Numerical Analysis of a Class of THM Coupled Model for Porous Materials

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Abstract. We consider the coupled models of the Thermo-hydro-mechanical (THM) problem for porous materials which arises in many engineering applications. Firstly, mathematical models of the THM coupled problem for porous materials were discussed. Secondly, for different cases, some numerical difference schemes of coupled model were constructed, respectively. Finally, assuming that the original water vapour effect is negligible and that the volume fraction of liquid phase and the solid phase are constants, the nonlinear equations can be reduced to linear equations. The discrete equations corresponding to the linear equations were solved by the Arnoldi method.

1. Introduction

The thermo-hydro-mechanical (THM) model describing the coupled physical phenomenon of porous materials is very important. An understanding of this model could lead to solutions to various engineering problems, such as exploitation of the physical phenomenon present in masonry materials[1], the poro-elastic and viscoelastic behaviour of articular cartilage[2], radioactive waste materials disposal[3], and so on[4-5]. After several decades of research on multifield coupling theory, significant achievements have been made in this field [4-7]. In general, the hybrid mixture theory (HMT) is available for the study of the interactions between soil phases under multifield coupled conditions. The approach method of nonlinear multifield coupled model was derived by Cai et al. using HMT [8]. It is very difficulty to obtain the solution of the THM coupled model. For obtaining the numerical solutions of the coupled problem, a numerical method of THM coupled model for porous materials is proposed in this paper.

2. THM Three Field Coupling Model

THM three field coupling model for porous materials consider the system of a solid skeleton, a liquid, and a gas, represented by s, l, and g, respectively. The mathematical model is shown as following.

$$p_s = (\rho_s) \frac{\partial A}{\partial \rho_s} \bigg|_{\rho=\rho_s} = (\rho_s) \frac{\partial A_s}{\partial \rho_s} = K_s \frac{\rho_s}{\rho_{s0}} + \lambda_s^\varepsilon I : \varepsilon_s^e - \lambda_s^c T \quad (2.1)$$

$$p_g = (\rho_g) \frac{\partial A_g}{\partial \rho_g} \bigg|_{\rho=\rho_g} = (\rho_g) \frac{\partial A_g}{\partial \rho_g} = K_g \frac{\rho_g}{\rho_{g0}} + \lambda_g^\varepsilon \varepsilon_g^e - \lambda_g^c T \quad (2.2)$$
\[ p_\beta - p_s = n_\beta \rho_\beta \frac{\partial A}{\partial n_\beta} = n_{p\beta} \Theta_\beta n_\beta + n_{p\beta} \lambda_\beta \frac{\rho_\beta}{\rho_{p\beta}} n_\beta \lambda_\beta T \]  
(2.3)

\[ n_{p\alpha} \frac{\partial \rho_\alpha}{\partial t} + \frac{\partial n_\alpha}{\partial t} + n_{p\alpha} \nabla \cdot \frac{\partial \mathbf{u}_s}{\partial t} = 0 \]  
(2.4)

\[ n_{p\beta} \lambda_\beta \frac{\rho_\beta}{\rho_{p\beta}} - n_{p\beta} \lambda_\beta^T T \left( \nabla n_\beta - \delta^{\nu_\beta, \epsilon_\beta^P} \epsilon^P_s - \delta^{\nu_\beta, \nabla T} \nabla T \right) \right] + n_\beta \nabla \cdot \frac{\partial \mathbf{u}_s}{\partial t} = 0 \]  
(2.5)

\[ \nabla \cdot \mathbf{t} + F = 0 \]  
(2.6)

\[ \epsilon_s = \epsilon_{s\text{\tiny un}} = \frac{\partial u_t}{\partial x} + \frac{\partial u_s}{\partial y} + \frac{\partial u_z}{\partial z} \]  
(2.7)

\[ T_0 \left[ \sum_{\alpha=\text{l},\text{g}} n_{\text{p}\alpha} \frac{c_{\alpha} T}{T_0} + \sum_{\alpha=\text{l},\text{g}} n_{\text{p}\alpha} \frac{\lambda_\alpha^T \lambda_\alpha^F}{\rho_{\text{p}\alpha}} + \alpha_s^T (3 \lambda_s^T + 2 \mu_s^T) \frac{\partial \epsilon^P}{\partial t} + \sum_{\alpha=\text{l},\text{g}} n_{\text{p}\alpha} \lambda_\alpha^T \frac{\partial n_\beta}{\partial t} \right] \]  
(2.8)

The number of unknowns in the these equations is 10, which includes fluid volume fraction \( n_\beta (\beta = \text{l}, \text{g}) \), the temperature \( T \), phase densities \( \rho_\alpha (\alpha = \text{s}, \text{l}, \text{g}) \), phase pressure \( p_\alpha (\alpha = \text{s}, \text{l}, \text{g}) \) and solid displacement \( \mathbf{u}_s \).

Where subscript ‘0’ respect the initial state, \( K_s \) is the bulk modulus, \( K_\beta \) is the bulk modulus of the fluid, \( c_s \) is the specific heat capacity, \( \lambda_s \) and \( \mu_s \) are the Lame constants of the soil skeleton, \( \lambda_\beta^T \) represents the thermal-mechanical coupling in the fluid, \( \lambda_\beta^F \) represents the coupling between the change in fluid content and the fluid compression, \( \lambda_\beta^T \) represents the coupling between the change in temperature and the fluid density, \( \lambda_\beta^F \) represents the temperature effect on the compression of the solid phase, and \( \lambda_\beta^P = 3 K_s \alpha_s^T \), \( \alpha_s^T \) is the thermal expansion coefficient of the soil skeleton, \( \Theta_\beta \) is the suction related coefficient, which describes the change in the fluid content and \( \epsilon^P \) represents plastic strain. All these coupling factors will degenerate into zero-order material parameters, which can be expressed by \( \lambda_\beta^P \), \( \delta^{\nu_\beta, \epsilon_\beta^P} \), \( \delta^{\nu_\beta, \nabla T} \), \( \delta^{\nu_\beta, \nabla T} \) and \( \delta^{\nu_\beta, \nabla T} \) when only linear coupling is considered.

Based on the HMT framework, the formulations of the THM coupling behavior for porous materials has been established. The closed field equations include 10 equations and 10 unknown variables. Then the number of unknown variables is equal to equations, thus the closure of this coupling problem is set up.

### 3. A Class of Degenerate THM Coupled Equations

Equation (2.5) is the control equation for fluid flow, according to the Darcy’s law; we can get that the following equation:
\[ v_{\beta,s} = \frac{1}{\delta_{\gamma,s}} \left[ n_{p} \nabla p_{\beta} - n_{p} \rho_{p} g_{\beta} + \left( n_{0} \Theta_{\beta}^{m} n_{p} + n_{0} \sigma_{m}^{\beta} \rho_{p} - n_{0} \lambda_{\beta}^{m} T \right) \nabla n_{p} \right] - \frac{1}{\delta_{\gamma,s}} \left[ \delta_{\gamma,s}^{\beta,\epsilon_{s}} \epsilon_{s}^{p} + \delta_{\gamma,s}^{\beta,T} \nabla T \right] \]

Where \( v_{\beta,s} \) is the relative velocity, and \( v_{\beta,s} = v_{\beta} - v_{s} \), so the equation (2.5) is an extension of the following equation:

\[ \frac{n_{0}}{\rho_{0}} \left( \frac{1}{K_{\beta}} \frac{\partial p_{\beta}}{\partial t} - \alpha_{\beta} \frac{\partial T}{\partial t} \right) + \frac{n_{0}}{\rho_{0}} \nabla \cdot v_{\beta,s} + n_{0} \nabla \cdot \frac{\partial u_{s}}{\partial t} = 0 \]  

Then the difference equation is obtained by the discretization of the equation (3.2).

\[ \frac{n_{0}}{\rho_{0}} \left[ \frac{1}{K_{\beta}} \left( p_{\beta,i+1,j,m} - p_{\beta,i,j,m} \right) - \alpha_{\beta} \frac{1}{\tau} \left( T_{i+1,j,m} - T_{i,j,m} \right) \right] + \frac{1}{\tau} \left( n_{0} k_{i+1,j,m} - n_{0} k_{i,j,m} \right) + \frac{n_{0}}{h} \left( v_{\beta,s,i+1,j,m} - v_{\beta,s,i,j,m} - v_{\beta,s,i,j,m+1} - v_{\beta,s,i,j,m} \right) \]

\[ \frac{n_{0}}{h} \left[ u_{s,i+1,j,m} - u_{s,i,j,m} - u_{s,i,j,m+1} - u_{s,i,j,m} \right] = 0 \]  

We can see that the discrete form of THM coupling model is a big nonlinear equations, and the solution is relatively complex, so we should solve its simplified form firstly.

Considering the complexity of the equation, in order to solve the solution easily, we make some assumptions about the equation under the actual situation. The volume fraction \( \eta_{\beta} \) of solid and liquid phase in ideal state is constant (that is \( n_{l} = n_{g} = n_{1} = n_{0} = n_{g} = n_{2} \)), elastic strain \( \epsilon_{e} \) and plastic strain \( \epsilon_{p} \) have the same stress effect, that is to say \( \epsilon_{e} = \epsilon_{p} = \epsilon_{s} = \frac{\partial u_{s}}{\partial x} + \frac{\partial u_{s}}{\partial y} + \frac{\partial u_{s}}{\partial z} \). The acting force of the liquid phase, we just consider the action of the water, the effect of steam we ignore (that is \( \rho_{\beta} = \rho_{l}, P_{\beta} = P_{l} \)). Considering the first boundary condition as an example, dividing \( x, y, z \) into \( N \) equal points, the grid division of the point

\[ x_{i} = i h, i = 0, 1, \ldots, N - 1; y_{j} = j h, j = 0, 1, \ldots, N - 1; z_{m} = m h, m = 0, 1, \ldots, N - 1 \]

in the three-dimensional space cube.

We have the following notation for unknowns in order to derive the matrix form of the equation easily.

**Table 1. New Notation for Unknowns**

| unknowns | \( \rho_{i} \) | \( p_{i} \) | \( u_{i} \) | \( T \) |
|----------|----------------|----------------|----------------|----------------|
| new notations | \( x_{1} \) | \( x_{2} \) | \( x_{3} \) | \( x_{4} \) | \( x_{5} \) |

Note: the unknowns \( x_{i} \) are vectors. So the original equations would be degenerated into the following equations.

\[ p_{s} = \frac{K_{s}^{s}}{\rho_{s0}^{s}} \rho_{s} + \lambda_{s}^{s} \mathbf{I} : \nabla u_{s} - \lambda_{s}^{s} T \]  

(3.4)
\[ p_\beta = \frac{K_\beta}{\rho_\beta} \rho_\beta + \lambda_\beta n_1 - \lambda_\beta \rho_\beta T \] \hfill (3.5)

\[ p_\beta - p_s = n_1^2 \Theta_0^s + \frac{n_1 \lambda_\beta}{\rho_\beta} \rho_\beta - n_1 \lambda_\beta T \] \hfill (3.6)

\[ n_2 \frac{\partial \rho_s}{\partial t} + n_2 \nabla \cdot \rho_s = 0 \] \hfill (3.7)

\[ \frac{n_1}{\rho_\beta} \left( \frac{1}{K_\beta} \frac{\partial p_\beta}{\partial t} - \alpha_\beta \frac{\partial T}{\partial t} \right) + \frac{n_1^2}{\delta_\beta} \frac{\partial \rho_\beta}{\partial T} \right) + \frac{n_1^2}{\delta_\beta} \frac{\partial g}{\partial \rho_\beta} \frac{\partial \rho_\beta}{\partial T} - \frac{n_1^2}{\delta_\beta} \frac{\partial \rho_\beta}{\partial T} = 0 \] \hfill (3.8)

\[ g(n_2 \rho_s + n_1 \rho_i) = 0 \] \hfill (3.9)

\[ \varepsilon_s = \varepsilon_{ijm} \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \right) = \nabla \cdot \mathbf{u} \] \hfill (3.10)

\[ T_0 \left( \sum_{a=j} n_{a} \frac{c_0}{T_{a0}} \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{u} \right) + \frac{n_1}{\rho_\beta} \left( \frac{\partial p_\beta}{\partial T} + \frac{\partial \rho_\beta}{\partial T} + \alpha_\beta \frac{\partial \rho_\beta}{\partial T} + \alpha_\beta \frac{\partial \rho_\beta}{\partial T} + \alpha_\beta \frac{\partial \rho_\beta}{\partial T} = 0 \right) \] \hfill (3.11)

The above eight equations are the degenerated equations, which are the linear equations, the equations are discretized by difference scheme.

\[ -\frac{K_x}{\rho_0} x_{1,jm}^k + x_{3,jm}^k + \lambda_\beta \rho_\beta + \frac{1}{h} \lambda_\beta \mathbf{I} : \left( x_{6,jt+1,jm}^k + x_{6,jt+1,jm}^k + x_{6,jt+1,jm}^k - 3x_{6,jt+1,jm}^k \right) = 0 \] \hfill (3.12)

\[ -\frac{K_1}{\rho_0} x_{2,jm}^k + x_{4,jm}^k + \lambda_\beta \rho_\beta = \lambda_\beta \rho_\beta \] \hfill (3.13)

\[ -\frac{n_1}{\rho_0} \lambda_\beta \rho_\beta + x_{3,jm}^k + x_{6,jm}^k - n_1 \lambda_\beta \rho_\beta = n_1 \frac{\partial \rho_\beta}{\partial T} = 0 \] \hfill (3.14)

\[ \frac{n_2}{h \tau} \left( x_{1,jm}^{k+1} - x_{1,jm}^k \right) + \frac{n_2}{h \tau} \left( x_{6,jt+1,jm}^k + x_{6,jt+1,jm}^k + x_{6,jt+1,jm}^k - 3x_{6,jt+1,jm}^k \right) = 0 \] \hfill (3.15)
\[
\frac{n_i}{\varphi_{0} K_i} x_{i,j}^{k+1} + \left( \frac{3 n_i g}{\delta^{\nu,\pi}} h - \frac{n_i}{\varphi_{0} K_i} \right) x_{i,j}^{k} - \frac{n_i^2 g}{\delta^{\nu,\pi}} h \left( x_{i,j+1}^{k} + x_{i,j-1}^{k} + x_{i,j}^{k} \right)
\]
\[
+ \left( \frac{n_i \alpha_{i,j}^{T}}{\varphi_{0}} + \delta^{\nu,\rho,\pi} \right) n_i \left( x_{i,j}^{k} + x_{i,j}^{k} \right) + \left( \frac{n_i}{h \tau} - \frac{6 \delta^{\nu,\rho,\pi}}{h^2} \right) \left( x_{i,j+1}^{k} + x_{i,j}^{k} \right) + \left( \frac{n_i}{h \tau} \right) \left( x_{i,j+1}^{k} + x_{i,j}^{k} \right)
\]
\[
- \frac{n_i \alpha_{i,j}^{T}}{\varphi_{0}} x_{i,j}^{k+1} \left( x_{i,j+1}^{k} + x_{i,j}^{k} + x_{i,j}^{k} \right) - \frac{n_i}{h \tau} \left( x_{i,j+1}^{k} + x_{i,j}^{k} + x_{i,j}^{k} \right)
\]
\[
+ x_{5,j+1}^{k} - 3x_{4,j}^{k+1} + \left( \frac{3 n_i g}{\delta^{\nu,\pi}} h - \frac{n_i}{\varphi_{0} K_i} \right) x_{i,j}^{k} = 0
\]  
(3.16)
\[
g \left( n_i x_{1,j}^{k} + n_i x_{2,j}^{k} \right) = 0
\]  
(3.17)

4. Matrix Form of Degenerated Equations

The above equations are converted into the form of matrix equations \( AX = B \), and the form of the unknown quantity matrix X is the following.
\[ X = \left( x_{1,jm}^{k}, x_{1,jm}^{k+1}, x_{2,jm}^{k}, x_{1,jm+1}^{k}, x_{2,jm}^{k+1}, x_{2,jm+1}^{k}, x_{3,jm}^{k}, x_{1,jm+1}^{k}, x_{3,jm+1}^{k}, x_{4,jm}^{k}, x_{1,jm+1}^{k}, x_{4,jm+1}^{k}, x_{5,jm}^{k}, x_{1,jm+1}^{k}, x_{5,jm+1}^{k}, x_{6,jm}^{k}, x_{1,jm+1}^{k}, x_{6,jm+1}^{k}, x_{7,jm}^{k}, x_{1,jm+1}^{k}, x_{7,jm+1}^{k}, x_{8,jm}^{k}, x_{1,jm+1}^{k}, x_{8,jm+1}^{k}, x_{9,jm}^{k}, x_{1,jm+1}^{k}, x_{9,jm+1}^{k}, x_{10,jm}^{k}, x_{10,jm+1}^{k}, x_{11,jm}^{k}, x_{11,jm+1}^{k}, x_{12,jm}^{k}, x_{12,jm+1}^{k} \right)^{T} \]

There are 34 different variables, so the corresponding matrix \( A^{K} \) is \( 7 \times 34 \) order form (given the number of discrete nodes, \( A \) is a large sparse matrix represented by thousands of nodes.). Some related coefficients are substituted in order to calculate easily.

### Table 2. Known parameter substitution

| original quantity | \( \lambda_{3}^{m} \) | \( \lambda_{3}^{p} \) | \( \lambda_{1}^{m} \) | \( \delta_{\nu,\sigma} \) | \( \delta_{\nu,\rho,\sigma} \) | \( \delta_{\nu,\rho,\nu,\sigma} \) | \( \delta_{\nu,\rho,\nu,\nu,\sigma} \) |
|-------------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| substituted quantity | \( a_{1} \) | \( a_{2} \) | \( a_{3} \) | \( r \) | \( b_{1} \) | \( b_{2} \) | \( b_{3} \) | \( b_{4} \) |

Denoting \( (3\lambda_{3} + 2\mu) = d \), we divide the matrix into seven columns due to the matrix is very long, in order to write conveniently. So the matrix is expressed as follows:

\[
A^{K} = \begin{bmatrix}
A_{11} & A_{12} & A_{13} & A_{14} & A_{15} & A_{16} \\
A_{21} & A_{22} & A_{23} & A_{24} & A_{25} & A_{26}
\end{bmatrix}
\]

Each small block matrix is represented as follows:

\[
A_{11} = \begin{bmatrix}
0 & -K_{0} & 0 & 0 & 0 & 0 \\
0 & \rho_{0} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
n_{2} & -n_{2} & 0 & 0 & 0 & 0
\end{bmatrix},
A_{12} = \begin{bmatrix}
0 & 1 & 0 & 0 & 0 & 0 \\
K_{1} & 0 & 0 & 0 & 0 & 1 \\
\rho_{0} & 0 & 0 & 0 & 0 & 1 \\
n_{2} & \rho_{0} & 0 & 0 & 0 & 0
\end{bmatrix}
\]

\[
A_{13} = \begin{bmatrix}
0 & a_{2} & 0 & 0 & 0 \\
0 & a_{2} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & -n_{2} & 0 & 0 & 0
\end{bmatrix}
\]

\[
A_{14} = \begin{bmatrix}
0 & -a_{2} & 0 & 0 & 0 \\
0 & -a_{2} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 3a_{2} & n_{2} & n_{2} & n_{2}
\end{bmatrix},
A_{15} = \begin{bmatrix}
0 & 0 & -a_{2} & 0 & 0 \\
0 & 0 & -a_{2} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]

\[
A_{16} = \begin{bmatrix}
-a_{2} & 3a_{2} & 0 & 0 & 0 \\
3a_{2} & h & 0 & 0 & 0 \\
h & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]

\[
A_{21} = \begin{bmatrix}
0 & 0 & n_{1} & 0 \\
0 & 0 & -n_{1} & 0 \\
0 & 0 & 0 & 0 \\
n_{1} & 0 & 0 & 0
\end{bmatrix}
\]

\[
A_{22} = \begin{bmatrix}
0 & gn_{2} & 0 & 0 \\
-\rho_{0} & \rho_{0} & 0 & 0 \\
n_{1} & n_{1} & 0 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}
\]

\[
A_{23} = \begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}
\]
Based on Arnoldi method and LD decomposition, the numerical solutions of the equation can be obtained. And matrix $A^k$ is the sub-matrix of $A$. The matrix that the equations present can be written as a square matrix to make $Ax = b$. Based on Arnoldi method and LD decomposition, and so on, the final numerical solutions of the equation can be obtained.

5. The Conclusion and Prospect
In this paper, the (THM) coupling model was established, and then analysis of the coupling equation of discrete format, and the block matrix forms of linear equations were obtained. In the future we’ll test the examples based on the numerical method.

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7. References
[1] Long N, Konke C, Bettzieche V and Lahmer T 2017 Numerical modeling and validation for 3D coupled-nonlinear thermo-hydro-mechanical problems in masonry dams *Comput Struct* **178** pp 143-54
[2] Behrou R, Foroughi H and Haghpanah F 2018 Numerical study of temperature effects on the poro-viscoelastic behavior of articular cartilage J Mech Behav Biomed 78 pp 214-23
[3] Carbol P, Wegen D, Wiss T and Fors P 2017 Spent nuclear fuel as waste material Mat Sci Eng Elsevier Current as of 24 May 2017
[4] Yu C 2011 Numerical analysis of heat and mass transfer for porous materials A theory of drying (Beijing: Tsinghua University Press) chapter 4 pp 153-215
[5] Chen X, Liu B and Xia X 2017 Analysis of thermocouple measurement error in high temperature porous materials Acta Energiae Solaris Sinica 38 pp 846-51
[6] Xie T , He Y, Wu M and He C 2014 Study on theoritical for the effective thermal conductivity of silia aerogel composite insulating materials J Eng Thermo phys-rus 35 pp 299-304
[7] ChenY, Zhou C,Tong F and Jing L 2009A numerical model for fully coupled THM processes Chinese Journal of Rock Mechanics and Engineering 28 pp 649-65
[8] Cai G, Sheng D, Sloan S and Zhao C 2013 Preliminary Study on Modeling Thermo-Hydro-Mechanical Coupling Behavior of Unsaturated Soils Based on Hybrid Mixture Theory. Biot Conference on Poromechanics 30, pp.1444-53