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DEVELOPMENT AND DEMONSTRATION OF MATERIAL PROPERTIES DATABASE AND SOFTWARE FOR THE SIMULATION OF FLOW PROPERTIES IN CEMENTITIOUS MATERIALS

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G.P. Flach

March 2015

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EXECUTIVE SUMMARY

This report describes work performed by the Savannah River National Laboratory (SRNL) in fiscal year 2014 to develop a new Cementitious Barriers Project (CBP) software module designated as FLOExcel. FLOExcel incorporates a uniform database to capture material characterization data and a GoldSim model to define flow properties for both intact and fractured cementitious materials and estimate Darcy velocity based on specified hydraulic head gradient and matric tension. The software module includes hydraulic parameters for intact cementitious and granular materials in the database and a standalone GoldSim framework to manipulate the data. The database will be updated with new data as it comes available. The software module will later be integrated into the next release of the CBP Toolbox, Version 3.0. This report documents the development efforts for this software module.

The FY14 activities described in this report focused on the following two items that form the FLOExcel package:

1) Development of a uniform database to capture CBP data for cementitious materials. In particular, the inclusion and use of hydraulic properties of the materials are emphasized.

2) Development of algorithms and a GoldSim User Interface to calculate hydraulic flow properties of degraded and fractured cementitious materials. Hydraulic properties are required in a simulation of flow through cementitious materials such as Saltstone, waste tank fill grout, and concrete barriers. At SRNL these simulations have been performed using the PORFLOW code as part of Performance Assessments for salt waste disposal and waste tank closure.

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LIST OF ABBREVIATIONS

CBP	Cementitious Barriers Partnership
DOE	Department of Energy
GTG	GoldSim Technology Group
LXO	LeachXS/Orchestra
SRNL	Savannah River National Laboratory
STADIUM	Software for Transport and Degradation in Unsaturated Materials

1.0 Introduction

Work was performed by SRNL in fiscal year 2014 to develop a software module for the CBP Toolbox named FLOExcel. The FLOExcel module includes a database of material properties for intact cementitious and granular materials, and a GoldSim model to manipulate this data. The model (described in Section 4) accesses the database of material properties (described in Section 2) to obtain hydraulic properties for cementitious and granular (soils and gravel) materials selected by the user. These materials can then be blended (i.e. hydraulic properties calculated for a composite material) to simulate cementitious material degradation or the material blend required to simulate specified fracture network parameters. The module will be integrated into the next release of the CBP Toolbox, Version 3.0. This report documents the development efforts for this software module.

2.0 FLOExcel Property Database

In Version 2.0 of the CBP Toolbox, the user primarily works in a copy of the **Template** subfolder which is created during Toolbox installation. Within the **Template** folder is a **Materials** subfolder containing three Microsoft Excel workbooks with composition and physical property data for concrete, salt waste, and soil. Contents of the current **Materials** folder are shown in Figure 2-1.

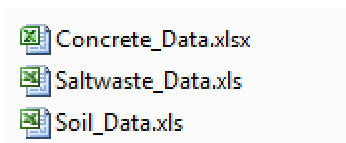

Figure 2-1. Contents of current materials folder

These Excel workbooks contain spreadsheets with material properties formatted for either STADIUM or LXO simulations. For example, STADIUM input is provided for Vault 1/4 and Vault 2 concrete, Type 1 and Type 2 Saltstone (SRS waste forms), and Type 1 soil. Vault 1/4 concrete is representative of the concrete used to build SRS Saltstone Disposal Units 1 and 4 while the Vault 2 concrete is representative of the concrete used for SRS Saltstone Disposal Units 2, 6 and related disposal units. The properties were obtained from the CBP Task 7 report prepared by SIMCO Technologies, Inc. (SIMCO, 2010) and (Protiere and Samson, 2014). The user can either use the preset material properties for simulations or manually change the properties in the spreadsheet so that, for example, when Type 1 concrete is selected for a STADIUM calculation, the properties will actually represent a different material that the user needs to evaluate.

Similarly, preset properties that can be used for LeachXS/ORCHESTRA (LXO) simulations are also provided. The STADIUM and LXO models have different input requirements. For example, STADIUM requires an initial concrete mineral composition and the chemical composition of fluid within the concrete pores along with certain material properties. On the other hand, LXO requires a leachate composition and concrete formulation. Therefore, while in some cases the behavior of the same concrete can be simulated with either code, input for the simulations are significantly different. The property data files were structured with the STADIUM data in the upper section and the LXO data below. This structure makes the files awkward to read and difficult to maintain.

To improve and expand the existing property data available for use in the CBP Toolbox, the three Excel files were consolidated into a single Excel file. The new Excel workbook named **Materialproperties.xls** has separate spreadsheets for STADIUM and LXO inputs and includes six additional spreadsheets providing: hydraulic properties of cementitious materials, binder and solution compositions, chemical compositions and molecular weights of minerals, atomic weights for the first 100 elements, and a list of references. This Excel file is conceived as a first step toward development of a relational CBP material property database.

The Materialproperties.xls database consolidated the data contained in the three Excel workbooks shown in Figure 2-1 into a single source. Input data required for the STADIUM and LXO codes were collected in separate worksheets for easier maintenance. These worksheets essentially reproduce the data in the original workbooks while including some additional information such as cement formulation. However, because these worksheets do not add any additional functionality to the CBP toolbox, they will not be discussed further. Similarly, several other worksheets were included in the database as placeholders for suggested data to include in a full CBP database. These other worksheets are:

1. **Binders** tab in the workbook which provides a listing of cement binder chemical compositions reported by SIMCO in their CBP studies (2010, 2014).
2. **Solutions** tab in the workbook which lists the composition of the salt solution simulant used in SIMCO testing of concrete used to construct SRS Saltstone Disposal Units 2 and 4.
3. **Minerals** tab in the workbook which gives a datasheet listing minerals, their chemical composition, and molecular weight. This list of minerals does not include all of the LeachXS/ORCHESTRA minerals currently available in the CBP Toolbox and will be expanded.
4. **Atomic Wts** tab in the workbook gives a table of atomic weights used to calculate mineral and chemical molecular weights.

For all of these datasheets, it is intended that the data will be expanded as new information is developed and new models are added to the CBP Toolbox. As with the existing version, the Toolbox user can overwrite any of the spreadsheet entries to enter properties for a different material not included in the ones provided. Again, since these worksheets do not add any additional functionality to the CBP Toolbox they will not be discussed further.

Figure 2-2 (**Hydraulic** tab in workbook) shows the list of hydraulic properties provided in the database. Properties for 15 cementitious materials and 11 soils used in SRS performance assessment calculations (Phifer et al., 2006) and 11 soils used in Hanford Performance assessments (Last et al., 2009) are available. The hydraulic properties provided are: horizontal and vertical saturated conductivity, effective diffusion coefficient, material bulk density and particle density, and van Genuchten parameters to allow the calculation of water retention curves. Combined with the FloExcel GoldSim module, this data set will add functionality to the CBP Toolbox. The use of this property data by the FloExcel GoldSim module is demonstrated in Section 4.

Figure 2-3 (**References** tab in workbook) shows the final Excel worksheet in the database which lists the original references used to obtain the data. A copy of this worksheet is included to provide a list of the data sources used to compile the material property database.

Index	SRS Cementitious Materials	Saturated Horizontal Hydraulic Conductivity	Saturated Vetical Hydraulic Conductivity	K_h/K_v	Saturated Effective Diffusion Coefficient	Total Porosity	Dry Bulk Density	Particle Density	Water Retention Curves - Van Genuchten Parameters				Reference
	Material	Kh (cm/s)	Kv (cm/s)	-	De (cm^2/s)	%	g/cm^3	g/cm^3	θ_r	θ_s	α (cm^{-1})	n	
1	E-Area Vault Concrete	1.0E-12	1.0E-12	1.0	5.0E-08	18.4	2.11	2.59	0	0.0820	2.0856E-06	1.9433	10
2	New E-Area CIG Grout-Low Quality Concrete	1.0E-08	1.0E-08	1.0	8.0E-07	21.1	2.06	2.61	0	0	7.6118E-06	1.3930	10
3	E-Area CLSM	1.9E-06	1.9E-06	1.0	4.0E-06	33.0	1.78	2.67	0.1724	0.2900	2.0007E-03	1.7000	10
4	Z-Area Vaults #1 and #4 Work Slab	5.0E-09	5.0E-09	1.0	1.0E-07	13.6	2.22	2.57	0	0.1190	2.8940E-06	1.6660	10
5	Z-Area Vault #1 Wall and Floor Concrete	2.0E-09	2.0E-09	1.0	5.0E-08	18.1	2.21	2.70	0	0.0820	2.0856E-06	1.9433	10
6	Z-Area Vault #1 Roof Concrete	5.0E-09	5.0E-09	1.9	1.0E-07	14.5	2.20	2.57	0	0.1190	2.8940E-06	1.6660	10
7	Z-Area Vault #4 Wall and Floor Concrete	1.0E-10	1.0E-10	1.0	5.0E-08	18.1	2.21	2.70	0	0.0820	2.0856E-06	1.9433	10
8	Z-Area Vault #4 Roof Concrete	5.0E-09	5.0E-09	1.0	1.0E-07	13.6	2.21	2.56	0	0.1190	2.8940E-06	1.6660	10
9	Z-Area Vault #2 and Future Vault Concrete	1.0E-10	1.0E-10	1.0	5.0E-08	18.4	2.11	2.59	0	0.0820	2.0856E-06	1.9433	10
10	Z-Area Saltstone	1.0E-11	1.0E-11	1.0	5.0E-09	42.3	1.26	2.18	0	0	3.2930E-07	1.6500	10
11	Z-Area Clean Cap	1.0E-11	1.0E-11	1.0	5.0E-09	42.3	1.26	2.18	0	0	3.2930E-07	1.6500	10
12	FTF Spec Fill Grout	3.60E-08	3.60E-08	1.0	8.0E-07	26.6	1.81	2.51	0.2142	0	1.1895E-02	1.2173	11
13	Fully Degraded FTF Spec Fill Grout	3.60E-06	3.60E-06	1.0	5.6E-06	26.6	1.81	2.51	0.2142	0	1.1895E-02	1.2173	11
14	FTF Aged Concrete	3.50E-08	3.50E-08	1.0	8.0E-07	16.8	2.06	2.51	0.2142	0	1.1895E-02	1.2173	11
15	Fully Degraded FTF Aged Concrete	3.50E-06	3.50E-06	1.0	5.6E-06	16.8	2.06	2.51	0.2142	0	1.1895E-02	1.2173	11

Index	SRS Vadose Zone Soil Materials	Saturated Horizontal Hydraulic Conductivity	Saturated Vertical Hydraulic Conductivity	K_h/K_v	Saturated Effective Diffusion Coefficient	Total Porosity	Dry Bulk Density	Particle Density	Water Retention Curves - Van Genuchten Parameters				Reference
	Material	Kh (cm/s)	Kv (cm/s)	-	De (cm^2/s)	%	g/cm^3	g/cm^3	θ_r	θ_s	α (cm^{-1})	n	
1	Upper Vadose Zone (Above 264 ft-msl in both E-Area and Z-Area)	6.2E-05	8.7E-06	7.1	5.3E-06	39	1.65	2.70	0.5050	0	6.0989E-03	1.3525	10
2	Lower Vadose Zone (Below 264 ft-msl in both E-Area and Z-Area)	3.3E-04	9.1E-05	3.6	5.3E-06	39	1.62	2.66	0.3665	0	1.4254E-02	1.3917	10
3	E-Area Operational Soil Cover Prior to Dynamic Compaction	1.2E-04	1.2E-04	1.0	5.3E-06	46	1.44	2.65	0.5050	0	7.8470E-03	1.3525	10
4	E-Area Operational Soil Cover after Dynamic Compaction	1.4E-05	1.4E-05	1.0	4.0E-06	27	1.92	2.65	0.5050	0	3.4821E-03	1.3525	10
5	Control Compacted Backfill	7.6E-05	4.1E-05	1.9	5.3E-06	35	1.71	2.63	0.3223	0	2.5460E-02	1.2199	10
6	IL Vault Permeable Backfill	1.4E-03	7.6E-04	1.9	8.0E-06	41	1.56	2.64	0.3905	0	1.9177E-02	2.1240	10
7	Single Vadose Zone	1.9E-04	3.0E-05	6.3	5.3E-06	39	1.63	2.67	0.4267	0	1.0291E-02	1.3772	10
8	Sand (<25% Mud)	5.0E-04	2.8E-04	1.8	8.0E-06	38	1.65	2.66	0.3100	0	1.8929E-02	1.3812	10
9	Clay-Sand (25-50% Mud)	8.3E-05	2.1E-05	4.0	5.3E-06	37	1.68	2.67	0.5110	0	6.3464E-03	1.4132	10
10	Clay (>50% Mud)	2.0E-06	9.5E-07	2.1	4.0E-06	43	1.52	2.67	0.5366	0	8.9327E-03	1.2074	10
11	Gravel	1.5E-01	1.5E-01	1.0	9.4E-06	30	1.82	2.60	0.0464	0	1.3877E-01	1.4516	10

Index	Hanford Vadose Zone Soil Materials	Saturated Horizontal Hydraulic Conductivity	Saturated Vertical Hydraulic Conductivity	K_h/K_v	Saturated Effective Diffusion Coefficient	Total Porosity	Dry Bulk Density	Particle Density	Water Retention Curves - Van Genuchten Parameters				Reference
	Material	Kh (cm/s)	Kv (cm/s)	-	De (cm^2/s)	%	g/cm^3	g/cm^3	θ_r	θ_s	α (cm^{-1})	n	
1	Backfill	5.98E-04	5.98E-04	1.0		21.0	1.94		0.030	0.262	1.90E-02	1.400	12
2	Hanford formation silty sand	8.58E-05	8.58E-05	1.0		44.8	1.61		0.072	0.445	8.00E-03	1.915	12
3	Hanford formation fine sand	3.74E-04	3.74E-04	1.0		40.6	1.60		0.032	0.379	2.70E-02	2.168	12
4	Hanford formation coarse sand	2.27E-03	2.27E-03	1.0		38.6	1.67		0.027	0.349	6.10E-02	2.031	12
5	Hanford formation gravelly sand	6.65E-04	6.65E-04	1.0		28.0	1.94		0.033	0.238	1.40E-02	2.120	12
6	Hanford formation sandy gravel	3.30E-04	3.30E-04	1.9		25.8	1.93		0.022	0.167	1.70E-02	1.725	12
7	Hanford formation gravel	1.46E-03	1.46E-03	1.0		25.9	1.97		0.020	0.102	7.00E-03	1.831	12
8	Cold Creek Unit slit	5.57E-05	5.57E-05	1.0		40.4	1.68		0.040	0.419	5.00E-03	2.249	12
9	Cold Creek Unit caliche	8.45E-04	8.45E-04	1.0		34.0	1.72		0.054	0.281	1.10E-02	1.740	12
10	Cold Creek Unit gravels	1.03E-03	1.03E-03	1.0					0.056	0.286	1.10E-02	1.750	12
11	Ringold Formation sandy gravel	4.13E-04	4.13E-04	1.0		29.3	1.84		0.026	0.177	8.00E-03	1.660	12

Figure 2-2. Hydraulic properties datasheet

	References
	SIMCO CBP Reports
1	Washington Savannah River Company, Subcontract No. AC48992N, Report Tasks 2 & 4 - "Experimental Results from Vault Concretes", SIMCO Technologies, Inc., July 10, 2009
2	Washington Savannah River Company, Subcontract No. AC48992N, Report Task 6 - "Characterization of a Saltstone mixture", SIMCO Technologies, Inc., July 10, 2009
3	Washington Savannah River Company, Subcontract No. AC48992N, Report Task 6 - "Characterization of a Wasteform Mixture", SIMCO Technologies, Inc., June 16, 2010
4	Washington Savannah River Company, Subcontract No. AC81850N, Report - "Vault Concrete Characterization", SIMCO Technologies, Inc., March, 2012
5	CPB-TR-2010-007-C3, Rev. 0 Cementitious Barriers Partnership Task 7 - "Demonstration of Stadium for the Performance Assessment of Concrete Low Activity Waste Storage Structures", E. Sampson, SIMCO Technologies, Inc. March 2010.
6	CPB-TR-2015-001, Rev. 0 Cementitious Barriers Partnership Task 12 - Experimental Study "OPC Paste Samples Exposed to Aggressive Solutions", Y. Protiere, E. Sampson, SIMCO Technologies, Inc. November 2015.
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	LeachXS/Orchestra CBP Reports
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11	WSRC-STI-2007-00369, K. Dixon and M.A. Phifer, "Hydraulic and Physical Properties of Tank Grouts For FTF Closure", Washington SRC, Aiken,SC, Revsion 0, October 2007. (see Table 20 for Reducing Gout and Base Mat Surrogate properties)
	PNNL Reports
12	PNNL-18564, G.V. Last., M.L. Rockhold, C.J. Murray and K.J. Cantrell, "Selection and Traceability of Parameters to Support Hanford-Specific RESRAD Analyses", July 2009.

Water Retention Equations
$m = 1 - 1/n$
$\beta(\psi) = 1 + (\alpha * \psi)^n$
$S(\psi) = \theta_r + (1 - \theta_r) / \beta^m$
$k_r(\psi) = [1 - (1 - 1/\beta)^m]^2 * \beta^{m/2}$

Figure 2-3. References datasheet

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3.0 FLOExcel Simulation Module

This section of the report describes a module developed for simulating flow properties in degraded and fractured cementitious materials. Hydraulic properties for cementitious materials of significance at the Savannah River Site (SRS) and soils at both SRS and Hanford have been included in the CBP Toolbox materials database as described in Section 2 (see Figure 2-2). These properties were obtained directly from documents published at the two sites. To demonstrate use of the FloExcel database to calculate property data, a stand-alone GoldSim model (FloExcel.gsm) was created to read hydraulic data from the database, calculate water retention curves using the tabulated van Genuchten parameters and output results to an Excel worksheet. Initially the model was intended to simply output water retention curves showing saturation, permeability and conductivity for the pure materials. The initial model has been extended to calculate water retention curves for blended material, such as an intact cementitious material and a granular material, to represent a fractured or otherwise degraded cementitious material.

To model the performance of degraded cementitious materials, Jordan and Flach (2013) used a composite material having hydraulic properties representing a blend of intact concrete with soil or gravel following the Equivalent Continuum Model concept (e.g. Altman et al. 1996). The saturation, relative permeability, and saturated conductivity of the composite material are calculated as:

$$S(\psi) = \frac{f_s\,\varepsilon_s\,S_s(\psi) + f_c\,\varepsilon_c\,S_c(\psi)}{f_s\,\varepsilon_s + f_c\,\varepsilon_c} \tag{1}$$

$$k_r(\psi) = \frac{f_s\,K_s\,k_{rs}(\psi) + f_c\,K_c\,k_{rc}(\psi)}{f_s\,K_s + f_c K_c} \tag{2a}$$

$$K = f_s\,K_s\ + f_c\,K_c \tag{2b}$$

Where:

f .... fraction of material in blend (-)
ε .... porosity (-)
K .... saturated hydraulic conductivity (cm/s)
k_r .... relative permeability (-)
S .... saturation (-)
ψ .... suction head (cm)

with subscripts denoting

s .... soil or gravel
c .... cementitious material.

This blending calculation has been included as part of the hydraulic property determination in the FLOExcel GoldSim module. Figure 3-1 shows the GoldSim dashboard developed as a user interface to access and blend hydraulic properties. On the left hand side of the screen, the user selects a cementitious material and a granular material (soil or, as in this case, gravel) from the materials available in the database (see Figure 2-4 in the previous section for a list of available materials and their hydraulic properties). The user then specifies the fraction of soil/gravel to be included in a composite material. Specifying a fraction of zero will produce the hydraulic properties for the (intact) cementitious material while specifying a soil/gravel fraction of 1.0 will produce the properties of the soil or gravel.

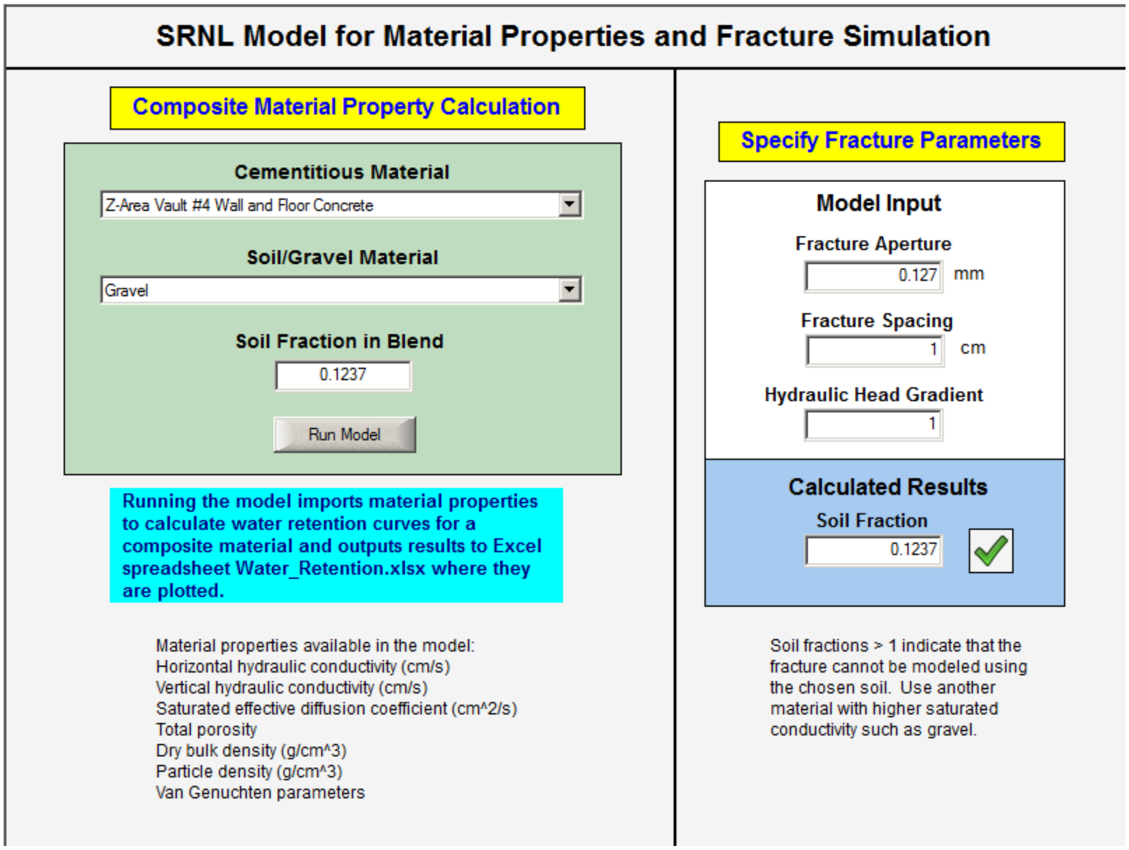


Figure 3-1. Dashboard user interface for hydraulic property calculation.

As an example application of this feature, Figure 3-2 shows hydraulic conductivity for various blends of SRS Vault 4 concrete with gravel. At low suction, blending even small amounts of gravel with the concrete to represent concrete degradation or fracturing has a significant effect on the hydraulic conductivity giving increased values. At high suction, the blends all tend to behave as concrete.

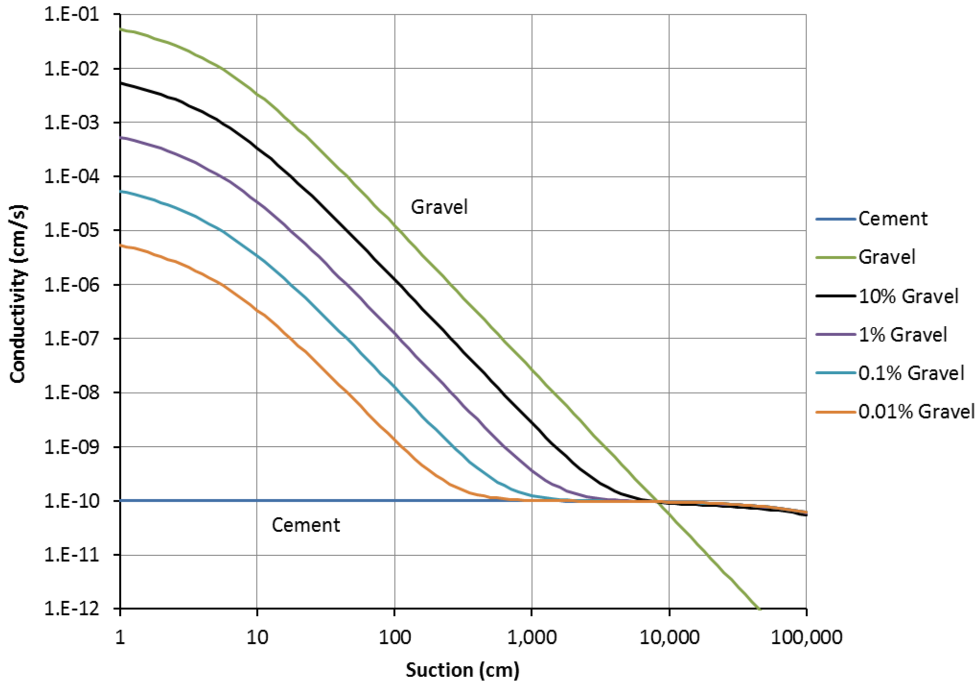


Figure 3-2. Hydraulic conductivity as a function of suction for blends of Vault 4 concrete with gravel.

3.1 Simulation of Fractured Materials

As an alternative approach to simulate the properties of specific fractures, the controls on the right hand side of the dashboard shown in Figure 3-1 allow the user to simulate a fractured concrete by specifying the fracture aperture in mm and spacing between fractures in cm. The model will then determine the fraction the soil material selected that must be blended with the selected concrete to simulate this fractured material. Calculation of the blending fraction is determined as described below.

An equivalent saturated hydraulic conductivity for the fracture is first calculated using the equation:

$$K_f = \frac{\rho\, g\, b^2}{12\, \eta} \tag{3}$$

Where:

ρ.......................liquid density (kg/m^3)
g ....gravitational acceleration (m/s^2)
b ....fracture aperture (m)
η.......................liquid viscosity (kg/m-s).

The effective saturated conductivity of the fractured porous matrix is then calculated as:

$$K_{eff} = \frac{b\, K_f + BK_m}{b + B} \approx \frac{b}{b + B} K_f \tag{4}$$

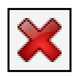
Where:

b ....fracture aperture (m)
B......................thickness of intact cementitious material (m)
K_m ....saturated hydraulic conductivity of cementitious material (m)

The approximation shown in Eq. (4) is useful for estimating the expected behavior and verifying trial calculations; however, the rigorous expression is used in the FLOExcel calculator. Using the result in Eq. (4), the model calculates the fraction of soil material needed to produce the required effective saturated conductivity for the two materials selected on the left hand side of the dashboard from the equation:

$$f_s = \frac{K_{eff} - K_c}{K_s - K_c} \tag{5}$$

A soil fraction greater than one means that the materials selected cannot be blended to produce the desired fracture properties. In this case, to alert the user than infeasible parameters have been specified, the check box display below the calculated soil fraction changes to the symbol:



If the suction head ψ and hydraulic gradient $|dh/dz|$ are known, the Darcy velocity (U, volumetric water flux) through the damaged material can be computed from the equation:

$$U = K k_r(\psi) \left|\frac{dh}{dz}\right| \tag{6}$$

The hydraulic gradient tends to asymptotically approach 1.0 in the subsurface moving upward from the water table, thus a value of 1.0 is a reasonable approximation for the vadose zone if the gradient is not precisely known. As shown in Figure 3-1, the properties dashboard allows the user to specify a hydraulic gradient. For demonstration purposes, the calculated Darcy velocity is output to an Excel spreadsheet. The method outlined in this section can be used within the CBP Toolbox to define a fractured material and calculate flow through the material. Figure 3-3 shows the hydraulic conductivity for the material blend that simulates the fracture properties specified in Figure 3-1. Figure 3-4 shows the Darcy velocity calculated for this material as a function of suction.

As an example application, the model described above could be used to support the LXO Percolation with Radial Diffusion model included in CBP Toolbox Version 2 (Brown et al., 2013). This model requires specification of the infiltration rate. The infiltration flow is the rate of water percolation in the axial direction through the material cracks whereas only radial solute diffusion occurs in the intact matrix (Sakar et al., 2013). In experimental applications the infiltration rate is typically controlled and known from measurement. In field applications, the infiltration rate is typically not measured. However, hydraulic gradient ($|dh/dz|$) and matric tension (ψ) are typically known or can be estimated from field measurements or system-level modeling. Based on the fracture spacing and matric tension, the saturated hydraulic conductivity and relative permeability of the percolation material can calculated from Eqs. (2a) and (2b). The volumetric infiltration flux (Darcy velocity) can then be computed from hydraulic head gradient using Eq. (6).

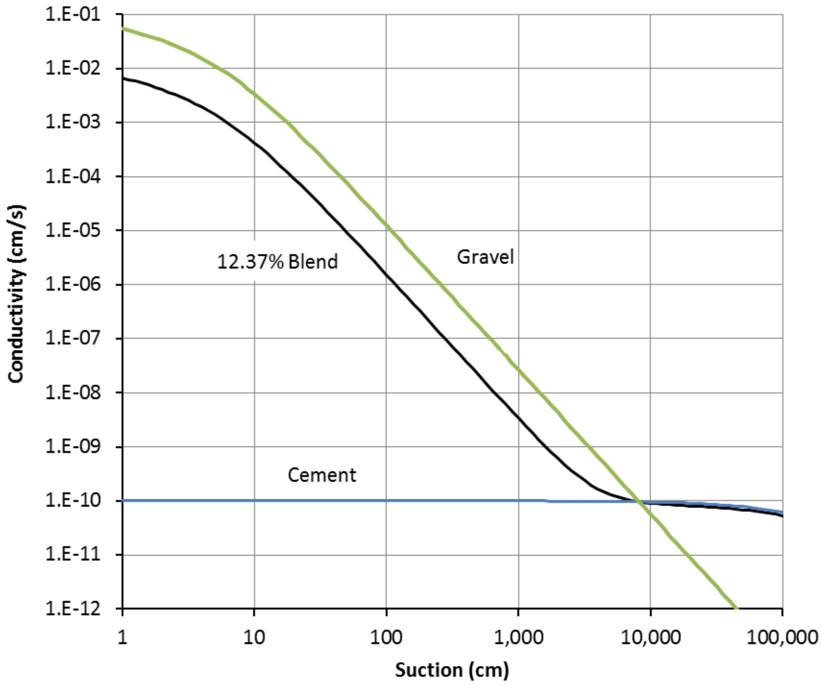


Figure 3-3. Hydraulic conductivity as a function of suction for Vault 4 concrete blended with gravel to simulate the fracture properties shown in Figure 3-1.

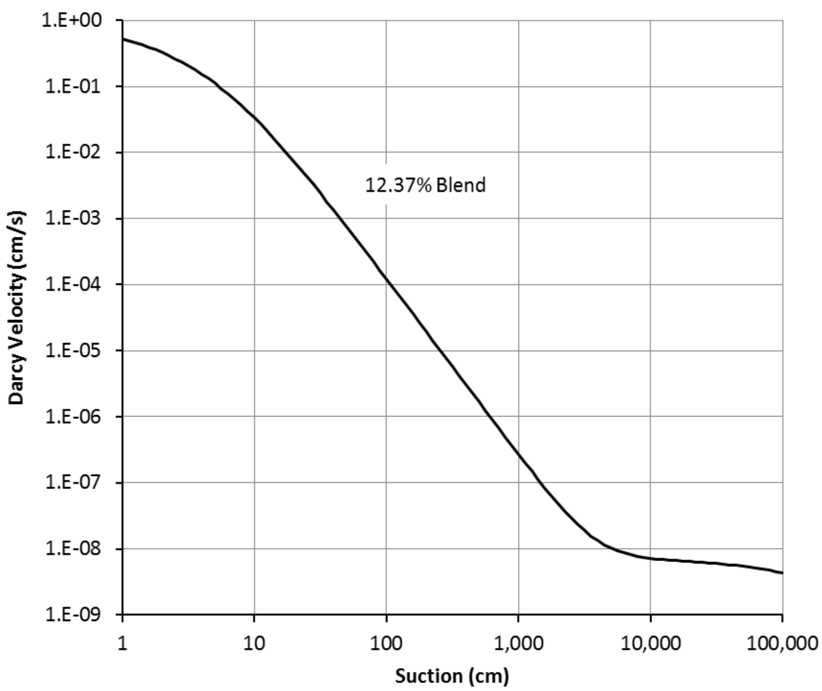


Figure 3-4. Darcy velocity as a function of suction for Vault 4 concrete blended with gravel to simulate the fracture properties shown in Figure 3-1.

4.0 Conclusions

The development work described in this report can be summarized as the following suggested changes to the CBP Toolbox:

1) Development of a uniform database to capture CBP data for cementitious materials including their hydraulic properties.

2) Development of a Software and GoldSim User Interface to calculate hydraulic flow properties of degraded and fractured cementitious materials and estimate Darcy velocity from matric tension and hydraulic gradient.

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