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GEOMECHANICAL FACIES CONCEPT AND THE APPLICATION OF HYBRID NUMERICAL AND ANALYTICAL TECHNIQUES FOR THE DESCRIPTION OF HTMC COUPLED TRANSPORT IN FRACTURED SYSTEMS

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ABSTRACT

Fractured rock provides the basic building blocks of enhanced geothermal systems (EGS). Mass and energy transport in the three dimensional fracture network is critical to the operating efficiency. Hydraulic, thermal, mechanical and chemical coupled processes under the typical geothermal environment conditions operate at different scales. Depending on whether the process is continuum dominated (e.g. transfer of stress in the rock body) or discontinuity dominated (e.g. hydraulic transport processes) different methods of numerically investigating and quantifying the system can be applied. A geomechanical facies approach provides the basis for large scale numerical analysis of the coupled processes and prediction of system response. However there is often a difficult balance between the numerical stability criteria of the different equation systems which need to be solved to describe the interaction of the dominant processes. The introduction of analytical solutions where possible, functional dependencies and multiple meshes provides an efficient method for the prediction of the effect of the *in situ* coupling.

INTRODUCTION

Quantification of mass and heat transport in fractured porous rocks is important to areas such as contaminant transport, storage and release in fractured rock aquifers, the migration and sorption of radioactive nuclides from waste depositories and the characterization of engineered heat exchangers in the context of enhanced geothermal systems. The large difference in flow and transport characteristics between fractures and the surrounding matrix rock mean models of such systems are forced to make a number of simplifications. Analytical approaches assume a homogeneous system, numerical approaches address the scale at which a process is operating, but may loose individual important processes due to averaging considerations. Numerical stability criteria limit the contrasts possible in defining material properties. Here a hybrid analytical numerical method to modeling flow, heat and mass transport in fractured media is presented using the advantages of both approaches. This approach is intimately linked to the geometry of the *in situ* deposits and their physical properties via the geomechancial facies concept. This modeling approach is illustrated for several different coupled scenarios including hydraulic, mechanical, thermal and reactive transport under geothermal conditions.

SYSTEM ANALYSIS

Addressing the response of geological deposits to the extraction, or storage of heat requires an understanding of the complex three dimensional geometry of the deposits. This geometry in reality is difficult to assess, especially as the scale of numerical and experimental investigation alters the size of the parameters measured. Upscaling is an ongoing relevant issue, e.g. [*Gräsle and Kessels*, 2003; *Lock, et al.*, 2004; *McDermott, et al.*, 2003; *Tidwell and Wilson*, 2000; *Zimmermann, et al.*, 2003].

The term rock mass was introduced to describe the large scale behavior of the fractured rock body. The rock mass includes the total *in situ* rock medium comprising the different geological units as well as the bedding planes, folds, faults, joints, shear zones and other structural features. Given the complicated and extensive variation in the elements comprising the rock mass, characterization of the rock mass in three dimensions is as expected difficult, e.g. [*Brady and Brown*, 2004]. For understanding the three dimensional rock mass system defining geothermal reservoirs it is necessary to have both a mechanical, geochemical and hydro-geological understanding of the geometrical structures present controlling the processes operating in the system.

Adding to the complexity of the system is the fact that the processes of interest, e.g. heat transport, hydraulic response, mechanical response and geochemical kinetics operate at different scales, Figure 1. Additionally [*Tsang*, 1991] identified the importance of examining the coupling of the dominant processes in geosystems. Since then there has been much work on coupling. Most recently results from the DECOVELEX project regarding coupling of THM processes and the various methods of evaluating the effects of the processes are introduced by a lead preface by [*Jing and Stephansson*, 2005] and includes contributions by [*Alonso, et al.*, 2005; *Blum, et al.*, 2005; *Cassiraga, et al.*, 2005; *Chan, et al.*, 2005; *Chan and Stanchell*, 2005; *Chijimatsu, et al.*, 2005; *Hsiung, et al.*, 2005; *Hudson, et al.*, 2005; *Millard, et al.*, 2005; *Min, et al.*, 2005; *Nguyen, et al.*, 2005; *Ohman, et al.*, 2005; *Olivella and Gens*, 2005; *Rutqvist, et al.*, 2005a; *Rutqvist, et al.*, 2005b; *Sonnenthal, et al.*, 2005; *Tsang, et al.*, 2005]. To address the understanding and predictive modeling of these systems it is necessary to have a holistic and multi-disciplinary approach.

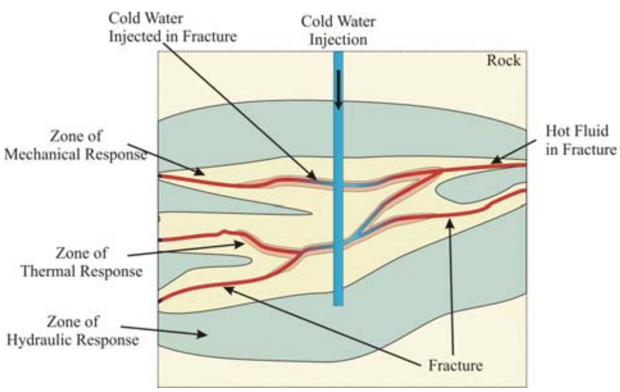

Figure 1 Different processes operate at different scales, example for hydraulic, mechanical and thermal processes.

Starting from the structure of the geological deposits, it is clear that they are not just randomly formed, but rather there is both depositional and structural process control on the *in situ* properties. This consideration has led to the concept of architectural elements within geological deposits, particularly sedimentary deposits, e.g. [*Hornung and Aigner*, 1999, 2002; *Klingbeil, et al.*, 1999; *Liu, et al.*, 2002; *Rea and Knight*, 1998; *Stephens*, 1994]. An architectural element defines a principle building block of the geological deposit being considered to which specific parameters are assigned. Adapting this for a hydrogeological and geo-mechanical situation, i.e. the coupling of hydraulic, mechanical, thermal and geochemical properties as necessary in the consideration of geothermal reservoirs, allows the definition of geomechanical facies as introduced by [*McDermott, et al.*, 2006a]. Recently the importance of the geomechanical facies approach for the comparison of the exploration and evaluation techniques of hot dry rock sites Soultz sous Forêts and Urach Spa [*Tenzer, et al.*, revision 2007].

A geomechanical facies approach allows the description of separate architectural elements of the geothermal reservoir in terms of the physical parameters of the process of interest, e.g. with definite flow, transport, chemical and mechanical characteristics. This approach provides both an up scaling concept for the parameters, an approach to experimentally quantify the reservoir material, a geometrical characterization of the reservoir and a method of numerically representing the reservoir (Figure 2). It is applicable in the predictive modeling of the coupled geosystem processes.

By defining the fundamental aspects of the responses of the geomechanical facies through modeling and where available the application of experimental data, so it becomes possible to construct small and large scale models where the responses of the various processes operating at different scales can be taken into account. The scale at which a process is operating is related to the Representative Elementary Volume, REV, [*Bear and Bachmat*, 1990] for that process, the characteristic response of the process is then included in the geomechanical facies model to provide a three dimensional scale dependent understanding of the fractured porous rock system. The response of the processes are then defined at the various scales by functional approximations where appropriate. These functions are combined over the geomechanical facies model to describe the response of the whole system. In effect it is a type of hybrid continuum approach to modeling, similar to approaches recently applied to complex flow and transport problems in porous rock, e.g. [*Helmig, et al.*, 2002].

An example of the application of the geomechanical facies approach is illustrated in Figure 3 for the division of the KTB site into the principle facies. The three dimensional combination of these facies is illustrated in Figure 4. The hydro-mechanical coupling response of these facies were included in the modeling via a geomechanical model and a functional approximation, $k = f(\sigma_n)$, illustrated in Figure 5. The effects of thermal stress on the solid properties of the system coupled with fluid properties dependent on the state variables and to some degree the salinity enabled the development of a coupled HTMC model for the Spa Urach, [*McDermott, et al.*, 2006b].

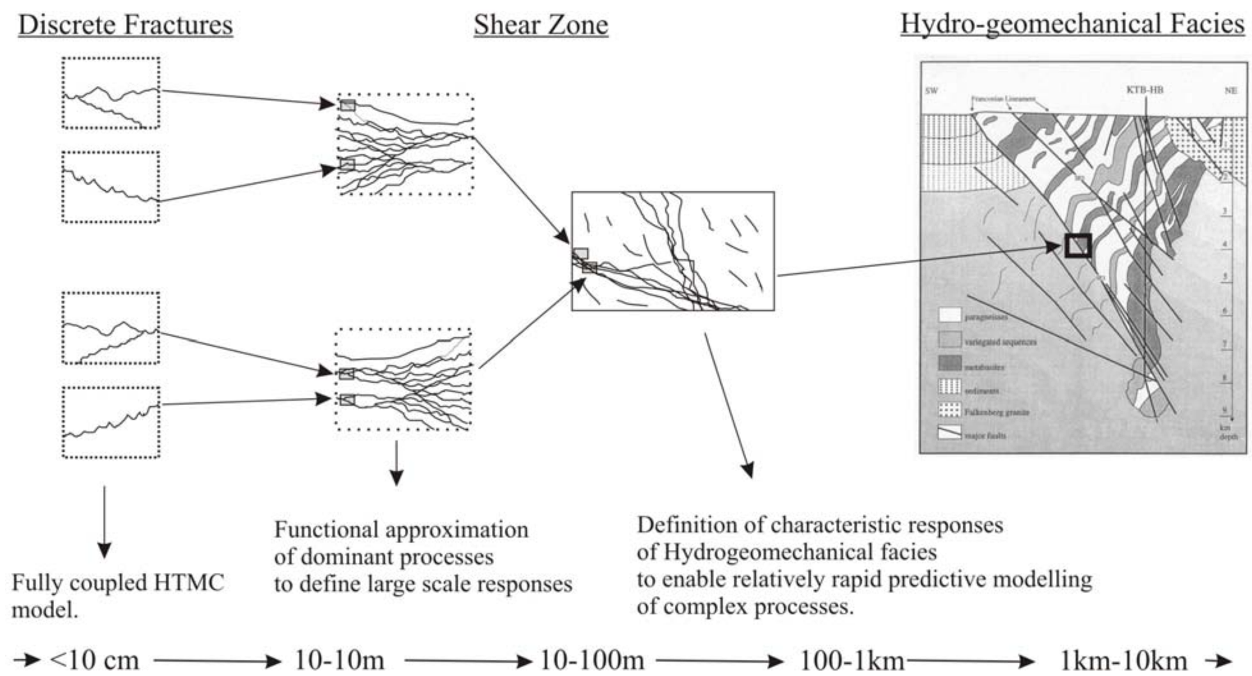

Figure 2 Geomechanical facies concept

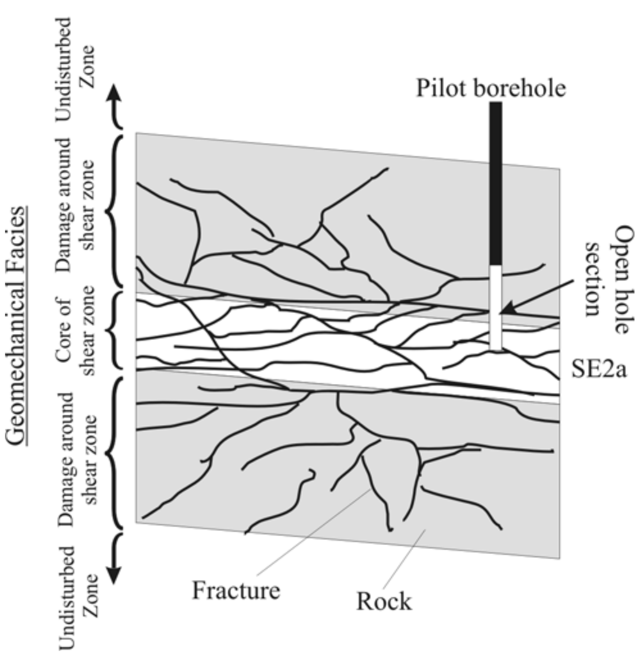

Figure 3 Example of the application of geomechanical facies, after [McDermott, et al., 2006a].

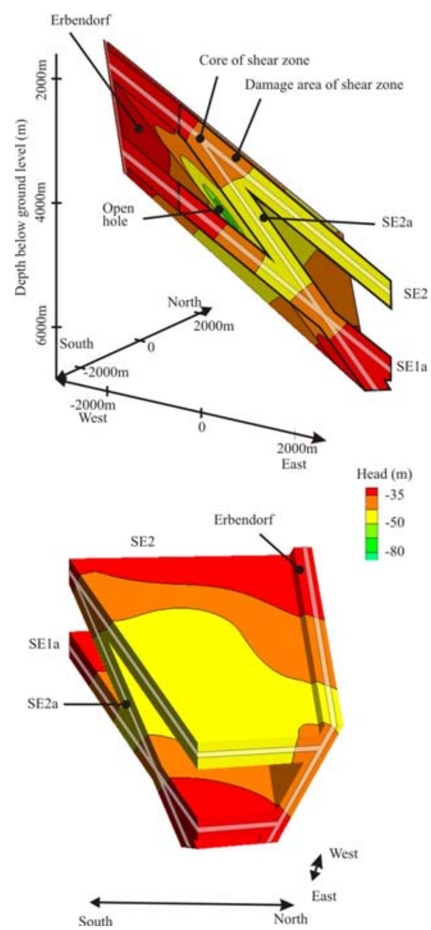

Figure 4 Three dimensional combination of the geomechanical facies at the KTB site, [McDermott, et al., 2006a].

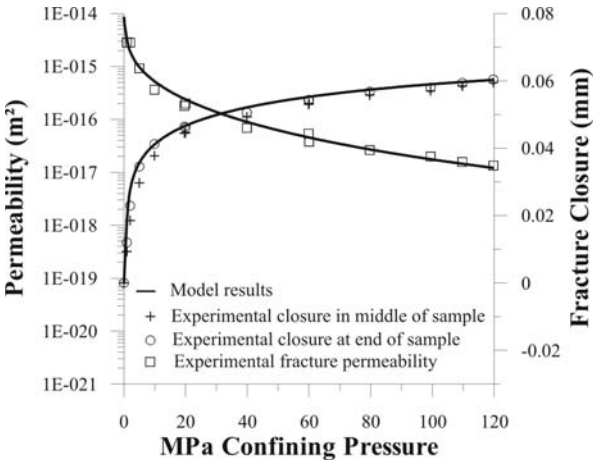

Figure 5 Functional approximation of permeability with stress.

ANALYTICAL AND NUMERICAL MODELS

Analytical models are only possible by oversimplifying the system, however such models have provided much insight into the key parameters and processes involved in defining the mass and heat transfer processes, e.g. [*Häfner, et al.*, 1992]. A key example is the work of [*Tang, et al.*, 1981] who provided a standard work on the mathematical description of the transport of a solute in a single fracture with matrix diffusion. However due to geometrical constraints, analytical models are only valid for a simplified investigation of processes, e.g. [*Carrera, et al.*, 1998].

To simulate complex *in situ* geometrical conditions of fracture networks, and the coupling of several processes, numerical techniques have to be applied. Simulating heat and mass transport in a fractured may be undertaken by several approaches, current trends are discussed in [*Neuman*, 2004]. Fracture surface heterogeneity or roughness, coupled thermal - hydro-mechanical behavior and complex 3D geometry make the meaningful solution of these systems using analytical solutions impossible.

On the other hand numerical simulations are complicated by the mathematical stability of the solution techniques, especially where large differences in material parameters are to be accounted for. Time dependent solution of advective and diffusive processes are controlled by different stability criteria, outlined for instance in [*Kolditz*, 1997]. When discretely modeling flow in fractured media, often the time step control of the diffusive processes is several orders of magnitude greater that that required for the stable solution of the advective transport, unless intricate and complex mesh refinement has been undertaken. Such mesh refinement leads to significantly increasing computational requirements, and consideration of grid adaptation algorithms, e.g. [*Haefner and Boy*, 2003]

Hybrid numerical and analytical models use the advantages of both numerical and analytical techniques to analyze flow heat and mass transport. [*McDermott, et al.*, 2007] developed such an approach to describe mass transfer in a system with material parameters varying by over 10 orders of magnitude. Here an example is given of such a hybrid model where the functional response of the matrix in a fractured system in terms of matrix diffusion for heat and storage of chemical species for reactive transport is replaced by a mathematical formulation for matrix diffusion. For simplified fracture geometries the approach is validated against the PICNIC code, [*Barten and Robinson*, 2001], illustrated for advection only, advection with matrix diffusion and advection with matrix diffusion and linear sorption in Figure 6.

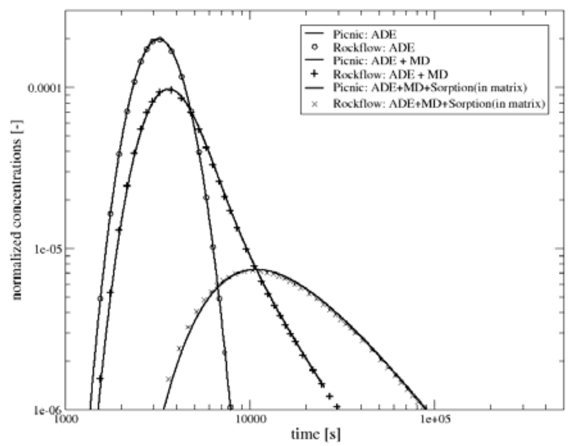

Figure 6 Validation of advection, advection and matrix diffusion, advection matrix diffusion and linear sorption.

SOLUTION OF FLOW, HEAT AND MASS TRANSPORT EQUATIONS AND COUPLING TO REACTIVE GEOCHEMISTRY.

The mass balance equation for fluid flow for a unit volume is given by (1).

$$S\frac{dh}{dt} - K\Delta h = Q \qquad (1)$$

The solution of (1) using the finite element technique is covered in standard works such as. Solving (1) [*Istok*, 1989; *Kolditz*, 2002; *Lewis and Schrefler*, 1998; *Zienkiewicz and Taylor*, 2005] provides the fluid head at each discrete node in the finite element model which then can be interpolated for the elements and converted into flow velocities v (m/s) via (4) in the elements.

$$v_{(x,y,z)} = K \,\mathrm{grad}\, h_{(x,y,z)} \qquad (2)$$

The flow velocities are then used to derive the solution of the mass transport equation (3) or heat transport equation (4) .

$$\frac{dC}{dt} = D\Delta C - \mathrm{div} vC - C_s \qquad (3)$$

$$c\rho \frac{dT}{dt} = D\Delta T - c^w \rho^w \mathrm{div} vT - T_s \qquad (4)$$

c	heat capacity medium (J/kg K)
c^w	heat capacity fluid (J/kg K)
C	concentration (kg/m³)
C_s	chemical source (kg/m³ s)
Dc	diffusion coefficient (m/s²)
Dt	thermal diffusion coefficient (J/K m s)
h	head (m)
Q	flow rate (m³/s)
K	hydraulic conductivity (m/s)
S	storage (–)
t	time (s)
T	Temperature (K)
T_s	Heatsource(J/kg K)
ρ	density medium (kg/m³)
ρ^w	density water (kg/m³)

Flow in fractured rock is characterized by advective dominated transport in the fractures and diffusive dominated transport in the matrix. To ensure the stability of the numerical solution of (3) and (4) the Courant and Neumann mesh stability criteria have to be observed [*Kolditz*, 1997]. The velocity of advective transport dominates the courant number, and the diffusion coefficient dominates the Neumann number. In fractures the advective velocity is several orders of magnitude larger than the matrix diffusion coefficients for typical contaminants. To solve such problem the mesh can be refined parallel to the diffusive flow [*Kolditz and Clauser*, 1998], this however leads to intensive computational requirements avoided by the hybrid approach.

COUPLING TO REACTIVE TRANSPORT

Applying the concept of the hybrid analytical numerical modeling to simplify the complexity numerical simulations to be undertaken allows us to determine the flow, heat and mass transport in the different geomechanical facies. System variable (Pressure, Temperature, Concentration) dependent material parameters such as fluid properties of density, heat capacity, viscosity, conductivity etc., can be included. The transport of the various chemical species to be considered in the fracture flow is calculated, then the temperature, pressure and concentration of the various species in the aqueous solution, as well and the phase limitations, e.g. whether gas is allowed to form or not, are exported to a geochemical solver. Equilibrium chemistry allows the use of standard Gibbs energy solution procedures, e.g. ChemApp, or GEMS, or Mass Action Solvers, e.g. Phreeqc. The thermodynamic data base used for the solution of the chemical mixture defines the results and the applicability of the data sets. Once the geochemical solver has predicted the concentrations of the various phases and species, this data is imported into the solution mass transport calculations.

APPLICATION.

To illustrate the above concepts on hand of an example based on reality we model the reactive transport and mixing of hot saline waters of seawater composition, [*Nordstrom, et al.*, 1979] and a typical geothermal chloride water, in this case as found in Wairakei, New Zealand [*Nicholson*, 1993]. We assume both waters have equilibrated with a carbonate / gypsum surrounding, and that the geothermal chloride water is injected at a temperature of 120°c into fractured rock containing the saline water at 40°c. The modeled fracture has dimensions of 12 cm width and 52 cm length, the permeability distribution in the fracture is dependent on the aperture distribution. The aperture distribution can be altered to fit the surface roughness of the fracture. Transport in the fracture where the aperture distribution is based on experimental measurement of shear zone material recovered from the Grimsel Rock Laboratory [*Mettier, et al.*, 2005 submitted] is illustrated in Figure 7. Here the effect of including the matrix diffusion discussed above is illustrated on an advecting radionucleid front.

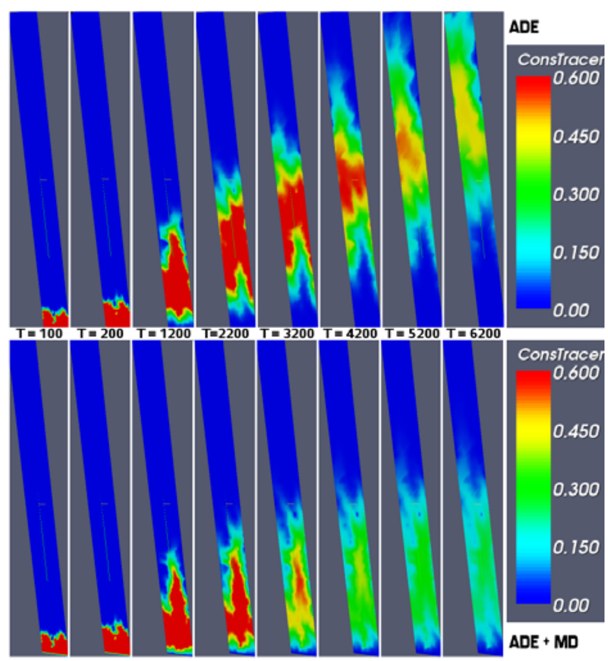

Figure 7 Realistic fracture profile, transport of a tracer with (lower) and without (upper) the influence of matrix diffusion.

For the geochemical analysis we assume a constant aperture for the purpose of demonstration, and examine the change of concentration of the various species along the length of the fracture during flow. Naturally it is possible to link the fracture aperture to some geochemical parameter, such as the amount of a solid phase present or being dissolved. Eleven processes are solved during this calculation, the species are listed in table 1.

Table 1: Geochemical components of two saline waters mixing.

Variable		***In situ* Sea Water**	**Geothermal Water**
Temperature °C		40	120
pH		6.7	7.9
Aqueous Component	**Aq. Diff. Coeff. m²/s**	**Moles**	**Moles**
H2O		55.56	55.56
Na<+>	1.33E-09	4.85E-01	4.67E-02
K<+>	1.96E-09	1.06E-02	2.62E-03
Cl<->	2.03E-09	5.66E-01	5.01E-02
Mg<2+>	7.06E-10	1.72E-02	9.62E-04
Ca<2+>	7.92E-10	4.69E-02	5.05E-04
(SO4)<2->	1.07E-09	2.81E-02	1.29E-03
(HCO3)<->	1.00E-09	1.58E-03	5.05E-04
Solid Phase			
Ca(SO4)_Anhydrite		0	1.999
Ca(CO3)_Calcite		0.9247	1.002
CaMg(CO3)2_Dolomite		1.038	0.9991
Ca(SO4):2H2O_Gypsum		2.001	0

A comparison of the preliminary calculations is provided in Figure 9 between flow, heat and mass transport for the above system with and without reactive geochemistry. There are several aspects which could be picked out from this comparison, which would take this paper beyond its current scope. Also we have limited the species being considered during transport to those listed above. Here we highlight the interaction of anhydrite and gypsum, and note that as the temperature front ingresses into the fracture that the gypsum converts to anhydrite. Coupling this with a porosity or fracture opening coupling would lead to the development of flow paths as the density of anhydrite is circa 25% higher than that of gypsum. This temperature dependent alteration could be interpreted as a functional response of the Geochemical system, which when integrated into a geomechancial facies concept could allow us to characterize the dominant Geochemical response of the system over a large scale.

CONCLUSIONS

Hybrid numerical analytical modeling approaches to geothermal systems linked with a geomechancial facies approach may provide a tool for a holistic multi-scaled modeling approach for complicated coupled systems, conceptually illustrated in Figure 8. Here this approach is illustrated on hand of work done at the KTB site, Grimsel, Soultz, Spa Urach and theoretical modeling work. The result is a model approach which allows predictive modeling of the operation of complicated geosystems.

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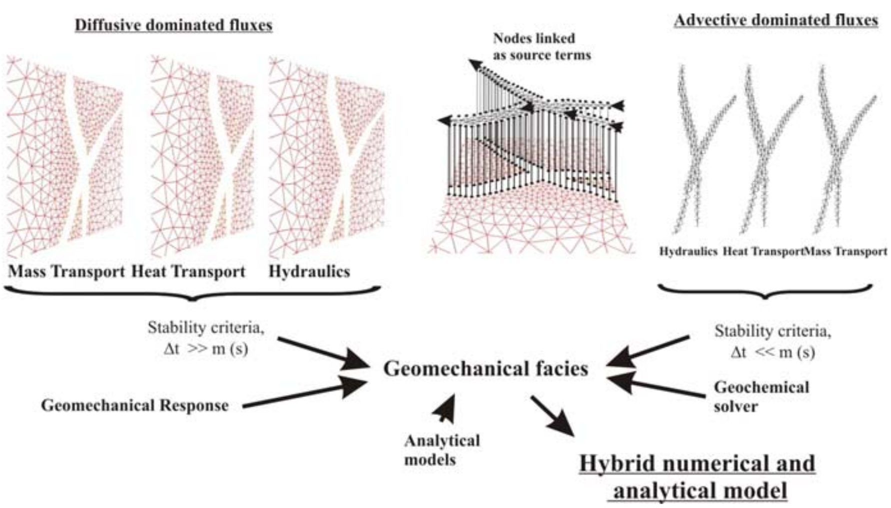

Figure 8 Conceptual illustration of a multiple mesh hybrid numerical analytical mdoel for HTMC coupling based on the geomechanical facies approach

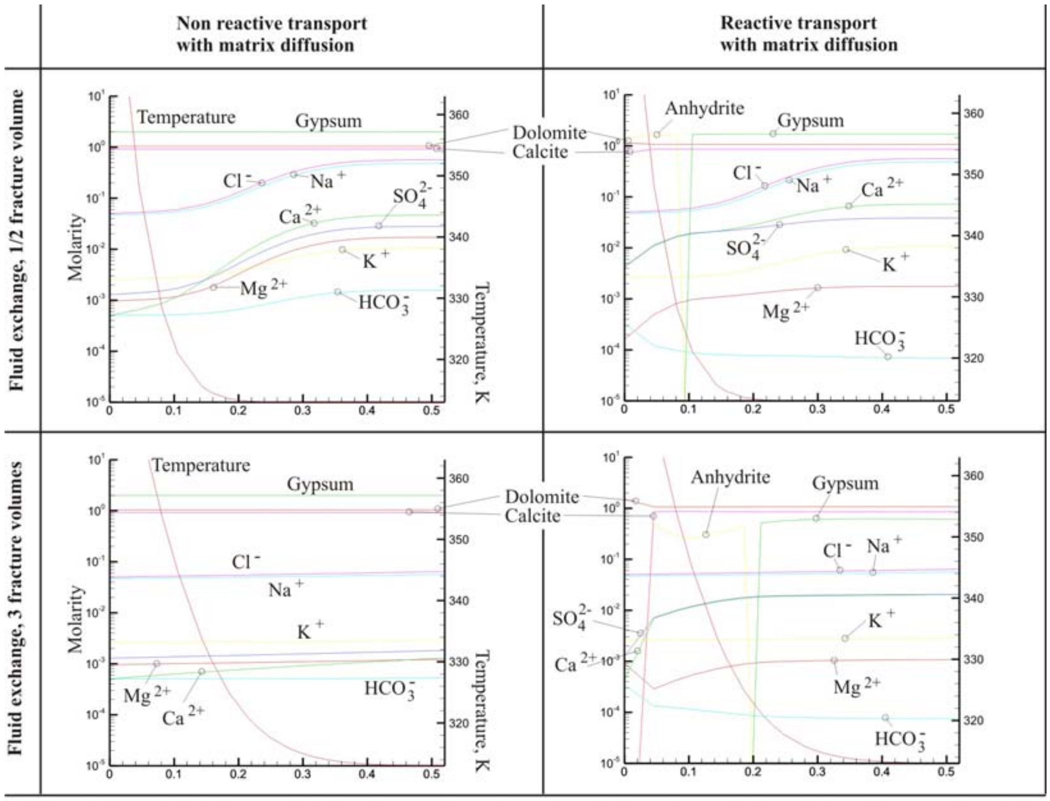

Figure 9 Comparison between non reactive and reactive transport modeling of the mixing of hot geothermal fluid and seawater in carbonate and gypsiferous fractured rock.

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