

Paper B

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Compositional IMPSAT
Formulation With Relaxed
Stability Constraints ***

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A Volume Balance Consistent Compositional IMPSAT Formulation With Relaxed Stability Constraints

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Abstract. A new and improved compositional IMPSAT formulation has been developed. The conventional compositional primary variables, pressure and mole numbers, are transformed into pressure, volumes and a set of complementary isochoric (constant volume) variables. Similarly, the component conservation equations are transformed into volume balance equations and complementary isochoric conservation equations. Pressure and saturations are treated implicitly, while the isochoric variables are treated explicitly. The approach is consistent, and yields a minimal overlap between the implicit volume solution and the explicit constant volume solution. In addition, a new approximate CFL stability criterion for the IMPSAT formulation is proposed. The new criterion may allow for significantly larger timesteps than the conventional IMPSAT stability criterion.

Numerical results which support the new formulation are shown.

Keywords: compositional model, IMPSAT formulation, volume balance, complementary isochoric variables and equations, relaxed stability constraints.

1. Introduction

The governing equations of a compositional model are nonlinear and coupled, both within and between gridblocks. The nonlinearities imply that the equations must be solved iteratively, for instance by the Newton-Raphson method. The couplings between gridblocks, which are due to the interblock flow terms, indicate that we should solve all equations in all gridblocks simultaneously (fully implicitly). Fully implicit formulations are unconditionally stable, but the computational costs per timestep often become prohibitively large.

A key to reducing computational costs is to evaluate the interblock flow terms with values of some of the primary variables from the previous time level. By such an explicit treatment of variables, the corresponding couplings between gridblocks vanish, and the corresponding equations can be solved one gridblock at a time (explicitly). The computational costs per timestep are thus reduced, but explicit treatment of variables introduces stability problems that restrict timestep size.

The conventional compositional approach is an IMPES approach. Pressure and component mole numbers are the primary variables, and a volume balance pressure equation and a set of component conservation equations are the primary equations. Only pressure is determined implicitly, and all the component mole numbers are treated explicitly. The motivation for determining pressure implicitly is that pressure changes spread instantaneously throughout the porous medium. IMPES is the fastest approach on a per-timestep basis, but the explicit treatment of mole numbers may introduce severe stability problems.

In an IMPSAT formulation, pressure and saturations are determined implicitly. As fluid flow in porous media is governed by Darcy's law, which is basically a relation in pressure and saturations, an implicit solve for pressure and saturations resolves the main features of flow. The chosen additional primary variables should have little influence on the interblock flow terms, so that explicit treatment of these variables, with relaxed stability constraints, is feasible. However, a completely satisfactory set of additional variables and equations for determining these has not yet been presented in the literature.

The IMPSAT (or IMPSAT-like) approaches that have been reported, [1–5], mainly differ in their choices of explicit variables and implicit and explicit equations.

In [1], Watts generalised the Volume Balance Method developed by Ács, Doleschall and Farkas, [6], and used weighted sums of the component conservation equations to form a set of volume balance pressure and saturation equations. The volume balance equations are conveniently solved implicitly for pressure and saturations, and Watts also showed that the saturation equations reduce to the conventional black-oil equations when used with black-oil fluid properties. However, Watts proposed a subsequent explicit update of all the overall mole fractions, based on the original component conservation equations. Consequently, the number of primary variables (pressure, saturations and the overall mole fractions) exceeds the number of primary equations. As Watts pointed out, this inherent inconsistency may lead to inaccuracies.

Quandalle and Savary, [2], addressed Watts' shortcoming by introducing a set of phase mole fractions as additional primary variables, thereby making the number of primary variables equal to the number of primary equations. They chose to treat all the phase mole fractions explicitly, and used a selection of component conservation equations as explicit equations, thus apparently introducing an overlap between the implicit and explicit system of equations.

The approaches of Branco and Rodríguez, [3], and Cao and Aziz, [4], are also based on using a set of phase mole fractions as primary variables. In addition, reduction of the linearised system of component

conservation equations is used to form implicit and explicit equations. Consequently, the overlap encountered in the approach of Quandalle and Savary is removed at the linearised level.

Cao and Aziz also presented an approximate CFL stability criterion for the IMPSAT formulation, and reported that their IMPSAT model is significantly more stable than the IMPES model, and in many cases substantially less expensive than the fully implicit model.

In [5], Haukås et al. aimed at minimising not only the overlap between the implicit and explicit equations at the nonlinear level, but also the overlap between pressure and saturations and the additional primary variables. Based on the theory of orthogonal complements in linear algebra, they presented a set of additional conservation equations that are complementary to the volume balance equations of Watts, and can be derived as weighted sums of the component conservation equations. In addition, they claimed that some selection of phase mole fractions should not be considered complementary to pressure and saturations, and defined their additional primary variables as weighted sums of phase mole fractions, based on a stability argument.

Haukås et al. presented results indicating improved convergence over the approach of Quandalle and Savary. However, they commented that a thermodynamic interpretation of their additional primary variables, and a natural relation between these variables and the additional conservation equations, is missing. In addition, we note that Haukås et al. chose to evaluate interblock flow terms with the additional variables from the previous iteration level and not from the previous time level. Consequently, at convergence, a fully implicit solution is obtained. Their scheme therefore corresponds to a quasi-Newton fully implicit scheme, and not a true IMPSAT scheme.

This paper is a continuation of the work done by Haukås et al. We argue that a reformulation of the component conservation equations is important for consistence, and use the same system of implicit and explicit equations as presented in [5]. However, due to the lack of a thermodynamic interpretation of the additional primary variables introduced in [5], we discard using weighted sums of phase mole fractions as primary variables. We claim that the stability properties of IMPSAT are easier to analyse if we introduce a set of explicit variables that can be interpreted as complementary to pressure and saturations. Consequently, a more precise stability criterion can be proposed. We also note that the use of complementary variables and equations makes the system better conditioned. In addition, we use a true IMPSAT scheme, in which the interblock flow terms are evaluated with explicit variables from the previous time level and not from the previous iteration level.

2. Background

2.1. GENERAL ISOTHERMAL COMPOSITIONAL MODEL

Compositional multiphase flow in porous media is governed by N_c component flow equations, where N_c is the number of chemical components in the system. The equations express conservation of the mass of each component within some (bulk) volume V_b . The i -th component conservation equation can be written in integral form as

$$\int_{V_b} \frac{\partial}{\partial t} \left(\frac{n_i}{V_b} \right) dV_b = \int_{V_b} \bar{q}_i dV_b - \int_{\mathcal{S}} \bar{f}_i d\mathcal{S}, \quad (1)$$

where n_i is the component mole number present in V_b , \bar{q}_i is the component source density within V_b per time, and \bar{f}_i is the component outflux density per time through the boundary \mathcal{S} of V_b .

In a control-volume discretisation, we refer to V_b as a control-volume. The control-volume is assumed to be fixed in time, and we interpret n_i as an average over the control-volume. For a timestep of size Δt , the control-volume discretised form of the i -th component conservation equation can then be written

$$g_i = \left(\frac{\delta n_i}{\delta t} - q_i + f_i \right) \Delta t = 0. \quad (2)$$

Here, $\delta n_i / \delta t$ is a discretisation of the time derivative $\partial n_i / \partial t$, while q_i is the total source of component i within the control-volume per time and f_i is the discretised net outflux through the boundary of the control-volume per time. If $\mathbf{u} = [u_1, \dots, u_N]^T$ denotes the set of primary variables, a possible time discretisation is

$$\frac{\delta n_i}{\delta t} = \sum_{k=1}^N \left(\frac{\partial n_i}{\partial u_k} \right)_{\mathbf{u}^{(k)}} \frac{\Delta u_k}{\Delta t}, \quad (3)$$

where the subscript $\mathbf{u}^{(k)}$ indicates that all primary variables except for u_k are kept fixed, and Δu_k is the change in u_k during the timestep Δt .

In an isothermal model, pressure p and the mole numbers $\mathbf{n} = [n_1, \dots, n_{N_c}]^T$ give a complete description of the system. However, the set (p, \mathbf{n}) must confine to the specified size V_b of the control-volume. This requirement is inherent in the compositional pressure equation, which expresses conservation of the total fluid volume V_T within V_b , and can be written in discretized form as, [1],

$$\left(V_b \frac{d\phi}{dp} - \left(\frac{\partial V_T}{\partial p} \right)_{\mathbf{n}} \right) \frac{\Delta p}{\Delta t} + \sum_{i=1}^{N_c} \left(\frac{\partial V_T}{\partial n_i} \right)_{p, \mathbf{n}^{(i)}} (f_i - q_i) = 0, \quad (4)$$

where ϕ is the porosity of the control-volume. The equation corresponds to $V_T - \phi V_b = 0$, and is unique, although it can be derived in a number of different ways, [7].

The conventional set of primary equations for an isothermal compositional model is the component conservation equations (2) plus the compositional pressure equation (4), and the conventional set of primary variables is (p, \mathbf{n}) . The time discretisation (3) then reduces to $\delta n_i / \delta t = \Delta n_i / \Delta t$.

Let N_p denote the number of fluid phases. The set of IMPSAT primary variables can generally be written as $(p, \mathbf{S}_p, \mathbf{x}_p)$, where \mathbf{S}_p is a set of $N_p - 1$ primary saturations, and \mathbf{x}_p is the set of $N_c - N_p$ additional primary variables. The similar set that corresponds to the conventional set (p, \mathbf{n}) is $(p, \mathbf{V}, \mathbf{x}_p)$, where \mathbf{V} contains the N_p fluid volumes. For both sets, $V_b = V_T / \phi$ is an inherent condition.

Generally, the variables \mathbf{x}_p must be defined so that a complete description of the system is preserved. In addition, to make explicit treatment of the variables \mathbf{x}_p feasible, the interblock flow terms should be only weakly dependent of \mathbf{x}_p . Since the interblock flow terms mainly depend on pressure and volumes, this is obtained if the variables \mathbf{x}_p are complementary to (p, \mathbf{V}) , which also implies that the set $(p, \mathbf{V}, \mathbf{x}_p)$ gives a complete description of the system. We will refer to the variables \mathbf{x}_p as the *isochoric* (constant volume) *variables*. The reason for this notion is given in section 4.2.

In addition, a set of conservation equations for determining the primary variables is needed. For consistence, there should be a minimum overlap between the pressure and saturation equations and the conservation equations that determine the isochoric variables, referred to as the *isochoric conservation equations* (see section 4.2). This is obtained if the isochoric conservation equations are complementary to the pressure and saturation equations.

We also note that the use of complementary variables and equations yields a better conditioned system.

3. Principles

In this section, we use the concept of complementary subspaces in linear algebra to define the isochoric variables \mathbf{x}_p and the isochoric conservation equations.

3.1. TRANSFORMATION FROM (p, \mathbf{n}) TO $(p, \mathbf{V}, \mathbf{x}_p)$

We consider a transformation from (p, \mathbf{n}) to $(p, \mathbf{V}, \mathbf{x}_p)$, i.e., a mapping that produces $(\mathbf{V}, \mathbf{x}_p)$ when applied to \mathbf{n} . The same transformation is applied to the component conservation equations to derive a pressure equation, $N_p - 1$ saturation equations and $N_c - N_p$ isochoric conservation equations. This provides a natural relation between the isochoric variables and the isochoric conservation equations.

We let \mathbf{W}_V and \mathbf{W}_x denote the transformations from \mathbf{n} to \mathbf{V} and from \mathbf{n} to \mathbf{x}_p , respectively, and write

$$\mathbf{V} = \mathbf{W}_V(\mathbf{n}), \quad \mathbf{W}_V : \mathbb{R}^{N_c} \rightarrow \mathbb{R}^{N_p}, \quad (5)$$

$$\mathbf{x}_p = \mathbf{W}_x(\mathbf{n}), \quad \mathbf{W}_x : \mathbb{R}^{N_c} \rightarrow \mathbb{R}^{N_c - N_p}. \quad (6)$$

If interpreted as matrices, \mathbf{W}_V is a $N_p \times N_c$ matrix, while \mathbf{W}_x is a $(N_c - N_p) \times N_c$ matrix. \mathbf{W}_V is referred to as the volume transformation, and \mathbf{W}_x is referred to as the isochoric transformation.

Letting \mathbf{r}_V denote the residuals of the pressure and saturation equations, and \mathbf{r}_x denote the residuals of the isochoric conservation equations, we write

$$\mathbf{r}_V = \mathbf{W}_V(\mathbf{g}), \quad \mathbf{r}_x = \mathbf{W}_x(\mathbf{g}), \quad (7)$$

where $\mathbf{g} = [g_1, g_2, \dots, g_{N_c}]^T$, g_i is defined by (2) and

$$\frac{\delta n_i}{\delta t} = \left(\frac{\partial n_i}{\partial p} \right)_{\mathbf{S}_p, \mathbf{x}_p} \frac{\Delta p}{\Delta t} + \left(\frac{\partial n_i}{\partial \mathbf{S}_p} \right)_{p, \mathbf{x}_p} \frac{\Delta \mathbf{S}_p}{\Delta t} + \left(\frac{\partial n_i}{\partial \mathbf{x}_p} \right)_{p, \mathbf{S}_p} \frac{\Delta \mathbf{x}_p}{\Delta t}, \quad (8)$$

according to (3).

We realise from (5), (6) and (7) that if \mathbf{W}_x is complementary to \mathbf{W}_V , the variables \mathbf{x}_p will be complementary to the variables \mathbf{V} , and the equations $\mathbf{r}_x = \mathbf{0}$ will be complementary to the equations $\mathbf{r}_V = \mathbf{0}$.

3.2. VOLUME TRANSFORMATION

The form of the volume transformation \mathbf{W}_V is derived from Euler's theorem for homogenous functions, [8]. Any volume V (phase volume or total volume) is a homogenous function of first degree in the mole numbers, and may therefore be expressed by

$$V = \sum_{i=1}^{N_c} \left(\frac{\partial V}{\partial n_i} \right)_{p, \mathbf{n}_{(i)}} n_i. \quad (9)$$

Consequently, the transformation from mole numbers \mathbf{n} to volumes \mathbf{V} is given by

$$\mathbf{W}_V = \left(\frac{\partial \mathbf{V}}{\partial \mathbf{n}} \right)_p. \quad (10)$$

If, for instance, $\mathbf{V} = [V_T, V^o, V^w]^T$, where V^o is the oil volume and V^w is the water volume, the transformation can be given in terms of the matrix

$$\mathbf{W}_V = \begin{bmatrix} \left(\frac{\partial V_T}{\partial n_1}\right)_{p, \mathbf{n}_{(1)}} & \left(\frac{\partial V_T}{\partial n_2}\right)_{p, \mathbf{n}_{(2)}} & \cdots & \left(\frac{\partial V_T}{\partial n_{N_c}}\right)_{p, \mathbf{n}_{(N_c)}} \\ \left(\frac{\partial V^o}{\partial n_1}\right)_{p, \mathbf{n}_{(1)}} & \left(\frac{\partial V^o}{\partial n_2}\right)_{p, \mathbf{n}_{(2)}} & \cdots & \left(\frac{\partial V^o}{\partial n_{N_c}}\right)_{p, \mathbf{n}_{(N_c)}} \\ \left(\frac{\partial V^w}{\partial n_1}\right)_{p, \mathbf{n}_{(1)}} & \left(\frac{\partial V^w}{\partial n_2}\right)_{p, \mathbf{n}_{(2)}} & \cdots & \left(\frac{\partial V^w}{\partial n_{N_c}}\right)_{p, \mathbf{n}_{(N_c)}} \end{bmatrix}. \quad (11)$$

It has been shown by Watts, [1], that the discretised form of the equations which result from applying (11) to the vector of component conservation equations, may be written

$$\left(V_b \frac{d\phi}{dp} - \left(\frac{\partial V_T}{\partial p}\right)_{\mathbf{n}}\right) \frac{\Delta p}{\Delta t} + \sum_{i=1}^{N_c} \left(\frac{\partial V_T}{\partial n_i}\right)_{p, \mathbf{n}_{(i)}} (f_i - q_i) = 0, \quad (12)$$

which is the compositional pressure equation, and

$$\phi V_b \frac{\Delta S^j}{\Delta t} + \left(\frac{d\phi}{dp} V_b S^j - \left(\frac{\partial V^j}{\partial p}\right)_{\mathbf{n}}\right) \frac{\Delta p}{\Delta t} + \sum_{i=1}^{N_c} \left(\frac{\partial V^j}{\partial n_i}\right)_{p, \mathbf{n}_{(i)}} (f_i - q_i) = 0, \quad (13)$$

which is the compositional saturation equation of phase j . Here S^j is the saturation of phase j , and V^j is the volume of phase j (in the above case, $j = o, w$).

The compositional pressure and saturation equations (12) and (13) express conservation of total volume and phase volumes, respectively, and will be referred to as the *volume balance equations*. Watts, [1], showed that the compositional saturation equations reduce to the conventional black-oil equations when used with black-oil fluid properties. Consequently, the volume balance equations form the basis for a unified black-oil and compositional model.

3.3. ISOCHORIC TRANSFORMATION

In order for the isochoric variables and equations to be complementary to pressure and saturations and to the volume balance equations, respectively, the isochoric transformation \mathbf{W}_x must be complementary to \mathbf{W}_V . In the following, we use the theory of orthogonal complements in linear algebra to obtain this.

The effect of the transformation \mathbf{W}_V can be described by the *range* of \mathbf{W}_V^T , which is a subspace of \mathbb{R}^{N_c} defined by

$$\pi_V = \mathcal{R}(\mathbf{W}_V^T) = \left\{ \mathbf{v} \in \mathbb{R}^{N_c} \mid \mathbf{v} = \mathbf{W}_V^T \mathbf{u} \text{ for } \mathbf{u} \in \mathbb{R}^{N_p} \right\}. \quad (14)$$

In words, the range of \mathbf{W}_V^T is the set of linear combinations of the rows of \mathbf{W}_V . The space π_V will be referred to as the *volume space*.

The *nullspace* (kernel) of \mathbf{W}_V , also a subspace of \mathbb{R}^{N_c} , is defined by

$$\mathcal{N}(\mathbf{W}_V) = \left\{ \boldsymbol{\omega} \in \mathbb{R}^{N_c} \mid \mathbf{W}_V \boldsymbol{\omega} = \mathbf{0} \right\}. \quad (15)$$

It can be shown that the nullspace of \mathbf{W}_V is the orthogonal complement of the range of \mathbf{W}_V^T , [9]. Consequently, \mathbf{W}_x is complementary to \mathbf{W}_V if and only if

$$\mathcal{R}(\mathbf{W}_x^T) = \left[\mathcal{R}(\mathbf{W}_V^T) \right]^\perp = \mathcal{N}(\mathbf{W}_V). \quad (16)$$

The space

$$\pi_x = \mathcal{R}(\mathbf{W}_x^T) = \mathcal{N}(\mathbf{W}_V) \quad (17)$$

will be referred to as the *isochoric space*.

If we give \mathbf{W}_x in terms of a matrix, the rows $\boldsymbol{\omega}_m^T$ of \mathbf{W}_x , with m ranging from 1 to $N_c - N_p$, must form a basis for the isochoric space, which means that the vectors $\boldsymbol{\omega}_m$ must be $N_c - N_p$ linearly independent solutions of the equations

$$\mathbf{W}_V \boldsymbol{\omega}_m = \mathbf{0}. \quad (18)$$

In other words, we require

$$\mathbf{W}_V \mathbf{W}_x^T = \mathbf{O}, \quad (19)$$

and that $\mathbf{W}_x \mathbf{W}_x^T$ is non-singular.

Although a basis is not unique, the equations (18) and the requirement of linear independence provide the essential properties of \mathbf{W}_x . An interpretation of the isochoric space π_x and the isochoric variables \mathbf{x}_p , defined by

$$\mathbf{x}_p = \mathbf{W}_x \mathbf{n}, \quad (\mathbf{x}_p)_m = \sum_{i=1}^{N_c} \omega_{m,i} n_i, \quad (20)$$

can therefore still be given.

We will return to the question of a unique definition of the elements of \mathbf{W}_x when considering the properties of the isochoric conservation equations, which can be written

$$\sum_{i=1}^{N_c} \omega_{m,i} \left(\frac{\partial n_i}{\partial t} + f_i - q_i \right) = 0, \quad (21)$$

or, by the discretisation (3) of the time derivative,

$$\sum_{i=1}^{N_c} \omega_{m,i} \left(\frac{\partial n_i}{\partial p} \Delta p + \frac{\partial n_i}{\partial \mathbf{S}_p} \Delta \mathbf{S}_p + \frac{\partial n_i}{\partial \mathbf{x}_p} \Delta \mathbf{x}_p + (f_i - q_i) \Delta t \right) = 0. \quad (22)$$

4. Interpretation

4.1. AN INTERPRETATION OF THE ISOCHORIC VARIABLES

In the following, we give an interpretation of the isochoric variables \mathbf{x}_p . We will here assume that the rows of \mathbf{W}_x form an orthogonal basis for the isochoric space π_x .

The existence of the two mutually orthogonal spaces π_V and π_x indicates that we may split the mole numbers in a volume part and an isochoric part without losing any information. We recall the orthogonal decomposition theorem of linear algebra, [9]:

THEOREM 1. *Let π be a subspace of \mathbb{R}^n . Then each \mathbf{y} in \mathbb{R}^n can be written uniquely in the form*

$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z}, \quad (23)$$

where $\hat{\mathbf{y}}$ is in π and \mathbf{z} is in π^\perp . In fact, if $\{\mathbf{u}_1, \dots, \mathbf{u}_p\}$ is any orthogonal basis of π , then

$$\hat{\mathbf{y}} = \text{proj}_\pi \mathbf{y} = \frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1} \mathbf{u}_1 + \dots + \frac{\mathbf{y} \cdot \mathbf{u}_p}{\mathbf{u}_p \cdot \mathbf{u}_p} \mathbf{u}_p, \quad (24)$$

and $\mathbf{z} = \mathbf{y} - \hat{\mathbf{y}}$.

The notion $\text{proj}_\pi \mathbf{y}$ is referred to as the orthogonal projection of \mathbf{y} onto π . We note that if the rows of a matrix \mathbf{W} form an orthonormal basis for π , which also means that π is the range of \mathbf{W}^T , the definition (24) reduces to

$$\text{proj}_\pi \mathbf{y} = \mathbf{W}^T \mathbf{W} \mathbf{y}. \quad (25)$$

Since the volume space π_V and the isochoric space π_x are orthogonal complements and subspaces of \mathbb{R}^{N_c} , any vector $\mathbf{n} \in \mathbb{R}^{N_c}$ can, according to the orthogonal decomposition theorem, be written as

$$\mathbf{n} = \text{proj}_{\pi_V} \mathbf{n} + \text{proj}_{\pi_x} \mathbf{n}. \quad (26)$$

If we choose the rows of the $(N_c - N_p) \times N_c$ matrix \mathbf{W}_x to form an orthonormal basis for π_x , we may conveniently calculate the isochoric part of \mathbf{n} as

$$\text{proj}_{\pi_x} \mathbf{n} = \mathbf{W}_x^T \mathbf{W}_x \mathbf{n}, \quad (27)$$

and the volume part as

$$\text{proj}_{\pi_V} \mathbf{n} = \mathbf{n} - \mathbf{W}_x^T \mathbf{W}_x \mathbf{n}. \quad (28)$$

By inserting (20) into (27), we find that

$$\text{proj}_{\pi_x} \mathbf{n} = \mathbf{W}_x^T \mathbf{x}_p. \quad (29)$$

Consequently, the isochoric variables \mathbf{x}_p are the coefficients of the linear combination of the rows of \mathbf{W}_x necessary to form the projection of \mathbf{n} onto the isochoric space. In other words, the variables \mathbf{x}_p identify the isochoric part of the mole numbers \mathbf{n} .

4.2. AN INTERPRETATION OF THE ISOCHORIC SPACE

We also give a physical interpretation of the isochoric space π_x , thus motivating the use of the notion isochoric.

The set (p, \mathbf{n}) gives a complete description of the system, and we may therefore write $\mathbf{V} = \mathbf{V}(p, \mathbf{n})$. Consequently, at constant pressure, $dp = 0$, we deduce that

$$d\mathbf{V} = \left(\frac{\partial \mathbf{V}}{\partial p} \right)_{\mathbf{n}} dp + \left(\frac{\partial \mathbf{V}}{\partial \mathbf{n}} \right)_p d\mathbf{n} = \mathbf{W}_V d\mathbf{n}. \quad (30)$$

Now if

$$d\mathbf{n} \sim \text{proj}_{\pi_x} \mathbf{n} = \mathbf{W}_x^T \mathbf{x}_p, \quad (31)$$

and pressure is kept fixed, we find that

$$d\mathbf{V} = \mathbf{W}_V d\mathbf{n} \sim \mathbf{W}_V \mathbf{W}_x^T \mathbf{x}_p = \mathbf{0}, \quad (32)$$

due to (19). In other words, (31) identifies a set of mole number changes that, under constant pressure, do not change any of the volumes.

When pressure is kept fixed, the dimension of the computational space (e.g., the mole numbers) is N_c . The requirement of constant volumes provides N_p conditions, and identifies a subspace of dimension $N_c - N_p$. The elements of the subspace are of the form (31). Consequently, the subspace coincides with the range of \mathbf{W}_x^T , which has been referred to as the isochoric space π_x . Based on the above analysis, the notions isochoric space, isochoric variables and isochoric conservation equations are well-founded.

The presence of an isochoric space seems reasonable, but studies of isobaric, isochoric processes have, to our knowledge, not been reported in the literature. However, an intuitive example of an isobaric, isochoric process can be given. If we keep pressure fixed and replace some amount of volatile components by a larger amount of less volatile components (corresponding to a $d\mathbf{n}$ of the form (31)), we may be able to preserve the phase volumes, as less volatile components generally occupy a smaller volume than volatile components.

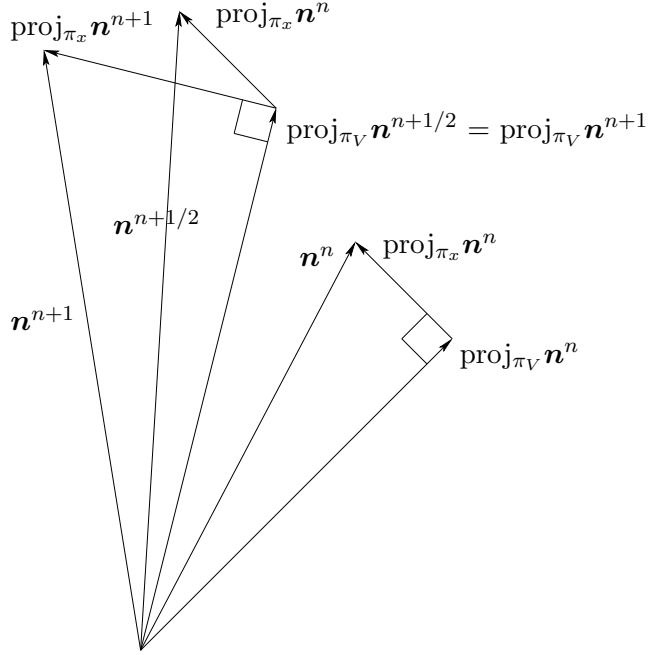


Figure 1. An interpretation of the IMPSAT scheme: the mole numbers evolve from time t^n (right) to time t^{n+1} (left) through one implicit volumetric step and one explicit isochoric step.

4.3. AN INTERPRETATION OF THE IMPSAT SCHEME

In an IMPSAT formulation, we treat the isochoric variables \mathbf{x}_p explicitly in the interblock flow terms, i.e., we fix the coefficients of the isochoric part of the interblock flow terms. The resulting scheme can be interpreted as follows, referring to Figure 1.

At time t^n , the state variables p^n and \mathbf{n}^n are known. The mole numbers \mathbf{n}^n can be decomposed into a volume part, $\text{proj}_{\pi_V} \mathbf{n}^n$, basically identified by the volumes \mathbf{V}^n , and an isochoric part, $\text{proj}_{\pi_x} \mathbf{n}^n$, identified by the isochoric variables \mathbf{x}_p^n .

The first step of IMPSAT, which corresponds to solving the volume balance equations implicitly with respect to pressure and saturations, establishes an intermediate state, referred to by superscripts $^{n+1/2}$. The isochoric variables \mathbf{x}_p are kept fixed, and we determine pressure $p^{n+1/2}$ and volumes $\mathbf{V}^{n+1/2}$. Consequently, the implicit step identifies the volume part $\text{proj}_{\pi_V} \mathbf{n}^{n+1/2}$ of the mole numbers, while the isochoric part is still $\text{proj}_{\pi_x} \mathbf{n}^n$, as shown in Figure 1.

According to Darcy’s law, the implicit step determines the dominant part of the interblock flow terms. Since the variables \mathbf{x}_p are treated explicitly, we regard the implicitly determined volume part and the isochoric part of the previous timestep as sufficient to establish the interblock flow terms. We note that this assumption is the one that may introduce stability problems.

In the second step of IMPSAT, we aim at determining the isochoric part of \mathbf{n}^{n+1} , i.e., $\text{proj}_{\pi_x} \mathbf{n}^{n+1}$. For this purpose we use the isochoric conservation equations, and determine the isochoric variables \mathbf{x}_p . As the interblock flow terms are determined by the implicit step, the second step only adjusts the isochoric state locally in each gridblock. This corresponds to an explicit solve.

Unfortunately, the implicit and explicit equations will not be completely decoupled, e.g., the volume derivatives $(\partial V/\partial p)_n$, present in the accumulation terms of the volume balance equations, will also depend on the isochoric variables \mathbf{x}_p . This is not avoidable, but since the isochoric variables are complementary to pressure and saturations, we argue that the overlap between the implicit volume solution and the explicit isochoric solution is minimal.

If the adjustment of the volume balance residuals due to the update of the isochoric variables is insignificant, the first implicit step actually yields the volume state and the interblock flow terms at time t^{n+1} . We may then set $p^{n+1} = p^{n+1/2}$ and $\mathbf{V}^{n+1} = \mathbf{V}^{n+1/2}$, which means that $\text{proj}_{\pi_V} \mathbf{n}^{n+1} = \text{proj}_{\pi_V} \mathbf{n}^{n+1/2}$. The explicit step then establishes the isochoric state $\text{proj}_{\pi_x} \mathbf{n}^{n+1}$, identified by the variables \mathbf{x}_p^{n+1} . This is illustrated in Figure 1.

On the other hand, if the adjustment is considerable, we must do new implicit and explicit steps until the explicit update of \mathbf{x}_p is insignificant for the volume solution.

5. Practical Considerations

5.1. CONSIDERING THE NEED FOR A UNIQUE DEFINITION OF \mathbf{W}_x

We have based our interpretations on the requirement that the rows of \mathbf{W}_x must form a basis for the nullspace of the volume transformation matrix \mathbf{W}_V , i.e.,

$$\mathbf{W}_V \mathbf{W}_x^T = \mathbf{O}, \quad (33)$$

where \mathbf{O} is a zero matrix of dimensions $N_p \times (N_c - N_p)$, and where the rows of \mathbf{W}_x must be linearly independent.

As mentioned, a basis is not unique. If the rows of \mathbf{W}_x form a basis for the nullspace, then so do the rows of $\mathbf{H}\mathbf{W}_x$, for any non-singular

matrix \mathbf{H} of dimensions $(N_c - N_p) \times (N_c - N_p)$, because

$$\mathbf{W}_V (\mathbf{H}\mathbf{W}_x)^\top = \mathbf{W}_V \mathbf{W}_x^\top \mathbf{H}^\top = \mathbf{O}. \quad (34)$$

Fortunately, we may show that the isochoric projection, defined by (27), is independent of the choice of orthonormal basis. If the rows of \mathbf{W}_x and $\mathbf{H}\mathbf{W}_x$ both form orthonormal bases for the nullspace, we know that

$$\mathbf{W}_x \mathbf{W}_x^\top = \mathbf{I}, \quad (\mathbf{H}\mathbf{W}_x) (\mathbf{H}\mathbf{W}_x)^\top = \mathbf{I}, \quad (35)$$

where \mathbf{I} is the identity matrix of dimensions $(N_c - N_p) \times (N_c - N_p)$. Consequently,

$$\mathbf{I} = (\mathbf{H}\mathbf{W}_x) (\mathbf{H}\mathbf{W}_x)^\top = \mathbf{H}\mathbf{W}_x \mathbf{W}_x^\top \mathbf{H}^\top = \mathbf{H}\mathbf{H}^\top, \quad (36)$$

which means that \mathbf{H} is a square orthonormal matrix with

$$\mathbf{H}^{-1} = \mathbf{H}^\top. \quad (37)$$

The expression (27), using the alternative basis $(\mathbf{H}\mathbf{W}_x)^\top$, therefore still reduces to

$$\text{proj}_{\pi_x} \mathbf{n} = (\mathbf{H}\mathbf{W}_x)^\top (\mathbf{H}\mathbf{W}_x) \mathbf{n} = \mathbf{W}_x^\top \mathbf{H}^\top \mathbf{H}\mathbf{W}_x \mathbf{n} = \mathbf{W}_x^\top \mathbf{W}_x \mathbf{n}. \quad (38)$$

However, the need for a unique definition of \mathbf{W}_x must also be considered with respect to the primary equations. We repeat the form of the isochoric conservation equations, (22), which are to be solved with respect to the isochoric variables \mathbf{x}_p :

$$\sum_{i=1}^{N_c} \omega_{m,i} \left(\frac{\partial n_i}{\partial p} \Delta p + \frac{\partial n_i}{\partial \mathbf{S}_p} \Delta \mathbf{S}_p + \frac{\partial n_i}{\partial \mathbf{x}_p} \Delta \mathbf{x}_p + (f_i - q_i) \Delta t \right) = 0. \quad (39)$$

The equations appear to be non-linear in \mathbf{x}_p , so that a Newton-Raphson linearisation may be necessary. We can show that the derivatives $\partial n_i / \partial u$, $u \in (p, \mathbf{S}_p, \mathbf{x}_p)$ generally depend on first derivatives of the rows of \mathbf{W}_x , referred to as the weight vectors ω_m^\top , with m ranging from 1 to $N_c - N_p$. The linearisation of (39) with respect to \mathbf{x}_p thus requires both first and second order derivatives of the weight vectors. To be able to carry out this differentiation, we need a unique definition of \mathbf{W}_x .

The equations (33) constitute $N_p(N_c - N_p)$ relations for determining the $N_c(N_c - N_p)$ elements of \mathbf{W}_x . Consequently, $(N_c - N_p)^2$ additional conditions, including conditions that impose linear independence, are needed. We note that the number of additional conditions is the same as the number of elements in \mathbf{H} .

Since the weight vectors $\boldsymbol{\omega}_m$ are supposed to span the isochoric space, it is natural to impose linear independence by requiring orthogonality between each pair of vectors $\boldsymbol{\omega}_m, \boldsymbol{\omega}_l$, i.e.,

$$\boldsymbol{\omega}_m^T \boldsymbol{\omega}_l = 0, \quad m \neq l. \quad (40)$$

The equations (40) correspond to $(1/2)(N_c - N_p)(N_c - N_p - 1)$ independent conditions. In addition, we may add $N_c - N_p$ scaling conditions to obtain an orthonormal basis, and thereby make the convenient relation (27) applicable.

The conditions of orthonormality are satisfied by a standard singular value decomposition of \mathbf{W}_V , which produces an orthonormal basis for the nullspace. However, $(1/2)(N_c - N_p)(N_c - N_p - 1)$ conditions still remain. The number of remaining conditions indicate that they should relate each pair of weight vectors, and thus provide an order of precedence for the weight vectors. Generally, we could write the remaining conditions as

$$F(\boldsymbol{\omega}_m, \boldsymbol{\omega}_l) = 0, \quad m \neq l, \quad (41)$$

but, unfortunately, the form of the ranking conditions is not evident.

In addition to the problem of specifying a full set of conditions, we realize that the calculation of derivatives of the weight vectors may become very time-consuming. Due to (18) and (11), the first and second derivatives of the weight vectors namely depend on second and third order derivatives of volumes, respectively.

However, we may show that both of the above problems are overcome if we assume the weight vectors to be constant over a timestep, i.e., if we assume that the isochoric space π_x does not change considerably during a timestep. Such an assumption seems plausible.

5.2. THE CONSEQUENCES OF USING CONSTANT WEIGHT VECTORS

In the following, we let the weight vectors $\boldsymbol{\omega}_m$ be mutually orthonormal. If the weight vectors are assumed constant, we may differentiate through (20) to find that

$$\frac{\partial(\mathbf{x}_p)_m}{\partial t} = \sum_{i=1}^{N_c} \omega_{m,i} \frac{\partial n_i}{\partial t}. \quad (42)$$

Consequently, by inserting relation (42) into equation (21), we find that the isochoric conservation equations reduce to the simple form

$$\frac{\partial(\mathbf{x}_p)_m}{\partial t} + \sum_{i=1}^{N_c} \omega_{m,i} (f_i - q_i) = 0. \quad (43)$$

We observe that all non-linearities in the accumulation term are eliminated, and recall that the interblock flow terms f_i are evaluated using values of the isochoric variables from the previous timestep. This means that a linearisation (which implies calculation of derivatives with respect to the isochoric variables \mathbf{x}_p) is necessary only in gridblocks containing a non-constant source term. However, since the isochoric projection of the mole numbers is the same, regardless of the actual definition of the orthonormal weight vectors, so is the solution of (43). The possible influence on the convergence rate of the iteration used to solve (43) is limited to a minor number of gridblocks (the well blocks), and will not be discussed.

However, the weight vectors also go into the calculation of partial derivatives with respect to (p, \mathbf{S}_p) , as the isochoric variables \mathbf{x}_p are to be kept constant in such a differentiation. Partial derivatives with respect to (p, \mathbf{S}_p) are required to solve the non-linear volume balance equations. In the following, we show that any set of basis vectors for the space π_x produce the same partial derivatives with respect to (p, \mathbf{S}_p) . Referring to (34), we show that the presence of the matrix \mathbf{H} does not affect the calculations.

Let $\mathbf{u} = (p, \mathbf{S}_p, \mathbf{x}_p)$ denote the set of primary variables for the compositional model. We find that the set

$$\mathbf{n}^j = \mathbf{n}^j(\mathbf{u}) = [n_1^1, \dots, n_{N_c}^1, n_1^2, \dots, n_{N_c}^2, \dots, n_1^{N_p}, \dots, n_{N_c}^{N_p}]^T, \quad (44)$$

where n_k^j is the mole number of component k in phase j , is a convenient set of secondary variables, since the conventional thermodynamic equation of state model is given in terms of the set (p, \mathbf{n}^j) . Consequently, any variable or relation h can be written as

$$h = h[\mathbf{u}, z(p, \mathbf{n}^j(\mathbf{u}))], \quad (45)$$

and all derivatives with respect to $v \in (p, \mathbf{S}_p)$ therefore depend on the $N_p N_c$ derivatives $\partial \mathbf{n}^j / \partial v$. To determine these derivatives, we need $N_p N_c$ secondary relations,

$$\mathbf{r}_s = \mathbf{r}_s[\mathbf{u}, z(p, \mathbf{n}^j(\mathbf{u}))] = \mathbf{0}. \quad (46)$$

The conditions of chemical equilibrium between the components of different phases j and l constitute $N_c(N_p - 1)$ independent relations, conveniently represented by fugacity equalities

$$f_i^j(p, \mathbf{n}^j) - f_i^l(p, \mathbf{n}^l) = 0. \quad (47)$$

In addition, we have a relation between pressure and density for each phase, represented by the equation of state relations

$$p\phi V_b S^j - n^j RT Z^j(p, \mathbf{n}^j) = 0, \quad (48)$$

where n^j is the total mole number of phase j , R is the universal gas constant, T is the absolute temperature and Z^j is the phase compressibility factor.

The remaining $N_c - N_p$ conditions assure that the derivatives confine to the definition of the isochoric variables \mathbf{x}_p ,

$$\sum_{i=1}^{N_c} \omega_{m,i} n_i(p, \mathbf{n}^j) - (\mathbf{x}_p)_m = 0, \quad (49)$$

where the coefficients $\omega_{m,i}$ now are assumed to be constant.

By differentiating through the relations (46) with respect to v , we obtain a linear system for determining $\partial \mathbf{n}^j / \partial v$:

$$\left(\frac{\partial \mathbf{r}_s}{\partial \mathbf{z}} \right)_u \left(\frac{\partial \mathbf{z}}{\partial \mathbf{n}^j} \right)_p \frac{\partial \mathbf{n}^j}{\partial v} = - \left(\frac{\partial \mathbf{r}_s}{\partial \mathbf{u}} \right)_z \frac{\partial \mathbf{u}}{\partial v} - \left(\frac{\partial \mathbf{r}_s}{\partial \mathbf{z}} \right)_u \left(\frac{\partial \mathbf{z}}{\partial p} \right)_{\mathbf{n}^j} \frac{\partial p}{\partial v}. \quad (50)$$

The system of equations can be written

$$\mathbf{A} \frac{\partial \mathbf{n}^j}{\partial v} = \mathbf{b}_v, \quad (51)$$

where

$$\mathbf{A} = \begin{bmatrix} \mathbf{B} \\ \mathbf{C} \end{bmatrix}, \quad \begin{array}{l} \mathbf{B} : (N_c N_p - (N_c - N_p)) \times N_c N_p, \\ \mathbf{C} : (N_c - N_p) \times N_c N_p, \end{array} \quad (52)$$

and only the part of the system involving the sub-matrix \mathbf{C} is influenced by the definition of the weight vectors ω_m .

We find that

$$\mathbf{C} = \left[\mathbf{C}^1 \ \mathbf{C}^2 \ \dots \ \mathbf{C}^{N_p} \right], \quad \mathbf{C}^j = \mathbf{W}_x, \quad (53)$$

where \mathbf{W}_x is a solution of (33) which has linearly independent rows. It is evident that $\mathbf{H}\mathbf{W}_x$ satisfies the same criteria as \mathbf{W}_x , so that \mathbf{C} could be replaced by $\mathbf{H}\mathbf{C}$.

We consider the two alternative system matrices for the system (51),

$$\mathbf{A} = \begin{bmatrix} \mathbf{B} \\ \mathbf{C} \end{bmatrix}, \quad \tilde{\mathbf{A}} = \begin{bmatrix} \mathbf{B} \\ \mathbf{H}\mathbf{C} \end{bmatrix}, \quad (54)$$

and let their inverses be given by

$$\mathbf{A}^{-1} = \left[\mathbf{E} \ \mathbf{F} \right], \quad \tilde{\mathbf{A}}^{-1} = \left[\tilde{\mathbf{E}} \ \tilde{\mathbf{F}} \right], \quad (55)$$

where

$$\begin{array}{l} \mathbf{E}, \tilde{\mathbf{E}} : N_c N_p \times (N_c N_p - (N_c - N_p)), \\ \mathbf{F}, \tilde{\mathbf{F}} : N_c N_p \times (N_c - N_p). \end{array} \quad (56)$$

Since $v \in (p, \mathbf{S}_p)$, the last $N_c - N_p$ elements of the right hand side \mathbf{b}_v of (51), corresponding to the relations (49), are zero. This reflects the fact that the derivatives $\partial(\mathbf{x}_p)_m/\partial v$ are zero. Consequently, the submatrices \mathbf{F} and $\tilde{\mathbf{F}}$ are immaterial; they will be multiplied by a zero vector when solving the system (51).

If we can show that $\tilde{\mathbf{E}} = \mathbf{E}$, the effect of the matrices \mathbf{A} and $\tilde{\mathbf{A}}$ will be the same, regardless of \mathbf{H} , and so will the derivatives $\partial \mathbf{n}^j / \partial v$, $v \in (p, \mathbf{S}_p)$. From

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{I} = \begin{bmatrix} \mathbf{B}\mathbf{E} & \mathbf{B}\mathbf{F} \\ \mathbf{C}\mathbf{E} & \mathbf{C}\mathbf{F} \end{bmatrix}, \quad (57)$$

we find that $\mathbf{B}\mathbf{E} = \mathbf{I}$ and that $\mathbf{C}\mathbf{E} = \mathbf{O}$, and from

$$\tilde{\mathbf{A}}\tilde{\mathbf{A}}^{-1} = \mathbf{I} = \begin{bmatrix} \mathbf{B}\tilde{\mathbf{E}} & \mathbf{B}\tilde{\mathbf{F}} \\ \mathbf{H}\mathbf{C}\tilde{\mathbf{E}} & \mathbf{H}\mathbf{C}\tilde{\mathbf{F}} \end{bmatrix}, \quad (58)$$

we deduce that $\mathbf{B}\tilde{\mathbf{E}} = \mathbf{I}$ and that $\mathbf{H}\mathbf{C}\tilde{\mathbf{E}} = \mathbf{O}$. Since \mathbf{H} is non-singular, the latter implies $\mathbf{C}\tilde{\mathbf{E}} = \mathbf{O}$. This means that

$$\mathbf{A}(\mathbf{E} - \tilde{\mathbf{E}}) = \mathbf{O}, \quad (59)$$

implying that $\mathbf{E} = \tilde{\mathbf{E}}$.

Consequently, we have shown that if we assume the changes in the isochoric space π_x with respect to time to be so small that the space may be considered constant during a timestep, the equations (18) and the requirement of linear independence (in our case, orthogonality) yield a sufficient set of conditions for identifying the transformation matrix \mathbf{W}_x . In other words, specifying any additional conditions will not affect the performance of the formulation. We can therefore simply use a standard singular value decomposition of \mathbf{W}_V to determine \mathbf{W}_x as an orthonormal basis for the nullspace of \mathbf{W}_V .

6. Stability Analysis

6.1. THE GENERAL CFL STABILITY CRITERION

The compositional flow equations form a system of hyperbolic conservation equations, written in differential form as

$$\mathbf{u}_t + \bar{\mathbf{f}}(\mathbf{u})_x = \mathbf{0}, \quad (60)$$

where \mathbf{u} are the solution variables, $\bar{\mathbf{f}}$ are the flow density rates, and subscripts t and x denote partial differentiation with respect to time and space, respectively.

If the system of equations is solved by an explicit finite-difference scheme, i.e., a finite-difference scheme where the flow terms are evaluated using values of \mathbf{u} from the previous timestep, timestep sizes must be restricted to avoid an unstable solution (a solution that experiences physically unreasonable, increasing oscillations).

Instabilities occur when the Courant-Friedrichs-Lewy (CFL) criterion is violated. The CFL criterion requires that the numerical domain of dependence must contain the domain of dependence of the associated system of partial differential equations. For a system of the form (60), the CFL criterion can be shown to be, [10],

$$\text{CFL} = \left\| \rho \left(\frac{\partial \bar{\mathbf{f}}}{\partial \mathbf{u}} \right) \right\|_{L_\infty} \frac{\Delta t}{V_b} \leq 1, \quad (61)$$

where ρ is the spectral radius of the matrix $\partial \bar{\mathbf{f}} / \partial \mathbf{u}$, while V_b is the size of the gridblock in which the system of equations is solved. If we assume V_b to be constant, and let $\mathbf{f} = V_b \bar{\mathbf{f}}$ denote the flow rates, we may write

$$\text{CFL} = \left\| \rho \left(\frac{\partial \mathbf{f}}{\partial \mathbf{u}} \right) \right\|_{L_\infty} \Delta t \leq 1. \quad (62)$$

If the system of equations is linear, e.g., $\mathbf{f} = \text{diag}(\lambda_i) \mathbf{u}$, where $\text{diag}(\lambda_i)$ is a diagonal matrix with entries λ_i on the diagonal, the CFL criterion reduces to

$$\text{CFL} = \max_i \lambda_i \Delta t \leq 1. \quad (63)$$

Here, $\text{diag}(\lambda_i)$ represents the ratio between the flow rate of \mathbf{u} and the value of \mathbf{u} in place in the gridblock. The physical interpretation of (63) is that the flow of \mathbf{u} out of a gridblock must not exceed the amount of \mathbf{u} present in the gridblock. A similar interpretation applies to (62), i.e., the largest stable timestep is the time the solution wave needs to travel through one gridblock.

If the system is non-linear, calculations of eigenvalues of the matrix $\partial \mathbf{f} / \partial \mathbf{u}$ for each timestep will be too expensive. We therefore look for an approximate CFL criterion. This may be achieved by simplifying assumptions that linearise the equations, and/or consideration of the physical interpretation of the CFL criterion.

6.2. EXPLICIT TREATMENT OF MOLE FRACTIONS

In [4], Cao and Aziz presented a CFL stability criterion for explicit treatment of the mole fraction c_i^j of component i in phase j ,

$$\text{CFL}_{c_i^j} = \frac{\Delta t \sum_{j=1}^{N_p} c_i^j \xi^j f^j}{\phi V_b \sum_{j=1}^{N_c} c_i^j \xi^j S^j} \leq 1, \quad (64)$$

where $\xi^j = n^j/V^j$ is the molar density of phase j , and f^j is the volumetric flow rate of phase j . The criterion is based on simplifying assumptions that linearise the component conservation equations, [11].

In the following, we let f_i denote the flow rate of component i , represented by the gross component outflux through the boundary of V_b . In practice, we calculate f_i by going through all interfaces γ of a gridblock, and summing the interface fluxes $f_{i,\gamma}^j$ of component i in phases j for which the gridblock is the upstream cell. We note that f_i coincides with the sum in the nominator of (64), and that the denominator of (64) is the amount of component i present in the pore volume ϕV_b . We therefore introduce the ratio

$$\beta_i = \frac{f_i}{n_i}, \quad (65)$$

and write criterion (64) more conveniently as

$$\text{CFL}_{c_i^j} = \beta_i \Delta t \leq 1. \quad (66)$$

For stability, criterion (66) must be fulfilled for every gridblock in which the mole fraction c_i^j is treated explicitly. The interpretation of the criterion is that, in a stable timestep, the amount of component i flowing out of a gridblock can not exceed the amount of that component in place in the gridblock. In other words, a component can not move more than one gridblock in a stable timestep.

In the IMPSAT formulation of Cao and Aziz, all of the component mole fractions are treated explicitly, which means that the corresponding approximate CFL stability criterion can be written

$$\text{CFL}_{CA} = \|\boldsymbol{\beta}\|_{\infty} \Delta t \leq 1, \quad (67)$$

where $\boldsymbol{\beta} = [\beta_1, \dots, \beta_{N_c}]^T$. The corresponding maximum stable timestep is

$$\max(\Delta t)_{CA} = \frac{1}{\|\boldsymbol{\beta}\|_{\infty}}. \quad (68)$$

By comparison to (62) we find that criterion (67) corresponds to approximating the spectral radius of the matrix $\partial \mathbf{f} / \partial \mathbf{n}$ by the maximum of the ratios f_i/n_i .

6.3. EXPLICIT TREATMENT OF THE ISOCHORIC VARIABLES \mathbf{x}_p

In order to find an approximate CFL criterion for explicit treatment of the isochoric variables \mathbf{x}_p , we look for a modification of the ratio (65). We note that the criterion of Cao and Aziz does not distinguish between the part of the mole numbers that is treated explicitly and the part

that is treated implicitly. Hence, it should be possible to derive a more precise, i.e., less restrictive, approximate CFL criterion for IMPSAT.

Explicit treatment of the isochoric variables corresponds to explicit treatment of the isochoric projection of the mole numbers, $\text{proj}_{\pi_x} \mathbf{n}$. The decomposition into a volume part and an isochoric part can be done not only for the mole numbers,

$$\mathbf{n} = \text{proj}_{\pi_V} \mathbf{n} + \text{proj}_{\pi_x} \mathbf{n}, \quad (69)$$

but also for the flow rates

$$\mathbf{f} = [f_1, \dots, f_{N_c}]^T = \text{proj}_{\pi_V} \mathbf{f} + \text{proj}_{\pi_x} \mathbf{f}. \quad (70)$$

Our experience with the IMPSAT formulation shows that instabilities (increasing oscillations) only appear in the isochoric part of the mole numbers and in the isochoric part of the flow terms. This suggests that the isochoric projections should be included in our modified ratio.

As a first approach, we introduce

$$\eta_i = \frac{(\text{proj}_{\pi_x} \mathbf{f})_i}{(\text{proj}_{\pi_x} \mathbf{n})_i}, \quad \boldsymbol{\eta} = [\eta_1, \dots, \eta_{N_c}]^T, \quad (71)$$

and the approximate CFL stability criterion

$$\text{CFL}_{\mathbf{x}_p}^\eta = \|\boldsymbol{\eta}\|_\infty \Delta t \leq 1. \quad (72)$$

The interpretation of criterion (72) is that the isochoric part of the outflux from a gridblock must not exceed the isochoric part of the mass in place in that gridblock. Unfortunately, experience shows that the criterion in many cases allows for an unstable solution, corresponding to a violation of the true CFL criterion. In other cases, it is more restrictive than the criterion of Cao and Aziz. The criterion is therefore of no use, and we must look for another modified ratio.

We know that instabilities arise from the hyperbolic part of the system. Consequently, the pressure (total volume) equation (12), which has an elliptic nature, should possibly be excluded from the stability analysis. This is not reflected in (71), as the volume space $\pi_V = \pi_x^\perp$, defined by (14), includes the total volume (pressure).

In order to obtain a modified volume space that only represents the hyperbolic part of the phase volumes, we exclude the total volume from the volume transformation (10), and introduce

$$\mathbf{W}_{\bar{V}^j} = \left(\frac{\partial \bar{V}^j}{\partial \mathbf{n}} \right)_p, \quad (73)$$

where $\mathbf{W}_{\overline{V}^j}$ contains all the fluid volumes except for that of phase j . We interpret $\mathbf{W}_{\overline{V}^j}$ as a $(N_p - 1) \times N_c$ matrix, and introduce $\mathbf{W}_{\overline{x}^j}$ as a $(N_c - N_p + 1) \times N_c$ matrix, the rows of which form an orthonormal basis for the nullspace of $\mathbf{W}_{\overline{V}^j}$.

We may then argue that the projection operator

$$\text{proj}_{\pi_{\overline{x}^j}} = \mathbf{W}_{\overline{x}^j}^T \mathbf{W}_{\overline{x}^j} \quad (74)$$

captures the explicit hyperbolic part of the system better than the operator proj_{π_x} , and that (71) should be replaced by

$$\nu_i^j = \frac{\left(\text{proj}_{\pi_{\overline{x}^j}} \mathbf{f} \right)_i}{\left(\text{proj}_{\pi_{\overline{x}^j}} \mathbf{n} \right)_i}, \quad \boldsymbol{\nu}^j = [\nu_1^j, \dots, \nu_{N_c}^j]^T. \quad (75)$$

Experience shows that some of the ratios (75) may be negative, indicating that the projected component flux is an influx rather than an outflux. The way we formulate the stability criterion, only outfluxes are used to limit the stability. We therefore only consider the positive components of $\boldsymbol{\nu}^j$, corresponding to a vector $\boldsymbol{\nu}^{j+}$.

In addition, we must choose which phase j should be left out in (73). In order for phase j to reflect the stability properties of the total volume (pressure), it should be chosen as the most stable phase. This corresponds to

$$\text{CFL}_{\mathbf{x}_p}^\nu = \min_j \left\| \boldsymbol{\nu}^{j+} \right\|_\infty \Delta t \leq 1, \quad (76)$$

and yields a maximum stable timestep of

$$\max(\Delta t)_{\mathbf{x}_p} = \frac{1}{\min_j \left\| \boldsymbol{\nu}^{j+} \right\|_\infty}. \quad (77)$$

The interpretation of criterion (76) is that the explicit hyperbolic part of the outflux from a gridblock must not exceed the explicit hyperbolic part of the mass in place in that gridblock. Consequently, we expect (76) to be closer to the true CFL criterion than the first approach, (72). However, the precision of the criterion depends on the assumption that phase j reflects the stability properties of the total volume, and its range of validity must be tested by numerical examples.

Finally, we note that (76) reduces to the criterion of Cao and Aziz, (67), in the single phase case. In that case, only pressure is treated implicitly, and the criterion should be interpreted as a compositional IMPES stability criterion.

7. Numerical Results

7.1. RESERVOIR AND FLUID DATA FOR TEST CASES

In order to investigate the properties of the presented IMPSAT formulation, we consider a reservoir where the fluids consist of four hydrocarbon components (C1, C2, nC4, nC7). We are not interested in single phase gridblocks, in which only pressure would be treated implicitly (IMPES), so we initialise with a two phase (gas/oil) chemical equilibrium and consider only horizontal flow (reservoir fluids are not subject to gravity segregation). We use a $25 \times 25 \times 1$ uniform orthogonal quadrilateral grid with gridblocks of dimensions $100 \text{ m} \times 100 \text{ m} \times 10 \text{ m}$. The porosity is set to $\phi = 0.2$ in all gridblocks, and we use a uniform permeability tensor of

$$\mathbf{K} = \begin{bmatrix} 100 & 0 & 0 \\ 0 & 100 & 0 \\ 0 & 0 & 10 \end{bmatrix} \text{ mD}. \quad (78)$$

We let the residual oil and gas saturations be zero, and use the simple gas and oil relative permeability relations

$$k_r^g = 0.4 \cdot (S^g)^2, \quad k_r^o = 0.4 \cdot (S^o)^2. \quad (79)$$

All thermodynamic calculations are based on the Peng-Robinson equation of state, [12], using component properties from Reid et. al., [13]. Phase viscosities are calculated by the approach of Lorentz et. al., [14]. The reservoir temperature is set to 420.0 K, and capillary pressure between the oil and gas phases is neglected. The initial pressure in all gridblocks is 40.0 bars.

A producer, controlled by a fixed bottom hole pressure of 30.0 bars, is located in gridblock (1,1,1).

To control timestep sizes, we use the formula

$$\Delta t^{n+1} = \min \left\{ \Delta t^n \min_u \left[\frac{(1 + \lambda)\Delta u^n}{\Delta u^* + \lambda\Delta u^n} \right], \alpha \cdot \max(\Delta t)_{x_p} \right\} \text{ days}, \quad (80)$$

where Δt^{n+1} is the next timestep, Δt^n is the previous timestep, Δu^n is the change in the variable u over the previous timestep, Δu^* is the target variable change during the next timestep, λ is a tuning factor and α is the CFL factor of (76). The leftmost part of the formula is due to Aziz and Settari, [16]. We use $\lambda = 0.5$, $\Delta p^* = 15.0$ bars, $\Delta S^{j,*} = 0.1$ and $\Delta c_i^{j,*} = 0.05$.

We note that instabilities may occur for $\alpha > 1$, but that the oscillations will eventually be damped due to the leftmost part of the timestep control formula. The initial timestep is 1 day.

7.2. TEST CASES

Case 1: Initial overall composition: $\mathbf{z} = [0.1, 0.1, 0.2, 0.6]^T$. Oil dominant, $S^o = 0.84905$ initially.

Case 2: Initial overall composition: $\mathbf{z} = [0.3, 0.2, 0.2, 0.3]^T$. Gas dominant, $S^g = 0.888087$ initially.

Case 3: Initial overall composition: $\mathbf{z} = [0.2, 0.05, 0.1, 0.65]^T$. Similar oil and gas volumes, $S^o = 0.547284$, $S^g = 0.452716$ initially.

7.3. VALIDATION

To check our results, we use the commercial compositional simulator Eclipse300, [15]. The Eclipse300 simulations are run in fully implicit mode (FIM).

7.4. COMPARED QUANTITIES

For each case, we first run our simulator through 50 timesteps controlled by (80) with $\alpha = 1$. We may then plot the maximum stable timestep during the simulation, both according to the criterion of Cao and Aziz, (68), and the new criterion, (77). We also plot the actual timestep taken due to the timestep control (80). We expect that the new approximate CFL criterion allows for larger timesteps than the criterion of Cao and Aziz, and we plot the relative timestep size improvement, calculated by

$$\kappa = \frac{\max(\Delta t)_{\mathbf{x}_p} - \max(\Delta t)_{CA}}{\max(\Delta t)_{CA}}. \quad (81)$$

The cases are then run using some $\alpha > 1$ in the timestep control, thus producing an unstable solution. We plot how the solution, represented by pressure, oil saturation and normalised mole numbers, evolves with time in the production block, according to the runs with $\alpha = 1$, the corresponding runs with Eclipse300, and the runs with $\alpha > 1$.

Finally, for a component amount n_i which experiences increasing oscillations, we plot its decomposition onto the volume space and the isochoric space,

$$n_i = \left(\text{proj}_{\pi_V} \mathbf{n} \right)_i + \left(\text{proj}_{\pi_x} \mathbf{n} \right)_i, \quad (82)$$

with respect to time.

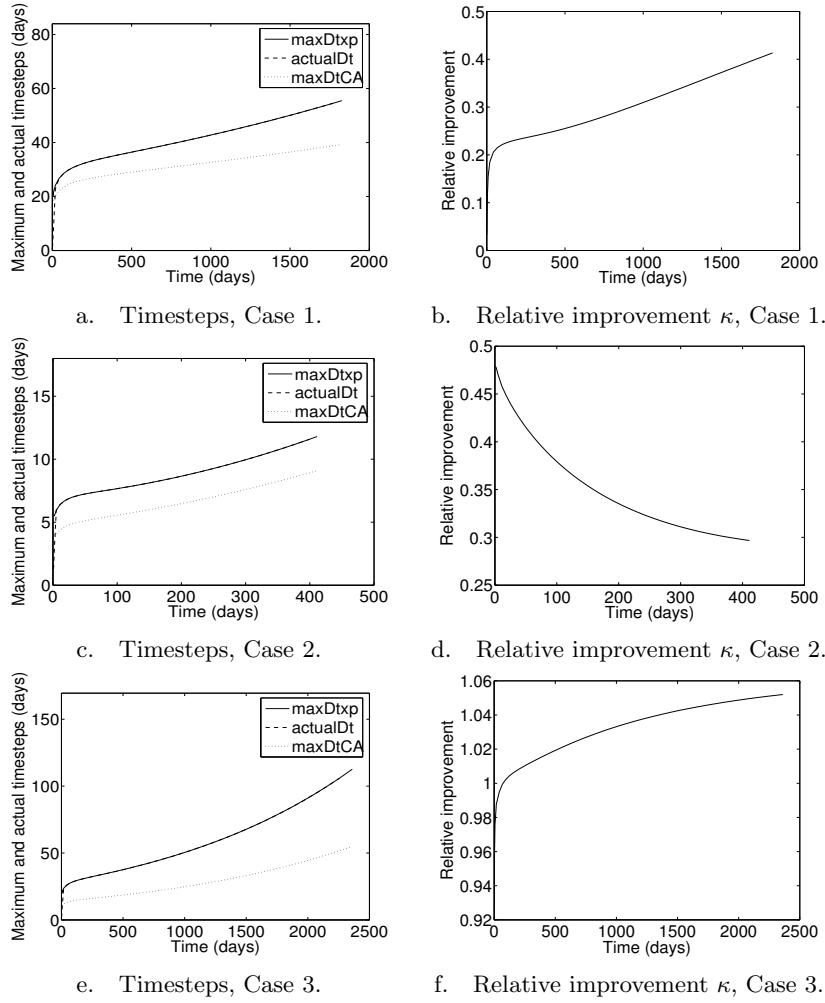


Figure 2. Timesteps and relative improvement for Cases 1, 2, 3. Here, 'maxDtxp' is the maximum stable timestep according to the new criterion (77), 'actualDt' is the actual timestep controlled by (80), while 'maxDtCA' is the maximum stable timestep according to the criterion of Cao and Aziz, (68).

7.5. COMPARING TIMESTEP SIZES

Figure 2 shows timesteps, timestep limits and relative improvements κ for Cases 1, 2, 3. Timesteps are controlled by the maximum stable timestep limit ('maxDtxp') during most of the simulations. The relative improvement κ is significant in all cases, and ranges from around 20-40 % in Cases 1 and 2, to around 100 % in Case 3. We note that, since (76) reduces to (67) in the single phase case, smaller values of κ are expected when the system is close to single phase (Cases 1 and 2).

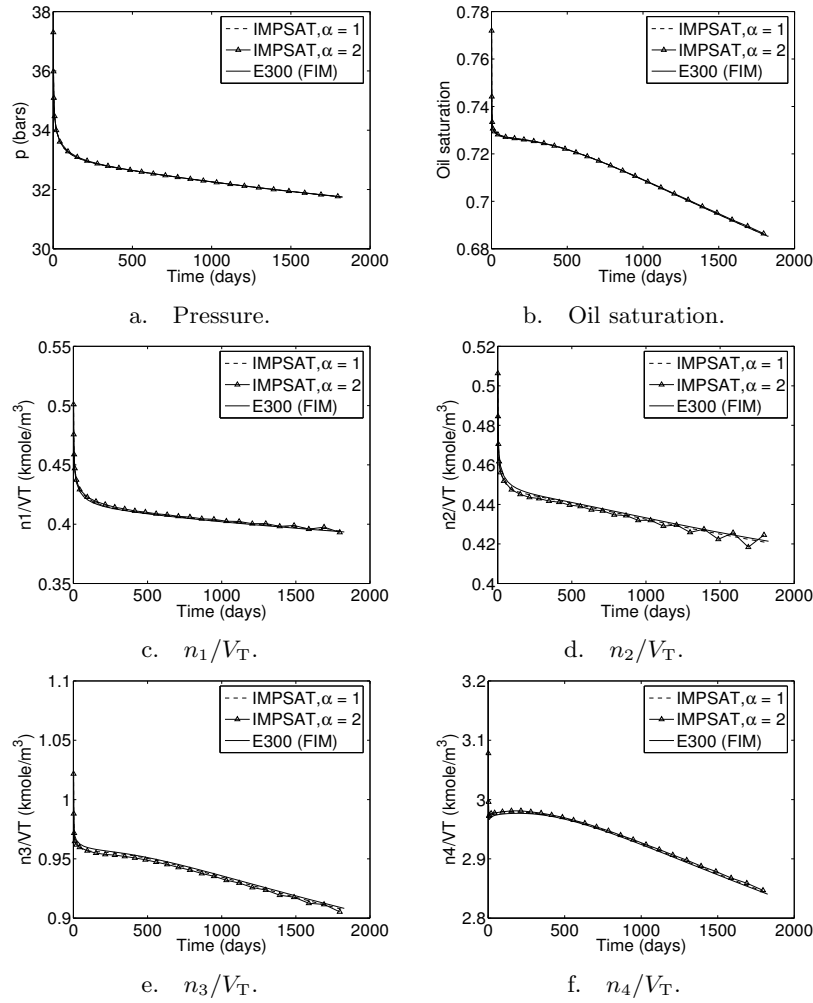


Figure 3. Production block results versus time, Case 1. Comparison of IMPSAT runs with CFL factors of $\alpha = 1$ and $\alpha = 2$ and a fully implicit Eclipse300 run.

7.6. PRODUCTION BLOCK RESULTS, CASE 1

Figure 3 shows production block results versus time for Case 1. We observe that the results of IMPSAT with a CFL factor of $\alpha = 1$ match the results of Eclipse300. However, for an IMPSAT run with a CFL factor of $\alpha = 2$, some of the normalised mole numbers experience increasing oscillations. An extra simulation with $\alpha = 1.9$ showed no sign of oscillations. We conclude that the stability limit for Case 1 corresponds to a CFL factor of (76) of around 2.0. Consequently, in Case 1, the approximate CFL criterion is reasonably precise.

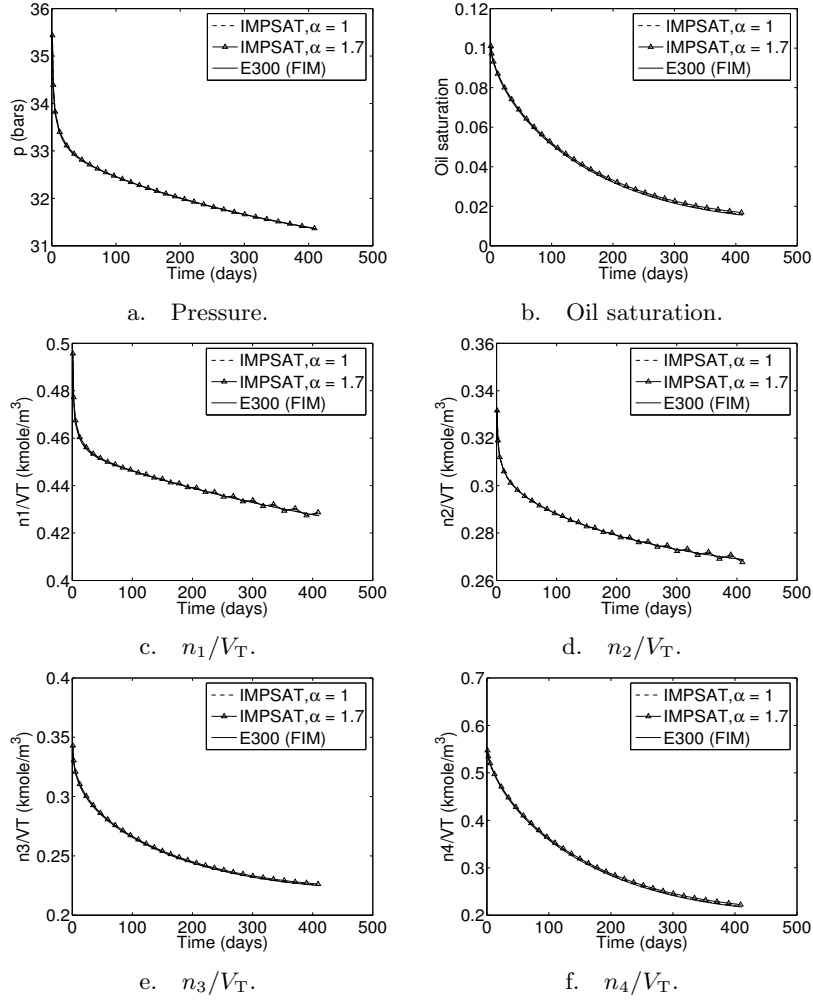


Figure 4. Production block results versus time, Case 2. Comparison of IMPSAT runs with CFL factors of $\alpha = 1$ and $\alpha = 1.7$ and a fully implicit Eclipse300 run.

7.7. PRODUCTION BLOCK RESULTS, CASE 2

Figure 4 shows production block results versus time for Case 2. The results of Eclipse300 and IMPSAT with a CFL factor of $\alpha = 1$ are very similar, but for a run with a CFL factor of $\alpha = 1.7$ the solution becomes unstable. Repeated runs leads us to conclude that the stability limit for Case 2 corresponds to a CFL factor of around 1.7. Consequently, the approximative CFL criterion is reasonably precise also in Case 2.

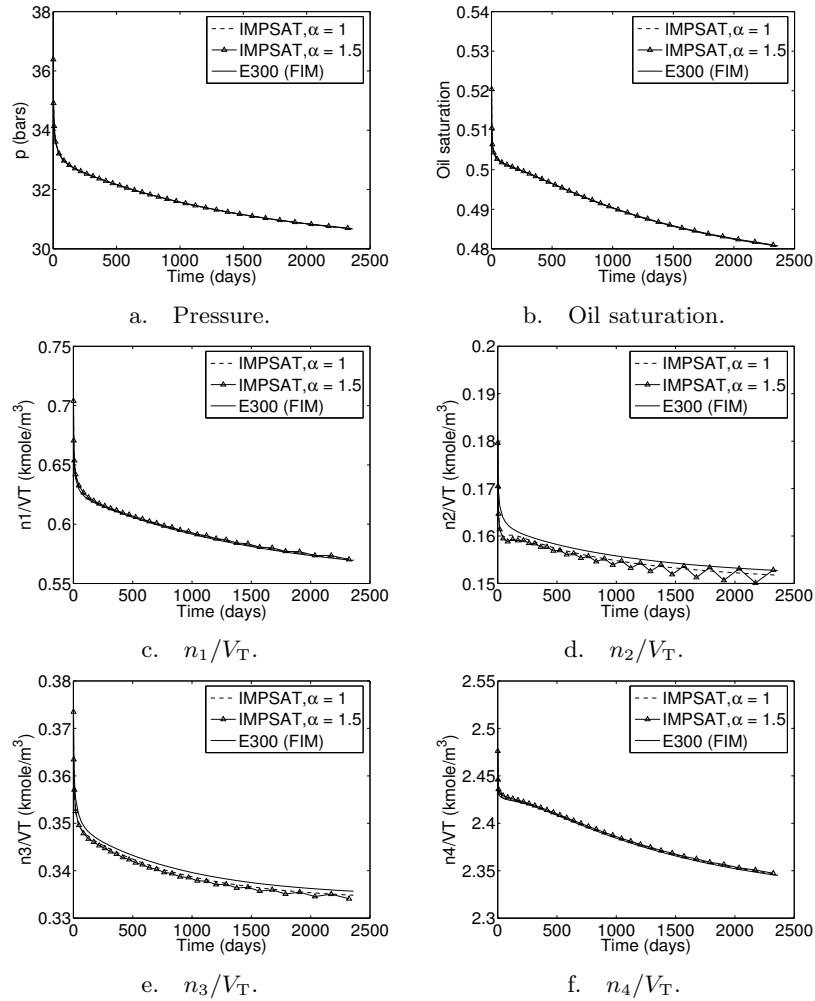


Figure 5. Production block results versus time, Case 3. Comparison of IMPSAT runs with CFL factors of $\alpha = 1$ and $\alpha = 1.5$ and a fully implicit Eclipse300 run.

7.8. PRODUCTION BLOCK RESULTS, CASE 3

Figure 5 shows production block results versus time for Case 3. We here observe a mismatch between the results of Eclipse300 and IMPSAT, but only for the components that contribute less to the saturations, i.e., the intermediate ones. A one-dimensional study shows that the corresponding component fronts are significantly more smeared by the Eclipse300 fully implicit solution. Consequently, the mismatch is reasonable.

For a run with a CFL factor of $\alpha = 1.5$ the solution becomes unstable. We conclude that the stability limit corresponds to a CFL factor of around 1.5, which makes (76) a quite precise estimate.

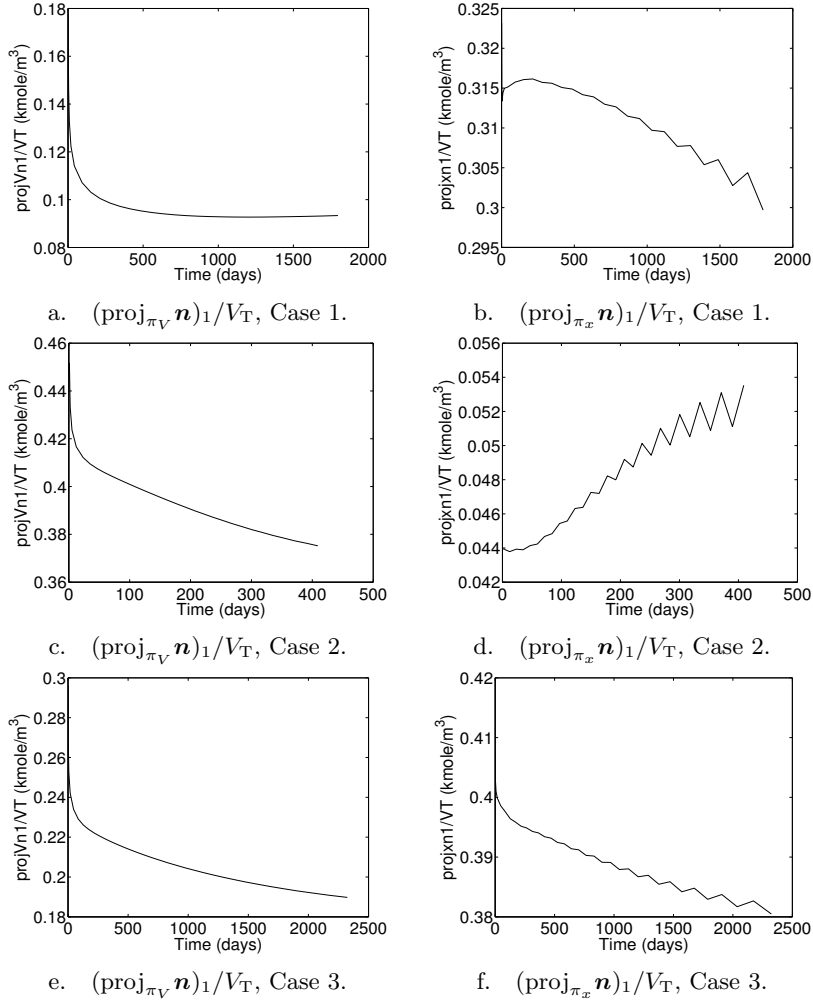


Figure 6. Volume part (left) and isochoric part (right) of the lightest component with respect to time in Cases 1, 2, 3, with CFL factor $\alpha = 2, 1.7$ and 1.5 , respectively.

7.9. INSTABILITIES

Figure 6 shows the volume part and the isochoric part of the lightest component versus time for Case 1, 2, 3, with $\alpha = 2$, $\alpha = 1.7$ and $\alpha = 1.5$, respectively. In all three cases, we observe that the increasing oscillations are isolated to the isochoric part. In addition, we note that similar behaviour is seen for the decomposition of the flow rate of component i ,

$$\mathbf{f}_i = (\text{proj}_{\pi_V} \mathbf{f})_i + (\text{proj}_{\pi_x} \mathbf{f})_i, \quad (83)$$

with respect to time.

8. Conclusions and Further Work

A new volume balance consistent compositional IMPSAT formulation has been developed and tested. It is based on transforming the conventional set of variables and equations into complementary sets: pressure, volumes and the volume balance equations on the one hand, and isochoric (constant volume) variables and isochoric conservation equations on the other hand. The approach yields a minimum overlap between the implicit volume solution and the explicit constant volume solution.

In addition, the new concepts of isochoric variables and spaces have been interpreted both mathematically and physically, leading to a better understanding of the stability of the IMPSAT formulation. Consequently, new approximate CFL stability criteria have been proposed and tested. Numerical results indicate that the new approach leads to a reasonable measure for the stability of IMPSAT. The predicted maximum stable timestep can in some cases be up to twice the timestep allowed by the conventional IMPSAT stability criterion of Cao and Aziz (corresponding to a relative improvement of 100 %). However, further testing is required to establish the range of validity of the new stability criterion.

The main focus of this paper has been the theory behind the volume balance consistent IMPSAT approach. Simulator performance has not been emphasised, but we have noted that the use of complementary variables and equations yields a better conditioned system. Comparisons to other IMPSAT formulations will be subject to future research.

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