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Subject: An overview of the BRAGFLO two-phase flow parameters used to model the run-of-mine salt panel closures implemented in the PCS-2012 PA

Introduction

BRAGFLO Version 6.0 is the WIPP PA code used in the PABC-2009 to calculate brine and gas flows in and around the repository. Version 6.0 is the most recent qualified version of BRAGFLO, and is the code version that will be used for the PCS-2012 PA. BRAGFLO assumes an immiscible water/gas system (Nemer 2007). Immiscible fluids are not capable of mixing and have interfaces across which pressure discontinuities exist. This interfacial tension produces a capillary pressure between the water and gas phases. Capillary pressure modeling is a component of the overall flow modeling implemented in BRAGFLO.

This memo describes the two-phase flow model and the parameters associated with the run-of-mine (ROM) salt panel closures to be implemented in the PCS-2012 (Camphouse et al 2012). Generally, the two-phase flow flags used in BRAGFLO specify the relative permeability model and whether the capillary pressure model is to be used or not for a given material. Capillary pressure, which is a function of saturation and threshold pressure, is used to constrain the brine and gas pressures. Parameters associated with these models must be chosen carefully as they can cause BRAGFLO numerical difficulties. In particular, capillary pressure modeling in BRAGFLO typically causes numerical difficulties when materials undergo instantaneous changes in permeability. Capillary pressure modeling in BRAGFLO is often disabled for these kinds of materials.

BRAGFLO Capillary Pressure Modeling

Several PA parameters are used as part of the capillary pressure modeling implemented in BRAGFLO. The threshold capillary pressure, P_T, characterizes the point at which gas, the non wetting phase, can start to flow in the porous media saturated with brine, and thus defines the capillary pressure at 100%

brine saturation. The capillary pressure must exceed the threshold capillary pressure before the gas phase can start to drain the porous medium and flow.

There are two BRAGFLO material parameters that are used to calculate the threshold capillary pressure for a given material. These two parameters are named PCT_A and PCT_EXP. In BRAGFLO, the practice has been to correlate the threshold capillary pressure to permeability according to (Vaughn 1996)

$$P_T = PCT\_A * k^{PCT\_EXP}, \quad \text{(Equation 1)}$$

where k is the brine permeability (m^2) in the x direction. A capability was included in BRAGFLO during the preparation of the CCA that provided a dependence of threshold capillary pressure on dynamic changes in permeability. The database parameter KPT is used as a flag that provides an instruction to BRAGFLO to dynamically update the threshold capillary pressure as k changes temporally. Setting KPT = 1 allows threshold capillary pressure to be updated if permeability changes in the material. The quantity P_T is not updated when KPT is set to 0. KPT has been set to 0 for all BRAGFLO materials in the CCA and every PA performed since, so threshold capillary pressure has never been dynamically updated in WIPP PA.

BRAGFLO solves a system of two mass balance equations for brine pressure and gas saturation as well as two constraint equations for saturation and capillary pressure in the calculation of two-phase flow (Nemer 2007). Instantaneous changes in permeability, due to material changes in a grid region, cause difficulty in numerically satisfying the convergence criterion for the capillary pressure constraint equation. When the convergence criterion cannot be satisfied, the capillary pressure model is disabled for the responsible materials so that a convergent solution can be obtained from BRAGFLO. The flag for this is to set PCT_A = 0, which results in the capillary pressure component being disabled. When this occurs, the convention is to also set PCT_EXP = 0.

BRAGFLO grid regions used to represent the ROM salt panel closures in the PCS-2012 will undergo instantaneous changes in permeability. Specifically, the permeability prescribed to these BRAGFLO grid regions will change instantaneously at 100 and 200 years as closure materials change from PCS_T1 to PCS_T2 and from PCS_T2 to PCS_T3 (Camphouse et al 2012). It is currently planned that capillary pressure modeling will be enabled for these materials. However if numerical convergence difficulties are encountered in BRAGFLO, then capillary pressure modeling will be disabled for them.

In addition to properties PCT_A and PCT_EXP, each material in BRAGFLO has a flag named CAP_MOD associated with it. A value of 1 or 2 is prescribed to CAP_MOD in WIPP PA for all BRAGFLO materials. As illustrated in the BRAGFLO Version 6.0 User's Manual (see e.g. Figure 18 and Figure 19), capillary pressure can be unbounded as a function of brine saturation, depending on the relative permeability model employed. A value of CAP_MOD = 2 results in the capillary pressure being bounded above by a maximum value which is assigned to material property PC_MAX. PC_MAX is 1×10^8 Pa by default for all materials in BRAGFLO. The convention used in WIPP PA is to set CAP_MOD = 1 for materials that have capillary pressure disabled, and to set CAP_MOD = 2 otherwise. That is, CAP_MOD = 1 for materials that also have PCT_A = 0. Thus, all BRAGFLO materials in which capillary pressure is used have a default value of 1×10^8 Pa specified for PC_MAX (and have since the CCA).

Property CAP_MOD is denoted as KPC inside the actual BRAGFLO Fortran code. There is a capillary pressure model number 3 (KPC = 3) included in the BRAGFLO Fortran code in which a minimum brine pressure is defined, denoted by P0_MIN. However, while the capillary pressure model 3 (CAP_MOD = 3) was developed and coded in BRAGFLO in preparation for the original certification of WIPP, it has never actually been used in any PA, including the original certification PA. Even though CAP_MOD = 3 has never been used in PA, BRAGFLO still expects a value to be specified for P0_MIN for all materials, so all BRAGFLO materials have a prescribed value of 1.01325×10^5 Pa for property PO_MIN,

A summary of the parameters used in BRAGFLO capillary pressure modeling is provided in the following bulleted list and Table 1:

- In WIPP PA, threshold capillary pressure is defined by Equation (1). The threshold capillary pressure is constant, based on the initial permeability of each material, and has never been dynamically updated as a function of temporal permeability changes. Material property flag KPT has been set to 0 for all BRAGFLO materials since the CCA.
- Capillary pressure modeling is disabled by setting PCT_A = 0. The convention used in PA is to set PCT_EXP = 0 when PCT_A = 0.
- The convention used in PA is to set CAP_MOD = 1 for materials that have the capillary pressure model disabled. CAP_MOD = 2 corresponds to capillary pressure being bounded above by PC_MAX. All BRAGFLO materials have a value of PC_MAX = 1×10^8 Pa prescribed to them.
- CAP_MOD = 3 corresponds to a capillary pressure model that depends on the minimum brine pressure P0_MIN. This model has never been used in any PA, including the original certification PA. BRAGFLO still expects a value to be specified for P0_MIN for all materials, however. The value used for P0_MIN is 1.01325×10^5 Pa.

Table 1: Parameters Used for BRAGFLO Capillary Pressure Modeling

Property	Description	Value Capillary Pressure Model Enabled	Value Capillary Pressure Model Disabled
PCT_A	Threshold Capillary Pressure Linear Parameter	Material Dependent Nonzero Value	0
PCT_EXP	Threshold Capillary Pressure Exponential Parameter	Material Dependent Nonzero Value	0
CAP_MOD	Capillary Pressure Model Number	2	1
PC_MAX (Pa)	Maximum Allowable Capillary Pressure	1×10^8	1×10^8
KPT	Flag for Permeability Determined Threshold Capillary Pressure	0	0
P0_MIN (Pa)	Minimum Brine Pressure for Capillary Pressure Model 3 (CAP_MOD = 3 has never been used in PA)	1.01325×10^5	1.01325×10^5

BRAGFLO Relative Permeability Modeling

The relative permeability model associated with a given material in BRAGFLO is specified by property RELP_MOD. BRAGFLO panel closure materials have been given a value of RELP_MOD = 4 in WIPP PA. RELP_MOD = 4 corresponds to the Second Modified Brooks-Corey Model illustrated in Figure 20 of the BRAGFLO Version 6.0 User's Manual (Nemer 2007) and the discussion pertaining to that figure. In this model, capillary pressure is a function of the effective saturation which depends on the current brine saturation and both the residual brine and gas saturations. The model also depends on a pore size distribution parameter, denoted as property PORE_DIS in WIPP PA. The run-of-mine (ROM) salt panel closures implemented in the PCS-2012 PA, specifically materials PCS_T1, PCS_T2, and PCS_T3, will be assigned a value of RELP_MOD = 4.

The DRZ has two components for the PCS-2012 PA: DRZ_1 and DRZ_PCS. The DRZ region overall (i.e. material DRZ_1) used a value of RELP_MOD = 4 in the PABC-2009. DRZ_PCS models the healed DRZ above and below panel closures, and also uses RELP_MOD = 4. The material properties assigned to material DRZ_PCS are exactly the same as those used for material DRZ_1, with the exception of permeability. The permeabilities are defined by their logarithm in the x, y, and z directions, and denoted by PRMX_LOG, PRMY_LOG, and PRMZ_LOG, respectively (Stein 2002). Materials DRZ_1 and DRZ_PCS will also be used in the PCS-2012 PA, and will use the same relative permeability model (RELP_MOD = 4) and permeability parameters as used in the PABC-2009.

References

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