Application of the density-enthalpy method to the multi-phase flow through a porous medium

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Summary

A new method to solve multi-phase fluid flow problems is developed at TNO and presented in [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 Chem. Eng., Glasgow, 2005] for spatially homogeneous systems. In the current paper, we apply this method for up to $2D$ fluid systems by using finite elements for spatial discretization. The density-enthalpy method eliminates the requirement of separate sets of equations for various phases and necessitates fewer parametric assumptions.

Keywords: multi-phase, porous medium, finite elements, density-enthalpy phase diagram

1.   Introduction

In this paper, a new method for modeling multi-phase flows, is presented for 0-, 1- and 2-dimensional fluid systems. We will call this method *the density-enthalpy method* because a density-enthalpy phase diagram (henceforth ρ-h diagram) plays an important role in it. Physical models for multi-phase fluid systems in porous media have applications in industrial processes such as drying, steam production, and freezing. These models are meant to simulate the processes and to enhance the quality of products. Food items, in general, can be considered as porous medium (bread, potato etc). In the context of the density-enthalpy method, Arendsen has presented many applications in his work [1, 2, 3] (a boiler system, potato drying etc). The so called Stefan problems are typically solved by methods such as the level-set, moving-grid, and the phase-field model. For the description, application, and the comparison of these models, see [6, 7, 8] and the references therein. Level-set and moving-grid models use a sharp interface between adjacent phases. In contrast, the phase-field model allows a diffuse region where, for example, the mass density between the two coexisting phases varies smoothly from one phase to the other [7]. Advantages and disadvantages of common approaches for modeling thermal processes with phase change are compared with the density-enthalpy method in [1, 2]. It is common practice to solve the heat or mass balance equations alone or to assume constant boiling pressure and temperature. Arendsen also explained that only taking heat or mass balance is valid for a limited range and that their physical basis is incomplete. Furthermore, the assumption of constant ambient pressure and a fixed phase-change temperature profile cannot always be justified [1, 4]. Another drawback of the aforementioned approaches is that they keep track of the phase change, which might take place only for a small time interval as compared to the whole process. Then these methods switch to another set of equations with a change in phase, which might cause numerical instabilities.

In this paper we use the mass and energy balances together and use density and enthalpy as our state variables. These coupled partial differential equations are solved by using finite elements, with a Streamline Upwind Petrov-Galerkin approach for the convective part. A ρ-h diagram is then used to determine temperature, pressure and mass fractions [1]. The obtained results are explained qualitatively on the basis of physical laws. This method does not require a constant ambient pressure or a constant phase change temperature. In our view, the density-enthalpy method is potentially a better approach to model multi-phase fluid systems.

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2. Problem Definition

We consider the flow of propane (C_3H_8) in a unit square and the ρ-h diagrams used are therefore only for this substance. The mathematical model for the two-dimensional system is given by the following partial differential equations.

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v}) = 0, \quad \underline{x} \in \Omega, \ t > t_0, \qquad \text{(mass conservation)}, \qquad (1)$$

$$\frac{\partial(\rho h)}{\partial t} + \vec{\nabla} \cdot (\rho h \vec{v}) = \vec{\nabla} \cdot (\lambda \vec{\nabla} T) + q, \quad \underline{x} \in \Omega, \ t > t_0, \qquad \text{(energy conservation)}, \qquad (2)$$

$$\vec{v} = -\frac{K}{\mu} \vec{\nabla} P, \qquad \text{(Darcy Law)}, \qquad (3)$$

where the permeability K, dynamic viscosity μ, and heat diffusivity λ are assumed to be constants and q is a heat source. We neglected gravitational effects. Density (ρ) and enthalpy (h) are taken as state variables. All other variables, temperature (T), pressure (P), and gas mass fraction (X_G) are computed by using the ρ-h diagram [1]. Along with initial conditions, we use Robin boundary conditions. The external mass transfer is proportional to the difference in the internal density (ρ) and the ambient density (ρ_a),

$$\rho \vec{v}.\vec{n} = k_m(\rho - \rho_a), \quad t > t_0, \ \underline{x} \in \Gamma,$$

where k_m is a mass transfer coefficient. The heat transport across the boundaries takes place if there is a difference in temperature or a difference in density, across boundaries, i.e.,

$$(\rho h)\vec{v}.\vec{n} = \begin{cases} h|_\Gamma k_m(\rho - \rho_a), & \text{if } \rho - \rho_a > 0 \text{ on } \Gamma, \\ h_a k_m(\rho - \rho_a), & \text{if } \rho - \rho_a < 0 \text{ on } \Gamma, \end{cases} \qquad \text{(heat transport, convective part)},$$

$$\lambda \vec{\nabla} T.\vec{n} = k_h(T - T_a), \qquad\qquad t > t_0, \ \underline{x} \in \Gamma, \ \text{(heat transport, diffusive part)},$$

where $\vec{n}$ is a unit vector normal to the boundary Γ and k_h is a heat transfer coefficient. For the one-dimensional case, we assume that there is no mass and heat gradient in y and z-directions.

3. Method Description

In the domain Ω, the density is approximated by,

$$\rho(\underline{x}, t) \approx \sum_{j=1}^{N} \rho_j(t)\phi_j(\underline{x}),$$

where $\phi_j(\underline{x})$ is a piecewise linear basis function and $\rho_j(t)$ is the nodal density. We take $s = \rho h$ and discretize all variables in a similar way. For the computation of the mass matrix $M^{(1)}$, the stiffness matrix $S^{(1)}$ and the vector $F^{(1)}$, we refer to [5]. The semi-discrete, weak form corresponding to equation (1) is given by,

$$M^{(1)}\frac{d\underline{\rho}}{dt} = S^{(1)}\underline{\rho} + \underline{F}^{(1)}.$$

Following similar arguments, the weak form resulted from equation (2) is given by,

$$M^{(2)}\frac{d\underline{s}}{dt} = S^{(2)}\underline{s} + \underline{F}^{(2)}.$$

The velocity $\vec{v}$ is determined as a post processing step. For the time discretization of the given matrix equations, we use a semi-implicit scheme.

Once the system given by equations (1)-(3) is solved for h and ρ, the ρ-h diagram is used to find P, T, and X_G.

4. Numerical Results

In our numerical experiments, we used various boundary and initial conditions to simulate several thermodynamic systems. This included, for example, an isolated system for mass and heat ($k_m = 0$, $k_h = 0$), open system for mass ($k_m \neq 0$), open system for heat ($k_h \neq 0$), and open system for mass and heat etc. Simulation results for one of the experiments are given in Figure 1. This system is open to mass, that is, mass can flow
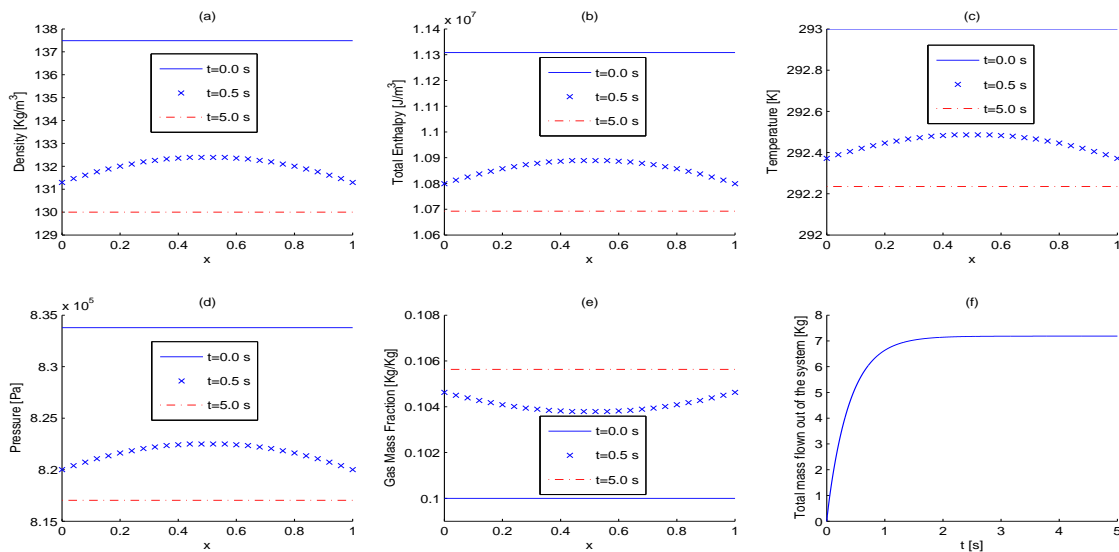

Figure 1: Plots of simulation results from a one-dimensional system open to mass, (a) density at t=0, 0.5, 5 sec, (b) total enthalpy, (c) temperature, (d) pressure, (e) gas mass fraction, and (f) total mass flown out of the system.

into the system or out of the system. In this experiment we use constant initial conditions, as shown in Figure 1(a)-(e). Since the density inside the system is higher than the ambient density, mass flows out. A decrease in density results in a decrease in total enthalpy (ρh) as well as in temperature (T) and pressure (P), as shown in Figure 1(b)-(d). An increase in the gas mass fraction (X_G) is the result of a decrease in the density (ρ). In Figure 1(f) a graph for the total mass transfer across the system boundaries is given. The time instant at which system's internal density becomes equal to the ambient density, mass transfer across boundaries stops. For the simulation of the two-dimensional fluid system, partially shown in Figure 2, we use the same initial and boundary conditions as we use for the one-dimensional configuration. In this figure, we have given graphs for ρ and h at various time instances (with a coarser grid). We do not observe a significant relative error when the numerical results obtained by using one-dimensional model are compared with the two-dimensional model.

As far as we know, an analytical solution of this system is not available. Numerical results, in general, are interpreted qualitatively on the basis of physical laws. In [1] a zero-dimensional system is compared with experimental data with a good matching. We also compared the zero-dimensional system with the one- and two-dimensional configurations (not shown in this abstract).

5. Conclusions and further work

It is concluded that the density-enthalpy method can successfully be applied, at least qualitatively, for multiphase fluid systems where we have certain spatial profiles for system variables. At this moment, the time discretization step Δt is too small, even with a coarse grid. An option is to use an adaptive Δt and an adaptive mesh. This is planned for future studies.
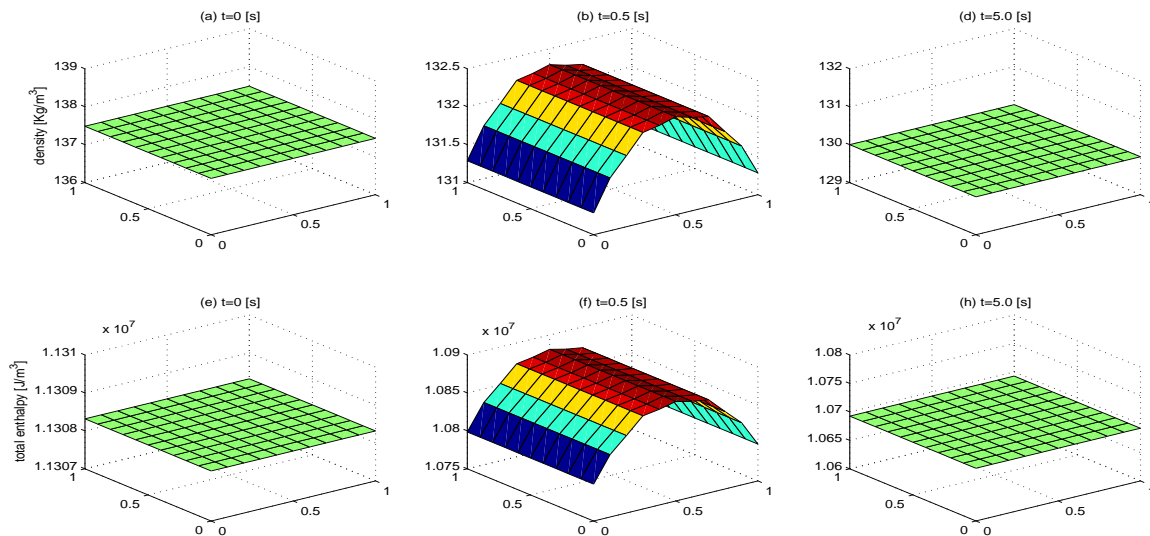
Figure 2: Plots of results from two-dimensional simulations for (up) the density at various instances, (down) total enthalpy.

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