AN OPEN FRAMEWORK FOR THE SIMULATION OF COUPLED THERMO-HYDRO-MECHANICAL PROCESSES IN DISCRETE ELEMENT SYSTEMS

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Abstract This paper outlines the theoretical framework and experimental validation of a fully Thermo-Hydro-Mechanical model, ThermalEngine, as part of the open source DEM software Yade. ThermalEngine is constructed on top of Yade’s existing thoroughly validated and well optimized Pore Finite Volume (PFV) scheme, which enables a highly efficient upwind forward finite difference advection scheme that reuses existing pore scale mass-fluxes to conserve pore energy. Conductive heat transfer within phases and between phases is solved explicitly in time by conserving energy and modeling heat fluxes with classic heat transfer models. In addition to advection and conduction, the thermo-mechanical component of ThermalEngine incorporates the thermal expansion or contraction of particles and pore fluids by estimating pore volume changes and adding them to the existing PFV mass balance. In addition to the theoretical framework, the experimental and numerical validation of the coupled THM ThermalEngine model is presented by heating a cylindrical rock specimen and observing interior cavity fluid pressure changes. Cavity fluid pressure changes follow experimental data closely; as rock temperature increases the cavity fluid expands resulting in an increased cavity pressure until pressure gradients direct fluid out of cavity allowing fluid pressure to stabilize back to initial conditions. It is clear that the foundational, easily modifiable, and open sourced THM-DEM framework presented within is applicable to a wide range of disciplines including geomechanics and powder technologies.

1 INTRODUCTION

Thermo-Hydro-Mechanical (THM) couplings in DEM are can be comprised of three heat transfer models: a particle-particle conduction model, a particle-fluid conduction model, and a heat advection model. In addition, the thermal mechanical models include the effect of fluid thermal expansion on fluid pressures and particle forces, while particle
thermal expansion also contributes to fluid pressure changes which ultimately affects the advection of heat in the particulate medium. Existing THM couplings in DEM contain some but not all of these features and can be found in commercial software PFC [11, 8] and Open LIGGGHTS CFDDEM [5]. Both softwares approach particle particle heat transfer as some variation of pipe networks transferring a magnitude of heat flux dependent on particle overlap presented in [1, 3, 7]. With respect to heat advection, PFC can be manually modified to include a 2D heat advection model [10], but at the time of this writing there is no publicly available code to do so and the commercial release does not include a 2D or 3D heat advection model. Meanwhile LIGGGHTS uses a computationally expensive CFD coupling that neglects thermal expansion and compressibility of fluid [5, 4]. Although the LIGGGHTS CFD coupling is advantageous for various high porosity particle applications and mass transfer models, there remains a need for an open sourced THM model focused on high efficiency in low porosity 3D DEM assemblies with a thermo-mechanical fluid component. Yade ThermalEngine fills this need with the introduction of a coupled THM model comprised of a pore scale advective heat transfer model and a particulate scale conduction model.

2 METHODS

2.1 Compressible Pore Finite Volume in DEM

Yade’s compressible Pore Finite Volume (PFV) scheme triangulates Discrete Element sphere locations to form a tetrahedral mesh. Following the original publication, [2], each tetrahedron is comprised of four discrete elements and represents a single pore comprised of solid and fluid fractions. The full tetrahedral network constitutes the pore network, which is used to establish a Stokes-flow based on the continuity equation represented by a contour integral:

\[
\int_{\Theta_i} \frac{1}{K} \frac{\partial p_i}{\partial t} = \int_{\partial \Theta_i} (u - v) \cdot n \ dS - \dot{V}_{p,i}
\]

where \(K\) is the fluid compressibility, \(\dot{V}_{p,i}\) is the rate of pore volume change, \(u\) is the fluid velocity relative to the contour velocity \(v\), and \(\partial \Theta_i\) is the pore contour. \(\partial \Theta_i\) can be reduced to only the fluid fractions \(S_{fij}\) of the pore contour. Thus, the integral can be represented as the sum of fluid fluxes exchanged by each pore and its four neighbors \((j=1 \text{ to } 4)\):

\[
\sum_{j=1}^{4} \int_{S_{fij}} (u - v) \cdot n \ dS = \sum_{j=1}^{4} q_{ij}
\]

The flux \((q_{ij})\) through the pore throat connecting pore \(i\) and \(j\) is approximated by a local pressure gradient which enables the final compressible flow approximation:

\[
\sum_{j=1}^{4} \int_{S_{fij}} (u - v) \cdot n \ dS = \sum_{j=1}^{4} q_{ij}
\]
\[ q_{ij} = k_{ij} \frac{p_i - p_j}{l_{ij}} \]  \hspace{1cm} (3)

\[ \sum_{j=1}^{4} q_{ij} = \dot{V}_{p,i} + \frac{\dot{p}_i V_{p,i}}{K} \]  \hspace{1cm} (4)

where \( p_i \) and \( p_j \) are the pressures of neighboring pores and \( l_{ij} \) is the length of the connecting pore throat. The matrix representation of the full linear system is simply the known conductivity matrix \( G \), the unknown vector of pressures \( p \), and the vector of rate of volume changes \( \dot{V} \). \( \dot{V} \) depends linearly on particles velocities, which can be expressed by an operator \( E \) such that \( \dot{V} = E\dot{x} \). The instantaneous pressures-velocities relation finally reads:

\[ Gp = E\dot{x} \]  \hspace{1cm} (5)

### 2.2 Conductive heat transfer

#### 2.2.1 Particle-particle conduction

Conductive heat transfer in ThermalEngine is simulated between interacting particles, between incident pores, and between pore fluid and incident particles. Simplifying assumptions include the negligence of radiation effects below 400°C, the resistance to heat transfer inside the particle is significantly smaller than between particles (\( Bi = \frac{2a}{\pi r} \ll 1 \)), and creep flow, 0<Re<100. Given these assumptions, the transient conservation of energy for a particle \( i \) can be written as:

\[ m_i c_{p,i} \frac{dT_i}{dt} = \sum_{j=1}^{N} \Phi_{i,j} + \sum_{k=1}^{M} \Phi_{i,k} \]  \hspace{1cm} (6)

where \( m_i \) is the mass of the particle, \( c_{p,i} \) is the heat capacity at constant pressure for the particle, \( T_i \) is the temperature of the particle, \( \Phi_{i,j} \) is the heat-flux between particle \( i \) and \( j \), \( \Phi_{i,k} \) is the heat-flux between particle \( i \) and pore \( k \), and \( N \) is the number of particles interacting with particle \( i \), while \( M \) is the number of cells interacting with particle \( i \). Conductive heat-flow between particles can be modelled using the contact area, as modeled in [7]:

\[ d = r_i + r_j - p_d \]  \hspace{1cm} (7)

\[ r_c = \sqrt{\frac{4d^2r_j^2 - (d^2 - r_i^2 + r_j^2)^2}{2d}} \]  \hspace{1cm} (8)

\[ \Phi_{i,j} = \frac{2r_i^2(k_i + k_j)}{d}(T_j - T_i) \]  \hspace{1cm} (9)
where \( d \) is the distance between particles less the overlap, \( p_d \), \( r \) is the particle radius, \( k \) is the particle thermal conductivity, and \( T \) is the particle temperature.

### 2.2.2 Particle-pore conduction

The estimate of heat-flux between the particles and the pores follows a traditional CFD-DEM approach [7]:

\[
\Phi_{i,k} = h_i A_i (T_k - T_i) \tag{10}
\]

where \( A_i \) is the particle surface interacting with the pore (spherical triangle shown in Fig. 1), \( T_k \) is the temperature of the pore, and the heat transfer coefficient, \( h_i \), is computed for a sphere based on the Nusselt \((Nu)\) number which can be empirically estimated using porosity \((0.35 < \epsilon < 1)\) and Reynolds number \((0 < Re < 10^2)\) [9]:

\[
Nu = (7 - 10\epsilon + 5\epsilon^2)(1 + 0.1Re^{0.2} Pr^{1/3}) + (1.33 - 2.19\epsilon + 1.15\epsilon^2) Re^{0.7} Pr^{1/3} \tag{11}
\]

where \( Pr \) is Prandtl’s number. The heat transfer coefficient becomes \( h_i = Nu \cdot k_f / d_i \), where \( k_f \) and \( d_i \) are the thermal conductivity of the fluid and the diameter of the particle of interest, respectively.

Given the particle-particle (\( \Phi_{i,j} \), Eq. 9) and particle-fluid (\( \Phi_{i,k} \), Eq. 10) heat flux approximations. Eq. 6 is approximated with a forward finite difference in time to estimate the particle temperature change:

\[
T_i^{t+\Delta t} = \frac{\Delta t}{m_i c_{p,i}} \left[ \sum_{j=1}^{N} \frac{2r_j^2 (k_i + k_j)}{d_i} (T_j^t - T_i^t) + \sum_{k=1}^{M} \frac{Nu k_f A_i}{d_i} (T_k^t - T_i^t) \right] + T_i^t \tag{12}
\]

### 2.2.3 Pore-pore conduction

Similar to the particle conductive heat transfer, the pores conduct heat between one another through a network of pipes. Each pipe is characterized by a thermal resistance, which determines the heat flux based on the temperature difference between pores:

\[
\Phi_{k,l} = \frac{k_f A_{k,l}}{d_{k,l}} (T_k - T_l) \tag{13}
\]
where \( d_{k,j} \) is the distance between pore \( k \) and pore \( j \) barycenters, \( T_k \) and \( T_j \) are the temperatures of the respective pores, and \( A_{k,l} \) is the fluid area shared by both pores.

### 2.3 Advective heat transfer

Heat advection in this model depends on the pressure field determined by Yade’s existing Pore Finite Volume scheme (PFV). Energy is conserved assuming thermal pressure changes are negligibly small, fluid movement energy is negligible for \( 0<\text{Re}<100 \), and pore fluid contains zero energy at absolute zero. Given these assumptions, each pore is treated as an open thermodynamic system where the change of internal energy is:

\[
\Delta U = Q + W + \Delta U_{\text{matter}}
\]

(14)

where \( Q \) is the heat-flux, \( W \) is the work done on or by the pore (neglected for small pressure changes), and \( \Delta U_{\text{matter}} \) is the change of internal energy due to matter entering or exiting the system. For each pore system, the reference energy is:

\[
U = c_{p,f} \rho_f V T_f
\]

(15)

where \( c_{p,f}, \rho_f, V, \) and \( T_f \) are the heat capacity at constant pressure (constant between 0-150°C), density, volume, and temperature of the pore fluid. The change of internal energy due to mass-flux and solid-fluid heat-flux can be expressed as a surface integral using the divergence theorem:

\[
\dot{U}_{p,i} = \int_S \mu \cdot \mathbf{n} \, dS + \int_P \Phi_q \cdot \mathbf{n} \, dP
\]

(16)

where \( S \) is the surface of pore \( i \), \( \mu \) is the mass-energy-flux, \( \mathbf{n} \) is the outward pointing unit vector, \( P \) is the solid-fluid surface, and \( \Phi_q \) is the heat-flux between the solid particles and the fluid pores. Starting with the advection term, each pore system abuts four neighboring pores \( (j=1 \text{ to } 4) \), which means the integral can be reduced to a summation:

\[
\int_S \mu \cdot \mathbf{n} \, dS = \sum_{j=1}^{4} \int_{s_i} \mu \cdot \mathbf{n} \, ds = \sum_{j=1}^{4} \mu_{ij}
\]

(17)

where the pore-pore mass-energy-flux between home pore \( i \) and neighbor pore \( j \), \( \mu_{ij} \), depends on the volumetric flow, \( q_{ij} = k_{ij} \frac{p_i - p_j}{l_{ij}} \), defined in Sec. 2.1.

\[
\mu_{ij} = q_{ij} c_{p,f} \rho_f T_i \text{ or } j
\]

(18)

where \( T_i \text{ or } j \) is the temperature of the home or neighbor pore depending on the flow direction. As shown in Sec. 2.1, hydraulic conductance, \( k_{ij}/l_{ij} \), is already constructed in the conductivity matrix \( ([G]) \) of the PFV scheme for the implicit solution of the pore.
An open framework for the simulation of coupled THM processes in discrete element systems

pressure vector, \( \mathbf{Gp} = \mathbf{E} \dot{\mathbf{x}} \). Therefore, the change of internal energy due to mass-energy-flux for all pores is explicitly integrated by augmenting \( [\mathbf{G}] \):

\[
\frac{U_{p,i}^{t+\Delta t} - U_{p,i}^t}{\Delta t} = c_p f \rho_f \sum_{j=1}^{4} T_{(i \text{ or } j)g_{ij}} (p_{i}^{t+\Delta t} - p_{j}^{t+\Delta t})
\]

(19)

where the augmented \( [\mathbf{G}] \) is:

\[
[\bar{\mathbf{G}}] = c_p f \rho_f \Delta t \sum_{j=1}^{4} T_{(i \text{ or } j)g_{ij}}.
\]

(20)

Meanwhile, the conductive heat-flux, \( \{\Phi\} \), exchanged between pore-particle and pore-pore is computed as shown below in Sec. 2.2.2 and Sec. 2.2.3. Finally, the internal energy, \( \{U^{t+\Delta t}\} \), is computed for all pores:

\[
\{U^{t+\Delta t}\} = [\bar{\mathbf{G}}] \{p\} + \{U^t\} + \{\Phi\} \Delta t
\]

(21)

and the temperature of the pores at \( t + \Delta t \) is:

\[
\{T^{t+\Delta t}\} = \frac{\{U^{t+\Delta t}\}}{c_p f \rho_f \{V^{t+\Delta t}\}}.
\]

(22)

2.4 Thermo-Hydro-Mechanical coupling

2.4.1 Hydro-Mechanical coupling

The advection and conduction scheme are both hydraulically and thermally coupled with the mechanical DEM scheme. The two way hydro-mechanical coupling was first developed and presented by [2], but a brief description is presented here for completeness. The hydraulic force exerted by the pore on the particle is decomposed into pressure and viscous forces. The pressure force, \( F_{p}^{i,j,k} \), is computed using the pressure difference along the pore throat between pores \( i \) and \( j \), \( (p_i - p_j) \), multiplied by the area of particle \( k \), \( A_{ij}^k \), exposed to the pore throat.

\[
F_{p}^{i,j,k} = A_{ij}^k (p_i - p_j) n_{ij}
\]

(23)

where \( n_{ij} \) is the unit vector pointing from \( P_i \) to \( P_j \). The total viscous force, \( F_{v}^{ij} \) is computed for the entire pore throat, and then the viscous force applied to each particle, \( F_{v}^{k} \), is simply proportional to the area of each particle, \( \gamma_{ij}^k \), comprising the total solid area of the pore throat, \( \sum_{k=1}^{3} \gamma_{ij}^k \):
\[ F_{ij}^V = A_{ij}^f (p_i - p_j) n_{ij} \] (24)
\[ F_{ij}^{V,k} = F_{ij}^V \frac{\gamma_{ij}^k}{\sum_{k=1}^3 \gamma_{ij}^k} \] (25)

### 2.4.2 Thermal-mechanical coupling

The thermal mechanical coupling explicitly models thermal expansion/contraction of fluid and particle by estimating volume changes and adding them to the existing rate of volume changes, \( \{\dot{E}x\} \), used within the implicit flow solution (Sec. 2.1). Thus, compressibility effects are handled inherently within the flow solver. For a given time-step, the heat exchanged by a pore and the four incident particles is estimated following Sec. 2.2.1. The temperature changes resulting from heat exchange with pores and particles for a single time step is used to estimate the thermal expansion/contraction of the particle:

\[ \Delta r_{ti, t+\Delta t} = r_{ti}^l \beta_p (T_{ti, t+\Delta t} - T_{ti, t}) \] (26)

where \( \beta_p \) is a coefficient of thermal expansion for the particle, \( r_i \) is the radius of particle \( i \), and \( T \) is the temperature of particle \( i \) before and after the exchange of heat for a single time step. These particle volume changes, \( \sum_{i=1}^4 \Delta v_i \), are used to compute the pore volume changes \( \Delta v_k \), which are added to the pore rate of volume changes, \( \{\dot{E}x\} \), used within the implicit flow solver:

\[ \Delta v_k = - \sum_{i=1}^4 \Delta v_i \] (27)
\[ \Delta v_k = - \sum_{i=1}^4 A_{sph,i}^3 4 \pi (r_{i,t, t+\delta t}^3 - r_{i,t}^3) \] (28)
\[ E\dot{x}_k =+ \frac{\Delta v_k}{\Delta t} \] (29)

where \( \Delta t \) is the thermal time step, \( A_{sph,i} \) and \( A_{tot,i} \) are the spherical area of incident particle \( i \) and the total surface area of particle \( i \), respectively. Similar to the particle thermal-mechanical coupling, the thermal pore fluid expansion/contraction also contributes to the pore rate of volume changes, \( \{\dot{E}x\} \):

\[ E\dot{x}_k =+ \frac{V_k \beta_f \Delta T}{\Delta t} \] (30)

where the temperature change \( \Delta T \) and the fluid volumetric coefficient of thermal expansion, \( \beta_f \) determine the thermal volume change of the pore.
2.5 Air-water mixture compressibility model

The equivalent compressibility of the air-water mixture ($C_{eq}$) depends on the fraction of air within the mixture ($\phi$) and the compressibility of that air ($C_a$) [6]:

\[ C_{eq} = \phi C_a + (1 - \phi) C_w \]  
\[ C_a = \frac{1}{P_a} \]  
\[ \phi = \frac{P_{a,0}}{P_a} \phi_0 \]

where $P_a$ is the absolute pressure of the air. $P_{a,0}$ and $\phi_0$ are the initial absolute air pressure and air fraction.

3 ANALYTICAL AND NUMERICAL VERIFICATIONS

ThermalEngine’s model was thoroughly verified and validated using a variety of uncoupled and coupled scenarios. Specifically, the conduction scheme was verified by comparing various thermal DEM simulations (neglecting mechanical interactions between particles) to the 1D heat equation. Advection, on the other hand, was verified numerically with FEM by passing cold fluid through a packing of 200 spheres. Only the fully coupled thermo-hydro-mechanical experimental and numerical verification is presented below.

4 EXPERIMENTAL AND NUMERICAL VALIDATION OF FULLY COUPLED THM MODEL

[6] performed two experiments on a 30 cm tall x 15 cm diameter cylindrical granite specimen containing an inner cylindrical cavity measuring 15 cm tall x 2.4 cm diameter. These experiments were also reproduced numerically by [6] using a fully coupled THM finite-element (COMSOL) model. The present study compares these experimental and numerical models to a DEM-THM model exhibiting the same cylindrical dimensions, boundary conditions, mechanical properties, and thermal properties as [6]’s granite specimen (Fig. 2). Micro DEM properties reported in Table 1 were calibrated using typical DEM compression tests, thermal diffusivity tests, and thermal expansivity tests.

The first experiment focused on deriving a permeability estimate based on the HM response of the granite specimen by pumping $3.333 \times 10^{-10}$ m$^3$/s of water into the fluid filled cavity. Cavity pressure was monitored during cavity pressurization until steady state was achieved. After one hour at steady state, flow was terminated and depressurization within the cavity was monitored. As shown in Fig. 3, air fractions ($\phi_0$) between $2.5 \times 10^{-5}$ and $3.75 \times 10^{-5}$ yielded the best match to experimental data. Similar to [6]’s FEM-HM model, higher $\phi_0$ yields better accuracy during pressurization, and the lower $\phi_0$ yields better accuracy during depressurization.
The second experiment presented by [6] focused on elucidating the THM response of the same granite specimen. During this experiment, the fully saturated granite rock specimen’s surface was heated from 25 to 70 °C over the course of one hour (Fig. 4a). The temperature was held at 70 °C for three hours, after which the surface temperature was reduced to 25 °C and held for eight additional hours. During the course of this 12 hour thermal response test, the cavity pressure and temperature were monitored. As shown in Fig. 3, application of the same experimental boundary temperatures to the DEM-THM results in the same experimental and numerical pressurization and depressurization trends reported by [6]. Specifically, cavity pressure increases with increasing temperature followed by a decrease to 0 kPa once the maximum temperature is achieved. As soon as the temperature begins to drop, the cavity pressure becomes negative and follows the reverse trend observed during heating. Numerical cavity temperatures also follow closely with experimental and numerical temperatures reported by [6], as shown in Fig. 4b.

5 CONCLUSION

The paper presented an open sourced framework for the simulation of coupled THM processes in discrete element systems. Heat advection between fluid pores and heat conduction between particles were built on top of the robust Yade DEM software and its well validated PFV scheme. In particular, ThermalEngine reuses existing pore scale fluid fluxes for its upwind forward difference advection scheme. Meanwhile, the explicit con-
Figure 3: Experimental and numerical cavity pressure curves a) permeability test b) thermal response test

Figure 4: a) Experimentally collected top and circumference specimen temperatures used as variable Dirichlet boundary conditions in FEM-HM [6] and the present study DEM-THM. b) Experimental and numerical cavity temperatures during thermal response test.
ductive heat transfer within phases and between phases follows traditional heat transfer models. In addition to advection and conduction, the thermo-mechanical coupling adjusts existing volume changes in the compressible PFV scheme according to particle and fluid thermal contraction/expansion. The full THM model was demonstrated in a geomechanical validation by comparing the current ThermalEngine to literature based experimental and numerical data based on granite cylinder THM behavior. Results show that the transient THM trends in Yade’s ThermalEngine follow closely to experimental and numerical trends. These results combine with an open sourced THM-DEM framework to make a useful tool for scientists from a variety of disciplines such as geomechanics and powder technologies.

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An open framework for the simulation of coupled THM processes in discrete element systems.

12


