# Compositional Reservoir Simulation With Emphasis on the IMPSAT Formulation

PhD Thesis

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# Preface

The work presented in this thesis is the partial fulfilment of the requirements for the degree of Doctor of Philosophy at the University of Bergen. The studies leading to the submission of the thesis started in March 2003, and have been done both at the Department of Mathematics at the University of Bergen, and at Centre for Integrated Petroleum Research.

Principal Researcher/VISTA Professor Ivar Aavatsmark has been the main advisor for the work, while Professor Magne Espedal and Researcher/Professor II Edel Reiso have been co-advisors. Norsk Hydro has provided funding for the project, under PhD scholarship agreement no. 2000771 between Norsk Hydro, the University of Bergen and Centre for Integrated Petroleum Research.

# Outline

The thesis consists of two parts. The first part focuses on motivation, background and objectives of research for the thesis, and includes the setup of a mathematical and a numerical model for multiphase, multicomponent fluid flow. Some calculation details are also given. These details serve as documentation of the in-house simulator XPSIM, which has been a by-product of the work presented in the thesis. The second part contains research papers stemming from the first part, and some ideas for further work.

A bibliography of references is included at the end of the thesis.

## Part I: The Development of a Reservoir Simulator

Chapter 1 gives the basic motivation for the work presented in the thesis, and a brief overview of the corresponding objectives of research.

The background for the thesis continues with Chapter 2, where a mathematical model for multiphase, multicomponent fluid flow is set up. We here outline the governing principles and the number of variables required to uniquely describe the reservoir state, and consider the black-oil and compositional fluid characterization models. Furthermore, the framework for a unified black-oil and compositional model is discussed. For the rest of the thesis, the focus is on a unified formulation, i.e., a compositional formulation which reduces to a black-oil formulation when used with black-oil fluid properties.

A numerical model is presented in Chapter 3. Here, discretization and initialization is considered, and iterative schemes for solving the governing equations are set up. In addition, possible reformulations of the fluid flow equations, e.g., volume balance equations, are presented. We also give an overview of different time schemes, including the IMPSAT scheme, which has been an important subject of research in the thesis. Finally, we briefly discuss timestep selection, convergence criteria and phase disappearance and reappearance.

Chapter 4 contains documentation of the in-house simulator XPSIM, and includes calculation details associated with the mathematical and numerical model presented in Chapters 2 and 3.

## Part II: Papers and Ideas for Further Work

Five research papers are included in the second part of the thesis, namely

**Paper A: A Black-Oil and Compositional IMPSAT Simulator With Improved Compositional Convergence**. J. Haukås, I. Aavatsmark and M. Espedal. Included in *Proceedings of the 9th European Conference on the Mathematics of Oil Recovery*, Cannes, France, 30 August – 2 September 2004.

**Paper B: A Volume Balance Consistent Compositional IMPSAT Formulation With Relaxed Stability Constraints**. J. Haukås, I. Aavatsmark, M. Espedal and E. Reiso. Submitted to *Computational Geosciences*, July 2005.

**Paper C: Exact Volume Balance Versus Exact Mass Balance in Compositional Reservoir Simulation**. J. Haukås, I. Aavatsmark, M. Espedal and E. Reiso. Submitted to *Computational Geosciences*, December 2005.

**Paper D: A Comparison of Two Different IMPSAT Models in Compositional Simulation**. J. Haukås, I. Aavatsmark, M. Espedal and E. Reiso. Submitted to *SPE Journal*, December 2005.

**Paper E: Isothermal Gravity/Chemical Equilibrium Calculations**. J. Haukås and S. G. Johnsen. Exam report for the summer school *Thermodynamic Models: Fundamentals and Computational Aspects*, IVC-SEP, Technical University of Denmark, August 9 – 27, 2004. Evaluated and accepted by Professors Michael L. Michelsen and Jørgen M. Mollerup at IVC-SEP.

An overview of the papers is given in Chapter 5, and some ideas for further work are presented in Chapter 6.

# Acknowledgements

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I am also very grateful for the project funding received from Norsk Hydro under PhD scholarship agreement no. 2000771 between Norsk Hydro, the University of Bergen and Centre for Integrated Petroleum Research. Working with a project which is of interest for the petroleum industry has been very motivating.

Centre for Integrated Petroleum Research (CIPR) has been my workplace for most of the PhD period. I would like to thank my friends and colleagues at CIPR for providing an interesting research environment and good company for lunch. I am happy that I will have the opportunity to remain associated with CIPR for some time after I have finished my PhD.

During the autumn of 2004, I visited IVC-SEP at the Technical University of Denmark for three months, and improved my knowledge of the fundamentals and computational aspects of thermodynamic models significantly. I thank my host there, Erling Stenby, for a pleasant and interesting stay.

Finally, I want to express my gratitude to family and friends, especially my wife Camilla, who has been a crucial support to me.

Jarle Haukås
Bergen, January 2006.

# Contents

# Part I

# The Development of a Reservoir Simulator

# Chapter 1

# Introduction

In this introductory chapter, we provide the basic motivation for the work presented in the thesis, and outline the corresponding objectives of research.

## 1.1 Basic Motivation

Reservoir simulation involves the use of computer programs (simulators) to describe the fluid flow processes in a reservoir. In the petroleum industry, predictions made by reservoir simulators are for instance used in well planning, e.g., to investigate the effect of different injection-production scenarios on the reservoir performance, in production planning and optimization, and in estimation of reservoir parameters, i.e., inverse problems/history matching. With the development of new and improved simulation techniques, and with more computational power at hand, reservoir simulation has become an increasingly useful tool. Today, nearly all major reservoir development decisions are based at least partially on simulation results, [1].

Although reservoir simulation is a quite mature field of research, there is still room for further improvements. However, we should keep in mind the trade-off between the precision and flexibility with which the fluid flow processes are described, and the computational effort needed for the calculations. From a mathematical and numerical point of view, it is therefore important to develop improved solution approaches that produce reliable results with reduced simulator runtime. This is also the basic motivation for the work presented in the thesis.

## 1.2 Objectives of Research

The objectives of research for the thesis are associated with the use of a compositional fluid characterization model, as motivated below. Important keywords are

flexibility, efficiency and numerical stability.

### 1.2.1 Black-oil vs. compositional fluid characterization

Real reservoir fluids consist of hundreds of chemical components. However, to limit the size of the computational system, components with similar chemical properties may be grouped into a pseudo component, treated as a single unity. With a black-oil fluid characterization model, the reservoir fluids other than water are assumed to consist of only two (pseudo) components, an oil component and a gas component. With a compositional fluid characterization model, the number of (pseudo) components is in principle arbitrary.

Traditionally, black-oil simulation has been preferred to compositional simulation. This is because of the prohibitively large runtimes with the conventional compositional simulators, mainly due to the large system of primary equations and variables, and the extensive computational effort required for the phase equilibrium calculations. With a black-oil fluid characterization model, these calculations can be done quite simply, as the fluid behaviour is less complex than with a compositional fluid characterization model.

However, in cases where compositional effects are important, e.g., in cases where the fluid composition varies significantly in the reservoir, and/or the injected fluids are very different from the fluids already present in the reservoir, reliable simulation results can only be obtained with a compositional model. The development of a more efficient numerical formulation for compositional fluid flow is therefore a crucial objective of research.

In addition, we note that black-oil and compositional simulations have traditionally been performed with separate reservoir simulators. The reason for this is the lack of a proper unified black-oil and compositional formulation, i.e., a compositional formulation which reduces to a black-oil formulation when used with black-oil fluid properties, and preserves the conventional efficiency. Having a unified formulation would lead to a significant reduction in simulator development and maintenance costs. Consequently, the development of a flexible, but efficient, unified black-oil and compositional formulation is another important objective of research.

### 1.2.2 The IMPSAT formulation

Many compositional formulations have been proposed in the literature, e.g., [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]. The formulations differ in their choices of primary variables and equations and approaches for solving the equations.

Experience shows that a solution of all primary equations with respect to all primary variables simultaneously (fully implicitly) may often be computationally

too demanding. The conventional compositional approach has therefore been an IMPES formulation, e.g., [2, 3, 5, 6, 8]. Here, pressure is determined separately (implicitly), while the other primary variables are determined by explicit updates. Unfortunately, the explicit determination of variables may lead to stability problems, i.e., unphysical oscillations in the solution. To avoid an unstable solution, timestep size must be restricted. Consequently, although IMPES is the fastest approach on a per-timestep basis, timestep restrictions often severely reduce its overall efficiency.

An alternative is the IMPSAT formulation. Here, pressure and saturations are determined implicitly, while the other primary variables are determined by explicit updates. An IMPSAT approach is significantly more stable than an IMPES approach, and may be substantially less expensive than a fully implicit approach, [15]. Furthermore, pressure and saturations are the conventional black-oil primary variables, and an IMPSAT formulation is thus the natural basis for a unified black-oil and compositional formulation. The development of an efficient IMPSAT formulation is therefore an interesting objective of research.

We note that, although some work on the IMPSAT formulation has been reported in the literature, e.g., [9, 10, 12, 15, 16], a completely satisfactory set of primary equations and variables in addition to the pressure and saturation part has not yet been presented. The choice of primary variables and equations for an IMPSAT formulation is an important issue in this thesis.

For completeness, we should also mention the adaptive implicit approach, which involves different formulations (fully implicit, IMPES, IMPSAT) in the solution of the fluid flow problem in different parts of the reservoir. Several authors discuss adaptive implicit methods, e.g., [15, 16, 17, 18, 19, 20], but such methods are not considered in this thesis.

Having outlined the motivation and objectives of research, the following chapters are supposed to provide a background for the research papers included in the thesis. The research papers focus on the development of a unified black-oil and compositional formulation, within the framework of an improved IMPSAT formulation. The background therefore includes the setup of a mathematical model for multiphase, multicomponent fluid flow, some details on the black-oil and compositional fluid characterization models, and the setup of a numerical model for solving the equations. In addition, calculation details necessary for the implementation of a compositional simulator are given.

# Chapter 2

# Mathematical Model

In this chapter, we give an overview of the mathematical basis for a reservoir simulator. We first present the governing principles, which are the general principles of conservation and phase equilibrium. Furthermore, we consider the number of variables required to uniquely determine the state of the reservoir system. We then present the characteristic features of the black-oil and compositional fluid characterization models, and let the framework for a unified black-oil and compositional model conclude the chapter.

## 2.1 Governing Principles

In the following, we outline the governing principles that are common to any reservoir simulator. The final form of the governing equations depends on the fluid characterization model, and will be given in section 2.3.

### 2.1.1 Conservation of mass

The mathematical description of fluid flow is based on the principle of mass conservation (mass balance), i.e., that the accumulation of mass in some domain is exactly balanced by the mass flowing through the boundary of the domain and the contribution of sources/sinks within the domain. In reservoir simulation, the principle applies to every (pseudo) component present in the fluids.

We let $N_{\mathrm{c}}$ denote the number of components, and write the $N_{\mathrm{c}}$ mass balance equations in the form

$$\int_{V_{\mathrm{b}}} \frac{\partial}{\partial t}\left(\phi \frac{\boldsymbol{n}}{V_{\mathrm{T}}}\right) dV - \int_{V_{\mathrm{b}}} \hat{\boldsymbol{q}}\, dV + \int_{S_{\mathrm{b}}} \hat{\boldsymbol{f}} \cdot \vec{n}\, dS = \mathbf{0}. \tag{2.1}$$

Here, $\phi$ is the porosity, $\boldsymbol{n}$ is the $N_{\mathrm{c}}$ vector of component amounts, $V_{\mathrm{T}}$ is the total fluid volume, $\hat{\boldsymbol{f}}$ contains the $N_{\mathrm{c}}$ component fluxes, $\hat{\boldsymbol{q}}$ is the $N_{\mathrm{c}}$ vector of source

density rates, while $V_\mathrm{b}$ is some (bulk) volume with surface $S_\mathrm{b}$. The unit normal of $S_\mathrm{b}$ is denoted $\vec{n}$. We note that each component flux in $\hat{\boldsymbol{f}}$ is a vector in space. The dot product in (2.1) is taken for each component flux, so that $\hat{\boldsymbol{f}} \cdot \vec{n}$ is a $N_\mathrm{c}$ vector.

The fluids should fill the pore space, i.e., $V_\mathrm{T} = \phi V_\mathrm{b}$, see section 2.1.4. Consequently, $\phi \boldsymbol{n}/V_\mathrm{T} = \boldsymbol{n}/V_\mathrm{b}$, and the leftmost integral in (2.1) properly represents the time derivative of the component amounts averaged over $V_\mathrm{b}$. Furthermore, the porosity $\phi$ is usually assumed to be a function of pressure $p$ and a (constant) rock compressibility $c_R$,

$$\phi = \tilde{\phi}\left[1 + c_R\left(p - \tilde{p}\right)\right]. \tag{2.2}$$

Here, $\tilde{\phi}$ is the reference porosity, given at some reference pressure $\tilde{p}$.

The discussion of sources/sinks is postponed to Chapter 3, while the general form of the flux term is outlined below.

### 2.1.2 Darcy's law

The components are distributed in fluid phases, e.g., oil, gas and water phases. Actually, fluid flow is characterized by flow of phases rather than flow of the individual components. Darcy's law is the relation between the gradient of the potential of a phase $j$ and the phase volumetric flow rate $u^j$, and can be written

$$u^j = -\frac{k_r^j}{\mu^j}\boldsymbol{K}\left(\nabla p + \nabla P_c^j - \rho^j g \nabla D\right). \tag{2.3}$$

Here, $\boldsymbol{K}$ is the absolute permeability (tensor), $k_r^j$ is the phase relative permeability, $\mu^j$ is the phase viscosity, $p$ is the pressure of one of the phases, $P_c^j$ is the capillary pressure between phase $j$ and the phase to which the pressure $p$ belongs, $\rho^j$ is the phase mass density, $g$ is the acceleration of gravity, and $D$ is the depth in the reservoir. Note that $u^j$ is associated with a direction in space.

Using Darcy's law, the $i$-th component flux in (2.1) can be expressed by

$$\hat{f}_i = \sum_{j=1}^{N_p} c_i^j \xi^j u^j = -\sum_{j=1}^{N_p} \frac{c_i^j \xi^j k_r^j}{\mu^j}\boldsymbol{K}\left(\nabla p + \nabla P_c^j - \rho^j g \nabla D\right), \tag{2.4}$$

where $N_\mathrm{p}$ is the number of phases, $c_i^j$ is the fraction of component $i$ in phase $j$, while $\xi^j$ is the phase density. Note that either mass fractions and mass densities or mole fractions and molar densities can be used. Consequently, the $i$-th mass balance equation can be given in the form

$$\begin{aligned} \int_{V_\mathrm{b}} \frac{\partial}{\partial t}\left(\phi \frac{n_i}{V_\mathrm{T}}\right) dV - \int_{V_\mathrm{b}} \hat{q}_i \, dV \\ - \int_{S_\mathrm{b}} \sum_{j=1}^{N_p} \frac{c_i^j \xi^j k_r^j}{\mu^j}\boldsymbol{K}\left(\nabla p + \nabla P_c^j - \rho^j g \nabla D\right) \cdot \vec{n} \, dS &= 0. \end{aligned} \tag{2.5}$$

The absolute permeability $\boldsymbol{K}$ is given as input to the reservoir simulator, while the relative permeabilities $k_r^j$ and the capillary pressures $P_c^j$ are (tabulated) functions of the saturations

$$S^j = \frac{V^j}{V_\mathrm{p}}. \tag{2.6}$$

Here, $V^j$ is the phase volume and $V_\mathrm{p}$ is the size of the pore volume. The calculation of the other terms in (2.5) depends on the fluid characterization model.

### 2.1.3 Conservation of energy

The principle of energy conservation governs temperature variations in the reservoir. However, in this work, we only consider isothermal reservoirs, i.e., reservoirs where the temperature is assumed to be constant. Consequently, the energy conservation equation is redundant.

### 2.1.4 Conservation of volume

The volume balance principle requires that the fluids must fill the pore volume exactly, i.e.,

$$V_\mathrm{T} = V_\mathrm{p} = \phi V_\mathrm{b}. \tag{2.7}$$

Using (2.6), we may alternatively express (2.7) by

$$\sum_{j=1}^{N_\mathrm{p}} S^j = 1. \tag{2.8}$$

### 2.1.5 Phase equilibrium

In addition to the conservation requirements, we require an instantaneous thermodynamic equilibrium locally in the reservoir. This requirement is due to the assumption that the distribution of components in phases at equilibrium is a much more rapid process than the fluid flow.

Generally, the conditions of thermodynamic equilibrium are based on the second law of thermodynamics, which implies that an equilibrium state is a stationary point of maximum entropy. Consequently, it can be shown that pressure, temperature and the $N_\mathrm{c}$ component chemical potentials must be uniform in all phases at thermodynamic equilibrium. This corresponds to $(N_\mathrm{p} - 1)(N_\mathrm{c} + 2)$ independent phase equilibrium conditions. Here, the influence of gravity and surface tension is neglected. For more details, see for instance [21, 22].

The form of the conditions of thermodynamic equilibrium depends on the fluid characterization model, see section 2.3.

## 2.2 State Variables

In the governing principles outlined above, many different variables are used to describe the state of the reservoir system, i.e., pressure, component amounts, volumes, densities, etc. However, due to the relations between the variables, e.g., the phase equilibrium relations, only a minimum number of independent state variables is required to uniquely determine the state.

The state variables are classified as either intensive or extensive variables. Extensive variables, for instance volumes and component amounts, depend on the extent of the system, while intensive variables, for instance pressure, mass/mole fractions and densities, do not.

In the following, we consider the number of independent state variables. We note that this number corresponds to the number of primary variables in the mathematical model.

### 2.2.1 Gibbs' phase rule

A thermodynamic postulate says that, in order to describe the state of a simple single-phase system of $N_{\mathrm{c}}$ components, we must give $N_{\mathrm{c}}+2$ independent variables. However, if we only want to describe the intensive properties, it is sufficient to give $N_{\mathrm{c}}+1$ independent intensive variables.

If $N_{\mathrm{p}}$ phases are at equilibrium, all of the intensive properties of all the phases will be determined by $N_{\mathrm{p}}(N_{\mathrm{c}}+1)$ intensive variables. At the same time, the $(N_{\mathrm{p}}-1)(N_{\mathrm{c}}+2)$ phase equilibrium conditions must be fulfilled. Consequently, the number of degrees of freedom is

$$N_{\mathrm{p}}(N_{\mathrm{c}}+1)-(N_{\mathrm{p}}-1)(N_{\mathrm{c}}+2)=N_{\mathrm{c}}-N_{\mathrm{p}}+2. \tag{2.9}$$

This is traditionally referred to as *Gibbs' phase rule*, [23]. By giving $N_{\mathrm{c}}-N_{\mathrm{p}}+2$ intensive variables, we may determine the intensive properties of all the phases.

However, we must also determine the relative amounts of each phase, e.g., the saturations. Due to the volume balance requirement (2.8), only $N_{\mathrm{p}}-1$ saturations are needed, and the number of independent variables becomes

$$N_{\mathrm{c}}-N_{\mathrm{p}}+2+(N_{\mathrm{p}}-1)=N_{\mathrm{c}}+1. \tag{2.10}$$

To determine extensive properties, another variable must be added, and at least one of the $N_{\mathrm{c}}+2$ independent variables must be an extensive one. For an isothermal model, where temperature is a constant parameter rather than a variable, these numbers reduce to $N_{\mathrm{c}}$ and $N_{\mathrm{c}}+1$.

In reservoir simulation, the bulk volume $V_{\mathrm{b}}$, which is an extensive quantity, is usually known. Consequently, for an isothermal model, the state is uniquely described in terms of $N_{\mathrm{c}}$ independent primary variables plus $V_{\mathrm{b}}$.

## 2.3 Fluid Characterization Models

Two different fluid characterization models are used in reservoir simulation, the black-oil model and the compositional model. In the following, we consider the characteristic features of these two models. For both models, we assume that the water phase only consists of water, and that the water component is not present in the oil and gas phases. Consequently, the only phase equilibrium that needs to be considered is the one between oil and gas.

### 2.3.1 The black-oil fluid characterization model

In a black-oil model, the number of components other than water is limited to two (pseudo) components, an oil component and a gas component. The oil, gas and water components are referred to by subscripts $o$, $g$ and $w$, respectively, while the oil, gas and water phases are referred to by superscripts $o$, $g$ and $w$, respectively.

In the classical black-oil model, see for instance [24, 25], the gas component is allowed to dissolve in the oil phase, but the oil component is not allowed to exist in the gas phase. However, in the modified black-oil model, e.g., [24, 26], the oil and gas components may be present in both the oil and gas phases. For generality, we consider the modified black-oil model, from which the classical black-oil model can be obtained by cancelling some of the terms.

#### Characteristic features

A characteristic feature of the black-oil model is the use of standard conditions, usually a pressure of 1 atmosphere and a temperature of 15.5 °C. At standard conditions, the oil component coincides with the oil phase, while the gas component coincides with the gas phase. The densities of oil, gas and water at standard conditions, $\xi_s^o$, $\xi_s^g$ and $\xi_s^w$, are given (input) parameters. We note that the conventional black-oil fluid characterization is in terms of masses and mass densities rather than moles and molar densities.

The oil and gas volumes at reservoir conditions are denoted $V_r^o$ and $V_r^g$, respectively. Taken to standard conditions, $V_r^o$ corresponds to an oil volume $V_s^o$ and a gas volume $V_s^{dg}$ (dissolved gas). This is due to the fact that gas boils out of the oil phase when pressure is lowered. As illustrated in the phase diagram in Figure 2.1, this process takes place to the left of the critical point.

Similarly, $V_r^g$ corresponds to a gas volume $V_s^g$ and an oil volume $V_s^{vo}$ (vaporized oil) at standard conditions. Here, oil appears from the gas phase when pressure is lowered. Referring to Figure 2.1, this process takes place in the region to the right of the critical point, often referred to as the retrograde gas condensate

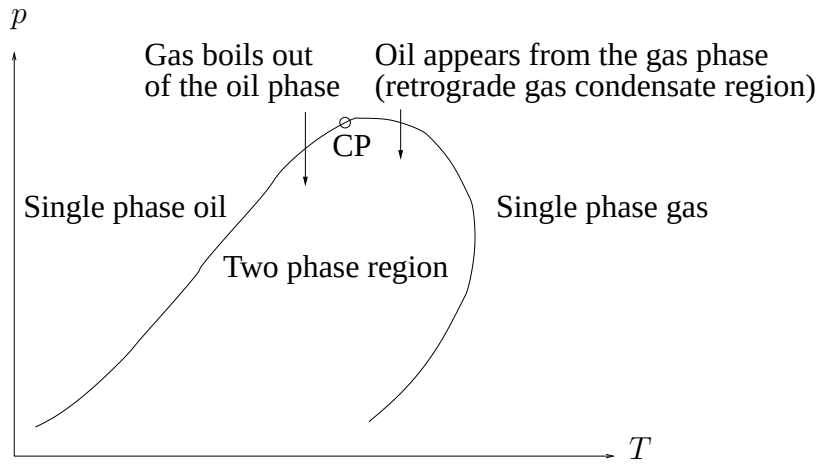



Figure 2.1: Phase diagram where $p$ is pressure and $T$ is the absolute temperature. At the critical point (CP), the phases are truly indistinguishable. Going from single phase to two phase by a lowering of the pressure corresponds to gas boiling out of the oil phase to the left of the critical point, and oil appearing from the gas phase to the right of the critical point, i.e., in the retrograde gas condensate region.

region. We note that retrograde gas condensate cases are included in the modified black-oil model, but not in the classical black-oil model.

For the water phase, the volumes at reservoir and standard conditions are denoted $V_r^w$ and $V_s^w$, respectively.

Based on the above notation, it is convenient to introduce the formation volume factors (FVFs),

$$B^o = \frac{V_r^o}{V_s^o}, \qquad B^g = \frac{V_r^g}{V_s^g}, \qquad B^w = \frac{V_r^w}{V_s^w}, \tag{2.11}$$

and the solution gas/oil ratio and the vaporized oil/gas ratio,

$$R_s = \frac{V_s^{dg}}{V_s^o}, \qquad R_v = \frac{V_s^{vo}}{V_s^g}, \tag{2.12}$$

respectively.

If both the oil and gas phases are present at reservoir conditions, the number of phases equals the number of components, and the intensive properties of the phases are determined by $N_\mathrm{c} - N_\mathrm{p} + 2 = 2$ intensive variables, according to (2.9). A natural choice of state variables is pressure and temperature, where temperature is constant for an isothermal model. Consequently, all the parameters (2.11), (2.12) can be given as functions of pressure. Here, the ratios (2.12) represent the

phase equilibrium conditions between oil and gas. The case where both oil and gas are present is referred to as the saturated black-oil case.

On the other hand, if the gas phase is absent at reservoir conditions, the remaining oil phase is referred to as undersaturated oil. We then need to specify three intensive variables to uniquely determine the intensive phase properties. A natural choice is pressure, temperature and the solution gas/oil ratio $R_s$, which represents the composition of the oil phase. Consequently, for undersaturated oil, the oil formation volume factor $B^o$ depends on both pressure and $R_s$.

Similarly, if the oil phase is absent at reservoir conditions, the remaining gas phase is referred to as supercritical or undersaturated gas. Here, the natural choice of independent state variables is pressure, temperature and the vaporized oil/gas ratio $R_v$, which represents the composition of the gas phase. For supercritical/undersaturated gas, the gas formation volume factor $B^g$ thus depends on both pressure and $R_v$.

### Black-oil primary variables

To determine the relative phase amounts, $N_\mathrm{p} - 1$ saturations $\boldsymbol{S}_\mathrm{p}$ are used. In addition, we assume that the bulk volume $V_\mathrm{b}$ is known. Hence, the conventional set of $N_\mathrm{c}$ black-oil primary variables is

$$\boldsymbol{u}_\mathrm{p} = \begin{bmatrix} p \\ \boldsymbol{S}_\mathrm{p} \\ R \end{bmatrix}, \tag{2.13}$$

where $R = R_s$ for undersaturated oil and $R = R_v$ for supercritical/undersaturated gas. In the saturated black-oil case, $R$ is redundant as a primary variable.

### Black-oil mass balance equations

The black-oil mass balance equations can be expressed explicitly in terms of pressure, FVFs, saturations and the ratios $R_s$ and $R_v$, as shown in the following.

At reservoir conditions, the oil phase contains some amount $n_g^o$ of the gas component, and some amount $n_o^o$ of the oil component, namely

$$n_g^o = \xi_s^g \, V_s^{dg} = \xi_s^g \, R_s \, \frac{V_r^o}{B^o}, \qquad n_o^o = \xi_s^o \, V_s^o = \xi_s^o \, \frac{V_r^o}{B^o}. \tag{2.14}$$

Correspondingly, the gas phase contains

$$n_g^g = \xi_s^g \, V_s^g = \xi_s^g \, \frac{V_r^g}{B^g}, \qquad n_o^g = \xi_s^o \, V_s^{vo} = \xi_s^o \, R_v \, \frac{V_r^g}{B^g}. \tag{2.15}$$

Furthermore, the water phase consists of water only, so that

$$n_w = n^w = \xi_s^w V_s^w = \xi_s^w \frac{V_r^w}{B^w}. \tag{2.16}$$

The oil, gas and water mass balance equations thus involve

$$\phi \frac{n_o}{V_\mathrm{T}} = \phi \frac{n_o^o + n_o^g}{V_\mathrm{T}} = \phi \left( \xi_s^o \frac{S^o}{B^o} + \xi_s^o R_v \frac{S^g}{B^g} \right) \tag{2.17}$$

$$\phi \frac{n_g}{V_\mathrm{T}} = \phi \frac{n_g^g + n_g^o}{V_\mathrm{T}} = \phi \left( \xi_s^g \frac{S^g}{B^g} + \xi_s^g R_s \frac{S^o}{B^o} \right), \tag{2.18}$$

$$\phi \frac{n_w}{V_\mathrm{T}} = \phi \, \xi_s^w \frac{S^w}{B^w}, \tag{2.19}$$

where (2.6) and (2.7) have been used. Furthermore, (mass) densities are given by

$$\xi^o = \frac{n_g^o + n_o^o}{V_r^o} = \frac{\xi_s^g R_s + \xi_s^o}{B^o}, \qquad \xi^g = \frac{n_g^g + n_o^g}{V_r^g} = \frac{\xi_s^g + \xi_s^o R_v}{B^g}, \tag{2.20}$$

$$\xi^w = \frac{n_w}{V_r^w} = \frac{\xi_s^w}{B^w}, \tag{2.21}$$

while the flux terms (2.4) depend on the calculation of

$$c_o^o \, \xi^o = \frac{n_o^o}{V_r^o} = \frac{\xi_s^o}{B^o}, \qquad c_o^g \, \xi^g = \frac{n_o^g}{V_r^g} = \frac{\xi_s^o R_v}{B^g}, \tag{2.22}$$

$$c_g^o \, \xi^o = \frac{n_g^o}{V_r^o} = \frac{\xi_s^g R_s}{B^o}, \qquad c_g^g \, \xi^g = \frac{n_g^g}{V_r^g} = \frac{\xi_s^g}{B^g}, \tag{2.23}$$

$$c_w^w \, \xi^w = \xi^w = \frac{\xi_s^w}{B^w}. \tag{2.24}$$

Consequently, using (2.5), the oil mass balance equation can be written

$$\begin{aligned} &\int_{V_\mathrm{b}} \frac{\partial}{\partial t} \left[ \phi \left( \xi_s^o \frac{S^o}{B^o} + \xi_s^o R_v \frac{S^g}{B^g} \right) \right] dV - \int_{V_\mathrm{b}} \hat{q}_o \, dV \\ &- \int_{S_\mathrm{b}} \frac{\xi_s^o k_r^o}{B^o \mu^o} \boldsymbol{K} \left( \nabla p + \nabla P_c^o - \frac{\xi_s^g R_s + \xi_s^o}{B^o} g \nabla D \right) \cdot \vec{n} \, dS \\ &- \int_{S_\mathrm{b}} \frac{\xi_s^o R_v k_r^g}{B^g \mu^g} \boldsymbol{K} \left( \nabla p + \nabla P_c^g - \frac{\xi_s^g + \xi_s^o R_v}{B^g} g \nabla D \right) \cdot \vec{n} \, dS \;\; = \;\; 0, \end{aligned} \tag{2.25}$$

the gas mass balance is expressed by

$$\begin{aligned}
&\int_{V_\mathrm{b}} \frac{\partial}{\partial t}\left[\phi\left(\xi_s^g\,\frac{S^g}{B^g}+\xi_s^g\,R_s\,\frac{S^o}{B^o}\right)\right]dV-\int_{V_\mathrm{b}}\hat{q}_g\,dV\\
&-\int_{S_\mathrm{b}}\frac{\xi_s^g k_r^g}{B^g\mu^g}\boldsymbol{K}\left(\nabla p+\nabla P_c^g-\frac{\xi_s^g+\xi_s^o\,R_v}{B^g}g\nabla D\right)\cdot\vec{n}\,dS\\
&-\int_{S_\mathrm{b}}\frac{\xi_s^g\,R_s k_r^o}{B^o\mu^o}\boldsymbol{K}\left(\nabla p+\nabla P_c^o-\frac{\xi_s^g\,R_s+\xi_s^o}{B^o}g\nabla D\right)\cdot\vec{n}\,dS \;=\; 0, \qquad (2.26)
\end{aligned}$$

while the water mass balance is given by

$$\begin{aligned}
&\int_{V_\mathrm{b}} \frac{\partial}{\partial t}\left[\phi\xi_s^w\,\frac{S^w}{B^w}\right]dV-\int_{V_\mathrm{b}}\hat{q}_w\,dV\\
&-\int_{S_\mathrm{b}}\frac{\xi_s^w k_r^w}{B^w\mu^w}\boldsymbol{K}\left(\nabla p+\nabla P_c^w-\frac{\xi_s^w}{B^w}g\nabla D\right)\cdot\vec{n}\,dS \;=\; 0. \qquad (2.27)
\end{aligned}$$

Here, porosity is given by (2.2), the densities at standard conditions are constant parameters, relative permeabilities and capillary pressures are functions of the saturations, while viscosities are given as (tabulated) functions of pressure. The phase equilibrium conditions are inherent in the parameters $R_s$ and $R_v$, while phase reappearance and disappearance can be controlled by tables of bubblepoint and dewpoint pressures. The black-oil mass balance equations are $N_\mathrm{c}$ primary equations to be solved with respect to the $N_\mathrm{c}$ primary variables (2.13).

We note that the oil, gas and water mass balance equations may be divided by the standard densities $\xi_s^o$, $\xi_s^g$ and $\xi_s^w$, respectively. The resulting equations then represent balances on "standard volumes" rather than mass balances, [24].

## 2.3.2 The compositional fluid characterization model

In a compositional model, the number of components is arbitrary. This allows for a more flexible fluid description than with a black-oil model, but adds complexity to the calculations, as shown in the following.

### General component characterization

The compositional fluid characterization model is based on a general component characterization. For a (pseudo) component present in the oil and gas phases, a sufficient set of characteristic component properties is

- critical temperature $T_{c,i}$,
- critical pressure $p_{c,i}$,

- critical molar volume $V_{c,i}$,
- molar mass $M_i$,
- acentric factor $\omega_i$,
- binary interaction coefficients $d_{i,k}$ between components $i$ and $k$.

For water, the required input properties are the molar mass $M_w$, the molar density $\tilde{\xi^w}$ at some reference pressure $\tilde{p}$ and the (constant) water compressibility $c_w$.

Tables of component properties can for instance be found in [27]. The properties are used as parameters in phase equilibrium calculations, density calculations and viscosity calculations, as outlined below.

### Phase equilibrium

In a compositional model, the number of (pseudo) components in the oil and gas phases exceeds two, and no simple equilibrium relations of the form (2.12) can be proposed. Consequently, the general phase equilibrium conditions, i.e., equalities of component chemical potentials in all phases, must be considered.

The chemical potential $\mu_i^j$ of component $i$ in phase $j$ can be expressed by

$$\mu_i^j = \mu_i^{\text{id}}(T, p_0) + RT \ln \frac{f_i^j}{p_0}, \tag{2.28}$$

where $\mu_i^{\text{id}}$ is the ideal-gas contribution, $R$ = 8.3145 J/(K mol) is the universal gas constant, $T$ is the absolute temperature, $f_i^j$ is the fugacity of component $i$ in phase $j$ and $p_0$ is some constant reference pressure, see for instance [21]. The fugacity $f_i^j$ is interpreted as the tendency of component $i$ to escape from phase $j$, and is often written in the form

$$f_i^j = pc_i^j \phi_i^j, \tag{2.29}$$

where $\phi_i^j$ denotes the fugacity coefficient of component $i$ in phase $j$.

For an equilibrium between two phases $o$ and $g$, the equality of chemical potentials is equivalent to the fugacity equality

$$f_i^o - f_i^g = 0, \tag{2.30}$$

and to the equality

$$\frac{c_i^g}{c_i^o} = \frac{\phi_i^o}{\phi_i^g}, \tag{2.31}$$

when (2.29) and the requirement of uniform pressure in the phases is used.

Expressions for chemical potentials, fugacities and fugacity coefficients are generally obtained from a state function, e.g., the Gibbs energy function or the

Helmholtz energy function, see [22]. However, the complexity of the general state functions has motivated the use of cubic equations of state, which approximate the thermodynamic behaviour and thereby the general state functions. A cubic equation of state for a phase $j$ can be written

$$\left(Z^j\right)^3 + c_2\left(Z^j\right)^2 + c_1 Z^j + c_0 = 0, \tag{2.32}$$

and is solved with respect to the so-called compressibility factor $Z^j$, defined by

$$Z^j = \frac{pV^j}{n^j RT}. \tag{2.33}$$

Here, $n^j$ is the number of moles of phase $j$. The coefficients $c_2$, $c_1$ and $c_0$ depend on pressure, temperature and phase mole fractions $c_i^j$, and are based on empirical component mixing rules that take the characteristic component properties into account. Consequently, the fugacities and fugacity coefficients of (2.29), calculated with the use of a cubic equation of state, also depend on pressure, temperature and phase mole fractions.

We note that (2.32) has three roots, some of them possibly complex. However, the equilibrium solution should correspond to a stationary point of minimum Gibbs energy, which is a equivalent to a entropy maximum, see [22]. Consequently, the smallest real root is usually chosen for the oil phase, while the largest real root is usually chosen for the gas phase.

Many different cubic equations of state have been proposed, and an overview can for instance be found in [26]. In reservoir simulation, the Peng-Robinson equation of state, [28], is commonly used. Details on the calculation of compressibility factors, fugacities and fugacity coefficients with the Peng-Robinson equation of state are provided in section 4.4.

### Density and viscosity calculations

In a compositional model, the molar densities and mass densities of the oil and gas phases are calculated by

$$\xi^j = \frac{n^j}{V^j} = \frac{p}{RTZ^j}, \qquad \rho^j = \xi^j \sum_{i=1}^{N_c} c_i^j M_i, \tag{2.34}$$

where (2.33) is used. Furthermore, water densities are calculated by

$$\xi^w = \tilde{\xi^w}\left(1 + c_w(p - \tilde{p})\right), \qquad \rho^w = M_w \xi^w. \tag{2.35}$$

The viscosities of the oil and gas phases are assumed to depend on pressure, temperature and phase mole fractions, and may for instance be calculated by the Lohrenz-Bray-Clark (LBC) method, [29]. Details on the LBC method are given in section 4.5. The water viscosity is most often assumed to be constant. Alternatively, it can be given as a function of pressure.

**Note** We note that fugacities, densities and viscosities are given in terms of pressure, temperature and the phase mole fractions $c_i^j$. Alternatively, since

$$c_i^j = \frac{n_i^j}{n^j}, \qquad n^j = \sum_{k=1}^{N_\mathrm{c}} n_k^j, \tag{2.36}$$

where $n_i^j$ is the mole number of component $i$ in phase $j$, we may express fugacities, densities and viscosities in terms of pressure, temperature and the mole numbers of the components in all the phases,

$$\boldsymbol{n^j} = \left[n_1^1, n_2^1, \ldots, n_{N_\mathrm{c}}^1, \ldots\ldots n_1^{N_\mathrm{p}}, n_2^{N_\mathrm{p}}, \ldots, n_{N_\mathrm{c}}^{N_\mathrm{p}}\right]^\mathrm{T}. \tag{2.37}$$

The mole fractions $c_i^j$ are required to sum to unity, while the mole numbers $n_i^j$ are not. Consequently, the use of (2.37) may be computationally convenient.

### Compositional mass balance equations

The compositional mass balance equations involve the calculation of

$$\phi \frac{n_i}{V_\mathrm{T}} = \frac{\phi}{V_\mathrm{T}} \sum_{j=1}^{N_\mathrm{p}} c_i^j \xi^j V^j = \phi \sum_{j=1}^{N_\mathrm{p}} c_i^j \xi^j S^j, \tag{2.38}$$

where (2.6) and (2.7) have been used. Consequently, (2.5) can be written

$$\begin{aligned} &\int_{V_\mathrm{b}} \frac{\partial}{\partial t} \left[\phi \sum_{j=1}^{N_\mathrm{p}} c_i^j \xi^j S^j\right] dV - \int_{V_\mathrm{b}} \hat{q}_i \, dV \\ &- \int_{S_\mathrm{b}} \sum_{j=1}^{N_p} \frac{c_i^j \xi^j k_r^j}{\mu^j} \boldsymbol{K} \left(\nabla p + \nabla P_c^j - \rho^j g \nabla D\right) \cdot \vec{n} \, dS \;\; = \;\; 0. \end{aligned} \tag{2.39}$$

Here, porosity is given by (2.2), densities are calculated by (2.34) and (2.35), relative permeabilities and capillary pressures are functions of the saturations, oil and gas viscosities may be calculated as functions of pressure, temperature and phase mole fractions, while the water viscosity is constant or a function of pressure. We note that the only non-zero $c_i^j$ in the water mass balance equation is the fraction of water in the water phase, $c_w^w = 1$.

Unfortunately, unlike the black-oil mass balance equations, the compositional mass balance equations cannot be written explicitly in terms of only $N_\mathrm{c}$ primary variables. This is due to the complexity and nonlinear nature of the phase equilibrium conditions (2.30). Consequently, the notion of primary and secondary variables must be introduced, as outlined below.

### Compositional primary and secondary variables

The mass balance equations (2.39) can clearly be written explicitly in terms of pressure, saturations and component mole fractions. An alternative set of variables is pressure and the phase mole numbers $\boldsymbol{n^j}$, due to (2.36) and

$$S^j = \frac{V^j}{V_\mathrm{p}} = \frac{n^j}{\xi^j \phi V_\mathrm{b}} = S^j\left(p, \boldsymbol{n^j}\right). \tag{2.40}$$

Generally, we let $\boldsymbol{u}$ contain a set of variables such that all properties (and equations) can be written explicitly in terms of $\boldsymbol{u}$. The set $\boldsymbol{u}$ can be separated into two parts,

$$\boldsymbol{u} = \begin{bmatrix} \boldsymbol{u}_\mathrm{p} \\ \boldsymbol{u}_\mathrm{s} \end{bmatrix}, \tag{2.41}$$

where $\boldsymbol{u}_\mathrm{p}$ contains $N_\mathrm{c}$ primary variables, while $\boldsymbol{u}_\mathrm{s}$ contains $N_\mathrm{s}$ secondary variables. We require that the primary variables are independent, i.e., that a primary variable cannot be expressed in terms of the other primary variables. In an isothermal model where the bulk volume $V_\mathrm{b}$ is known, the $N_\mathrm{c}$ primary variables then uniquely determine all the properties of the system, as outlined in section 2.2.1. However, the determination of the secondary variables $\boldsymbol{u}_\mathrm{s}$ depends on $N_\mathrm{s}$ relations

$$\boldsymbol{r}_\mathrm{s}\left(\boldsymbol{u}\right) = \boldsymbol{0}, \tag{2.42}$$

which, due to the phase equilibrium relations, contain inherent nonlinearities.

The solution of a set of nonlinear equations requires an iterative approach. With such an approach, the $N_\mathrm{c}$ primary variables can be determined by solving the $N_\mathrm{c}$ mass balance equations, while the $N_\mathrm{s}$ secondary variables can be determined by solving the $N_\mathrm{s}$ secondary relations (2.42). Iterative solution schemes are discussed in section 3.3.

The need for an iterative solution of the phase equilibrium equations is a characteristic feature of the compositional model, and is one of the reasons why black-oil simulators may be significantly more efficient than compositional simulators.

**Note** We note that there is a certain amount of freedom involved in the choice of $\boldsymbol{u}$. The only requirements on $\boldsymbol{u}$ are that the primary variables must be independent, that there must exist $N_\mathrm{s}$ independent relations of the form (2.42) that relate the secondary variables to the primary variables, and that we must be able to express all properties explicitly in terms of $\boldsymbol{u}$. The choice of primary variables $\boldsymbol{u}_\mathrm{p}$ is especially important, as it determines the properties of the iterative scheme for solving the fluid flow equations.

## 2.4 Unified Black-Oil and Compositional Model

Although the phase equilibrium is treated differently in the black-oil and compositional models, the primary equations of both models are mass balance equations. However, the conventional compositional primary variables are pressure and component mole numbers (or overall mole fractions), e.g., [6], while the conventional black-oil primary variables are given by (2.13). Both sets are chosen for computational efficiency. Still, the development of an efficient unified black-oil and compositional model is an important objective of research, since such a model would reduce the simulator development and maintenance costs significantly. A framework for a unified black-oil and compositional model is given below.

### 2.4.1 General framework

For a unified black-oil and compositional model, the compositional primary variables must include the set (2.13). This is obtained by

$$\boldsymbol{u}_{\mathrm{p}} = \begin{bmatrix} p \\ \boldsymbol{S}_{\mathrm{p}} \\ \boldsymbol{x}_{\mathrm{p}} \end{bmatrix}, \tag{2.43}$$

where $\boldsymbol{S}_{\mathrm{p}}$ contains $N_{\mathrm{p}} - 1$ saturations, while $\boldsymbol{x}_{\mathrm{p}}$ contains $N_{\mathrm{c}} - N_{\mathrm{p}}$ additional variables. Here, the general black-oil case is included, provided that $\boldsymbol{x}_{\mathrm{p}}$ reduces to the solution gas/oil ratio $R_s$ in the undersaturated oil case, and to the vaporized oil/gas ratio $R_v$ in the supercritical/undersaturated gas case.

The choice of $\boldsymbol{x}_{\mathrm{p}}$ for the compositional part of the model is one of the main issues in this thesis. Generally, we may assume that

$$\boldsymbol{x}_{\mathrm{p}} = \boldsymbol{x}_{\mathrm{p}}\left(p, \boldsymbol{n}^{\boldsymbol{j}}\right), \tag{2.44}$$

since all properties can be written explicitly in terms of pressure and the phase mole numbers. The variables $\boldsymbol{x}_{\mathrm{p}}$ should ideally be chosen so that the efficiency of the resulting iterative scheme is comparable to or better than the efficiency of the conventional compositional scheme. Different choices of $\boldsymbol{x}_{\mathrm{p}}$ are discussed in Papers A and B, included at the end of the thesis.

In addition to the choice of primary variables (2.43), we must choose a set of $N_{\mathrm{s}}$ secondary variables $\boldsymbol{u}_{\mathrm{s}}$ so that all properties can be written explicitly in terms of the primary and secondary variables. One alternative is to choose

$$\boldsymbol{u}_{\mathrm{s}} = \boldsymbol{n}^{\boldsymbol{j}}. \tag{2.45}$$

With this choice, $N_{\mathrm{s}} = N_{\mathrm{p}}\, N_{\mathrm{c}}$. The $N_{\mathrm{s}}$ required relations (2.42) could then be the $(N_{\mathrm{p}} - 1)\, N_{\mathrm{c}}$ phase equilibrium conditions, the $N_{\mathrm{p}}$ volume relations

$$\phi V_{\mathrm{b}} S^j - \frac{n^j}{\xi^j} = 0, \qquad j = 1, \ldots, N_{\mathrm{p}}, \tag{2.46}$$

plus the $N_{\mathrm{c}} - N_{\mathrm{p}}$ relations (2.44). However, other sets of secondary variables and equations may of course be used.

We note that the specification of the $N_{\mathrm{s}}$ relations (2.42) may imply a choice between exact volume balance and exact mass balance, as discussed in Paper C.

For the rest of the thesis, the main focus is on the compositional part of a unified black-oil and compositional model. Consequently, we do not discuss the black-oil model any further, but assume that the compositional model reduces to the conventional black-oil model when used with black-oil fluid properties.

We also note that the mathematical model presented above is complete once a set of initial and boundary conditions are given. Initialization is discussed in section 3.2, and we use no-flow boundary conditions.

# Chapter 3

# Numerical Model

In this chapter, we present a numerical model for solving the equations presented in Chapter 2. We first set up a discretization of the mass balance equations, and outline a procedure for determining the initial state. We then propose an iterative solution of the equations. In addition, we consider a reformulation of the mass balance equations into volume balance equations and additional conservation equations, and different time schemes, i.e., fully implicit (FIM), pressure implicit (IMPES) and pressure and saturation implicit (IMPSAT). Finally, we discuss timestep selection, convergence criteria and phase disappearance/reappearance.

## 3.1 Discretization

In the following, we present a discretization of the mass balance equations (2.1) in time and space, including a general flux discretization and a simple well discretization. The framework is a general control-volume discretization.

### 3.1.1 Control-volume discretization

In a control-volume discretization, the reservoir is divided into gridblocks, generally of varying size $V_{\mathrm{b}}$. The mass balance equations (2.1) apply to every gridblock, and the same expression for the flux through an interface is used for both gridblocks incident on the interface. Consequently, the discretization yields both local and global mass conservation.

Furthermore, the variables of a gridblock are assumed to represent an average over the gridblock, and are assigned to the centre of the gridblock. Assuming $V_{\mathrm{b}}$ to be fixed in time, the accumulation term of (2.1) becomes

$$\int_{V_{\mathrm{b}}} \frac{\partial}{\partial t}\left(\phi \frac{\boldsymbol{n}}{V_{\mathrm{T}}}\right) dV = \frac{\partial}{\partial t}\left(\phi \frac{\boldsymbol{n}}{V_{\mathrm{T}}}\right) \int_{V_{\mathrm{b}}} dV = \frac{\partial}{\partial t}\left(\phi \frac{\boldsymbol{n}}{V_{\mathrm{T}}}\right) V_{\mathrm{b}} = \frac{\partial \boldsymbol{n}}{\partial t}, \qquad (3.1)$$

where $V_\mathrm{T} = \phi V_\mathrm{b}$ has been used. The other terms in (2.1) are

$$\boldsymbol{f} = \int_{S_\mathrm{b}} \hat{\boldsymbol{f}} \cdot \vec{n}\, dS, \qquad \boldsymbol{q} = \int_{V_\mathrm{b}} \hat{\boldsymbol{q}}\, dV = \hat{\boldsymbol{q}}\, V_\mathrm{b}. \tag{3.2}$$

Consequently, $\boldsymbol{f}$ and $\boldsymbol{q}$ are $N_\mathrm{c}$ vectors of component flow rates and source rates, respectively. Discretizations of these terms are outlined in sections 3.1.3 and 3.1.4.

### 3.1.2 Time discretization

We assume that the reservoir state is known at some time $t^{n-1}$, possibly by the initialization procedure presented in section 3.2, and aim at determining the state at a later time $t^n = t^{n-1} + \Delta t$, where $\Delta t$ is the timestep. The conventional mass conservative discretization of the time derivative (3.1) is

$$\frac{\partial \boldsymbol{n}}{\partial t} \simeq \frac{\Delta \boldsymbol{n}}{\Delta t} = \frac{\boldsymbol{n}^n - \boldsymbol{n}^{n-1}}{\Delta t}, \tag{3.3}$$

where superscripts $n$ and $n-1$ denote evaluation at time levels $t^n$ and $t^{n-1}$, respectively. Consequently, the discretized version of (2.1) can be written

$$\boldsymbol{r}_\mathrm{c} = \Delta \boldsymbol{n} + (\boldsymbol{f} - \boldsymbol{q})\, \Delta t = \boldsymbol{0}. \tag{3.4}$$

The source terms $\boldsymbol{q}$ are usually evaluated at time level $t^n$. The time level at which the interblock flow terms $\boldsymbol{f}$ are evaluated is discussed in section 3.5.

### 3.1.3 Flux discretization

According to (2.4), the interblock flow terms $\boldsymbol{f} = [f_1, \ldots, f_{N_\mathrm{c}}]^\mathrm{T}$ are given by

$$f_i = \int_{S_\mathrm{b}} \hat{f}_i \cdot \vec{n}\, dS = -\int_{S_\mathrm{b}} \sum_{j=1}^{N_p} \frac{c_i^j \xi^j k_r^j}{\mu^j} \left(\boldsymbol{K} \nabla \Psi^j\right) \cdot \vec{n}\, dS, \tag{3.5}$$

where

$$\nabla \Psi^j = \nabla p + \nabla P_c^j - \rho^j g \nabla D. \tag{3.6}$$

We assume that the surface $S_\mathrm{b}$ consists of interfaces $S_\gamma$ with unit normals $\vec{n}_\gamma$. For each interface, we let the discretized flow rate $f_{i,\gamma}^j$ of component $i$ in phase $j$ be denoted

$$f_{i,\gamma}^j = \Lambda_{i,\gamma}^j T_\gamma^j\,, \tag{3.7}$$

and calculate the discretized component flow rate $f_i$ as the sum of (3.7) over all phases and interfaces. Here, $\Lambda_{i,\gamma}^j$ is the generalized mobility over the interface, defined by

$$\Lambda_{i,\gamma}^j = \frac{c_i^j \xi^j k_r^j}{\mu^j}. \tag{3.8}$$

For stability reasons, the generalized mobility is evaluated upstream, i.e., in the gridblock for which $f^j_{i,\gamma}$ is an outflux. Consequently, it is taken outside the integral sign of (3.5). Furthermore, $T^j_\gamma$ is referred to as the phase flow factor through the interface, and defines an integral approximation

$$T^j_\gamma = \sum_{\eta \in \mathcal{I}_\gamma} t_{\eta,\gamma} \Psi^j_{\eta,\gamma} \approx - \int_{\mathcal{S}_\gamma} \left( \mathbf{K} \nabla \Psi^j \right) \cdot \vec{n}_\gamma \, dS. \tag{3.9}$$

The index set $\mathcal{I}_\gamma$ represents the set of gridblocks used in the approximation, referred to as the flux molecule of the interface. The quantity $t_{\eta,\gamma}$ is called the transmissibility of gridblock $\eta$ in the flux molecule, while

$$\Psi^j_{\eta,\gamma} = p_\eta + P^j_{c,\eta} - \rho^j_\gamma \, g \, D_\eta. \tag{3.10}$$

Here, $p_\eta$ is the pressure of gridblock $\eta$, while $P^j_{c,\eta}$ is the capillary pressure of phase $j$ in that gridblock, $g$ is the acceleration of gravity and $D_\eta$ is the gridblock depth. The quantity $\rho^j_\gamma$ should be a representative mass density of phase $j$ flowing through the interface. A proper choice is the saturation weighted average of the mass densities in the two gridblocks incident on the interface, here denoted with subscripts $\alpha$ and $\beta$, i.e.,

$$\rho^j_\gamma = \frac{S^j_\alpha \, \rho^j_\alpha + S^j_\beta \, \rho^j_\beta}{S^j_\alpha + S^j_\beta}. \tag{3.11}$$

The transmissibilities $t_{\eta,\gamma}$ depend on the absolute permeabilities of the gridblocks in the flux molecule and the grid geometry of the flux molecule, and can for instance be calculated by the multipoint flux approximation (MPFA) O-method, [30]. For a quadrilateral grid, this method generally leads to a 6-point flux molecule in 2D and an 18-point flux molecule in 3D. Consequently, since the interblock flow terms $\boldsymbol{f}$ involve a sum of contributions from all interfaces of a gridblock, these terms may depend on potential values (3.10) from 9 gridblocks in 2D and from 27 gridblocks in 3D.

The MPFA O-method handles grid skewness and heterogeneities and anisotropies in the permeability field in a proper way. For details, see [30].

### 3.1.4 Well discretization

The source terms $\boldsymbol{q} = [q_1, \ldots, q_{N_c}]^{\mathrm{T}}$ in (3.4) are due to wells in the reservoir. For simplicity, we only consider vertical wells with a single block-centred connection, and two types of well control, fixed bottom hole pressure (for production wells) and fixed single phase surface rate (for injection wells).

The flow path between the well bore of a well and a gridblock in which the well is completed is called a well connection. The component source rate due to

a well connection $w$ can generally be written

$$q_i = -\sum_{j=1}^{N_\mathrm{p}} \Lambda_{wi}^j T_w \left(p + P_c^j - p_w - p_h\right), \tag{3.12}$$

where $\Lambda_{wi}^j$ is the generalized mobility of the connection, $T_w$ is the connection transmissibility factor, $p$ is the gridblock pressure, $P_c^j$ is the gridblock capillary pressure of phase $j$, while $p_w$ is the well bottom hole pressure and $p_h$ is the well bore pressure head between the connection and the bottom hole datum depth. For wells with a single block-centred connection, the location of the connection coincides with the bottom hole datum depth, and $p_h$ is zero. For simplicity, we also neglect capillary pressures.

For production wells, the generalized mobility $\Lambda_{wi}^j$ of the connection equals the generalized mobility of the gridblock,

$$\Lambda_{wi}^j = \frac{c_i^j \xi^j k_r^j}{\mu^j}, \tag{3.13}$$

corresponding to an upstream evaluation. For injection wells, it is calculated as the total generalized mobility of the injected phases in the gridblock,

$$\Lambda_{wi}^j = \sum_{k=1}^{N_\mathrm{p,inj}} \frac{c_i^k \xi^k k_r^k}{\mu^k}. \tag{3.14}$$

For both types of wells, the connection transmissibility factor is given by

$$T_w = \frac{2\pi Kh}{\ln\left(r_0/r_w\right)}, \tag{3.15}$$

where $2\pi$ indicates that the connection is block-centred, $Kh$ is the effective permeability times net thickness of the connection, $r_0$ is the so-called pressure equivalent radius and $r_w$ is the well bore radius.

For vertical wells, the effective permeability is calculated as the geometric mean of the $x$- and $y$-direction permeabilities, $K_x$ and $K_y$, and the net thickness is represented by the vertical dimension of the gridblock, $\Delta z$, so that

$$Kh = \left(K_x K_y\right)^{1/2} \Delta z. \tag{3.16}$$

The pressure equivalent radius $r_0$ is defined as the distance from the well at which the local pressure equals the (average) gridblock pressure, and is given by, [31],

$$r_0 = 2 \cdot 0.1403649 \cdot \frac{\left[\Delta x^2 (K_y/K_x)^{1/2} + \Delta y^2 (K_x/K_y)^{1/2}\right]^{1/2}}{(K_y/K_x)^{1/4} + (K_x/K_y)^{1/4}}. \tag{3.17}$$

The expression (3.17), referred to as Peaceman's formula, is valid for rectangular gridblocks in which the anisotropies in the permeability are aligned with the grid, and the well is assumed to penetrate the full thickness of the block, perpendicularly to two of its faces, [31, 32]. Here, $\Delta x$ and $\Delta y$ are the horizontal dimensions of the gridblock.

#### Fixed bottom hole pressure control (production wells)

For production wells, we may specify a fixed value of the bottom hole pressure $p_w$ which is below the gridblock pressure $p$. Consequently, if the state of the gridblock is known, component source rates are readily calculated from (3.12), with $p_h = 0$ and $P_c^j = 0$.

#### Fixed single phase surface rate control (injection wells)

For injection wells, we may specify a single phase volumetric rate $Q_s^k$ at surface conditions, together with the overall composition $\boldsymbol{z} = [z_1, \ldots, z_{N_c}]^{\mathrm{T}}$ of the injected phase $k$. Here, $z_i$ is the fraction of component $i$ to the total amount of injected fluid. Surface conditions usually refer to a pressure of 1 atmosphere and a temperature of 15.5 °C. By a conventional phase equilibrium calculation with $\boldsymbol{z}$ and the surface conditions, see section 3.2.2, we may determine the density $\xi_s^k$, and thereby the component rates

$$q_i = z_i \, \xi_s^k \, Q_s^k. \tag{3.18}$$

We note that the component rates are the same at both surface conditions and reservoir conditions.

## 3.2 Initialization

Before we can start a simulation run, we must specify the initial reservoir state, as outlined in the following.

### 3.2.1 General requirements

For a proper initialization, the phases should be at thermodynamic equilibrium, and no fluid flow should occur unless wells are introduced in the reservoir.

The phase equilibrium is determined by (2.30). In addition, due to Darcy's law (2.3), the hydrostatic equilibrium condition

$$\Delta p - \rho^j g \, \Delta D = 0 \tag{3.19}$$

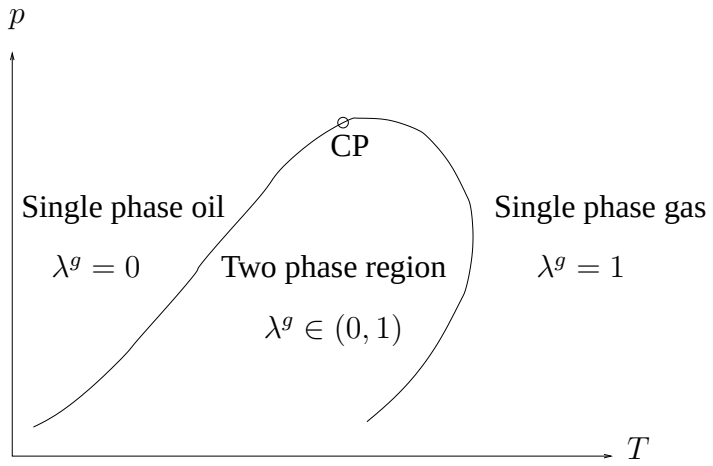



Figure 3.1: Phase diagram for some overall mole fractions $\boldsymbol{z}$. The critical point (CP) is the point at which the phases are truly indistinguishable.

must also be fulfilled. In (3.19), the operator $\Delta$ gives the difference between values of two neighbouring gridblocks, and we have neglected capillary pressures.

If gravity is not included, e.g., for horizontal flow, (3.19) requires the initial pressure to be uniform in the reservoir. Consequently, only the phase equilibrium condition (2.30) must be considered, and we may use a conventional two-phase equilibrium calculation for the initialization of the oil and gas phases. In addition, the initial water saturation must be specified. However, if gravity is included, we should use a gravity/chemical equilibrium calculation. Both procedures are discussed below.

### 3.2.2 Conventional two-phase equilibrium

A conventional two-phase equilibrium calculation is based on a specification of pressure, temperature and the overall mole fractions $\boldsymbol{z}$ of the components that may be present in the two phases. The result of the calculations are the overall phase fractions $\boldsymbol{\lambda} = [\lambda^o, \lambda^g]^{\mathrm{T}}$ and the phase mole fractions $\boldsymbol{c} = [\boldsymbol{c}^o, \boldsymbol{c}^g]$, where

$$\lambda^j = \frac{n^j}{n^o + n^g}, \qquad \boldsymbol{c}^j = \left[c_1^j, \ldots, c_{N_c}^j\right]^{\mathrm{T}}. \tag{3.20}$$

The phase fraction $\lambda^g$ can be illustrated in a phase diagram for the overall mole fractions $\boldsymbol{z}$, see Figure 3.1. We observe that $\lambda^g$ is determined by a specification of pressure and temperature in the phase diagram.

### The Rachford-Rice equation

The overall mole fractions $\boldsymbol{z} = [z_1, \ldots, z_{N_c}]^{\mathrm{T}}$ can be expressed by

$$z_i = \lambda^o c_i^o + \lambda^g c_i^g = (1 - \lambda^g)\, c_i^o + \lambda^g c_i^g = (1 - \lambda^g + \lambda^g K_i)\, c_i^o, \tag{3.21}$$

where we have introduced the K-values

$$K_i = \frac{c_i^g}{c_i^o}. \tag{3.22}$$

From (3.21) we deduce that

$$c_i^o = \frac{z_i}{1 + (K_i - 1)\, \lambda^g}. \tag{3.23}$$

Furthermore, since the phase mole fractions must sum to unity, we find that

$$\sum_{i=1}^{N_c} (c_i^o - c_i^g) = 0 \;\Leftrightarrow\; \sum_{i=1}^{N_c} (K_i - 1)\, c_i^o = 0, \tag{3.24}$$

which may be combined with (3.21) to yield

$$\sum_{i=1}^{N_c} \frac{(K_i - 1)\, z_i}{1 + (K_i - 1)\, \lambda^g} = 0. \tag{3.25}$$

Equation (3.25) is often referred to as the Rachford-Rice equation, due to [33].

### Successive substitution

According to (2.31), the phase equilibrium is determined by

$$K_i = \frac{\phi_i^o}{\phi_i^g}, \tag{3.26}$$

where (3.22) has been used. If an estimate for the K-values is known, we may determine $\lambda^g$ from (3.25) and phase mole fractions from (3.23) and (3.22). Consequently, we have an estimate of the phase equilibrium.

Initial K-values can be obtained with the Wilson correlation,

$$\ln K_i = \ln \frac{p_{c,i}}{p} + 5.373\,(1 + \omega_i) \left(1 - \frac{T_{c,i}}{T}\right), \tag{3.27}$$

see for instance [22], while subsequent K-value estimates can be obtained by calculating the fugacity coefficients $\phi_i^j$ as functions of pressure, temperature and phase mole fractions, see section 4.4, and using (3.26).

However, we note that $\lambda^g$ as determined by (3.25) may not be in $(0,1)$. If $\lambda^g \leq 0$, we should set $\lambda^g = 0$ and conclude that the equilibrium is a single phase oil equilibrium, i.e., $c_i^o = z_i$. If $\lambda^g \geq 1$, we should set $\lambda^g = 1$ and conclude that the equilibrium is a single phase gas equilibrium, i.e., $c_i^o = z_i$. Due to the nonlinear nature of (3.25), a careful solution strategy is required, see [22].

The approach outlined above is referred to as successive substitution, and experience shows that the estimates eventually converge to the proper equilibrium solution. Unfortunately, the convergence may be slow, especially near the critical point. Some acceleration techniques have therefore been proposed. Alternatively, the successive substitution approach can be used to obtain a proper initial estimate for a solution of (2.30) by Newton's method. For further details on (accelerated) successive substitution and other methods for efficient calculation of a two-phase equilibrium, we refer to [22].

**Note** To determine the oil and gas saturations, we use (2.33) in the form

$$n^j = \frac{p\phi V_{\mathrm{b}} S^j}{RTZ^j} \tag{3.28}$$

and the definition of $\lambda^j$ in (3.20) to derive

$$\lambda^g Z^g S^o - \lambda^o Z^o S^g = 0. \tag{3.29}$$

Here, $Z^j = Z^j\left(p, \boldsymbol{c}^j\right)$ is determined by a solution of the cubic equation of state (2.32). Since the saturations must sum to unity, we find that

$$S^j = \frac{\lambda^j Z^j}{\lambda^o Z^o + \lambda^g Z^g}\left(1 - S^w\right). \tag{3.30}$$

for $j = o, g$, where $S^w$ is given as input. Consequently, since pressure, saturations and the phase mole fractions are known, all fluid properties can be calculated.

### 3.2.3 Gravity/chemical equilibrium

In a reservoir at gravity/chemical equilibrium, the components and phases are distributed with depth according to their (average) molar mass. Consequently, the gas phase is situated above the oil and water phases, and the oil phase is situated above the water phase. The interface between the gas and oil phases is referred to as the gas-oil contact (GOC), while the interface between the oil phase and the water phase is referred to as the water-oil contact (WOC).

In the following, for simplicity, we neglect capillary pressures. Consequently, the contacts between the phases are sharp, and there is no two-phase equilibrium

in the reservoir initially. Furthermore, all saturations attain their maximum values wherever they are present. The positions of the gas-oil and water-oil contacts are required as input for the initialization.

For the oil and gas phases, the distribution of components with depth $D$ within the reservoir is determined by

$$f_i^j(D) - f_i^j(D_{\text{ref}})\, e^{\frac{M_i g}{RT}(D-D_{\text{ref}})} = 0, \tag{3.31}$$

where $f_i^j(D)$ is the fugacity at depth $D$, while $f_i^j(D_{\text{ref}})$ is a known fugacity at some reference depth $D_{\text{ref}}$. A derivation of (3.31) from a general thermodynamic equilibrium requirement is given in Paper E, which is included at the end of the thesis. The relations (3.31) can be linearized and solved with respect to pressure and the overall mole fractions at depth $D$. Here, the calculation of reference fugacities relies on a specification of pressure and mole fractions at depth $D_{\text{ref}}$.

Actually, a solution of (3.31) satisfies the hydrostatic equilibrium condition (3.19). Furthermore, the amount of heavier components increases with depth, while the amount of lighter components decreases with depth. For further details, we refer to Paper E.

Below the water-oil contact, we may solve (3.19) directly with respect to pressure, since the water density is given as a linear function of pressure, (2.35).

**Note** A stringent gravity/chemical equilibrium with the use of (3.31) is not always considered in a reservoir simulator. More commonly, the initial overall composition versus depth and pressure at some reference depth are given, and an approximate solution of (3.19) is sought by a successive substitution approach, i.e., by repeated estimates of pressure and densities, see for instance [16]. Consequently, if the given overall composition versus depth is in accordance with (3.31), the corresponding initial equilibrium is good. Otherwise, for instance if the same initial overall composition is used for all depths, the initial state may be far from equilibrium. A poor initial equilibrium could lead to initial convergence problems when solving the mass balance and phase equilibrium equations.

## 3.3 Iterative Solution Schemes

A characteristic feature of the compositional mass balance and phase equilibrium equations presented in Chapter 2 is that they are nonlinear with respect to any set of state variables. Consequently, in order to solve the equations, we must linearize them and use an iterative solution approach.

In the following, we present a general Newton-Raphson scheme for solving the nonlinear equations that determine the reservoir state. We present one version

which includes both primary and secondary equations and variables in a simultaneous iteration, and another version which involves a splitting of the scheme into a primary and a secondary iteration.

### 3.3.1 Simultaneous Newton-Raphson iteration

With no lack of generality, we use the notation introduced in section 2.3.2 and assume that all of the equations can be expressed explicitly in terms of

$$\boldsymbol{u} = \begin{bmatrix} \boldsymbol{u}_\mathrm{p} \\ \boldsymbol{u}_\mathrm{s} \end{bmatrix}, \tag{3.32}$$

where $\boldsymbol{u}_\mathrm{p}$ is a $N_\mathrm{c}$ vector of primary variables, while $\boldsymbol{u}_\mathrm{s}$ is a $N_\mathrm{s}$ vector of secondary variables. Furthermore, we assume that $N_\mathrm{c}$ primary equations

$$\boldsymbol{r}_\mathrm{p}(\boldsymbol{u}) = \boldsymbol{0} \tag{3.33}$$

are chosen, together with $N_\mathrm{s}$ secondary relations

$$\boldsymbol{r}_\mathrm{s}(\boldsymbol{u}) = \boldsymbol{0}. \tag{3.34}$$

The primary equations are the discretized mass balance equations (3.4), possibly reformulated, see section 3.4. The secondary relations contain the phase equilibrium conditions (2.30) and possibly some other relations, see section 2.4.

In order to set up a Newton-Raphson scheme, we assume that some guess $\boldsymbol{u}^{(k)}$ for the solution of (3.33) and (3.34) is known. The guess could for instance be the current state. We then linearize the equations in a neighbourhood $\boldsymbol{u}^{(k+1)} = \boldsymbol{u}^{(k)} + \Delta\boldsymbol{u}^{(k+1)}$ of the guess, i.e.,

$$\boldsymbol{r}_\mathrm{p}^{(k+1)} = \boldsymbol{r}_\mathrm{p}^{(k)} + \left(\frac{\partial \boldsymbol{r}_\mathrm{p}}{\partial \boldsymbol{u}_\mathrm{p}}\right)_{\boldsymbol{u}_\mathrm{s}}^{(k)} \Delta\boldsymbol{u}_\mathrm{p}^{(k+1)} + \left(\frac{\partial \boldsymbol{r}_\mathrm{p}}{\partial \boldsymbol{u}_\mathrm{s}}\right)_{\boldsymbol{u}_\mathrm{p}}^{(k)} \Delta\boldsymbol{u}_\mathrm{s}^{(k+1)} + \boldsymbol{\epsilon}_\mathrm{p}, \tag{3.35}$$

$$\boldsymbol{r}_\mathrm{s}^{(k+1)} = \boldsymbol{r}_\mathrm{s}^{(k)} + \left(\frac{\partial \boldsymbol{r}_\mathrm{s}}{\partial \boldsymbol{u}_\mathrm{p}}\right)_{\boldsymbol{u}_\mathrm{s}}^{(k)} \Delta\boldsymbol{u}_\mathrm{p}^{(k+1)} + \left(\frac{\partial \boldsymbol{r}_\mathrm{s}}{\partial \boldsymbol{u}_\mathrm{s}}\right)_{\boldsymbol{u}_\mathrm{p}}^{(k)} \Delta\boldsymbol{u}_\mathrm{s}^{(k+1)} + \boldsymbol{\epsilon}_\mathrm{s}. \tag{3.36}$$

Here, subscripts $\boldsymbol{u}_\mathrm{s}$ and $\boldsymbol{u}_\mathrm{p}$ indicates which variables are kept fixed in the partial differentiation. The terms $\boldsymbol{\epsilon}_\mathrm{p}$ and $\boldsymbol{\epsilon}_\mathrm{s}$ are of order

$$\mathcal{O}\left(\left(\Delta\boldsymbol{u}^{(k+1)}\right)^2\right). \tag{3.37}$$

Furthermore, by setting $\boldsymbol{r}_\mathrm{p}^{(k+1)} = \boldsymbol{0}$ and $\boldsymbol{r}_\mathrm{s}^{(k+1)} = \boldsymbol{0}$ and neglecting $\boldsymbol{\epsilon}_\mathrm{p}$ and $\boldsymbol{\epsilon}_\mathrm{s}$, we obtain

$$\left(\frac{\partial \boldsymbol{r}_\mathrm{p}}{\partial \boldsymbol{u}_\mathrm{p}}\right)_{\boldsymbol{u}_\mathrm{s}}^{(k)} \Delta\boldsymbol{u}_\mathrm{p}^{(k+1)} + \left(\frac{\partial \boldsymbol{r}_\mathrm{p}}{\partial \boldsymbol{u}_\mathrm{s}}\right)_{\boldsymbol{u}_\mathrm{p}}^{(k)} \Delta\boldsymbol{u}_\mathrm{s}^{(k+1)} = -\boldsymbol{r}_\mathrm{p}^{(k)}, \tag{3.38}$$

and

$$\left(\frac{\partial \boldsymbol{r}_\mathrm{s}}{\partial \boldsymbol{u}_\mathrm{p}}\right)_{\boldsymbol{u}_\mathrm{s}}^{(k)} \Delta \boldsymbol{u}_\mathrm{p}^{(k+1)} + \left(\frac{\partial \boldsymbol{r}_\mathrm{s}}{\partial \boldsymbol{u}_\mathrm{s}}\right)_{\boldsymbol{u}_\mathrm{p}}^{(k)} \Delta \boldsymbol{u}_\mathrm{s}^{(k+1)} = -\boldsymbol{r}_\mathrm{s}^{(k)}. \tag{3.39}$$

Equations (3.38) and (3.39) are $N_\mathrm{c}+N_\mathrm{s}$ linear equations in the $N_\mathrm{c}+N_\mathrm{s}$ solution changes $\Delta \boldsymbol{u}^{(k+1)}$, and can be used to determine a new solution guess $\boldsymbol{u}^{(k+1)}$. If the new guess is not a satisfactory solution, we proceed to the next iteration level, thus repeating the linearization and determining yet another solution guess.

Provided that the initial guess $\boldsymbol{u}^{(0)}$ is sufficiently close to the solution of (3.33) and (3.34), the Newton-Raphson scheme (3.38) and (3.39) converges to the solution of these equations. Furthermore, provided that the derivatives of $\boldsymbol{r}_\mathrm{p}$ and $\boldsymbol{r}_\mathrm{s}$ are calculated correctly (analytically),

$$\Delta \boldsymbol{u}^{(k+1)} = \mathcal{O}\left(\left(\Delta \boldsymbol{u}^{(k)}\right)^2\right), \tag{3.40}$$

i.e., the convergence is quadratic.

### 3.3.2 Primary and secondary Newton-Raphson iteration

The Newton-Raphson scheme (3.38), (3.39) solves both the primary and secondary equations simultaneously. Alternatively, we may use the implicit relationship

$$\boldsymbol{u}_\mathrm{s} = \boldsymbol{u}_\mathrm{s}\left(\boldsymbol{u}_\mathrm{p}\right) \tag{3.41}$$

to split the scheme into a primary and a secondary iteration.

Let us assume that $\boldsymbol{u}$, consisting of $\boldsymbol{u}_\mathrm{p}$ and $\boldsymbol{u}_\mathrm{s}$, corresponds to a solution of the secondary equations (3.34), but not necessarily to a solution of the primary equations (3.33). By differentiating through (3.34) with respect to $\boldsymbol{u}_\mathrm{p}$, taking advantage of (3.41), we find that

$$\left(\frac{\partial \boldsymbol{r}_\mathrm{s}}{\partial \boldsymbol{u}_\mathrm{p}}\right)_{\boldsymbol{u}_\mathrm{s}} + \left(\frac{\partial \boldsymbol{r}_\mathrm{s}}{\partial \boldsymbol{u}_\mathrm{s}}\right)_{\boldsymbol{u}_\mathrm{p}} \frac{d\boldsymbol{u}_\mathrm{s}}{d\boldsymbol{u}_\mathrm{p}} = \boldsymbol{0}. \tag{3.42}$$

Equation (3.42) can be solved with respect to $d\boldsymbol{u}_\mathrm{s}/d\boldsymbol{u}_\mathrm{p}$, which are the total derivatives of the secondary variables with respect to the primary variables.

With the use of (3.41), we may also write the residuals of the primary equations as

$$\boldsymbol{r}_\mathrm{p} = \boldsymbol{r}_\mathrm{p}\left(\boldsymbol{u}_\mathrm{p}, \boldsymbol{u}_\mathrm{s}\left(\boldsymbol{u}_\mathrm{p}\right)\right), \tag{3.43}$$

so that the Newton-Raphson iteration for determining the primary variables $\boldsymbol{u}_\mathrm{p}$ becomes

$$\left[\left(\frac{\partial \boldsymbol{r}_\mathrm{p}}{\partial \boldsymbol{u}_\mathrm{p}}\right)_{\boldsymbol{u}_\mathrm{s}} + \left(\frac{\partial \boldsymbol{r}_\mathrm{p}}{\partial \boldsymbol{u}_\mathrm{s}}\right)_{\boldsymbol{u}_\mathrm{p}} \frac{d\boldsymbol{u}_\mathrm{s}}{d\boldsymbol{u}_\mathrm{p}}\right]^{(k)} \Delta \boldsymbol{u}_\mathrm{p}^{(k+1)} = -\boldsymbol{r}_\mathrm{p}^{(k)}. \tag{3.44}$$

Here, the term in brackets is the total derivative of $\boldsymbol{r}_\mathrm{p}$ with respect to $\boldsymbol{u}_\mathrm{p}$.

Furthermore, at the end of each iteration step with (3.44), the residuals of the secondary equations can be written

$$\boldsymbol{r}_\mathrm{s} = \boldsymbol{r}_\mathrm{s}\left(\boldsymbol{u}_\mathrm{p}^{(k+1)}, \boldsymbol{u}_\mathrm{s}^{(k)}\right), \tag{3.45}$$

where the primary variables $\boldsymbol{u}_\mathrm{p}^{(k+1)}$ are known. A Newton-Raphson scheme for determining $\boldsymbol{u}_\mathrm{s}^{(k+1)}$ is then

$$\left(\frac{\partial \boldsymbol{r}_\mathrm{s}}{\partial \boldsymbol{u}_\mathrm{s}}\right)_{\boldsymbol{u}_\mathrm{p}}^{(l)} \Delta \boldsymbol{u}_\mathrm{s}^{(l+1)} = -\boldsymbol{r}_\mathrm{s}^{(l)}. \tag{3.46}$$

The secondary iteration (3.46) is carried out until convergence, with the primary variables kept fixed. A proper initial guess is

$$\boldsymbol{u}_\mathrm{s}^{(l=0)} = \boldsymbol{u}_\mathrm{s}^{(k)} + \left(\frac{d\boldsymbol{u}_\mathrm{s}}{d\boldsymbol{u}_\mathrm{p}}\right)^{(k)} \Delta \boldsymbol{u}_\mathrm{p}^{(k+1)}. \tag{3.47}$$

Consequently, at the end of the secondary iteration (3.46), we have determined

$$\boldsymbol{u}^{(k+1)} = \begin{bmatrix} \boldsymbol{u}_\mathrm{p}^{(k+1)} \\ \boldsymbol{u}_\mathrm{s}^{(k+1)} \end{bmatrix}, \tag{3.48}$$

which is a solution of the secondary equations (3.34), but not necessarily a solution of the primary equations (3.33). The total derivatives $d\boldsymbol{u}_\mathrm{s}/d\boldsymbol{u}_\mathrm{p}$ can then be determined from (3.42), and we may proceed with the primary iteration (3.44) until a satisfactory solution of the primary equations is obtained. Provided that all derivatives are calculated correctly (analytically), convergence of both the primary and the secondary iteration will be quadratic near the true solution.

We refer to the scheme outlined above as the *splitted scheme*. An advantage of the splitted scheme is that the challenges of the secondary equations, e.g., the phase equilibrium challenges, are left out of the primary iteration. Consequently, fewer iteration steps may be required for the primary iteration, which, due to the interblock couplings of the flow equations, is expected to be the most costly of the two iterations.

In addition, the splitted scheme is convenient when dealing with reformulations of the mass balance equations and different time schemes. As will be shown in section 3.4, a volume balance reformulation is based on the calculation of partial molar volumes. Such a calculation is outlined in section 4.10, and requires that the phase equilibrium is determined at every stage, i.e., that the secondary equations are solved at every primary iteration step. Furthermore, a rigorous evaluation of terms with primary variables at different time levels requires the use of a relation of the form (3.41), as shown in section 3.5.

### 3.3.3 A comment on exact fulfilment

Due to the nonlinear nature of the equations, an iterative scheme usually determines the reservoir state only within some tolerance. However, for some relations, exact fulfilment can be obtained. Typically, exact volume balance,

$$\sum_{j=1}^{N_{\mathrm{p}}} S^j = 1, \tag{3.49}$$

is obtained by determining $N_{\mathrm{p}} - 1$ saturations $\boldsymbol{S}_{\mathrm{p}}$ and calculating the remaining saturation directly from (3.49). On the other hand, exact mass balance can be obtained by determining the interblock flow terms $\boldsymbol{f}$ and the source terms $\boldsymbol{q}$ from the primary variables, and using the direct update

$$\boldsymbol{n} = \boldsymbol{n}^{n-1} - (\boldsymbol{f} - \boldsymbol{q})\,\Delta t \tag{3.50}$$

when determining the secondary variables. However, exact mass balance and exact volume balance cannot be obtained simultaneously. Exact mass balance versus exact volume balance is discussed in Paper C.

## 3.4 Reformulation of Mass Balance Equations

For improved performance of the iterative schemes presented above, there should be a natural relation between the primary variables and the primary equations. Such natural relations are also the basis for a sequential solution approach, where the system of primary equations is divided into parts that are solved separately.

An illustrative example of a natural relation is the relation between the component amounts and the mass balance equations. In the following, we consider a reformulation of the mass balance equations into alternative primary equations that are naturally related to pressure, saturations $\boldsymbol{S}_{\mathrm{p}}$ and the variables $\boldsymbol{x}_{\mathrm{p}}$, which are the primary variables introduced in section 2.4. For other discussions related to equation reformulations, we refer to [34, 35, 36].

### 3.4.1 Volume balance equations

Pressure and saturations are naturally related to the total volume $V_{\mathrm{T}}$ and the phase volumes, respectively. If we assume that $\boldsymbol{S}_{\mathrm{p}}$ contains the oil and water saturations, the volumes that naturally relate to $(p, \boldsymbol{S}_{\mathrm{p}})$ are

$$\boldsymbol{V} = \begin{bmatrix} V_{\mathrm{T}} \\ V^o \\ V^w \end{bmatrix}. \tag{3.51}$$

Since pressure and the component mole numbers $\boldsymbol{n}$ are $N_\mathrm{c}+1$ independent variables that give a complete description of all extensive and intensive properties of the system, see section 2.2, we may write $\boldsymbol{V}=\boldsymbol{V}\left(p,\boldsymbol{n}\right)$. Furthermore, we note that volumes are homogeneous functions of first degree in the mole numbers, i.e.,

$$\boldsymbol{V}\left(p,\nu\boldsymbol{n}\right)=\nu\boldsymbol{V}\left(p,\boldsymbol{n}\right), \tag{3.52}$$

for some scalar $\nu$. Consequently, by differentiating through (3.52) with respect to $\nu$, we find that

$$\boldsymbol{V}=\left(\frac{\partial\boldsymbol{V}}{\partial\boldsymbol{n}}\right)_{p}\boldsymbol{n}=\boldsymbol{W}_{V}\,\boldsymbol{n}, \tag{3.53}$$

where the $N_\mathrm{p}\times N_\mathrm{c}$ matrix $\boldsymbol{W}_V$ contains the partial molar volumes. A calculation of partial molar volumes is outlined in section 4.10. We note that this calculation requires that the phase equilibrium equations are fulfilled, e.g., that the splitted Newton-Raphson scheme presented in section 3.3.2 is used.

The relation (3.53) motivates a reformulation of the mass balance equations (3.4), denoted $\boldsymbol{r}_\mathrm{c}=\boldsymbol{0}$, into volume balance equations by

$$\boldsymbol{r}_\mathrm{VBE}=\boldsymbol{W}_{V}\,\boldsymbol{r}_\mathrm{c}=\boldsymbol{0}. \tag{3.54}$$

The differential form of the volume balance equations (3.54) was derived by Watts, [9], extending the work of Ács, Doleschall and Farkas, [8]. Watts' starting point was the differential form of the mass balance equations,

$$\frac{\partial}{\partial t}\left(\phi\frac{\boldsymbol{z}}{v_\mathrm{T}}\right)+\nabla\cdot\hat{\boldsymbol{f}}-\hat{\boldsymbol{q}}=\boldsymbol{0}, \tag{3.55}$$

where $\boldsymbol{z}=\left(1/n_\mathrm{T}\right)\boldsymbol{n}$ is the overall composition, $v_\mathrm{T}=V_\mathrm{T}/n_\mathrm{T}$ is the total specific volume and $n_\mathrm{T}$ is the total amount of components. The form (3.55) is derived from the integral form (2.1) by writing the surface integral as a volume integral and requiring the overall volume integrand to be zero, based on an assumption of continuity. We note that $\nabla\cdot$ is taken for each component of $\hat{\boldsymbol{f}}$.

Watts showed that a weighting of (3.55) by the total partial molar volumes $\left(\partial V_\mathrm{T}/\partial\boldsymbol{n}\right)_p$ yields a pressure equation of the form

$$\frac{\partial\phi}{\partial t}-\frac{\phi}{v_\mathrm{T}}\left(\frac{\partial v_\mathrm{T}}{\partial p}\right)_{\boldsymbol{z}}\frac{\partial p}{\partial t}+\left(\frac{\partial V_\mathrm{T}}{\partial\boldsymbol{n}}\right)_{p}\left(\nabla\cdot\hat{\boldsymbol{f}}-\hat{\boldsymbol{q}}\right)=0, \tag{3.56}$$

while a weighting by $\left(\partial V^j/\partial\boldsymbol{n}\right)_p$, yields a saturation equation of the form

$$\frac{\partial}{\partial t}\left(\phi S^j\right)-\frac{\phi}{v_\mathrm{T}}\left(\frac{\partial v^j}{\partial p}\right)_{\boldsymbol{z}}\frac{\partial p}{\partial t}+\left(\frac{\partial V^j}{\partial\boldsymbol{n}}\right)_{p}\left(\nabla\cdot\hat{\boldsymbol{f}}-\hat{\boldsymbol{q}}\right)=0, \tag{3.57}$$

where $v^j = V^j/n_{\mathrm{T}}$ is the specific volume of phase $j$.

The equations (3.56) and (3.57) are easily interpreted as volume balance equations, as they are written in terms of changes to the pore volume, volume changes due to the fluid compressibility and volume changes due to fluxes and source terms. For a discussion of the use of the volume balance equations in an iterative scheme, we refer to Paper C.

### 3.4.2 Additional conservation equations

The volume balance reformulation (3.54) is naturally related to the volumes $\boldsymbol{V}$, and thereby to pressure and saturations. A similar reformulation, e.g.,

$$\boldsymbol{r}_{\mathrm{ACE}} = \boldsymbol{W}_x \, \boldsymbol{r}_{\mathrm{c}} = \boldsymbol{0}, \tag{3.58}$$

where $\boldsymbol{W}_x$ is a $(N_{\mathrm{c}} - N_{\mathrm{p}}) \times N_{\mathrm{c}}$ matrix, could be used to derive $N_{\mathrm{c}} - N_{\mathrm{p}}$ additional conservation equations that are naturally related to the $N_{\mathrm{c}} - N_{\mathrm{p}}$ variables $\boldsymbol{x}_{\mathrm{p}}$. The natural relation is clearly obtained if

$$\boldsymbol{x}_{\mathrm{p}} = \boldsymbol{W}_x \, \boldsymbol{n}, \tag{3.59}$$

but the form of the matrix $\boldsymbol{W}_x$ is not evident.

However, we note that the equations (3.54) and (3.58) lead to the total reformulation

$$\begin{bmatrix} \boldsymbol{r}_{\mathrm{VBE}} \\ \boldsymbol{r}_{\mathrm{ACE}} \end{bmatrix} = \begin{bmatrix} \boldsymbol{W}_V \\ \boldsymbol{W}_x \end{bmatrix} \boldsymbol{r}_{\mathrm{c}} = \boldsymbol{W} \, \boldsymbol{r}_{\mathrm{c}} = \boldsymbol{0} \tag{3.60}$$

of the system of mass balance equations. Here, $\boldsymbol{W}$ is a $N_{\mathrm{c}} \times N_{\mathrm{c}}$ matrix. For (3.60) to preserve the properties of the original conservation system, $\boldsymbol{W}$ must be non-singular.

Possible definitions of the variables $\boldsymbol{x}_{\mathrm{p}}$ and the matrix $\boldsymbol{W}_x$ are presented in Papers A and B, while the form of the additional conservation equations (3.58) is an issue in Papers B and C. We note that, in Paper A, the alternative notations $\boldsymbol{W}_{\mathrm{VBE}}$ and $\boldsymbol{W}_{\mathrm{ACE}}$ are used for the matrices $\boldsymbol{W}_V$ and $\boldsymbol{W}_x$, respectively, and the definition of $\boldsymbol{x}_{\mathrm{p}}$ is not of the form (3.59).

### 3.4.3 A comment on sequential solution approaches

Sequential solution approaches are attempts of simplifying the iterative solution of the primary equations by solving the equations stepwise. Examples of sequential approaches are given in [9, 37].

Here, we note that the volume balance pressure equation, e.g., (3.56), may possibly be separated from the rest of the equations, and solved with respect to

pressure only. Furthermore, the volume balance saturation equations, e.g., (3.57), may possibly be separated from the remaining part of the system, and solved with respect to saturations only. Alternatively, we could solve the volume balance equations with respect to both pressure and saturations simultaneously. Finally, we could solve the additional conservation equations, e.g., (3.58). Such an approach is used in Paper A.

Generally, sequential solution approaches may involve a considerable amount of iteration steps due to the couplings between the equations, especially for the interblock flow terms. However, if parts of the interblock flow terms are not updated during the iteration (evaluated at the previous time level), the efficiency may be improved. This is discussed below.

## 3.5 Different Time Schemes

So far, we have not specified the time level at which the flow terms $\boldsymbol{f}$ of (3.4) are evaluated. In the following, we consider three different choices for the evaluation of $\boldsymbol{f}$, the fully implicit approach (FIM), the pressure implicit approach (IMPES) and the pressure and saturations implicit approach (IMPSAT). Throughout the section, we assume that the splitted scheme presented in section 3.3.2 is used for solving the primary and secondary equations. For a supplement on linearization techniques for different time schemes, we refer to [38, 39].

### 3.5.1 Fully implicit (FIM)

A fully implicit formulation of (3.4) can be written

$$\boldsymbol{r}_{\mathrm{c}}^{\mathrm{FIM}} = \boldsymbol{n}^{n} - \boldsymbol{n}^{n-1} + \left[\boldsymbol{f}^{n} - \boldsymbol{q}^{n}\right]\Delta t = \boldsymbol{0}. \tag{3.61}$$

When setting up the primary Newton-Raphson scheme (3.44), the differentiation is with respect to variables at time level $t^n$, and derivatives of terms evaluated at the previous time level $t^{n-1}$ vanish. Consequently, if the form (3.61) is used for the primary equations, the iterative scheme (3.44) becomes

$$\left\{\frac{d\boldsymbol{n}}{d\boldsymbol{u}_{\mathrm{p}}} + \left[\frac{d\boldsymbol{f}}{d\boldsymbol{u}_{\mathrm{p}}} - \frac{d\boldsymbol{q}}{d\boldsymbol{u}_{\mathrm{p}}}\right]\Delta t\right\}^{(k)} \Delta\boldsymbol{u}_{\mathrm{p}}^{(k+1)} = -\left(\boldsymbol{r}_{\mathrm{c}}^{\mathrm{FIM}}\right)^{(k)}, \tag{3.62}$$

where the derivatives with respect to $\boldsymbol{u}_{\mathrm{p}}$ are total derivatives, i.e.,

$$\frac{d}{d\boldsymbol{u}_{\mathrm{p}}}(\,\cdot\,) = \frac{\partial}{\partial\boldsymbol{u}_{\mathrm{p}}}(\,\cdot\,)_{\boldsymbol{u}_{\mathrm{s}}} + \frac{\partial}{\partial\boldsymbol{u}_{\mathrm{s}}}(\,\cdot\,)_{\boldsymbol{u}_{\mathrm{p}}}\frac{d\boldsymbol{u}_{\mathrm{s}}}{d\boldsymbol{u}_{\mathrm{p}}}. \tag{3.63}$$

Due to the interblock flow terms, (3.62) contains couplings between equations of different gridblocks. The corresponding Jacobian is a matrix of dimensions

$$N_{\mathrm{b}} N_{\mathrm{c}} \times N_{\mathrm{b}} N_{\mathrm{c}}. \tag{3.64}$$

Here, $N_{\mathrm{b}}$ is the total number of gridblocks. Actually, the Jacobian is a $N_{\mathrm{b}} \times N_{\mathrm{b}}$ block matrix with blocks of size $N_{\mathrm{c}} \times N_{\mathrm{c}}$ and $N_{\Gamma}$ non-zero diagonals, where $N_{\Gamma}$ is the number of gridblocks involved in the discretization of $\boldsymbol{f}$ for a gridblock. Using a multipoint flux approximation (MPFA), $N_{\Gamma}$ can be 9 in 2D and 27 in 3D.

The size of the Jacobian and the large number of derivatives to be calculated could make the fully implicit approach prohibitively costly on a per-timestep basis. However, fully implicit approaches are unconditionally stable, i.e., there are no other restrictions on the timestep sizes than those necessary to ensure convergence of the Newton-Raphson scheme.

### 3.5.2 Pressure implicit (IMPES)

An IMPES formulation of (3.4) can be written

$$\boldsymbol{r}_{\mathrm{c}}^{\mathrm{IMPES}} = \boldsymbol{n}^{n} - \boldsymbol{n}^{n-1} + \left[\boldsymbol{f}\left(p^{n}, \boldsymbol{S}_{\mathrm{p}}^{n-1}, \boldsymbol{x}_{\mathrm{p}}^{n-1}\right) - \boldsymbol{q}^{n}\right] \Delta t = \boldsymbol{0}. \tag{3.65}$$

In (3.65), the interblock flow terms are evaluated with pressure at the current time level, but with saturations and the variables $\boldsymbol{x}_{\mathrm{p}}$ at the previous time level. This is referred to as implicit treatment of pressure and explicit treatment of saturations and the variables $\boldsymbol{x}_{\mathrm{p}}$.

The evaluation is done rigorously with the splitted iterative scheme, as the interblock flow terms can be expressed explicitly in terms of

$$\boldsymbol{u} = \begin{bmatrix} \boldsymbol{u}_{\mathrm{p}} \\ \boldsymbol{u}_{\mathrm{s}}\left(\boldsymbol{u}_{\mathrm{p}}\right) \end{bmatrix}. \tag{3.66}$$

Here, the secondary variables $\boldsymbol{u}_{\mathrm{s}}$ correspond to a solution of the secondary equations with the primary variables $\boldsymbol{u}_{\mathrm{p}}$ specified. When evaluating the interblock flow terms, we use

$$\boldsymbol{u} = \begin{bmatrix} p^{n} \\ \boldsymbol{S}_{\mathrm{p}}^{n-1} \\ \boldsymbol{x}_{\mathrm{p}}^{n-1} \\ \boldsymbol{u}_{\mathrm{s}}\left(p^{n}, \boldsymbol{S}_{\mathrm{p}}^{n-1}, \boldsymbol{x}_{\mathrm{p}}^{n-1}\right) \end{bmatrix}, \tag{3.67}$$

while all other terms in (3.65) are evaluated with

$$\boldsymbol{u} = \begin{bmatrix} p^n \\ \boldsymbol{S}_{\mathrm{p}}^n \\ \boldsymbol{x}_{\mathrm{p}}^n \\ \boldsymbol{u}_{\mathrm{s}}\left(p^n, \boldsymbol{S}_{\mathrm{p}}^n, \boldsymbol{x}_{\mathrm{p}}^n\right) \end{bmatrix}. \tag{3.68}$$

If the original mass balance equations are used as primary equations, the system is still coupled, and all equations must be solved simultaneously. However, by a proper reformulation, i.e., by a volume balance pressure equation in which the accumulation term depends on pressure only, pressure may be determined by a separate iterative scheme. The pressure scheme has a Jacobian of dimensions

$$N_{\mathrm{b}} \times N_{\mathrm{b}}, \tag{3.69}$$

which is significantly smaller than (3.64). Then, since the interblock flow terms are determined by pressure only, the other variables $(\boldsymbol{S}_{\mathrm{p}}, \boldsymbol{x}_{\mathrm{p}})$ can be determined gridblock by gridblock, with local Jacobians of dimensions $(N_{\mathrm{c}} - 1) \times (N_{\mathrm{c}} - 1)$.

We note that, for gridblocks containing fully implicit and variable source terms $\boldsymbol{q}$, the pressure equation may possibly not be decoupled from the rest of the equations, and a simultaneous solution of all the primary equations could be required. However, the number of such gridblocks is small, and the corresponding increased size of the Jacobian is negligible compared to $N_{\mathrm{b}}$.

Unfortunately, the IMPES approach is associated with stability limitations that restrict timestep size. These limitations are mainly due to the explicit treatment of saturations, which contribute strongly to the nonlinearities of the interblock flow terms through relative permeabilities and capillary pressures. Consequently, the timestep restrictions may be severe.

For discussions of proper stability criteria, we refer to [40, 41, 42, 43, 44].

### 3.5.3 Pressure and saturations implicit (IMPSAT)

An IMPSAT formulation of (3.4) can be written

$$\boldsymbol{r}_{\mathrm{c}}^{\mathrm{IMPSAT}} = \boldsymbol{n}^n - \boldsymbol{n}^{n-1} + \left[\boldsymbol{f}\left(p^n, \boldsymbol{S}_{\mathrm{p}}^n, \boldsymbol{x}_{\mathrm{p}}^{n-1}\right) - \boldsymbol{q}^n\right] \Delta t = \boldsymbol{0}. \tag{3.70}$$

In (3.70), the interblock flow terms are evaluated with pressure and saturations at the current time level, but with the variables $\boldsymbol{x}_{\mathrm{p}}$ at the previous time level. In other words, pressure and saturations are treated implicitly, while the variables $\boldsymbol{x}_{\mathrm{p}}$ are treated explicitly.

The evaluation of interblock flow terms is here done rigorously with

$$\boldsymbol{u} = \begin{bmatrix} p^n \\ \boldsymbol{S}_{\mathrm{p}}^n \\ \boldsymbol{x}_{\mathrm{p}}^{n-1} \\ \boldsymbol{u}_{\mathrm{s}}\left(p^n, \boldsymbol{S}_{\mathrm{p}}^n, \boldsymbol{x}_{\mathrm{p}}^{n-1}\right) \end{bmatrix}, \tag{3.71}$$

while all other terms in (3.70) are evaluated with (3.68).

By a proper reformulation, i.e., by volume balance pressure and saturation equations in which the accumulation terms depend on pressure and saturations only, we may determine pressure and saturations by a separate iterative scheme. The pressure and saturation scheme has a Jacobian of dimensions

$$N_{\mathrm{b}}N_{\mathrm{p}} \times N_{\mathrm{b}}N_{\mathrm{p}}, \tag{3.72}$$

which may still be significantly smaller than (3.64). Furthermore, the $N_{\mathrm{c}} - N_{\mathrm{p}}$ variables $\boldsymbol{x}_{\mathrm{p}}$ can be determined gridblock by gridblock, with systems of size $(N_{\mathrm{c}} - N_{\mathrm{p}}) \times (N_{\mathrm{c}} - N_{\mathrm{p}})$. We note, however, that the comment on fully implicit and variable source terms $\boldsymbol{q}$ made for IMPES still applies.

With the IMPSAT formulation, the nonlinearities in the interblock flow terms due to relative permeabilities and capillary pressures are taken into account. Consequently, IMPSAT is more stable than IMPES. However, there are still stability limitations due to the explicit treatment of the variables $\boldsymbol{x}_{\mathrm{p}}$.

The stability properties of the IMPSAT approach are investigated in Paper B and in Paper D. Other references on IMPSAT stability are [15, 16].

## 3.6 Additional Simulation Issues

Finally, to complete the numerical model, we discuss some simulation issues, including timestep selection, convergence criteria and phase disappearance and reappearance.

### 3.6.1 Timestep selection

Generally, we may let timesteps be governed by the formula

$$\Delta t^{n+1} = \Delta t^n \min_u \left[ \frac{(1+\lambda)\Delta u^n}{\Delta u^* + \lambda \Delta u^n} \right], \tag{3.73}$$

where $\Delta t^{n+1}$ is the next timestep, $\Delta t^n$ is the previous timestep, $\Delta u^n$ is the change in the variable $u$ over the previous timestep, $\Delta u^*$ is the target variable change during the next timestep and $\lambda$ is a tuning factor. The formula is due to [25].

The timestep control parameters, e.g., $\lambda$, $\Delta u^*$ and the initial timestep $\Delta t^0$, must be specified as input to the simulator. Typically, target changes are specified for pressure, saturations and/or phase mole fractions. Furthermore, we could specify a maximum timestep.

With proper timestep control, convergence of the Newton-Raphson scheme is assured. In addition, for IMPES or IMPSAT, a timestep restriction due to stability limitations must be added.

### 3.6.2 Convergence criteria

Convergence criteria must be set for both primary and secondary equations. For the mass balance equations, we could use the criterion

$$r_c^{(k)} = \left\| \boldsymbol{r}_c^{(k)} \right\|_\infty < \epsilon_c, \qquad \boldsymbol{r}_c^{(k)} = \max \left| \left( \frac{\Delta \boldsymbol{n} + (\boldsymbol{f} - \boldsymbol{q})\,\Delta t}{\boldsymbol{n}} \right)^{(k)} \right|, \tag{3.74}$$

and for the phase equilibrium equations, we could use

$$r_f^{(k)} = \left\| \boldsymbol{r}_f^{(k)} \right\|_\infty < \epsilon_f, \qquad \boldsymbol{r}_f^{(k)} = \max \left| \left( \frac{\boldsymbol{f}^o - \boldsymbol{f}^g}{\boldsymbol{f}^g} \right)^{(k)} \right|, \tag{3.75}$$

where $\boldsymbol{f}^j$ contains the fugacities of phase $j$. We note that the maximum is taken over all gridblocks, and that fractions of vectors are taken component-wise.

In addition, we could require that the changes to the variables during an iteration step must be below some tolerance for convergence. A quite general set of convergence criteria is provided in Paper C.

### 3.6.3 Phase disappearance and reappearance

During a simulated timestep, a phase may disappear or reappear in a gridblock. Consequently, since the number of phases $N_\mathrm{p}$ changes, so does the number of saturations $\boldsymbol{S}_\mathrm{p}$ and the number of variables $\boldsymbol{x}_\mathrm{p}$.

Phase disappearance is indicated by a negative saturation value when determining the primary variables $(p, \boldsymbol{S}_\mathrm{p}, \boldsymbol{x}_\mathrm{p})$. The saturation of the disappeared phase should then be set to zero, the remaining saturations should be adjusted to sum to unity, and the variables $\boldsymbol{x}_\mathrm{p}$ should be updated according to their definition.

Phase reappearance implies reappearance of gas or oil in a gridblock where only undersaturated oil or supercritical/undersaturated gas has been present. To check for phase reappearance, a conventional phase equilibrium calculation of the current pressure and overall composition can be performed in those gridblocks,

see section 3.2.2. The phase equilibrium calculation determines if the phase fraction $\lambda^g$ has returned to the interval $(0, 1)$. If this is the case, the reappeared phase saturation is calculated, and the state, including the variables $\boldsymbol{x}_{\mathrm{p}}$, can be updated.

We note that a useful supplement to the conventional phase equilibrium is a phase stability test. If the stability test suggests that a phase remains absent, no phase equilibrium calculations need to be performed. For details on phase stability tests, we refer to [22] and Paper E. However, to calculate the properties of a reappeared phase, a full phase equilibrium calculation must be applied.

# Chapter 4

# XPSIM Documentation

In this chapter, we give an overview of the calculations involved in the compositional reservoir simulator XPSIM, which has been the by-product of the work presented in this thesis.

## 4.1 Introduction

The main objective of the simulator is to solve the $N_{\mathrm{c}}$ mass balance equations

$$\Delta \boldsymbol{n} + (\boldsymbol{f} - \boldsymbol{q})\,\Delta t = \boldsymbol{0}, \tag{4.1}$$

and the $(N_{\mathrm{hp}} - 1)\,N_{\mathrm{hc}}$ phase equilibrium equations

$$\boldsymbol{f}^o - \boldsymbol{f}^g = \boldsymbol{0}, \tag{4.2}$$

in an efficient manner, using ideas presented in this thesis. Here, $N_{\mathrm{hp}}$ is the number of phases other than water, $N_{\mathrm{hc}}$ is the number of components other than water, and $\boldsymbol{f}^j$ contains the fugacities of the components present in phase $j$. Additional equations are

$$\phi V_{\mathrm{b}} S^j - \frac{n^j}{\xi^j} = 0, \tag{4.3}$$

for each phase $j$, representing $N_{\mathrm{p}}$ volume relations, and

$$\boldsymbol{x}_{\mathrm{p}} - \boldsymbol{W}_x\,\boldsymbol{n} = \boldsymbol{0}, \tag{4.4}$$

representing the definition of the $N_{\mathrm{c}} - N_{\mathrm{p}}$ variables $\boldsymbol{x}_{\mathrm{p}}$.

The definition of the $(N_{\mathrm{c}} - N_{\mathrm{p}}) \times N_{\mathrm{c}}$ matrix $\boldsymbol{W}_x$ is given in Paper B, and makes $\boldsymbol{W}_x$ complementary to the $N_{\mathrm{p}} \times N_{\mathrm{c}}$ matrix

$$\boldsymbol{W}_V = \left(\frac{\partial \boldsymbol{V}}{\partial \boldsymbol{n}}\right)_p, \tag{4.5}$$

where $\boldsymbol{V}$ represents the $N_\mathrm{p}$ phase volumes. The matrices $\boldsymbol{W}_V$ and $\boldsymbol{W}_x$ are used to reformulate the $N_\mathrm{c}$ mass balance equations into $N_\mathrm{p}$ volume balance equations and $N_\mathrm{c} - N_\mathrm{p}$ additional conservation equations, see section 3.4 and Paper C.

The chosen $N_\mathrm{c}$ primary variables,

$$\boldsymbol{u}_\mathrm{p} = \begin{bmatrix} p \\ \boldsymbol{S}_\mathrm{p} \\ \boldsymbol{x}_\mathrm{p} \end{bmatrix}, \tag{4.6}$$

form the basis for a unified black-oil and compositional formulation, and are used in both a fully implicit scheme and an IMPSAT scheme. The chosen secondary variables are

$$\boldsymbol{u}_\mathrm{s} = \boldsymbol{n}^{\boldsymbol{j}}. \tag{4.7}$$

We note that the number of secondary variables is $N_\mathrm{s} = (N_\mathrm{hp} - 1)\, N_\mathrm{hc} + N_\mathrm{c}$, which equals the number of relations (4.2), (4.3) and (4.4). In the determination of the secondary variables, XPSIM offers a choice between exact volume balance and exact mass balance, see Paper C.

Various modules are involved in the setup of the equations, including input and preprocessing, initialization, thermodynamics, calculation of variable properties and calculation of interblock flow terms and source terms. Furthermore, for an iterative solution of the equations, a broad range of derivatives must be calculated. The different modules included in XPSIM are discussed below.

## 4.2 Input and Preprocessing Module

We start by reading input parameters from file. These include

- grid specification, i.e., input of gridblock cornerpoint coordinates,
- absolute permeability tensor for each gridblock,
- reference porosity for each gridblock, plus a reference pressure,
- component properties (see section 2.3.2), temperature, rock compressibility, tabulated relative permeability and capillary pressure functions, initial conditions (pressure, overall mole fractions, water saturation, fluid contact locations),
- injection rates and production bottom hole pressures (fixed),
- time scheme (fully implicit or IMPSAT), exact conservation (mass or volume), convergence limits and timestep control parameters.

The preprocessing part includes calculations that can be done before the start of the simulation run. Using the grid input, we determine interfaces between gridblocks and gridblock volumes. Furthermore, with the use of absolute permeabilities and grid geometry, transmissibilities are calculated by the MPFA O-method, [30]. Here, no-flow boundary conditions are applied. Finally, the initialization module outlined below is invoked.

## 4.3 Initialization Module

For cases of horizontal flow, the initialization is done by a conventional phase equilibrium calculation with the input pressure and overall mole fractions, see section 3.2.2. Here, access to a module for calculation of compressibility factors and fugacity coefficients is required. This module is outlined in section 4.4.

On the other hand, if the effect of gravity is included, a gravity/chemical equilibrium calculation is performed. If a gas-oil contact is specified in the reservoir, XPSIM assumes that the input pressure is an estimate of the pressure at the gas-oil contact, and that the input overall mole fractions are the overall mole fractions at the gas-oil contact. Capillary pressures are neglected. Consequently, the pressure at the gas-oil contact should equal a saturation pressure, i.e., a point on the boundary of the two phase region. Saturation point calculations are discussed in Paper E. However, if no gas-oil contact exists in the reservoir, the input pressure is not adjusted, and the input overall mole fractions are assumed to represent single phase oil or gas at some reference depth.

Subsequently, pressure and the overall mole fractions are used to calculate reference fugacities, and the gravity/chemical equilibrium calculation outlined in section 3.2.3 is carried out. Above the gas-oil contact, XPSIM determines the pressure and the mole fractions of the gas phase. Below the gas-oil contact and above the water-oil contact, the pressure and the mole fractions of the oil phase are determined. For further details, we refer to Paper E. Below the water-oil contact, the pressure is determined directly by the hydrostatic equilibrium condition (3.19).

The gravity/chemical equilibrium initialization must have access to modules which calculate fugacities and derivatives of these with respect to pressure and phase mole numbers, see sections 4.4 and 4.7, respectively.

## 4.4 Thermodynamics Module

The thermodynamics module calculates compressibility factors, fugacity coefficients and fugacities. XPSIM uses the Peng-Robinson equation of state, [28], for

these calculations. Consequently, the coefficients of

$$\left(Z^j\right)^3 + c_2\left(Z^j\right)^2 + c_1 Z^j + c_0 = 0 \tag{4.8}$$

are given by

$$c_2 = -(1 - B^j), \tag{4.9}$$

$$c_1 = A^j - 3\left(B^j\right)^2 - 2B^j, \tag{4.10}$$

$$c_0 = -A^j B^j + \left(B^j\right)^2 + \left(B^j\right)^3, \tag{4.11}$$

$$A^j = \left[\sum_{i=1}^{N_{\rm hc}}\sum_{m=1}^{N_{\rm hc}} c_i^j c_k^j \sqrt{a_i a_k}\,(1 - d_{i,k})\right]\frac{p}{R^2T^2}, \qquad B^j = \left[\sum_{i=1}^{N_{\rm hc}} c_i^j b_i\right]\frac{p}{RT}, \tag{4.12}$$

$$a_i = \Omega_A\left[1 + \kappa_i\left(1 - \sqrt{T/T_{c,i}}\right)\right]^2 \frac{R^2T_{c,i}^2}{p_{c_i}}, \qquad b_i = \Omega_B\frac{RT_{c,i}}{p_{c,i}}, \tag{4.13}$$

$$\Omega_A = 0.457235529, \qquad \Omega_B = 0.077796074, \tag{4.14}$$

$$\kappa_i = \begin{cases} 0.37464 + 1.54226\,\omega_i - 0.26992\,\omega_i^2, & \omega_i \le 0.49, \\ 0.379642 + 1.48503\,\omega_i - 0.164423\,\omega_i^2 + 0.016666\,\omega_i^3, & \omega_i > 0.49. \end{cases} \tag{4.15}$$

The cubic equation of state can be solved analytically with respect to the compressibility factors $Z^j$, defined by (2.33). The three roots are

$$Z_1^j = \frac{1}{6}\left(\beta^{1/3} - \frac{12c_1 - 4c_2^2}{\beta^{1/3}} - 2c_2\right), \tag{4.16}$$

$$Z_2^j = -\frac{1}{12}\left[\beta^{1/3} - \frac{12c_1 - 4c_2^2}{\beta^{1/3}} + 4c_2 - i\sqrt{3}\left(\beta^{1/3} + \frac{12c_1 - 4c_2^2}{\beta^{1/3}}\right)\right], \tag{4.17}$$

$$Z_3^j = -\frac{1}{12}\left[\beta^{1/3} - \frac{12c_1 - 4c_2^2}{\beta^{1/3}} + 4c_2 + i\sqrt{3}\left(\beta^{1/3} + \frac{12c_1 - 4c_2^2}{\beta^{1/3}}\right)\right], \tag{4.18}$$

where

$$i = \sqrt{-1}, \tag{4.19}$$

$$\beta = 36c_1c_2 - 108c_0 - 8c_2^3 + 12\sqrt{\alpha}, \tag{4.20}$$

$$\alpha = 12c_1^3 - 3c_1^2c_2^2 - 54c_1c_2c_0 + 81c_0^2 + 12c_0c_2^3. \tag{4.21}$$

The solution of the cubic equation of state should represent a minimum of the Gibbs energy, [22]. Consequently, the largest real root is chosen for the gas phase, while the smallest real root is chosen for the oil phase.

Furthermore, the calculation of fugacities and fugacity coefficients is done by

$$f_i^j = pc_i^j\phi_i^j, \qquad \phi_i^j = \frac{\exp(B_i^j(Z^j-1))}{Z^j - B^j}\left(\frac{Z^j - (\sqrt{2}-1)B^j}{Z^j + (\sqrt{2}+1)B^j}\right)^{\frac{A^j(A_i^j - B_i^j)}{2\sqrt{2}B^j}}, \tag{4.22}$$

respectively, where

$$A_i^j = \frac{\sum_{k=1}^{N_{\mathrm{hc}}} 2c_k^j\sqrt{a_ia_k}\,(1-d_{i,k})}{\sum_{k=1}^{N_{\mathrm{hc}}}\sum_{l=1}^{N_{\mathrm{hc}}} c_k^jc_l^j\sqrt{a_ka_l}\,(1-d_{k,l})}, \qquad B_i^j = \frac{b_i}{\sum_{m=1}^{N_{\mathrm{hc}}} c_k^jb_k}. \tag{4.23}$$

## 4.5 Variables Module

As mentioned in section 2.3.2, all variable properties can be expressed explicitly in terms of $\left(p, \boldsymbol{n^j}\right)$. However, during a simulation run, we also work in terms of the primary variables $(p, \boldsymbol{S}_{\mathrm{p}}, \boldsymbol{x}_{\mathrm{p}})$. The iterative scheme ensures that the two sets $\left(p, \boldsymbol{n^j}\right)$ and $(p, \boldsymbol{S}_{\mathrm{p}}, \boldsymbol{x}_{\mathrm{p}})$ are in accordance. Consequently, the variables module takes the entire set $\left(p, \boldsymbol{S}_{\mathrm{p}}, \boldsymbol{x}_{\mathrm{p}}, \boldsymbol{n^j}\right)$ as input for the calculation of quantities in the primary and secondary equations.

Most of the calculations have been outlined in Chapter 2, including the calculation of porosity

$$\phi = \tilde{\phi}\left(1 + c_R\left(p - \tilde{p}\right)\right), \tag{4.24}$$

and densities

$$\xi^w = \tilde{\xi^w}\left(1 + c_w\left(p - \tilde{p}\right)\right), \qquad \xi^j = \frac{p}{RTZ^j}, \tag{4.25}$$

$$\rho^w = M_w\xi^w, \qquad \rho^j = \xi^j\sum_{i=1}^{N_{\mathrm{hc}}} c_i^jM_i. \tag{4.26}$$

Here, the thermodynamics module must be invoked to determine $Z^j$.

Furthermore, volumes can be calculated by either of the two expressions

$$V^j = \phi V_{\mathrm{b}}S^j, \qquad V^j = \frac{n^j}{\xi^j}. \tag{4.27}$$

The expression to the left is used with the exact volume balance scheme, while the expression to the right is used with the exact mass balance scheme, see Paper C.

Relative permeabilities and capillary pressures are given functions of saturations, water viscosity is assumed to be constant, while the oil and gas viscosities are calculated by the LBC method, [29], as outlined below.

In the LBC method, the low-pressure, pure-component gas viscosities $\mu_i^*$ are given by

$$\mu_i^*\zeta_i = \begin{cases} 34\cdot 10^{-5}T_{ri}^{0.94} & , \quad T_{ri} < 1.5, \\ 17.78\cdot 10^{-5}(4.58T_{ri}-1.67)^{\frac{5}{8}} & , \quad T_{ri} > 1.5, \end{cases} \qquad \zeta_i = \frac{T_{c,i}^{1/6}}{M_i^{1/2}p_{c,i}^{2/3}}, \tag{4.28}$$

where $T_{ri} = T/T_{c,i}$ denotes the reduced temperature. Subsequently, the viscosity of phase $j$ is calculated by

$$\mu^j = (\mu^j)^* + \frac{1}{\zeta^j}\left[-10^{-4} + \left(\chi^j\right)^4\right], \tag{4.29}$$

where

$$(\mu^j)^* = \frac{\sum_{i=1}^{N_{\rm hc}} c_i^j \mu_i^* \sqrt{M_i}}{\sum_{i=1}^{N_{\rm hc}} c_i^j \sqrt{M_i}}, \qquad \zeta^j = \frac{\left(\sum_{i=1}^{N_{\rm hc}} c_i^j T_{c,i}\right)^{1/6}}{\left(\sum_{i=1}^{N_{\rm hc}} c_i^j M_i\right)^{1/2}\left(\sum_{i=1}^{N_{\rm hc}} c_i^j p_{c,i}\right)^{2/3}}, \tag{4.30}$$

$$\chi^j = 0.1023 + 0.023364\,\xi_r^j + 0.058533\,(\xi_r^j)^2 - 0.040758\,(\xi_r^j)^3 + 0.0093324\,(\xi_r^j)^4, \tag{4.31}$$

and

$$\xi_r^j = \xi^j \sum_{i=1}^{N_{\rm hc}} c_i^j V_{c,i}. \tag{4.32}$$

We note that, if temperatures are in Kelvin, molar masses are in g/mol, and pressures are in atmospheres, the resulting viscosities are in cP (= $10^{-3}$ Pa s).

## 4.6 Interblock Flow and Source Module

The interblock flow and source module calculates interblock flow terms and source terms according to the discretization given in sections 3.1.3 and 3.1.4.

### 4.6.1 Interblock flow term calculations

Going through all interfaces $\gamma$ of the grid, XPSIM calculates

$$T_\gamma^j = \sum_{\eta \in \mathcal{I}_\gamma} t_{\eta,\gamma} \left( p_\eta + P_{c,\eta}^j - \frac{\rho_\alpha^j S_\alpha^j + \rho_\beta^j S_\beta^j}{S_\alpha^j + S_\beta^j} g D_\eta \right), \quad \Lambda_{i,\gamma}^j = \left( \frac{c_i^j \xi^j k_r^j}{\mu^j} \right)_\gamma, \tag{4.33}$$

$$f_{i,\gamma}^j = \Lambda_{i,\gamma}^j T_\gamma^j. \tag{4.34}$$

Subsequently, the net flow rate out of each gridblock is calculated by assembling the interface flow rates (4.34). We note that the sign of $T_\gamma^j$ determines in which of the two cells $\alpha$ and $\beta$ incident on the interface the generalised mobility is evaluated, i.e., the upstream cell.

If an IMPSAT scheme is used, the interblock flow terms are evaluated with $p^n$, $\boldsymbol{S}_{\mathrm{p}}^n$ and $\boldsymbol{n^j} = \boldsymbol{n^j}\left(p^n, \boldsymbol{S}_{\mathrm{p}}^n, \boldsymbol{x}_{\mathrm{p}}^{n-1}\right)$, while if a FIM scheme is used, the interblock flow terms are evaluated with $p^n$, $\boldsymbol{S}_{\mathrm{p}}^n$ and $\boldsymbol{n^j} = \boldsymbol{n^j}\left(p^n, \boldsymbol{S}_{\mathrm{p}}^n, \boldsymbol{x}_{\mathrm{p}}^n\right)$

### 4.6.2 Source term calculations

For injection wells, XPSIM calculates

$$q_i = z_i \xi_s^k Q_s^k, \tag{4.35}$$

where $z_i$ and $Q_s^k$ are input parameters (overall composition and rate of injected fluid), while $\xi_s^k$ is determined by a conventional phase equilibrium calculation of the overall composition and the surface conditions, see section 3.2.2. Since the injection rates are fixed, (4.35) is calculated only once, i.e., initially.

For production wells, XPSIM calculates

$$q_i = -\sum_{j=1}^{N_{\mathrm{p}}} \Lambda_{wi}^j T_w \left(p - p_w\right), \qquad \Lambda_{wi}^j = \frac{c_i^j \xi^j k_r^j}{\mu^j}. \tag{4.36}$$

Here, $p_w$ is provided from input, while $T^w$ is given by (3.15).

## 4.7 Basic Derivatives Module

Since all variables and equations can be written explicitly in terms of $\left(p, \boldsymbol{n^j}\right)$, calculation of derivatives with respect to these variables, referred to as basic derivatives, is required.

We here focus on the basic derivatives of compressibilities and fugacities, which are important in the initialization module and in the calculation of total derivatives and volume derivatives, see sections 4.8 and 4.10, respectively.

**Notation** Compressibilities and fugacities can actually be written explicitly in terms of pressure and the phase mole numbers $\boldsymbol{n}^j$ of the phase to which they belong. We note that $\boldsymbol{n}^j$ is different from $\boldsymbol{n^j}$, which denotes the mole numbers of all phases. For brevity of notation, we consider differentiation with respect to $u \in (p, \boldsymbol{n}^j)$. For differentiation with respect to pressure, we use the interpretation

$$\frac{\partial}{\partial u}\left(\,\cdot\,\right) = \frac{\partial}{\partial p}\left(\,\cdot\,\right)_{\boldsymbol{n}^j}, \tag{4.37}$$

and note that

$$\frac{\partial p}{\partial u} = \left(\frac{\partial p}{\partial p}\right)_{\boldsymbol{n}^j} = 1, \qquad \frac{\partial c_i^j}{\partial u} = \left(\frac{\partial c_i^j}{\partial p}\right)_{\boldsymbol{n}^j} = 0. \tag{4.38}$$

For differentiation with respect to $\boldsymbol{n}^j$, we use the interpretation

$$\frac{\partial}{\partial u}\left(\,\cdot\,\right) = \frac{\partial}{\partial n_k^j}\left(\,\cdot\,\right)_{p,\boldsymbol{n}_{(k)}^j}, \tag{4.39}$$

and note that

$$\frac{\partial p}{\partial u} = \left(\frac{\partial p}{\partial n_k^j}\right)_{p,\boldsymbol{n}_{(k)}^j} = 0, \qquad \frac{\partial c_i^j}{\partial u} = \left(\frac{\partial c_i^j}{\partial n_k^j}\right)_{p,\boldsymbol{n}_{(k)}^j} = \frac{\delta_{i,k} n^j - n_i^j}{\left(n^j\right)^2} = \frac{\delta_{i,k} - c_i^j}{n^j}, \tag{4.40}$$

where $\delta_{i,k}$ is Kronecker's delta, i.e., $\delta_{i,k} = 1$ if $i = k$ and $\delta_{i,k} = 0$ if $i \neq k$.

Here, subscripts on the partial differentiation indicate which variables are kept fixed, and subscript $\boldsymbol{n}_{(k)}^j$ indicates that all mole numbers of phase $j$ except for $n_k^j$ are kept fixed.

### 4.7.1 Compressibility factor derivatives

By inserting the Peng-Robinson coefficients (4.9), (4.10) and (4.11) into the cubic equation of state (4.8) and differentiating through with respect to $u$, we find that

$$\begin{aligned} \tfrac{\partial Z^j}{\partial u}\left(3\left(Z^j\right)^2 - 2\left(1 - B^j\right)Z^j + A^j - 3\left(B^j\right)^2 - 2B^j\right) &= \tfrac{\partial A^j}{\partial u}\left(B^j - Z^j\right) \\ &\quad - \tfrac{\partial B^j}{\partial u}\left(\left(Z^j\right)^2 - \left(6B^j + 2\right)Z^j - A^j + 2B^j + 3\left(B^j\right)^2\right), \end{aligned} \tag{4.41}$$

which yields

$$\frac{\partial Z^j}{\partial u} = \frac{\tfrac{\partial A^j}{\partial u}\left(B^j - Z^j\right) - \tfrac{\partial B^j}{\partial u}\left(\left(Z^j\right)^2 - \left(6B^j + 2\right)Z^j - A^j + 2B^j + 3\left(B^j\right)^2\right)}{3\left(Z^j\right)^2 - 2\left(1 - B^j\right)Z^j + A^j - 3\left(B^j\right)^2 - 2B^j}. \tag{4.42}$$

Here,

$$\frac{\partial A^j}{\partial u} = \frac{A^j}{p}\frac{\partial p}{\partial u} + \left[\sum_{i=1}^{N_{\rm hc}}\sum_{m=1}^{N_{\rm hc}}\left(c_m^j\frac{\partial c_i^j}{\partial u} + c_i^j\frac{\partial c_m^j}{\partial u}\right)\sqrt{a_i a_m}\,(1-d_{i,m})\right]\frac{p}{R^2T^2}, \tag{4.43}$$

$$\frac{\partial B^j}{\partial u} = \frac{B^j}{p}\frac{\partial p}{\partial u} + \left[\sum_{i=1}^{N_{\rm hc}}\frac{\partial c_i^j}{\partial u}b_i\right]\frac{p}{RT}. \tag{4.44}$$

### 4.7.2 Fugacity derivatives

By introducing

$$w^j = \frac{Z^j - \left(\sqrt{2}-1\right)B^j}{Z^j + \left(\sqrt{2}+1\right)B^j}, \quad v_i^j = \frac{A^j\left(A_i^j - B_i^j\right)}{2\sqrt{2}B^j}, \quad y_i^j = \frac{\exp\left(B_i^j\left(Z^j-1\right)\right)}{Z^j - B^j}, \tag{4.45}$$

in (4.22), we may express the fugacity of component $i$ in phase $j$ by

$$f_i^j = pc_i^j y_i^j \left[w^j\right]^{v_i^j}. \tag{4.46}$$

Differentiation with respect to a variable $u$ then yields

$$\begin{aligned}\frac{\partial f_i^j}{\partial u} &= c_i^j\left[w^j\right]^{v_i^j}\frac{\partial p}{\partial u} + p\left[w^j\right]^{v_i^j}\frac{\partial c_i^j}{\partial u} + pc_i^j\frac{\partial y_i^j}{\partial u}\left[w^j\right]^{v_i^j} + \\ &\quad pc_i^j y_i^j\left[w^j\right]^{v_i^j}\left(\frac{\partial v_i^j}{\partial u}\ln w^j + \frac{v_i^j}{w^j}\frac{\partial w^j}{\partial u}\right),\end{aligned} \tag{4.47}$$

where we have used so-called logarithmic differentiation of $g_i^j = [w^j]^{v_i^j}$, i.e.,

$$\begin{aligned}\ln g_i^j &= v_i^j \ln w^j, \\ \frac{1}{g_i^j}\frac{\partial g_i^j}{\partial u} &= \frac{\partial v_i^j}{\partial u}\ln w^j + v_i^j\frac{1}{w^j}\frac{\partial w^j}{\partial u}, \\ \frac{\partial g_i^j}{\partial u} &= g_i^j\left(\frac{\partial v_i^j}{\partial u}\ln w^j + \frac{v_i^j}{w^j}\frac{\partial w^j}{\partial u}\right).\end{aligned} \tag{4.48}$$

To calculate (4.47), we must determine

$$\frac{\partial y_i^j}{\partial u} = -\frac{y_i^j}{Z^j - B^j}\left(\frac{\partial Z^j}{\partial u} - \frac{\partial B^j}{\partial u}\right) + y_i^j\left(\frac{\partial B_i^j}{\partial u}\left(Z^j-1\right) + B_i^j\frac{\partial Z^j}{\partial u}\right), \tag{4.49}$$

$$\frac{\partial v_i^j}{\partial u} = \frac{B^j \left[\frac{\partial A^j}{\partial u}\left(A_i^j - B_i^j\right) + A^j\left(\frac{\partial A_i^j}{\partial u} - \frac{\partial B_i^j}{\partial u}\right)\right] - A^j\left(A_i^j - B_i^j\right)\frac{\partial B^j}{\partial u}}{2\sqrt{2}\left(B^j\right)^2}, \quad (4.50)$$

$$\frac{\partial w^j}{\partial u} = \frac{2\sqrt{2}B^j\frac{\partial Z^j}{\partial u} - 2\sqrt{2}Z^j\frac{\partial B^j}{\partial u}}{\left(Z^j + \left(\sqrt{2}+1\right)B^j\right)^2}, \quad (4.51)$$

$$\begin{aligned}\frac{\partial A_i^j}{\partial u} &= \frac{\sum_{k=1}^{N_{\rm hc}} 2\frac{\partial c_k^j}{\partial u}\sqrt{a_i a_k}\left(1-d_{i,k}\right)}{\sum_{k=1}^{N_{\rm hc}}\sum_{l=1}^{N_{\rm hc}} c_k^j c_l^j \sqrt{a_k a_l}\left(1-d_{k,l}\right)} \\ &\quad - \frac{A_i^j}{\sum_{k=1}^{N_{\rm hc}}\sum_{l=1}^{N_{\rm hc}} c_k^j c_l^j \sqrt{a_k a_l}\left(1-d_{k,l}\right)} \cdot \\ &\quad \left(\sum_{k=1}^{N_{\rm hc}}\sum_{l=1}^{N_{\rm hc}}\left(c_k^j\frac{\partial c_l^j}{\partial u} + c_l^j\frac{\partial c_k^j}{\partial u}\right)\sqrt{a_k a_l}\left(1-d_{k,l}\right)\right), \end{aligned} \quad (4.52)$$

$$\frac{\partial B_i^j}{\partial u} = -\frac{b_i\sum_{k=1}^{N_{\rm hc}}\frac{\partial c_k^j}{\partial u}b_k}{\left(\sum_{k=1}^{N_{\rm hc}} c_k^j b_k\right)^2}. \quad (4.53)$$

In addition, we make use of the relations (4.42), (4.43) and (4.44).

## 4.8 Total Derivatives Module

Total derivatives are derivatives with respect to the primary variables $\boldsymbol{u}_{\rm p}$. If the total derivatives of a property $h$ cannot be determined directly, we use

$$\frac{dh}{d\boldsymbol{u}_{\rm p}} = \left(\frac{\partial h}{\partial p}\right)_{\boldsymbol{n^j}}\frac{dp}{d\boldsymbol{u}_{\rm p}} + \left(\frac{\partial h}{\partial \boldsymbol{n^j}}\right)_p\frac{d\boldsymbol{n^j}}{d\boldsymbol{u}_{\rm p}}. \quad (4.54)$$

The derivatives with respect to $\left(p, \boldsymbol{n^j}\right)$ are basic derivatives, see section 4.7, while $\partial p/\partial v$, where $v \in (p, \boldsymbol{S}_{\rm p}, \boldsymbol{x}_{\rm p})$, is unity for $v = p$ and zero otherwise. The calculation of $d\boldsymbol{n^j}/d\boldsymbol{u}_{\rm p}$ is outlined below.

To calculate the derivatives of the oil and gas phase mole numbers $\boldsymbol{n}^o$ and $\boldsymbol{n}^g$ with respect to $v \in (p, \boldsymbol{S}_{\rm p}, \boldsymbol{x}_{\rm p})$, we use the system of equations

$$\begin{bmatrix} \boldsymbol{f}^o - \boldsymbol{f}^g \\ \phi V_{\rm b} S^o - n^o/\xi^o \\ \phi V_{\rm b} S^g - n^g/\xi^g \\ \boldsymbol{x}_{\rm p} - \boldsymbol{W}_x\,\boldsymbol{n} \end{bmatrix} = \boldsymbol{0}, \quad (4.55)$$

where $\xi^j = p/\left(RTZ^j\right)$. Here, $p$, $\phi$, $S^j$ and $\boldsymbol{x}_\mathrm{p}$ are given explicitly in terms of the primary variables, and differentiation of these with respect to $v$ is straightforward. For the other terms, which may be given in terms of $(p, \boldsymbol{n}^o, \boldsymbol{n}^g)$, we use the form (4.54) for differentiation with respect to $v$. Consequently, by differentiating through (4.55) with respect to $v \in (p, \boldsymbol{S}_\mathrm{p}, \boldsymbol{x}_\mathrm{p})$ and rearranging terms, we obtain

$$\begin{bmatrix} \frac{\partial \boldsymbol{f}^o}{\partial \boldsymbol{n}^o} & -\frac{\partial \boldsymbol{f}^g}{\partial \boldsymbol{n}^g} \\ -\frac{\partial (n^o/\xi^o)}{\partial \boldsymbol{n}^o} & \mathbf{0}^\mathrm{T} \\ \mathbf{0}^\mathrm{T} & -\frac{\partial (n^g/\xi^g)}{\partial \boldsymbol{n}^g} \\ -\frac{\partial (\boldsymbol{W}_\mathrm{x}\,\boldsymbol{n})}{\partial \boldsymbol{n}^o} & -\frac{\partial (\boldsymbol{W}_\mathrm{x}\,\boldsymbol{n})}{\partial \boldsymbol{n}^g} \end{bmatrix} \begin{bmatrix} \frac{\partial \boldsymbol{n}^o}{\partial v} \\ \frac{\partial \boldsymbol{n}^g}{\partial v} \end{bmatrix} = \begin{bmatrix} \left(\frac{\partial \boldsymbol{f}^g}{\partial p}\right)_{\boldsymbol{n}^o} \frac{\partial p}{\partial v} - \left(\frac{\partial \boldsymbol{f}^o}{\partial p}\right)_{\boldsymbol{n}^g} \frac{\partial p}{\partial v} \\ -V_\mathrm{b} S^o \frac{\partial \phi}{\partial p}\frac{\partial p}{\partial v} - \phi V_\mathrm{b} \frac{\partial S^o}{\partial v} \\ -V_\mathrm{b} S^g \frac{\partial \phi}{\partial p}\frac{\partial p}{\partial v} - \phi V_\mathrm{b} \frac{\partial S^g}{\partial v} \\ \left(\frac{\partial (\boldsymbol{W}_\mathrm{x}\,\boldsymbol{n})}{\partial p}\right)_{\boldsymbol{n}^o,\boldsymbol{n}^g} - \frac{\partial \boldsymbol{x}_\mathrm{p}}{\partial v} \end{bmatrix}. \quad (4.56)$$

We observe that basic derivatives of fugacities and compressibility factors are needed in the calculation of both the system matrix and the right hand side. Furthermore, we note that derivatives of $\boldsymbol{W}_x$ vanish if $\boldsymbol{W}_x$ is kept fixed during a timestep, as suggested in Paper B.

The system matrix of (4.56) is independent of $v$, so that only a single inversion is necessary to calculate all the derivatives $\partial \boldsymbol{n}^o/\partial v$ and $\partial \boldsymbol{n}^g/\partial v$. In addition, the water mole numbers $n^w$ can be written as an explicit function of pressure and water saturation only, so that the calculation of $\partial n^w/\partial v$ is straight-forward. Consequently, the calculation of $d\boldsymbol{n^j}/d\boldsymbol{u}_\mathrm{p}$ is complete.

## 4.9 Flow and Source Derivatives Module

A separate module calculates total derivatives of interblock flow terms and source terms with respect to $(p, \boldsymbol{S}_\mathrm{p}, \boldsymbol{x}_\mathrm{p})$.

### 4.9.1 Flux derivatives

Using subscript $\nu$ to denote a cell in the flux molecule of some interface $\gamma$, we do differentiation of (4.34) with respect to $v_\nu \in (p, \boldsymbol{S}_\mathrm{p}, \boldsymbol{x}_\mathrm{p})_\nu$ by

$$\frac{\partial f^j_{i,\gamma}}{\partial v_\nu} = \frac{\Lambda^j_{i,\gamma}}{\partial v_\nu} T^j_\gamma + \Lambda^j_{i,\gamma} \frac{\partial T^j_\gamma}{\partial v_\nu}, \quad (4.57)$$

where

$$\frac{\partial \Lambda^j_{i,\gamma}}{\partial v_\nu} = \begin{cases} \xi^j \frac{k^j_r}{\mu^j}\frac{\partial c^j_i}{\partial v_\nu} + c^j_i \frac{k^j_r}{\mu^j}\frac{\partial \xi^j}{\partial v_\nu} + c^j_i \xi^j \frac{1}{\mu^j}\frac{\partial k^j_r}{\partial v_\nu} - c^j_i \xi^j \frac{k^j_r}{(\mu^j)^2}\frac{\partial \mu^j}{\partial v_\nu}, & \nu = \nu^*, \\ 0, & \nu \neq \nu^*, \end{cases} \quad (4.58)$$

$$\frac{\partial T_\gamma^j}{\partial v_\nu} = \sum_{\eta\in\mathcal{I}_\gamma} t_{\eta,\gamma}\frac{\partial}{\partial v_\nu}\left(p_\eta + P_{c,\eta}^j - \frac{\rho_\alpha^j S_\alpha^j + \rho_\beta^j S_\beta^j}{S_\alpha^j + S_\beta^j} g D_\eta\right). \tag{4.59}$$

and $\nu^*$ denotes the upstream cell. We note that derivatives with respect to $\boldsymbol{x}_\mathrm{p}$ are omitted (set to zero) if an IMPSAT scheme is used.

Derivatives of phase mole fractions and densities are obtained with the form (4.54), while derivatives of relative permeabilities and capillary pressures, which are functions of saturations only, are straight-forward. However, the calculation of viscosity derivatives is more involved. We use (4.29) to find

$$\frac{\partial \mu^j}{\partial v} = \frac{\partial (\mu^j)^*}{\partial v} - \frac{1}{(\zeta^j)^2}\left[-10^{-4} + \left(\chi^j\right)^4\right]\frac{\partial \zeta^j}{\partial v} + \frac{4}{\zeta^j}\left(\chi^j\right)^3 \frac{\partial \chi^j}{\partial \xi_r^j}\frac{\partial \xi_r^j}{\partial v}, \tag{4.60}$$

where

$$\begin{aligned}\frac{\partial (\mu^j)^*}{\partial v} &= \frac{\sum_{i=1}^{N_{hc}} \frac{\partial c_i^j}{\partial v}\mu_i^*\sqrt{M_i}}{\sum_{i=1}^{N_{hc}} c_i^j\sqrt{M_i}} - \frac{(\mu^j)^*\sum_{i=1}^{N_{hc}}\frac{\partial c_i^j}{\partial v}\sqrt{M_i}}{\sum_{i=1}^{N_{hc}} c_i^j\sqrt{M_i}} \\ &= \frac{\sum_{i=1}^{N_{hc}}((\mu_i)^* - (\mu^j)^*)\sqrt{M_i}\frac{\partial c_i^j}{\partial v}}{\sum_{i=1}^{N_{hc}} c_i^j\sqrt{M_i}},\end{aligned} \tag{4.61}$$

$$\begin{aligned}\frac{\partial \zeta^j}{\partial v} &= \left[\left(\sum_{i=1}^{N_{hc}} c_i^j M_i\right)^{1/2}\left(\sum_{i=1}^{N_{hc}} c_i^j p_{c,i}\right)^{2/3}\right]^{-1} \cdot \\ &\quad \left[\frac{1}{6}(\sum_{i=1}^{N_{hc}} c_i^j T_{c,i})^{-5/6}\sum_{i=1}^{N_{hc}}\frac{\partial c_i^j}{\partial v}T_{c,i}\right. \\ &\quad -\frac{1}{2}\zeta^j(\sum_{i=1}^{N_{hc}} c_i^j M_i)^{-1/2}(\sum_{i=1}^{N_{hc}}\frac{\partial c_i^j}{\partial v}M_i)(\sum_{i=1}^{N_{hc}} c_i^j p_{c,i})^{2/3} \\ &\quad \left.-\frac{2}{3}\zeta^j(\sum_{i=1}^{N_{hc}} c_i^j p_{c,i})^{-1/3}(\sum_{i=1}^{N_{hc}}\frac{\partial c_i^j}{\partial v}p_{c,i})(\sum_{i=1}^{N_{hc}} c_i^j M_i)^{1/2}\right],\end{aligned} \tag{4.62}$$

$$\frac{\partial \chi^j}{\partial \xi_r^j} = 0.023364 + 2\cdot 0.058533\xi_r^j - 3\cdot 0.040758(\xi_r^j)^2 + 4\cdot 0.0093324(\xi_r^j)^3, \tag{4.63}$$

$$\frac{\partial \xi_r^j}{\partial v} = \frac{\partial \xi^j}{\partial v}\sum_{i=1}^{N_{hc}} c_i^j V_{c,i} + \xi^j\sum_{i=1}^{N_{hc}}\frac{\partial c_i^j}{\partial v}V_{c,i}. \tag{4.64}$$

We observe that derivatives of phase mole fractions and densities, obtained with the form (4.54), are involved in the calculation of viscosity derivatives.

### 4.9.2 Source derivatives

Source terms are also differentiated with respect to $v \in (p, \boldsymbol{S}_\mathrm{p}, \boldsymbol{x}_\mathrm{p})$. If the source comes from an injector with constant injection rate,

$$\frac{\partial q_i}{\partial v} = 0, \tag{4.65}$$

while if the source corresponds to a producer with fixed bottom hole pressure,

$$\frac{\partial q_i}{\partial v} = -\sum_{j=1}^{N_\mathrm{p}} \left( \frac{\partial \Lambda_{w,i}^j}{\partial v} T_w \left(p - p_w\right) + \Lambda_{w,i} T_w \frac{\partial p}{\partial v} \right), \tag{4.66}$$

where

$$\frac{\partial \Lambda_{i,w}^j}{\partial v} = \xi^j \frac{k_r^j}{\mu^j} \frac{\partial c_i^j}{\partial v} + c_i^j \frac{k_r^j}{\mu^j} \frac{\partial \xi^j}{\partial v} + c_i^j \xi^j \frac{1}{\mu^j} \frac{\partial k_r^j}{\partial v} - c_i^j \xi^j \frac{k_r^j}{(\mu^j)^2} \frac{\partial \mu^j}{\partial v}. \tag{4.67}$$

Here, the derivatives outlined for the flux terms are used.

## 4.10 Volume Derivatives Module

The reformulation of mass balance equations into volume balance equations, see section 3.4, requires the calculation of derivatives of volumes with respect to $(p, \boldsymbol{n})$. So does the definition

$$\boldsymbol{x}_\mathrm{p} = \boldsymbol{W}_x \, \boldsymbol{n} \tag{4.68}$$

and the reformulation of mass balance equations into additional conservation equations, as the matrix $\boldsymbol{W}_x$ is to be complementary to the matrix

$$\boldsymbol{W}_V = \left( \frac{\partial \boldsymbol{V}}{\partial \boldsymbol{n}} \right)_p \tag{4.69}$$

of partial molar volumes, see Papers B and C.

### 4.10.1 Water volume derivatives

For the water phase, the calculations are quite simple, as

$$V^w = \frac{n_w}{\xi^w}, \tag{4.70}$$

where $\xi^w$ is a function of pressure only, according to (2.35). Consequently,

$$\left( \frac{\partial V^w}{\partial n_w} \right)_p = \frac{1}{\xi^w}, \qquad \left( \frac{\partial V^w}{\partial p} \right)_{n_w} = -\frac{n_w \tilde{\xi^w} c_w}{\left(\xi^w\right)^2}. \tag{4.71}$$

### 4.10.2 Oil and gas volume derivatives

The gas and oil volumes are differentiated with respect to $y \in (p, \boldsymbol{n})$ by

$$\frac{\partial V^j}{\partial y} = \left(\frac{\partial V^j}{\partial p}\right)_{\boldsymbol{n}^j} \frac{\partial p}{\partial y} + \left(\frac{\partial V^j}{\partial \boldsymbol{n}^j}\right)_{p} \frac{\partial \boldsymbol{n}^j}{\partial y}. \tag{4.72}$$

Since

$$V^j = \frac{n^j RT Z^j}{p} \tag{4.73}$$

can be obtained from (2.33), we find that

$$\left(\frac{\partial V^j}{\partial p}\right)_{\mathbf{n}^j} = \frac{n^j RT}{p}\left(\frac{\partial Z^j}{\partial p}\right)_{\mathbf{n}^j} - \frac{n^j RT Z^j}{p^2}. \tag{4.74}$$

$$\left(\frac{\partial V^j}{\partial n_k^j}\right)_{p,\boldsymbol{n}^j_{(k)}} = \frac{RT Z^j}{p} + \frac{n^j RT}{p}\left(\frac{\partial Z^j}{\partial n_k^j}\right)_{p,\boldsymbol{n}^j_{(k)}}, \tag{4.75}$$

where the derivatives of $Z^j$ are given by (4.42). Furthermore, $\partial p/\partial y$ equals unity when $y = p$ and zero when $y \in \boldsymbol{n}$.

To calculate derivatives of $\boldsymbol{n}^j$ with respect to $v \in (p, \boldsymbol{n})$, we utilize the system of equations

$$\begin{bmatrix} \boldsymbol{f}^o - \boldsymbol{f}^g \\ \boldsymbol{n}^o + \boldsymbol{n}^g - \boldsymbol{n} \end{bmatrix} = \mathbf{0}. \tag{4.76}$$

By using expressions similar to (4.72) to differentiate through (4.76) with respect to $v \in (p, \boldsymbol{n})$, we obtain

$$\begin{bmatrix} \frac{\partial \boldsymbol{f}^o}{\partial \boldsymbol{n}^o} & -\frac{\partial \boldsymbol{f}^g}{\partial \boldsymbol{n}^g} \\ \boldsymbol{I} & \boldsymbol{I} \end{bmatrix} \begin{bmatrix} \frac{\partial \boldsymbol{n}^o}{\partial y} \\ \frac{\partial \boldsymbol{n}^g}{\partial y} \end{bmatrix} = \begin{bmatrix} \left(\frac{\partial \boldsymbol{f}^g}{\partial p}\right)_{\boldsymbol{n}^o} \frac{\partial p}{\partial y} - \left(\frac{\partial \boldsymbol{f}^o}{\partial p}\right)_{\boldsymbol{n}^g} \frac{\partial p}{\partial y} \\ \frac{\partial \boldsymbol{n}}{\partial y} \end{bmatrix}, \tag{4.77}$$

where $\boldsymbol{I}$ are unity matrices of suitable dimensions. We observe that the system matrix is independent of $y$, so that only a single inversion is necessary to calculate all derivatives of $\boldsymbol{n}^o$ and $\boldsymbol{n}^g$ with respect to $y$.

We note that (4.76) should be fulfilled whenever the volume derivatives are calculated. Consequently, the phase equilibrium should be solved at every iteration level. This is obtained with the splitted scheme introduced in section 3.3.2.

## 4.11 Iterative Scheme Module

In the iterative scheme module, the primary and secondary equations are solved with respect to the primary and secondary variables by the splitted scheme. The calculations involved in one primary iteration step are:

1. Linearise the mass balance equations, i.e., set up the Jacobian and the right hand side. Reformulate the equations into volume balance equations and additional conservation equations, as shown in Paper C. Total derivatives are required for the linearization, while volume derivatives are required for the reformulation. With $\boldsymbol{r}_{\mathrm{p}}$ denoting the residuals of the reformulated equations, the resulting system can be written

$$\left(\frac{d\boldsymbol{r}_{\mathrm{p}}}{d\boldsymbol{u}_{\mathrm{p}}}\right)^{(k)} \Delta\boldsymbol{u}_{\mathrm{p}}^{(k+1)} = -\boldsymbol{r}_{\mathrm{p}}^{(k)}. \tag{4.78}$$

2. Solve the linear system (4.78) with respect to changes in the primary variables. If an IMPSAT scheme is used, only pressure and saturations changes must be determined simultaneously in all gridblocks, while the variables $\boldsymbol{x}_{\mathrm{p}}$ are determined gridblock by gridblock. XPSIM uses a GMRES linear solver, [45], to solve the part of (4.78) that contains interblock couplings.

3. Keep the primary variables fixed and solve the secondary equations $\boldsymbol{r}_{\mathrm{s}} = \boldsymbol{0}$ with respect to the secondary variables by

$$\left(\frac{\partial\boldsymbol{r}_{\mathrm{s}}}{\partial\boldsymbol{u}_{\mathrm{s}}}\right)^{(l)}_{\boldsymbol{u}_{\mathrm{p}}} \Delta\boldsymbol{u}_{\mathrm{s}}^{(l+1)} = -\boldsymbol{r}_{\mathrm{s}}^{(l)}, \tag{4.79}$$

   until convergence, e.g.,

$$\left\|\frac{\boldsymbol{f}^o - \boldsymbol{f}^g}{\boldsymbol{f}^g}\right\|_\infty^{(l)} < \epsilon_f, \quad \left|\phi V_{\mathrm{b}} S^j - \frac{n^j}{\xi^j}\right|^{(l)} < \epsilon_v, \quad \|\boldsymbol{x}_{\mathrm{p}} - \boldsymbol{W}_x\,\boldsymbol{n}\|_\infty^{(l)} < \epsilon_x. \tag{4.80}$$

   Here, basic derivatives are required, and either exact mass balance or exact volume balance can be obtained, see Paper C.

4. Update primary equation residuals and check for convergence, e.g.,

$$\left\|\frac{\Delta\boldsymbol{n} + (\boldsymbol{f} - \boldsymbol{q})\,\Delta t}{\boldsymbol{n}}\right\|_\infty^{(k)} < \epsilon_c. \tag{4.81}$$

5. In addition, the simulator must keep track of phase disappearance and reappearance during the iteration.

## 4.12 Main Program

The main program governs all the modules described above. In a typical simulation run, XPSIM goes through the following:

1. Read input data and do the preprocessing.
2. Initialize the system at equilibrium.
3. Decide on the size of the next timestep by

$$\Delta t^{n+1} = \Delta t^n \min_u \left[ \frac{(1+\lambda)\Delta u^n}{\Delta u^* + \lambda \Delta u^n} \right], \tag{4.82}$$

   plus timestep restrictions. The initial timestep is required as input.
4. Go through the iterative scheme until convergence.
5. When converged, return to 3., or end the simulation run.
6. If requested, XPSIM gives output of results suitable for analysis and plotting, i.e., gridblock values at certain time levels or with respect to time, injection bottom hole pressures, production rates, etc.

**Note** XPSIM is still under development. Possible extensions include modules for taking input of black-oil fluid properties into account, and implementation of IMPES and AIM schemes. The ideas for further work discussed in Chapter 6 are also a natural part of improving XPSIM.

# Part II

# Papers and Ideas for Further Work

# Chapter 5

# Overview of Papers

This chapter gives an overview of the research papers included in the thesis.

## Paper A

A Black-Oil and Compositional IMPSAT Simulator With Improved Compositional Convergence.
Jarle Haukås, Ivar Aavatsmark and Magne Espedal.
Included in *Proceedings of the 9th European Conference on the Mathematics of Oil Recovery*, Cannes, France, 30 August – 2 September 2004.

Paper A focuses on the development of a unified black-oil and compositional simulator. The objective is to obtain an improved compositional formulation that reduces to a black-oil formulation when used with black-oil fluid properties.

For a unified formulation, pressure and saturations are chosen as primary variables, and the volume balance equations, [9], are used as primary equations. The improvements of the compositional formulation are related to new choices of additional primary equations and variables in an IMPSAT formulation.

The main idea of the paper is that convergence can be improved by the use of additional equations that are complementary to the volume balance equations. Like the volume balance equations, the additional equations are proposed as weighted sums of the component mass balance equations. The notion complementary is related to linear algebra, and involves the choice of equation weights that are orthogonal to the weights of the volume balance method. In addition, weighted sums of phase mole fractions are used as additional primary variables. The choice of mole fraction weights is based on a stability argument.

The results of the paper show some indications of improved convergence. However, the new approach lacks interpretation of the equation weights and mole

fraction weights, and a natural relation between equations and variables. In addition, the interblock flow terms are evaluated with additional variables from the previous iteration level rather than from the previous time level (sequential approach). Further speedup could be expected with a true IMPSAT approach.

The inclusion of an extra implicit variable in the case of an absent hydrocarbon phase is mentioned as an interesting subject of further research. Some ideas in this direction are outlined in section 6.1.

# Paper B

A Volume Balance Consistent Compositional IMPSAT Formulation With Relaxed Stability Constraints.
Jarle Haukås, Ivar Aavatsmark, Magne Espedal and Edel Reiso.
Submitted to *Computational Geosciences*, July 2005.

Paper B gives an extension of the work presented in paper A. Here, interpretation of the additional primary variables and equations is emphasized. Furthermore, a true IMPSAT approach is used, rather than a sequential approach, and a new IMPSAT stability criterion is developed.

A new idea in Paper B is to use the same weights for both equations and variables, and let the weighted variables be component mole numbers rather than phase mole fractions. Then, since the weighted equations are component equations, a natural relation between the additional variables and equations is obtained. The common weights are the equation weights introduced in Paper A.

Thermodynamic analysis shows that the new additional variables represent the part of the system that may change even though pressure and the phase volumes remain fixed. Consequently, the new variables are interpreted as isochoric variables, i.e., volume complementary variables. In addition, the analysis illuminates the fact that the component mole numbers can be decomposed into a volume part (volume projection) and an isochoric part (isochoric projection).

Since a true IMPSAT approach is used, where interblock flow terms are evaluated with isochoric variables from the previous time level, stability is limited. Actually, the isochoric projection of the mole numbers identifies the unstable part. The development of a new IMPSAT stability criterion, based on isochoric projections, is an important contribution to Paper B.

An unresolved issue in the paper is the non-unique definition of the weights used to form isochoric variables and equations. The isochoric interpretation only requires the vectors of weights to form an orthonormal basis for a space. However, since a basis is not unique, the weights are not uniquely defined. Unless some additional conditions on the weight vectors are provided, the weights cannot be differentiated, and must be kept fixed during a timestep.

In the paper, some effort is spent on showing that the actual choice of basis does not affect the calculations if the weights are kept fixed during a timestep. Some new ideas on the definition of weights are outlined in section 6.2.

**Note** In Paper B, the suggested discretization of the time derivative in the mass balance equations is

$$\frac{\partial \boldsymbol{n}}{\partial t} \approx \frac{\partial \boldsymbol{n}}{\partial \boldsymbol{u}_{\mathrm{p}}} \frac{\Delta \boldsymbol{u}_{\mathrm{p}}}{\Delta t} = \frac{\partial \boldsymbol{n}}{\partial p} \frac{\Delta p}{\Delta t} + \frac{\partial \boldsymbol{n}}{\partial \boldsymbol{S}_{\mathrm{p}}} \frac{\Delta \boldsymbol{S}_{\mathrm{p}}}{\Delta t} + \frac{\partial \boldsymbol{n}}{\partial \boldsymbol{x}_{\mathrm{p}}} \frac{\Delta \boldsymbol{x}_{\mathrm{p}}}{\Delta t}, \tag{5.1}$$

where $\Delta \boldsymbol{u}_{\mathrm{p}}$ denotes the change in the primary variables $\boldsymbol{u}_{\mathrm{p}}$ over the timestep $\Delta t$. The same form is mentioned in Paper A, and (5.1) is consistent with the use of

$$\left( V_{\mathrm{b}} \frac{\partial \phi}{\partial p} - \left( \frac{\partial V_{\mathrm{T}}}{\partial p} \right)_{\boldsymbol{n}} \right) \frac{\Delta p}{\Delta t} + \left( \frac{\partial V_{\mathrm{T}}}{\partial \boldsymbol{n}} \right)_{p} (\boldsymbol{f} - \boldsymbol{q}) = 0, \tag{5.2}$$

$$\phi V_{\mathrm{b}} \frac{\Delta S^j}{\Delta t} + \left( \frac{\partial \phi}{\partial p} V_{\mathrm{b}} S^j - \left( \frac{\partial V^j}{\partial p} \right)_{\boldsymbol{n}} \right) \frac{\Delta p}{\Delta t} + \left( \frac{\partial V^j}{\partial \boldsymbol{n}} \right)_{p} (\boldsymbol{f} - \boldsymbol{q}) = 0, \tag{5.3}$$

as discretizations of the volume balance differential equations (3.56) and (3.57).

However, the conventional mass conservative time discretization is

$$\frac{\partial \boldsymbol{n}}{\partial t} \approx \frac{\Delta \boldsymbol{n}}{\Delta t}, \tag{5.4}$$

and a solution obtained with (5.1) may be different from a solution obtained with (5.4), especially for large timesteps.

The basic ideas and results presented in Papers A and B do not rely on the use of (5.1). However, to obtain a solution that is fully consistent with (5.4), an alternative form of the volume balance equations must be used, and the additional primary equations must be adjusted accordingly. A proper reformulation of the mass balance equations which includes (5.4) is given in Paper C.

# Paper C

Exact Volume Balance Versus Exact Mass Balance in Compositional Reservoir Simulation.
Jarle Haukås, Ivar Aavatsmark, Magne Espedal and Edel Reiso.
Submitted to *Computational Geosciences*, December 2005.

Paper C deals with different reformulations of the mass balance equations, including the weighted sums encountered in Paper A and Paper B. The reformulations may be used to obtain either exact mass balance or exact volume balance.

The background for Paper C is the observation that a combined volume/isochoric balance requirement is a consistent alternative to the conventional mass balance requirement. Consequently, the isochoric variables and equations illuminate the difference between exact mass balance and exact volume balance.

The equations of the volume balance method, [9], are a natural part of the discussion. By an extended version of the original volume balance method, the conventional mass balance,

$$\Delta \boldsymbol{n} + (\boldsymbol{f} - \boldsymbol{q})\,\Delta t = \boldsymbol{0}, \tag{5.5}$$

is imposed by a direct (exact) update of the mole numbers, while volume/isochoric discrepancies govern the iterative scheme. Alternatively, a modified form of the volume balance equations can be used, where volume balance is imposed directly (exactly), while mass balance discrepancies govern the iterative scheme. Details are provided in the paper.

Paper C also gives a comparison of the performance of an exact mass balance scheme to the performance of an exact volume balance scheme. The numerical results are in favour of exact volume balance, but it is noted that the conclusion may be implementation dependent. However, the important part of the paper is the volume/isochoric reformulation of the mass balance equations and the clarification of the difference between exact volume balance and exact mass balance.

# Paper D

A Comparison of Two Different IMPSAT Models in Compositional Simulation.
Jarle Haukås, Ivar Aavatsmark, Magne Espedal and Edel Reiso.
Submitted to *SPE Journal*, December 2005.

Paper D is a comparison paper. Here, the IMPSAT formulation with isochoric variables and equations presented in Papers B and C is compared to an IMPSAT formulation with phase mole fractions and a selection of component conservation equations as the additional variables and equations, [15, 16].

A key issue in the paper is that the isochoric IMPSAT approach allows for a consistent update of interblock flow terms, and thereby quadratic convergence of the Newton-Raphson iterative scheme. In addition, the stability criteria of the two IMPSAT formulations are compared.

Numerical results indicate that the consistent update of interblock flow terms may improve the convergence significantly, and that the stability criterion of Paper B may allow for significantly larger timesteps. However, retrograde gas condensate cases impose particular severe stability limitations on the isochoric IMPSAT formulation. Here, the interpretation of the isochoric variables presented

in Paper B is useful. For retrograde gas condensate cases, the isochoric part experiences more rapid changes compared to the volumetric part than for other cases. The corresponding stability limitations are therefore reasonable.

Improving the stability of IMPSAT by explicit treatment of other variables than the isochoric variables is an interesting subject of further research. A brief comment in this direction is given in section 6.3.

# Paper E

Isothermal Gravity/Chemical Equilibrium Calculations.
Jarle Haukås and Sverre Gullikstad Johnsen.
Exam report for the summer school
*Thermodynamic Models: Fundamentals and Computational Aspects*,
IVC-SEP, Technical University of Denmark, August 9 – 27, 2004. Evaluated and accepted by Professors M. L. Michelsen and J, M. Mollerup at IVC-SEP.

Paper E is a report on gravity/chemical equilibrium calculations, and is associated with an assignment given at the IVC-SEP Summer School 2004, at the Technical University of Denmark. The assignment was to implement a computer program for determining the pressure and phase composition above and below a given reference depth in a reservoir fluid column, and for determining whether a gas-oil contact could exist within a specified depth range in the column.

In the paper, the conditions for steady state phase equilibrium in a gravity field are derived. Furthermore, different aspects of gravity/chemical equilibrium calculations are discussed, including phase stability analysis and saturation point calculations. Phase stability tests are used to discover two-phase gas-oil interfaces, which correspond to a saturated gas-oil contact. Saturation point calculations are necessary to discover undersaturated gas-oil contacts, for which no two-phase behaviour can be observed. In addition, a Newton-Raphson scheme and various successive substitution schemes for solving the equations are presented.

The paper provides useful guidelines for initialization of a reservoir system under the influence of gravity. In addition, the presented plots give insight into the thermodynamic interpretation of gas-oil contacts.

# Chapter 6

# Ideas for Further Work

This chapter contains some ideas for further work, stemming from the research papers included in the thesis.

## 6.1 Extra Implicit Undersaturated Variable

The development of a unified black-oil and compositional simulator is an important issue in the research papers. For a compositional IMPSAT formulation that reduces to a fully implicit black-oil formulation in the saturated black-oil case, the key is to use pressure and saturations as implicit primary variables.

However, for undersaturated oil, the solution gas/oil ratio $R_s$ is included as an implicit variable in the conventional black-oil formulation, and so is the the vaporized oil/gas ratio $R_v$ in the supercritical/undersaturated gas case. Here, the conventional IMPSAT formulation still only treats pressure and saturations implicitly. An extended IMPSAT formulation that reduces to a fully implicit black-oil formulation regardless of the black-oil fluid properties, must include an extra implicit variable in the undersaturated oil and supercritical/undersaturated gas cases.

A possible approach is to define the extra implicit variable in the form

$$R = \boldsymbol{\omega}^{\mathrm{T}} \boldsymbol{n}, \tag{6.1}$$

where $\boldsymbol{\omega}$ is a $N_{\mathrm{c}}$ vector of weights. Furthermore, we could set up the $(N_{\mathrm{p}}+1)\times N_{\mathrm{c}}$ matrix

$$\boldsymbol{W}_V^+ = \begin{bmatrix} \left(\frac{\partial \boldsymbol{V}}{\partial \boldsymbol{n}}\right)_p \\ \boldsymbol{\omega}^{\mathrm{T}} \end{bmatrix}, \tag{6.2}$$

and determine the variables other than pressure, saturations and the extra implicit variable $R$ by

$$\boldsymbol{x}_{\mathrm{p}}^+ = \boldsymbol{W}_x^+ \boldsymbol{n}, \tag{6.3}$$

where the $(N_\mathrm{c} - N_\mathrm{p} - 1) \times N_\mathrm{c}$ matrix $\boldsymbol{W}_x^+$ is complementary to $\boldsymbol{W}_V^+$. With such an approach, the variable $R$ fits into the framework presented in Paper B, and the ideas of Paper B may be used to propose a modified stability criterion for explicit treatment of the variables $\boldsymbol{x}_\mathrm{p}^+$.

If used with black-oil fluid properties, $R$ should reduce to the solution gas/oil ratio for undersaturated oil and to the vaporized oil/gas ratio for supercritical/undersaturated gas. However, for an undersaturated compositional case, $R$ could be used to increase the stability of the extended IMPSAT formulation. For instance, we could let $R$ represent the least stable part of the isochoric variations in the system. This part could possibly be identified by its large contribution to the timestep restriction presented in Paper B.

## 6.2 Unique/Explicit Definition of Weights

In Paper B, the isochoric variables are defined by

$$\boldsymbol{x}_\mathrm{p} = \boldsymbol{W}_x \, \boldsymbol{n}, \tag{6.4}$$

where the $(N_\mathrm{c} - N_\mathrm{p}) \times N_\mathrm{c}$ matrix $\boldsymbol{W}_x$ is complementary to the $N_\mathrm{p} \times N_\mathrm{c}$ matrix

$$\boldsymbol{W}_V = \left( \frac{\partial \boldsymbol{V}}{\partial \boldsymbol{n}} \right)_p, \tag{6.5}$$

i.e., the rows of $\boldsymbol{W}_x$ form an orthonormal basis for the nullspace of $\boldsymbol{W}_V$. We note that

$$\boldsymbol{V} = \boldsymbol{W}_V \, \boldsymbol{n}, \tag{6.6}$$

since volumes are homogeneous functions of first degree in the mole numbers.

The definition of the matrix $\boldsymbol{W}_V$ is unique, as the partial molar volumes can be calculated from

$$V^j = V^j \left( p, \boldsymbol{n^j} \right) = \frac{n^j}{\xi^j}, \tag{6.7}$$

taking the phase equilibrium conditions (2.30) into account, see section 4.10. However, the definition of $\boldsymbol{W}_x$ is not unique. As noted in Paper B, the requirement that the rows of $\boldsymbol{W}_x$ should form an orthonormal basis for the nullspace of $\boldsymbol{W}_V$ corresponds to $(1/2)\,(N_\mathrm{c} - N_\mathrm{p})\,(N_\mathrm{c} + N_\mathrm{p} + 1)$ conditions on the $(N_\mathrm{c} - N_\mathrm{p})\,N_\mathrm{c}$ elements of $\boldsymbol{W}_x$. Consequently, $(1/2)\,(N_\mathrm{c} - N_\mathrm{p})\,(N_\mathrm{c} - N_\mathrm{p} - 1)$ conditions remain unspecified. We note that the number of unspecified conditions corresponds to one relation for each pair of rows in $\boldsymbol{W}_x$.

Evidently, to obtain a unique definition of $\boldsymbol{W}_x$, we could look for a specification of the remaining conditions. However, even if a set of such relations is found,

the resulting $(N_\mathrm{c} - N_\mathrm{p})\, N_\mathrm{c}$ conditions are nonlinear in the elements of $\boldsymbol{W}_x$, and an iterative solution is required to determine $\boldsymbol{W}_x$.

An alternative idea is to seek an explicit relation

$$\boldsymbol{x}_\mathrm{p} = \boldsymbol{x}_\mathrm{p}\left(p, \boldsymbol{n^j}\right), \tag{6.8}$$

defining $\boldsymbol{x}_\mathrm{p}$ as a homogeneous functions of first degree in the mole numbers, i.e.,

$$\boldsymbol{x}_\mathrm{p} = \left(\frac{\partial \boldsymbol{x}_\mathrm{p}}{\partial \boldsymbol{n}}\right)_p \boldsymbol{n}. \tag{6.9}$$

With such an approach, the matrix $\boldsymbol{W}_x$ would be uniquely defined by

$$\boldsymbol{W}_x = \left(\frac{\partial \boldsymbol{x}_\mathrm{p}}{\partial \boldsymbol{n}}\right)_p. \tag{6.10}$$

The explicit relation (6.8) could possibly be based on an equation of state relation, and should take the phase equilibrium into account. In addition, it should be consistent with the interpretation of the variables $\boldsymbol{x}_\mathrm{p}$ as isochoric variables. Here, thermodynamic analysis is necessary.

It is not clear if the requirement that the matrices $\boldsymbol{W}_x$ and $\boldsymbol{W}_V$ should be complementary can be made inherent in an explicit relation of the form (6.8). In any case, great care must be taken to ensure that the $N_\mathrm{c} \times N_\mathrm{c}$ matrix

$$\begin{bmatrix} \boldsymbol{W}_V \\ \boldsymbol{W}_x \end{bmatrix} = \begin{bmatrix} \left(\frac{\partial \boldsymbol{V}}{\partial \boldsymbol{n}}\right)_p \\ \left(\frac{\partial \boldsymbol{x}_\mathrm{p}}{\partial \boldsymbol{n}}\right)_p \end{bmatrix} \tag{6.11}$$

is non-singular.

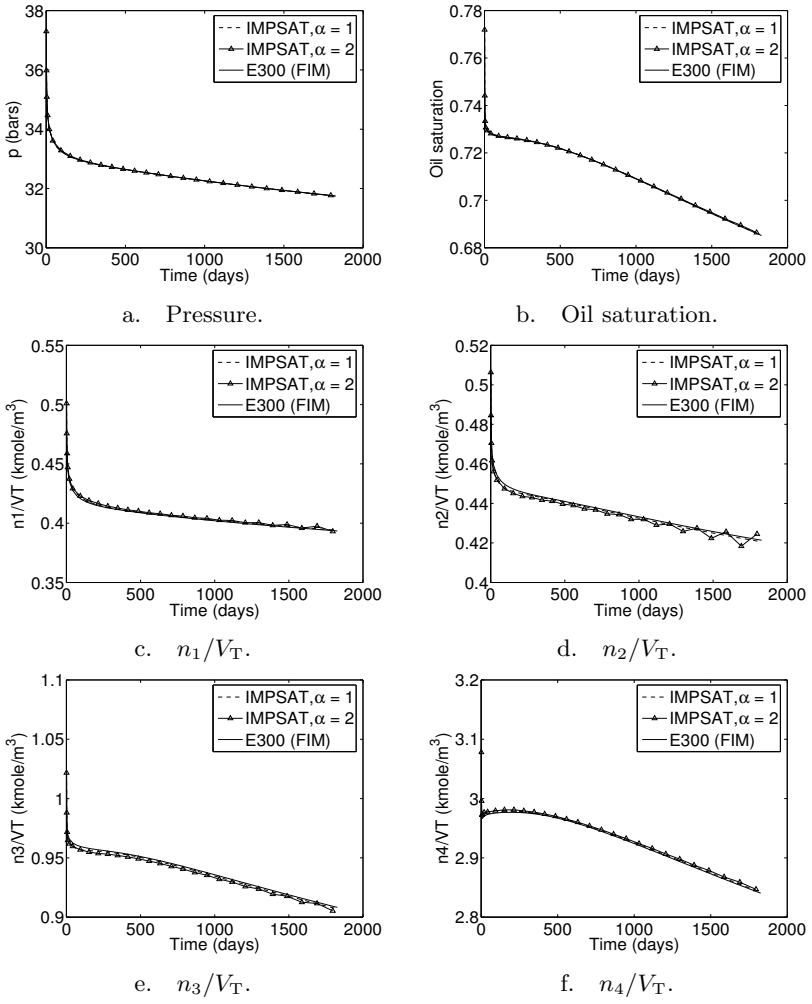
## 6.3 Stability Considerations

In Paper D, it is noted that the stability limitations due to explicit treatment of isochoric variables are especially severe in retrograde gas condensate cases. This suggests that the stability of IMPSAT in such cases can be improved by explicit treatment of variables $\boldsymbol{x}_\mathrm{p}$ that are not isochoric variables.

Generally, we could still use the definition

$$\boldsymbol{x}_\mathrm{p} = \boldsymbol{W}_x\, \boldsymbol{n}. \tag{6.12}$$

However, instead of defining the variables $\boldsymbol{x}_\mathrm{p}$ as isochoric variables, we could look for variables $\boldsymbol{x}_\mathrm{p}$ that yield the optimal IMPSAT stability. The stability properties of different choices of $\boldsymbol{x}_\mathrm{p}$ could be evaluated by the corresponding IMPSAT stability criterion, e.g., a criterion similar to the one proposed in Paper B.




a. Pressure. b. Oil saturation.

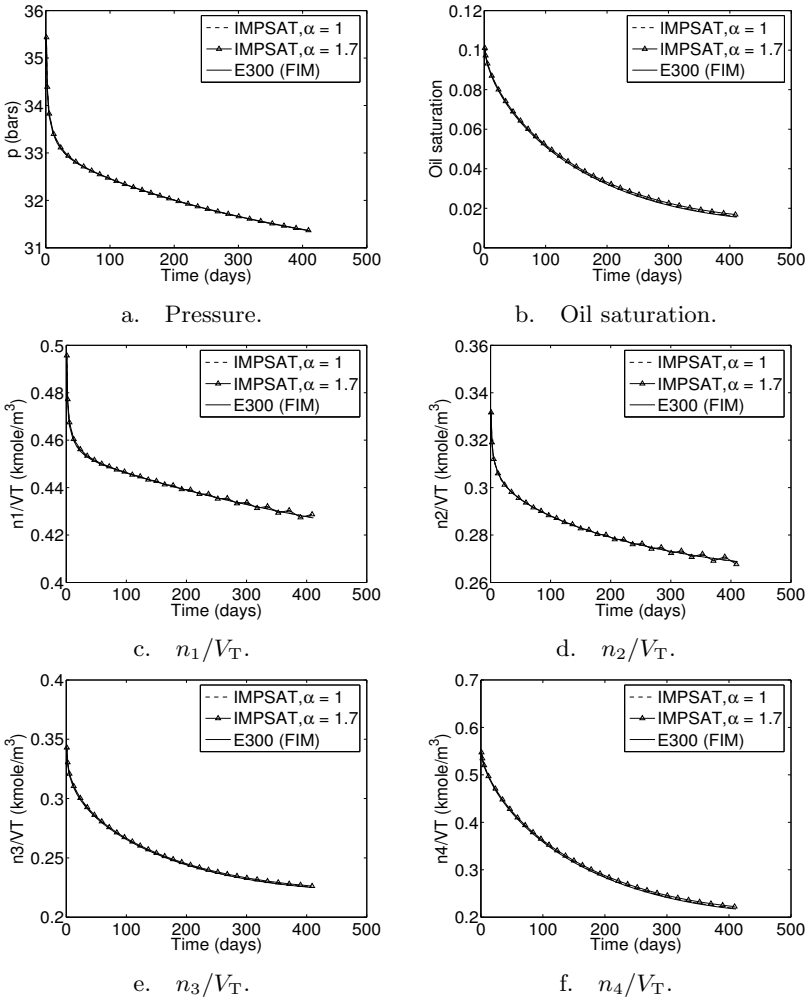
c. $n_1/V_{\mathrm{T}}$. d. $n_2/V_{\mathrm{T}}$.

e. $n_3/V_{\mathrm{T}}$. f. $n_4/V_{\mathrm{T}}$.

*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.




a. Pressure. b. Oil saturation.

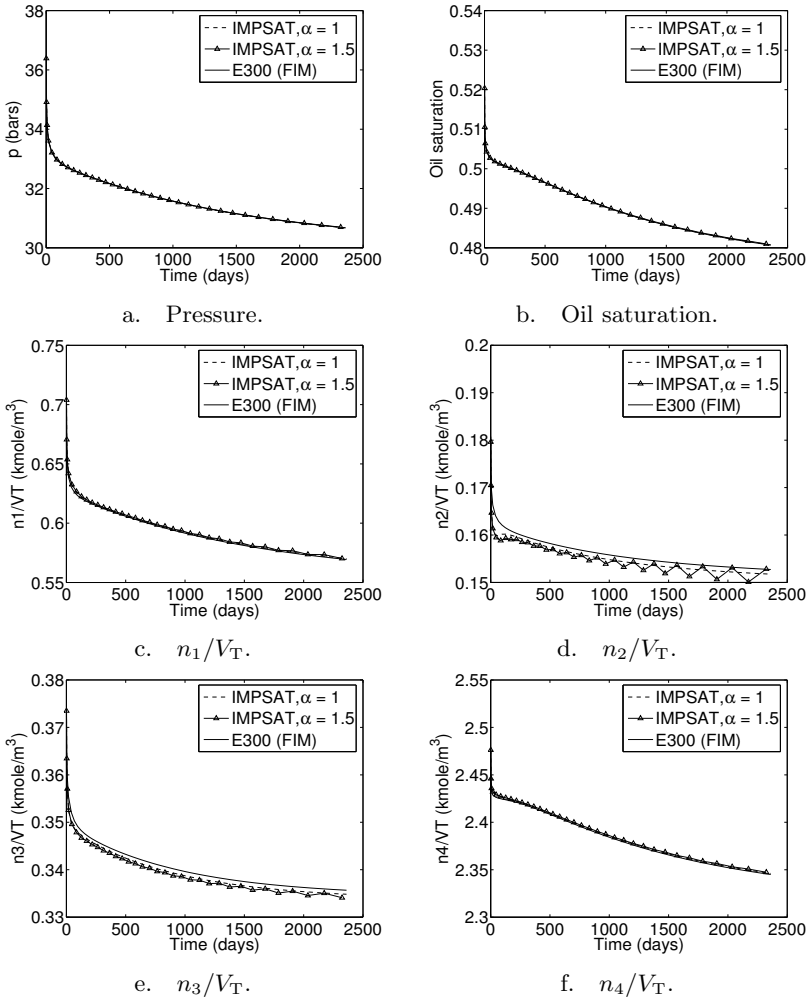
c. $n_1/V_{\mathrm{T}}$. d. $n_2/V_{\mathrm{T}}$.

e. $n_3/V_{\mathrm{T}}$. f. $n_4/V_{\mathrm{T}}$.

*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.




a. Pressure. b. Oil saturation.

c. $n_1/V_{\mathrm{T}}$. d. $n_2/V_{\mathrm{T}}$.

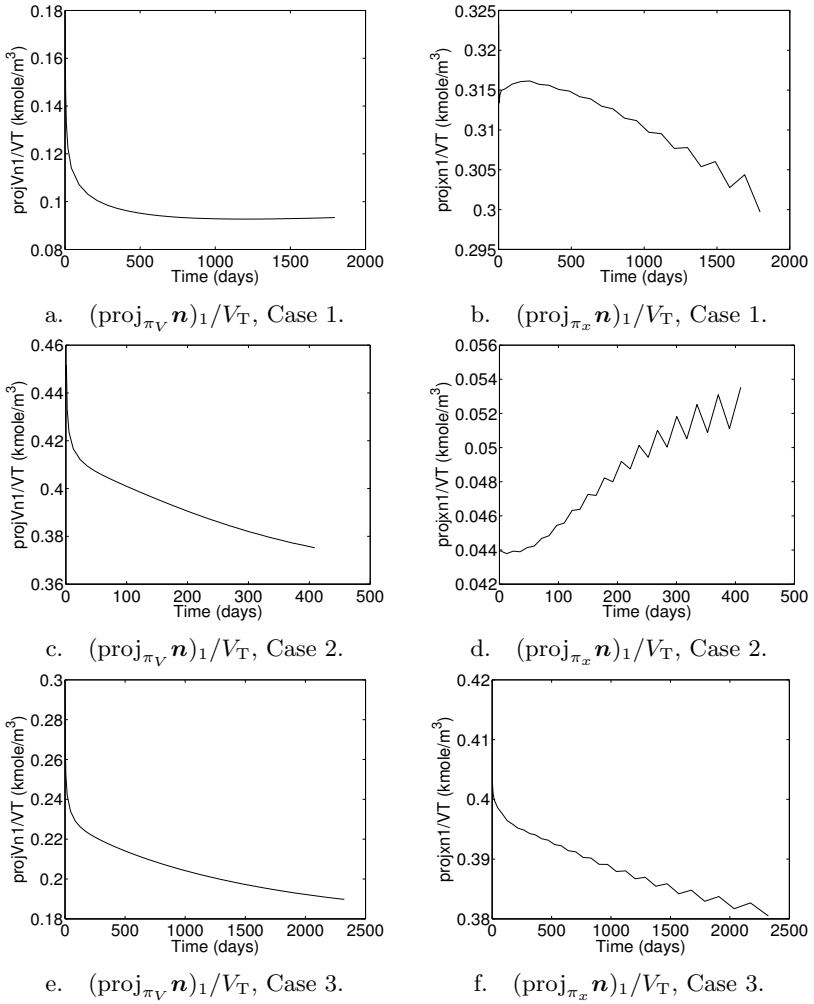
e. $n_3/V_{\mathrm{T}}$. f. $n_4/V_{\mathrm{T}}$.

*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.




a. $(\mathrm{proj}_{\pi_V}\boldsymbol{n})_1/V_\mathrm{T}$, Case 1. b. $(\mathrm{proj}_{\pi_x}\boldsymbol{n})_1/V_\mathrm{T}$, Case 1.

c. $(\mathrm{proj}_{\pi_V}\boldsymbol{n})_1/V_\mathrm{T}$, Case 2. d. $(\mathrm{proj}_{\pi_x}\boldsymbol{n})_1/V_\mathrm{T}$, Case 2.

e. $(\mathrm{proj}_{\pi_V}\boldsymbol{n})_1/V_\mathrm{T}$, Case 3. f. $(\mathrm{proj}_{\pi_x}\boldsymbol{n})_1/V_\mathrm{T}$, Case 3.

*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 $i$,

$$f_i = \left(\mathrm{proj}_{\pi_V}\boldsymbol{f}\right)_i + \left(\mathrm{proj}_{\pi_x}\boldsymbol{f}\right)_i, \tag{83}$$

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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