Simulation of Channelized Gas Flow Pattern in Heterogeneous Porous Media: A Feasibility Study of Continuum Simulation at Bench Scale

Shirin Samani* and Helmut Geistlinger

In remediation technologies, air or O₂ gas is injected into a polluted aquifer to remove organic contaminants. A gas injection process is also applied in enhanced oil recovery and CO₂ sequestration. The wide range of gas injection processes into porous media necessitates accurate gas flow modeling. The focus of this study was to determine whether a continuum model with stochastic parameters can represent the properties of gas flow patterns. We applied stochastic heterogeneity in TOUGH2 simulation and used the experimental observations to validate simulation results. We created two types of stochastic heterogeneity: correlated heterogeneity, generated by an assigned covariance function, and uncorrelated heterogeneity, which distributes uniformly. We used Euler characteristics to quantify the gas channel properties and to determine whether the heterogeneity applied in a continuum model can represent gas channel properties. The results of this investigation confirm that the continuum model, which includes correlated heterogeneity, can predict the quantitative properties of gas flow, such as gas volume. Also, it can create gas channels that have Euler characteristics close to those obtained by experimental observation. In conclusion, the continuum model can predict the properties of gas flow if the spatial variability and correlation structure of the characteristic properties applied to the model are representative of the medium.

Abbreviations: GBS, glass ballotine spheres.

Compartmentalized lumped-parameter models and multiphase flow models are mostly used in gas injection modeling (McCray, 2000). Compartmentalized lumped-parameter models separate fluid phases into different compartments and simulate the mass transfer between them by lumping the mass transfer into bulk parameters. Lumped-parameter models are simpler to use and appropriate for field screening, but they cannot predict the gas pressure or subsurface gas saturation (McCray, 2000).

On the other hand, multiphase flow models have the potential to provide more accurate representations of gas pressures and gas saturations, but they require a considerable amount of data collection (McCray, 2000). Multiphase modeling is based on the continuum assumption, in which the macroscopic value of each variable is obtained by averaging the microscopic values of this variable across a certain volume of the porous medium, which is called the representative elementary volume (Bachmat and Bear, 1986).

McCray (2000) and Thomson and Johnson (2000) reviewed the results of many multiphase flow models and emphasized the accuracy of the continuum assumption in representing the bulk distribution of gas flow (e.g., gas plume size and plume shape) and the effect of bulk heterogeneity. However, they did not report the accuracy of continuum models in presenting details about discrete gas channels. To examine the accuracy of continuum modeling, Selker et al. (2007) referred to the argument of Brooks et al. (1999), who questioned the continuum assumption for low flow rates. Selker et al. (2007) declared that a dense gas flow network at a high flow rate is sufficient for utilizing the continuum assumption. They explained that when injected gas does not occupy all the equiprobable channel realizations of a porous medium (i.e., a few gas channels are distributed
We used Euler number calculations and measured gas volumes to 6
Therefore, it is critical to apply the appropriate heterogeneity in  
Radii exhibit lognormal distributions (Kosugi, 1996).

Geistlinger et al. (2006) performed by Geistlinger et al. (2006) for 1-mm glass ballotine
3-mm spheres (GBS) and used the TOUGH2 program (Pruess et al., 1999) as a continuum model to simulate their experimental results. We applied different types of stochastic heterogeneity (Gaussian and uniformly distributed heterogeneity) in simulations and determined how stochastic heterogeneity can indicate gas phase connectivity.

The novelty of this work is the application of different degrees of heterogeneity in continuum simulations to test which is representative of the actual heterogeneity of the medium, along with the use of quantified simulation results to characterize gas channels using Euler numbers.

**Experimental Setup**

Geistlinger et al. (2006) used a two-dimensional Plexiglas flow cell with inner dimensions of $L_x$ by $L_y$ by $L_z$ = 40 by 1.2 by 45 cm to conduct gas injection experiments. They gradually poured wet glass beads into the flow cell to a height of 35 cm and then covered the glass beads with 6 cm of lead spheres as a lithostatic layer to prevent bead rearrangement. Figure 1 shows the specifications of the flow cell and injection point. Geistlinger et al. (2006) used three different classes of glass beads—0.5-, 1-, and 2-mm GBS—and published the experimental results of the 0.5-mm GBS in detail (Geistlinger et al., 2009). We emphasize that the focus of our work is quantifying the gas channels of 1-mm GBS in both experimental images and simulation results. Geistlinger et al. (2006) measured the porosity ($\phi$), permeability ($k_{\exp}$), and entry capillary pressure ($P_e$) values for 1-mm GBS in a series of experiments. The averaged values of these parameters are summarized in Table 1. Geistlinger et al. (2006) equipped their experimental setup with two measuring systems: an optical system that recorded the gas distribution with time, and a gravimetric system that measured the weight of the displaced water. Figure 2 shows experimental images of the gas distribution in 1 mm-GBS for injection rates ($Q_g$) of 70, 809, and 2417 mL min$^{-1}$. The experimental flow pattern shows a few distinct gas channels at $Q_g$ = 70 mL min$^{-1}$, whereas a higher gas injection rate creates a denser gas channel network. By considering the flow cell as a volumetric system, the volume of displaced water is equal to the injected gas volume. Table 2 summarizes the steady-state values of capillary pressure ($P_c$) and gas volume ($P'_{c}$) for each injection rate.

The 1-mm GBS beads are characterized by a size interval of 0.75 to 1 mm, which makes the sediment packing a heterogeneous medium. The maximum and minimum pore radius values, $r_{\max}$ and $r_{\min}$, that exist within the 1-mm GBS were calculated according to Busch et al. (1993):

$$r_{\max} = (0.458...0.732)r_{k}$$

$$r_{\min} = (0.155...0.414)r_{k}$$

where $r_{k}$ is the mean particle-size radius. For 1-mm GBS, the maximum and minimum pore radii values were calculated to be 0.260 and 0.124 mm, respectively. For a pore size distribution that
varies between \( r_{\text{min}} \) and \( r_{\text{max}} \), the smallest pore radii occur in pore throats and the larger pore radii are those of the pore bodies.

Using the pore size distribution, we calculated the capillary pressure–saturation relationship for 1-mm GBS and calibrated it by the observed experimental entry pressure. We used the Brooks and Corey (1966) capillary pressure curve model, which is mainly used in the literature (Ippisch et al., 2006). Table 3 summarizes the corresponding parameters: \( P_{\text{e}} \), \( \lambda \), \( S_{\text{wr}} \), and \( S_{\text{m}} \) that are the entry pressure, pore size distribution index, water residual saturation, and maximum water saturation, respectively. Appendix A provides a summary of the equations used in the Brooks and Corey (1966) model.

**Continuum Modeling of Channelized Gas Flow Pattern**

As our numerical model, we used the TOUGH2 program (Pruess et al., 1999) to simulate gas injection in 1-mm GBS. Appendix B introduces the TOUGH2 program and presents the mathematical equations for multiphase flow that are used in this program. Since the Brooks and Corey (1966) model is not implemented in the original version of the TOUGH2 program, we modified the source code of the TOUGH2 program to apply the relative permeability and capillary pressure equations of the Brooks–Corey model.

Geistlinger et al. (2006) captured experimental images at the surface of the Plexiglas wall. The width of the flow cell was 1.2 cm, which is very small compared with its length and height, which were 40 and 45 cm, respectively (see Fig. 1). Therefore, we assumed that a gas injection into the flow cell behaves like two-dimensional fluid flow, and the gas flow through glass beads can be represented by the observed flow pattern at the wall.

In our model, the grid blocks have the dimensions \( l_x = l_y = 0.5 \) cm and \( l_z = 1.2 \) cm. This cell size creates a two-dimensional model consisting of 102, 81, and 1 grid blocks in the \( x \), \( y \), and \( z \) directions, respectively. To confirm that the flow characteristics are not discretization artifacts, we decreased the size of the grid blocks several times. The smaller grid size in the simulation led to the same gas plume shape and gas volume, so we used this grid size for all the simulations.

In the experiment, excess water leaked outside the flow cell through the overflow system at the side walls. For modeling, we applied a no-flow condition at the bottom and fixed-pressure boundary conditions at the top, left, and right sides of the model. This set of boundary conditions allows water to flow through the sides and prevents increases in the water table during gas injection. We obtained the initial condition of the simulation model by applying the capillary–gravity equilibrium, in which the constant pressure at the top is equal to the atmospheric pressure.

**Applying Stochastic Heterogeneity**

The experimental glass beads are not all the same size, which consequently creates different pore sizes (see Eq. [1]). The capillary pressure is inversely dependent on the pore radius and is related to permeability by the Leverett J-function (Leverett, 1941). In the TOUGH2 program, macroscopic heterogeneity can be implemented by permeability modifiers. The permeability modifier of grid block \( n \) is defined as

\[
\zeta_n = \frac{k_n'}{k_n}
\]

where \( \zeta_n \) is a permeability modifier of the \( n \)th grid block (dimensionless), \( k_n' \) is the modified permeability of the \( n \)th grid block [L\(^2\)], and \( k_n \) is the absolute permeability value of the \( n \)th grid block [L\(^2\)].
TOUGH2 uses the Leverett J-function (Leverett, 1941) to apply the effect of heterogeneous permeability to the capillary pressure field. In one rock type, in which the interfacial tension and contact angle remain constant, the permeability and capillary pressure are dependent according to

\[ P_{c,n} = \frac{P_{c,n}}{\sqrt{n}} \]  

where \( P_{c,n} \) is the modified capillary pressure of the \( n \)th grid block \([M L^{-1} T^{-2}]\), and \( P_{c,n} \) is the capillary pressure of the \( n \)th grid block \([M L^{-1} T^{-2}]\).

In this work, we used the pore radii realizations \( (R) \) generated by the Hydro-Gen program (Bellin and Rubin, 1996). Each pore radii realization includes a set of random values for pore radii \( (r) \) in two dimensions, which Hydro-Gen generates using the assigned grid spacing, correlation length, mean value, variance value, and covariance type.

We forced Hydro-Gen to use a Gaussian function as the covariance type (i.e., correlation function). We input the correlation length value that determines which pores are correlated to each other. Hydro-Gen takes the grid spacing and the field dimensions and creates random pore radii values for each grid. The pore radii that are in the range of the correlation length are correlated to each other. Hydro-Gen creates an independent set of pore radii values as one realization (i.e., \( R \)), in which every grid block has one pore radius value.

We calculated the capillary pressure of each grid block using the Laplace–Young equation. Therefore, we applied pore radii heterogeneity to the capillary pressure value that varies with \( r^{-1} \). Furthermore, we scaled the permeability value for each grid block by assuming that the mean permeability value corresponds to the mean pore radius and this changes with \( r^2 \). Therefore, we applied pore radii heterogeneity to the permeability field.

We considered 1-mm GBS to be an isotropic porous medium with a correlation length equal to 2 cm in the horizontal and vertical directions (i.e., correlation length is 5% of the horizontal length of a flow cell that is 40 cm long).

We created 10 different Gaussian-distributed pore radii realizations \( (R1–R10) \) to show that the results are independent of the realization number. Figure 3 shows three stochastic permeability fields \( (R1, R5, \text{and } R10) \) for 1-mm GBS with cell dimensions of \( l_x \) by \( l_y \) by \( l_z \) = 0.5 by 0.5 by 1.2 cm. For these three Gaussian-distributed pore radii realizations, the averaged mean permeability value is \( k_{\text{mean}} = 5.5 \times 10^{-10} \text{ m}^2 \), which is equal to the experimental value (see Table 1).

Figure 4 presents the numerical results of applying the stochastic permeability fields shown in Fig. 3 at three injection rates of 70, 809, and 2417 mL min\(^{-1}\). A comparison of the numerical results in Fig. 4 with the experimental images in Fig. 2 reveals that Gaussian-distributed heterogeneity can represent the average geometry of the gas distribution. Without considering the uniformity of the gas distribution within the gas plume, all the numerical gas saturation results are parabolic in shape, which is also the case in all the experimental images. To quantify these parabolic shapes, we extracted the outer boundary of the gas plumes, where the gas saturation threshold is 10%. We then compared the shape and the fitted parabolic curves to the boundary lines in the experimental and numerical results shown in Fig. 5. The first row of Fig. 5 shows the outer boundary of the numerical gas plume for 10 realizations and the experimental image. The second row shows the corresponding parabolic equation that is fitted to the experimental boundary line and the average boundary line calculated for the 10 realizations. Although the fitting is poor at the low injection rate of 70 mL min\(^{-1}\), the parabolic equations are very close at the higher injection rates. To measure the accuracy, in the second row of Fig. 5, we calculated the relative error between the locations of the outer boundaries. The numerical model predicted the width of the gas plume with 80% accuracy for the gas distribution of the low injection rate \( (e.g., Q_g = 70 \text{ mL min}^{-1}) \). The measured width reached 90 and 97% accuracies for the higher injection rates of 809 and 2417 mL min\(^{-1}\), respectively. This means that the simulations at the higher injection rates have higher accuracies in predicting the shape and boundary line of the gas plume than those at the low injection rate, which develops more distinct gas channels.

Also, we calculated the numerical gas volumes by integrating the gas saturation in the simulation model. The averaged gas

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![Fig. 3. Stochastic permeability fields created using a Gaussian distribution in Hydro-Gen for pore radii realizations R1, R5, and R10.](image-url)
volumes for realizations $R_1$ to $R_{10}$ with correlated permeability were 20.89, 65.5, and 111.35 cm$^3$ at gas injection rates of 70, 809, and 2417 mL min$^{-1}$ (average $\sigma_k = 0.14 \times 10^{-10}$ m$^2$). A quantitative comparison of the measured gas volumes in the experiments (Table 2) and those calculated for the numerical results confirms that the continuum model can predict the average gas volume with 90% accuracy for all the injection rates.

In conclusion, the continuum model has reasonable accuracy in predicting the integral properties of the experiments, e.g., the gas volume and plume shape of the gas distribution.

**Calculation of Euler Number**

Compared with the experimental images in Fig. 2, stochastic heterogeneity can create distinct gas channels at all injection rates.
We used the Euler number to characterize the connected gas channels (clusters) in the TOUGH2 simulation results and compared them with the Euler numbers calculated for the gas distributions of the experimental images.

The Euler number is a scalar indicator obtained when a threshold is defined for the Euler characteristic. The Euler characteristic is a topological function used to characterize the number of clusters and to measure the number of channels and their connectivity (Renard and Allard, 2013). In two dimensions, the Euler number is defined by subtracting the number of holes from the number of clusters, whereas in three dimensions, it is defined as the summation of the number of clusters and holes minus the number of handles (Renard and Allard, 2013).

The calculation of the Euler number is based on the decomposition of the field into two sets by applying a threshold value. To quantify the gas channels, we calculated Euler numbers for the experimental images and compared them with the Euler numbers calculated for the numerical simulations. We used MATLAB (The MathWorks) to calculate the Euler numbers and considered the whole range of saturation levels (i.e., 0.001–1) for the threshold. In each step, the Euler number indicates the connectivity of the grids that have gas saturations equal to or higher than the specified threshold value. Therefore, the calculation of the Euler numbers builds a characteristic curve for the medium.

Figure 6 shows a comparison of the Euler numbers calculated for 10 realizations ($R_1$–$R_{10}$) with those determined from the experimental images. We can see that the simulated and experimental Euler numbers follow the same trend at all three injection rates. This means that for any threshold saturation, the number of connected gas clusters minus the number of holes is similar in both the stochastic simulation results and the experimental images. However, having a similar Euler number does not guarantee equal gas-channel length or similarity of gas-channel location.

The results reveal that the Euler number first increases with gas saturation and then decreases. The maximum Euler number values occur at 15 to 18, 25 to 30, and 35 to 40% gas saturations at

![Fig. 5. Saturation boundary lines of experimental and numerical gas plumes for gas injection rates $Q_g = 70, 809,$ and 2417 mL min$^{-1}$ when correlated permeability fields (i.e., pore radii realizations $R_1$–$R_{10}$) are used.](image-url)
injection rates of 70, 809, and 2417 mL min$^{-1}$, respectively. At the lower injection rate of 70 mL min$^{-1}$, the Euler number reaches zero at 30% gas saturation. In this case, all the grids with gas saturations \( \leq 30\% \) are connected. In other words, the maximum gas saturation within the porous medium can reach 30% at an injection rate of 70 mL min$^{-1}$. This number increases at injection rates of 809 and 2417 mL min$^{-1}$ to 40 and 50%, respectively.

The number of channels and the maximum gas saturation value within the porous medium increase with the injection rate. This means that the injection rate of 2417 mL min$^{-1}$ has the highest Euler number.

The Euler numbers for the simulation results fluctuated at lower gas saturation values at injection rates of 809 and 2417 mL min$^{-1}$ (Fig. 6). This is because when gas is injected at a high rate, it first fills many grids that may be connected to other gas channels or it may vanish as the injection continues. Therefore, the gas flows through the more established channels. The Euler numbers of the experimental images show no fluctuation and change more smoothly than those in the simulation results. This is because the experimental images have limited accuracy in capturing gas saturation values. Changes in the gas channels captured in the experimental images were not at high resolution. Therefore, the changes in the Euler numbers are greater in the experimental images than in the simulation results, for which the accuracy of gas saturation measurement was very high.

Next, we fit one Kernel distribution to the gas saturation data at every injection rate. Figure 7 shows the cumulative distribution function (CDF) of the fitted Kernel distributions for the experimental and simulation results. The CDF does not show the connectivity of the gas channels but reflects the cumulative probability of reaching gas saturation within the model. Every gas saturation value in the simulation results has a higher CDF value, which means that there is higher probability of having saturation values that are lower than or equal to this saturation value in the simulation results than in the experimental images.

Many researchers, for example Geistlinger et al. (2009) and Selker et al. (2007), have argued that a continuum model cannot predict gas channels, but they did not apply stochastic heterogeneity. The results presented below show that stochastic heterogeneity, which is created by experimental variance, can represent the parabolic shape of the gas distribution and the topology of connected gas channels. Although stochastic simulations cannot predict the exact location of gas channels, they can accurately predict the average gas flow pattern and number of gas channels.

**Applying Uncorrelated Heterogeneity**

Although most of the pore radii distributions are reported to be lognormal Gaussian distributions, Stauffer et al. (2009) argued...
that they had captured the effect of heterogeneity by applying the uncorrelated, uniformly distributed, random pore radii.

To investigate the validity of the argument of Stauffer et al. (2009), we generated five different realizations (R1–R5) of pore radii distributions for 1-mm GBS using the minimum and maximum pore radius values. We created the permeability and capillary pressure fields using the pore radius distribution and applying the approach described for applying stochastic heterogeneity. The corresponding uncorrelated permeability fields have an averaged mean value and averaged standard deviation of $k_{\text{mean}} = 5.50 \times 10^{-10}$ m$^2$ and $\sigma_k = \pm 3.67 \times 10^{-10}$ m$^2$, respectively. The mean value is equal to the mean permeability of the 1-mm GBS, which is measured experimentally, but the standard deviation is 26-fold higher than the experimental value (see Table 1). This means that the heterogeneous permeability field created using the uncorrelated uniformly distributed pore radii is much stronger than that of the experimental observation.

Figure 8 shows the uncorrelated stochastic permeability fields for two out of the five realizations (R1 and R4), created using uniformly distributed pore radii. Unlike the smooth permeability distribution in Fig. 3, which is close to the mean permeability value, the heterogeneity in Fig. 8 is a random distribution of the smallest and largest permeability values, which only infrequently match the mean permeability value.

Figure 9 shows the numerical gas distribution results at steady state when the uncorrelated heterogeneities of R1 and R4 are applied at injection rates of 70, 809, and 2417 mL min$^{-1}$. The numerical results in Fig. 9 show that uncorrelated random heterogeneity creates distinct stochastic gas channels but cannot represent the parabolic shape of the gas plume observed experimentally.

The uncorrelated heterogeneity of the pore radii results in a highly stochastic capillary pressure field. Because a high capillary force dominates the buoyancy force, the stochastic gas channels develop more in the horizontal direction, which results in a wide gas distribution. This effect is noticeable at the injection rate of 2417 mL min$^{-1}$ in Fig. 9.

The averaged gas volumes for realizations R1 to R5 with uncorrelated permeability were 65.99, 177.88, and 274.66 cm$^3$ at gas injection rates of 70, 809, and 2417 mL min$^{-1}$ (average $\sigma_k = 3.67 \times 10^{-10}$ m$^2$). A comparison of these gas volumes with those in Table 2 reveals that the uncorrelated heterogeneity yields an integral gas volume much higher than the experimental values. This is because the strong capillary force causes the gas phase to accumulate, prevents gas movement, and creates high saturation of the trapped gas. On the one hand, uncorrelated heterogeneity generates distinct gas channels. On the other hand, strong heterogeneity leads to high gas volumes in the model.

Figure 10 shows the Euler numbers calculated in the simulation of the five uncorrelated pore radii realizations compared with the experimental values. The Euler numbers of the numerical gas distributions are much higher than the experimental Euler numbers, where the difference escalates with increases in the gas injection rate. The trapped gas in the numerical results creates higher channel numbers at any gas saturation than that in the experimental results.

In conclusion, the lognormal distribution function can describe the pore size distribution more accurately than other functions like the uncorrelated uniform pore distribution. Furthermore, heterogeneity in the permeability and capillary pressure should be applied in simulations, and it is important to consider a reasonable heterogeneity that satisfies the experimental observations.

**Conclusions**

There is controversy in the literature regarding whether continuum modeling can describe channelized flow patterns. Based on the Brooks et al. (1999) condition, the continuum approach can be expected to describe gas flow patterns at high flow rates, whereas it fails to describe sparse gas channel networks observed at low flow rates. In this study, we conducted a set of numerical simulations to show how applying representative heterogeneity and related parameters in a continuum model can capture the gas channels.

Because the structure of a heterogeneous field is, however, rarely known, the model parameters must be estimated based on
limited knowledge. Therefore, an important question is how a heterogeneous structure is best characterized and what are the key features that should be captured.

In this study, we showed that applying correlated heterogeneity in the permeability and capillary pressure fields, which are obtained experimentally, can capture the dynamic features of the experimental gas flow pattern. However, the uncorrelated heterogeneity predictions deviate from the quantitative values of the experimental gas distribution.

In conclusion, the continuum model can describe a gas flow pattern if the key parameters of the porous medium, like representative capillary pressure and permeability, are estimated and applied. A calibrated model that includes the experimental heterogeneity can predict average flow properties, such as the gas

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**Fig. 9.** Numerical gas distributions for gas injection rates $Q_g = 70$, 809, and 2417 mL min$^{-1}$ when the uncorrelated permeability fields of Fig. 8 are applied in TOUGH2 modeling.

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**Fig. 10.** Euler number calculations for experimental images and numerical gas distributions of the uncorrelated permeability fields of pore radii realizations $R1$ to $R5$ for gas injection rates $Q_g = 70$, 809, and 2417 mL min$^{-1}$.
injection volume. This is because it is developed based on the continuum assumption, which applies the effective properties at the representative elementary volume. Furthermore, connectivity metrics like the Euler number provide a practical method for quantifying gas channels and measuring the properties of gas flow channels.

Appendix A

Brooks and Corey (1966) proposed the following function to express the capillary pressure–saturation relationship:

\[ P_e = P_m S_e^{-(3/\lambda)} \]  \hspace{1cm}  \text{[A1]}

where \( P_e \) is the entry pressure [\( \text{M L}^{-1} \text{T}^{-2} \)], \( \lambda \) is the pore size distribution index (dimensionless), and \( S_e \) is the effective saturation of the wetting phase (dimensionless), which is equal to

\[ S_e = \frac{S_w - S_{wr}}{S_m - S_{wr}} \]

where \( S_w \) is saturation of the wetting phase (dimensionless), \( S_{wr} \) is residual saturation of the wetting phase (dimensionless), \( S_m = 1 - S_{nw} \) is maximum saturation of the wetting phase (dimensionless), and \( S_{nw} \) is residual saturation of the non-wetting phase (dimensionless).

The relative permeability functions of wetting and non-wetting phases are derived by substituting Eq. [A1] in the Burdine (1953) approach. The relative permeability functions of the Brooks–Corey model are

\[ k_{r,w} = S_e^{(2+3\lambda)/\lambda} \]  \hspace{1cm}  \text{[A2]}

\[ k_{r,nw} = (1 - S_e) \left[ 1 - S_e^{(2+3\lambda)/\lambda} \right] \]  \hspace{1cm}  \text{[A3]}

where \( k_{r,w} \) is the relative permeability of the wetting phase (dimensionless), and \( k_{r,nw} \) is the relative permeability of the non-wetting phase (dimensionless).

In this work, the wetting and non-wetting phases are water and the gas phase, respectively.

Appendix B

The TOUGH2 program (Pruess et al., 1999) is a multidimensional, multiphase model to simulate the fluid and heat flow of a multicomponent system. The accuracy of the TOUGH2 program has been tested and verified with respect to different analytical and numerical solutions and the results of different laboratory experiments (Pruess et al., 1999). The TOUGH2 program has a modular source code written in FORTRAN77 that facilitates user-defined changes in different modules.

The TOUGH2 program solves the integral form of mass continuity and energy balance equations, in which the fluid advection flow is described by a generalized Darcy’s law and diffusive transport can exist in all phases. A general mathematical mass- and energy-balance equation for a multiphase flow model, solved by TOUGH2 (Pruess et al., 1999), is

\[ \frac{d}{dt} \int_{V} M K dV = \int_{V} F K nd\Gamma_n + \int_{V} q dV \]  \hspace{1cm}  \text{[B1]}

where \( t \) is time [T], \( M \) is the mass or energy per volume [\( \text{M L}^{-3} \)], \( V \) is an arbitrary subdomain of the flow system [\( \text{L}^3 \)], \( F \) is mass or heat flux [\( \text{M L}^{-2} \text{T}^{-1} \)], \( K \) is the mass component (e.g., water, air, or solutes) and counts from 1 to \( N_K \) (dimensionless), \( n \) is a normal vector on surface element \( d\Gamma_n \) (dimensionless), pointing into \( V_n \), \( \Gamma_n \) is a closed surface bounding \( V_n \) [\( \text{L}^2 \)], and \( q \) is the sink or source rate within the volume [\( \text{M L}^{-3} \text{T}^{-1} \)].

The mass accumulation in Eq. [B1] is

\[ M^K = \sum_i \rho_i X^K_i \]  \hspace{1cm}  \text{[B2]}

where \( \phi \) is the porosity (dimensionless), \( i \) is the phase (e.g., liquid, gas, or a nonaqueous-phase liquid) (dimensionless), \( S \) is saturation (dimensionless), \( \rho \) is density [\( \text{M L}^{-3} \)], and \( X^K \) is the mass fraction of the \( K \)th component (dimensionless).

The mass flux in Eq. [B1] is the sum of mass fluxes across the phases, where the individual phase flux is obtained by a generalized Darcy law:

\[ F^K_i = \sum_j X^K_j F_j \]  \hspace{1cm}  \text{[B3]}

\[ F_i = -k_i \frac{\rho_i}{\mu_i} (\nabla P_i - \rho_i g) \]  \hspace{1cm}  \text{[B4]}

where \( k \) is absolute permeability [\( \text{L}^2 \)], \( \mu_i \) is relative permeability of the \( i \)th phase (dimensionless), \( \mu \) is viscosity [\( \text{M L}^{-1} \text{T}^{-1} \)], \( P_i \) is pressure of the \( i \)th phase [\( \text{M L}^{-1} \text{T}^{-2} \)], and \( g \) is gravitational acceleration [\( \text{L T}^{-2} \)].

By neglecting heat transfers (isothermal condition), phase change effect, and the gas pressure gradient, a simplified version of Eq. [B1] is obtained for liquid-phase flow in the unsaturated zone. Hence, the flow equations of the water and gas phases within a gas–water flow system become

\[ \frac{\partial}{\partial t} (\rho w S_w \phi) + \nabla \cdot (-\rho w k_{r,w} \nabla (P_w - \rho w g z)) = I_w \]  \hspace{1cm}  \text{[B5]}

\[ \frac{\partial}{\partial t} (\rho g S_g \phi) + \nabla \cdot (-\rho g k_{r,g} \nabla (P_g - \rho g g z)) = I_g \]  \hspace{1cm}  \text{[B6]}

where \( \rho_w \) is the density of the water phase [\( \text{M L}^{-3} \)], \( S_w \) is water saturation (dimensionless), \( k_{r,w} \) is the relative permeability function of the water phase (dimensionless), \( \mu_w \) is the dynamic viscosity of the water phase (dimensionless), \( P_w \) is the pressure of water [\( \text{M L}^{-1} \text{T}^{-2} \)], \( z \) is elevation [\( \text{L} \)], \( I_w \) is the volumetric mass rate of production and injection of the water phase [\( \text{M L}^{-3} \text{T}^{-1} \)], \( \rho_g \) is the density of the gas phase [\( \text{M L}^{-3} \)], \( S_g \) is gas saturation (dimensionless), \( k_{r,g} \) is the relative permeability function of the gas phase (dimensionless), \( \mu_g \)
is the dynamic viscosity of the gas phase $[M \cdot L^{-1} \cdot T^{-1}]$, $P_g$ is gas pressure $[M \cdot L^{-1} \cdot T^{-2}]$, and $I_g$ is the volumetric mass rate of production and injection of the gas phase $[M \cdot L^{-3} \cdot T^{-1}]$.

In this system, the water and gas phases fill all the pore spaces, in which the following constraints hold:

$$S_w + S_g = 1.0 \quad [B7]$$

$$P_c(S_w) = P_g - P_w \quad [B8]$$

where $P_c$ is the capillary pressure $[M \cdot L^{-1} \cdot T^{-2}]$.

For solving the equation in TOUGH2, it is assumed that water is an incompressible fluid (i.e., $\rho_w$ is constant) and the compressibility of the pore space is negligible (i.e., $\partial \phi / \partial P \approx 0$). The partial differential equations consist of two equations and two independent variables, $P_w$ and $S_w$, and can be solved by using analytical or numerical methods when the values of independent variables are known under initial conditions or $t = 0$ and at the boundaries in each dimension (i.e., boundary conditions).

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