Comparing Equations for Two-Phase Fluid Flow in Porous Media

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Abstract: Various types of equation system formulations for modelling two-phase flow in porous media using the finite element method have been investigated. The system of equations consists of mass balances, partial differential equations (PDE) that describe the accumulation, transport and injection/production of the phases in the model. In addition, several auxiliary equations (eg. hydraulic properties) apply to the system, coupling the different phases in the system together. This set of equations, PDEs and auxiliary equations, allows for equation manipulation such that the main differences between the formulations are the dependent variables that are solved for. Here we have tested five different formulations for 2D simulations and one for 1D; the Buckley-Leverett equation. The various formulations are compared with regards to numerical performances like robustness (numerical stability) and solving time. The purpose of the investigation is to identify a preferred formulation that will be best suited for more complicated modelling, by for instance taking into account poroelasticity, energy balance, chemical reactions, dissolution of the phases, etc. The tests performed strongly suggest that the fractional flow formulation is the fastest and most robust formulation.

Keywords: Two-phase flow, porous media, finite element method

1. Introduction

Multi-phase flow, like two-phase flow, is often strongly convection-dominated (as opposed to diffusive flow). Pure convective transport is discontinuous, convection-dominated flow exert some diffusion, but still has a very sharp front of the intruding phase that needs to be numerically resolved and therefore can be very difficult, sometimes even impossible, to solve with the finite element method. A possible remedy to this is to use stabilization techniques, for instance artificial diffusion, but there are big uncertainties and controversy about the accuracy obtained by using these methods.

As a consequence of this, using the best suitable and most robust method for solving the problem from a wide variety of choices can be crucial. There are many alternative numerical methods to be used when solving two-phase flow problem, but the finite element method has some very appealing advantages, one of them being the flexible meshing and discretization and hence the ability to deal with complicated geometric structures.

Using the finite element method, in two-phase flow the system of equations consists of mass balances; partial differential equations (PDE) that describe the accumulation, transport and injection/production of the phases in the model. In addition, several auxiliary equations describing for instance hydraulic properties, apply to the system, coupling the different phases and enabling equation manipulation thus the main differences between the formulations are the dependent variables that are solved for. Using the finite element method, there are many ways to solve two-phase flow problems, in the next section six various formulations will be presented.

2. Equations

See appendix A for description of the symbols and variables.

The background equations for all versions of two-phase flow equations presented here are derived from the fluid phase mass balance equations, of each phase:

$$\frac{\partial}{\partial t}(\phi\rho_\alpha S_\alpha) - \nabla\cdot[\rho_\alpha\lambda_\alpha\mathbf{K}(\nabla p_\alpha + \gamma_\alpha\nabla z)] = \rho_\alpha q_\alpha \quad (1)$$

where the Darcy velocity can be defined by:

$$v_{\alpha i} = -\lambda_{\alpha ij}K_{ij}\left(\frac{\partial p_\alpha}{\partial x_j} - \gamma\nabla z\right) \quad (2)$$

here the indices *i* and *j* refer to the axes directions; x- and y-axes direction, respectively.

In addition to the mass balance, several auxiliary relations apply to complete the two-

phase flow formulation. Among these is the continuity of fluid saturation:

$$S_w + S_n = 1 \,, \tag{3}$$

and the capillary pressure defined as:

$$p_c = p_n - p_w \,. \tag{4}$$

Capillary pressure-saturation relationships and relative permeability can be expressed by for instance Van Genuchten or Brooks-Corey. Here the latter is used, see eq. B.1-5.

2.2. Formulations of two-phase flow

In this section various formulations for 2D two-phase flow will be reviewed. They will be applied on a simple geometry so they can be compared with a solution obtained using the Buckley-Leverett equation for two-phase flow in 1D. Also, the methods are ranked with regards to the numerical performance; degrees of freedom solved per second, but also robustness. Even though the various formulations describe the same phenomenon by different equations only, the models are solved numerically and are therefore subjected to varying degree of numerical stability.

Note that we are here concerned with isothermic, immiscible displacement of two, incompressible fluids in an incompressible solid matrix. These requirements induce certain implications on the equations: The temperature is constant in the system, the fluid properties (eg. density) of the two phases are considered constant and not depending on pressure and the solid matrix is not poroelastic; meaning that the available pore space (porosity) is constant. Also, for simplicity, gravity is ignored.

The main types of equation system formulations presented here are termed:

Buck - Buckley-Leverett equation
Part - Partial pressure formulation
Flod - Flooding formulation
Phas - Phase pressure-saturation formulation
Frac - Fractional flow formulation
Weig - Weighted pressure formulation

The names above for the various formulations are in some cases typical names often referred to in the literature and others somewhat arbitrary chosen to clearly distinguish the various formulations. The main differences are the dependent PDE variables that are solved for.

Of the six types presented above, Part and Flod are so-called pressure based formulations and the others are saturation based formulations. The following indices n and w indicate the phase; non-wetting and wetting, respectively, p represents the pressure and S the saturation.

Part solve for p_n and p_w, Flod solve for p_c (= p_n - p_w) and p_s (= p_n + p_w), Phas solve for (p_n,S_w) or (p_w,S_n), Frac solve for (p_s,S_w) or (p_s,S_n) and Weig is similar to Frac, except that the total pressure p_s stems from a different definition.

2.3. Part; partial pressure formulation, [1, 4, 6, 12, 13, 14]

In the two-pressure approach the governing equations are written in terms of the pressures in each of the two phases through a straightforward substitution of Darcy's equation into the mass balance equations for each phase; p_n and p_w for non-wetting and wetting phase, respectively.

The wetting saturation is calculated via inversion of the Van Genuchten capillary pressure function; $S_w = f^{-1}(p_c)$. See appendix B for further details.

Two-phase flow in porous media follows separate equations for the wetting and non-wetting phase, substituting eq. 3 into eq. 1 (for the wetting phase), using the definition of the capillary pressure, eq. 4, and fluid capacity:

$$C = -\phi \frac{\partial S_w}{\partial p_c} \tag{5}$$

results in the two PDEs:

$$C\left[\frac{\partial p_n}{\partial t} - \frac{\partial p_w}{\partial t}\right] - \nabla \cdot \left(\lambda_w \mathbf{K} \nabla p_w\right) = q_w \tag{6}$$

$$-C\left[\frac{\partial p_n}{\partial t} - \frac{\partial p_w}{\partial t}\right] - \nabla \cdot \left(\lambda_n \mathbf{K} \nabla p_n\right) = q_n \tag{7}$$

2.4. Flod; flooding formulation, [8]

Flooding formulation is a pressure based formulation. The formulation is traditionally used in flooding problems, hence the name. The depedent variables solved for are the global

pressure p_s and the capillary pressure p_c. Also, using that:

$$\phi_\alpha \frac{\partial}{\partial t} S_\alpha = \phi_\alpha \frac{\partial S_\alpha}{\partial p_c} \frac{\partial p_c}{\partial t} = \phi_\alpha S_\alpha^{'} \frac{\partial p_c}{\partial t} \tag{8}$$

and adding and subtracting the two equations of eq. 1 for each phase and doing some equation manipulation results in the two PDEs to be solved for:

$$\frac{\partial}{\partial x}\left(\Lambda_s \frac{\partial p_s}{\partial x} + \Lambda_c \frac{\partial p_c}{\partial x}\right) + \frac{\partial}{\partial y}\left(\Lambda_s \frac{\partial p_s}{\partial y} + \Lambda_c \frac{\partial p_c}{\partial y}\right) = q_{ps} \tag{9}$$

$$-2C\frac{\partial p_c}{\partial t} + \frac{\partial}{\partial x}\left(\Lambda_s \frac{\partial p_c}{\partial x} + \Lambda_c \frac{\partial p_s}{\partial x}\right) + \frac{\partial}{\partial y}\left(\Lambda_s \frac{\partial p_c}{\partial y} + \Lambda_c \frac{\partial p_s}{\partial y}\right) = q_{pc} \tag{10}$$

where Λ_c and Λ_s are defined as:

$$\Lambda_s = \Lambda_{sxx} = \Lambda_{syy} = 1/2\left(\lambda_n + \lambda_w\right)\mathbf{K} \tag{11}$$

$$\Lambda_c = \Lambda_{cxx} = \Lambda_{cyy} = 1/2\left(\lambda_n - \lambda_w\right)\mathbf{K} \tag{12}$$

2.5. Phas; phase pressure-saturation formulation, [1, 5]

Since the saturation can be expressed as a function of the capillary pressure it is possible to reformulate the governing equations in terms of saturation of one of the phases and the phase pressure of the other phase. Hence, there are two main versions of this formulation; the (p_n,S_w)- and the (p_w,S_n)-systems that are directly derived from eq. 1, the former is:

$$\nabla \cdot \left(\lambda_w p^{'}_c K \nabla S_w - \lambda K \nabla p_n + \lambda K \mathbf{G}\right) = q_w + q_n \tag{13}$$

$$\phi \frac{\partial S_w}{\partial t} + \nabla \cdot \left(\lambda_w K(\rho_w \mathbf{g} - \nabla p_n) + \lambda_w p^{'}_c K \nabla S_w\right) = q_w \tag{14}$$

Note here that a typical abbreviation is used:

$$p^{'}_c = \partial p_c / \partial S_w \tag{15}$$

2.6. Frac; fractional flow formulation, [1, 2, 3, 5, 6, 7, 9, 10, 11, 15, 16]

The fractional flow approach originated in the petroleum engineering literature, and employs the saturation of one of the phases and a global/total pressure as the dependent variables. The fractional flow approach treats the multi-phase flow problem as a total fluid flow of a single mixed fluid, and then describes the individual phases as fractions of the total flow. This approach leads to two equations; the global pressure equation; and the saturation equation.

The equations can be found by 1: adding the mass balances and do some numerical manipulation; the pressure equation. 2: subtract the mass balances and do some numerical manipulation; saturation equation:

$$\nabla \cdot \mathbf{u} = q_w + q_n \tag{16}$$

$$\phi \frac{\partial (S_\alpha)}{\partial t} + \nabla \cdot \mathbf{u}_\alpha = q_\alpha \tag{17}$$

Using expressions for the total velocity eq. C.3 and phase velocities eq. C.1-2

2.7. Weig; weighted pressure formulation, [3, 15]

The weighted pressure formulation is an alternative to the fractional flow where one of the dependent variable is the total pressure. Then, applying the same algebraic manipulations as in deriving the fractional flow formulation results in a new definition of the total velocity, eq. C.4. The mass balances are the same as for the fractional flow formulation; eq. 15 and eq. 16.

2.8. Buck; Buckley-Leverett equation, [17]

The Buckley–Leverett is used to model two-phase flow in porous media in 1D:

$$\frac{\partial S_w}{\partial t} = u \frac{\partial f_w}{\partial x} = \frac{q_t}{\phi A} \frac{\partial f_w}{\partial S_w} \frac{\partial S_w}{\partial x} \tag{18}$$

where u is the front velocity [m/s] of the fluids at saturation S_w. Considering the saturation equation in the fractional flow formulation, eq. 17, eq. 18 can be derived, given mass conservation, ignoring capillary pressure and gravity. When including capillary pressure, the Buckley-Leverett equation can be defined as:

$$\phi \frac{\partial S_w}{\partial t} + \left(f_w q_t - D_w \frac{\partial S_w}{\partial x}\right) \frac{\partial}{\partial x} = 0 \tag{19}$$

where

$$D_w = \frac{\lambda_w \lambda_n}{\lambda_w + \lambda_n} \frac{dp_c}{dS_{ew}} \tag{20}$$

This equation is used when comparing the various 2D two-phase flow formulations.

3. Model definition

The geometry used to solve the Buckley-Leverett equation is a 1D geometry, see figure 1 for geometry and initial and boundary conditions.

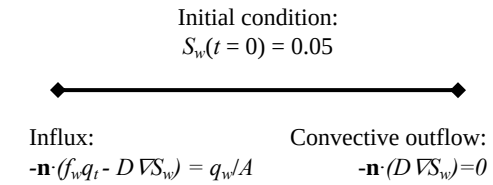

Figure 1. 1D geometry, initial condition and boundary conditions used for solving Buckley-Leverett equation. Length of geometry is 100 m. Here **n** is the outward pointing normal vector.

Similarly, the geometry and initial and boundary conditions used to solve the 2D equations are given in figure 2.

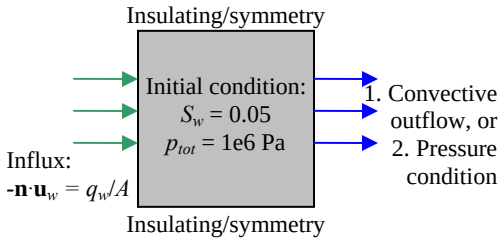

Figure 2. The 2D geometry, initial and boundary conditions used for solving the various two-phase flow formulations. The geometry is a square with 100 m width. Here **n** is the outward pointing normal vector. Where applicable, outlet boundary condition 1. is used, or else outlet boundary condition 2. is used

A small residual of the wetting phase is present initially; a fraction of 0.05. This is to insure that both phases in all formulations will be present and properly defined.

Because of the nature of the various formulations, some have a convective and a diffusive term in the PDEs, for example the saturation based formulations. For the pressure based formulations, which are strictly diffusive in nature, the geometry is 'stretched' in the length direction of the inflow (geometry is a rectangle 100mx200m) and a pressure condition equal to the initial pressure condition is applied on the outlet boundary. Where needed, the initial pressure conditions are all derived from the initial total pressure condition and using capillary pressure-saturation functions. For more model properties, see appendix Model properties.

4. Simulations and results

All formulations where solved and compared for different model setups, given in table 1. To compare the performance of the formulations, a value corresponding to number of degrees of freedom (dofs) solved per second was chosen. This is not a perfect criterion, since solution time is not linear with the workload (dofs). However, it gives, at least, a rough indication of the performance.

The results of the simulations for the various formulations and different setups are given in table 2.

Table 1: Model setups used to compare the various formulations. The parameter in setup 2-4 that is different than in setup 1 is indicated in bold.

Parameter	Setup			
	1	2	3	4
Intrinsic permeability, [m^2], **K**	1e-10	**1e-11**	1e-10	1e-10
Entry pressure, [Pa], p_d	1e4	1e4	**1e3**	1e4
Influx wetting phase, [m^3/s], q_w	1e-2	1e-2	1e-2	**1e-1**

Table 2: Results of the simulations for the various formulations and setups. Multiple values for each setup are given where multiple runs with different meshes where performed. The highest score for each run is indicated in bold.

Equation formulation	Setup, dofs/sec			
	1	2	3	4
Buck	6	4,4,5	5,3,3	6,4,5
Frac	**96**	**70,55,57**	**56,61,68**	**33,56,55**
Part	69,88	42,16,12	8,18,22	8,8,12
Flod	59,49	42,19,13	13,19,28	10,10,13
Phas	90	62,52,54	50,60,62	31,49,49
Weig	94	49[1)],50,52	50,53[1)],59[1)]	32,47,48

[1)] Needed a denser mesh than the other formulations

Figure 3 a-d show the effective wetting saturation along the x-axis for the Buckley-Leverett equation (thick black line) and the

various formulations for model setups 1-4, respectively. The color-code for the other formulations are given in table 3.

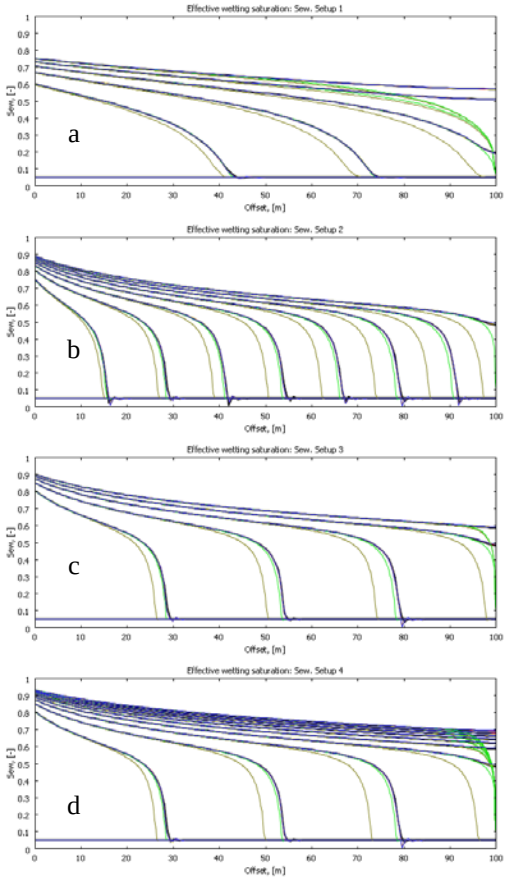

Figure 3. The plots show the effective wetting saturation as function of offset along the x-axis for the Buckley-Leverett equation (thick black line) and the other formulations. See table 3 for color-code explanation. (a) setup 1. (b) setup 2. (c) setup 3. (d) setup 4.

Table 3: Corresponding color-code and formulation in the result plots, figure 3 a-d.

color	Formulation	color	Formulation
Red	Frac	Yellow	Phas
Brown	Part	Blue	Weig
Green	Flod	Black	Buck

5. Discussion and conclusion

When it comes to numerical speed (solution time), the differences between the various formulations are noticeable, even for simple cases like setup 1 (table 2). When the model becomes more physically complicated to solve (due to low permeability, high injection rate, low entry pressure, etc.) the robustness of the formulation becomes important and the solution times differ even more. Also, when the values become more critical, some of the formulations need a denser mesh to get a solution at all. One method seems to be faster, when looking at the results in table 2, and more robust than the others (requires little or no tuning of mesh, etc.); the fractional flow formulation.

The results in figure 3 show consistent results for all formulations, except for the pressure formulations. The curves for Buck, Frac, Phas and Weig all coincide into one line, visible as the thick black line in figure 3. The pressure formulations (green and brown curve) show some deviation, particularly Part (brown curve). This is believed partly to be due to the different boundary conditions applied on the outlet boundary for the various formulations; the saturation based formulations have convective outflows on the outlet while the pressure based formulations have applied pressure conditions (corresponding to initial pressure conditions) since they do not have the convective outflow condition. The result of this pressure condition can be seen as the steep dips in the wetting saturation curves close to the outlet, in figure 3, as the pressure condition forces the saturation to initial value (here 0.05). However, it would be reasonable to expect Part to behave similarly to Flod, this seems not to be the case and need more investigation to fully understand. A conclusion to this is that the deviation in Part is too big to be explained by the boundary conditions alone, hence there is something not correct in the partial pressure based formulation. In addition to this, an explanation to the poor performances of the pressure based formulations in general is that if one of the saturations is very small then the pressure in that phase will be poorly defined and could be numerically difficult to solve.

For the other formulations, particularly Frac and Weig, even if one phase is to disappear (S_w or S_n is zero, or small) there is still a non-zero smooth variable for the global pressure p, a general advantage and intuitively a reason to choose one of these formulations.

Concerning robustness, for setup 2 and 3, Weig did not solve with the same settings as the others. It needed a denser mesh before it would

solve. It's a general requirement that the mesh needs to properly resolve the model compared to the front velocity of the injected phase, but Weig seemed particularly sensitive to this. The limit to how sensitive is not investigated.

The results for the Buckley-Leverett is not directly comparable to the others; first it's 1D and second it only solves one equation; for the wetting saturation. Because it solves much less dofs for a comparable model (same problem definition and same mesh resolution), it's much faster and therefore is a good choice for 1D problems.

Finally, a literature study and comparison of documented equation formulations for modelling two-phase flow have been performed. The objective has not been to go into the details of the numerical benefits and drawback of the various formulations, but find a formulation that is best suited for further development by including effects like thermodynamics, poroelasticity, chemistry, etc. The criteria of selection are numerical speed and robustness. For 2D problems, based on the analysis performed here, the favorite formulation is the fractional flow formulation.

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Appendix A. Nomenclature

p_α	partial/phase pressure, [Pa]
t	time, [s]
α	represents the fluid phases (wetting – w, non-wetting – n)
S_α	saturation of phase α, [-]
$S_{\alpha r}$	residual saturation of phase α, [-]
ρ_α	fluid density, [kg/m^3]
$\mathbf{K}$	intrinsic permeability tensor, [m^2]
ϕ	dimensionless porosity, [-]
γ_α	fluid specific weight or gradient due to gravitation, = $\rho_\alpha \cdot \mathbf{g}$, [Pa/m]
λ_α	phase mobility, [1/Pa·s], $\lambda_\alpha = k_{r\alpha} / \mu_\alpha$
λ	total mobility, [1/Pa·s], $\lambda = \lambda_w + \lambda_n$
z	positive upward vertical direction, [-]
$\mathbf{g}$	gravity vector, [m/s^2]
q_α	volumetric flux source term, [m^3/s]
f_α	fractional flow, [-], $f_\alpha = \lambda_\alpha / \lambda$
$k_{r\alpha}$	relative permeability, [-]
μ_α	dynamic viscosity, [Pa·s]
p_c	capillary pressure, [Pa], $p_c = p_n - p_w$

Appendix B. Van Genuchten relations

The advantage of using van Genuchten vs. Brooks-Corey functions is that the derivatives are continuous, improving numerical stability.

Capillary pressure vs. saturation function:

$$p_c(S_w) = \frac{1}{\alpha}\left(S_{ew}^{-\frac{1}{m}} - 1\right)^{\frac{1}{n}} \qquad \text{(B.1)}$$

The effective wetting saturation, S_{ew}, is given by:

$$S_{ew} = \frac{S_w - S_{wr}}{1 - S_{wr} - S_{nr}} \qquad \text{(B.2)}$$

where $S_{ew} \in [0,1]$.

The derivative is analytically derived:

$$\frac{\partial p_c}{\partial S_w} = -\frac{1}{\alpha}\cdot\frac{1}{n}\left(S_{ew}^{-\frac{1}{m}} - 1\right)^{\frac{m-1}{m}} \cdot \frac{1}{m} S_{ew}^{-\frac{1+m}{m}} \qquad \text{(B.3)}$$

Saturation vs. capillary pressure function:

$$S_{ew}(p_c) = \left((\alpha p_c)^n + 1\right)^{-m} \qquad \text{(B.4)}$$

The derivative is analytically derived:

$$\frac{dS_{ew}}{dp_c} = \left(-\left((\alpha p_c)^n + 1\right)^{-m}\right) m (\alpha p_c)^n \frac{n}{p_c\left((\alpha p_c)^n + 1\right)} \qquad \text{(B.5)}$$

Note: Here α is model parameter, related to the entry pressure, p_d, eg. $\alpha = 1/p_d$

Appendix C. Velocity vectors

The saturation based formulations uses these velocity vector expressions, depending on the phase described:

$$\mathbf{u}_w = f_w \mathbf{u} + \lambda_n f_w K\left(\nabla p_c + (\rho_w - \rho_n)\mathbf{g}\right) \qquad \text{(C.1)}$$

$$\mathbf{u}_n = f_n \mathbf{u} - \lambda_w f_n K\left(\nabla p_c + (\rho_w + \rho_n)\mathbf{g}\right) \qquad \text{(C.2)}$$

In addition, formulations Frac and Phas use this expression for the total velocity:

$$\mathbf{u} = -\mathbf{K}\left(\lambda \nabla p - (\lambda_w \rho_w + \lambda_n \rho_n)\mathbf{g}\right) \qquad \text{(C.3)}$$

The Weig formulation uses a different definition of the total pressure and hence a different expression for the total velocity:

$$\mathbf{u} = -\mathbf{K}\left(\lambda \nabla p + (S\lambda - \lambda_w)\nabla p_c + \lambda p_c \nabla S - (\lambda_w \rho_w + \lambda_n \rho_n)\mathbf{g}\right) \qquad \text{(C.4)}$$

Appendix D. Model parameters

Table D.1. Model parameters.

Description, variable	Unit	Value
Porosity, ϕ	[-]	0.2
Intrinsic permeability, tensor, $\mathbf{K}$	[m^2]	1e-10
Dynamic viscosity, wetting, μ_w	[kg/ms]	1e-3
Dynamic viscosity, non-wetting, μ_n	[kg/ms]	2e-2
In-flux, wetting phase, q_w	[m^3/s]	1e-2
In-flux, non-wetting phase, q_n	[m^3/s]	0
Total volumetric flux, $q_t = q_w + q_n$	[m^3/s]	1e-2
Total pressure, p_s	[Pa]	1e6
Residual wetting sat., S_{wr}	[-]	0
Residual non-wetting sat., S_{nr}	[-]	0
Model parameter, m	[-]	2/3
Model parameter, n	[-]	1/(1-m)
Model parameter, α	[1/Pa]	1e-4
Model parameter, ε	[-]	1/2
Model parameter, γ	[-]	1/3
Entry pressure, p_d	[Pa]	1e4
Initial saturation, S_{w0}	[-]	0.05