



Sandia National Laboratories

Operated for the U.S. Department of Energy
by

Sandia Corporation

4100 National Parks Highway
Carlsbad, NM 88220

Phone: (505) 234-0013
Fax: (505) 234-0061
Internet: djclayt@sandia.gov

545764

Date: April 10, 2007

To: Eric Vugrin, 6711

From: Dan Clayton, 6711

Technical Review: Eric Vugrin, 6711

QA Review: Mario Chavez, 6710

Management Review: Moo Lee, 6711

Subject: Justification of Relative Permeability and Capillary Pressure Model Parameters for Use
by BRAGFLO Version 6.0

1.0 Introduction

Analysis Plan for the 2009 Compliance Recertification Application Performance Assessment, AP-132 (Vugrin and Nemer 2007) describes an analysis that will include several enhancements to performance assessment (PA) models. The code BRAGFLO Version 6.0 is currently being developed for use in this analysis. The purpose of this document is to justify the values of the parameters that will be used by the code for the AP-132 analysis. Because the modification of these parameters was not explicitly listed in AP-132, this document represents a deviation from that analysis.

2.0 Open Cavities

Nemer (2007) recommends a new model, $KRP=11$, for the capillary pressure and relative permeability of the open cavities, which removes the capillary pressure effects from the relative permeability. The model is applicable to open cavities during operational period of the repository, CAVITY_1, CAVITY_2, CAVITY_3 and CAVITY_4, as well as the open cavities which persist after closure, OPS_AREA and EXP_AREA.

3.0 Waste Area

In running BRAGFLO version 5.0, the capillary pressure-saturation relationships were typically turned off in waste-filled regions because they caused the numerical solver in the code to take

very small time steps when the saturation levels approached the residual brine saturation. When the Jacobian is calculated, derivatives with respect to saturation are taken so as not to cross residual brine saturation. Nonetheless the Newton-Raphson solver can have difficulty finding a solution around the discontinuous derivative in capillary pressure when capillary pressure is capped at a maximum. In past calculations this situation has occurred when iron corrosion (which consumes water) reduced the saturation below residual saturation in the waste-filled regions. Furthermore, in BRAGFLO Version 6.0 the chemical reactions in the waste area use a cutoff saturation to determine when the computational cell is effectively dry and no chemical reactions are taking place (Nemer 2007). This increases the code robustness and reduced computational time.

A modified capillary pressure and relative permeability model, KRP=12, was developed such that the model would be independent of the cutoff saturation, as well as to account for the discontinuous derivative in the previous capillary pressure model (KRP=4) (Nemer 2007). The relative permeability model in the KRP=12 model is unchanged from the KRP=4 model. The KRP=12 model should be applied to the WAS_AREA and REPOSIT materials.

4.0 Parameter Summary

In order to use the aforementioned capillary pressure and relative permeability model parameters in the AP-132 calculations, parameters must be entered into the PA parameter database (PAPDB). This section lists the MATERIAL:PROPERTY and values that will be assigned. Table 1 lists all of the values of the capillary pressure and relative permeability model parameters that need to be modified to be used in the AP-132 BRAGFLO calculations. The KRP BRAGFLO variable is labeled in the PAPDB as the RELP_MOD property for each material.

Table 1. Relative Permeability Parameters Modifications. All properties are constant and dimensionless.

MATERIAL	PROPERTY	VALUE
CAVITY_1	RELP_MOD	11
CAVITY_2	RELP_MOD	11
CAVITY_3	RELP_MOD	11
CAVITY_4	RELP_MOD	11
OPS_AREA	RELP_MOD	11
EXP_AREA	RELP_MOD	11
WAS_AREA	RELP_MOD	12
REPOSIT	RELP_MOD	12

References

Nemer, M. B. 2007. Design Document for BRAGFLO Version 6.0. Sandia National Laboratories, Carlsbad, NM. ERMS 545015.

Vugrin, E. D. and M. B. Nemer. 2007. Analysis Plan for the 2009 Compliance Recertification Application Performance Assessment, AP-132. Sandia National Laboratories, Carlsbad, NM. ERMS 545496.