

COUPLED MULTIFLUX-TOUGH2-TOUGHREACT T-H-M-C MODEL FOR EGS STUDIES

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ABSTRACT

We have developed a coupled numerical model for simulating flows of coolant mass, as well as transport of heat and chemical species, in Enhanced Geothermal System (EGS) reservoirs with discrete fractures. A Computational Fluid Dynamics (CFD) submodel in MULTIFLUX solves for laminar or turbulent flows in any planar-, penny-, or lens-shaped fracture. The CFD submodel includes advective, convective, and diffusive transport of heat and mass in a multicomponent mixture within a fracture. Discrete fractures may form a network of planar fractures and connecting conduits. The fracture aperture of each planar configuration is variable with space and time, due to (a) thermal dilatation of the strata, (b) elastic deformation by hydraulic pressure in the fracture system, and (c) geochemical precipitation and dissolution.

The new concept is used in the formulation of a mechanical model for aperture variation in a self-propped fracture with hydrodynamic pressure and temperature. The CFD submodel is coupled to the submodel for the host geothermal formation, a porous, fractured, and jointed rock mass. Multiphase, multicomponent heat and fluid flow simulations are provided by TOUGH2 and/or TOUGHREACT in the geologic submodel. Coupling of the overlain fracture network system in the CFD model-element to the host geothermal formation involves the Numerical Transport Code Functionalization (NTCF) technique, a modeling accelerator of the iterations in MULTIFLUX.

Our new model can be used to interpret short-term injectivity test results and help in evaluating fracture aperture and planar extension. An industrial application example (and validation) of the model is provided for the Desert Peak EGS site in Nevada, operated by ORMAT. The model is also applicable to long-term thermal drawdown simulations and life-cycle studies.

INTRODUCTION

Advanced numerical models currently applied to thermal-hydrologic-chemical (T-H-C) component transport in a geologic formation assume a porous matrix for the media with equivalent-continuum porosity and permeability, overlain with equivalent-continuum fractures in the geologic media. Such models include TOUGH (Pruess et al., 1999), NUFT (Nitao, 2000), and UDEC (Itasca, 2009). Blackwell and McKenna used TOUGH to demonstrate transient and steady-state heat flow fields for a typical basin over hundreds of thousands of years (McKenna and Blackwell, 2003). However, their model used only a single fault with a rather coarse discretization and with a 10^{-14} m² permeability, contrasted with 10^{-20} m² in the bedrock. TOUGHREACT (Xu, et al., 2004) with reactive chemistry was utilized (Xu and Pruess, 2001) to model 3-D multiphase fluid flow and reaction of hot brine injection wells. Individual fractures and/or faults represent a challenge for porous-media models. A set of discrete fractures is used by researchers at National Energy Technology Laboratory (NETL) (Brohmal, et. al, 2011) for modeling the flow field in a natural geothermal system at the Brady's Hot Springs site, operated by ORMAT Technologies in Nevada, USA. This model, however, deals only with flows and does not have T-H-M-C capabilities.

What has not been seen in the literature is a numerical model for flow, heat, and mass transport for a single fracture or a system of single fractures, fully coupled to the rock mass with its porous and finely distributed continuum fractures. To serve the needs and overcome the difficulties listed in the foregoing, we have developed a new, fully-coupled T-H-M-C model, using a discrete fracture or fractures with autonomous, planar flow and aperture variation characteristics, as well as connections to the surrounding rock mass.

TIME-DEPENDENT MODEL-ELEMENTS FOR T-H-M-C PROCESSES

Time-Dependent Coolant Loss or Gain

Coolant fluid in the fracture may be lost or gained. The coolant mass flux from or to the rock mass is by Darcy flow (Bird and Stewart, 1960; Welty et al., 1984; Danko, 2011). The coolant fluid mass-flux density, q_{mF} , in $[kg/(m^2s)]$ units may be written as an advective flux component across a unit wall surface area of the fracture opening:

$$q_{mF} = k/v \text{ grad}(P)|_w \quad (1)$$

In Eq. (1), k in $[m^2]$ and v in $[m^2/s]$ are the rock-mass permeability and coolant-fluid kinematic viscosity, respectively. The $\text{grad}(P)$ term denotes the gradient (which, in a one-dimensional case, is a simple differential with respect to distance from the wall) of the flow pressure in the rock-mass pores and fractures within close proximity of the fracture wall.

Applying the NTCF model solution to Eq. (1), the time-dependent coolant-fluid flux density, q_{mF} , may be expressed in a matrix-vector equation, as follows (Danko, 2011):

$$[q_{mF}] = [q_{mF}^c] + [[M_P]] [P - P^c] \quad (2)$$

In Eq. (2), the bracketed variables are vectors composed of the sampled values of the variables taken at pre-selected time instants. Vectors $[q_{mF}^c]$, and $[P^c]$ are “central” values around which the linearized model in Eq. (2) is valid and defined during model identification. Matrix $[[M_P]]$ is a dynamic admittance operator of constant coefficients that are identified by the NTCF procedure.

Time-Dependent Rockmass Heat Flux

The total heat flux density, $[q_h]$ from the rock mass at the fracture wall boundary is the sum of the conduction and advection components. The following boundary equation can be written (Bird and Stewart, 1960; Welty et al., 1984; Danko, 2011):

$$q_h = \rho c_p a \text{ grad}(T)|_w + q_{hc}|_w \quad (3)$$

In Eq. (3), ρ in $[kg/(m^3)]$, c_p in $[J/(kg K)]$, a in $[m^2/s]$, and T in $[K]$ are density, specific heat, and thermal diffusivity, respectively. The last term,

$q_{hc}|_w$, in $[W/m^2]$ is the advective component of heat-flux density due to convective, Darcy-flow transport of all mass fluxes entering the fracture space from the rock mass. The time-dependent temperature gradient, $\text{grad}(T)$, and the pressure-driven, advective Darcy flux components are expressed with analytical matrix-vector equations using a mathematical-numerical technique called Numerical Transport Code Functionalization (NTCF) (Danko 2006). The corresponding NTCF model to Eq. (1) is as follows (Danko, 2011):

$$[q_h] = [q_h^c] + [[H_T]] [T - T^c] + [[H_P]] [P - P^c] \quad (4)$$

In Eq. (4), the bracketed variables are vectors composed of the sampled values for the temperature, T , and pressure, P , variables taken at pre-selected time instants. Time-dependency of q_h in Eq. (4) is in its vector form as a list of n values taken at n increasing time instants over a time interval. Vectors $[q_h^c]$, $[T^c]$, and $[P^c]$, also n -vectors, are “central” values around which the linearized model in Eq. (4) is defined during model setup. Matrices $[[H_T]]$ and $[[H_P]]$, all $n \times n$ in size, are dynamic admittance operators of constant coefficients that are identified by the NTCF procedure. This procedure employs system identification of the heat-transport process from the rock mass using a numerical transport model (i.e., a code such as TOUGH; Pruess, et al., 1999) with a set of pre-determined test boundary conditions as input histories with time.

Eq. (4) may be viewed as the algebraic, general representation of the differential model given in Eq. (3). The gradients, as driving forces of the diffusive and advective flux components, are replaced with finite differences, varying directly with time through the time-series of sampled boundary values given by vectors $[T]$ and $[P]$. The obvious advantage of using Eq. (4) is that the boundary values $[T]$ and $[P]$ can be calculated or modeled from the ventilation air temperature and pressure, and can even be measured for verification. In contrast, the $\text{grad}(T)|_w$ and $q_{hc}|_w$ are unknown and difficult-to-capture variables, dependent on time and the boundary conditions of T and P on the bounding wall.

In Eq.(4), the dynamic admittance matrices $[[H_T]]$, and $[[H_P]]$ may be determined

against model identification runs, using the thermal-hydrologic model of the rock mass, e.g., applying a TOUGH2 model (Pruess, et al., 1999). The advantage of using a rock-mass heat-transport model in the form of Eq. (4) is its accuracy in true time-dependent tasks, as well as its computational efficiency in iterative calculations.

Time-Dependent Chemical Species Flux

Chemical species may escape from the rock mass and flow into the coolant fluid in the fracture. Mass transport may occur by diffusion and advection. The rock mass is formed of porous and fractured geologic deposits and gives off its stored aqueous species by diffusion and advection. Additionally, dissolution or deposition may occur at the surface layer of the fracture wall. According to the basic governing laws introduced by Fick and Darcy (Danko, 2011; Danko, 2006; Pruess et al., 1999), the mass flux density, q_m , in $[kg/(m^2s)]$ units, may be written as the sum of the diffusive and advective flux components across a unit wall surface area of the fracture opening, and added to the source or sink term, q_{mS} :

$$q_{mC} = \rho D_m \text{grad}(c)|_w + c q_{mF} + q_{mS} \quad (5)$$

In Eq. (5), ρ in $[kg/(m^3)]$, D_m in $[m^2/s]$, c in $[kg/kg]$, and q_{mF} are the mixture density, species diffusion coefficient, concentration, and coolant-fluid loss or gain to or from the rock mass, respectively. The $\text{grad}(c)$ term denotes the gradient (which, in a one-dimensional case, is a simple differential with respect to distance from the wall) of the concentration of aqueous species in the rock-mass pores and fractures in close proximity to the fracture wall.

Applying the NTCF model solution to Eq. (5), the time-dependent species flux density, q_m , may be expressed in a matrix-vector equation as follows (Danko, 2006):

$$[q_{mC}] = [q_{mC}^c] + [[M_c]] [c - c^c] + [(c - c^c) q_{mF}] + [q_{mS}] \quad (6)$$

In Eq. (6), the bracketed variables are vectors composed of the sampled values for the variables taken at pre-selected time instants. Vectors $[q_{mC}^c]$, and $[c^c]$, are “central” values around which the linearized model in Eq. (6) is valid and defined during model identification. Matrix $[[M_c]]$ is a

dynamic admittance operator of constant coefficients that are identified by the NTCF procedure. The source or sink term, $[q_{mS}]$, may be temperature- and concentration-dependent, requiring modeling. The estimation of $[q_{mC}]$ may require another expansion of Eq. (6), with the use of the $[[M_T]]$ admittance operator for the temperature effect:

$$[q_{mC}] = [q_{mC}^c] + [[M_c]] [c - c^c] + [(c - c^c) q_{mF}] + [[M_T]] [T - T^c] \quad (7)$$

The boundary values, $[c]$, and $[T]$ can be calculated and/or modeled from the fracture-flow model. The dynamic admittance matrices in Eq. (7) can be determined from pre-selected model runs using (for example) TOUGHREACT for a given rock mass.

A simplified treatment of the temperature-dependent source term, q_{mS} , for a single-component reactive species, such as quartz, is as follows:

$$q_{ms} = A^* M / A [1 - (Q/K)] k_{25} \exp\left[\frac{-E}{R} \left(\frac{1}{T} - \frac{1}{298.15}\right)\right] \quad (8)$$

Equation (8) is based on the reaction-rate model used in TOUGHREACT (Xu et al., 2006) with some commonly accepted simplification, most notably, the omission of pressure dependency. In Equation (8), the following notations are used:

- r reaction mass flux (also called kinetic rate, of which positive values indicate dissolution, and negative values precipitation), in $[kg/(s-m^2)]$
- A^* total available reactive specific surface area (surface area per mol amount of mineral species), in $[m^2/mol]$
- M molar weight (mass) of the mineral species, in $[kg/mol]$
- A transport model surface area (bounding surface area per mol amount of mineral species) in $[m^2/mol]$
- Q reaction quotient for the mineral-water reaction at the interface between the mineral-species layer and the solution. The unit of Q depends on the chemical species involved in the reaction. Note that in simple reactions with only one aqueous species, such as with quartz, Q equals the concentration, $Q = c$ in $[kg/kg]$

K equilibrium constant for the mineral–water reaction. It is a function of temperature, defined by Equation (10). K has the same unit as Q and also depends on the chemical species involved in the reaction.

k_{25} Reaction-rate constant (mole mass per unit mineral surface area and unit time), taken at 25°C, in [mol/(s·m²)]

E activation energy for the reaction in [J/mol]

R gas constant in [J/(mol·K)]

T absolute temperature of the surface layer in [K]

The equilibrium constant, K , is as follows for any species

$$\log(K) = C_1 + C_2 \cdot \ln(T) + C_3 \cdot T + C_4 \cdot T^{-1} + C_5 \cdot T^{-2} \quad (9)$$

where C_1, C_2, C_3, C_4 and C_5 are constants and $\log(K)$ is the 10-based logarithm of K . The A^*/A surface ratio in Equation (9) may be viewed as a “projection” of the total reactive surface of a mole amount (or 1 kg amount, for that matter) of mineral crystals to the plane of the mass-transport surface of the rock mass in the reactive transport model.

TIME-DEPENDENT MODEL-ELEMENTS FOR COOLANT FLOW, HEAT, AND CHEMICAL SPECIES TRANSPORT IN A FRACTURE

Time-Dependent Coolant-Flow Model

The *bulk* flow in the fracture is modeled as a discretized fluid network. The flow is governed by the Navier-Stokes equation (Danko, 2008). In its simplified form for flow channels along given grid lines; it reads:

$$\rho(\partial v_x / \partial t + \mathbf{v} \cdot \nabla v_x) = \rho g_x - \partial Pb / \partial x + F_x \quad (10)$$

$$\rho(\partial v_y / \partial t + \mathbf{v} \cdot \nabla v_y) = \rho g_y - \partial Pb / \partial y + F_y \quad (11)$$

$$\rho(\partial v_z / \partial t + \mathbf{v} \cdot \nabla v_z) = \rho g_z - \partial Pb / \partial z + F_z, \quad (12)$$

where v_x, v_y, v_z are velocity components of *vector* \mathbf{v} ; g_x, g_y, g_z are gravitational forces that include buoyancy in $x, y,$ and z directions, Pb is total mixture pressure and F_x, F_y, F_z are viscous and kinetic dissipation terms. Note that the $\partial v_x / \partial t, \partial v_y / \partial t,$ and $\partial v_z / \partial t$ terms in Eqs. (10)–(12), accounting for the inertia forces accelerating or

stopping coolant flow, may be insignificant and omitted in slow transients.

The viscous dissipation terms are calculated from Moody's friction-resistance coefficient, while the kinetic dissipation terms are evaluated using fitting loss coefficients at network branch connections. The network-solution equation corresponding to Eqs. (10)–(12) for the flow total pressure, Pb , as a function of the bulk branch mass flow rate, qa , is as follows (Danko, 2008):

$$iRSa \cdot Pb = qa + iRSag \cdot Pbg - iRRSa \cdot Z \cdot g + iRRSag \cdot Zg \cdot g \quad (13)$$

Time-Dependent Heat Transport in the Fracture Flow

The heat balance for fracture flow is governed by Fourier's second law, as follows (Welty et al., 1984):

$$\rho c \frac{\partial T}{\partial t} + \rho c p v_i \frac{\partial T}{\partial x} = \rho c p^a \frac{\partial^2 T}{\partial x^2} + \rho c p^a \frac{\partial^2 T}{\partial y^2} + \rho c p^a \frac{\partial^2 T}{\partial z^2} + q_h \quad (14)$$

where q_h is the heat dissipation in the dx, dy, dz gridblock due to heat exchange on the rock-mass interface as well as viscous dissipation and expansion or compression work. The differential equation may be integrated over a finite element to form an integrated-parameter CFD solution. This approach allows for reducing the number of discretization elements in the computational domain. A mass, energy, and momentum network-solution method is implemented in MULTIFLUX (Danko, 2008). The network-solution equation corresponding to Eq. (14) for the time-dependent temperature field, T , is as follows:

$$iRSh \cdot T = qh + qh_n + qL + qVD + qCE + iRShg \cdot TG + ICgh \quad (15)$$

Time-Dependent Chemical Species Transport in Fracture Flow

The species concentration model in the fracture void space may be described by Fick's second law, as follows (Welt et al., 1984):

$$\rho \frac{\partial c}{\partial t} + \rho v_i \frac{\partial c}{\partial x} = \rho D \frac{\partial^2 c}{\partial x^2} + \rho D \frac{\partial^2 c}{\partial y^2} + \rho D \frac{\partial^2 c}{\partial z^2} + q_{mC} \quad (16)$$

where ρ is density of the bulk flow mixture in the void space; x, y, z are Cartesian coordinates; t is time; $c, D,$ and q_{mC} are respectively concentration, diffusion coefficient, and mass flux source of a given species; and v_i is the bulk velocity in flow channel i in a discretized flow network model. The network solution equation corresponding to Eq. (16) for the time-dependent concentration field c is as follows:

$$iRSc^*c = qmC + qc_n + iRScg.^*c_G + ICgc \quad (17)$$

ROCK MECHANICS MODEL FOR THE ROCK MASS

A new approach is a conceptual fracture-aperture construct with tunable constants for a self-propped fracture model that can be calibrated against either (a) field measurements of injection rate and wellhead pressure, or (b) against a three-dimensional (3-D) rock-mass model, e.g., in 3DEC (Itasca, 2009). Figures 1 and 2 show the self-propped fracture model element of a pixel for an open, planar fracture. The flow channels are assumed to be among “self-propping” islands.” The concept is very different from assuming an open planar fracture with a “penny-shaped” or “lens-shaped” cavity with free-hanging walls. The detailed solution for the self-propped fracture model is described in a separate paper (Danko and Bahrami, 2012). The final solution for the aperture of each fracture pixel is as follows:

$$\delta(X) = \delta_0 + C^p [\overline{Pb}(X) - \overline{Pb}_0(X)] + C^T \Delta L [T(X) - T_0(X)] \quad (18)$$

In Eq. (18), $X=(x,y,z,t)|_{\Delta A}$ denotes any point over the planar fracture at a grid of ΔA and at any instant in the simulation time interval. The bars in Eq. (18) indicate grid-averaged values in the (x,y,z) plane at any point over a ΔA surface. Term δ_0 is a small initial aperture that remains open under hydrostatic pressure when $\overline{Pb}(X) = \overline{Pb}_0(X)$. The scale factors, called pressure and thermal aperture coefficients, C^p , and C^T , respectively, are as follows:

$$C^p = \frac{\delta_p}{E_F} \quad \text{and} \quad C^T = C^p \frac{E_R}{L} \quad (19)$$

Notations:

- δ : Hydrodynamic fracture aperture under load, pressure, flow, and thermal effects
- δ_p : Fracture aperture under hydrostatic (no-flow) pressure
- S : Static deformation of L due to in situ stress
- $\Delta L(T)$: Total, integrated thermal contraction of the rock strata, function of temperature, T
- σ : in situ stress
- p : Hydrodynamic pressure in the fracture
- E_F : Self-propped fracture layer elastic modulus
- E_R : Rock mass elastic modulus

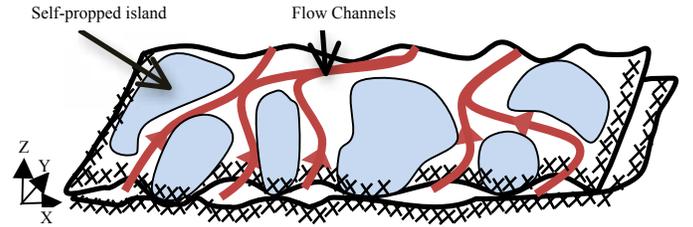


Figure 1. Self-propped fracture with flow channels and support islands.

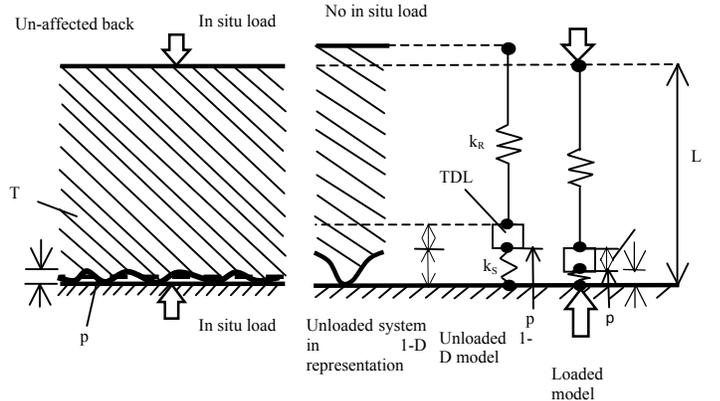


Figure 2. Thermal-hydraulic conceptualization of the fracture aperture change.

COUPLED SOLUTION FOR FLOW AND TRANSPORT PROCESSES BETWEEN THE ROCK MASS AND FRACTURE FLOW

The NTCF model elements for the rock mass and the CFD model elements for the fracture are coupled by an iterative procedure in MULTILUX (Dank, 2008). Figure 3 is a solution flowchart showing the coupling process by the Direct Iteration and Successive Approximation coupler (DISAC) module. DISAC matches temperature (T), heat flux (q_h), concentration (c), species flux (q_{mC}), and bulk flow flux (q_{mF}) on the boundary

surface node and time instance during simulation. The coupled simulation results are processed and saved by the DISAC module.

Three iteration loops are used in the Internal Balance Iteration (IBI) cycle to balance rock mass and airway transport processes, starting from the first innermost loop to the third outermost loop:

- Bulk flow calculation in the discretized fracture network system assuming an initial temperature, pressure, and concentration distribution.
- Heat-flow-balance iteration between the NTCF and airway CFD models for each time division.
- Chemical species mass-flow-balance iteration between the NTCF and fracture CFD models for each time division.

The three iteration loops are executed until no significant change is observed in the results between consecutive iterations. While the CFD model-element is solved within MULTIFLUX, the NTCF model elements are only surrogate models for the rock mass. TOUGH2 may be used as an independent solver for the heat and bulk coolant-transport processes in the rock mass. TOUGHREACT may be used as an independent solver for the chemical species transport. At high-temperature, strongly nonlinear applications, the NTCF model parameters must be refreshed during coupling iterations (Danko, 2006).

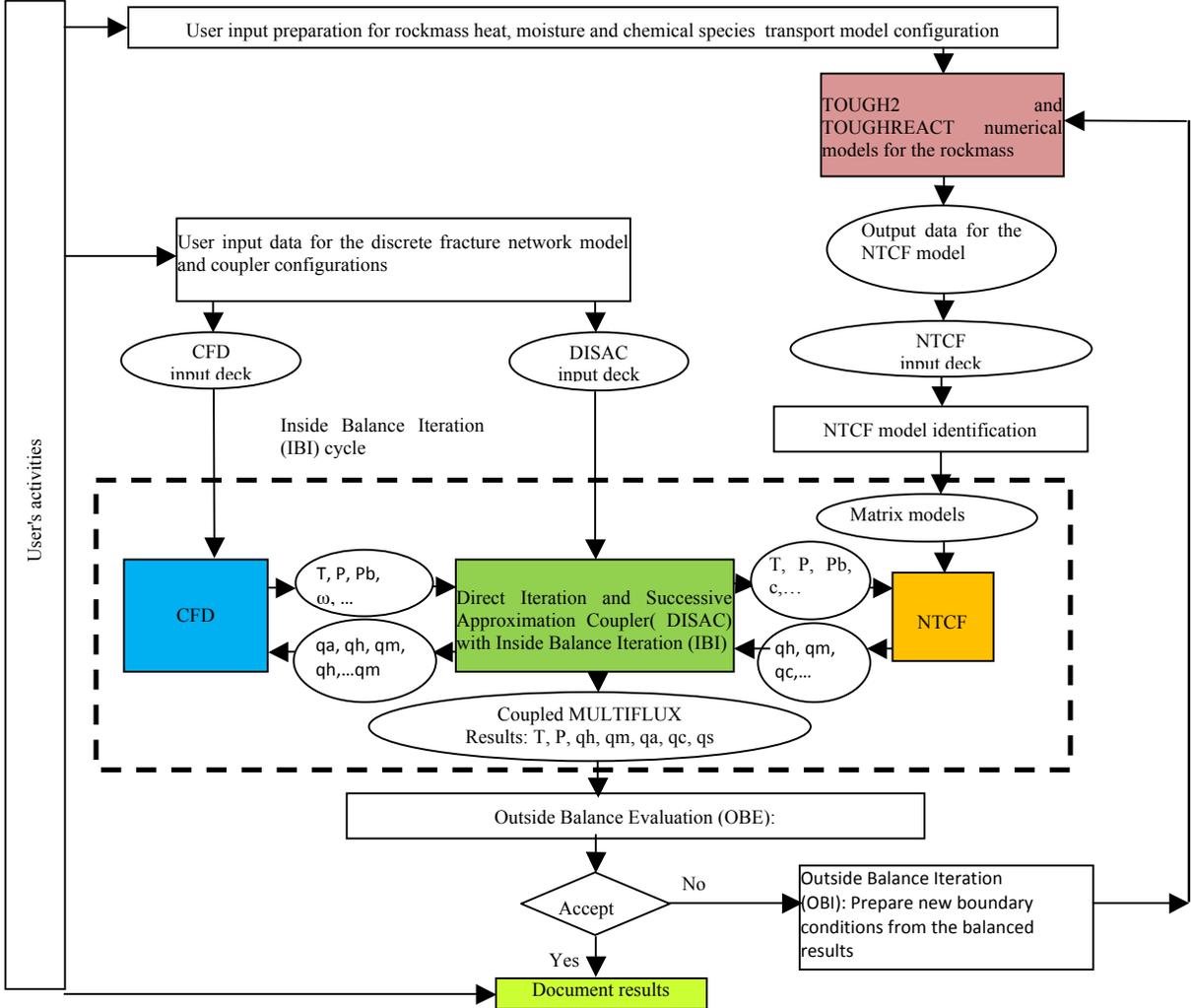


Figure 3. Solution of the coupled flow and transport processes between the rock mass and the discrete fracture.

MODEL APPLICATION EXAMPLE FOR THE DESERT PEAK EGS SITE

Here we use the MULTIFLUX model to characterize the EGS fracture at ORMAT's Desert Peak site in terms of fracture size from a single, short-time pumping test. A Rapid T-H-M process model is configured in MULTIFLUX for the explanation of the measurement results shown in Figure 4.

Application of the T-H-M model to interpret injection test results

The hypothesis of fracture-aperture variation according to Eq. (7) in a self-similar fracture over its entire spatial domain can be tested using the coupled T-H-M model in MULTIFLUX against injection pressure, flow, and thermal drawdown-measurement results.

For short-time, high-pressure-peak injections, it is necessary to use a transient model of fracture flow in the fracture plane surrounded with the porous media, filled with compressible fluid. Even if an EGS fracture were isolated with no connection to a production well or natural fracture and/or faults draw, fluid would flow into the rock mass due to elastic storativity. We modeled this flow process using TOUGH2, and results from TOUGH2 are imported via an NTCF model element. The rapid T-H-M process part of the curve is redrawn and restored by removing the interruption spike for model matching, shown in Figure 5.

The numerical model in MULTIFLUX is configured to deal with the storativity of pores and micro-fractures within the rock mass, and the storativity of the injection fluid in the EGS fracture void, due to the change in the fracture aperture and the extension of the opened fracture area. The changing size of the planar (penny or lens-shaped) EGS fracture in its extent (radius) and surface area is modeled by adjusting the fracture aperture according to Eq. (18)

Determination of the pressure coefficient, C^P , was accomplished using measured data from the short-term pumping test shown in Figure 5. The matching is achieved using 20 points along the curve, also shown in Figure 5. In the first step, the

self-propped pressure coefficient is determined as a variable for each pumping time instant, while the thermal coefficient is kept at zero ($C^T=0$) due to the short time period with negligible thermal penetration and thermal contraction. The variable C^P over time is shown in Figure 6. As depicted, the variation disappears after a few hours, and C^P becomes near-constant.

In the second step, a constant pressure coefficient value of $2.3597e-11$ for C^P is used for the entire time period of 10 hours. The wellhead pressure variation from the T-H-M model when using this constant and the self-propped fracture model is shown in Figure 7.

Figures 8 and 9 show the magnitude of the fracture-flow velocity and the hydrodynamic pressure in the EGS fracture according to the self-propped model, respectively. As depicted, the flow field does not completely occupy the available fracture extension to $R=700$ m, although this size would be available for flow in the fracture plane according to the envelope of the fracture in the model configuration.

Figures 10 and 11 show the hydrodynamic pressure and the self-adjusting fracture aperture profiles, respectively, across one cross section as a function of radius at three selected time instants.

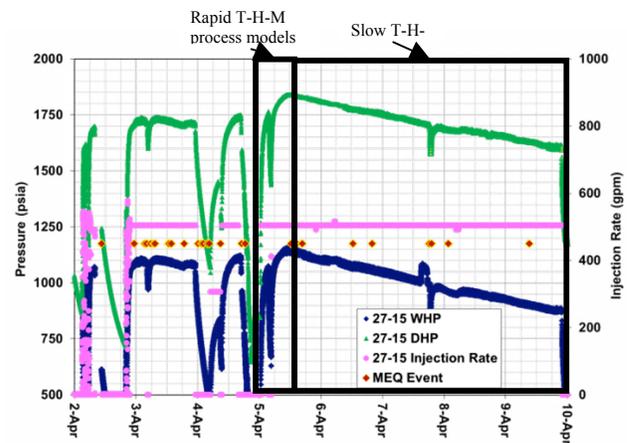


Figure 4. Short-time injection pressure and flow rate data from the pumpability tests at Desert Peak, ORMAT

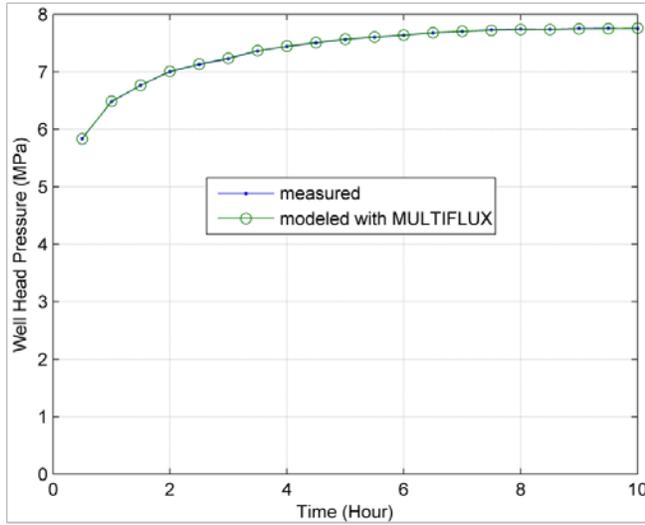


Figure 5. Comparison between measured and modeled results with variable C^P coefficient.

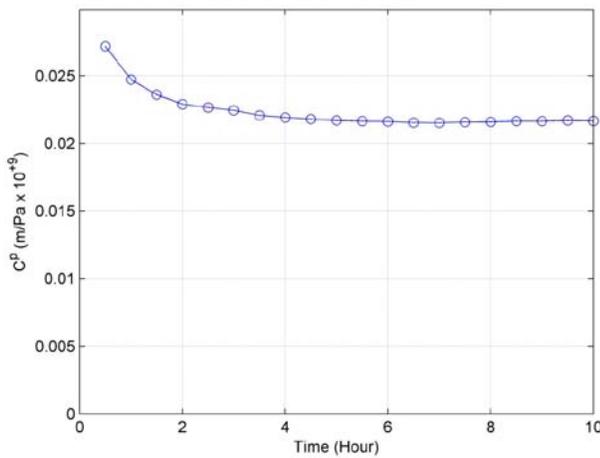


Figure 6. Variation of C^P with time for a perfect match in the wellhead pressure between model and measurement shown in Figure 5.

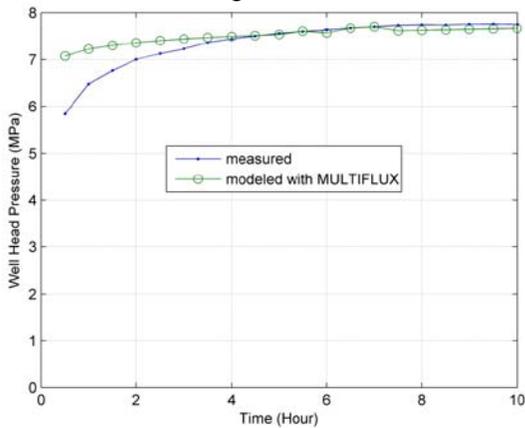


Figure 7. Wellhead pressure match between measurement and model simulation with a constant pressure coefficient of $C^P=2.3597e-11$.

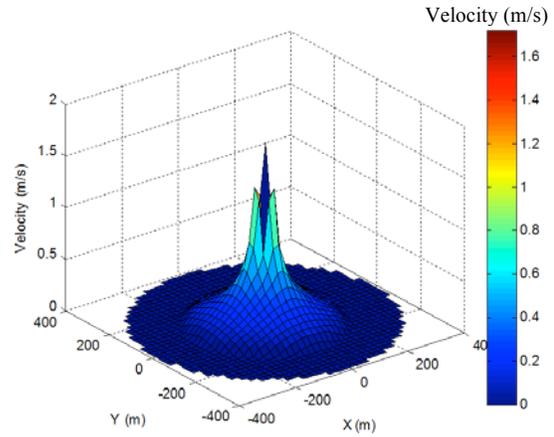


Figure 8. Distribution of the magnitude of the fracture flow velocity at time=10 hr.

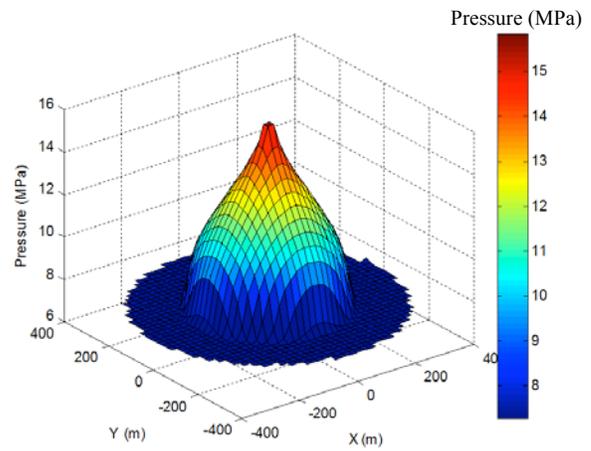


Figure 9. Distribution of the hydrodynamic pressure under flow condition at time=10 hr.

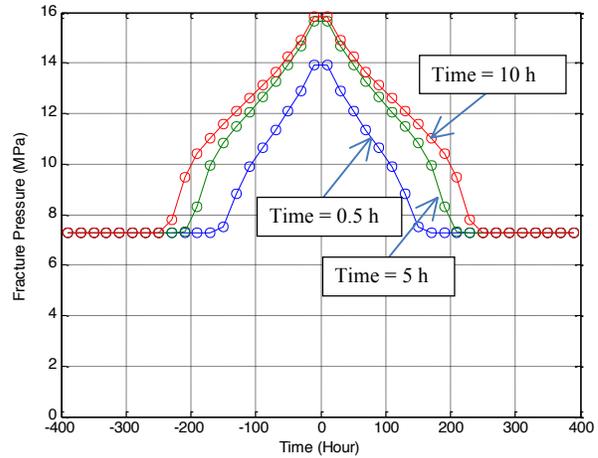


Figure 10. Hydrodynamic pressure profile at three selected time periods during the pumping test.

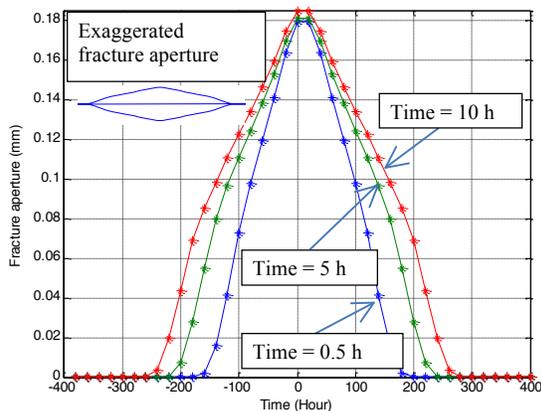


Figure 11. Fracture aperture profile at three selected time periods during the pumping test.

CONCLUSIONS

- We present a new T-H-M-C model for an EGS reservoir.
- The model describes the fracture aperture variation as it evolves under the injection pressure using a self-propped fracture model-element with self-similarity over the entire fracture envelope.
- There is no need to predetermine the extent of the fracture radius along its plane. The outer radius is self-determined by the model, governed by the force and mass balance of the system.
- The fracture-aperture model parameters, such as initial, open aperture as well as pressure and thermal coefficients in Eq. (18), can be uniquely identified from the measurement data of a single injection test.
- The MULTIFLUX model, with its new fracture-aperture model element, matches very well with published results from an EGS well at Desert Peak, operated by ORMAT.

ACKNOWLEDGEMENT

The financial support of DOE under grant number EE0002759 is appreciated. The in-kind support provided by ORMAT, the project's industrial partner, is also appreciated.

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