\beta S_\beta u_\beta^2 = \rho_m u_m^2 + \frac{S_G \rho_G \rho_L \rho_m}{(1 - S_G)\rho_m^{*2}} \left[(C_0 - 1)^2 u_m^2 + 2(C_0 - 1)u_m u_d + u_d^2 \right] =$$
$$= \rho_m u_m^2 + \frac{S_G \rho_G \rho_L \rho_m}{(1 - S_G)\rho_m^{*2}} \left[(C_0 - 1)u_m + u_d \right]^2 = \rho_m u_m^2 + \gamma$$

(A14)

Note that eq. (A8) is equivalent to the mixture momentum equation for the drift-flux model proposed by Hibiki and Ishii (2003) when the axial stress terms are assumed negligible. When all phases travel at the same velocity (i.e., $C_0 = 1 \; and \; u_d = 0$), γ will become zero and Eq. (A8) will reduce to the same momentum equation as a single phase flow.

Appendix B. Make file

```
# Microsoft Developer Studio Generated NMAKE File, Based on WellBore.dsp
!IF "$(CFG)" == ""
CFG=WellBore - Win32 Debug
!MESSAGE No configuration specified. Defaulting to WellBore - Win32 Debug.
!ENDIF


!IF "$(CFG)" != "WellBore - Win32 Release" && "$(CFG)" != "WellBore - Win32 Debug"
!MESSAGE Invalid configuration "$(CFG)" specified.
!MESSAGE You can specify a configuration when running NMAKE
!MESSAGE by defining the macro CFG on the command line. For example:
!MESSAGE
!MESSAGE NMAKE /f "WellBore.mak" CFG="WellBore - Win32 Debug"
!MESSAGE
!MESSAGE Possible choices for configuration are:
!MESSAGE
!MESSAGE "WellBore - Win32 Release" (based on "Win32 (x86) Console Application")
!MESSAGE "WellBore - Win32 Debug" (based on "Win32 (x86) Console Application")
!MESSAGE
!ERROR An invalid configuration is specified.
!ENDIF


!IF "$(OS)" == "Windows_NT"
NULL=
!ELSE
NULL=nul
!ENDIF


!IF  "$(CFG)" == "WellBore - Win32 Release"

OUTDIR=.\Release
INTDIR=.\Release
# Begin Custom Macros
OutDir=.\Release
# End Custom Macros

ALL : "$(OUTDIR)\WellBore.exe"


CLEAN :
	-@erase "$(INTDIR)\agra.obj"
	-@erase "$(INTDIR)\DFM.OBJ"
	-@erase "$(INTDIR)\DraftFluxModel.mod"
	-@erase "$(INTDIR)\eco2n_well.obj"
	-@erase "$(INTDIR)\meshm.obj"
```

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```
        -@erase "$(INTDIR)\mudfv.obj"
        -@erase "$(INTDIR)\SurfaceTension.mod"
        -@erase "$(INTDIR)\t2cg22x.obj"
        -@erase "$(INTDIR)\t2f.obj"
        -@erase "$(INTDIR)\t2solv.obj"
        -@erase "$(OUTDIR)\WellBore.exe"


"$(OUTDIR)" :
    if not exist "$(OUTDIR)/$(NULL)" mkdir "$(OUTDIR)"


F90=df.exe
F90_PROJ=/assume:dummy_aliases /automatic /compile_only /nologo /real_size:64 /recursive
/warn:nofileopt /module:"Release/" /object:"Release/"
F90_OBJS=.\Release/


.SUFFIXES: .fpp


.for{$(F90_OBJS)}.obj:
    $(F90) $(F90_PROJ) $<


.f{$(F90_OBJS)}.obj:
    $(F90) $(F90_PROJ) $<


.f90{$(F90_OBJS)}.obj:
    $(F90) $(F90_PROJ) $<


.fpp{$(F90_OBJS)}.obj:
    $(F90) $(F90_PROJ) $<


CPP=cl.exe
CPP_PROJ=/nologo /ML /W3 /GX /O2 /D "WIN32" /D "NDEBUG" /D "_CONSOLE" /D "_MBCS"
/Fp"$(INTDIR)\WellBore.pch" /YX /Fo"$(INTDIR)\\" /Fd"$(INTDIR)\\" /FD /c


.c{$(INTDIR)}.obj::
    $(CPP) @<<
    $(CPP_PROJ) $<
<<


.cpp{$(INTDIR)}.obj::
    $(CPP) @<<
    $(CPP_PROJ) $<
<<


.cxx{$(INTDIR)}.obj::
    $(CPP) @<<
    $(CPP_PROJ) $<
<<
```

```
.c{$(INTDIR)}.sbr::
   $(CPP) @<<
   $(CPP_PROJ) $<
<<


.cpp{$(INTDIR)}.sbr::
   $(CPP) @<<
   $(CPP_PROJ) $<
<<


.cxx{$(INTDIR)}.sbr::
   $(CPP) @<<
   $(CPP_PROJ) $<
<<


RSC=rc.exe
BSC32=bscmake.exe
BSC32_FLAGS=/nologo /o"$(OUTDIR)\WellBore.bsc"
BSC32_SBRS= \


LINK32=link.exe
LINK32_FLAGS=kernel32.lib /nologo /subsystem:console /incremental:no
/pdb:"$(OUTDIR)\WellBore.pdb" /machine:I386 /out:"$(OUTDIR)\WellBore.exe"
LINK32_OBJS= \
       "$(INTDIR)\agra.obj" \
       "$(INTDIR)\DFM.OBJ" \
       "$(INTDIR)\eco2n_well.obj" \
       "$(INTDIR)\meshm.obj" \
       "$(INTDIR)\mudfv.obj" \
       "$(INTDIR)\t2f.obj" \
       "$(INTDIR)\t2solv.obj" \
       "$(INTDIR)\t2cg22x.obj"

"$(OUTDIR)\WellBore.exe" : "$(OUTDIR)" $(DEF_FILE) $(LINK32_OBJS)
    $(LINK32) @<<
  $(LINK32_FLAGS) $(LINK32_OBJS)
<<


!ELSEIF  "$(CFG)" == "WellBore - Win32 Debug"


OUTDIR=.\Debug
INTDIR=.\Debug
# Begin Custom Macros
OutDir=.\Debug
# End Custom Macros
```

```
ALL : "$(OUTDIR)\WellBore.exe"


CLEAN :
        -@erase "$(INTDIR)\agra.obj"
        -@erase "$(INTDIR)\DF60.PDB"
        -@erase "$(INTDIR)\DFM.OBJ"
        -@erase "$(INTDIR)\eco2n_well.obj"
        -@erase "$(INTDIR)\meshm.obj"
        -@erase "$(INTDIR)\mudfv.obj"
        -@erase "$(INTDIR)\t2cg22x.obj"
        -@erase "$(INTDIR)\t2f.obj"
        -@erase "$(INTDIR)\t2solv.obj"
        -@erase "$(OUTDIR)\WellBore.exe"
        -@erase "$(OUTDIR)\WellBore.pdb"

"$(OUTDIR)" :
    if not exist "$(OUTDIR)/$(NULL)" mkdir "$(OUTDIR)"


F90=df.exe
F90_PROJ=/automatic /check:power /compile_only /dbglibs /debug:full /fpe:0
/fpscomp:filesfromcmd /nologo /real_size:64 /recursive /traceback
/warn:argument_checking /warn:nofileopt /warn:unused /module:"Debug/" /object:"Debug/"
/pdbfile:"Debug/DF60.PDB"
F90_OBJS=.\Debug/

.SUFFIXES: .fpp

.for{$(F90_OBJS)}.obj:
   $(F90) $(F90_PROJ) $<


.f{$(F90_OBJS)}.obj:
   $(F90) $(F90_PROJ) $<


.f90{$(F90_OBJS)}.obj:
   $(F90) $(F90_PROJ) $<


.fpp{$(F90_OBJS)}.obj:
   $(F90) $(F90_PROJ) $<


CPP=cl.exe
CPP_PROJ=/nologo /MLd /W3 /Gm /GX /ZI /Od /D "WIN32" /D "_DEBUG" /D "_CONSOLE" /D
"_MBCS" /Fp"$(INTDIR)\WellBore.pch" /YX /Fo"$(INTDIR)\\" /Fd"$(INTDIR)\\" /FD /GZ /c

.c{$(INTDIR)}.obj::
   $(CPP) @<<
   $(CPP_PROJ) $<
```

```
<<

.cpp{$(INTDIR)}.obj::
    $(CPP) @<<
    $(CPP_PROJ) $<
<<

.cxx{$(INTDIR)}.obj::
    $(CPP) @<<
    $(CPP_PROJ) $<
<<

.c{$(INTDIR)}.sbr::
    $(CPP) @<<
    $(CPP_PROJ) $<
<<

.cpp{$(INTDIR)}.sbr::
    $(CPP) @<<
    $(CPP_PROJ) $<
<<

.cxx{$(INTDIR)}.sbr::
    $(CPP) @<<
    $(CPP_PROJ) $<
<<

RSC=rc.exe
BSC32=bscmake.exe
BSC32_FLAGS=/nologo /o"$(OUTDIR)\WellBore.bsc"
BSC32_SBRS= \

LINK32=link.exe
LINK32_FLAGS=kernel32.lib /nologo /subsystem:console /incremental:no
/pdb:"$(OUTDIR)\WellBore.pdb" /debug /machine:I386 /out:"$(OUTDIR)\WellBore.exe"
/pdbtype:sept
LINK32_OBJS= \
        "$(INTDIR)\agra.obj" \
        "$(INTDIR)\DFM.OBJ" \
        "$(INTDIR)\eco2n_well.obj" \
        "$(INTDIR)\meshm.obj" \
        "$(INTDIR)\mudfv.obj" \
        "$(INTDIR)\t2f.obj" \
        "$(INTDIR)\t2solv.obj" \
        "$(INTDIR)\t2cg22x.obj"

"$(OUTDIR)\WellBore.exe" : "$(OUTDIR)" $(DEF_FILE) $(LINK32_OBJS)
```

```
    $(LINK32) @<<
  $(LINK32_FLAGS) $(LINK32_OBJS)
<<

!ENDIF


!IF "$(NO_EXTERNAL_DEPS)" != "1"
!IF EXISTS("WellBore.dep")
!INCLUDE "WellBore.dep"
!ELSE
!MESSAGE Warning: cannot find "WellBore.dep"
!ENDIF
!ENDIF


!IF "$(CFG)" == "WellBore - Win32 Release" || "$(CFG)" == "WellBore - Win32 Debug"
SOURCE=..\wellbore_code\Code_T2Well_core\agra.f

"$(INTDIR)\agra.obj" : $(SOURCE) "$(INTDIR)"
        $(F90) $(F90_PROJ) $(SOURCE)


SOURCE=..\wellbore_code\Code_T2Well_core\DFM.F

!IF  "$(CFG)" == "WellBore - Win32 Release"

F90_MODOUT=\
        "DraftFluxModel"


"$(INTDIR)\DFM.OBJ" "$(INTDIR)\DraftFluxModel.mod" : $(SOURCE) "$(INTDIR)"
"$(INTDIR)\SurfaceTension.mod"
        $(F90) $(F90_PROJ) $(SOURCE)


!ELSEIF  "$(CFG)" == "WellBore - Win32 Debug"


"$(INTDIR)\DFM.OBJ" : $(SOURCE) "$(INTDIR)"
        $(F90) $(F90_PROJ) $(SOURCE)


!ENDIF

SOURCE=..\wellbore_code\eco2n_well.f
```

```
!IF  "$(CFG)" == "WellBore - Win32 Release"

F90_MODOUT=\
        "SurfaceTension"


"$(INTDIR)\eco2n_well.obj" "$(INTDIR)\SurfaceTension.mod" : $(SOURCE) "$(INTDIR)"
        $(F90) $(F90_PROJ) $(SOURCE)


!ELSEIF  "$(CFG)" == "WellBore - Win32 Debug"


"$(INTDIR)\eco2n_well.obj" : $(SOURCE) "$(INTDIR)"
        $(F90) $(F90_PROJ) $(SOURCE)



!ENDIF

SOURCE=..\wellbore_code\Code_T2Well_core\meshm.f

"$(INTDIR)\meshm.obj" : $(SOURCE) "$(INTDIR)"
        $(F90) $(F90_PROJ) $(SOURCE)


SOURCE=..\wellbore_code\Code_T2Well_core\mudfv.f

"$(INTDIR)\mudfv.obj" : $(SOURCE) "$(INTDIR)" "$(INTDIR)\SurfaceTension.mod"
"$(INTDIR)\DraftFluxModel.mod"
        $(F90) $(F90_PROJ) $(SOURCE)


SOURCE=..\wellbore_code\Code_T2Well_core\t2cg22x.f

"$(INTDIR)\t2cg22x.obj" : $(SOURCE) "$(INTDIR)"
        $(F90) $(F90_PROJ) $(SOURCE)


SOURCE=..\wellbore_code\Code_T2Well_core\t2f.f

"$(INTDIR)\t2f.obj" : $(SOURCE) "$(INTDIR)" "$(INTDIR)\DraftFluxModel.mod"
        $(F90) $(F90_PROJ) $(SOURCE)


SOURCE=..\wellbore_code\Code_T2Well_core\t2solv.f

"$(INTDIR)\t2solv.obj" : $(SOURCE) "$(INTDIR)"
```

```
    $(F90) $(F90_PROJ) $(SOURCE)



!ENDIF
```