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Introducing PFLOTRAN's New Geothermal Fracture Model for Simulation of Geothermal Systems

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ABSTRACT

In this paper, a new PFLOTRAN process model which simulates variable density, multiphase fluid flow and reactive transport with energy through an equivalent continuum porous media (ECPM) representation of a discrete fracture network, is introduced. PFLOTRAN is a well-established, parallelized subsurface simulator that has been used previously to study problems in subsurface flow and transport, including CO_2 sequestration, geothermal processes, radioactive waste repositories, and other hydrogeological systems. Because it is open-source software, with active developer and user communities, PFLOTRAN is an ideal platform in which to develop advanced simulation capabilities for modeling enhanced geothermal systems, while ensuring broad benefits to future researchers interested in using or expanding on the current development work. Moreover, its reactive transport and geochemistry capabilities are unmatched by any other community-based, research-class simulator, and thus PFLOTRAN provides a wealth of modeling capabilities for treating the complex geochemistry inherent in geothermal systems.

The new PFLOTRAN "Geothermal Fracture Model", developed at Sandia National Laboratories, allows users to define an ECPM representation of discrete fracture networks, directly in the PFLOTRAN input file, consisting of any combination of individually defined fractures with specified fracture parameters (i.e., deterministic) or fracture families defined by sampling from statistical distributions of key fracture parameters (i.e., stochastic). Key fracture parameters include: (1) the fracture spatial orientation, in terms of the fracture center location and fracture plane normal vector, (2) fracture spatial extent, in terms of the maximum lengths along all 3 dimensions, and (3) fracture aperture size. Once an initial ECPM representation of the discrete fracture network is defined, fracture permeability can evolve in time throughout the simulation as a result of two key processes: (1) changes in fracture aperture due to thermal expansion and/or contraction of the host rock matrix, and (2) geochemical processes such as mineral dissolution and precipitation. Changes in fracture permeability are sequentially coupled to both the flow and reactive transport process models at every time-step.

More information and documentation on PFLOTRAN is available at https://www.pflotran.org, and the software can be downloaded for free at https://bitbucket.org/pflotran/pflotran. PFLOTRAN is an open-source software which can be distributed and/or modified under the terms of the GNU Lesser General Public License (version 2.1 or later) as published by the Free Software Foundation.

1. INTRODUCTION

1.1 Equivalent Continuous Porous Media Representation of a Discrete Fracture Network

An equivalent continuous porous media (ECPM) representation of a discrete fracture network (DFN) is a modeling approach that simplifies the complex geometry and flow dynamics of fractures into a continuum framework. This representation allows for the integration of the effects of fractures on fluid flow, transport, and energy processes within a porous continuum by averaging the properties of the fractured system. By employing effective medium theories, the ECPM captures the influence of fracture density, orientation, and connectivity on the overall hydraulic conductivity (or intrinsic permeability) and porosity of the continuous medium. This approach facilitates the simulation of subsurface flow in fractured environments, enabling more efficient numerical modeling while retaining essential characteristics of the DFN. Ultimately, it provides a practical means to analyze and predict fluid behavior in complex geological formations relevant to most geothermal systems.

Moreover, an ECPM representation of a DFN enables the simulation of heat transfer by integrating the thermal properties of both the matrix and fluids within fractures into a unified continuum model. This approach allows for the application of continuum heat transfer equations, which can efficiently capture the effects of conduction, convection, and thermal dispersion across the entire domain, allowing for the calculation of the exchange of heat between the matrix rock and the fluid within fractures. In contrast, pure DFN simulations cannot accurately model heat transfer between the host matrix and the fluids due to the absence of the matrix rock in the formulation of the governing equations (typically, only fluid pressures within the fracture network are solved for). Although the ECPM representation of a DFN simplifies the representation of a fractured subsurface environment, the advantage that is gained allows simulation of heat transfer processes, facilitating the analysis of thermal behavior in fractured systems. Consequently, this method enhances the ability to predict temperature distributions and thermal responses in subsurface environments, which is critical for applications such as enhanced geothermal systems.

1.2 Thermal Short Circuiting Due to Matrix Rock Thermal Expansion/Contraction

Thermal expansion or contraction of a host rock matrix in an enhanced geothermal system (EGS) can lead to thermal short circuiting by altering the flow paths of the circulating fluid. As the temperature of the rock matrix changes, it expands if it is heated or contracts if it is cooled, potentially creating new fractures or altering existing ones through changes in the fracture apertures. These processes can enhance fluid flow in certain regions (due to matrix rock contraction and subsequent fracture aperture expansion) while restricting it in others (due to matrix rock expansion and subsequent fracture aperture contraction). Eventually, these processes can lead to uneven distributions of fracture permeability and can result in preferential flow pathways with further consequences on heat transfer, leading to "thermal short circuiting" and inefficient heat extraction. Consequently, the effectiveness of the geothermal system is compromised, as the heat exchange between the fluid and the rock matrix deteriorates. Understanding these dynamics is crucial for optimizing EGS design and operation to ensure effective heat recovery and resource sustainability. For a more in depth understanding of thermal short circuiting, we refer the reader to previous work in this field by Fu *et al.* (2013), and Sonnenthal *et al.* (2015).

1.3 The PFLOTRAN Simulator

PFLOTRAN, which is short for Parallel FLOw and TRANsport, is a highly versatile, open-source simulation code designed for modeling subsurface flow and transport processes in porous media, with a particular emphasis on multiphase and multicomponent systems (Lichtner, Hammond, et al.). It employs a finite volume method to solve the governing equations of fluid flow, heat transfer, and solute transport, accommodating complex geological formations and varying boundary conditions. PFLOTRAN is capable of simulating a wide range of applications, including groundwater flow, contaminant transport, and geothermal systems, while also incorporating reactive transport processes that account for chemical interactions between fluids and geological materials. The code supports parallel computing, enabling efficient simulations of large-scale problems, and features a modular architecture that allows users to customize and extend its capabilities for specific research needs. Additionally, PFLOTRAN's integration with advanced pre- and post-processing tools facilitates the visualization and analysis of simulation results, making it a powerful resource for researchers in the field of subsurface hydrology and geoscience.

Because it is open-source software, with active developer and user communities, PFLOTRAN is an ideal platform in which to develop advanced simulation capabilities for modeling enhanced geothermal systems, while ensuring broad benefits to future researchers interested in using or expanding on the current development work. Moreover, its reactive transport and geochemistry capabilities are unmatched by any other community-based, research-class simulator, and thus PFLOTRAN provides a wealth of modeling capabilities for treating the complex geochemistry inherent in geothermal systems. In this paper, a new PFLOTRAN process model, called the Geothermal Fracture Model, is introduced. It simulates variable density, multiphase fluid flow and reactive transport with energy through an ECPM representation of a DFN and includes the effects of matrix rock thermal expansion/contraction for the study of thermal short circuiting.

2. DESCRIPTION OF THE GEOTHERMAL FRACTURE MODEL IN PFLOTRAN

2.1 General Process Model Architecture

The Geothermal Fracture Model, or GFM going forward, is a process model written within a module of the PFLOTRAN code base. If used, it is sequentially coupled with a PFLOTRAN flow process model and a reactive transport process model, as the last process model in the coupled list. The GFM has several functions, outside of the flow and transport process models, but which influence flow and transport in the domain. It is primarily responsible for: (1) the interface which allows a user to define sets of deterministic and/or stochastic fractures in the input deck, (2) the automatic translation of the user-defined sets of fractures into an ECPM representation, in terms of the overall intrinsic permeability and porosity fields in the domain, (3) the calculation of the thermal expansion/contraction of the surrounding host rock after each flow and transport step based on the updated temperature field, (4) the calculation of the resulting change in fracture aperture and the modification to the permeability of the ECPM domain within grid cells that contain at least one fracture at the end of each time step, and lastly, (5) the additional modification to the permeability within grid cells that contain at least one fracture where mineral precipitation or dissolution also occurs.

2.2 Defining Sets of Deterministic Fractures or Stochastic Fracture Families

The PFLOTRAN GFM allows users to define fracture networks, directly in the PFLOTRAN input file, consisting of any combination of individually defined fractures with specified fracture parameters (i.e., deterministic) or fracture families defined by sampling from statistical distributions of key fracture parameters (i.e., stochastic). Key fracture parameters include: (1) the fracture spatial orientation, in terms of the fracture center location given as a coordinate point (x,y,z) and fracture plane normal vector, (2) fracture spatial extent, in terms of the maximum lengths along all 3 dimensions, and (3) initial fracture aperture size. The fractures generated take a rectangular shape.

Any number of deterministic or stochastic fractures can be defined. Deterministic fractures are defined individually, while stochastic fractures are defined in family sets. For stochastic fracture family sets, the total number of fractures within a fracture family must be specified in addition to the statistical distribution desired and the relevant statistical distribution parameters (such as the mean and standard deviation) of each key parameter. In the current version of the PFLOTRAN GFM, a Normal Gaussian distribution is assumed for simplicity, although any other distribution can be added. Furthermore, the specified statistical distribution may be truncated to ensure physically realistic values. For example, the distributions for fracture spatial extents and fracture hydraulic aperture values are truncated so that they are positive. Additionally, for each stochastic fracture family, a seed can be specified which kicks off the distribution sampling algorithm. Because the sampling algorithm is based on a random number generator, specifying a seed ensures repeatability between simulations (as opposed to selecting a seed based on the computer's clock as is typically implemented), guaranteeing the same random sequence of numbers are generated.

2.3 Automatic Translation of Discrete Fractures into the ECPM Representation

An ECPM domain within PFLOTRAN consists of grid cells, which can be structured or unstructured, and inside a defined boundary. Within each grid cell, the material is treated as a continuum, with material properties consistent with a porous media. Therefore, for each grid cell there exists a porosity and permeability value, in addition to other relevant material properties such as the thermal conductivity, specific heat, bulk density, anisotropy, etc. Within each grid cell, the material is considered fractured or unfractured, based on whether or not a fracture (as defined by the user) happens to pass through the grid cell. For grid cells which contain one or more fractures, the initial porosity and permeability are modified as a function of the fracture orientation and/or the fracture aperture. For unfractured grid cells, the porosity and permeability remain unaltered.

For grid cells which contain a fracture, the initial porosity is modified according to,

$$\emptyset^f = \emptyset + \boldsymbol{\alpha/\mathcal{L}} \qquad \textbf{Equation 1}$$

where $\emptyset$ and $\emptyset^f$ are the unfractured and fractured porosity in units of void volume per grid cell volume (unitless), α is the initial fracture hydraulic aperture in units of meters, and $\mathcal{L}$ is the characteristic grid cell length in units of meters. The characteristic grid cell length is calculated as the cube root of the grid cell volume,

$$\boldsymbol{\mathcal{L} = \sqrt[3]{\mathcal{V}}} \qquad \textbf{Equation 2}$$

where $\mathcal{V}$ is the grid cell volume. This is valid for grid cells which are not overly distorted and contain LxWxD dimensions that are roughly equal. Therefore, the user is encouraged to create grids with cells as close to cubes as possible. For grid cells which contain more than one fracture, the user can additionally specify whether the sum of or maximum of $\alpha/\mathcal{L}$ is used. No further changes are made to the porosity of the domain beyond the initial modification to the porosity, even though it is possible for the hydraulic aperture to evolve during the course of a simulation. This is a known limitation of the current model and improvements will be forthcoming.

For grid cells which contain a fracture, the initial permeability field, K_0^d, is also modified. PFLOTRAN accounts for permeability in all three dimensions, and the permeability is described as a three-dimensional tensor. Only the diagonal components of the permeability tensor are considered, however, in the calculation of flow in the reservoir or domain. First, the fracture permeability, in the orientation of the fracture plane that was defined by the fracture normal vector by the user, is calculated according to a function of the fracture hydraulic aperture and grid cell characteristic length, as,

$$\boldsymbol{K_{xx}^f = K_{yy}^f = \frac{1}{12}\frac{\alpha^3}{\mathcal{L}}\,; \quad K_{zz}^f = 0} \qquad \textbf{Equation 3}$$

where K_{xx}^f and K_{yy}^f are parallel to the fracture plane and K_{zz}^f is perpendicular to the fracture plane. Note that fracture permeability is always zero perpendicular to the fracture plane, and all off-diagonal components of K^f are also zero.

Next, the fracture permeability K^f is rotated to the orientation of the computational domain. This is accomplished with the definition of a rotation matrix, $\mathbb{M}$, which applies a rotation by an angle θ about an axis $\boldsymbol{u} = (u_x, u_y, u_z)$ where its unit vector is $u_x^2 + u_y^2 + u_z^2 = 1$. In this case, the axis $\boldsymbol{u}$ is a vector parallel to the fracture plane, and the angle θ is the angle between the fracture plane and the domain. The rotation matrix is defined by (Palazzolo 1976),

$$\mathbb{M} = \begin{bmatrix} \boldsymbol{u_x^2(1-cos\theta)+cos\theta} & \boldsymbol{u_xu_y(1-cos\theta)-u_zsin\theta} & \boldsymbol{u_xu_z(1-cos\theta)+u_ysin\theta} \\ \boldsymbol{u_xu_y(1-cos\theta)+u_zsin\theta} & \boldsymbol{u_y^2(1-cos\theta)+cos\theta} & \boldsymbol{u_yu_z(1-cos\theta)-u_xsin\theta} \\ \boldsymbol{u_xu_z(1-cos\theta)-u_ysin\theta} & \boldsymbol{u_yu_z(1-cos\theta)+u_xsin\theta} & \boldsymbol{u_z^2(1-cos\theta)+cos\theta} \end{bmatrix}. \qquad \textbf{Equation 4}$$

Finally, the domain permeability, K^d, is calculated according to,

$$\boldsymbol{K^d = \mathbb{M}K^f\mathbb{M}^{-1} + K_0^d} \qquad \textbf{Equation 5}$$

where K_0^d is the initial domain permeability. For grid cells which contain more than one fracture, the user can additionally specify whether the sum of or maximum of $\mathbb{M}K^f\mathbb{M}^{-1}$ is used.

2.4 Calculation of Matrix Rock Thermal Expansion/Contraction

As the temperature of the matrix rock evolves, it will expand or contract relative to its original volume. The thermal expansion coefficient, δ, measures how much a material expands or contracts in response to a change in temperature and has units of $^oC^{-1}$. Specifically, it quantifies the fractional change in size (length, area, or volume) of a material per degree change in temperature. The change in length of the matrix rock, ΔL, within a grid cell given a change in temperature of the grid cell, ΔT, is calculated according to,

$$\boldsymbol{\Delta L = \mathcal{L}\delta\Delta T} \qquad \textbf{Equation 6}$$

where $\mathcal{L}$ is the characteristic grid cell length as previously defined in **Equation 2.** From this change in length, a change in fracture aperture can be calculated at the end of the time step. Currently, the PFLOTRAN GFM is limited in the sense that it only considers the characteristic

grid cell length of the grid cell in which the fracture occupies when calculating the change in length of the rock matrix. In reality, the distance over which to consider matrix rock temperature change is likely much longer, potentially several grid cells perpendicular to the fracture plane. Assuming that the injection of cold fluid into the reservoir flowing within the fractures is the source of the temperature change in the matrix rock, the majority of the temperature change will occur in the grid cell in which the fracture occupies, with diminishing temperature change expected in the adjacent grid cells in the direction perpendicular to the fracture. A temporary work around to this limitation in the model is to assign a slightly larger value for the thermal expansion coefficient, δ, than is realistic for the matrix rock being simulated. Improvements to the model are forthcoming.

2.5 Calculation of the Fracture Aperture and Permeability Field

Once the change in length of the matrix rock is calculated for each grid cell that contains a fracture, the change in fracture aperture is calculated according to,

$$\boldsymbol{\alpha^{t+1} = \alpha^{t} - \Delta L} \qquad \textbf{Equation 7}$$

where the superscript indicates the time step. Note the length change is subtracted from the current aperture to calculate the aperture for the next time step, since an expansion of the rock matrix results in a decrease in fracture aperture, and a contraction of the rock matrix results in an increase in fracture aperture. The new fracture permeability is then calculated according to **Equation 3**, and the new domain permeability is updated according to **Equation 5**.

An additional limitation of the PFLOTRAN GFM when calculating the matrix rock thermal expansion or contraction and the resulting fracture aperture change is that no consideration of the background *in situ* stress field is possible. Unlike other models, such as that presented in Fu *et al.* (2013) or Sonnenthal *et al.* (2015), the PFLOTRAN GFM is not coupled to a geomechanical model which can solve for stress in the rock matrix. Therefore, for scenarios where a geothermal reservoir is placed within a host rock that is stressed in addition to the overburden stress (in shear for example), the fracture aperture change may be influenced by the background stress in addition to thermal changes in the reservoir. In these scenarios, we note the PFLOTRAN GFM will not be as accurate as a model which also solves geomechanical constitutive equations as part of the fracture aperture calculations.

2.6 Modification to the Permeability Field Due to Geochemistry

If the user optionally includes geochemistry in the simulation within the transport process model, there may be additional changes to the permeability due to mineral dissolution and/or precipitation. These changes are preserved and considered additive to the changes in permeability due to fracture aperture changes from matrix rock thermal expansion or contraction. For example, injection of cold mineral-rich fluids will result in thermal contraction of the surround rock matrix, increasing fracture aperture and increasing permeability. At the same time, if mineral precipitation occurs out of the mineral-rich fluid, the change in mineral porosity of the fracture will decrease, resulting in decreasing permeability. In this purely hypothetical example, it is possible that the increase in permeability from fracture aperture expansion and decrease in permeability due to mineral porosity reduction may cancel each other out.

Changes in the permeability from geochemistry follow PFLOTRAN's standard approach in the Reactive Transport Process Model. Documentation for PFLOTRAN's Reactive Transport Process Model can be found online at the following site: https://documentation.pflotran.org/theory_guide/mode_reactive_transport.html.

2. DEMONSTRATION OF THE GEOTHERMAL FRACTURE MODEL IN PFLOTRAN

In this section, the new capabilities of the PFLOTRAN GFM are demonstrated. Further examples of the GFM in use can be seen in the companion paper submitted by Gatz-Miller, et al. (2025).

2.1 Automatic Creation of an ECPM Representation of a DFN

The following example provides a demonstration of the automatic process for creating an ECPM representation of a DFN for a 2-D domain with dimensions of 100m by 100m. In this example, five fractures were specified in the input deck (as specified in **Table 1**). All fractures were assigned the same fracture aperture, and because the grid consists of regular cuboid grid cells of identical dimensions (1m by 1m in x and z), the fracture permeability along the fracture plane (as assigned in **Equation 3**) is identical for all five fractures. Only the fracture orientation differs between fractures, therefore when the fracture is rotated into the orientation of the domain, the domain permeability and porosity are modified in the grid cells which contain a fracture. The background matrix rock was assigned an isotropic permeability value of 1.0e-13 m^2 in this example.

In **Figure 1** and **Figure 2**, the domain permeability is shown in the x-, y-, and z-directions. The only difference between the two figures is how the permeability is treated at the fracture intersections. In **Figure 1**, the maximum fracture permeability of all intersecting fractures is applied at fracture intersections, whereas in **Figure 2**, the sum of all intersecting fractures is applied at fracture intersections. Because this is a 2-D problem, there is no difference in the y-direction permeability because the fractures are oriented perpendicular to the page. However, permeability differences can be seen in the x- and z-directions. The more vertical a fracture is, the larger the z-direction permeability is and the lower the x-direction permeability is. Likewise, the more horizontal a fracture is, the larger the x-direction permeability is and the lower the z-direction permeability is. For fractures which are roughly tilted at 45 degrees, the x- and z-direction permeability will be roughly equal.

Table 1. List of five fractures and their properties for the example that provides a demonstration of the automatic process for creating an ECPM representation of a DFN.

FRACTURE #	FRACTURE CENTER (X,Z)	FRACTURE NORMAL VECTOR	FRACTURE APERTURE
1	(40, -25) m	1.1x + 0.9z	7.0e-3 m
2	(45, -50) m	0.8x + 1.0z	7.0e-3 m
3	(65, -45) m	-0.8x + 1.1z	7.0e-3 m
4	(45, -45) m	-0.8x + 0.1z	7.0e-3 m
5	(45, -45) m	-0.2x + 1.0z	7.0e-3 m

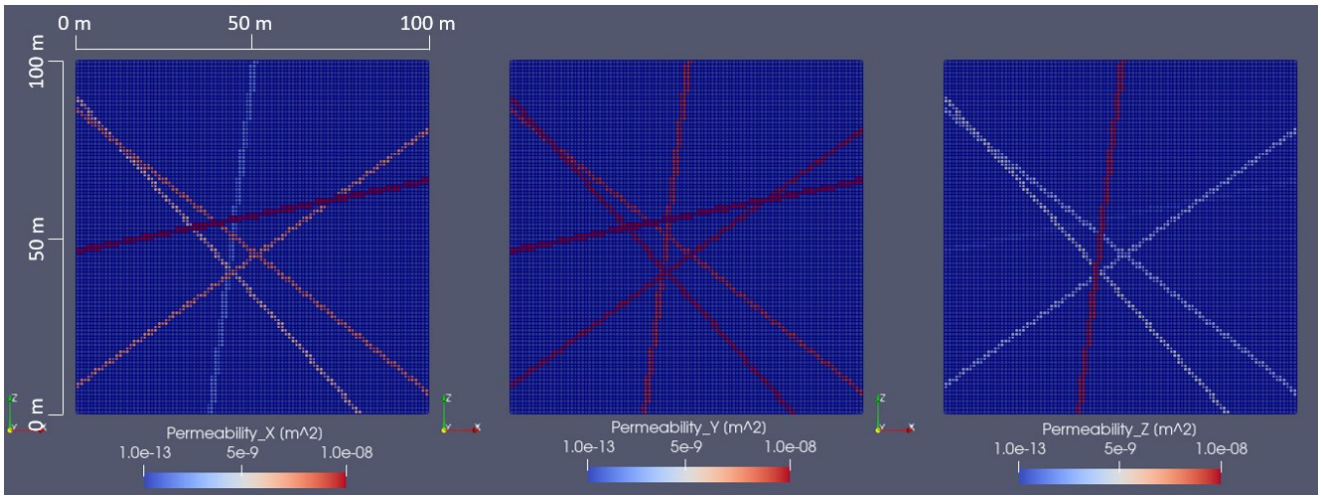

Figure 1. Domain permeability in the x, y, and z directions, showing five fractures. At fracture intersections, the maximum fracture permeability is applied.

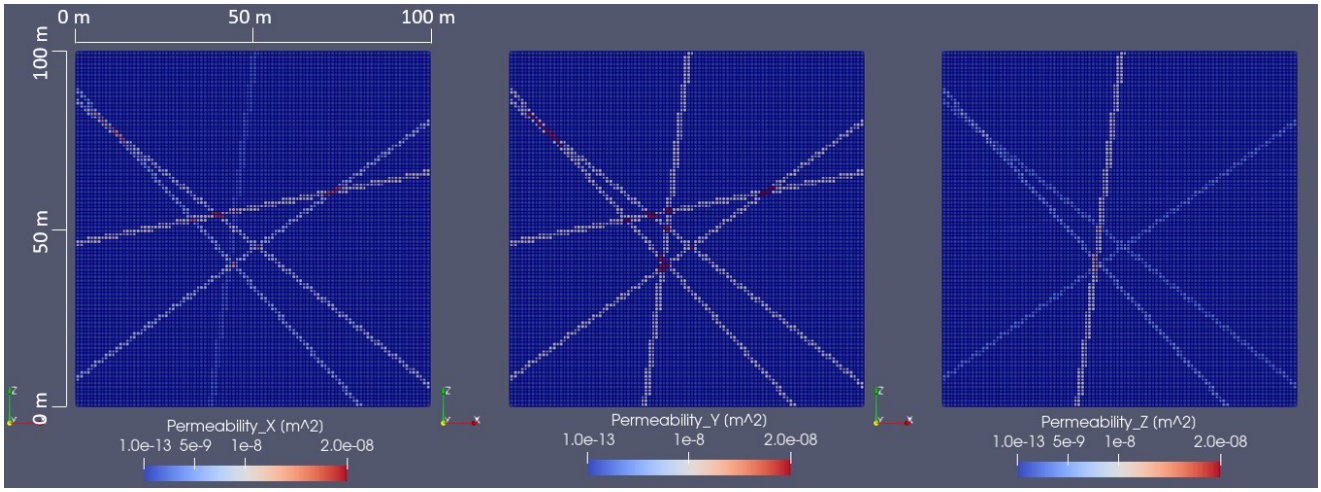

Figure 2. Domain permeability in the x, y, and z directions, showing five fractures. At fracture intersections, the sum of the fracture permeability is applied.

2.2 Change in Permeability in Fractures Due to Rock Matrix Cooling

The second example demonstrates the PFLOTRAN GFM's ability to simulate thermal short circuiting. In this example, a network of fractures is placed in the same 2-D domain with dimensions of 100m by 100m. All sides of the domain have no flow boundary conditions except for the top boundary, which is set to a hydrostatic pressure gradient allowing flow in or out of this boundary. The initial temperature of the domain is 80 ºC with pressure set to hydrostatic. The background matrix rock was assigned an isotropic permeability value of 1.0e-18 m^2. All fractures were assigned a hydraulic aperture identical to the previous example, i.e. 7.0e-3 m.

One fracture within the small network is dominantly vertical, and cold fluid at a temperature of 10 ºC is injected into the dominantly vertical fracture at the bottom of the domain at a rate of 0.01 kg/sec. The cold fluid is forced upwards and into the fracture network, thereby cooling the surrounding rock matrix. As the rock matrix cools, the fracture permeability increases due to thermal contraction of the rock matrix and expansion of the fracture aperture. The evolution of the temperature and permeability field within the domain are shown in **Figure 3**, **Figure 4**, and **Figure 5**.

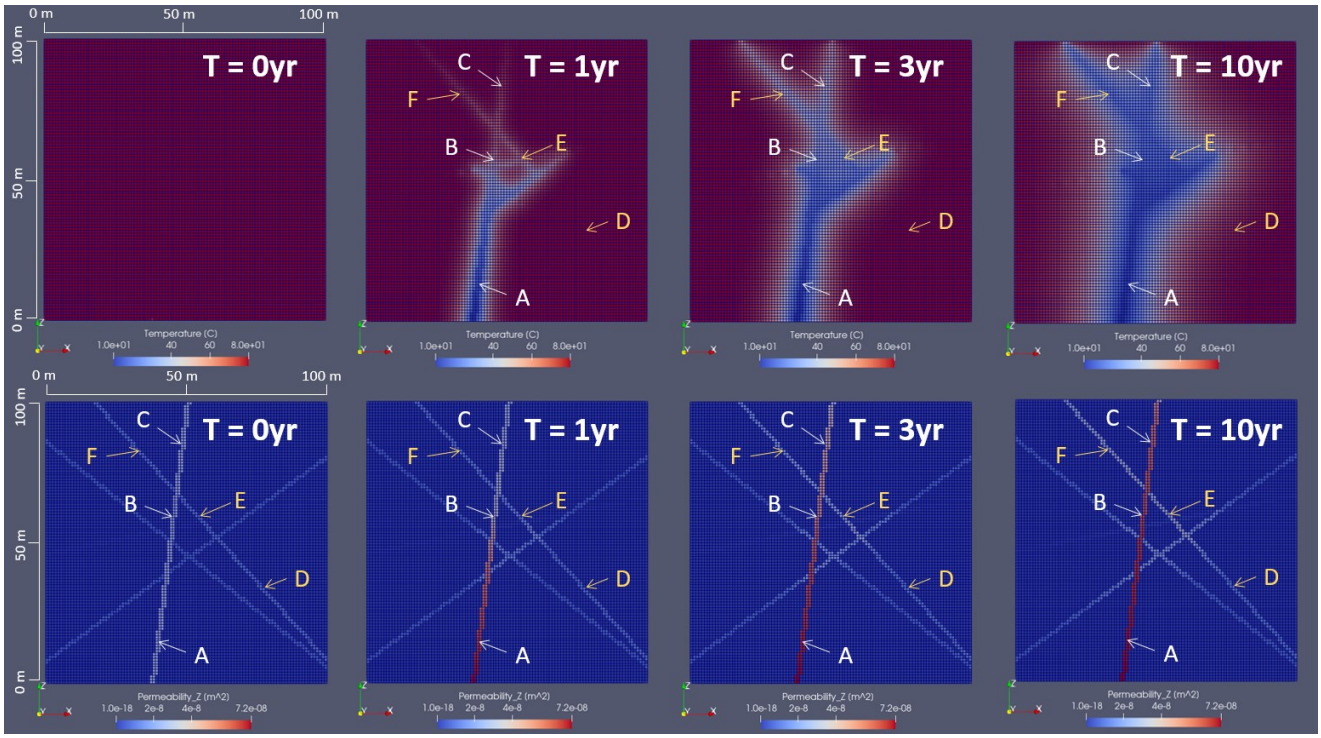

Figure 3. Evolution of the temperature (top row) and domain permeability in the z-direction (bottom row) over time, from t = 0yr to t = 10yr. Cold fluid at 10 ºC is injected from the bottom of the domain into the most vertical fracture. As fluid moves up and into the fracture network, the rock matrix cools over time, which causes thermal contraction and an increase in the fracture permeability. Letters A, B, C, D, E, and F correspond to locations along two fractures for plots in Figure 4 and Figure 5.

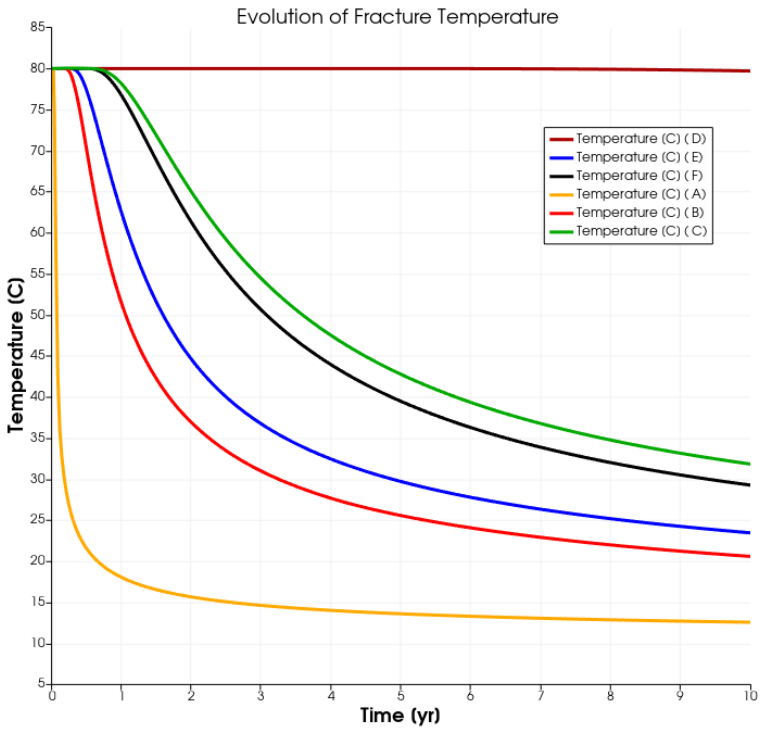

Figure 4. Evolution of the temperature at 6 points in the domain (labeled A, B, C, D, E, and F; locations of these points are originally shown in Figure 3). Temperature cools most quickly in the location nearest the fluid injection location (point A), and negligible cooling occurs at point D, which is along a dead end of a fracture where fluid does not flow.

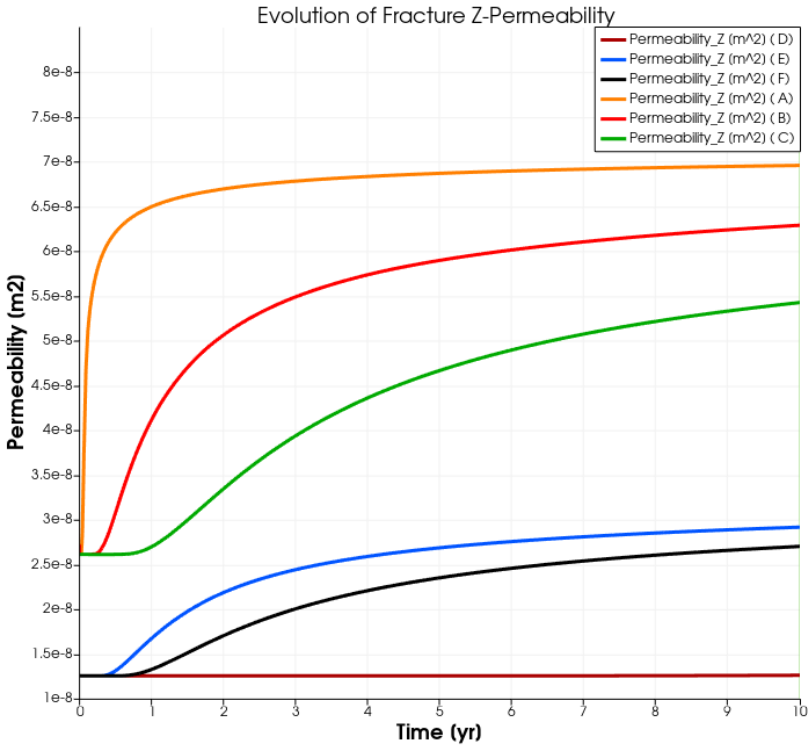

Figure 5. Evolution of the z-direction permeability at 6 points in the domain (labeled A, B, C, D, E, and F; locations of these points are originally shown in Figure 3). The largest increase in permeability occurs where temperature cools most rapidly (point A). Negligible change from initial permeability occurs at point D, which is along a dead end of a fracture.

3. CONCLUSIONS

In this paper, a new PFLOTRAN process model which simulates variable density, multiphase fluid flow and reactive transport with energy through an equivalent continuum porous media representation of a discrete fracture network, is introduced. The new PFLOTRAN "Geothermal Fracture Model", developed at Sandia National Laboratories, allows users to define an equivalent continuum porous media representation of discrete fracture networks, directly in the PFLOTRAN input file, consisting of any combination of individually defined fractures with specified fracture parameters (i.e., deterministic) or fracture families defined by sampling from statistical distributions of key fracture parameters (i.e., stochastic). Key fracture parameters include: (1) the fracture spatial orientation, in terms of the fracture center location and fracture plane normal vector, (2) fracture spatial extent, in terms of the maximum lengths along all 3 dimensions, and (3) fracture aperture size. Once an initial equivalent continuum porous media representation of the discrete fracture network is defined, fracture permeability can evolve in time throughout the simulation as a result of two key processes: (1) changes in fracture aperture due to thermal expansion and/or contraction of the host rock matrix, and (2) geochemical processes such as mineral dissolution and precipitation. Changes in fracture permeability are sequentially coupled to both the flow and reactive transport process models at every time-step.

More information and documentation on PFLOTRAN is available at https://www.pflotran.org, and the software can be downloaded for free at https://bitbucket.org/pflotran/pflotran. PFLOTRAN is an open-source software which can be distributed and/or modified under the terms of the GNU Lesser General Public License (version 2.1 or later) as published by the Free Software Foundation.

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