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1

STABILITY ANALYSIS OF THE NUMERICAL DENSITY-ENTHALPY MODEL

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ABSTRACT. In [5], we numerically solved a fluid system by using the numerical density-enthalpy model which consists of mass and energy conservation laws, Darcy's Law and other thermodynamics relations. In the current report, the convergence behavior of this model is investigated. We transform the original model to two-equation system. Which is further approximated by a linear model. The eigenvalues of the linear model are used to estimate convergence of the original model.

1. INTRODUCTION

In the density-enthalpy model, we solve a thermodynamic multi-phase flow system by considering density and enthalpy as state variables and compute rest of the system variables as a post processing step. We refer to [1,2,3,4], for more detail about the usage of numerical density-enthalpy phase diagrams (in short, ρ-h diagrams) and merits of this approach. Here, enthalpy h is actually the specific enthalpy with units $[J/k_g]$. However, we will use ρ and s as our state variables in this report, where s represents the total enthalpy with units $[J/m^3]$. In Figure

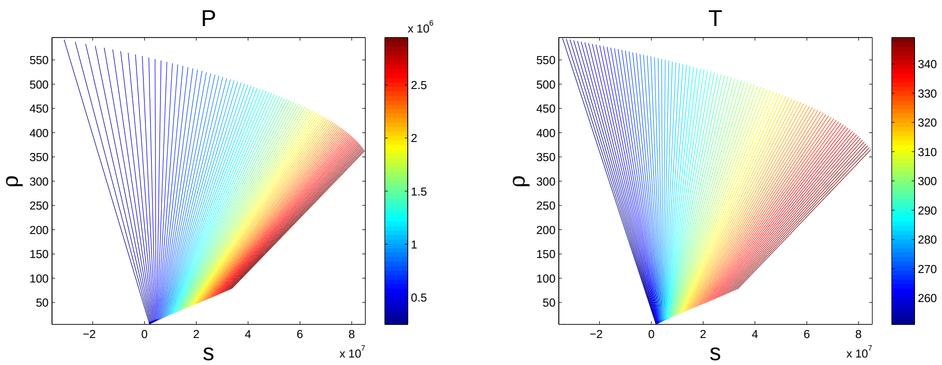

FIGURE 1. Partially negative total-enthalpy values corresponding to (left) pressure and (right) temperature.

1, two $(\rho,\ s)$ phase diagrams are shown for P and T. However, we observe that these values are valid for a certain temperature values. To make this point clear, s is plotted as a function of T at constant X_G in Figure 2. From this graph (and other experiments), we conclude that currently available (ρ, s) or equivalently (ρ, h) diagrams are valid approximately for $275 \leq T \leq 360$.

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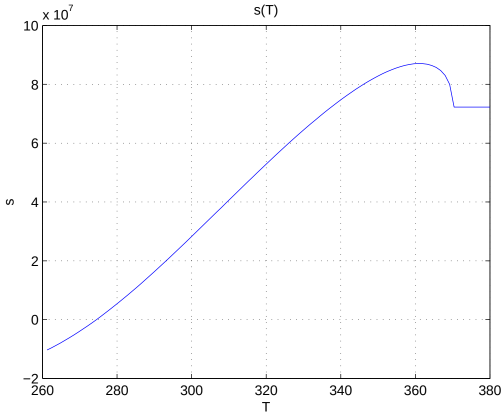

FIGURE 2. A plot of total enthalpy s as a function of T at constant X_G.

2. Two Equations Approach

In [25], we numerically solved a fluid flow system in a porous medium. The mathematical model for the one-dimensional system is given by the following equations.

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v)}{\partial x} = 0, \qquad x \in \Omega,\ t > 0,\ \text{(mass conservation)}, \tag{1}$$

$$\frac{\partial s}{\partial t} + \frac{\partial(sv)}{\partial x} - \lambda \frac{\partial^2 T}{\partial x^2} = q, \qquad x \in \Omega,\ t > 0,\ \text{(energy conservation)}, \tag{2}$$

$$v + \frac{K}{\mu}\frac{\partial P}{\partial x} = 0, \qquad x \in \Omega,\ t > 0, \text{(Darcy's law)}, \tag{3}$$

$$T = T(\rho, h), \qquad x \in \Omega,\ t > 0, \text{(thermodynamical relation)}, \tag{4}$$

$$P = P(\rho, h), \qquad x \in \Omega,\ t > 0, \text{(thermodynamical relation)}, \tag{5}$$

$$s = \rho h, \qquad x \in \Omega,\ t > 0, \text{(total enthalpy)}, \tag{6}$$

$$X_G = X_G(\rho, h), \qquad x \in \Omega,\ t > 0, \text{(thermodynamical relation)}, \tag{7}$$

where the permeability K, dynamic viscosity μ, and heat diffusivity λ are assumed to be constants and q is a heat source. The initial and boundary conditions are given as follows

$$T(x, 0) = T_0(x), \qquad x \in \Omega,$$

$$X_G(x, 0) = X_{G,0}(x), \qquad x \in \Omega,$$

$$\rho v = 0, \qquad x \in \Gamma,\ t > 0 \qquad \text{(zero mass flux)}\ , \tag{8}$$

$$-\lambda \frac{\partial T}{\partial x} + sv = 0, \qquad x \in \Gamma,\ t > 0 \qquad \text{(zero energy flux)}\ . \tag{9}$$

This system is solved and discussed in [25]. We give the numerical solution results for this system in Figure 3 (with a reduced resolution for fast printing). Later on this figure is used for comparison with other simulation results. We transform the model to two equations in a specific format. This approach helps in analyzing system stability.

2.1. **Transformation to two equations.** Consider the mass equation and substitute v by its value as given by the Darcy's law, we obtain

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\left[-\frac{K}{\mu}\rho\frac{\partial P}{\partial x}\right] = 0.$$

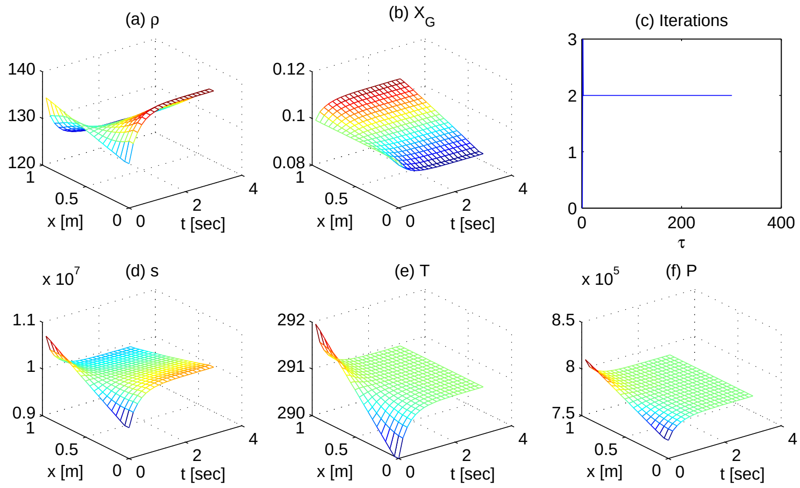

FIGURE 3. The original model. $\Delta t = 0.01$, $\Delta x = 0.01$. The plots of (a) ρ, (b) X_G, (c) Newton iterations/timestep (d) s, (e) T, and (f) P.

Now, using the value of $\frac{\partial P}{\partial x}$, i.e.,

$$\frac{\partial P}{\partial x} = \frac{\partial P}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial P}{\partial s}\frac{\partial s}{\partial x},$$

into the above equation, we realize

$$\frac{\partial \rho}{\partial t} - \frac{K}{\mu}\frac{\partial}{\partial x}\left[\rho\left(\frac{\partial P}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial P}{\partial s}\frac{\partial s}{\partial x}\right)\right] = 0. \tag{10}$$

By making similar substitutions of v, $\frac{\partial P}{\partial x}$, and $\frac{\partial T}{\partial x}$, the energy equation can be written as

$$\frac{\partial s}{\partial t} - \frac{K}{\mu}\frac{\partial}{\partial x}\left[s\left(\frac{\partial P}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial P}{\partial s}\frac{\partial s}{\partial x}\right)\right] - \lambda\frac{\partial}{\partial x}\left[\frac{\partial T}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial T}{\partial s}\frac{\partial s}{\partial x}\right] = 0. \tag{11}$$

Hence the many-equation system given by equations (1) to (6) is written in the following two-equation format

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left[D_{11}\frac{\partial \rho}{\partial x} + D_{12}\frac{\partial s}{\partial x}\right], \tag{12}$$

$$\frac{\partial s}{\partial t} = \frac{\partial}{\partial x}\left[D_{21}\frac{\partial \rho}{\partial x} + D_{22}\frac{\partial s}{\partial x}\right], \tag{13}$$

where D_{ij} are given by

$$D_{11} = \frac{K}{\mu}\rho\frac{\partial P}{\partial \rho}, \qquad D_{21} = \frac{K}{\mu}s\frac{\partial P}{\partial \rho} + \lambda\frac{\partial T}{\partial \rho},$$

$$D_{12} = \frac{K}{\mu}\rho\frac{\partial P}{\partial s}, \qquad D_{22} = \frac{K}{\mu}s\frac{\partial P}{\partial s} + \lambda\frac{\partial T}{\partial s}.$$

The boundary conditions are given by

$$\frac{K}{\mu}\rho\left(\frac{\partial P}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial P}{\partial s}\frac{\partial s}{\partial x}\right) = 0, \tag{14}$$

$$\frac{K}{\mu}s\left(\frac{\partial P}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial P}{\partial s}\frac{\partial s}{\partial x}\right) - \lambda\left(\frac{\partial T}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial T}{\partial s}\frac{\partial s}{\partial x}\right) = 0. \tag{15}$$

3. Numerical solution algorithm

To verify that the two approaches (many-equations versus two-equations model) are indeed equivalent, we solve the system given by equation (12) and (13) by Standard Galerkin Algorithm, as follows.

3.1. **The mass equation.** We start the solution algorithm by considering the transformed mass equation (i.e., equation (10)) and write down its linearized weak form

$$\int_\Omega \frac{\partial \rho}{\partial t}\phi d\Omega - \frac{K}{\mu}\int_\Omega \frac{\partial}{\partial x}\left[\rho\left(\frac{\partial P}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial P}{\partial s}\frac{\partial s}{\partial x}\right)\right]\phi d\Omega = 0.$$

Apply the product rule to the second integral

$$\int_\Omega \frac{\partial \rho}{\partial t}\phi d\Omega - \left[\frac{K}{\mu}\rho\left(\frac{\partial P}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial P}{\partial s}\frac{\partial s}{\partial x}\right)\phi\right]_0^1 + \frac{K}{\mu}\int_\Omega \rho\left(\frac{\partial P}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial P}{\partial s}\frac{\partial s}{\partial x}\right)\frac{d\phi}{dx}d\Omega = 0.$$

The boundary term vanishes (see equation (14)). By using Euler Backward time integration, the above equation is written as

$$\frac{1}{\Delta t}\int(\rho^\tau - \rho^{\tau-1})\phi dx + \frac{K}{\mu}\int_\Omega \rho^\tau \frac{\partial P^\tau}{\partial \rho}\frac{\partial \rho^\tau}{\partial x}\frac{d\phi}{dx}dx + \frac{K}{\mu}\int_\Omega \rho^\tau \frac{\partial P^\tau}{\partial s}\frac{\partial s^\tau}{\partial x}\frac{d\phi}{dx}dx = 0.$$

For brevity, we use a different convention for $\frac{\partial P}{\partial \rho}$, $\frac{\partial P}{\partial s}$, $\frac{\partial T}{\partial \rho}$, and $\frac{\partial T}{\partial s}$ terms such as the following

$$\begin{aligned}
&\frac{\partial P^\tau}{\partial \rho} \text{ for } \frac{\partial P}{\partial \rho}(\rho^\tau, s^\tau),\\
&\frac{\partial P^k}{\partial \rho} \text{ for } \frac{\partial P}{\partial \rho}(\rho^{\tau,k}, s^{\tau,k}),\\
&\frac{\partial P_i^k}{\partial \rho} \text{ for } \frac{\partial P}{\partial \rho}(\rho_i^{\tau,k}, s_i^{\tau,k}).
\end{aligned}$$

The convention used for $\frac{\partial P}{\partial s}$, $\frac{\partial T}{\partial \rho}$, and $\frac{\partial T}{\partial s}$ is analogous. The linearization about ρ^k and s^k is given by the following equation where we omit the index τ for brevity, except for explicit terms and use the notation $\delta\rho = \rho^{k+1} - \rho^k$ and $\delta s = s^{k+1} - s^k$.

$$\begin{aligned}
&\frac{1}{\Delta t}\int(\rho^k - \rho^{\tau-1} + \delta\rho)\phi dx\\
&+ \frac{K}{\mu}\int_\Omega \left[\rho^k \frac{\partial P^k}{\partial \rho}\frac{\partial \rho^k}{\partial x} + \delta\rho\frac{\partial P^k}{\partial \rho}\frac{\partial \rho^k}{\partial x} + \rho^k\left(\frac{\partial P^{k+1}}{\partial \rho} - \frac{\partial P^k}{\partial \rho}\right)\frac{\partial \rho^k}{\partial x} + \rho^k\frac{\partial P^k}{\partial \rho}\frac{\partial(\delta\rho)}{\partial x}\right]\frac{d\phi}{dx}dx\\
&+ \frac{K}{\mu}\int \left[\rho^k \frac{\partial P^k}{\partial s}\frac{\partial s^k}{\partial x} + \delta\rho\frac{\partial P^k}{\partial s}\frac{\partial s^k}{\partial x} + \rho^k\left(\frac{\partial P^{k+1}}{\partial s} - \frac{\partial P^k}{\partial s}\right)\frac{\partial s^k}{\partial x} + \rho^k\frac{\partial P^k}{\partial s}\frac{\partial(\delta s)}{\partial x}\right]\frac{d\phi}{dx}dx\\
&= 0. \qquad (16)
\end{aligned}$$

We use central difference approximations for the density and enthalpy derivatives, given by the following expressions.

$$\begin{aligned}
\frac{\partial P_i^k}{\partial \rho} &= \frac{\partial P}{\partial \rho}(\rho_i^k, s_i^k) = \frac{1}{2\epsilon_\rho}[P(\rho_i^k + \epsilon_\rho, s_i^k) - P(\rho_i^k - \epsilon_\rho, s_i^k)],\\
\frac{\partial^2 P_i^k}{\partial \rho^2} &= \frac{1}{\epsilon_\rho^2}[P(\rho_i^k + \epsilon, s_i^k) - 2P(\rho_i^k, s_i^k) + P(\rho_i^k - \epsilon, s_i^k)],\\
\frac{\partial^2 P_i^k}{\partial \rho \partial s} &= \frac{1}{4\epsilon_\rho\epsilon_s}[P(\rho_i^k + \epsilon_\rho, s_i^k + \epsilon_s) - P(\rho_i^k + \epsilon_\rho, s_i^k - \epsilon_s)\\
&\quad - P(\rho_i^k - \epsilon_\rho, s_i^k + \epsilon_s) + P(\rho_i^k - \epsilon_\rho, s_i^k - \epsilon_s)],
\end{aligned}$$

where ϵ_ρ and ϵ_s are suitable small numbers (in our case, $\epsilon_\rho = 0.1$ and $\epsilon_s = 100$). The approximations for $\frac{\partial P_i^k}{\partial s}$ and $\frac{\partial^2 P_i^k}{\partial s^2}$ are analogous. The approximation for $\frac{\partial P}{\partial \rho}$ from Taylor series expansion about $(\rho^k,\, s^k)$ leads to

$$\frac{\partial P^{k+1}}{\partial \rho} - \frac{\partial P^k}{\partial \rho} = (\rho^{k+1} - \rho^k)\frac{\partial^2 P^k}{\partial \rho^2} + (s^{k+1} - s^k)\frac{\partial^2 P^k}{\partial \rho \partial s}.$$

The expression $\left(\frac{\partial T^{k+1}}{\partial s} - \frac{\partial T^k}{\partial s}\right)$ is defined in a similar way. Using these values in equation (16), we get

$$\begin{aligned}
&\frac{1}{\Delta t}\int (\rho^k - \rho^{\tau-1} + \delta\rho)\phi dx \\
&+ \frac{K}{\mu}\int_\Omega \left[\rho^k \frac{\partial P^k}{\partial \rho}\frac{\partial \rho^k}{\partial x} + \frac{\partial P^k}{\partial \rho}\frac{\partial \rho^k}{\partial x}\delta\rho \right.\\
&\left. + \rho^k \frac{\partial \rho^k}{\partial x}\left(\delta\rho \frac{\partial^2 P^k}{\partial \rho^2} + \delta s \frac{\partial^2 P^k}{\partial \rho \partial s}\right) + \rho^k \frac{\partial P^k}{\partial \rho}\frac{\partial(\delta\rho)}{\partial x}\right]\frac{d\phi}{dx}dx \\
&+ \frac{K}{\mu}\int_\Omega \left[\rho^k \frac{\partial P^k}{\partial s}\frac{\partial s^k}{\partial x} + \frac{\partial P^k}{\partial s}\frac{\partial s^k}{\partial x}\delta\rho \right.\\
&\left. + \rho^k \frac{\partial s^k}{\partial x}\left(\delta\rho \frac{\partial^2 P^k}{\partial \rho \partial s} + \delta s \frac{\partial^2 P^k}{\partial s^2}\right) + \rho^k \frac{\partial P^k}{\partial s}\frac{\partial(\delta s)}{\partial x}\right]\frac{d\phi}{dx}dx = 0.
\end{aligned}$$

Now, we rearrange these terms into explicit and implicit parts

$$\begin{aligned}
&\frac{1}{\Delta t}\int \delta\rho\phi dx + \frac{K}{\mu}\int_\Omega \left(\frac{\partial P^k}{\partial \rho}\frac{\partial \rho^k}{\partial x}\delta\rho + \rho^k \frac{\partial \rho^k}{\partial x}\frac{\partial^2 P^k}{\partial \rho^2}\delta\rho + \rho^k \frac{\partial P^k}{\partial \rho}\frac{\partial(\delta\rho)}{\partial x}\right.\\
&\left.+ \frac{\partial P^k}{\partial s}\frac{\partial s^k}{\partial x}\delta\rho + \rho^k \frac{\partial s^k}{\partial x}\frac{\partial^2 P^k}{\partial \rho \partial s}\delta\rho\right)\frac{d\phi}{dx}dx \\
&+ \frac{K}{\mu}\int_\Omega \left(\rho^k \frac{\partial \rho^k}{\partial x}\frac{\partial^2 P^k}{\partial \rho \partial s}\delta s + \rho^k \frac{\partial s^k}{\partial x}\frac{\partial^2 P^k}{\partial s^2}\delta s + \rho^k \frac{\partial P^k}{\partial s}\frac{\partial(\delta s)}{\partial x}\right)\frac{d\phi}{dx}dx \\
&+ \frac{1}{\Delta t}\int (\rho^k - \rho^{\tau-1})\phi dx + \frac{K}{\mu}\int_\Omega \left(\rho^k \frac{\partial P^k}{\partial \rho}\frac{\partial \rho^k}{\partial x} + \rho^k \frac{\partial P^k}{\partial s}\frac{\partial s^k}{\partial x}\right)\frac{d\phi}{dx}dx = 0.
\end{aligned}$$

We apply the Standard Galerkin discretization by using approximations, $\delta\rho \approx \sum_{j=1}^N \delta\rho_j \phi_j$, $\delta s \approx \sum_{j=1}^N \delta s_j \phi_j$ and choosing $\phi \approx \phi_i$

$$\begin{aligned}
&\frac{1}{\Delta t}\sum_{j=1}^N \delta\rho_j \int \phi_i\phi_j dx + \frac{K}{\mu}\sum_{j=1}^N \delta\rho_j \int_\Omega \left(\frac{\partial P^k}{\partial \rho}\frac{\partial \rho^k}{\partial x}\phi_j + \rho^k \frac{\partial \rho^k}{\partial x}\frac{\partial^2 P^k}{\partial \rho^2}\phi_j + \rho^k \frac{\partial P^k}{\partial \rho}\frac{d\phi_j}{dx}\right.\\
&\left.+ \frac{\partial P^k}{\partial s}\frac{\partial s^k}{\partial x}\phi_j + \rho^k \frac{\partial s^k}{\partial x}\frac{\partial^2 P^k}{\partial \rho \partial s}\phi_j\right)\frac{d\phi_i}{dx}dx \\
&+ \frac{K}{\mu}\sum_{j=1}^N \delta s_j \int_\Omega \left(\rho^k \frac{\partial \rho^k}{\partial x}\frac{\partial^2 P^k}{\partial \rho \partial s}\phi_j + \rho^k \frac{\partial s^k}{\partial x}\frac{\partial^2 P^k}{\partial s^2}\phi_j + \rho^k \frac{\partial P^k}{\partial s}\frac{d\phi_j}{dx}\right)\frac{d\phi_i}{dx}dx \\
&+ \frac{1}{\Delta t}\int (\rho^k - \rho^{\tau-1})\phi_i dx + \frac{K}{\mu}\int_\Omega \left(\rho^k \frac{\partial P^k}{\partial \rho}\frac{\partial \rho^k}{\partial x} + \rho^k \frac{\partial P^k}{\partial s}\frac{\partial s^k}{\partial x}\right)\frac{d\phi_i}{dx}dx = 0.
\end{aligned}$$

The equivalent matrix form of the above equation is given by

$$S_{11}\ \boldsymbol{\delta\rho} + S_{12}\ \boldsymbol{\delta s} + \boldsymbol{f}_1 = \boldsymbol{0}. \tag{17}$$

The element matrices are defined as

$$S_{11_e} = \frac{1}{\Delta t}\frac{\Delta x}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \frac{K}{2\mu}\frac{\partial \rho^k}{\partial x_i}\begin{bmatrix} -\frac{\partial P^k_{i-1}}{\partial \rho} & -\frac{\partial P^k_{i}}{\partial \rho} \\ \frac{\partial P^k_{i-1}}{\partial \rho} & \frac{\partial P^k_{i}}{\partial \rho} \end{bmatrix}$$
$$+ \frac{K}{2\mu}\frac{\partial \rho^k}{\partial x_i}\begin{bmatrix} -\rho^k_{i-1}\frac{\partial^2 P^k_{i-1}}{\partial \rho^2} & -\rho^k_{i}\frac{\partial^2 P^k_{i}}{\partial \rho^2} \\ \rho^k_{i-1}\frac{\partial^2 P^k_{i-1}}{\partial \rho^2} & \rho^k_{i}\frac{\partial^2 P^k_{i}}{\partial \rho^2} \end{bmatrix} + \frac{K}{2\mu\ \Delta x}\left(\rho^k_i\frac{\partial P^k_i}{\partial \rho} + \rho^k_{i-1}\frac{\partial P^k_{i-1}}{\partial \rho}\right)\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$
$$+ \frac{K}{2\mu}\frac{\partial s^k}{\partial x_i}\begin{bmatrix} -\frac{\partial P^k_{i-1}}{\partial s} & -\frac{\partial P^k_{i}}{\partial s} \\ \frac{\partial P^k_{i-1}}{\partial s} & \frac{\partial P^k_{i}}{\partial s} \end{bmatrix} + \frac{K}{2\mu}\frac{\partial s^k}{\partial x_i}\begin{bmatrix} -\rho^k_{i-1}\frac{\partial^2 P^k_{i-1}}{\partial \rho\ \partial s} & -\rho^k_{i}\frac{\partial^2 P^k_{i}}{\partial \rho\ \partial s} \\ \rho^k_{i-1}\frac{\partial^2 P^k_{i-1}}{\partial \rho\ \partial s} & \rho^k_{i}\frac{\partial^2 P^k_{i}}{\partial \rho\ \partial s} \end{bmatrix},$$

where $\frac{\partial \rho^k}{\partial x_i} = \frac{\rho^k_i - \rho^k_{i-1}}{\Delta x}$ and $\frac{\partial s^k}{\partial x_i} = \frac{s^k_i - s^k_{i-1}}{\Delta x}$.

$$S_{12_e} = \frac{K}{2\mu}\frac{\partial \rho^k}{\partial x_i}\begin{bmatrix} -\rho^k_{i-1}\frac{\partial^2 P^k_{i-1}}{\partial \rho\ \partial s} & -\rho^k_{i}\frac{\partial^2 P^k_{i}}{\partial \rho\ \partial s} \\ \rho^k_{i-1}\frac{\partial^2 P^k_{i-1}}{\partial \rho\ \partial s} & \rho^k_{i}\frac{\partial^2 P^k_{i}}{\partial \rho\ \partial s} \end{bmatrix} + \frac{K}{2\mu}\frac{\partial s^k}{\partial x_i}\begin{bmatrix} -\rho^k_{i-1}\frac{\partial^2 P^k_{i-1}}{\partial s^2} & -\rho^k_{i}\frac{\partial^2 P^k_{i}}{\partial s^2} \\ \rho^k_{i-1}\frac{\partial^2 P^k_{i-1}}{\partial s^2} & \rho^k_{i}\frac{\partial^2 P^k_{i}}{\partial s^2} \end{bmatrix}$$
$$+ \frac{K}{2\mu\ \Delta x}\left(\rho^k_i\frac{\partial P^k_i}{\partial s} + \rho^k_{i-1}\frac{\partial P^k_{i-1}}{\partial s}\right)\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix},$$

$$f^i_1 = \frac{1}{\Delta t}\int(\rho^k - \rho^\tau)\phi_i dx + \frac{K}{\mu}\int_\Omega\left(\rho^k\frac{\partial P^k}{\partial \rho}\frac{\partial \rho^k}{\partial x} + \rho^k\frac{\partial P^k}{\partial s}\frac{\partial s^k}{\partial x}\right)\frac{d\phi_i}{dx}dx,$$
$$\boldsymbol{f}_{1_e} = \frac{1}{\Delta t}\frac{\Delta x}{2}\begin{bmatrix} \rho^k_{i-1} - \rho^{\tau-1}_{i-1} \\ \rho^k_i - \rho^{\tau-1}_i \end{bmatrix} + \frac{K}{2\mu}\Bigg[\frac{\partial \rho^k}{\partial x_i}\left(\rho^k_i\frac{\partial P^k_i}{\partial \rho} + \rho^k_{i-1}\frac{\partial P^k_{i-1}}{\partial \rho}\right)$$
$$+\frac{\partial s^k}{\partial x_i}\left(\rho^k_i\frac{\partial P^k_i}{\partial s} + \rho^k_{i-1}\frac{\partial P^k_{i-1}}{\partial s}\right)\Bigg]\begin{bmatrix} -1 \\ 1 \end{bmatrix}.$$

3.2. **The energy equation.** As a next step, we treat the transformed energy equation (equation (11)) and write down its weak formulation

$$\int_\Omega \frac{\partial s}{\partial t}\phi d\phi - \frac{K}{\mu}\int_\Omega \frac{\partial}{\partial x}\left[s\left(\frac{\partial P}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial P}{\partial s}\frac{\partial s}{\partial x}\right)\right]\phi d\Omega$$
$$-\lambda\int_\Omega \frac{\partial}{\partial x}\left[\frac{\partial T}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial T}{\partial s}\frac{\partial s}{\partial x}\right]\phi d\Omega = 0.$$

Applying the product rule to second and third integral in the above equation, we have

$$\int_\Omega \frac{\partial s}{\partial t}\phi d\phi + \frac{K}{\mu}\int_\Omega\left[s\left(\frac{\partial P}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial P}{\partial s}\frac{\partial s}{\partial x}\right)\right]\frac{d\phi}{dx}d\Omega + \lambda\int_\Omega\left[\frac{\partial T}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial T}{\partial s}\frac{\partial s}{\partial x}\right]\frac{d\phi}{dx}d\Omega$$
$$+\frac{K}{\mu}\left[s\left(\frac{\partial P}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial P}{\partial s}\frac{\partial s}{\partial x}\right)\phi\right]_0^1 - \lambda\left[\frac{\partial T}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial T}{\partial s}\frac{\partial s}{\partial x}\right]_0^1 = 0.$$

The boundary terms vanish by applying the boundary conditions (equation (15)). For the time integration, we use Euler Backward formula

$$\frac{1}{\Delta t}\int_\Omega(s^\tau - s^{\tau-1})\phi dx + \frac{K}{\mu}\int_\Omega s^\tau\frac{\partial P^\tau}{\partial \rho}\frac{\partial \rho^\tau}{\partial x}\frac{d\phi}{dx}dx + \frac{K}{\mu}\int_\Omega s^\tau\frac{\partial P^\tau}{\partial s}\frac{\partial s^\tau}{\partial x}\frac{d\phi}{dx}dx$$
$$+\lambda\int_\Omega\frac{\partial T^\tau}{\partial \rho}\frac{\partial \rho^\tau}{\partial x}\frac{d\phi}{dx}dx + \lambda\int_\Omega\frac{\partial T^\tau}{\partial s}\frac{\partial s^\tau}{\partial x}\frac{d\phi}{dx}dx = 0.$$

Using linearization about ρ^k and s^k.

$$\frac{1}{\Delta t}\int_\Omega \left(s^k+\delta s - s^{\tau-1}\right)\phi dx$$
$$+\frac{K}{\mu}\int_\Omega \left[s^k\frac{\partial P^k}{\partial \rho}\frac{\partial \rho^k}{\partial x}+\delta s\frac{\partial P^k}{\partial \rho}\frac{\partial \rho^k}{\partial x}+s^k\left(\delta\rho\frac{\partial^2 P^k}{\partial \rho^2}+\delta s\frac{\partial^2 P^k}{\partial \rho\partial s}\right)\frac{\partial \rho^k}{\partial x}+s^k\frac{\partial P^k}{\partial \rho}\frac{\partial (\delta\rho)}{\partial x}\right]\frac{d\phi}{dx}dx$$
$$+\frac{K}{\mu}\int_\Omega \left[s^k\frac{\partial P^k}{\partial s}\frac{\partial s^k}{\partial x}+\delta s\frac{\partial P^k}{\partial s}\frac{\partial s^k}{\partial x}+s^k\left(\delta\rho\frac{\partial^2 P^k}{\partial \rho\partial s}+\delta s\frac{\partial^2 P^k}{\partial s^2}\right)\frac{\partial s^k}{\partial x}+s^k\frac{\partial P^k}{\partial s}\frac{\partial (\delta s)}{\partial x}\right]\frac{d\phi}{dx}dx$$
$$+\lambda\int_\Omega \left[\frac{\partial T^k}{\partial \rho}\frac{\partial \rho^k}{\partial x}+\left(\delta\rho\frac{\partial^2 T^k}{\partial \rho^2}+\delta s\frac{\partial^2 T^k}{\partial \rho\partial s}\right)\frac{\partial \rho^k}{\partial x}+\frac{\partial T^k}{\partial \rho}\frac{\partial (\delta\rho)}{\partial x}\right]\frac{d\phi}{dx}dx$$
$$+\lambda\int_\Omega \left[\frac{\partial T^k}{\partial s}\frac{\partial s^k}{\partial x}+\left(\delta\rho\frac{\partial^2 T^k}{\partial \rho\partial s}+\delta s\frac{\partial^2 T}{\partial s^2}\right)\frac{\partial s^k}{\partial x}+\frac{\partial T^k}{\partial s}\frac{\partial (\delta s)}{\partial x}\right]\frac{d\phi}{dx}dx=0.$$

Rearranging this equation so that the terms containing $\delta\rho$ come first, then the terms having δs, and lastly the explicit terms.

$$\frac{K}{\mu}\int\left(s^k\delta\rho\frac{\partial^2 P^k}{\partial \rho^2}\frac{\partial \rho^k}{\partial x}+s^k\frac{\partial P^k}{\partial \rho}\frac{\partial (\delta\rho)}{\partial x}+s^k\delta\rho\frac{\partial^2 P^k}{\partial \rho\partial s}\frac{\partial s^k}{\partial x}\right)\frac{d\phi}{dx}dx$$
$$+\lambda\int\left(\delta\rho\frac{\partial^2 T^k}{\partial \rho^2}\frac{\partial \rho^k}{\partial x}+\delta\rho\frac{\partial^2 T^k}{\partial \rho\partial s}\frac{\partial s^k}{\partial x}+\frac{\partial T^k}{\partial \rho}\frac{\partial (\delta\rho)}{\partial x}\right)\frac{d\phi}{dx}dx$$
$$+\frac{1}{\Delta t}\int\delta s\ \phi dx+\frac{K}{\mu}\int\left(\delta s\ \frac{\partial P^k}{\partial \rho}\frac{\partial \rho^k}{\partial x}+s^k\delta s\frac{\partial^2 P^k}{\partial \rho\partial s}\frac{\partial \rho^k}{\partial x}\right.$$
$$\left.+\delta s\frac{\partial P^k}{\partial s}\frac{\partial s^k}{\partial x}+s^k\delta s\frac{\partial^2 P^k}{\partial s^2}\frac{\partial s^k}{\partial x}+s^k\frac{\partial P^k}{\partial s}\frac{\partial (\delta s)}{\partial x}\right)\frac{d\phi}{dx}dx$$
$$+\lambda\int\left(\frac{\partial^2 T^k}{\partial \rho\partial s}\frac{\partial \rho^k}{\partial x}+\frac{\partial^2 T^k}{\partial s^2}\frac{\partial s^k}{\partial x}\right)\delta s\frac{d\phi}{dx}dx+\lambda\int\frac{\partial T^k}{\partial s}\frac{\partial (\delta s)}{\partial x}\frac{d\phi}{dx}dx$$
$$+\frac{1}{\Delta t}\int(s^k-s^{\tau-1})\phi dx+\frac{K}{\mu}\int s^k\left(\frac{\partial P^k}{\partial \rho}\frac{\partial \rho^k}{\partial x}+\frac{\partial P^k}{\partial s}\frac{\partial s^k}{\partial x}\right)\frac{d\phi}{dx}dx$$
$$+\lambda\int\left(\frac{\partial T^k}{\partial \rho}\frac{\partial \rho^k}{\partial x}+\frac{\partial T^k}{\partial s}\frac{\partial s^k}{\partial x}\right)\frac{d\phi}{dx}dx=0.$$

Applying the approximation for $\delta\rho$ and δs as defined in the case of mass equation, we have

$$\frac{K}{\mu}\sum_{j=1}^N\delta\rho_j\int\left(s^k\frac{\partial^2 P^k}{\partial \rho^2}\frac{\partial \rho^k}{\partial x}\phi_j+s^k\frac{\partial P^k}{\partial \rho}\frac{\partial \phi_j}{\partial x}+s^k\frac{\partial^2 P^k}{\partial \rho\partial s}\frac{\partial s^k}{\partial x}\phi_j\right)\frac{d\phi_i}{dx}dx$$
$$+\lambda\sum_{j=1}^N\delta\rho_j\int\left(\frac{\partial^2 T^k}{\partial \rho^2}\frac{\partial \rho^k}{\partial x}+\frac{\partial^2 T^k}{\partial \rho\partial s}\frac{\partial s^k}{\partial x}\right)\phi_j\frac{d\phi_i}{dx}dx+\lambda\sum_{j=1}^N\delta\rho_j\int\frac{\partial T^k}{\partial \rho}\frac{d\phi_i}{dx}\frac{d\phi_j}{dx}dx$$
$$+\frac{1}{\Delta t}\sum_{j=1}^N\delta s_j\int\phi_i\phi_j dx+\frac{K}{\mu}\sum_{j=1}^N\delta s_j\int\left(\frac{\partial P^k}{\partial \rho}\frac{\partial \rho^k}{\partial x}\phi_j+s^k\frac{\partial^2 P^k}{\partial \rho\partial s}\frac{\partial \rho^k}{\partial x}\phi_j\right.$$
$$\left.+\frac{\partial P^k}{\partial s}\frac{\partial s^k}{\partial x}\phi_j+s^k\frac{\partial^2 P^k}{\partial s^2}\frac{\partial s^k}{\partial x}\phi_j+s^k\frac{\partial P^k}{\partial s}\frac{\partial \phi_j}{\partial x}\right)\frac{d\phi_i}{dx}dx$$
$$+\lambda\sum_{j=1}^N\delta s_j\int\left(\frac{\partial^2 T^k}{\partial \rho\partial s}\frac{\partial \rho^k}{\partial x}+\frac{\partial^2 T^k}{\partial s^2}\frac{\partial s^k}{\partial x}\right)\phi_j\frac{d\phi_i}{dx}dx+\lambda\sum_{j=1}^N\delta s_j\int\frac{\partial T^k}{\partial s}\frac{d\phi_i}{dx}\frac{d\phi_j}{dx}dx$$
$$+\frac{1}{\Delta t}\int(s^k-s^{\tau-1})\phi_i dx+\frac{K}{\mu}\int\left(s^k\frac{\partial P^k}{\partial \rho}\frac{\partial \rho^k}{\partial x}+s^k\frac{\partial P^k}{\partial s}\frac{\partial s^k}{\partial x}\right)\frac{d\phi_i}{dx}dx$$
$$+\lambda\int\left(\frac{\partial T^k}{\partial \rho}\frac{\partial \rho^k}{\partial x}+\frac{\partial T^k}{\partial s}\frac{\partial s^k}{\partial x}\right)\frac{d\phi_i}{dx}dx=0.$$

The equivalent matrix form is given by

$$S_{21}\ \boldsymbol{\delta\rho} + S_{22}\ \boldsymbol{\delta s} + \boldsymbol{f}_2 = 0. \tag{18}$$

The element matrices are defined as

$$\begin{aligned} S_{21}^{ij} =& \frac{K}{\mu} \int \left(s^k \frac{\partial^2 P^k}{\partial \rho^2} \frac{\partial \rho^k}{\partial x} \phi_j + s^k \frac{\partial P^k}{\partial \rho} \frac{\partial \phi_j}{\partial x} + s^k \frac{\partial^2 P^k}{\partial \rho \partial s} \frac{\partial s^k}{\partial x} \phi_j \right) \frac{d\phi_i}{dx} dx \\ &+ \lambda \int \left(\frac{\partial^2 T^k}{\partial \rho^2} \frac{\partial \rho^k}{\partial x} + \frac{\partial^2 T^k}{\partial \rho \partial s} \frac{\partial s^k}{\partial x} \right) \phi_j \frac{d\phi_i}{dx} dx + \lambda \int \frac{\partial T^k}{\partial \rho} \frac{d\phi_i}{dx} \frac{d\phi_j}{dx} dx \end{aligned}$$

or

$$\begin{aligned} S_{21_e} =& \frac{K}{2\Delta x\ \mu} \left(s_{i-1}^k \frac{\partial P_{i-1}^k}{\partial \rho} + s_i^k \frac{\partial P_i^k}{\partial \rho} \right) \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} + \frac{K}{2\mu} \frac{\partial \rho_i^k}{\partial x} \begin{bmatrix} -s_{i-1}^k \frac{\partial^2 P_{i-1}^k}{\partial \rho^2} & -s_i^k \frac{\partial^2 P_i^k}{\partial \rho^2} \\ s_{i-1}^k \frac{\partial^2 P_{i-1}^k}{\partial \rho^2} & s_i^k \frac{\partial^2 P_i^k}{\partial \rho^2} \end{bmatrix} \\ &+ \frac{K}{2\mu} \frac{\partial s_i^k}{\partial x} \begin{bmatrix} -s_{i-1}^k \frac{\partial^2 P_{i-1}^k}{\partial \rho \partial s} & -s_i^k \frac{\partial^2 P_i^k}{\partial \rho \partial s} \\ s_{i-1}^k \frac{\partial^2 P_{i-1}^k}{\partial \rho \partial s} & s_i^k \frac{\partial^2 P_i^k}{\partial \rho \partial s} \end{bmatrix} + \frac{\lambda}{2} \frac{\partial \rho_i^k}{\partial x} \begin{bmatrix} -\frac{\partial^2 T_{i-1}^k}{\partial \rho^2} & -\frac{\partial^2 T_i^k}{\partial \rho^2} \\ \frac{\partial^2 T_{i-1}^k}{\partial \rho^2} & \frac{\partial^2 T_i^k}{\partial \rho^2} \end{bmatrix} \\ &+ \frac{\lambda}{2} \frac{\partial s_i^k}{\partial x} \begin{bmatrix} -\frac{\partial^2 T_{i-1}^k}{\partial \rho \partial s} & -\frac{\partial^2 T_i^k}{\partial \rho \partial s} \\ \frac{\partial^2 T_{i-1}^k}{\partial \rho \partial s} & \frac{\partial^2 T_i^k}{\partial \rho \partial s} \end{bmatrix} + \frac{\lambda}{2\Delta x} \left(\frac{\partial T_{i-1}^k}{\partial \rho} + \frac{\partial T_i^k}{\partial \rho} \right) \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}. \end{aligned}$$

Similarly, the element matrix for S_{22} is computed as

$$\begin{aligned} S_{22}^{ij} =& \frac{1}{\Delta t} \int \phi_i \phi_j dx + \frac{K}{\mu} \int \left(\frac{\partial P^k}{\partial \rho} \frac{\partial \rho^k}{\partial x} \phi_j + s^k \frac{\partial^2 P^k}{\partial \rho \partial s} \frac{\partial \rho^k}{\partial x} \phi_j \right. \\ &+ \left. \frac{\partial P^k}{\partial s} \frac{\partial s^k}{\partial x} \phi_j + s^k \frac{\partial^2 P^k}{\partial s^2} \frac{\partial s^k}{\partial x} \phi_j + s^k \frac{\partial P^k}{\partial s} \frac{\partial \phi_j}{\partial x} \right) \frac{d\phi_i}{dx} dx \\ &+ \lambda \int \left(\frac{\partial^2 T^k}{\partial \rho \partial s} \frac{\partial \rho^k}{\partial x} + \frac{\partial^2 T^k}{\partial s^2} \frac{\partial s^k}{\partial x} \right) \phi_j \frac{d\phi_i}{dx} dx + \lambda \int \frac{\partial T^k}{\partial s} \frac{d\phi_i}{dx} \frac{d\phi_j}{dx} dx \end{aligned}$$

or

$$\begin{aligned} S_{22_e} =& \frac{1}{\Delta t} \frac{\Delta x}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \frac{K}{2\Delta x\ \mu} \left(s_{i-1}^k \frac{\partial P_{i-1}^k}{\partial s} + s_i^k \frac{\partial P_i^k}{\partial s} \right) \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \\ &+ \frac{K}{2\mu} \frac{\partial \rho_i^k}{\partial x} \begin{bmatrix} -\frac{\partial P_{i-1}^k}{\partial \rho} & -\frac{\partial P_i^k}{\partial \rho} \\ \frac{\partial P_{i-1}^k}{\partial \rho} & \frac{\partial P_i^k}{\partial \rho} \end{bmatrix} + \frac{K}{2\mu} \frac{\partial \rho_i^k}{\partial x} \begin{bmatrix} -\frac{\partial^2 - s_{i-1}^k P_{i-1}^k}{\partial \rho \partial s} & -s_i^k \frac{\partial^2 P_i^k}{\partial \rho \partial s} \\ \frac{\partial^2 s_{i-1}^k P_{i-1}^k}{\partial \rho \partial s} & s_i^k \frac{\partial^2 P_i^k}{\partial \rho \partial s} \end{bmatrix} \\ &+ \frac{K}{2\mu} \frac{\partial s_i^k}{\partial x} \begin{bmatrix} -\frac{\partial P_{i-1}^k}{\partial s} & -\frac{\partial P_i^k}{\partial s} \\ \frac{\partial P_{i-1}^k}{\partial s} & \frac{\partial P_i^k}{\partial s} \end{bmatrix} + \frac{K}{2\mu} \frac{\partial s_i^k}{\partial x} \begin{bmatrix} -s_{i-1}^k \frac{\partial^2 P_{i-1}^k}{\partial s^2} & -s_i^k \frac{\partial^2 P_i^k}{\partial s^2} \\ s_{i-1}^k \frac{\partial^2 P_{i-1}^k}{\partial s^2} & s_i^k \frac{\partial^2 P_i^k}{\partial s^2} \end{bmatrix} \\ &+ \frac{\lambda}{2} \frac{\partial \rho_i^k}{\partial x} \begin{bmatrix} -\frac{\partial^2 T_{i-1}^k}{\partial \rho \partial s} & -\frac{\partial^2 T_i^k}{\partial \rho \partial s} \\ \frac{\partial^2 T_{i-1}^k}{\partial \rho \partial s} & \frac{\partial^2 T_i^k}{\partial \rho \partial s} \end{bmatrix} + \frac{\lambda}{2} \frac{\partial s_i^k}{\partial x} \begin{bmatrix} -\frac{\partial^2 T_{i-1}^k}{\partial s^2} & -\frac{\partial^2 T_i^k}{\partial s^2} \\ \frac{\partial^2 T_{i-1}^k}{\partial s^2} & \frac{\partial^2 T_i^k}{\partial s^2} \end{bmatrix} \\ &+ \frac{\lambda}{2\Delta x} \left(\frac{\partial T_{i-1}^k}{\partial s} + \frac{\partial T_i^k}{\partial s} \right) \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}. \end{aligned}$$

The element vector, containing the explicit terms, is given by

$$\begin{aligned} f_2^i =& \frac{1}{\Delta t} \int (s^k - s^{\tau-1}) \phi_i dx + \frac{K}{\mu} \int \left(s^k \frac{\partial P^k}{\partial \rho} \frac{\partial \rho^k}{\partial x} + s^k \frac{\partial P^k}{\partial s} \frac{\partial s^k}{\partial x} \right) \frac{d\phi_i}{dx} dx \\ &+ \lambda \int \left(\frac{\partial T^k}{\partial \rho} \frac{\partial \rho^k}{\partial x} + \frac{\partial T^k}{\partial s} \frac{\partial s^k}{\partial x} \right) \frac{d\phi_i}{dx} dx = 0, \end{aligned}$$

or

$$\boldsymbol{f}_{2_e} = \frac{1}{\Delta t}\frac{\Delta x}{2}\left[\begin{array}{c} s_{i-1}^k - s_{i-1}^{\tau-1} \\ \\ s_i^k - s_i^{\tau-1} \end{array}\right] + \frac{K}{2\mu}\frac{\partial \rho_i^k}{\partial x}\left(s_{i-1}^k \frac{\partial P_{i-1}^k}{\partial \rho} + s_i^k \frac{\partial P_i^k}{\partial \rho}\right)\left[\begin{array}{c} -1 \\ 1 \end{array}\right]$$
$$+ \frac{K}{2\mu}\frac{\partial s_i^k}{\partial x}\left(s_{i-1}^k \frac{\partial P_{i-1}^k}{\partial s} + s_i^k \frac{\partial P_i^k}{\partial s}\right)\left[\begin{array}{c} -1 \\ 1 \end{array}\right] + \frac{\lambda}{2}\frac{\partial \rho_i^k}{\partial x}\left(\frac{\partial T_{i-1}^k}{\partial \rho} + \frac{\partial T_i^k}{\partial \rho}\right)\left[\begin{array}{c} -1 \\ 1 \end{array}\right]$$
$$+ \frac{\lambda}{2}\frac{\partial s_i^k}{\partial x}\left(\frac{\partial T_{i-1}^k}{\partial s} + \frac{\partial T_i^k}{\partial s}\right)\left[\begin{array}{c} -1 \\ 1 \end{array}\right].$$

3.3. **Comparison of numerical results from two approaches.** Equations (17) and (18) can be written in the following matrix form

$$\left[\begin{array}{cc} S_{11} & S_{12} \\ S_{21} & S_{22} \end{array}\right]\left[\begin{array}{c} \boldsymbol{\delta\rho} \\ \boldsymbol{\delta s} \end{array}\right] = -\left[\begin{array}{c} \boldsymbol{f}_1 \\ \boldsymbol{f}_2 \end{array}\right]. \tag{19}$$

or

$$\boldsymbol{G}^{k+1} = \boldsymbol{G}^k - J^{-1}\boldsymbol{F}, \tag{20}$$

where J is the Jacobian matrix. Furthermore

$$J = \left[\begin{array}{cc} S_{11} & S_{12} \\ S_{21} & S_{22} \end{array}\right], \qquad \boldsymbol{F} = \left[\begin{array}{c} \boldsymbol{f}_1 \\ \boldsymbol{f}_2 \end{array}\right], \qquad \boldsymbol{G}^k = \left[\begin{array}{c} \rho^k \\ s^k \end{array}\right].$$

Equation (20) is solved by a direct method (Gaussian elimination). Here, we give a comparison between the two-equation approach and the original 6-equation system. In Figure 4, the relative difference of density, total enthalpy, and temperature are provided. The number of Newton iteration per time step is also presented. From these results, we conclude that the two-equation model is an equivalent representation of the system given by equations (1) to (6).

4. Approximation by a linear system

We approximate the two-equation model by a linear system in the following way. As a first step, the constants a, b, c, and d are computed from $\{(T, X_G)|280 \le T \le 360,\ 0 \le X_G \le 1\}$. Their value is given by

$$A = \left[\begin{array}{cc} a & b \\ c & d \end{array}\right] = \left[\begin{array}{cc} D_{11} & D_{12} \\ D_{21} & D_{22} \end{array}\right] = \left[\begin{array}{cc} \frac{K}{\mu}\rho\frac{\partial P}{\partial \rho} & \frac{K}{\mu}\rho\frac{\partial P}{\partial s} \\ \frac{K}{\mu}s\frac{\partial P}{\partial \rho} + \lambda\frac{\partial T}{\partial \rho} & \frac{K}{\mu}s\frac{\partial P}{\partial s} + \lambda\frac{\partial T}{\partial s} \end{array}\right].$$

These constants are used in the approximate system, given as

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left(a\frac{\partial \rho}{\partial x} + b\frac{\partial s}{\partial x}\right),$$
$$\frac{\partial s}{\partial t} = \frac{\partial}{\partial x}\left(c\frac{\partial \rho}{\partial x} + d\frac{\partial s}{\partial x}\right).$$

We compute the eigenvalues of A to determine the stability of this linear system. Let λ be an eigenvalue of A, then it is computed as

$$|A - \lambda I| = 0,$$

where I is a unity matrix of 2×2. Hence, we solve

$$(a - \lambda)(d - \lambda) - bc = 0,$$
$$\lambda^2 - (a + d)\lambda + ad - bc = 0.$$

The solution is given by

$$\lambda = \frac{1}{2}\left(a + d \pm \sqrt{(a + d)^2 - 4(ad - bc)}\right).$$

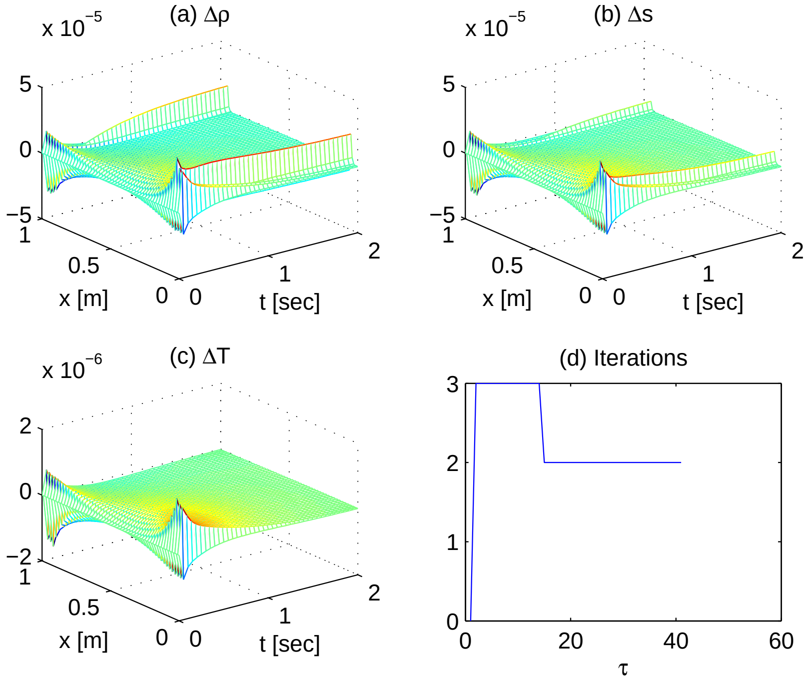

FIGURE 4. Comparison of two-equation model with the original system. The solution plots are (a) $\frac{\rho_j^{(1)}-\rho_j^{(2)}}{\rho_j^{(1)}}$, for $1 \le j \le 100$ and $0 \le t \le 2$ [*sec*], (b) $\frac{s_j^{(1)}-s_j^{(2)}}{s_j^{(1)}}$, (c) $\frac{T_j^{(1)}-T_j^{(2)}}{T_j^{(1)}}$, and (d) Newton iterations/timestep

We show that $ad = bc$ in the following expressions. Here we make use of the fact that $P = P(T)$, i.e., $\frac{\partial P}{\partial \rho} = \frac{\partial P}{\partial T}\frac{\partial T}{\partial \rho}$ and $\frac{\partial P}{\partial s} = \frac{\partial P}{\partial T}\frac{\partial T}{\partial s}$.

$$\begin{aligned} ad &= \frac{K}{\mu}\rho\frac{\partial P}{\partial \rho}\left(\frac{K}{\mu}s\frac{\partial P}{\partial s} + \lambda\frac{\partial T}{\partial s}\right), \\ &= \frac{K^2}{\mu^2}\rho s\frac{\partial P}{\partial \rho}\frac{\partial P}{\partial s} + \lambda\frac{K}{\mu}\rho\frac{\partial P}{\partial \rho}\frac{\partial T}{\partial s}, \\ &= \frac{K^2}{\mu^2}\rho s\frac{\partial P}{\partial \rho}\frac{\partial P}{\partial s} + \lambda\frac{K}{\mu}\rho\frac{\partial P}{\partial T}\frac{\partial T}{\partial \rho}\frac{\partial T}{\partial s}. \end{aligned} \tag{21}$$

Similarly

$$\begin{aligned} bc &= \frac{K}{\mu}\rho\frac{\partial P}{\partial s}\left(\frac{K}{\mu}s\frac{\partial P}{\partial \rho} + \lambda\frac{\partial T}{\partial \rho}\right), \\ &= \frac{K^2}{\mu^2}\rho s\frac{\partial P}{\partial s}\frac{\partial P}{\partial \rho} + \lambda\frac{K}{\mu}\rho\frac{\partial P}{\partial s}\frac{\partial T}{\partial \rho}, \\ &= \frac{K^2}{\mu^2}\rho s\frac{\partial P}{\partial s}\frac{\partial P}{\partial \rho} + \lambda\frac{K}{\mu}\rho\frac{\partial P}{\partial T}\frac{\partial T}{\partial s}\frac{\partial T}{\partial \rho}. \end{aligned} \tag{22}$$

Comparing expressions (21) and (22), we have

$$ad = bc.$$

Therefore, the eigen values of A are given by $\{0,\ \frac{K}{\mu}\rho\frac{\partial P}{\partial \rho} + \frac{K}{\mu}s\frac{\partial P}{\partial s} + \lambda\frac{\partial T}{\partial s}\}$ or equivalently

$$\lambda = \begin{cases} \{0,\ 0\} & \text{for } a+d = 0, \\ \{0,\ a+d\} & \text{for } a+d \neq 0. \end{cases}$$

It is difficult to find $a+d$ analytically. We numerically computed this value for the entire $(\rho,\ s)$-diagram, and it is given by $0.073 < a+d < 2.344$ for $0 \leq X_G \leq 1$ and $280 \leq T \leq 360$. Hence, the original system is unconditionally stable because $\lambda = \{0,\ \text{a positive value}\}$.

4.1. **Possibility of one state variable.** One of the two eigenvalues is zero for the entire phase diagram, hence the approximated linear system can be reformulated such that only one variable is sufficient to describe system dynamics. This can be achieved by diagonalization of A. Such conclusion can only be drawn for a linear system. However, we checked the possibility of one state variable, experimentally. Using the following initial conditions

$$T(x,0) = \begin{cases} 290 & \text{for } x \in [0, 0.05], \\ 290 + \frac{20}{9}x - \frac{1}{9} & \text{for } x \in]0.05, 0.95], \\ 292 & \text{for } x \in]0.95, 1], \end{cases}$$

$$X_G(x,0) = 0.2,$$

$$\Delta t = 1/100\ [s] \qquad \text{(time step)},$$

$$N = 100 \qquad \text{(mesh size)},$$

$$\Delta x = 1/(N-1) \qquad \text{(spatial step)},$$

$$\epsilon_r = 10^{-6} \qquad \text{(error tolerance on } \rho \text{ and } h),$$

$$K = 5 \times 10^{-11}\ [m^2],$$

$$\mu = 5 \times 10^{-5}\ [P_a\ s],$$

$$\lambda = 0.05\ [W/m/K],$$

$$t_{max} = 3.0\ [s] \qquad \text{(process time)}.$$

Figure 5 shows the relative difference between the initial and steady state value of

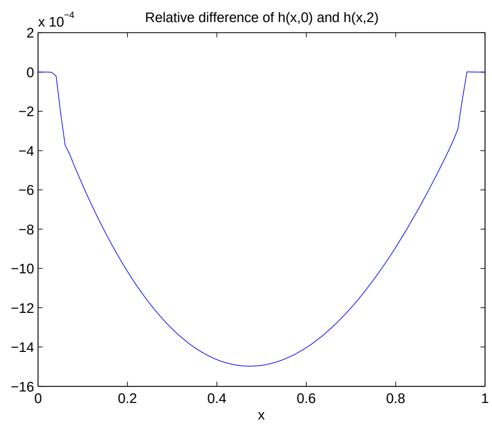

FIGURE 5. Relative difference between initial and steady-state h for original system.

h, when the above initial conditions are used by the original (6-equation) model. We do not observe a significant relative difference between the two values.

In an another experiment, we take only one equation i.e., the mass equation and ignore the energy equation. In other words, the original system is approximated by one equation only. The simulation results are comparable to the original model and they are given in Figure 6.

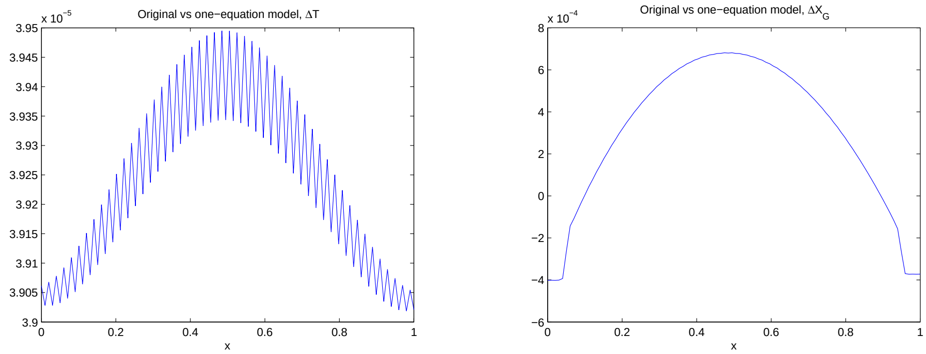

FIGURE 6. Comparison of variables from the original system and one-equation model at steady-state. (left) Relative difference in T and (right) relative difference in X_G.

4.2. **Gibbs Phase Rule.** Gibbs Phase Rule is given by the following relation

$$F = C + \Phi - 2,$$

where

F = number of degrees of freedom,

C = number of component (or substances),

Φ = number of phases in thermodynamic equilibrium with each other.

For our system, $C = 1$ because the only substance here is Propane, $\Phi = 2$, for a two phase flow. Therefore, the results we obtained are consistent with Gibbs Phase Rule i.e., one equation is sufficient to solve the system for a two phase flow.

5. CONCLUSIONS

The original system can be transformed to two-equation model. Which can further be approximated by a linear two-equation system. The eigenvalues of the linear system suggest that the original nonlinear system is stable for the given range of T and X_G. We also conclude that the system obeys Gibbs Phase Rule, at least for a two-phase flow.

REFERENCES

[1] A. R. J. Arendsen, A. I. van Berkel, A. B. M. Heesink, and G. F. Versteeg. Dynamic modelling of thermal processes with phase transitions by means of a density-enthalpy phase diagram. 7th World Congress of Chemical Engineering, Glasgow, Scotland, 2005.

[2] Ibrahim, F. J. Vermolen, and C. Vuik. Application of the numerical density-enthalpy method to the multi-phase flow through a porous medium. Procedia Computer S, cience 1 (2010) 781-790, Amsterdam, The Netherlands, 2010.

[3] A. R. J. Arendsen and G. F. Versteeg. Dynamic modelling of refrigeration cycles using density and enthalpy as state variables. 17th International Congress of Chemical and Process Engineering, Prague, The Czech Republic, 2006.

[4] A. R. J. Arendsen and G. F. Versteeg. Dynamic Thermodynamics with Internal Energy, Volume, and Amount of Moles as States: Application to Liquefied Gas Tank. Ind. Eng. Chem. Res. 2009, 48, 3167-3176.

[5] M. Fabbri and V. R. Voller. The Phase-Field Method in the Sharp-Interface Limit: A comparison between Model Potentials. Journal of Computational Physics, 1997.

[6] A. Abouhafç. Finite Element Modeling Of Thermal Processes With Phase Transitions. Master Thesis, 2007, Delft University of Technology.

[7] Ibrahim, C. Vuik, F.J. Vermolen, D. Hegen. Numerical Methods for Industrial Flow Problems. Delft University of Technology, Report 08-13, 2008.

[8] E. Javierre, C. Vuik, F. J. Vermolen, S. van der Zwaag. A comparison of numerical models for one-dimensional Stefan problems. J. Comp. Appl. Math., 2006, 192, 445-459.

[9] H. Emmerich. The Diffuse Interface Approach in Materials Science, Thermodynamic Concepts and Applications of Phase-Field Models. Springer, Berlin, 2003.

[10] J.H. Brusche, A. Segal, and C. Vuik. An efficient numerical method for solid-liquid transitions in optical rewritable recording. International Journal for Numerical Methods in Engineering, 77, pp. 702-718, 2009.

[11] O.C. Zienkiewicz, R.L. Taylor, & J.Z. Zhu. The Finite Element Method, Its Basis & Fundamentals. 6e, Butterworth-Heinemann, 2005.

[12] K. A. Hoffmann. Computational Fluid Dynamics, Vol I. 4e, EES, Wichita, USA, 2000.

[13] J. van Kan, A Segal, F. Vermolen. Numerical Methods in Scientific Computing. VSSD, 2004.

[14] R. J. Leveque. Finite Volume Methods for Hyperbolic Problems. Cambridge University Press, USA, 2002.

[15] J.N. Reddy. An Introduction to the Finite Element Method. 2e, McGraw-Hill, 1993.

[16] Ibrahim, C. Vuik, F.J. Vermolen, D. Hegen. Numerical Methods for Industrial Flow Problems. Delft University of Technology, Report 09-10, 2009.

[17] H. S. Udaykumar, R. Mittal, and Wei Shyy. Computation of SolidLiquid Phase Fronts in the Sharp Interface Limit on Fixed Grids. Journal of Computational Physics, 153, 1999, 535574.

[18] H. S. Udaykumar, R. Mittal, and W. Shyy. Computation of SolidLiquid Phase Fronts in the Sharp Interface Limit on Fixed Grids. Journal of Computational Physics 153, 1999, 535-574.

[19] S. Chen , B. Merriman , S. Osher , P. Smereka. A simple level set method for solving Stefan problems. Journal of Computational Physics, v.135 n.1, p.8-29, July 15, 1997.

[20] S. Osher , J. A. Sethian. Fronts propagating with curvature-dependent speed: algorithms based on Hamilton-Jacobi formulations. Journal of Computational Physics, v.79, pp.12-49, Nov. 1988.

[21] A. Faghri, Y. Zhang, J. Howell. Advanced Heat and Mass Transfer. Global Digital Press, 2010.

[22] B. Nedjar. An enthalpy-based finite element method for nonlinear heat problems involving phase change. Comput. Struct. 80 (2002) 9-21.

[23] G. Comini, S. DelGiudice, B. W. Lewis, O. C. Zienkiewicz. Finite element solution of non-linear heat conduction problems with special reference to phase change. Int. J. Numer. Meth. Engng., 8, pp. 613624, 1974.

[24] G. Segal, C. Vuik and F. J. Vermolen. A conserving discretization for the free boundary in a two-dimensional Stefan problem. J. Comp. Phys., 141, pp. 1-21, 1998.

[25] Ibrahim, F. J. Vermolen, C. Vuik. Numerical Methods for Industrial Flow Problems. Delft University of Technology, Report 10-23, 2010.