

The mathematical structure of multiphase thermal models of flow in porous media

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This article is concerned with the formulation and numerical solution of equations for modelling multicomponent, two-phase, thermal fluid flow in porous media. The fluid model consists of individual chemical component (species) conservation equations, Darcy's law for volumetric flow rates and an energy equation in terms of enthalpy. The model is closed with an equation of state and phase equilibrium conditions that determine the distribution of the chemical components into phases. It is shown that, in the absence of diffusive forces, the flow equations can be split into a system of hyperbolic conservation laws for the species and enthalpy and a parabolic equation for pressure. This decomposition forms the basis of a sequential formulation where the pressure equation is solved implicitly and then the component and enthalpy conservation laws are solved explicitly. A numerical method based on this sequential formulation is presented and used to demonstrate some typical flow behaviour that occurs during fluid injection into a reservoir.

Keywords: porous media flow, multiphase flow, multicomponent flow, phase equilibrium, conservation laws

1. Introduction

This article is concerned with the mathematical formulation and numerical solution of systems of partial differential equations for multicomponent, two phase flow in porous media that include thermal effects. The latter are important in the numerical simulation of enhanced oil recovery processes such as steam flooding and *in situ* combustion. Relevant methodologies have been reported in recent papers by Liu *et al.* (2007), Huang *et al.* (2007), Pasarai *et al.* (2005), Nilsson *et al.* (2005) and Christensen *et al.* (2004). Thermal process simulation also plays an important role in the modelling of geothermal reservoirs (the reader is referred to the recent survey by O'Sullivan *et al.* 2001). Modelling the behaviour and evaluating cleanup strategies for contaminants can also require the treatment of thermal processes, see for example Class *et al.* (2002) and the references cited therein for a survey of this type of application.

The development of solution methodologies for the simulation of complex subsurface thermal processes often leads to a compromise between accuracy and stabil-

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ity. Many of these thermal processes are characterised by sharp fronts propagating through the medium, which places stringent requirements on spatial and temporal resolution. However, the simulations also rely on an accurate coupling of a number of different processes, which places stringent requirements on process coupling and stability. The trend in recent years has been to place an emphasis on stability rather than spatial accuracy. Consequently, most approaches to thermal simulations are based on a fully-implicit formulation with lower-order implicit spatial differencing. Most of the approaches in the literature cited above are based on this type of strategy. It is also worth mentioning the work of Christensen *et al.* (2004) and Nilsson *et al.* (2005), who utilise adaptive mesh techniques to improve spatial resolution.

The goal of the present work is to develop an algorithm for modelling multiphase, multicomponent non-isothermal reacting flows that achieves a better balance between stability and accuracy. As part of this development, we will examine the mathematical structure of these types of flows which provides the basis for applying contemporary high-resolution upwind methodology in this context. Examples of this type of approach for the black-oil model are discussed in Bell *et al.* (1989). Similar types of discretization procedures are considered for compositional models in Mallison *et al.* (2003).

The approach taken here was used previously to analyse the structure of black-oil (Trangenstein & Bell 1989*a*) and compositional (Trangenstein & Bell 1989*b*) models for reservoir simulation. It represents a generalisation of the classical derivation of the Buckley-Leverett equation, see for example Peaceman (1977). As in the development of compositional models by Trangenstein & Bell (1989*b*) the following analysis relies heavily on the mathematical structure of the multiphase multicomponent phase behaviour. The treatment of phase behaviour for non-isothermal systems using an optimisation framework is discussed in Brantferger (1991*a*) as part of the development of a fully implicit thermal-compositional solver and in Michelsen (1999).

The rest of the paper is structured as follows. In section 2, we review the basic equations for multiphase, non-isothermal flow in porous media and discuss the structure of the phase equilibrium problem. In section 3 the sequential splitting of the flow equations is introduced. This sequential form separates the system into a parabolic pressure equation and a system of conservation laws for the chemical constituents of the fluid and the enthalpy of the rock / fluid system. We show in section 4 that, in the absence of capillary pressure and diffusive transport, this system of conservation laws is hyperbolic. We develop a numerical algorithm based on this formulation in section 5. Finally we present numerical results based on the sequential formulation that illustrate the behaviour of the interacting waves encountered in the system. These examples serve to validate the sequential formulation and illustrate the types of wave behaviour associated with this type of system.

2. Mathematical formulation

In this section, we present the basic flow equations describing non-isothermal, multiphase, multicomponent flows in heterogeneous porous media. The porosity of the medium is denoted by ϕ , and the phase volume of each phase per pore volume is denoted u_α . Greek subscripts refer to mobile phases. (The medium itself, which can be viewed as a solid phase is given a distinguished treatment since it is immobile.)

The multicomponent mixture is composed of N components (or lumped pseudo-components) and we define \mathbf{n}_α as the vector of moles of each component in phase α divided by the pore volume. Thus, $\sum_\alpha \mathbf{n}_\alpha \equiv \mathbf{n}$ is the total number of moles per pore volume of these components in the combined fluid system. (Mineral content of the solid is, of course, important for geochemistry but is not included in these definitions.)

Flow equations

The flow is governed by the equations of mass and energy conservation and by Darcy's law, which gives the volumetric flow rate, \vec{v}_α , of each phase in terms of the phase pressure, p_α

$$\vec{v}_\alpha = -\frac{Kk_{r,\alpha}}{\eta_\alpha}(\nabla p_\alpha - \rho_\alpha \vec{g}) \equiv -\lambda_\alpha(\nabla p_\alpha - \rho_\alpha \vec{g}) \quad (2.1)$$

where K is the permeability of the medium, $k_{r,\alpha}$ is the relative permeability, which expresses the modification of the flow rate from multiphase effects, η_α and ρ_α are the phase viscosity and density, respectively, and \vec{g} is the gravitational force. Here $\lambda_\alpha \equiv Kk_{r,\alpha}/\eta_\alpha$ is the phase mobility. The pressure in each phase is related to a reference pressure, p (typically taken to be the most wetting phase), by a capillary pressure, $p_{c,\alpha} = p_\alpha - p$, which is a function of saturation.

Conservation of mass for each component is given by

$$\frac{\partial(\phi \mathbf{n})}{\partial t} + \nabla \cdot \sum_\alpha \frac{\mathbf{n}_\alpha}{u_\alpha} \vec{v}_\alpha = \nabla \cdot \mathbf{D} + \mathbf{R}_n \quad (2.2)$$

Here \mathbf{D} are diffusive terms that include multiphase molecular diffusion and dispersion and \mathbf{R}_n are reaction terms. Both the diffusion and reaction terms can be quite complex, depending on the particular problem, see for example Chen *et al* (2006) for a detailed discussion of these terms.

For non-isothermal systems it is necessary to include the energy conservation in the system of equations. The overall energy balance must include energy in the solid phase. If we assume that the porous medium and the fluids are in thermal equilibrium, the energy balance is of the form

$$\frac{\partial H_t}{\partial t} + \nabla \cdot \sum_\alpha \frac{\vec{v}_\alpha}{u_\alpha} \mathbf{n}_\alpha^T \mathbf{h}_\alpha = \nabla \cdot \vec{q} + R_H \quad , \quad (2.3)$$

where $H_t = (1 - \phi)\rho_r H_r + \phi \sum_\alpha \mathbf{n}_\alpha^T \mathbf{h}_\alpha$ is the total enthalpy of the system, \mathbf{h}_α are the partial molar phase enthalpies, H_r the enthalpy of the medium and ρ_r the density of the medium. Here \vec{q} represents diffusive energy transport processes such as thermal conduction and R_H represents energy release from reactions and external heating. If one does not assume the porous medium and the fluid are in thermal equilibrium, R_H will contain relaxation terms that equilibrate the two temperatures. In the above formulation we have omitted a term from the right hand side of the form

$$\frac{\partial \sum_\alpha p_\alpha u_\alpha}{\partial t} + \sum_\alpha \vec{v}_\alpha \cdot \nabla p_\alpha \quad .$$

Omitting this term implicitly assumes that the change in phase pressures is slow so that these terms can be ignored. We note that formulations based on internal energy make a similar assumption by dropping a term of the form

$$\sum_{\alpha} \vec{v}_{\alpha} \cdot \nabla p_{\alpha}$$

from the energy equation. For a more detailed derivation and discussion, the reader should refer to Burger *et al* (1985).

Phase behaviour

The component conservation and energy equations express the change in total mass of each component due to advection, diffusion and chemical reactions. Since components are being transported in phases, it is necessary to know the composition of the phases before we can solve the flow equations. This decomposition is referred to as the phase behaviour of the system. The phase behaviour is determined by saying that the equilibrium state of the mixture occurs at the point of maximum entropy. The entropy of the phases is derived from the chemical potential μ_{α} . These chemical potentials are typically specified in terms of an equation of state to model the dependence of pressure on temperature, composition and specific volume of the phase. For a more detailed discussion see Michelson & Mollerup (2004) and Brantferger *et al.* (1991b).

The chemical potentials μ_{α} are functions of p_{α} , T , and phase composition \mathbf{n}_{α} . Note that we have preserved the role of capillary pressure in determining the thermodynamic behaviour of the system. One simplification is to define the thermodynamics in terms of the reference pressure and retain capillary pressure effects only in the definition of phase velocities, see Brantferger *et al.* (1991b). Furthermore the major thermodynamic variables describing each phase can all be expressed in terms of the phase's chemical potential. In particular, the partial molar entropies are given by

$$\mathbf{s}_{\alpha} = - \left(\frac{\partial \mu_{\alpha}}{\partial T} \right)_{\mathbf{x}_{\alpha}, p_{\alpha}} \quad (2.4)$$

where $\mathbf{x}_{\alpha} = \mathbf{n}_{\alpha} / \mathbf{e}^T \mathbf{n}_{\alpha}$ are the mole fractions, $\mathbf{e} = (1, 1, \dots, 1)^T$, and the partial molar enthalpies are given by

$$\mathbf{h}_{\alpha} = (\mu_{\alpha} + T \mathbf{s}_{\alpha}) \quad . \quad (2.5)$$

Here the phase equilibrium problem is to determine the composition of the phases \mathbf{n}_{α} given the total moles \mathbf{n} , pressure P and the total enthalpy H_t . The equilibrium distribution of the components is given by minimising the negative entropy of the system. In a two-phase liquid and vapour case this becomes

$$\min [-S = -(\mathbf{n}_l^T \mathbf{s}_l + \mathbf{n}_v^T \mathbf{s}_v)]$$

subject to

$$\mathbf{n} = \mathbf{n}_l + \mathbf{n}_v$$

and

$$H_t = (1 - \phi) \rho_r h_r + \phi (\mathbf{n}_l^T \mathbf{h}_l + \mathbf{n}_v^T \mathbf{h}_v)$$

along with inequality constraints ($\mathbf{n}_\alpha \geq 0$) guaranteeing non-negativity of the compositions and thermal stability of the fluid ($\mathbf{n}_\alpha^T \frac{\partial \mathbf{h}_\alpha}{\partial T} > 0$). As noted above, if we do not consider the solid and the fluids to be in thermal equilibrium then we hold the total fluid enthalpy, $H_f = \mathbf{n}_l^T \mathbf{h}_l + \mathbf{n}_v^T \mathbf{h}_v$, constant rather than the total enthalpy.

Treatment of this minimisation problem, *i.e.* the so-called isenthalpic flash calculation, has been presented in the literature (Michelsen & Mollerup (2004); Michelsen (1999); Brantferger (1999a)) and will not be discussed in detail here. There are, however, a couple of key observations about the structure of the minimisation that will play a role later in the development of the sequential discretization. Firstly, the Hessian of the negative entropy is a rank one perturbation of the Hessian of the Gibbs free energy, which is minimised in an isothermal flash calculation. Consequently, it is computationally simple to compute one of these matrices given the other. Secondly, at equilibrium the chemical potentials are equal, *i.e.*,

$$\frac{1}{T} \boldsymbol{\mu}_l(\mathbf{x}_l, T, p_l) = \frac{1}{T} \boldsymbol{\mu}_v(\mathbf{x}_v, T, p_v) \quad (2.6)$$

Here, the chemical potentials are typically specified in terms of mole fractions rather than moles; however, we can use the definition of mole fractions to express them in this form.

In addition to determining the composition of the phases and the temperature, the phase behaviour also determines the properties of the phases. In particular, given pressure, temperature and component mass densities, we can compute the volume occupied by the phases. To complete the mathematical formulation of the system we require that the sum of the phase volumes match the available pore volume, which we will represent as

$$1 = U(p, T, \mathbf{n}) = \sum_{\alpha} u_{\alpha}(p_{\alpha}, T, \mathbf{n}_{\alpha}) \quad . \quad (2.7)$$

This equation plays the role of an equation of state that constrains the evolution of the component conservation and energy equations. Here we have implicitly used the capillary pressure to relate the phase pressures to the reference pressure.

3. The sequential formulation

In this section we present a sequential formulation of the above thermal / compositional model. This approach, based on a total velocity splitting with a pressure equation determined by differentiating the equation of state (2.7) was first introduced by Acs & Dolschal (1985). The methodology introduced here follows the development in Trangenstein & Bell (1989b) and, as such, represents a generalisation of that work to a non-isothermal setting. As in Brantferger (1991a), we will use pressure, total enthalpy and molar densities as the primary unknowns. The use of enthalpy as a primary unknown instead of temperature reflects its role as the conserved variable in the energy equation. This choice also avoids issues related to the Gibbs phase rule that can occur if there are more phases than components, in which case pressure and temperature cannot vary independently. However, it also introduces some complexity because many of the thermodynamic variables are given in terms of the temperature, T . In particular, the functional form of the enthalpy

is given by

$$H_t = H_t(\mathbf{n}, T, p) \quad . \quad (3.1)$$

We view this relationship as implicitly defining the temperature as a function of the molar densities, pressure and the enthalpy. We also note that for some of the analysis it will be convenient to derive an equation for temperature; however, in the numerical method, the enthalpy is the quantity that is advanced in time.

Formally, the dynamics evolves conservation equations for the chemical components and energy with phase velocities given by Darcy's law. The entire evolution is constrained by the equation of state.

Pressure equation

As in Acs & Dolshal (1985) and Trangenstein & Bell (1989b), we first derive a pressure equation to satisfy the total volume balance by taking the first order Taylor expansion in time of the pore volume constraint (equation of state)

$$1 = U(t + \delta t) = U(t) + \Delta t \frac{\partial U}{\partial t} + O(\Delta t^2) \quad . \quad (3.2)$$

Using the functional dependence of U on \mathbf{n} , p and H_t , we can express the constraint as

$$\left(\frac{\partial U}{\partial p} \right)_{\mathbf{n} H_t} \frac{\partial p}{\partial t} + \left(\frac{\partial U}{\partial \mathbf{n}} \right)_{p H_t} \frac{\partial \mathbf{n}}{\partial t} + \left(\frac{\partial U}{\partial H_t} \right)_{\mathbf{n} p} \frac{\partial H_t}{\partial t} = \frac{1 - U(t)}{\Delta t} \quad (3.3)$$

The pressure equation expresses how the pressure needs to change to enforce the equation of state, (2.7). Because of splitting errors, U is not necessarily unity at time t and the right hand side includes a forcing term that attempts to correct errors from previous times. It is more natural to rewrite equation (3.3) in terms of (T, p, \mathbf{n}) since many of the thermodynamic quantities are explicit functions of (T, p, \mathbf{n}) . Relationships between the partial derivatives can be derived by inverting the Jacobian matrix of the change of variables from (H_t, p, \mathbf{n}) to (T, p, \mathbf{n}) . This transformation is described in detail in appendix A. Using this transformation, we can rewrite equation (3.3) as

$$\begin{aligned} & - \left(\phi \left(\frac{\partial U}{\partial p} - \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \frac{\partial H_t}{\partial p} \right) - \frac{d\phi}{dp} \left(\frac{\partial U}{\partial \mathbf{n}} - \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \frac{\partial H_t}{\partial \mathbf{n}} \right) \mathbf{n} \right) \frac{\partial p}{\partial t} = \\ & \left(\frac{\partial U}{\partial \mathbf{n}} - \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \frac{\partial H_t}{\partial \mathbf{n}} \right) \frac{\partial(\phi \mathbf{n})}{\partial t} + \phi \left(\left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \right) \frac{\partial H_t}{\partial t} - \phi \frac{(1-U(t))}{\Delta t} \end{aligned} \quad (3.4)$$

where we have dropped the indices that indicated which variables are constant in the partial derivatives since it is always some combination of p, T and \mathbf{n} .

If we use the evolution equations for enthalpy and molar densities to substitute for the time derivatives on the right hand side of (3.4) we obtain the pressure equation

$$\begin{aligned} & - \left(\phi \left(\frac{\partial U}{\partial p} - \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \frac{\partial H_t}{\partial p} \right) - \frac{d\phi}{dp} \left(\frac{\partial U}{\partial \mathbf{n}} - \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \frac{\partial H_t}{\partial \mathbf{n}} \right) \mathbf{n} \right) \frac{\partial p}{\partial t} = \\ & - \left(\frac{\partial U}{\partial \mathbf{n}} - \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial H_t}{\partial \mathbf{n}} \frac{\partial U}{\partial T} \right) (\nabla \cdot \sum_{\alpha} \frac{\bar{v}_{\alpha}}{u_{\alpha}} \mathbf{n}_{\alpha} - \nabla \cdot \mathbf{D} - \mathbf{R}_n) \\ & - \phi \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} (\nabla \cdot \sum_{\alpha} \frac{\bar{v}_{\alpha}}{u_{\alpha}} \mathbf{n}_{\alpha}^T \mathbf{h}_{\alpha} - \nabla \cdot \vec{q} - R_H) - \phi \frac{(1-U(t))}{\Delta t} \end{aligned} \quad (3.5)$$

If we now express the phase velocities in terms of the pressure gradient, we obtain

$$\begin{aligned}
 & - \left(\phi \left(\frac{\partial U}{\partial p} - \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \frac{\partial H_t}{\partial p} \right) - \frac{d\phi}{dp} \left(\frac{\partial U}{\partial \mathbf{n}} - \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \frac{\partial H_t}{\partial \mathbf{n}} \right) \mathbf{n} \right) \frac{\partial p}{\partial t} = \\
 & \left(\frac{\partial U}{\partial \mathbf{n}} - \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \frac{\partial H_t}{\partial \mathbf{n}} \right) (\nabla \cdot \sum_{\alpha} \frac{\mathbf{n}_{\alpha} \lambda_{\alpha}}{u_{\alpha}} (\nabla p + \nabla p_{c,\alpha} - \rho_{\alpha} \vec{g}) - \nabla \cdot \mathbf{D} - \mathbf{R}_n) + \\
 & \phi \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} (\nabla \cdot \sum_{\alpha} \frac{\mathbf{n}_{\alpha}^T \mathbf{h}_{\alpha} \lambda_{\alpha}}{u_{\alpha}} (\nabla p + \nabla p_{c,\alpha} - \rho_{\alpha} \vec{g}) - \nabla \cdot \vec{q} - R_H) - \phi \frac{(1-U(t))}{\Delta t}
 \end{aligned} \tag{3.6}$$

This expresses the pressure equation in a form that is formally parabolic. A more detailed analysis of this equation is given below.

Component and energy conservation equations

In the incompressible case where ϕ and U are independent of pressure, it is possible to define the notion of a ‘‘total velocity’’ that allows us to decompose the dynamics into an elliptic pressure equation and, ignoring diffusion, a system of hyperbolic conservation laws. To preserve this behaviour in the more general compressible case we again split the equations by computing the total velocity \vec{v}_T . We can then re-express the phase velocities in terms of the total velocity and eliminate the explicit dependence of the phase velocities on the pressure gradient in the conservation equations. First we define \vec{v}_T as

$$\vec{v}_T \equiv \sum_{\alpha} \vec{v}_{\alpha} = - \sum_{\alpha} \lambda_{\alpha} (\nabla p_{\alpha} - \rho_{\alpha} \vec{g}) . \tag{3.7}$$

Then solving for ∇p in terms of \vec{v}_T , we express the phase velocity in terms of the total velocity,

$$\vec{v}_{\alpha} = \frac{\lambda_{\alpha}}{\lambda_T} \vec{v}_T + \lambda_{\alpha} \left(\rho_{\alpha} - \sum_{\beta} \frac{\lambda_{\beta} \rho_{\beta}}{\lambda_T} \right) \vec{g} - \lambda_{\alpha} \left(\nabla p_{c,\alpha} - \sum_{\beta} \frac{\lambda_{\beta} \nabla p_{c,\beta}}{\lambda_T} \right) , \tag{3.8}$$

where $\lambda_T = \sum_{\alpha} \lambda_{\alpha}$ is the total mobility. Finally writing the conservation equations in terms of the total velocity yields the fractional flow form of the chemical component conservation equations

$$\begin{aligned}
 & \frac{\partial(\phi \mathbf{n})}{\partial t} + \nabla \cdot \sum_{\alpha} \frac{\mathbf{n}_{\alpha}}{u_{\alpha}} \left[\frac{\lambda_{\alpha}}{\lambda_T} \vec{v}_T + \lambda_{\alpha} \left(\rho_{\alpha} - \sum_{\beta} \frac{\lambda_{\beta} \rho_{\beta}}{\lambda_T} \right) \vec{g} \right] = \\
 & \nabla \cdot \sum_{\alpha} \frac{\mathbf{n}_{\alpha}}{u_{\alpha}} \lambda_{\alpha} \left(\nabla p_{c,\alpha} - \sum_{\beta} \frac{\lambda_{\beta} \nabla p_{c,\beta}}{\lambda_T} \right) + \nabla \cdot \mathbf{D} + \mathbf{R}_n .
 \end{aligned} \tag{3.9}$$

and a fractional flow form of the energy conservation equation,

$$\begin{aligned}
 & \frac{\partial H_t}{\partial t} + \nabla \cdot \sum_{\alpha} \frac{\mathbf{n}_{\alpha}^T \mathbf{h}_{\alpha}}{u_{\alpha}} \left[\frac{\lambda_{\alpha}}{\lambda_T} \vec{v}_T + \lambda_{\alpha} \left(\rho_{\alpha} - \sum_{\beta} \frac{\lambda_{\beta} \rho_{\beta}}{\lambda_T} \right) \vec{g} \right] = \\
 & \nabla \cdot \sum_{\alpha} \frac{\mathbf{n}_{\alpha}^T \mathbf{h}_{\alpha}}{u_{\alpha}} \lambda_{\alpha} \left(\nabla p_{c,\alpha} - \sum_{\beta} \frac{\lambda_{\beta} \nabla p_{c,\beta}}{\lambda_T} \right) + \nabla \cdot \vec{q} + R_H .
 \end{aligned} \tag{3.10}$$

In this form the component conservation and energy equations form a system of nonlinear advection-diffusion equations where the diffusion is typically small relative to the advection.

4. Analysis of the sequential formulation

In the limit of no capillary pressure, diffusion or reactions, the sequential formulation discussed above splits the dynamics into a formally-parabolic pressure equation and a system of first-order conservation laws for the component conservation and energy equations. For this decomposition to be well-posed, we need to show that the pressure equation is, in fact, parabolic and show that the conservation laws for components and energy form a hyperbolic system. The wave structure associated with the hyperbolic system is also useful in the construction of high-resolution discretizations.

Thermodynamic derivatives

The structure of the equations is tightly coupled to the phase behaviour. Consequently, we need to understand how perturbations in the state variables are reflected in changes in the phase behaviour. In this section, we derive a number of useful relationships that will be needed later in the analysis. For a more detailed discussion of these derivations see Trangenstein & Bell (1989*b*) and Brantferger (1991*a*).

As in the case of the derivation of the pressure equation, the analysis is simplified by treating perturbations of the system in terms of p , \mathbf{n} and T rather than p , \mathbf{n} and H_t . When T is fixed instead of H_t , phase equilibrium perturbations in \mathbf{n} correspond to minimization of the Gibbs free energy rather than negative entropy. However, the similarity in structure of the different types of equilibrium computations makes it easy to obtain the necessary structure about the isothermal flash and no additional minimisation need occur.

From the phase equilibrium we define

$$M = \left. \frac{\partial \mathbf{n}_l}{\partial \mathbf{n}} \right|_{T,p}, \quad I - M = \left. \frac{\partial \mathbf{n}_v}{\partial \mathbf{n}} \right|_{T,p}$$

$$\mathbf{m}_T = \left. \frac{\partial \mathbf{n}_l}{\partial T} \right|_{\mathbf{n},p}, \quad \mathbf{m}_T = - \left. \frac{\partial \mathbf{n}_v}{\partial T} \right|_{\mathbf{n},p}$$

and

$$\mathbf{m}_p = \left. \frac{\partial \mathbf{n}_l}{\partial p} \right|_{\mathbf{n},T}, \quad \mathbf{m}_p = - \left. \frac{\partial \mathbf{n}_v}{\partial p} \right|_{\mathbf{n},T}$$

From the Gibbs-Duhem equation M is symmetric, $M\mathbf{n}_l = \mathbf{n}_l$ and $M\mathbf{n}_v = 0$.

Since the phase potentials are equal at equilibrium, we can differentiate (2.6) with respect to T to obtain

$$G\mathbf{m}_T = \left(\frac{\partial \mu_v}{\partial T} \right)_{p, \mathbf{n}_v} - \left(\frac{\partial \mu_l}{\partial T} \right)_{p, \mathbf{n}_l} = \frac{1}{T}(\mathbf{h}_l - \mathbf{h}_v) \quad (4.1)$$

where

$$G = \frac{\partial \mu_l}{\partial \mathbf{n}_l} + \frac{\partial \mu_v}{\partial \mathbf{n}_v}$$

Similarly,

$$G\mathbf{m}_p = \left(\frac{\partial \mu_v}{\partial p} \right)_{T, \mathbf{n}_v} - \left(\frac{\partial \mu_l}{\partial p} \right)_{T, \mathbf{n}_l} = -(\boldsymbol{\nu}_l - \boldsymbol{\nu}_v)$$

where ν_α are the phase specific volumes.

Other useful thermodynamic relationships are a consequence of first-degree homogeneity. A thermodynamic property is homogeneous of first degree if a multiplication of the composition by a scalar changes the property by the same scalar. Such quantities are typically expressed in the form

$$\Xi_\alpha = \mathbf{n}_\alpha^T \boldsymbol{\chi}_\alpha$$

and first degree homogeneity implies

$$\mathbf{n}_\alpha^T \frac{\partial \Xi_\alpha}{\partial \mathbf{n}_\alpha} = 0$$

First degree homogeneity holds for enthalpy, phase volumes, and phase specific volumes.

Parabolicity of the pressure equation

Using these relationships we can now analyse the pressure equation and the component conservation equations. Certain technical assumptions, which are typically true, are needed for the analysis. These additional assumptions will be noted in the discussion. To analyse the pressure equation, we need to first show that the coefficient multiplying $\frac{\partial p}{\partial t}$ in (3.6),

$$-\phi \left(\frac{\partial U}{\partial p} - \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \frac{\partial H_t}{\partial p} \right) + \frac{d\phi}{dp} \left(\frac{\partial U}{\partial \mathbf{n}} - \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \frac{\partial H_t}{\partial \mathbf{n}} \right) \mathbf{n}$$

is positive.

Mechanical and thermal stability of the fluid guarantee that

$$\frac{\partial U}{\partial p} \leq 0$$

and

$$\frac{\partial H_t}{\partial T} \geq 0$$

We expect that both $\frac{\partial H_t}{\partial p}$ and $\frac{\partial U}{\partial T}$ to be non negative. Thus, for validity of the present model we need to assume that

$$\frac{\partial U}{\partial p} - \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \frac{\partial H_t}{\partial p} \leq 0 \quad (4.2)$$

It is mentioned (see for example O'Connell & Haile (2005)) that the thermal expansion coefficient $\alpha = \frac{1}{U} \frac{\partial U}{\partial T}$ is in general positive for gases and liquids, except for water under 4°C and at atmospheric pressure. For low density gases $\alpha \approx \frac{1}{T}$ and it decreases with increasing pressure. For liquids α has values an order of magnitude smaller than $\frac{1}{T}$ and they are nearly constant over modest changes of temperature and pressure. One can also derive, using the Maxwell relations, that $\frac{\partial H_t}{\partial p} = U(1 - \alpha T)$ and thus for most liquids and gases $\frac{\partial H_t}{\partial p} > 0$ and $\frac{\partial U}{\partial T} > 0$.

Using first-degree homogeneity, the coefficient of $\frac{d\phi}{dp}$ can be rewritten as

$$U - \phi \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} H_f$$

since $\frac{d\phi}{dp} \geq 0$, we also need this term to be positive or dominated by the first term. U is approximately 1, but there is not enough information to deduce the sign of the RHS term. Thus, we need to assume that this term is positive as well or that the medium is incompressible or that the compressibility is sufficiently small to guarantee parabolicity of the pressure equation.

We must also show that the coefficient of the second-order term on the right hand side of 3.6,

$$\left(\frac{\partial U}{\partial \mathbf{n}} - \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \frac{\partial H_t}{\partial \mathbf{n}} \right) \nabla \cdot \sum_{\alpha} \frac{\mathbf{n}_{\alpha} \lambda_{\alpha}}{u_{\alpha}} \nabla p + \phi \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \nabla \cdot \sum_{\alpha} \frac{\mathbf{n}_{\alpha}^T \mathbf{h}_{\alpha} \lambda_{\alpha}}{u_{\alpha}} \nabla p, \quad (4.3)$$

defines a second-order elliptic equation. First we note that

$$\begin{aligned} & - \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \frac{\partial H_t}{\partial \mathbf{n}} \nabla \cdot \sum_{\alpha} \frac{\mathbf{n}_{\alpha} \lambda_{\alpha}}{u_{\alpha}} \nabla p + \phi \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \nabla \cdot \sum_{\alpha} \frac{\mathbf{n}_{\alpha}^T \mathbf{h}_{\alpha} \lambda_{\alpha}}{u_{\alpha}} \nabla p = \\ & \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \nabla \cdot \left[- \sum_{\alpha} \frac{\partial H_t}{\partial \mathbf{n}} \frac{\mathbf{n}_{\alpha} \lambda_{\alpha}}{u_{\alpha}} + \phi \sum_{\alpha} \frac{\mathbf{n}_{\alpha}^T \mathbf{h}_{\alpha} \lambda_{\alpha}}{u_{\alpha}} \right] \nabla p + \\ & \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \nabla \frac{\partial H_t}{\partial \mathbf{n}} \cdot \sum_{\alpha} \frac{\lambda_{\alpha}}{u_{\alpha}} \mathbf{n}_{\alpha} \nabla p = \left(\frac{\partial H_t}{\partial T} \right)^{-1} \frac{\partial U}{\partial T} \nabla \frac{\partial H_t}{\partial \mathbf{n}} \cdot \sum_{\alpha} \frac{\lambda_{\alpha}}{u_{\alpha}} \mathbf{n}_{\alpha} \nabla p \end{aligned}$$

which is a lower order term that does not effect parabolicity. Thus, the leading order term on the right hand side of the equation is

$$\begin{aligned} & \frac{\partial U}{\partial \mathbf{n}} \nabla \cdot \sum_{\alpha} \frac{\mathbf{n}_{\alpha} \lambda_{\alpha}}{u_{\alpha}} \nabla p = \nabla \cdot \frac{\partial U}{\partial \mathbf{n}} \sum_{\alpha} \frac{\mathbf{n}_{\alpha} \lambda_{\alpha}}{u_{\alpha}} \nabla p - \nabla \frac{\partial U}{\partial \mathbf{n}} \cdot \sum_{\alpha} \frac{\mathbf{n}_{\alpha} \lambda_{\alpha}}{u_{\alpha}} \nabla p = \\ & \nabla \cdot \lambda_T \nabla p - \nabla \frac{\partial U}{\partial \mathbf{n}} \cdot \sum_{\alpha} \frac{\mathbf{n}_{\alpha} \lambda_{\alpha}}{u_{\alpha}} \nabla p \end{aligned}$$

Thus the leading term on the right hand side of the pressure equation is $\nabla \cdot \lambda_T \nabla p$ so that right hand side of the pressure equation (3.6) is elliptic.

Hyperbolic structure

If we ignore the capillary pressure terms, the fractional flow form of the equations forms a nonlinear system of conservation laws for the enthalpy and the molar densities. The capillary pressure terms introduce a nonlinear diffusion term that is typically fairly small so that the behaviour of the system is typically transport dominated. For incompressible two-phase, two-component systems the fractional flow form of the equations reduces to the familiar Buckley-Leverett equation. For a solution and discussion see Collins (1961). The work of Trangenstein & Bell (1989a, b) shows that for both the three-phase black-oil model and for a two-phase compositional model the conservation laws resulting from a total velocity splitting, form a hyperbolic system in the limit of vanishing capillary pressure (subject to well-posedness conditions on the three-phase fractional flow modelling in the black-oil case). In this section, we demonstrate that the total velocity splitting leads to hyperbolicity in the compositional / thermal model as well. As in the case of isothermal compositional flow, the hyperbolicity is directly linked to thermodynamic consistency of the phase behaviour.

In this analysis we look at the component conservation equations (2.2) and the energy equation (2.3) in the absence of capillary pressure and other diffusion terms as well as reactions. In the sequential formulation, we view the pressure and total velocity as specifying a prescribed spatial dependence of the flux. In one space dimension, we can write the conservation equations in the form

$$\phi \frac{\partial \mathbf{n}}{\partial t} + \frac{\partial(\mathbf{n}_l \sigma_l + \mathbf{n}_v \sigma_v)}{\partial x} = l.o.t. \quad (4.4)$$

and

$$\frac{\partial H_t}{\partial t} + \frac{\partial(\mathbf{n}_l^T \mathbf{h}_l \sigma_l + \mathbf{n}_v^T \mathbf{h}_v \sigma_v)}{\partial x} = l.o.t \quad (4.5)$$

where the

$$\sigma_\alpha = \frac{1}{u_\alpha} \left[\frac{\lambda_\alpha}{\lambda_T} v_T + \lambda_\alpha (\rho_\alpha - \sum_\beta \frac{\lambda_\beta \rho_\beta}{\lambda_T}) \vec{g} \cdot \vec{e}_x \right]$$

represent the phase velocities and *l.o.t* denotes lower order terms that arise from dependence of the flux on the spatial coordinate either directly or through the spatial dependence on pressure and total velocity. These lower order terms do not affect hyperbolicity.

To show that the system is hyperbolic, we need to show that the eigenvalues of the linearised system, which correspond to wave speeds, are real. Although the dependent variables are the molar densities and enthalpy, it is more natural to perform the characteristic analysis in terms of the molar densities and the temperature. The characteristic structure can also be used to develop numerical discretization for the conservation laws.

When we recast the equations in terms of \mathbf{n} and T , we need to be able to perturb the species at constant temperature, not at constant enthalpy. As noted above, having already determined temperature from an isenthalpic flash calculation, we note that an isothermal flash at that specified temperature will produce the same phase compositions and will also satisfy equality of the phase potentials.

We can now linearize equation (4.4) ignoring lower order terms to obtain

$$\begin{aligned} \phi \frac{\partial \mathbf{n}}{\partial t} + \left[M \sigma_l + (I - M) \sigma_v + \mathbf{n}_l \frac{\partial \sigma_l}{\partial \mathbf{n}} + \mathbf{n}_v \frac{\partial \sigma_v}{\partial \mathbf{n}} \right] \frac{\partial \mathbf{n}}{\partial x} \\ + \left[(\sigma_l - \sigma_v) \mathbf{m}_T + \mathbf{n}_l \frac{\partial \sigma_l}{\partial T} + \mathbf{n}_v \frac{\partial \sigma_v}{\partial T} \right] \frac{\partial T}{\partial x} = 0 \end{aligned} \quad (4.6)$$

Similarly, linearization of the enthalpy equation without lower order terms leads to

$$\begin{aligned} \left[(1 - \phi) \rho_r \frac{\partial H_r}{\partial T} + \phi (\mathbf{n}_l^T \frac{\partial \mathbf{h}_l}{\partial T} + \mathbf{n}_v^T \frac{\partial \mathbf{h}_v}{\partial T} + (\mathbf{h}_l^T - \mathbf{h}_v^T) \mathbf{m}_T) \right] \frac{\partial T}{\partial t} \\ + \left[\sigma_l \mathbf{n}_l^T \frac{\partial \mathbf{h}_l}{\partial T} + \sigma_v \mathbf{n}_v^T \frac{\partial \mathbf{h}_v}{\partial T} + (\sigma_l \mathbf{h}_l^T - \sigma_v \mathbf{h}_v^T) \mathbf{m}_T + \mathbf{n}_l^T \mathbf{h}_l \frac{\partial \sigma_l}{\partial T} + \mathbf{n}_v^T \mathbf{h}_v \frac{\partial \sigma_v}{\partial T} \right] \frac{\partial T}{\partial x} \\ + \left[\sigma_l \mathbf{h}_l^T M + \sigma_v \mathbf{h}_v^T (I - M) + \mathbf{n}_l^T \mathbf{h}_l \frac{\partial \sigma_l}{\partial \mathbf{n}} + \mathbf{n}_v^T \mathbf{h}_v \frac{\partial \sigma_v}{\partial \mathbf{n}} \right] \frac{\partial \mathbf{n}}{\partial x} \\ + \phi [\mathbf{h}_l^T M + \mathbf{h}_v^T (I - M)] \frac{\partial \mathbf{n}}{\partial t} = 0 \end{aligned} \quad (4.7)$$

where we have used homogeneity of degree 1 of the partial molar enthalpies. We now substitute for $\frac{\partial \mathbf{n}}{\partial t}$ in equation (4.7) to obtain

$$c_p \frac{\partial T}{\partial t} + [(\sigma_l - \sigma_v)(\mathbf{h}_l^T - \mathbf{h}_v^T)M(I - M)] \frac{\partial \mathbf{n}}{\partial x} + \left[\sigma_l \mathbf{n}_l^T \frac{\partial \mathbf{h}_l}{\partial T} + \sigma_v \mathbf{n}_v^T \frac{\partial \mathbf{h}_v}{\partial T} + (\mathbf{h}_l^T - \mathbf{h}_v^T)(\sigma_l(I - M) + \sigma_v M) \mathbf{m}_T \right] \frac{\partial T}{\partial x} = 0 \quad (4.8)$$

where

$$c_p = (1 - \phi)c_p^r + \phi c_p^f = ((1 - \phi)\rho_r \frac{\partial h_r}{\partial T} + \phi(\mathbf{n}_l^T \frac{\partial \mathbf{h}_l}{\partial T} + \mathbf{n}_v^T \frac{\partial \mathbf{h}_v}{\partial T} + (\mathbf{h}_l^T - \mathbf{h}_v^T) \mathbf{m}_T))$$

Here we have used $M\mathbf{n}_l = \mathbf{n}_l$ and $M\mathbf{n}_v = \mathbf{0}$. (The definition of c_p above does not correspond to a standard definition of specific heat at constant pressure because it includes a mass scaling.)

The system can now be re-written in the following form

$$\begin{bmatrix} \phi & 0 \\ 0 & c_p \end{bmatrix} \begin{pmatrix} \mathbf{n} \\ T \end{pmatrix}_t + A \begin{pmatrix} \mathbf{n} \\ T \end{pmatrix}_x = 0 \quad (4.9)$$

where A is

$$A = \begin{pmatrix} [M\sigma_l + (I - M)\sigma_v + \mathbf{n}_l \frac{\partial \sigma_l}{\partial \mathbf{n}} + \mathbf{n}_v \frac{\partial \sigma_v}{\partial \mathbf{n}}] \\ [(\sigma_l - \sigma_v)(\mathbf{h}_l^T - \mathbf{h}_v^T)M(I - M)] \\ [\sigma_l \mathbf{n}_l^T \frac{\partial \mathbf{h}_l}{\partial T} + \sigma_v \mathbf{n}_v^T \frac{\partial \mathbf{h}_v}{\partial T} + (\mathbf{h}_l^T - \mathbf{h}_v^T)(\sigma_l(I - M) + \sigma_v M) \mathbf{m}_T] \end{pmatrix}$$

Hyperbolicity depends on A having real eigenvalues. There are two cases to consider, one in which only one phase is formed and a second in which both phases are formed. Before discussing these cases, we note that in specifying the system, we have overdetermined the system. One could, for example, eliminate one of the molar densities from the system and solve for the missing variable from the equation of state using the pressure, temperature and other densities. However, because of the splitting errors this approach is not conservative. By carrying all of the molar densities and H_t we are carrying some redundant information. This redundancy manifests itself as a fictitious wave that essentially only carries information about the consistency of the over specified system. In the present case, following Trangenstein & Bell (1989b), we have defined the decomposition so that the fictitious wave moves with zero speed.

Single phase fluid

For the case of single phase flow, which we arbitrarily pick to be liquid here, the matrix A takes the form

$$A = \begin{pmatrix} (I - \frac{\mathbf{n}}{u_l} \frac{\partial u_l}{\partial \mathbf{n}}) & -\frac{1}{u_l} \frac{\partial u_l}{\partial T} \mathbf{n} \\ 0 & \mathbf{n}^T \frac{\partial \mathbf{h}_l}{\partial T} \end{pmatrix} \frac{v_T}{u_l} \quad (4.10)$$

where $\mathbf{n}_l = \mathbf{n}$. The upper left hand corner is a rank one perturbation of the identity matrix. This corresponds to a projection onto the space orthogonal to \mathbf{n} since

$\frac{\partial u_l}{\partial \mathbf{n}} \mathbf{n}_l = u_l$ which follows from the homogeneity of degree one of the phase volumes. This corresponds to the fictitious wave that reflects the redundancy in the equation. Thus, A has a single eigenvalue of 0 corresponding to a right eigenvector $(\mathbf{n}, 0)$ and $N - 1$ eigenvalues of $\frac{v_T}{u_l}$ corresponding to right eigenvectors $(\mathbf{n}^\perp, 0)$ with $\frac{\partial u_l}{\partial \mathbf{n}} \mathbf{n}^\perp = 0$. Given the scaling in (4.9) this corresponds to wave speeds of $\frac{v_T}{\phi u_l}$.

The eigenvalue corresponding to the lower right hand corner of A is $c_p^f \frac{v_T}{u_l}$ with eigenvector $(\alpha \mathbf{n}_l, 1)^T$ where $\alpha = -\frac{1}{u_l c_p^f} \frac{\partial u_l}{\partial T}$. Given the scaling in (4.9) this corresponds to a wave speed of $\frac{c_p^f}{c_p} \frac{v_T}{u_l}$. This implies that the thermal wave will be lagged as a result of the heat capacity of the medium. We also note that in the case in which the fluid and the porous medium are not assumed to be in thermal equilibrium, the thermal wave speed is $\frac{v_T}{\phi u_l}$.

(i) *Two phase fluid*

The characteristic analysis of the two-phase flow case requires showing that A can be transformed into a symmetric matrix. This is not straightforward but the derivation can be considerably simplified by noticing that since we are doing the characteristic analysis in terms of \mathbf{n} and T , the upper left hand corner of A corresponds to the quasilinear form of the molar conservation equations in the compositional model analysed by Trangenstein & Bell (1989b). This motivates the following similarity transformation of A :

$$\tilde{A} = \begin{pmatrix} R_M^{-1} & 0 \\ 0 & 1 \end{pmatrix} A \begin{pmatrix} R_M & 0 \\ 0 & 1 \end{pmatrix},$$

where R_M is the matrix of right eigenvectors of M so that

$$M R_M = R_M \Lambda_M, \quad ,$$

and Λ_M is the diagonal matrix of eigenvalues.

Following Trangenstein and Bell, R_M can be defined as:

$$R_M = \left(\frac{\mathbf{n}_l}{u_l}, \frac{\mathbf{n}_v}{u_v}, \bar{R}_M \right)$$

In addition, we know that $R_M^{-1} \mathbf{n}_l = u_l \mathbf{e}_1$, $R_M^{-1} \mathbf{n}_v = u_v \mathbf{e}_2$, and

$$\Lambda_M = \begin{pmatrix} 1 & & \\ & 0 & \\ & & \Lambda_{\bar{K}} \end{pmatrix}.$$

We note that the eigenvectors corresponding to eigenvalues in $\Lambda_{\bar{K}}$ represent perturbations in composition, $\delta \mathbf{n}_l$, that are split between liquid and vapour phases such that

$$\delta n_k = \delta n_{k,l} + \delta n_{k,v}$$

where

$$\delta n_{k,l} = \lambda_k \delta n_k$$

Stability of the mixture with respect to composition implies $0 \leq \lambda_k \leq 1$ so that all of the entries in Λ_M are between zero and one. Applying this similarity transform to A , yields:

$$\tilde{A} = \begin{pmatrix} \sigma_l \Lambda_M + \sigma_v (I - \Lambda_M) + R_M^{-1} (\mathbf{n}_l \frac{\partial \sigma_l}{\partial \mathbf{n}} + \mathbf{n}_v \frac{\partial \sigma_v}{\partial \mathbf{n}}) R_M \\ (\sigma_l - \sigma_v) (\mathbf{h}_l^T - \mathbf{h}_v^T) R_M \Lambda_M (I - \Lambda_M) \\ \left[\sigma_l \mathbf{n}_l^T \frac{\partial \mathbf{h}_l}{\partial T} + \sigma_v \mathbf{n}_v^T \frac{\partial \mathbf{h}_v}{\partial T} + (\mathbf{h}_l^T - \mathbf{h}_v^T) (\sigma_l (I - M) + \sigma_v M) \mathbf{m}_T \right] \end{pmatrix}$$

Finally, \tilde{A} can be re-written:

$$\tilde{A} = \begin{pmatrix} V & Q & \mathbf{b} \\ 0 & \bar{\Lambda} & \mathbf{c} \\ \mathbf{0}^T & \mathbf{d}^T & e \end{pmatrix}, \quad (4.11)$$

where

$$\begin{aligned} V &= \begin{pmatrix} \sigma_l & 0 \\ 0 & \sigma_v \end{pmatrix} + u_l \mathbf{e}_1 \frac{\partial \sigma_l}{\partial \mathbf{n}} N D_u^{-1} + u_v \mathbf{e}_1 \frac{\partial \sigma_v}{\partial \mathbf{n}} N D_u^{-1} \\ Q &= u_l \mathbf{e}_1 \frac{\partial \sigma_l}{\partial \mathbf{n}} \bar{R}_M + u_v \mathbf{e}_2 \frac{\partial \sigma_v}{\partial \mathbf{n}} \bar{R}_M \\ \bar{\Lambda} &= \sigma_l \Lambda_{\bar{K}} + \sigma_v (I - \Lambda_{\bar{K}}) \\ \mathbf{b} &= \begin{pmatrix} u_l \frac{\partial \sigma_l}{\partial T} + \mathbf{e}_1^T (\sigma_l - \sigma_v) R_M^{-1} \mathbf{m}_T \\ u_v \frac{\partial \sigma_v}{\partial T} + \mathbf{e}_2^T (\sigma_l - \sigma_v) R_M^{-1} \mathbf{m}_T \end{pmatrix} \\ \mathbf{c} &= (\sigma_l - \sigma_v) P_R R_M^{-1} \mathbf{m}_T \\ \mathbf{d}^T &= (\sigma_l - \sigma_v) (\mathbf{h}_l^T - \mathbf{h}_v^T) R_M \Lambda_M (I - \Lambda_M) P_R^T \\ e &= \sigma_l \mathbf{n}_l^T \frac{\partial \mathbf{h}_l}{\partial T} + \sigma_v \mathbf{n}_v^T \frac{\partial \mathbf{h}_v}{\partial T} + (\mathbf{h}_l^T - \mathbf{h}_v^T) (\sigma_l (I - M) + \sigma_v M) \mathbf{m}_T, \end{aligned}$$

and $P_R = [\mathbf{0}, \mathbf{0}, I]$ is a $((n_c - 2) \times n_c)$ projection operator.

In Trangenstein & Bell (1989b), it was shown that there is a similarity transformation that diagonalises V , and its eigenvalues are real. One of these eigenvalues is zero and corresponds to the fictitious wave. The other is $\frac{\partial \sigma_v}{\partial S_v}$ where $S_v = u_v / (u_l + u_v)$ is the vapour saturation. This corresponds to the Buckley-Leverett-type wave. We now need to prove that there is a similarity transformation that symmetries the sub-matrix:

$$\tilde{A}_{sub} = \begin{pmatrix} \bar{\Lambda} & \mathbf{c} \\ \mathbf{d}^T & e \end{pmatrix}$$

from which we conclude that the eigenvalues of this sub-matrix should also be real. Thus, all eigenvalues of \tilde{A} would be real and the hyperbolicity is proved.

Substituting $\mathbf{h}_l^T - \mathbf{h}_v^T = T \mathbf{m}_T^T G$ into the expression for \mathbf{d}^T , we obtain

$$\mathbf{d}^T = T (\sigma_l - \sigma_v) \mathbf{m}_T^T G R_M \Lambda_M (I - \Lambda_M) P_R^T$$

Next we make use of the the following result, which can be derived by using several similarity transformations described in Trangenstein & Bell (1989b)

$$R_M^T G R_M = D^2, \quad ,$$

where D is

$$D \equiv \begin{pmatrix} \lambda_l & 0 & 0 \\ 0 & \lambda_v & 0 \\ 0 & 0 & I \end{pmatrix}$$

This result is then used to further re-write $\mathbf{m}_T^T G R_M$ as

$$\mathbf{m}_T^T G R_M = \mathbf{m}_T^T R_M^{-T} R_M^T G R_M = \mathbf{m}_T^T R_M^{-T} D^2 .$$

\tilde{A}_{sub} has now become

$$\tilde{A}_{sub} = \begin{pmatrix} \bar{\Lambda} & (\sigma_l - \sigma_v) P_R \mathbf{x} \\ T(\sigma_l - \sigma_v) \mathbf{x}^T D_s^2 P_R^T & e \end{pmatrix} ,$$

where $D_s = D \sqrt{\Lambda_M(I - \Lambda_M)}$, and $\mathbf{x} = R_M^{-1} \mathbf{m}_T$. Since the matrix $\sqrt{\frac{1}{T}} P_R D_s^{-1} P_R^T$ is non-singular, we can use it to define a final similarity transformation:

$$\hat{A}_{sub} = \begin{pmatrix} \left(\sqrt{\frac{1}{T}} P_R D_s^{-1} P_R^T \right)^{-1} & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix} \tilde{A}_{sub} \begin{pmatrix} \sqrt{\frac{1}{T}} P_R D_s^{-1} P_R^T & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix} ,$$

which results in

$$\hat{A}_{sub} = \begin{pmatrix} \bar{\Lambda} & \sqrt{T}(\sigma_l - \sigma_v) P_R D_s \mathbf{x} \\ \sqrt{T}(\sigma_l - \sigma_v) \mathbf{x}^T D_s P_R^T & e \end{pmatrix} \quad (4.12)$$

\hat{A}_{sub} is a symmetric matrix, therefore it has real eigenvalues and the system of linearised conservation laws is hyperbolic. This completes the derivation of hyperbolicity for the two-phase flow.

5. Discretization issues

In this section we present a numerical method for solving the thermal/compositional model described above. The intent here is to use the method to elucidate some of the wave phenomena associated with this type of system. For this reason we focus on a simplified version of the model. We consider only one-dimensional flows without gravity. We also assume that there is no capillary pressure or diffusive transport and that there are no reactions. With these assumptions we solve the conservation laws and the pressure equation on a uniform grid using a finite volume approach. A mesh is defined in the (x, t) -plane. The computational domain is restricted to $x \in [0, L]$. The points on the mesh are at locations $(x_i = i\Delta x, t^n = n\Delta t)$ with $i = 0, \dots, N_x$ and $n = 0, \dots, N_t$. The discrete values of $\vec{Q}(x, t)$ at $(i\Delta x + \Delta x/2, n\Delta t)$ will be denoted by \vec{Q}_i^n .

Pressure, enthalpy and component molar densities are defined on cell centres and the total velocity is defined on cell faces. In outline semi-discrete form, the algorithm for solving the conservation laws for components and enthalpy, equations (3.9,3.10), and the pressure equation (3.6) looks like:

1. Given a solution at t^n : $(p^n, H_t^n, \mathbf{n}^n)$, calculate phase equilibrium and hence $(T^n, \mathbf{n}_l^n, \mathbf{n}_v^n, V_l^n, V_v^n, \dots)$.

2. Solve pressure equation implicitly.

$$\frac{\partial p}{\partial t} + \dots = \frac{(1 - u_l^n - u_v^n)}{\Delta t} + \dots \text{ gives } p^{n+1}$$

3. Calculate v_T using p^{n+1} .

4. Solve component and enthalpy conservation eqs.

$$\begin{aligned} \frac{\partial \mathbf{n}}{\partial t} + \dots &= \dots \text{ gives } \mathbf{n}^{n+1} \\ \frac{\partial H_t}{\partial t} + \dots &= \dots \text{ gives } H_t^{n+1} \end{aligned}$$

5. Set $(p^n, H^n, \mathbf{n}^n) = (p^{n+1}, H^{n+1}, \mathbf{n}^{n+1})$ and go to STEP 1.

The different steps are described in more detail as follows:

Step 1: For the phase equilibrium calculation, an isenthalpic flash algorithm developed by Michelsen (1999) is used. The algorithm currently considers the fluid enthalpy, not the total enthalpy, in the minimisation of negative entropy, therefore we have incorporated an outer iteration to solve the full minimisation problem. In particular, we added an outer iteration to find T such that

$$H_t = (1 - \phi) c_p^r (T - T_{ref}^r) + \phi H_f \quad (5.1)$$

where H_f is at the minimum negative entropy. This nonlinear equation is solved using the secant method. Details of this additional step are described in appendix Appendix B.

Step 2: The pressure equation is treated implicitly, thus using a central-difference approximation equation (3.5) becomes

$$\begin{aligned} & \left[\phi \frac{\partial U}{\partial p} \right]_i^n \frac{p_i^{n+1} - p_i^n}{\Delta t} + \frac{1}{\Delta x^2} \left[\frac{\partial U}{\partial \mathbf{n}} \right]_i^n \left[\left(\sum_{\alpha=l,v} \frac{\mathbf{n}_\alpha}{u_\alpha} \frac{K k_{r,\alpha}}{\eta_\alpha} \right)_{i+\frac{1}{2}}^n (p_{i+1}^{n+1} - p_i^{n+1}) - \right. \\ & \left. \left(\sum_{\alpha=l,v} \frac{\mathbf{n}_\alpha}{u_\alpha} \frac{K k_{r,\alpha}}{\eta_\alpha} \right)_{i-\frac{1}{2}}^n (p_i^{n+1} - p_{i-1}^{n+1}) \right] + \phi \left[\frac{\partial U}{\partial H_t} \right]_i^n \frac{1}{\Delta x^2} \left[\left(\sum_{\alpha=l,v} \frac{\mathbf{n}_\alpha^T \mathbf{h}_\alpha}{u_\alpha} \frac{K k_{r,\alpha}}{\eta_\alpha} \right)_{i+\frac{1}{2}}^n \right. \\ & \left. (p_{i+1}^{n+1} - p_i^{n+1}) - \left(\sum_{\alpha=l,v} \frac{\mathbf{n}_\alpha^T \mathbf{h}_\alpha}{u_\alpha} \frac{K k_{r,\alpha}}{\eta_\alpha} \right)_{i-\frac{1}{2}}^n (p_i^{n+1} - p_{i-1}^{n+1}) \right] = \phi_i^n \frac{1 - U_i^n}{\Delta t} \end{aligned}$$

Quantities at the cell faces, *i.e.* $(\cdot)_{i+\frac{1}{2}}^n$, are calculated as an average of their respective cell centre values $(\cdot)_{i+\frac{1}{2}}^n = \frac{1}{2}((\cdot)_i^n + (\cdot)_{i+1}^n)$, hence no extra phase equilibrium calculation is needed. The discretized system is solved with a tridiagonal matrix solver.

Step 3: To calculate v_T the variables at time n are used except for calculating the pressure gradient in the definition of v_T , for which the pressure at time $n + 1$ is used. Consequently, the total velocity is discretized as

$$[v_T]_{i+\frac{1}{2}}^n = [\lambda_T]_{i+\frac{1}{2}}^n \frac{p_{i+1}^{n+1} - p_i^{n+1}}{\Delta x}$$

Step 4: This is a system of hyperbolic equations and we have used a simple first order (in time and space) conservative upwind scheme to solve it since our numerical examples are designed in such a way that all the eigenvalues are positive. Hence, the system of conservation laws

$$\frac{\partial Q}{\partial t} + \frac{\partial(Fv_T)}{\partial x} = 0$$

where

$$Q = \begin{pmatrix} \phi \mathbf{n} \\ H_t \end{pmatrix}, \quad F = \frac{1}{\lambda_T} \begin{pmatrix} \sum_{\alpha} \frac{\lambda_{\alpha}}{u_{\alpha}} \mathbf{n}_{\alpha} \\ \sum_{\alpha} \mathbf{h}_{\alpha}^T \mathbf{n}_{\alpha} \frac{\lambda_{\alpha}}{u_{\alpha}} \end{pmatrix}$$

is discretized using the first-order Godunov approach

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} \left([v_T]_{i+\frac{1}{2}}^n F_{i+\frac{1}{2}}^n - [v_T]_{i-\frac{1}{2}}^n F_{i-\frac{1}{2}}^n \right)$$

where strictly upwind fluxes are used

$$F_{i+\frac{1}{2}}^n = F_i^n$$

The above forms a basis for higher order discretisations; we will present appropriate methodologies in a future communication.

6. Numerical examples

In order to give a more quantitative description of the types of waves that can form in a realistic situations where flow velocities depend on pressure gradients, four test cases are calculated. They correspond to particular situations occurring during thermal recovery processes: hot gas, hot liquid and hot two-phase mixture injection.

In all four test cases the following parameters are used: number of grid points $N_x = 400$, reservoir length $L = 7620.0 [cm]$, permeability $\kappa = 2 \cdot 10^{-8} [cm^2]$, relative permeability $k_{r,\alpha} = s_{\alpha}^2$, rock reference temperature $T_{ref}^{rock} = 293 [K]$, liquid viscosity $\eta_l = 0.001 [Pa \cdot s]$, vapour viscosity $\eta_v = 6 \cdot 10^{-5} [Pa \cdot s]$. The values for other parameters like binary interaction parameters and critical properties etc. used in the Peng-Robinson equation of state can be found in Danesh (1998).

It is sometimes necessary to dampen the influence of the pressure correction term in the pressure equation (3.6) by a factor f_{press} ; e.g., use $f_{press} \cdot (1 - u_l - u_v)$ for the correction term. Normally we take $f_{press} = 1$. In Table (1) the values for pressure correction factor f_{press} , time step Δt and simulation time t are given.

The eigenvalues can be calculated in two ways. First, one can use the matrix A defined in equation (4.9), rescaled by ϕ, C_p . The other option is to use matrix \hat{A} in equation (4.11). The eigenvalues of matrix V are zero and the Buckley-Leverett wave which is $\frac{1}{\phi U} \frac{\partial v_v}{\partial s_v}$. Subsequently, only the eigenvalues of the matrix \hat{A}_{sub} in equation (4.12) are needed. The second system is a two by two system and can easily be solved analytically.

In the single phase case there are $N - 1$ essentially linearly degenerate waves with wave speed $\frac{v_T}{\phi u_l}$ and one linearly degenerate wave with wave speed zero. The ‘‘energy’’ wave with wave speed $\frac{v_T}{u_l C_p} \mathbf{n}_l^T \frac{\partial \mathbf{h}_l}{\partial T}$ is also nearly linearly degenerate but propagates at a reduced speed. If $\phi = 1$ then the thermal wave speed is also $\frac{v_T}{u_l}$.

In Figures 1, 2, 3 and 4 a number of quantities (component densities, total enthalpy, pressure, eigenvalues, total velocity, saturation and deviation of the equation of state from unity) are presented as a function of position in the reservoir, for test cases 1, 2, 3 and 4 respectively. The error in the equation of state, which takes the form of a volume discrepancy, remains small in all cases as the calculations show.

In Test 1 a hot vapour containing 95% methane, 4.9% butane 0.1% nonane is injected into a liquid containing 20% methane, 20% butane, 60% nonane. The details of the initial and boundary conditions of the reservoir are summarised in table 2. The results are plotted in figure 1. The solution structure for this problem consists of two discontinuous waves that connect the single phase vapour injection mixture to the single phase liquid initially in the reservoir. The slower wave corresponds to the transition from a single-phase region to a two-phase region. At these transition regions, the flux function is not differentiable and there are discontinuous changes in the eigenstructure. This type of structure is fundamentally different than the behaviour of Buckley-Leverett because of mass-transfer effects between phases and consequently, we do not see the long rarefaction associated with the simpler system. The faster discontinuity is a shock wave from the λ_1 family.

In Test 2 the same configuration as in Test 1 is considered but now with $\phi = 0.4$. The results are plotted in figure 2. The introduction of the rock heat capacity results in significant changes in the flow field. The extent of the two phase region is much larger and shows a typical Buckley-Leverett rarefaction-shock pattern in λ_1 for $x > 2000$, [cm]. We again see a discontinuous wave separating the single-phase vapour region from the two-phase region; however, in this case it is considerably slower. Within the two phase region, we also see an additional weak wave at approximately $x = 1600$, [cm]. The interaction between the waves inside the two-phase region is also more complex. Inside the two-phase region the compound wave consists of a constant state, a contact discontinuity and a rarefaction wave. We also note that λ_1 crosses the other waves at around $x = 1000$ [cm] indicating a loss of strict hyperbolicity.

In Test 3 a hot liquid containing 10% methane, 20% butane 70% nonane is injected into a liquid containing 80% methane, 10% butane, 10% nonane and the details of the initial reservoir and boundary conditions are summarised in table 3. The results are plotted in figure 3. This is a single phase liquid simulation. Because of the presence of the porous medium there are two distinct wave speeds. This results in a slow wave in the λ_3 at around $x = 1500$ [cm] separated by a constant state and followed by a faster wave at approximately $x = 1500$ [cm]. The faster wave corresponding to λ_1, λ_2 is essentially a contact discontinuity. Curiously, the slower wave is also essentially linearly degenerate. The structure in this case is carried by the change in the total velocity and reflects a change in density resulting from changes in compressibility as a function of temperature.

Test 4 is an example of a hot two-phase mixture containing 40% methane, 10% butane, 50% nonane being injected into a colder two-phase mixture containing 80% methane, 10% butane, 10% nonane. The details of the initial reservoir and boundary conditions are summarised in table 3. The results, see figure 4, show a rather complex behaviour. The hot two-phase mixture first condenses in a small region ahead of the propagating hot front. This is a result of the lagged behaviour of the thermal wave arising because of the heat capacity of the rock. The transition again shows the compound wave behaviour typical of Buckley-Leverett. The mixture then transitions back into a two-phase mixture with transition between phases accompanied by another Buckley-Leverett shock. This multiplicity of waves is made possible by the loss of strict hyperbolicity shown by the crossing of the eigenvalue curves.

7. Summary and Conclusions

A system of equations describing the flow of non-isothermal multicomponent two-phase fluids in a porous medium has been developed and analysed. The equations governing the system are an extension of the compositional solver developed in (Trangenstein & Bell 1989*b*). It is shown that the system of equations can be split into a hyperbolic system of conservation laws for component density and enthalpy and a parabolic pressure equation that constrains the volume of fluids to the available pore volume. This procedure of decoupling the fundamental equations forms the basis of a sequential numerical algorithm. The sequential method is then applied to study four test cases of multi-phase flows that can be encountered in thermal recovery processes. They demonstrate that the method can resolve the interacting waves present in the flow field and can shed new light into the understanding of the solution structure. The analysis presented here can also form the basis for the development of higher-order approaches for the component and energy conservation equations and for including additional physical phenomena such as capillary pressure, diffusion and reactions.

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Appendix A. Partial Derivatives

It is simpler to define the partial derivatives of equation (3.3) at constant T than at constant H_t since the equation of state is an explicit function of (T, p, \mathbf{n}) . Here, we present in detail the transformation (based on change of variables) to compute $\left(\frac{\partial U}{\partial p}\right)_{\mathbf{n} H_t}$ assuming that $\left(\frac{\partial U}{\partial p}\right)_{\mathbf{n} T}$ is known, by using the fact that:

$$dU = \left(\frac{\partial U}{\partial p}\right)_{\mathbf{n} H_t} dp + \left(\frac{\partial U}{\partial \mathbf{n}}\right)_{p H_t} d\mathbf{n} + \left(\frac{\partial U}{\partial H_t}\right)_{\mathbf{n} p} dH_t \quad (\text{A } 1)$$

Dividing equation (A 1) by dp and taking T constant then gives

$$\left(\frac{\partial U}{\partial p}\right)_T = \left(\frac{\partial U}{\partial p}\right)_{\mathbf{n} H_t} + \left(\frac{\partial U}{\partial \mathbf{n}}\right)_{p H_t} \left(\frac{\partial \mathbf{n}}{\partial p}\right)_T + \left(\frac{\partial U}{\partial H_t}\right)_{\mathbf{n} p} \left(\frac{\partial H_t}{\partial p}\right)_T \quad (\text{A } 2)$$

Finally, if one also takes \mathbf{n} constant, equation (A 2) reduces to

$$\left(\frac{\partial U}{\partial p}\right)_{\mathbf{n} H_t} = \left(\frac{\partial U}{\partial p}\right)_{T \mathbf{n}} - \left(\frac{\partial U}{\partial H_t}\right)_{\mathbf{n} p} \left(\frac{\partial H_t}{\partial p}\right)_{T \mathbf{n}} \quad (\text{A } 3)$$

Equation (A 3) gives the required transformation to compute $\left(\frac{\partial U}{\partial p}\right)_{\mathbf{n} H_t}$. A similar transformation to compute $\left(\frac{\partial U}{\partial H_t}\right)_{\mathbf{n} p}$ can also be obtained by dividing equation (A 1) by dT and taking \mathbf{n} and p constant

$$\left(\frac{\partial U}{\partial T}\right)_{\mathbf{n} p} = \left(\frac{\partial U}{\partial H_t}\right)_{\mathbf{n} p} \left(\frac{\partial H_t}{\partial T}\right)_{\mathbf{n} p} \quad (\text{A } 4)$$

With the help of the above expression, equation (A 3) can now be rewritten as a function of the primitive variables \mathbf{n} , p and T and can be calculated explicitly.

$$\left(\frac{\partial U}{\partial p}\right)_{\mathbf{n} H_t} = \left(\frac{\partial U}{\partial p}\right)_{T \mathbf{n}} - \left(\frac{\partial H_t}{\partial T}\right)_{\mathbf{n} p}^{-1} \left(\frac{\partial H_t}{\partial p}\right)_{\mathbf{n} T} \left(\frac{\partial U}{\partial T}\right)_{\mathbf{n} p} \quad (\text{A } 5)$$

In a similar way one can derive

$$\left(\frac{\partial U}{\partial \mathbf{n}}\right)_{p H_t} = \left(\frac{\partial U}{\partial \mathbf{n}}\right)_{T p} - \left(\frac{\partial H_t}{\partial T}\right)_{\mathbf{n} p}^{-1} \left(\frac{\partial H_t}{\partial \mathbf{n}}\right)_{p T} \left(\frac{\partial U}{\partial T}\right)_{\mathbf{n} p} \quad (\text{A } 6)$$

and

$$\left(\frac{\partial U}{\partial H_t}\right)_{p \mathbf{n}} = \left(\frac{\partial H_t}{\partial T}\right)_{\mathbf{n} p}^{-1} \left(\frac{\partial U}{\partial T}\right)_{\mathbf{n} p} \quad (\text{A } 7)$$

In order to compute (A 5), (A 6) and (A 7), the partial derivatives of H_t with respect to T , p and \mathbf{n} are required. Since H_t is the total enthalpy of the system, the enthalpy of the surrounding rock should be taken into account. Therefore H_t can be expressed as:

$$H_t = (1 - \phi)H_s + \phi H_f, \quad H_s = \rho_r H_r, \quad H_f = \mathbf{n}_l^T \mathbf{h}_l + \mathbf{n}_v^T \mathbf{h}_v \quad (\text{A } 8)$$

Assuming that $\phi = \phi(p)$ and $H_s = H_s(T)$, then the partial derivatives of H_t with respect to the primitive variables now become:

$$\left(\frac{\partial H_t}{\partial T}\right)_{\mathbf{n} p} = (1 - \phi) \left(\frac{\partial H_s}{\partial T}\right)_{\mathbf{n} p} + \phi \left(\frac{\partial H_f}{\partial T}\right)_{\mathbf{n} p} \quad (\text{A } 9)$$

$$\left(\frac{\partial H_t}{\partial p}\right)_{\mathbf{n} T} = -\frac{d\phi}{dp} H_s + \frac{d\phi}{dp} H_f + \phi \left(\frac{\partial H_f}{\partial p}\right)_{\mathbf{n} T} \quad (\text{A } 10)$$

$$\left(\frac{\partial H_t}{\partial \mathbf{n}}\right)_{p T} = \phi \left(\frac{\partial H_f}{\partial \mathbf{n}}\right)_{p T} \quad (\text{A } 11)$$

Appendix B. Secant Method

In order to solve equation (5.1) the Secant method is used. In the following the term *flash* is used to refer to a phase equilibrium calculation at given (\mathbf{n}, p) . Given an initial enthalpy H_1 and temperature T_1 the algorithm looks like:

$$H_f^1 = \frac{1}{\phi}(H_1 - (1 - \phi) C_p^{rock}(T_1 - T_{ref}^{rock}))$$

$$flash(H_f^1) \rightarrow \tilde{T}$$

$$f_1 = H_1 - (1 - \phi) C_p^{rock}(\tilde{T} - T_{ref}^{rock}) - \phi H_f^1 = (1 - \phi) C_p^{rock}(T_1 - \tilde{T})$$

$$T_2 = T_1 + \Delta T$$

$$H_f^2 = \frac{1}{\phi}(H_1 - (1 - \phi) C_p^{rock}(T_2 - T_{ref}^{rock}))$$

$$flash(H_f^2) \rightarrow \tilde{T}$$

$$f_2 = H_1 - (1 - \phi) C_p^{rock}(\tilde{T} - T_{ref}^{rock}) - \phi H_f^2 = (1 - \phi) C_p^{rock}(T_2 - \tilde{T})$$

$$T_3 = T_2 - \frac{(T_2 - T_1)}{(f_2 - f_1)} f_2$$

for $l = 1$ to N_{iter} **do**

$$H_f^3 = \frac{1}{\phi}(H_1 - (1 - \phi) C_p^{rock}(T_3 - T_{ref}^{rock}))$$

$$flash(H_f^3) \rightarrow \tilde{T}$$

$$f_3 = H_1 - (1 - \phi) C_p^{rock}(\tilde{T} - T_{ref}^{rock}) - \phi H_f^3 = (1 - \phi) C_p^{rock}(T_3 - \tilde{T})$$

$$T_4 = T_3 - \frac{(T_3 - T_2)}{(f_3 - f_2)} f_3$$

$$err = \left\| \frac{T_4 - T_3}{T_3} \right\|$$

if $err < \epsilon$ **then**

stop

end if

$$T_2 = T_3$$

$$f_2 = f_3$$

$$T_3 = T_4$$

end for

In the numerical simulations described in Section 6 $\Delta T = 10. [K]$ and $\epsilon = 1 \cdot 10^{-6}$.

Table 1. Simulation details for the different test cases.

	Test 1	Test 2	Test 3	Test 4
f_{press}	1.	1.	1.	0.6
Δt	500 Δx	500 Δx	1000 Δx	5 Δx
$t[s]$	1.E8	3.E7	5.E6	5.E5

Table 2. Injection and reservoir condition for Test cases one and two.

	Test 1		Test 2	
	Injection	Reservoir	Injection	Reservoir
$n_{C_1} [mol/cm^3]$	0.005385	0.001365	0.005385	0.001365
$n_{C_4} [mol/cm^3]$	0.000277	0.001365	0.000277	0.001365
$n_{C_9} [mol/cm^3]$	5.6684E-6	0.004096	5.6684E-6	0.004096
ϕ	1.	1.	0.4	0.4
$C_p^{rock} [J/cm^3/K]$	0.	0.	1.5	1.5
$P [MPa]$	13.80331E6	13.78952E6	13.80331E6	13.78952E6
$T [K]$	800.	344.3	800.	344.3
$H [J/cm^3]$	56.7385	-127.7710	478.9954	-4.9384

Table 3. Injection and reservoir condition for Test cases three and four.

	Test 3		Test 4	
	Injection	Reservoir	Injection	Reservoir
$n_{CO_2} [mol/cm^3]$	0.000284	0.010603	0.000246	0.002109
$n_{C_4} [mol/cm^3]$	0.000567	0.001325	0.000616	0.000264
$n_{C_9} [mol/cm^3]$	0.001985	0.001325	0.001601	0.000264
ϕ	0.4	0.4	0.4	0.4
$C_p^{rock} [J/cm^3/K]$	1.5	1.5	0.25	0.25
$P [MPa]$	6.9E6	6.8E6	3.9E6	3.8E6
$T [K]$	600.	300.	550.	300.
$H [J/cm^3]$	335.8399	-59.1795	75.6951	-6.2640

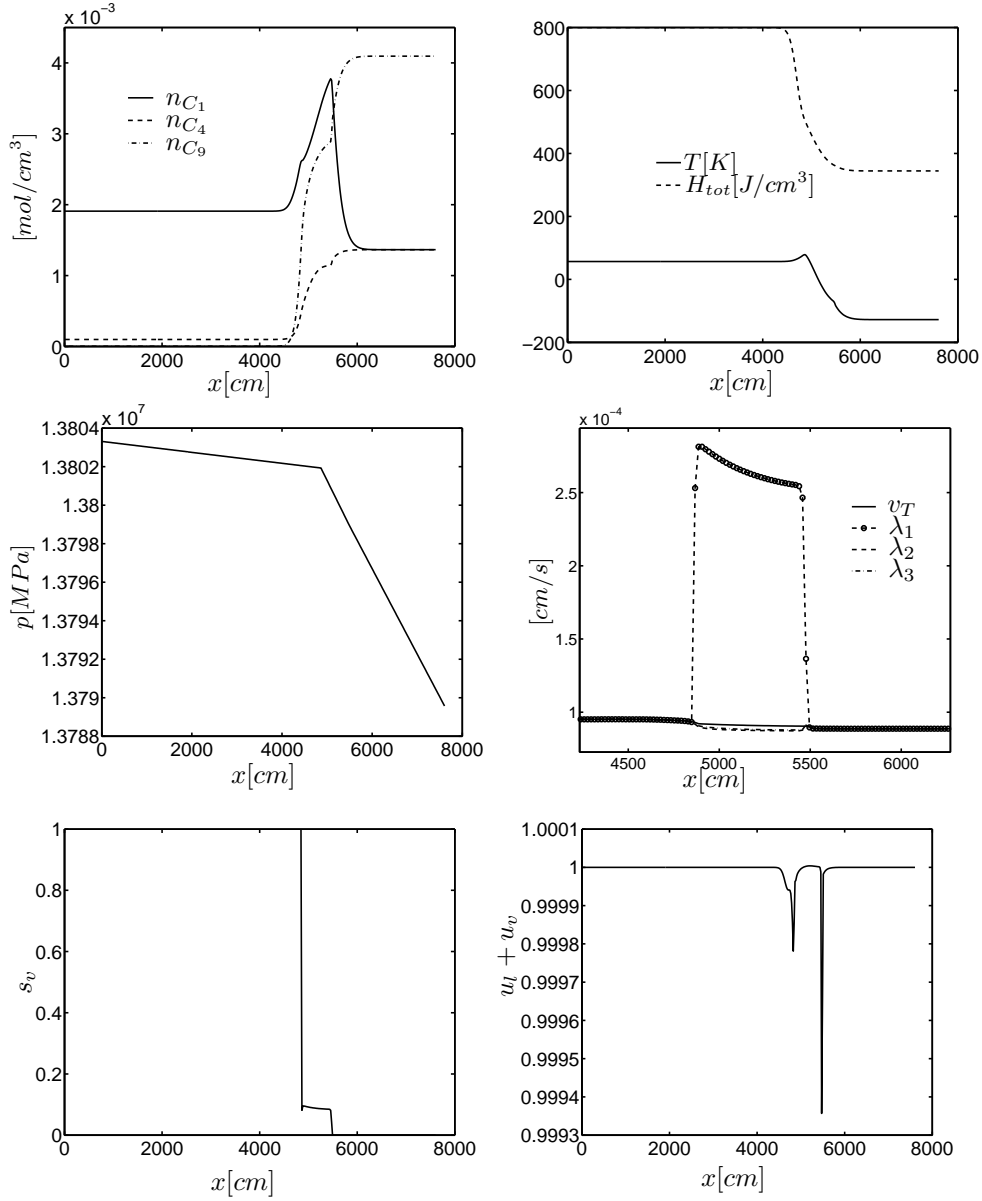


Figure 1. Test case 1: Injection of a hot vapour containing 95% C_1 -4.9% C_4 -0.1% C_9 into a liquid containing 20% C_1 -20% C_4 -60% C_9 . $C_p = 0$. [$\frac{\text{J}}{\text{cm}^3\text{K}}$], $\phi = 0.4$, $t = 1.E8$ [s]. From the top left to the bottom right the following variables are plotted: component molar densities, temperature and enthalpy, pressure, total velocity and eigenvalues, vapour saturation, volume filling condition.

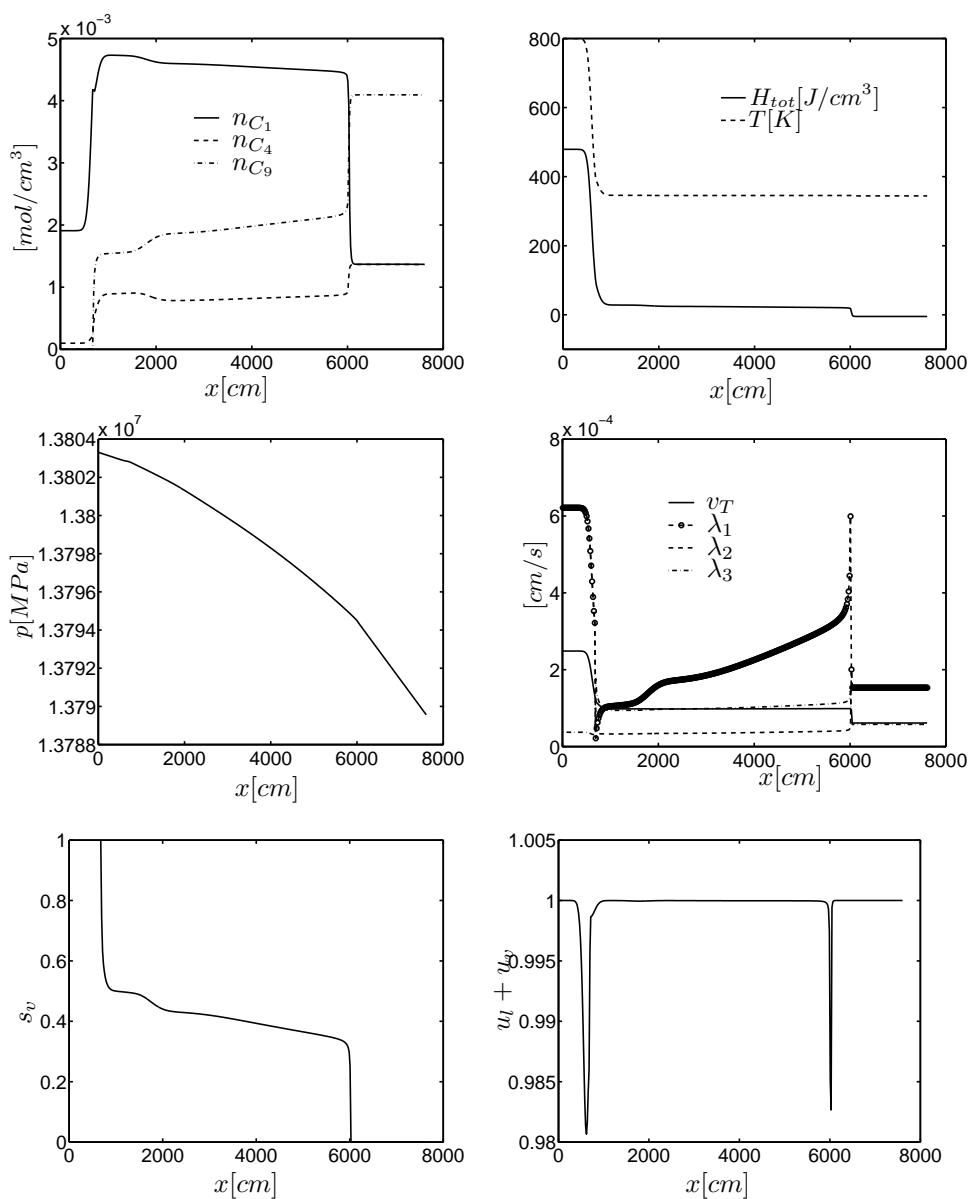


Figure 2. Test case 2: Injection of a hot vapour containing 95% C_1 -4.9% C_4 -0.1% C_9 into a liquid reservoir containing a mixture of 20% C_1 -20% C_4 -60% C_9 . $C_p = 1.5 [\frac{\text{J}}{\text{cm}^3\text{K}}]$, $\phi = 0.4$, $t = 3.E7$ [s]. From the top left to the bottom right the following variables are plotted: component molar densities, temperature and enthalpy, pressure, total velocity and eigenvalues, vapour saturation, volume filling condition.

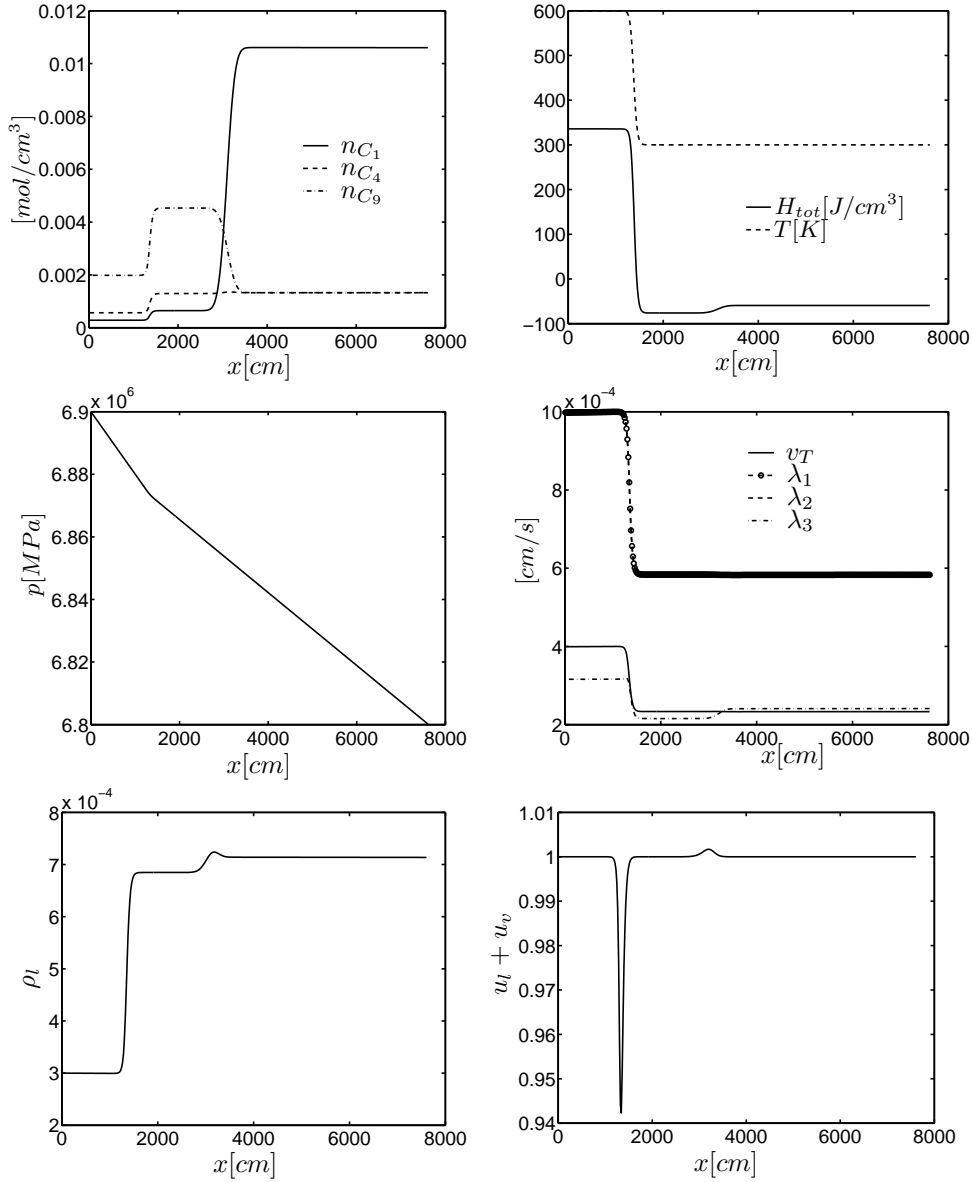


Figure 3. Test case 3: Injection of a hot liquid containing 10%CO₂-20%C₄-70%C₉ into a liquid containing 80%CO₂-10%C₄-10%C₉. $s_v = 0$ in the whole domain. $C_p = 1.5 \left[\frac{\text{J}}{\text{cm}^3 \text{K}} \right]$, $\phi = 0.4$, $t = 5.E6$ [s]. From the top left to the bottom right the following variables are plotted: component molar densities, temperature and enthalpy, pressure, total velocity and eigenvalues, liquid density, volume filling condition. The eigenvalues λ_1 and λ_2 are on top of each other.

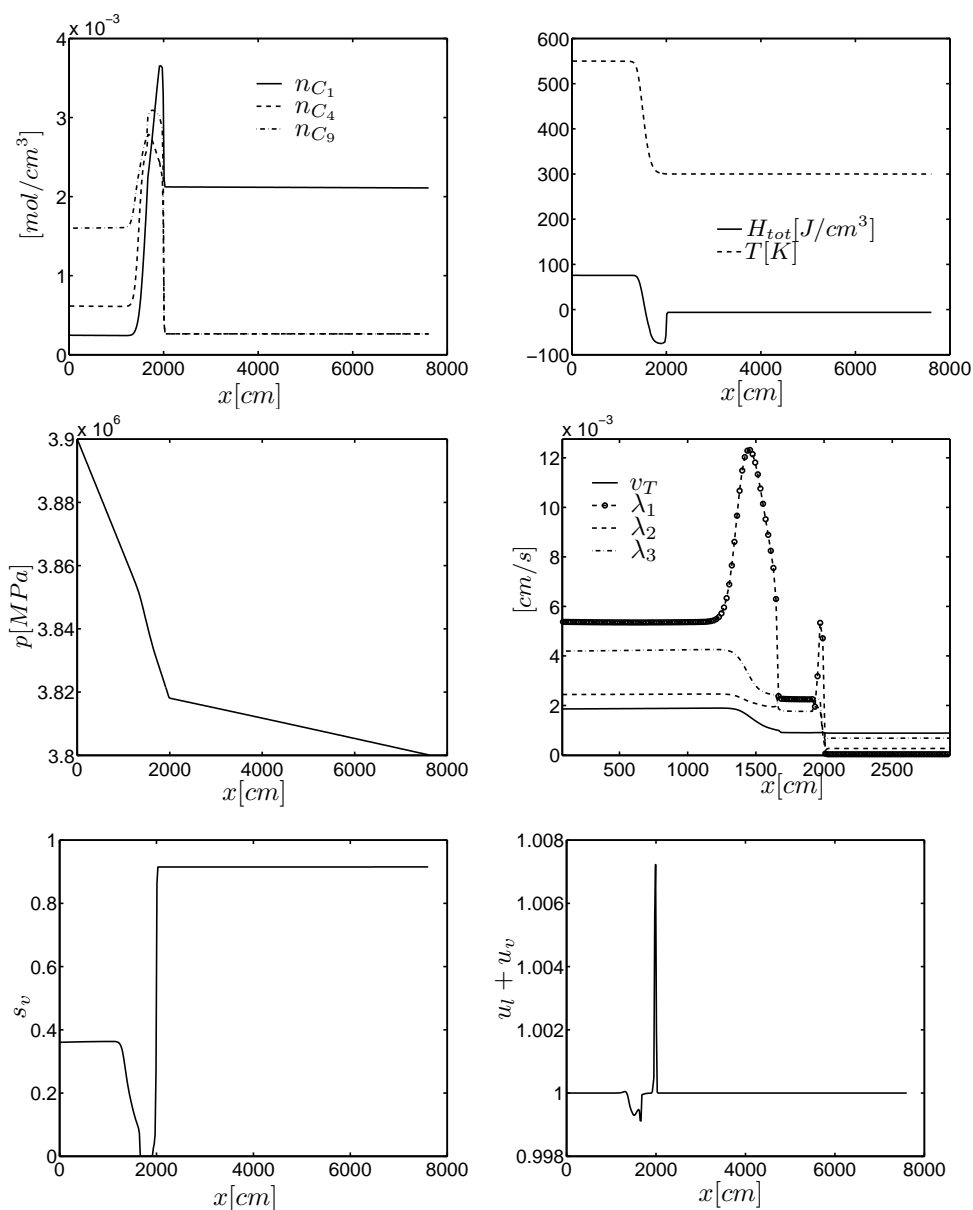


Figure 4. Test case 4: Injection of a hot mixture containing 40%CO₂-10%C₄-50%C₉ into a mixture containing 80%CO₂-10%C₄-10%C₉. $C_p = 0.25 \left[\frac{\text{J}}{\text{cm}^3 \text{K}} \right]$, $\phi = 0.4$, $t = 5.E5$ [s]. From the top left to the bottom right the following variables are plotted: component molar densities, temperature and enthalpy, pressure, total velocity and eigenvalues, vapour saturation, volume filling condition.