THERMAL ADAPTIVE IMPLICIT RESERVOIR SIMULATION

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Abstract

The Fully Implicit Method (FIM) is widely used in numerical reservoir simulation due to its unconditional stability, which allows for arbitrarily large time steps. However, FIM is computationally expensive per time step, especially for large numbers of components and highly detailed reservoir models. IMPEST (Implicit Pressure, Explicit Saturations, Temperature and mole fractions), on the other hand, is computationally inexpensive, but only conditionally stable. For large-scale heterogeneous models, the allowable stable time step of IMPEST may be extremely small. In the Adaptive Implicit Method (AIM), only a subset of the primary variables is treated implicitly. AIM offers a balance between FIM and IMPEST by employing implicit treatment only when and where necessary. The challenge with AIM is to: (1) find robust and sharp stability criteria that can be used to choose an optimal time step size, and (2) devise an efficient switching algorithm to dynamically label variables in gridblocks implicit or explicit.

The objective of this thesis is to formulate, implement, and validate an efficient Thermal Adaptive Implicit Method (TAIM) that is capable of solving the nonlinear system of algebraic equations efficiently using the minimum number of implicit variables for a given time step. TAIM includes the stability criteria for the selection of the time step size and a switching algorithm to label the variables as either implicit or explicit.

The TAIM stability criteria are obtained using the von Neumann approach. The derivation of the criteria is obtained using a comprehensive linear stability analysis that takes into account the complex physics being modeled, including mass and heat convection, thermal conduction, phase change, and gravity. The criteria were implemented and evaluated using Stanford’s General Purpose Research Simulator (GPRS). The stability criteria serve as an input to a switching algorithm that calculates the maximum possible time step size for which a stable solution for explicit saturation, temperature, and compositions in a gridblock is
guaranteed. We implemented two switching algorithms in GPRS, namely, percentage-based and variable-based. In the percentage-based approach, the user specifies the percentage break-up between various implicit schemes. Since an arbitrary percentage break-up in difficult problems can lead to extremely small time steps, thereby rendering the TAIM method infeasible, a more optimal solution is for the user to specify a desired time step size, and let the TAIM switching algorithm decide on the implicit/explicit labeling of variables in the gridblocks. We formulated this algorithm and refer to this approach as the variable-based TAIM.

We demonstrate that a TAIM-based approach is a promising technique for the simulation of thermal-compositional displacement processes of practical interest. TAIM simulations are not only more accurate than their FIM counterparts due to reduced numerical diffusion, but TAIM also offers an efficient numerical simulation method that uses time steps comparable to those used in FIM, while treating a large subset of the variables explicitly. In this thesis, we derive the thermal-compositional stability criteria that provide the CFL (Courant-Friedrichs-Lewy) numbers to obtain the maximum allowable time steps. The criteria are used in conjunction with a variable-based switching algorithm that labels the variables as implicit/explicit, which can vary both in space and time. We found the stability criteria to be sharp, i.e., when convection is the dominant mechanism, mild violations of the stability limits lead to unstable solutions both in the saturation and temperature profiles. In our numerical experiments, small violations of the CFL numbers lead to significant deviations from the reference solutions; for larger CFL violations, severe oscillations were observed in the explicit variables. When thermal conduction is dominant over convection, the stability criteria restrict the allowable time steps to impractically small values, when temperature is treated explicitly. The variable-based TAIM method accurately captures the countercurrent shocks and their reflection in the gravity segregation problems by treating the saturation around sharp gradients implicitly. TAIM is effective in reducing the number of implicit variables considerably from the fully implicit set, and it allows the use of time steps that are comparable to FIM for large problems.
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Chapter 1

Introduction

Conventional primary and secondary recovery operations often leave two thirds of the oil in the reservoir. In the United States, Enhanced Oil Recovery (EOR) methods have the potential to recover an estimated 200 billion barrels of the remaining oil resource [3]. EOR processes involve injecting a fluid into the reservoir to increase reservoir pressure, or reduce oil viscosity, in order to mobilize the oil. Injectants include steam (thermal processes), polymers and gels (chemical processes), carbon dioxide, nitrogen, and natural gas (gas processes). Gas injection and thermal recovery by steam injection are the most utilized EOR processes [40], [41], [2].

Oil and gas field development projects require significant investment of up-front capital to drill wells and build facilities for fluid processing. Investment decisions are often made with limited data and considerable uncertainty in the reservoir parameters. Reservoir simulation has become a standard industry tool for evaluating the effects of uncertainty on field performance and investment requirements. Management decision makers require reservoir simulation studies to support decisions on large capital investment. Reservoir simulation is used throughout the life cycle of a field from making early investment decisions to developing plans to optimize field performance at later stages of development. Efficient numerical techniques are required to enable effective application of reservoir simulation. Numerical reservoir simulation involves simultaneous solution of the nonlinear governing equations that account for the various physical behaviors in the reservoir.

The governing equations that describe multiphase flow in reservoirs are nonlinear and coupled. The discrete form of the equations can be represented as an algebraic system of
equations, which are linearized using the Newton method. The matrix of the linearized system is called the Jacobian, and the RHS consists of the residual vector. In the Fully Implicit Method (FIM), all the primary variables are treated implicitly. To further reduce the cost of simulation, we can treat some primary variables explicitly and reduce the number of implicit unknowns per gridblock. Normally, such models are much more computationally efficient than FIM models, especially for highly detailed models with large numbers of components. However, explicit treatment of some primary variables limits the maximum time step size that can be used. The solution of nonlinear fluid flow problems in reservoirs using FIM is unconditionally stable, but computationally expensive per time step. The IMPEST method (Implicit Pressure, Explicit Saturation, and Temperature), on the other hand, decouples the pressure equation and solves it implicitly. The pressure solution is then used to obtain the saturations and temperature explicitly, cell by cell. IMPEST is computationally inexpensive, but only conditionally stable, and the maximum stable time step can be extremely small. When it is stable, IMPEST yields a more accurate solution of the saturation distribution and breakthrough times compared with FIM, because it has less numerical dispersion. A variation of the IMPEST method is the IMPTES (Implicit Pressure and Temperature, Explicit Saturation) method, where pressure and temperature are treated implicitly, and the saturations (and compositions) are subsequently updated explicitly.

The Thermal Adaptive Implicit Method (TAIM) is a reservoir simulation method that treats some primary variables as implicit and others as explicit. In other words, on a gridblock basis, TAIM treats some gridblocks using FIM, while the others are treated with IMPEST, or IMPTES. For example, flow around a wellbore requires rigorous analysis, since large changes in pressure, saturation, and temperature take place in the vicinity of the well. In contrast, changes away from wells tend to be small enough, such that using FIM is a waste of computational effort. In such regions, the IMPEST method should suffice. TAIM attempts to find a balance between the FIM, IMPTES and IMPEST schemes in order to yield solutions that are both accurate and efficient. TAIM is conditionally stable, and its time steps can be controlled using the linear stability criteria described in this work.


1.1 Objectives

The objective of this thesis is to formulate, implement, and validate an efficient Thermal Adaptive Implicit Method (TAIM) for thermal-compositional reservoir simulation. The TAIM framework must be capable of solving the nonlinear system of equations with the smallest set of implicit variables, while taking into account the complex physics in the reservoir. The decision to label a variable in a gridblock as implicit or explicit is made using stability criteria and a switching algorithm. The key goals of this thesis are:

1. Formulation of thermal-compositional stability criteria and the development of a variable-based switching algorithm: The goal is to derive comprehensive stability criteria for thermal-compositional flows, extensible to multiple dimensions, and that account for all the major mechanisms governing fluid flow, namely, viscous, capillary, buoyancy, as well as, heat convection and conduction. In addition, an efficient approach for labeling the gridblock variables as implicit or explicit is required at each time step.

2. Implementation of TAIM in GPRS: Stanford’s General Purpose Research Simulator (GPRS) [11], [25], [26] is an actively used research platform for petroleum reservoir simulation. As part of this research, the goal is to extend GPRS for Thermal AIM, which includes implementation of the stability criteria and effective switching algorithms that use the criteria to decide on the time step size.

3. Validation of the criteria for complex thermal-compositional recovery processes: The stability criteria depend on complex nonlinear physical behaviors. The goal of the thesis is to validate the derived stability criteria using several test cases that capture the complex behaviors associated with thermal-compositional displacements.

1.2 Thesis Contributions

Stability Criteria and Switching Algorithm Formulation

The stability conditions are derived using the von Neumann method [44], [23], [29], which has been used to analyze isothermal systems [9], [15], [16], [17], [22], [38], [46]. The von Neumann method tests the linear stability of the discretization with respect to time. Even though thermal-compositional simulation involves highly complex nonlinear physical behaviors, the
derived linear-stability criteria serve as a necessary requirement for the stability of the discrete nonlinear problem. The linear-stability criteria account for all major mechanisms governing thermal-compositional fluid flow. The criteria are easily extensible to multiple dimensions and reduce to the isothermal stability criteria given by Coats [16]. We obtain the stable limit for each variable, and this is used in a switching algorithm for adaptive implicit simulation. The derived stability conditions are tested using a simple MATLAB-based simulator [33], [6] and the General Purpose Research Simulator (GPRS) [11], [25], [26] using thermal and isothermal test cases involving complex physical behaviors.

In addition to the stability criteria, we developed a variable-based TAIM technique that employs a user specified time step size, and depending on the stability limit of each variable in each gridblock, the variable is labeled implicit or explicit. This method is particularly effective in large-scale thermal-compositional applications, where different parts of the reservoir are dominated by different mechanisms, e.g., conduction or convection. The variable-based approach avoids the stringent stability restrictions (i.e., severe limits on the time step size) associated with explicit treatment of temperature in conduction dominated systems.

**TAIM Implementation in GPRS**

GPRS is a general-purpose research tool for reservoir simulation. GPRS is currently capable of handling all major mechanisms of isothermal multi-component, multiphase flow, namely, convection, capillarity, gravity and compressibility. GPRS can solve the reservoir simulation model fully implicitly for any number of phases but has been limited to two-phase flows for adaptive implicit solutions. GPRS supports the energy-balance equation for thermal systems [45] and has the capability to run thermal-compositional simulations with heat conduction.

As part of this research, we have added modules to implement TAIM (Thermal Adaptive Implicit Method), which compute the CFL numbers at each time step for each explicit variable and implement the corresponding switching algorithm. As a result of this work, GPRS is now capable of running TAIM simulations with up to three phases, given a fixed percentage of the various implicit-level schemes or a user-specified time step, with fluid and heat convection, and heat conduction. The gridblock assignment to different levels of
implicitness can be also decided on a fixed percentage-basis or using an improved variable-based strategy. The different levels of implicitness are: (i) only pressure is implicit; (ii) both pressure and temperature are implicit with explicit saturations and compositions; (iii) both pressure and saturations are implicit with explicit temperature and compositions; and (iv) pressure, temperature, saturations are implicit with only compositions explicit.

Validation for Complex Physics in Reservoirs

The thermal stability criteria depend on the nature of the nonlinear physical processes in the system. These include, but are not limited to, fluid and heat convection, thermal conduction, phase change phenomena, gravity effects, and capillarity. The factors affecting fluid convection primarily are (i) the fractional flow curves which include relative permeability and viscosity relations; and (ii) permeability. Heat convection, in addition to the parameters for fluid convection, also depends on (i) fluid density and (ii) fluid heat capacity. Thermal conduction is affected by (i) rock heat capacity and (ii) conduction of the porous medium. Phase change phenomena are observed while modeling (i) solution gas for black oil systems; and (ii) vapor-liquid equilibrium behavior of compositional problems. Gravitational effects can be dominant when there is a large contrast in fluid densities. Each of the parameters – permeability, relative permeability, fluid and rock heat capacities, densities and conduction transmissibility – vary in space and time with pressure, temperature, fluid saturations, and compositions (mole fractions). This makes the system of equations highly coupled and nonlinear. The stability criteria derived from the set of governing equations thus depend on all of the above factors and are complicated due to the coupled nature of the system of equations.

We validate the accuracy of the derived thermal stability criteria using synthetic test cases in one-dimension using a MATLAB simulator [7]. In these tests, we studied the effect of violating the Courant-Friedrichs-Lewy (CFL) [18] criteria for saturation and temperature on computed numerical solutions. For small violations of the saturation CFL (CFLS) criterion, we observed small deviations from the fully implicit water saturation ($S_w$) front. For large violations of CFLS, we observed oscillations around the saturation front leading to non-monotonic and physically unacceptable results.

We extended GPRS to employ TAM. For that purpose, we applied the thermal stability criteria and the percentage-based and the variable-based switching algorithms to Thermal
GPRS. The validation is performed using one- and two-dimensional test cases that incorporate fluid and heat convection, heat conduction, temperature dependent fluid densities and viscosities, constant rock and fluid heat capacities. Black-oil and compositional problems were tested as part of this effort. We studied the $S_{iw}$ fronts for various schemes such as FIM (fully implicit method), IMPEST (only pressure implicit) and TAIM, and we compared their time stepping behaviors for stable solutions. Thermal conduction is best studied in 2-D, where it is easy to distinguish between the effects of conduction and convection in the reservoir. In 2-D thermal displacement problems, we observed that in regions where conduction is more dominant compared to convection, strict conditions on explicit treatment of temperature can lead to very small (global) time steps. Therefore, when thermal conduction is high compared to convection, temperature should be treated implicitly using a variable-based switching algorithm.

1.3 Outline of the Thesis

The thesis is organized as follows: Chapter 2 describes related work. Chapter 3 covers the mathematical formulation of the governing equations including the derivation of the stability criteria using the von Neumann method. Details of the percentage-based and the variable-based switching algorithms are covered in Chapter 4. The implementation details of the criteria and switching algorithms are described in Chapter 5, which also briefly summarizes the relevant GPRS details. Chapter 6 describes the results and explains the major findings of this investigation. The tests were designed in order to study the accuracy of the thermal stability criteria for various physical mechanisms. The thesis concludes with Chapter 7 summarizing the conclusions and future recommendations for TAIM simulation research.
Chapter 2

Related Work

Adaptive implicit methods were first used in reservoir simulation in 1983 through the work of Thomas and Thurnau [43]. In their work, they developed the mathematical procedure that involves labeling some variables as implicit while others are classified as explicit. The method provides a changing level of implicitness from explicit to implicit (but not vice versa) in space and time and is done on a cell-by-cell basis. They used user supplied threshold criteria, which did not assess the stability of the discretization. They presented the savings in computational time and storage using a black-oil model example.

Forsyth and Sammon [20] noted that the criteria presented by Thomas and Thurnau for selecting implicit cells are not straightforward. They presented methods utilizing different degrees of implicitness on a cell by cell basis, and they developed an iterative matrix solution technique for the adaptive implicit Jacobian using incomplete LU factorization. Forsyth and Sammon showed that an approximate Jacobian can be constructed, which could be used to solve the fully implicit system, instead of using the fully implicit Jacobian. They showed significant computing time reductions.

Russell [38], developed a switching criterion for black-oil models based on the CFL stability condition that determines whether an unknown is implicit or explicit. Further, the CFL criterion was also used for time step control in IMPES models and was extensible to compositional simulation. It was observed that AIM provided more accurate answers than FIM through the reduction of numerical dispersion. In that work, pressure was treated implicitly owing to the near elliptic nature of the equation, whereas saturations and compositions were treated explicitly where possible, as the equations are near hyperbolic in nature.
Russell extended the one-dimensional problem to multiple space dimensions, and obtained the multi-dimensional CFL condition in terms of the one-dimensional CFL numbers.

Grabenstetter et al. [22], extended Russell’s CFL based criteria to compositional reservoir simulation. They derived the criteria for the case of a single spatial dimension and no capillary pressure. Subsequently, they showed the effect of capillarity as deviations from hyperbolicity of the conservation law. Grabenstetter et al. [22] concluded that the parabolic character introduced to the set of equations does not pose any deficiency as far as the derivation of the criteria is concerned. For multiple dimensions, they employed a different form of the criteria compared to the one presented by Russell.

Young and Russell [47] applied AIM to compositional simulation and observed that greater efficiency is obtained when less than 5 percent of the gridblocks are treated implicitly. The switching logic was based on the CFL analysis of Russell [38]. Young and Russell tested various problems and concluded that AIM did not show dramatic efficiency improvement compared with IMPES, but that AIM is a good alternative to FIM for problems where IMPES is inadequate. They also concluded that AIM appears to benefit compositional models more than black-oil models.

Coats [15] derived stability criteria for multidimensional three-phase flow for black-oil and compositional models. The criteria could be used to set the time steps for IMPES or as switching criteria for AIM. The criteria accounted for three-phase flow, including capillarity, gravity and viscous forces with cocurrent and countercurrent flow configurations. Coats expressed the stability conditions in terms of a function, $F_i$, which had a different expression for different flow mechanisms. He distinguished between oscillatory and non-oscillatory stability depending upon the CFL numbers being larger or smaller than unity, respectively. Coats [17] concluded that for reservoir problems, non-oscillatory stability is required.

Cao, in his Ph.D dissertation [11], developed techniques for general purpose simulation. He developed the first version of GPRS, the General Purpose Reservoir Simulator, where he proposed and implemented new AIM techniques that make use of FIM, IMPSAT (implicit pressure and saturation, explicit compositions) and IMPES combinations. Today, GPRS is a general purpose reservoir simulator that can handle both black-oil and compositional models for isothermal simulation on unstructured grids [26]. Cao and Aziz [12] developed the IMPSAT related stability criteria for isothermal compositional simulations using a CFL
based approach. Their criteria reduce to Coats’ analysis [15] for explicit mole fractions.

Wan et al. [46] presented general stability criteria for compositional and black-oil models taking into account all of the major mechanisms governing fluid flow, i.e., convection, diffusion, capillary forces, gravity, fluid and rock compressibility, vapor-liquid equilibrium in compositional models and solubility in black-oil models. The black-oil model was treated as a special case of the compositional model.

The stability criteria for this research on Thermal AIM are derived using the von Neumann method, which is a linear stability analysis based on Fourier series expansions. The CFL-condition (Courant-Friedrichs-Lewy condition) is commonly used to denote the stability criteria for linear hyperbolic systems of equations. Even though our equations are not strictly hyperbolic, we will refer to the stability criteria using the term CFL. The stability analyses performed by Russell [38], [47], Grabenstetter et al. [22], Coats [16], [17], Cao and Aziz [11], and Wan et al. [46] for isothermal systems are in this category.

The adaptive implicit method has been applied to thermal simulation as well. Tan [42] used pre-estimates of the changes in the variables, post-correction, flux volume, and residual error methods to determine explicit and implicit labeling. The method did not assess the stability of the discretization.

Fung et al. [21] developed stability criteria for isothermal black-oil simulations using matrix stability analysis. The criteria could switch variables from implicit to explicit and vice versa, but their approach required evaluation of norms of very large matrices. In order to simplify the stability analysis, Fung et al. dropped the \( n^{th}\)-time-level accumulation terms from the conservation equations. Their justification for reducing the system to a local one is not clear, especially for complicated three-phase, thermal-compositional systems as pointed out by Peaceman [35]. Oballa et al. [32] applied the criteria developed by Fung et al. to thermal applications. They neglected heat conduction in their stability analysis, and they considered only convection-dominated flows. They found that in steam injection processes, the implicit/explicit switching in AIM is triggered either by the appearance of gas or by a moving temperature front in heavy-oil reservoirs.

This thesis derives the stability criteria using the linear von Neumann approach for thermal-compositional models taking into account the major mechanisms governing fluid flow. The CFL-based thermal criteria test the stability of the numerical discretization
scheme and are validated using a comprehensive set of test cases involving nonlinear behaviors due to the coupled nature of the mass and energy conservation equations, the thermodynamic phase behavior, and gravity. This work extends the previous research on the derivation of CFL-based stability criteria for isothermal systems done by Russell [38], [47], Grabenstetter et al. [22], Coats [13], [16], [17], Cao and Aziz [11], and Wan et al. [46], to a thermal-compositional formulation. The thermal stability criteria are employed in Stanford’s General Purpose Research Simulator (GPRS).
Chapter 3

Stability Criteria

We derive the linear stability criteria for thermal-compositional displacements in porous media. We make the following assumptions:

- Source and sink terms are treated implicitly.
- Density $\rho$ and viscosity $\mu$ are functions of pressure and temperature.
- Specific heat is constant.
- Relative permeability is a function of saturation only.
- Rock porosity $\phi$ is constant.
- Heat loss to the reservoir surroundings is ignored.

3.1 Governing equations

The Darcy equations for non-isothermal gas, oil, and water flow are given as follows:

$$
\mathbf{u}_g = -\frac{k}{\mu_g} \left( \nabla P_g - \gamma_g \nabla Z \right), \\
\mathbf{u}_o = -\frac{k}{\mu_o} \left( \nabla P_o - \gamma_o \nabla Z \right), \\
\mathbf{u}_w = -\frac{k}{\mu_w} \left( \nabla P_w - \gamma_w \nabla Z \right),
$$

(3.1) (3.2) (3.3)
where subscripts $g$, $o$, and $w$ refer to the gas, oil and water phases, respectively, $k$ is the permeability, and $k_r$ is the relative permeability. The phase velocities can be written as functions of the total velocity $u_t$, fractional flows, $f_p$ and an average mobility defined by $\bar{\lambda}_{pq} = \frac{\lambda_p \lambda_q}{\lambda_t}$. For the three-phase case, fractional flows and phase velocities can be written as:

\[ f_g = \frac{\lambda_g}{\lambda_t} \left( 1 + \frac{(\lambda_t - \lambda_g) \bar{\rho}_g - \lambda_o \bar{\rho}_o - \lambda_w \bar{\rho}_w}{u_t} g k \frac{\partial D}{\partial x} \right), \]  

\[ f_o = 1 - f_g - f_w, \]  

and

\[ f_w = \frac{\lambda_w}{\lambda_t} \left( 1 + \frac{(\lambda_t - \lambda_w) \bar{\rho}_w - \lambda_o \bar{\rho}_o - \lambda_g \bar{\rho}_g}{u_t} g k \frac{\partial D}{\partial x} \right). \]  

The bar above the density $\bar{\rho}_p$ means it is an average density over the vertical distance $D$.

\[ u_g = u_t f_g - \bar{\lambda}_{gw} k \frac{\partial P_{cWO}}{\partial x} - (\bar{\lambda}_{go} + \bar{\lambda}_{gw}) \frac{\partial P_{cGO}}{\partial x}, \]  

\[ u_o = u_t f_o - \bar{\lambda}_{ow} k \frac{\partial P_{cWO}}{\partial x} + \bar{\lambda}_{go} k \frac{\partial P_{cGO}}{\partial x}, \]  

and

\[ u_w = u_t f_w + (\bar{\lambda}_{gw} + \bar{\lambda}_{ow}) k \frac{\partial P_{cWO}}{\partial x} + \bar{\lambda}_{gw} k \frac{\partial P_{cGO}}{\partial x}. \]  

Conservation of mass for each phase can be expressed as follows:

\[ \phi \frac{\partial}{\partial t} [\rho_g S_g] = -\frac{\partial}{\partial x} [\rho_g u_g] \]
oil:

\[
\phi \frac{\partial}{\partial t} [\rho_o S_o] = - \frac{\partial}{\partial x} [\rho_o u_o] \quad (3.14)
\]

water:

\[
\phi \frac{\partial}{\partial t} [\rho_w S_w] = - \frac{\partial}{\partial x} [\rho_w u_w] \quad (3.15)
\]

Conservation of energy is given by

\[
\phi \frac{\partial}{\partial t} \left( \rho_g U_g S_g + \rho_o U_o S_o + \rho_w U_w S_w \right) + (1 - \phi) \frac{\partial}{\partial t} (\rho_R U_R) \nonumber
\]

\[
= - \frac{\partial}{\partial x} \left( \rho_g H_g u_g + \rho_o H_o u_o + \rho_w H_w u_w \right) + \kappa \frac{\partial^2 T}{\partial x^2} \quad (3.16)
\]

where,

\[
H_p = U_p + \alpha \frac{P_p}{\rho_p}, \quad (3.17)
\]

and

\[
U_p = C_{p_p} (T - T_i). \quad (3.18)
\]

Here, the unit of \( C_{p_p} \) is BTU/lb-F and \( T \) is in °F. \( T_i \) is the initial temperature in the gridblock. Using consistent field unit conversion factors, we get \( \alpha = 0.18504 \). We can write \( \frac{\partial P_{cwo}}{\partial x} \) as follows:

\[
\frac{\partial P_{cwo}}{\partial x} = p'_c \frac{\partial S_w}{\partial x}, \quad (3.19)
\]

where \( p'_c \) is the derivative of \( P_{cwo} \) with respect to water saturation, \( S_w \). The differential form of the mass conservation equations for the water, \( w \), and the oil, \( o \), in a dead-oil model are as follows:

\[
\frac{\partial}{\partial t} (\phi \rho_w S_w) + \frac{\partial}{\partial x} (\rho_w u_w) = 0, \quad (3.20)
\]

\[
\frac{\partial}{\partial t} (\phi \rho_o S_o) + \frac{\partial}{\partial x} (\rho_o u_o) = 0, \quad (3.21)
\]

where \( \phi \) is the porosity of the rock, and the corresponding differential form of the energy
conservation equation is given by:

\[ \phi \frac{\partial}{\partial t} (\rho_w S_w U_w + \rho_o S_o U_o) + (1 - \phi) \frac{\partial U_R}{\partial t} - \Upsilon_c \frac{\partial^2 T}{\partial x^2} + \frac{\partial}{\partial x} (\rho_w u_w H_w + \rho_o u_o H_o) = 0, \]

(3.22)

where \( U_R \) is the rock internal energy, \( \Upsilon_c \) is the heat conductivity, \( H_n \) and \( U_n \) are the enthalpy and the internal energy of phase \( n \) respectively.

In order to derive the stability criteria for the IMPEST (implicit pressure, explicit saturations, temperature and mole fractions) formulation, the saturation equation must be derived from Eq.(3.20) and Eq.(3.21), and the temperature equation is obtained from Eq.(3.20) and Eq.(3.22). The details are given in Appendix A. The IMPEST stability criteria specify the maximum CFL for the saturation, temperature and mole fractions. In order to derive the saturation and the temperature equations from the coupled system of equations described above, a few assumptions are made, including that the phase densities \( \rho_n \), are functions of average pressure within the gridblock. This implies that \( \rho_n \) is independent of the spatial variable \( x \), but its time dependence is retained. This is reasonable as we are only concerned with a stability analysis with respect to time. Moreover, the rock porosity, \( \phi \), is assumed to be constant with respect to time, \( t \).

We obtain the following system of equations after eliminating the pressure derivative terms from Eqs.(3.20),(3.21) and (3.22):

\[ A \Delta t S_w + B \Delta t T = \left[ -C \Delta_x n S_w + D \Delta_{xx} n S_w - E \Delta_x n T \right] \Delta t, \]

(3.23)

and

\[ F \Delta t S_w + G \Delta t T = \left[ -H \Delta_x n S_w + I \Delta_{xx} n S_w - J \Delta_x n T + K \Delta_{xx} n T \right] \Delta t. \]

(3.24)

The above Eqs. (3.23) and (3.24) are explicitly discretized using the following definitions.
based on phase-based upwind discretization for the first order spatial derivative terms [9]. For simplicity, we assume the flow is from left to right and central discretization of the second order spatial derivatives of saturation and temperature:

\[
\begin{align*}
\Delta_t S_w &= S_{w,j+1}^n - S_{w,j}^n, \\
\Delta_t T &= T_{w,j+1}^n - T_{w,j}^n, \\
\Delta^x_n S_w &= \frac{\Delta x}{S_{w,j}^n - S_{w,j-1}^n}, \\
\Delta^x_n T &= \frac{\Delta x}{T_{w,j}^n - T_{w,j-1}^n}, \\
\Delta^xx_n S_w &= \frac{S_{w,j+1}^n - 2S_{w,j}^n + S_{w,j-1}^n}{(\Delta x)^2}, \\
\Delta^xx_n T &= \frac{T_{w,j+1}^n - 2T_{w,j}^n + T_{w,j-1}^n}{(\Delta x)^2}.
\end{align*}
\]

A von Neumann analysis is performed on this discretized set of equations and is described in more detail in the next section.

### 3.2 von Neumann method for stability analysis

The primary goal of a finite-difference scheme is to obtain a solution that is as close as possible to the true analytical (free of numerical dispersion) solution. Two aspects that ensure this are [29]:

1. Consistency – Locally the finite-difference scheme must approximate the differential equation, i.e., a numerical scheme is consistent if the discrete numerical equation tends to the exact differential equation as the mesh size (represented by \(\Delta x\) and \(\Delta t\)) tends to zero,

2. Stability – A finite-difference scheme is stable if the errors made at one time step of the calculation do not cause the errors to increase as the computations are continued. If the errors decay and eventually damp out, the numerical scheme is said to be stable.

We have a nonlinear system of equations, which is linearized with respect to time using constant coefficients. The von Neumann method is the most commonly applied procedure
for performing a local analysis using frozen coefficients. For deriving stability criteria of nonlinear equations, we must make sure that we (at least) honor linear stability. Therefore, we use this method to study the stability characteristics of our finite-difference scheme. The procedure is based on performing a spatial Fourier transform along all spatial dimensions, thereby reducing the finite difference scheme to a time recursion in terms of a spatial Fourier transform of the system.

The system of equations given by Eq.(3.23) and Eq.(3.24) can be written in matrix form as follows:

\[
X \begin{pmatrix} \Delta_t S_w \\ \Delta_t T \end{pmatrix} = Y \begin{pmatrix} \Delta^n S_w \\ \Delta^n_{xx} S_w \\ \Delta^n_x T \\ \Delta^n_{xx} T \end{pmatrix},
\]

(3.25)

where

\[
X = \begin{pmatrix} A & B \\ F & G \end{pmatrix},
\]

and

\[
Y = \begin{pmatrix} C & D & E & 0 \\ H & I & J & K \end{pmatrix}.
\]

We can solve the matrix equation given by Eq.(3.25) and obtain the coefficients \(A_1, A_2, B_1, B_2, C_1, C_2, D_1\) and \(D_2\), such that

\[
\begin{pmatrix} -A_1 & A_2 & -B_1 & B_2 \\ -C_1 & C_2 & -D_1 & D_2 \end{pmatrix} = X^{-1} Y,
\]

After solving for \(\Delta_t S_w\) and \(\Delta_t T\), we can replace the discrete values in Eq.(3.25) by their generalized Fourier component:

\[
S^n_{w,j} = \xi^n_S e^{i \beta S j},
\]

(3.26)

and
Using the above approach and the identity \( e^{i\beta j} = \cos \beta j + i \sin \beta j \), the following coupled system of error propagation equations is obtained from Eqs. (3.23), (3.24) and (3.25):

\[
\begin{align*}
\xi_{S}^{n+1} &= \xi_{S}^{n} \left[ 1 - \left( \frac{A_1 \Delta t}{\Delta x} + \frac{2 A_2 \Delta t}{\Delta x^2} \right) \left(1 - \cos \beta_S \right) \right] \\
&\quad - \xi_{S}^{n} \left[ i \frac{A_1 \Delta t}{\Delta x} \sin \beta_S \right] \\
&\quad + \xi_{T}^{n} \left[ - \left( \frac{B_1 \Delta t}{\Delta x} + \frac{2 B_2 \Delta t}{\Delta x^2} \right) \left(1 - \cos \beta_T \right) \right] \\
&\quad - \xi_{T}^{n} \left[ i \frac{B_1 \Delta t}{\Delta x} \sin \beta_T \right],
\end{align*}
\]

(3.28)

and

\[
\begin{align*}
\xi_{T}^{n+1} &= \xi_{T}^{n} \left[ 1 - \left( \frac{D_1 \Delta t}{\Delta x} + \frac{2 D_2 \Delta t}{\Delta x^2} \right) \left(1 - \cos \beta_T \right) \right] \\
&\quad - \xi_{T}^{n} \left[ i \frac{D_1 \Delta t}{\Delta x} \sin \beta_T \right] \\
&\quad + \xi_{S}^{n} \left[ - \left( \frac{C_1 \Delta t}{\Delta x} + \frac{2 C_2 \Delta t}{\Delta x^2} \right) \left(1 - \cos \beta_S \right) \right] \\
&\quad - \xi_{S}^{n} \left[ i \frac{C_1 \Delta t}{\Delta x} \sin \beta_S \right],
\end{align*}
\]

(3.29)

where the subscript \( S \) refers to saturation, and the subscript \( T \) refers to temperature. The maximum eigenvalues of the above error propagation system of equations given by Eqs. (3.28) and (3.29) are obtained for \( \beta_S = n \pi \) and \( \beta_T = n \pi \) as described in Appendix C. Thus, the above system of equations is reduced to the following:

\[
\begin{align*}
\xi_{S}^{n+1} &= \xi_{S}^{n} \left[ 1 - 2 \left( \frac{A_1 \Delta t}{\Delta x} + \frac{2 A_2 \Delta t}{(\Delta x)^2} \right) \left(1 - \cos \beta_S \right) \right] \\
&\quad + \xi_{T}^{n} \left[ -2 \left( \frac{B_1 \Delta t}{\Delta x} + \frac{2 B_2 \Delta t}{(\Delta x)^2} \right) \left(1 - \cos \beta_T \right) \right],
\end{align*}
\]

(3.30)
and

\[
\xi^{n+1}_T = \xi^n_S \left[ -2 \left( \frac{C_1 \Delta t}{\Delta x} + \frac{2 C_2 \Delta t}{(\Delta x)^2} \right) \right] + \xi^n_T \left[ 1 - 2 \left( \frac{D_1 \Delta t}{\Delta x} + \frac{2 D_2 \Delta t}{(\Delta x)^2} \right) \right].
\]  

(3.31)

Writing the above equations in matrix form gives:

\[
\begin{bmatrix}
\xi^{n+1}_S \\
\xi^{n+1}_T
\end{bmatrix} = \begin{pmatrix}
1 - \alpha & -\beta \\
-\gamma & 1 - \delta
\end{pmatrix} \begin{bmatrix}
\xi^n_S \\
\xi^n_T
\end{bmatrix},
\]  

(3.32)

where

\[
\alpha = 2 \left( \frac{A_1 \Delta t}{\Delta x} + \frac{2 A_2 \Delta t}{(\Delta x)^2} \right),
\]

\[
\beta = 2 \left( \frac{B_1 \Delta t}{\Delta x} + \frac{2 B_2 \Delta t}{(\Delta x)^2} \right),
\]

\[
\gamma = 2 \left( \frac{C_1 \Delta t}{\Delta x} + \frac{2 C_2 \Delta t}{(\Delta x)^2} \right),
\]

and

\[
\delta = 2 \left( \frac{D_1 \Delta t}{\Delta x} + \frac{2 D_2 \Delta t}{(\Delta x)^2} \right).
\]

The non-oscillatory stability condition requires that the spectral radius of the error propagation matrix given by Eq.(3.32) be less than unity. The above statement is true only for amplification factors of single equations or normal matrices. Thus, we have:

\[
\left| 2 - \alpha - \delta \pm \sqrt{(\alpha - \delta)^2 + 4 \beta \gamma} \right| < 2.
\]  

(3.33)

The above expression reduces to:

\[
\alpha + \delta \pm \sqrt{(\alpha - \delta)^2 + 4 \beta \gamma} < 4.
\]  

(3.34)

The various parameters in the above equation are complicated expressions given by Eqs. (A.4)-(A.8) and Eqs. (A.11)-(A.16).
3.3 Decoupling the Temperature CFL

The stability criteria derived above are very complicated with lengthy expressions due to the algebra involved in solving for the eigenvalues of the system of equations. The analysis leads to two eigenvalues for the two-phase thermal case, one corresponding to the CFL number for saturation (CFLS) and the other for temperature (CFLT). If we had a-priori knowledge that both saturation and temperature needed to be treated implicitly or explicitly, we would not need to evaluate the CFLS and CFLT individually. However, for a variable-based TAIM, we need the individual CFL numbers in order to decide whether saturation or temperature, or both, need to be explicit or implicit in a gridblock.

In order to be able to handle TAIM in a more efficient manner as described above, we need to decouple the energy equation and obtain the temperature CFL number (CFLT). In order to achieve that we make a few assumptions:

- Phase density is nonzero, $\rho_p \neq 0$.
- Neglect the pressure derivatives in the flux terms.
- The total-velocity spatial variation is zero, $\frac{\partial u_T}{\partial x} \approx 0$.
- The capillary pressures in the accumulation term are neglected.

Moncorgé and Tchelepi [31] showed that we get a convection-dispersion equation in temperature only, which can be written as:

$$
\phi \gamma_s \frac{\partial T}{\partial t} = -\gamma_f \frac{\partial T}{\partial x} + \kappa \frac{\partial^2 T}{\partial x^2}
$$

(3.35)

where, $\gamma_s = \sum_p \rho_p \frac{\partial H_p}{\partial T} S_p + \frac{1 - \phi}{\phi} (\rho_R U_R)$

$$
- \sum_p \rho_p \frac{\partial H_p}{\partial T} S_p - 0.1838 \left( \sum_p \frac{1}{\rho_p} \frac{\partial \rho_p}{\partial T} S_p \right)
$$

and $\gamma_f = \sum_p \rho_p \frac{\partial H_p}{\partial T} u_p - \sum_p \frac{\partial H_p}{\partial T} S_p + 0.1838 \left( \sum_p \frac{1}{\rho_p} \frac{\partial \rho_p}{\partial T} u_p \right)$.

From Eq. (3.35), we can compute the CFLT number easily, and the expression is given as:
### Extension to multiple dimensions

For multiple dimensions, we compute the one-dimensional CFL numbers over all the edges between the blocks in the reservoir model and allocate the value to the upstream block [38]. Therefore, in multiple dimensions, the CFL of a block is a sum of one dimensional CFL numbers. This can be written as:

\[ \text{CFL}_i = \text{CFL}_{x_i} + \text{CFL}_{y_i} + \text{CFL}_{z_i} \]  

(3.37)

In case the fluid phases do not flow in the same direction, we cannot determine which block is upstream and which is downstream. In such cases, a conservative approach that honors stability is used, where we allocate the CFL to both the upstream and downstream blocks of the edge.

### 3.4 Stability Analysis for Two Phase Isothermal Systems

We use the Von Neumann method to derive the required stability criteria for non-oscillatory stability. The analysis for two-phase isothermal systems using this method has been previously performed by Coats [15], [16], Grabenstetter et al. [22], Russell [38], Wan et al. [46]. The term non-oscillatory stability refers to the case in which all eigenvalues are positive and less than unity. For example, the following 1-D water saturation equation

\[ \frac{\partial S_w}{\partial t} = -C \frac{\partial S_w}{\partial x} + D \frac{\partial^2 S_w}{\partial x^2}, \]

(3.38)

can be discretized explicitly as follows:

\[ \frac{S_{w_{j+1}}^{n+1} - S_{w_j}^n}{\Delta t} = -C \left[ \frac{S_{w_j}^n - S_{w_{j-1}}^n}{\Delta x} \right] + D \left[ \frac{S_{w_{j+1}}^{n+1} - 2S_{w_j}^n + S_{w_{j-1}}^n}{\Delta x^2} \right], \]

(3.39)
where flow is assumed from cell $j - 1$ to cell $j$. The discrete value in the difference equation is replaced by its generalized Fourier component:

\[ S_{w_j}^n = \xi^n e^{i \beta j}. \]  \hspace{1cm} (3.40)

Substitution of Eq. 3.40 in Eq. 3.39 results in the following equation:

\[ \frac{\xi^{n+1}}{\xi^n} = 1 - \left( \frac{C \Delta t}{\Delta x} + \frac{2 D \Delta t}{\Delta x^2} \right) (1 - \cos \beta) - i \frac{C \Delta t}{\Delta x} \sin \beta, \]  \hspace{1cm} (3.41)

where $\frac{\xi^{n+1}}{\xi^n}$ is the amplification factor. For non-oscillatory stability, the sufficient condition is:

\[ |\frac{\xi^{n+1}}{\xi^n}| < 1. \] \hspace{1cm} (3.42)

From Eq. (3.41), this amplification factor can be written as:

\[ |\lambda|^2 = \left| \frac{\xi^{n+1}}{\xi^n} \right|^2 = \left[ 1 - \left( \frac{C \Delta t}{\Delta x} + \frac{2 D \Delta t}{\Delta x^2} \right) (1 - \cos \beta) \right]^2 + \left[ \frac{C \Delta t}{\Delta x} \sin \beta \right]^2. \]  \hspace{1cm} (3.43)

The maximum value of the amplification factor is obtained by using the criteria:

\[ \frac{d}{d \beta} \left( |\lambda|^2 \right) = 0, \] \hspace{1cm} (3.44)

which is satisfied for

\[ \beta = n \pi. \] \hspace{1cm} (3.45)

Combining Eq. (3.42) and Eq. (3.43), we have:

\[ \left| 1 - 2 \left( \frac{C \Delta t}{\Delta x} + \frac{2 D \Delta t}{\Delta x^2} \right) (1 - \cos \beta) \right| < 1. \] \hspace{1cm} (3.46)

We thus arrive at the following stability condition:

\[ 0 < \frac{C \Delta t}{\Delta x} + \frac{2 D \Delta t}{\Delta x^2} < 1. \] \hspace{1cm} (3.47)

The general stability condition for isothermal two-phase oil-water flow in the presence of capillary effects is given by:
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\[ 0 < \left[ \frac{q_t \frac{\partial f_w}{\partial S_w}}{V \phi} - \frac{2 \Upsilon G \bar{\lambda} P'_w \Delta t}{V \phi} \right] \left[ \begin{array}{c} \frac{\rho_o}{S_o} + \frac{\rho_w}{S_w} \\ \frac{-P'_c}{S_w} \end{array} \right] < 1, \]  

(3.48)

where

\[ q_t = A u_t, \]
\[ V = A \Delta x, \]
\[ \text{and } \Upsilon_G = \frac{k A}{\Delta x}, \]

where \( A \) is the cross-sectional area, and \( \Upsilon_G \) is the geometric transmissibility. Thus, we have

\[ CFLS = \left[ \frac{q_t \frac{\partial f_w}{\partial S_w} \Delta t}{V \phi} - \frac{2 \Upsilon G \bar{\lambda} P'_w \Delta t}{V \phi} \right] \left[ \begin{array}{c} \frac{\rho_o}{S_o} + \frac{\rho_w}{S_w} \\ \frac{-P'_c}{S_w} \end{array} \right] < 1. \]  

(3.49)

From the expression of CFLS given by Eq. 3.49, we can calculate the maximum allowable time step size. If the capillary pressure term is dropped, this expression becomes

\[ CFLS = \frac{q_t \frac{\partial f_w}{\partial S_w} \Delta t}{V \phi}. \]  

(3.50)

which is the well known CFL condition based on the throughput and fractional flow [16], [9].

The CFL for the explicit treatment of saturations in a three-phase system is expressed as the maximum of the eigenvalues of a two-by-two matrix, given as follows:

\[ CFLS = \frac{q_t F \Delta t}{V \phi}, \]  

(3.51)

where

\[ F = \begin{pmatrix} \frac{\partial f_s}{\partial S_s} & \frac{\partial f_s}{\partial S_w} \\ \frac{\partial f_w}{\partial S_s} & \frac{\partial f_w}{\partial S_w} \end{pmatrix}. \]  

(3.52)
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The two eigenvalues correspond to each unknown saturation variable. We use the maximum of the two values and obtain the saturation CFL number. The assumption in determining the CFL number using the above mentioned eigenvalue matrix is that the eigenvalues of Eq. 3.52 must be bounded and the matrices should be normal. We will check for these assumptions using a three-phase test case in Chapter 6, and we verify that the stability analysis works even when the two-by-two matrix is not normal, which is the case for highly nonlinear relative permeability functions.

3.5 Steam Formulation

Thermal simulation with steam is a challenging problem because of the strong coupling of the mass and energy conservation equations and the nonlinear behavior of steam injection processes. Steam injection gives rise to various physical phenomena such as viscosity reduction, distillation, miscible mixing, thermal expansion, wettability changes, cracking and lowered oil-water interfacial tension [28]. The major computational challenge with steam is due to the fact that water exists as both liquid and gas. Phases can appear, or disappear, due to changes in the thermodynamic state (overall composition, pressure, temperature), where components can be transferred across fluid phases, or due to displacement processes. Thus, the choice of the primary variables in a gridblock depends on the phase-state in that block. To decide which phase-state is valid, we use a variable substitution strategy [14], [13]. Therefore, the stability criteria and switching algorithms for steam simulation must account for the complex physical behavior of steam.

We use the von Neumann linear stability analysis. However, we should note the limitation that we are obtaining the criteria for a very nonlinear system by a linear method. So, we may require additional analysis in order to accurately design the TAIM method. The governing equations for derivation of stability criteria for the steam injection problem with distillation, neglecting source/sink terms and heat loss, are summarized below.

Mass Balances on Hydrocarbon Components:

\[
\phi \frac{\partial}{\partial t} [\rho_o S_o x_i + \rho_g S_g y_i] = -\frac{\partial}{\partial x} [\rho_o u_o x_i + \rho_g u_g y_i],
\]

where \( i = 1, ..., n_c \), where \( n_c \) is the number of components, and \( u_g \) and \( u_o \) are given by
Eqs. 3.1 and 3.2, respectively. The liquid phase \((x_i)\) and the gas phase \((y_i)\) hydrocarbon mole fractions are related through equilibrium \((K_i)\) values as follows:

\[
y_i = K_i (P, T) x_i.
\] (3.54)

**Mass Balance on Water:**

\[
\phi \frac{\partial}{\partial t} \left[ \rho_w S_w + \rho_g S_g y_s \right] = -\frac{\partial}{\partial x} \left[ \rho_w u_w + \rho_g u_g y_s \right],
\] (3.55)

where \(y_s\) is the steam mole fraction and is equal to \(\frac{P}{P_{\text{sat}}}\). \(P_{\text{sat}}\) is the steam saturation pressure and is a function of temperature.

**Energy Balance:**

\[
\phi \frac{\partial}{\partial t} \left( \rho_g U_g S_g + \rho_o U_o S_o + \rho_w U_w S_w \right) + (1 - \phi) \frac{\partial}{\partial t} \left( \rho_R U_R \right)
= -\frac{\partial}{\partial x} \left( \rho_g H_g u_g + \rho_o H_o u_o + \rho_w H_w u_w \right) + \kappa \frac{\partial^2 T}{\partial x^2}.
\] (3.56)

The water and steam internal energies, \(U_w\) and \(U_s\), and the steam enthalpy, \(H_s\), are taken from steam tables [36], [4] and are functions of temperature. The oil and gas phase internal energies and enthalpies are calculated as follows [1]:

\[
U_o = \sum_i x_i C_p i \Delta T,
\] (3.57)

\[
U_g = \sum_i y_i C_p i \Delta T + y_s U_s,
\] (3.58)

\[
H_o = U_o + W T \frac{P_o}{\rho_o},
\] (3.59)

and

\[
H_g = \sum_i y_i C_p i \Delta T + W T \frac{P_g}{\rho_g} + y_s H_s.
\] (3.60)

We apply the von Neumann analysis to the above system of governing equations to obtain the stability criteria for explicit saturations, mole fractions, and temperature. Note
that the energy equation is the same as that described earlier in Eq. 3.22. The definitions of internal energy and enthalpy for the gas phase are different in order to account for the steam contributions. This is done using the steam mole fraction. The mass conservation equations for hydrocarbon mole fractions given by Eq. 3.53 have been described by Cao [11], and the stability criteria for explicit mole fractions (IMPSAT) can be evaluated using the von Neumann method [11], [12]. The stability criteria for saturation are derived using Eq. 3.55. The expressions for the criteria for explicit saturations when steam is present are different from those given by Eq. 3.49, due to the presence of water in the gas phase. When there is no steam in the gridblock, \( y_s = 0 \), the expressions reduce to the thermal-compositional derivation described in Appendix A.

The second important aspect in the AIM formulation is the switching algorithm. It is not only important to correctly assign the implicit and explicit variables in a gridblock based on the stability limits, but it is also critical to be consistent with the variable substitution algorithm. This means we need to keep track of the phase state and the corresponding distinct set of primary variables in each gridblock. An important thermodynamic quantity in steam simulation is the saturation vapor-pressure, which can be expressed as a function of temperature. Therefore, the temperature CFL number need not be calculated, if there is a nonzero steam mole fraction. This is because restraining the time step size based on an explicit temperature variable will hamper the performance of AIM unnecessarily, when it is not required by the physics. Similarly, when the steam has condensed completely into hot water, temperature becomes independent of pressure, and we must evaluate the stability criteria for the explicit treatment of temperature. Therefore, it is important to provide the simulator with the appropriate phase-change logic for switching the primary variables.
Chapter 4

Switching Algorithm

In addition to the stability criteria, we require a switching algorithm that instructs the simulator to decide on the time step size and label the variables as implicit or explicit. In this chapter, we explain in detail the two switching algorithms in GPRS that are used to determine the time step size and for assigning the implicit level for each gridblock.

4.1 Percentage-Based Switching

In this algorithm, the simulation begins with input from the user, namely \( x\% \) IMPEST (Implicit Pressure, Explicit Saturation, Temperature and mole fractions), \( y\% \) IMPTES (Implicit Pressure and Temperature, Explicit Saturation and mole fractions) and \( z\% \) FIM (Fully Implicit), where \( x + y + z = 1 \). In order to determine the maximum stable time step size that can be taken for the given percentage break-up, the gridblocks are arranged according to their CFL numbers in a monotonic order. The stable time step size, which can satisfy the given percentage is then evaluated. Subsequently, a gridblock is labeled implicit if the CFL number is bigger than the CFL limit and explicit otherwise. This is the method that is currently implemented in GPRS for isothermal and thermal AIM. The flowchart showing the steps to get the stable time step size is shown in Figure 4.1.

One disadvantage of this method is that for some situations, a pre-specified fixed percentage of an explicit scheme can lead the simulator to take extremely tiny time steps, resulting in a significant waste of computational time. To motivate the need for a better switching algorithm, consider the following synthetic example of a 10 block dead-oil system.
START

Invoke ThermalCFL() constructor

Generate CFL Arrays without \( \Delta t \)

Sort arrays in ascending order (for TAIM)

Find Max(\( \Delta t \)) using CFL_Limit for TAIM & single implicit level (\( \Delta t \))

If

\[
dt > \text{max}_{\Delta t} \text{ (user input)}
\]

\[\Delta t = \text{max}_{\Delta t}\]

END

Figure 4.1: Flowchart for calculation of time step size using the percentage-based algorithm.

Table 4.1 gives the CFLS and CFLT numbers without the time step size \( (\Delta t) \) at a certain time, and we want to find the new time step size based on a 70% IMPEST and a 30% FIM distribution. After arranging the CFLS column, we find that the time step size should be 2.6 days based on a CFL limit of unity. Thus, we label gridblocks 4, 5 and 6 FIM, and the rest IMPEST. Even though temperature could be treated explicitly in all blocks, we have to solve it implicitly in the FIM blocks due to the fixed percentages of IMPEST and FIM. We could take \( \Delta t = 3.8 \) days for a 60% IMPEST and 40% FIM distribution, and a \( \Delta t \) of
5 days for a 50% IMPEST and 50% FIM distribution for the given CFL values. Thus, as we increase the FIM percentage, we can take larger time steps; however, we have to treat temperature implicitly when it is not required by stability considerations.

<table>
<thead>
<tr>
<th>gridblock</th>
<th>$CFL_S$</th>
<th>$CFL_T$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1</td>
<td>0.02</td>
</tr>
<tr>
<td>2</td>
<td>0.19</td>
<td>0.021</td>
</tr>
<tr>
<td>3</td>
<td>0.26</td>
<td>0.022</td>
</tr>
<tr>
<td>4</td>
<td>0.38</td>
<td>0.02</td>
</tr>
<tr>
<td>5</td>
<td>0.41</td>
<td>0.018</td>
</tr>
<tr>
<td>6</td>
<td>0.45</td>
<td>0.02</td>
</tr>
<tr>
<td>7</td>
<td>0.1</td>
<td>0.019</td>
</tr>
<tr>
<td>8</td>
<td>0</td>
<td>0.021</td>
</tr>
<tr>
<td>9</td>
<td>0</td>
<td>0.022</td>
</tr>
<tr>
<td>10</td>
<td>0</td>
<td>0.019</td>
</tr>
</tbody>
</table>

Table 4.1: CFLS and CFLT values without $\Delta t$ to illustrate percentage-based and variable-based switching algorithms.

We observe that the percentage-based scheme is arbitrary and can lead to larger, or smaller, time steps based on the numerical values of the CFL numbers. In Chapter 6, a similar example arises when the percentage of IMPEST blocks chosen is smaller than the regions with strong heat conduction resulting in explicit treatment of temperature, which leads to tiny time steps. However, if temperature is treated implicitly everywhere in that case, the simulation runs a lot faster. Therefore, it is purely trial-and-error on the part of the user to specify the breakdown correctly so as to allow for reasonably large time steps while maintaining stability. Hence, there is a need for a better technique to handle the assignment of implicit levels in the gridblocks.

### 4.2 Variable-Based Switching

The variable-based switching approach for TAIM [8] provides a flexible strategy for selecting an optimal percentage breakdown between varying levels of implicitness, and that helps to improve the overall computational efficiency of the simulator. For a user specified time step size, we assign the implicit level for each variable in each gridblock according to the stability
criterion (CFL number of the variable in the gridblock) for that variable. This means we treat a variable implicitly only when it is required by the stability criterion. This method is straightforward, and the percentage of gridblocks for each scheme can change between time steps.

The procedure to find the implicit level structure honoring stability and using a large time step is:

1. Use the pressure, saturations, compositions and temperature for each gridblock, and evaluate the phase velocities from the petro-physical data.

2. Calculate the CFL numbers using the stability criteria with the given time step size, $\Delta t$.

3. In each gridblock, label the variables as implicit if their corresponding CFL is greater than the CFL limit.

4. Using this implicit level structure and the time step, perform the computations.

Using the above procedure for the previous example, and taking a time step size of 5 days, we observe that we only need to treat saturation implicitly in gridblocks 3, 4, 5 and 6, and the saturation in the rest of the blocks and the temperature in all the blocks are treated explicitly. Thus, we reduce the number of implicit variables, and we are able to take a larger time step size compared to the percentage-based case. A comparison of the implicit variables and time step sizes for the illustrated example is shown in Table 4.2.

<table>
<thead>
<tr>
<th>Scheme</th>
<th># Imp Vars</th>
<th>$\Delta t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>variable-TAIM</td>
<td>4</td>
<td>5</td>
</tr>
<tr>
<td>70 IMPEST-30 FIM</td>
<td>6</td>
<td>2.6</td>
</tr>
<tr>
<td>60 IMPEST-40 FIM</td>
<td>8</td>
<td>3.8</td>
</tr>
<tr>
<td>50 IMPEST-50 FIM</td>
<td>10</td>
<td>5</td>
</tr>
</tbody>
</table>

Table 4.2: Comparison of the total number of implicit variables taken and time step size in the percentage-based and variable-based switching algorithms.

A percentage-based algorithm can match the variable-based algorithm’s time step size; however, it is nontrivial to determine such a distribution a-priori. Moreover, $\Delta t$ depends on the governing CFL numbers, which vary both in space and time, such that a fixed
distribution may not be suitable for the entire simulation. Note that the percentage of the implicit level schemes in the variable switching will be different at each time step. The advantage of this method is that the user can specify the desired time step size, and the simulator controls the percentage distribution. So if the time step is too aggressive, we solve the system in FIM mode; otherwise, we save computational time by maximizing the use of AIM. Comparisons of the two switching algorithms are performed in Chapter 6.
Chapter 5

Implementation in GPRS

Stanford’s General Purpose Research Simulator (GPRS) [11], [25], [26] is a research tool with extensible software design that incorporates simulation techniques for structured and unstructured grids, network modeling, two-point and multi-point flux calculations for black-oil and compositional reservoir simulation. This chapter describes the implementation of TAIM (Thermal Adaptive Implicit Method) in GPRS. We start by giving the relevant details of the original isothermal GPRS and its thermal extension. Later, we describe the implementation of the derived stability criteria for thermal compositional reservoir simulation, as well as, the percentage-based and variable-based switching algorithms.

Figure 5.1: Key modules in existing GPRS code (Courtesy: GPRS manual [11]).
5.1 Current GPRS

GPRS was developed as an isothermal reservoir simulator for solving mass balance equations for both compositional and black-oil models. In evolving from black-oil to compositional models, the number of equations increases, and this strongly influences the computational performance of the simulator. The solution of the nonlinear system of equations is performed iteratively using a Jacobian and residual by the Newton-Raphson method. The terms in the Jacobian are partial derivatives of the mass conservation equations with respect to each unknown variable, and the terms can be evaluated at the current time (value of the variable is not known) or at the previous time (value is known). The unknown variables are termed implicit, when the Jacobian coefficients are evaluated at the current time, whereas they are called explicit when we use values from a previous time step. When all the variables are implicit, it is considered to be a fully implicit Jacobian, and hence a larger system must be solved. The key modules and the high level C++ class structure of GPRS are shown in Figure 5.1. Additional implementation details of these modules are explained in Cao’s PhD thesis [11], Jiang’s MS report [25], and Jiang’s PhD thesis [26].

In order to explain the structure of the Jacobian matrix, we consider a simple two-well example. The grid is shown in Figure 5.2. Well 1 is completed in gridblock 1, and well 2 is completed in gridblock 5. The corresponding Jacobian matrix for this system is shown in Figure 5.3, where green represents a term generated by the accumulation part, blue represents a term generated by the flux part, and orange represents a term generated by the well part.

![Figure 5.2: An example grid for illustrating the Jacobian structure.](image)

Now consider the case when only \( P \) and \( T \) are implicit. The flux term derivatives of the mass balance and energy balance equations with respect to the explicit variables will
Figure 5.3: Jacobian matrix for the example grid shown in Figure 5.2. This is the Jacobian matrix structure for all variables implicit.

become zero, and the Jacobian structure for the example of Figure 5.2 is shown in Figure 5.4. Comparison of Figures 5.3 and 5.4 shows the reduction in the size of the Jacobian by reducing the number of variables that are treated implicitly. This reduction of the Jacobian leads to a direct reduction in computational time. The remaining explicit variables can be updated after the implicit variables have been solved. But explicit treatment requires certain stability restrictions that need to be followed, which limit the time step size that can be taken compared to a fully implicit solution. The adaptive implicit solution technique in GPRS has previously been used only for the solution of two-phase isothermal systems without phase change [11].

GPRS has been extended to account for the energy-balance equation [45]. Each block of the Jacobian is expanded to include a row for the extra (energy) equation and a column for the extra variable (temperature). The location of this additional row and column in the Jacobian is specified using the parameter $nIns$ for each gridblock. For example, if
the isothermal Jacobian has a variable line-up that includes pressure $P$, saturations of one less than the total number of phases (e.g., $S_g$, $S_o$), and mole fractions $y_1$, $y_2$, then after the addition of the energy equation, the primary variable line-up becomes $P$, $S_g$, $T$ and the remaining mole fractions $y_i$. The energy equation in this case is inserted at location $nIns$ equal to two in the original isothermal Jacobian. The parameter $nIns$ can be assigned any value between one and the number of primary variables, $nPri$, for each gridblock individually for cases where there is no phase disappearance or reappearance. For problems with phase change, Thermal GPRS sets $nIns = 1$ in all the gridblocks, so that disappearance, or reappearance, of saturations and mole fractions does not affect the rearrangement of the primary variables in the Jacobian. Once the energy equation is included in the Jacobian and the residual, we can solve the nonlinear system of equations for each time step, update the solution, and go to the next time step. In problems with phase change, since the primary variables in a gridblock change dynamically, we need to implement a robust $nIns$ logic in Thermal GPRS that can take any value between one and
For schemes that are not fully implicit, we need to specify the number of implicit variables ($nImpVars$) for each gridblock in the reservoir. The primary variables in GPRS are arranged, such that the first $nImpVars$ variables are implicit and the remaining ones are explicit. For example, in a two-phase black-oil thermal case, we have primary variables as $P$, $S$, and $T$. If $nIns$ is one, the order would be $P, T, S$, and if $nImpVars$ is two, only $P$ and $T$ are implicit, whereas $S$ is explicit. The parameter $nIns$ is particularly useful in a variable-based Thermal AIM algorithm implementation, because it can take on a different value for different gridblocks. All primary variables lined up before the $nIns$ location would be implicit and the rest explicit. Thus, in the current example, if only $P$ and $S$ are treated implicitly, $nIns$ takes the value of two. That is, the energy equation and the temperature are placed last in the Jacobian, whereas, if $P$ and $T$ are treated implicitly, $nIns$ would be equal to one.

5.2 TAIM in GPRS

To improve the balance between timestep size and computational cost, we implement a Thermal Adaptive Implicit method (TAIM) that uses a switching algorithm, where some unknowns are treated implicitly, while others are treated with explicit schemes such as IMPEST. The switching algorithm decides on the time step size according to the stability criteria derived in Chapter 3.

5.2.1 Thermal Stability Criteria Implementation

$ThermalCFL$ class: The derived thermal stability criteria are implemented as a separate $ThermalCFL$ module in GPRS. The class diagram is shown in Figure 5.5, and the details are explained below:

- Extract data from the DataPool class [$initializeParameters(DataPool* mDataPool)$]: This allows isolating the ThermalCFL class for future code changes in GPRS. Adding new variables will simply require updating the initialization of the local arrays.

- Calculate the total flow rate from a cell [$calcQpV(DataPool* mDataPool)$]: The
Figure 5.5: ThermalCFL class in GPRS to provide the thermal stability criteria for TAIM.

calculation is done based on upstream analysis allowing extensibility to multiple dimensions.

• Calculate the total-heat transmissibility using \[\text{calcmHT}_V(DataPool * mDataPool)\].

• Populate the matrices for calculating CFL numbers \([\text{populateMatrices()}]\): There are separate functions depending on the number of explicit variables and existing phases in a block. The function evaluates the CFL numbers and stores them in an array for time step calculation and assignment of implicit levels to the gridblocks.

Treatment of transmissibility: In order to solve a nonlinear system of equations using an adaptive implicit strategy, we reduce the implicit level of the fully implicit system in two steps. First, we set all the derivatives of flux terms in the mass balance and energy balance equations with respect to the explicit variables to zero. Next, we decouple the implicit variables from the explicit variables using standard decoupling methods, such as the Householder reflection (QR decomposition) method [27]. This is discussed in detail in the GPRS manual [11].

Flux terms contain transmissibility, which is a function of phase saturation and temperature. When either of these variables is explicit, we can either fix the value at the old
time level, or update it iteration by iteration. GPRS originally was designed for isothermal systems and had various options for treating the saturation variable implicitly or explicitly in the transmissibility. With the addition of the energy equation in Thermal GPRS, we implemented a new parameter $\text{transImpT}$ for each gridblock that defines how derivatives of the transmissibility would be treated with respect to temperature. The parameter $\text{transImpT}$ can take one of two possible values: (i) zero when temperature is explicit, or (ii) one when temperature is implicit. Essentially, this means that derivatives with respect to temperature will be evaluated only when $\text{transImpT}$ is unity; otherwise, temperature is treated explicitly.

5.2.2 Switching Algorithms

The switching algorithms give information about the implicit and explicit variables in each gridblock depending on the stability criteria. This is done using the function $\text{SimMaster :: assignImpLevels()}$. The details of each of these switching algorithms are described next.

Percentage-Based TAIM

The first step in this algorithm is to find the stable time step size given the percentage break up of the various implicit level schemes. This is done in the $\text{SimMaster :: calcDt(double maxdt)}$ function. Recall from the algorithm described in the previous chapter that CFL numbers are evaluated without any time step size. Thus, after rearranging the CFL array in an ascending order, the stable time step size is calculated based on the fact that all gridblocks must stay stable honoring the given percentage break up. Once the time step size is known, the CFL array is multiplied with this time step to obtain the CFL numbers.

The next step is to label the gridblocks with the implicit level scheme. In the $\text{SimMaster :: assignImpLevels()}$ function, for each gridblock the minimum implicit level is assigned. Then, we check if the CFL number violates the maximum CFL limit. If it does, the implicit level is changed, and the information is passed onto the Jacobian.
Variable-Based TAIM

The primary-variables array in GPRS is such that we always keep pressure, $P$, as the first variable, followed by saturations and then compositions. We can use the parameter $nIns$ as discussed earlier in this chapter and place temperature for thermal simulations wherever we want. The parameter $nImpVars$ gives the number of implicit variables in a gridblock, and it arranges the variables in a given order starting with pressure. Thus we can use $nIns$ to be the position at which variables become explicit. This means temperature can be implicit or explicit irrespective of the saturations. We assume that if compositions are implicit, saturations must be implicit as well, but if the compositions are explicit, the saturations can be either implicit or explicit.

The time step size is specified by the user in the variable-based algorithm. In the $[SimMaster :: assignImpLevels()$] function, we check for the CFL number for each variable, such as saturation, temperature, and composition, in each gridblock. If a criterion is violated, the variable is labeled implicit, and the information is passed onto the Jacobian. We can see that if the time step size exceeds the maximum CFL limit for all variables, the gridblock becomes fully implicit.

5.3 Additional Modules

The reservoir simulation equations are highly nonlinear. Due to the complexity of the physics involved, taking into account the phase change behavior for compositional systems leads to difficulty in obtaining convergence of the nonlinear loop. Thus, even though, the time step size is stable with respect to the linear stability criteria, the Newton iterations may not converge, and the simulator chops the time step size. This leads to a loss in computational effort, as the Newton iterations are wasted. In cases where the saturations are explicit, saturations may have values that make them immobile. This creates convergence problems, as the solver gets confused about the disappearance or reappearance of a phase, leading to a smaller time step in order to be able to avoid sudden changes across phase boundaries. We implemented the Appleyard Chop algorithm in GPRS for improving the $[newtonUpdate()$] function. The Appleyard Chop algorithm is a heuristic that controls saturation changes by modifying the Newton update on a cell-by-cell basis [5]. An additional challenge with AIM is the computation of non-monotonic solutions, even when the implicit
levels are assigned appropriately and the time step is within the linear stability limit. This happens due to AIM discretization errors. These are discussed next.

5.3.1 Appleyard Chop

In this algorithm, we do a cell-wise modification of the Newton solution update, such that if a saturation changes from mobile to immobile, or vice versa, it is set to be just mobile. We observed that making this modification impacts the performance of the simulation significantly. Time step chops are usually not required because the nonlinear loop does not alternate between the two states of presence and disappearance of a phase. This is especially true for compositional simulations with gas injection, where phase behavior is more nonlinear compared to black-oil models. Using the Appleyard chop not only improves the AIM simulations, but is also quite effective in FIM simulations. However, the algorithm is not used frequently in many FIM simulations as the saturations tend to be mobile due to the increased numerical diffusion associated with FIM. The Appleyard algorithm is implemented in the $mthCompFlowEqnModel::appleyardChop()$ function in GPRS.

5.3.2 AIM Discretization Error Handler

During AIM simulations, at the boundary of implicit and explicit blocks, we observed that the saturation profile had a little kink. This did not lead to any oscillations, but it represents a non-physical behavior. The kink occurs because an upstream implicit gridblock allows any throughput to its downstream neighbor, without the implicit level information of the downstream gridblock. When the downstream gridblock is explicit, due to stability restrictions, it cannot pass on the higher throughput received to the next downstream block. Thus, an accumulation of saturation occurs at the implicit-explicit gridblock boundary, which appears as a kink in the saturation profile. The kink travels with the front, eventually decreasing in magnitude [19]. The problem is visible in the region downstream of a well block. We can overcome this problem by assigning downstream gridblocks that would have been labeled explicit as implicit depending on the saturation CFL number of the upstream implicit gridblock. Using this algorithm, we can smooth out the non-physical kink in the saturation profile.

Figure 5.6 shows the saturation profile for a simple 1-D simulation with 20 gridblocks.
The first eight gridblocks are implicit according to the stability criteria, and the remaining twelve are explicit. We observe a kink in the saturation at the boundary, which disappears when gridblocks nine and ten are labeled implicit.

Additionally, the issue of the AIM discretization error can also be handled by computing the CFL numbers based on inflow as opposed to outflow fluxes. This method is conservative because the time step size would be calculated based on the throughput a gridblock gets from its neighboring connections. The following example shows the results that we obtained using this modification. The domain is a horizontal 20 gridblock reservoir, and we inject water in block 1. Water invades the domain from left to right. Figure 5.7 shows the water saturation profile for the AIM simulations. Gridblocks 10 and 11 have CFL numbers greater than unity and form an implicit-explicit boundary. Thus, saturation builds up in blocks 11 and 12 during this time step. When we use the AIM discretization heuristic, the kink in the saturation profile is removed. This is shown by the line labeled as *heuristic*. The *Inflow-Based* plot shows the saturation profile when throughput into the gridblock is used to compute the CFL numbers. This is a more conservative strategy, but it does not require a heuristic treatment. Thus, we can use either of the two methods to eliminate the AIM discretization-error problem.
Figure 5.7: Water saturation profile showing AIM discretization error and the correction by two different methods.
Chapter 6

Validation Using GPRS

This chapter describes the simulation results for the stability criteria and the switching algorithms implemented in Stanford’s General Purpose Research Simulator (GPRS). In order to determine the correctness of the criteria, the reservoir model was made progressively more complex by including the following physical phenomena:

- Fluid and heat convection: This is the most common mechanism for mass and heat transfer occurring in reservoirs. The convective flux is the first order term in the mass and energy differential equations.

- Thermal conduction: Heat transfer in the reservoir takes place due to conduction through rock and fluids. This is dependent upon the conductivity of the medium and is the second order diffusive term in the energy balance.

- Phase changes: The disappearance and reappearance of the phases in the reservoir is due to changes in overall composition, temperature, and pressure. Phase changes lead to the removal, or addition, of primary variables from the discrete system.

- Gravity: Flow in the reservoir due to density differences between the fluids is an important mechanism and is a challenge for the AIM approach, especially when counter-current flow is dominant.
6.1 Fluid and Heat Convection

The evaluation is done using a hot-water injection simulation using the Thermal Adaptive Implicit Method (TAIM). The physical set-up is a 1-D horizontal two-component dead-oil reservoir 300 ft in length divided equally into 20 gridblocks, with water injection in block 1 and production from block 20, with both these blocks treated fully implicitly. Water is injected in the reservoir at a temperature much higher than the initial reservoir temperature at a constant volumetric rate. Initial water saturation in the reservoir is 0.2. The dimensionless time in pore volumes injected (PVI) is given by

\[ PVI = \frac{Q_{inj} \cdot t}{\phi V_{res}}, \]

where \( Q_{inj} \) is the hot-water volumetric injection rate in \( ft^3/day \), \( t \) is time in \( days \), \( \phi \) is porosity, and \( V_{res} \) is the volume of the reservoir in \( ft^3 \). The water injection rate was chosen such that we achieve a water advance of about 1 ft/day, a value typical of field scale waterfloods. The value of the heat conduction coefficient, \( \gamma_C = 40 \) BTU/ft-day-F is such that the contribution of heat conduction is much smaller than heat convection. This is a common value of conductivity for berea sandstones [37]. The details of the oil and water physical data for all tests are given in Appendix B. Figure 6.1 shows the fractional flow curves. As shown, the solid line represents a unit end-point mobility ratio and the dotted line is an end-point mobility ratio of 30, where the mobility ratio is defined as the ratio of the mobility of the displacing fluid to that of the displaced fluid. The mobility of a fluid is given by its relative permeability divided by its viscosity. The end-point mobility ratio is unity for this test case.

We compare the TAIM simulation with FIM (everything implicit), and IMPEST (only P implicit). The results are also compared with FIM using the same time steps as the IMPEST run. The TAIM simulation has two implicit levels (IMPEST 70% and FIM 30%) with their percentage breakdown decided in advance for the entire simulation. Figure 6.2 shows the time stepping behavior. FIM takes time steps that grow with time. The time step size is calculated using changes in the saturation variable for the FIM scheme. We observe that as we decrease the IMPEST percentage of the TAIM scheme, larger time step sizes are taken eventually approaching the size used for the FIM scheme.

To study the level of diffusion and the correspondence between \( S_{sw} \) and CFLS, we consider
CHAPTER 6. VALIDATION USING GPRS

Figure 6.1: Water fractional flow for two mobility ratios.

Figure 6.2: Time step size in cell PVI (CPVI) vs. time for different schemes. FIM takes time step sizes that grow with time, whereas time steps in the semi-explicit schemes are limited due to stability.
a low mobility-ratio \((M = 1)\) case. As shown in Figure 6.3(a), the TAIM model has less numerical dispersion compared with the FIM result using large time steps; moreover, TAIM has a sharp front, similar to that of IMPEST. In order to make a direct comparison of the diffusion levels, the simulator was forced to take the same time steps in FIM as those in IMPEST (labeled as \textit{FIM small dt} in Figure 6.3(a)). The IMPEST solution has a sharper front as expected; however, due to the explicit treatment of saturation and temperature, smaller time steps are allowed compared to the TAIM and FIM solutions. Section 6.2 covers the results for a high mobility-ratio \((M = 30)\) case typically observed for medium heavy-oil reservoirs [30], [37]. From Figures 6.3(a) and 6.3(b), we observe a correspondence between the saturation front and the governing saturation CFL. Note that the CFLS number is largest around the water front where the shock travels with the maximum speed. This follows from the expression of CFLS given by Eq. 3.49.

In order to establish the correctness of the TAIM solution, we compare the results with the analytical solution obtained using the fractional flow curve shown in Figure 6.1 for the low mobility ratio case. The TAIM solution is compared with the analytical solution for two times, namely 0.2 and 0.3 PVI. These are shown in Figures 6.4(a) and 6.4(b), respectively. We observe that the TAIM solution is more accurate and is closer to the analytical solution.
compared to the FIM solution. For the FIM solution, we used the same small time steps as were taken by the TAIM solution.

The TAIM saturation fronts are much sharper compared with the FIM solution. The effect of refining the grid is studied for this case. We evaluate the saturation profiles for the 20-gridblock case using FIM and the percentage-based TAIM. Figure 6.5 shows the water saturation profile as a function of the distance from the injector for the coarse-grid FIM (20 gridblocks), medium-grid FIM (60 gridblocks), fine-grid FIM (100 gridblocks) and the TAIM solution for the 20-gridblock coarse-grid and the 60-gridblock medium-grid. We observe that the level of diffusion in the TAIM coarse profile is comparable to that when we refined the FIM grid by three times. Also, the TAIM medium-grid profile matches with the FIM fine-grid profile. Thus, TAIM on the coarse-grid fares better than FIM on a much finer grid, by producing more accurate solutions.

Thermal conductivity is an important aspect as it affects the transfer of heat through the rock. The most common value of thermal conductivity in reservoir formations like Berea sandstone is between 20 and 40 BTU/ft-day-F \cite{37}. The heat conductivity value varies insignificantly with saturation changes. Hence, it is a valid engineering assumption to use a constant value for thermal conductivity ($\kappa$) within this range. It has been observed that
as the water saturation decreases, thermal conductivity values decrease [37]. A decrease in $\kappa$ leads to larger allowable time step sizes. This follows from the temperature CFL expression given by Eq. 3.36. We study thermal conduction in detail in the next section. The value of $\kappa$ used for this simulation is 40 BTU/ft-day-F. Figure 6.3(b) shows a comparison between CFLS and CFLT at 0.4 PVI. We observe that the CFLS values are much larger than the CFLT values implying that temperature is rarely the governing CFL number for time step selection. Additionally, the highest CFLS value occurs near the water saturation front, which coincides with the maximum change in $S_w$. (Refer to the IMPEST profile in Figure 6.3(a).)

### 6.2 Thermal Conduction

Thermal conduction effects are evaluated using the following three simulations: First, we study the effects of thermal conduction and convection on the CFLT number using a 2-D setting. Then, we study the influence of rock heat capacity compared to conduction. Finally, we consider TAIM with variable-based switching, and we compare it with the percentage-based switching strategy for a 2-D tertiary hot-water flooding problem.
The physical set-up consists of a quarter of a five-spot pattern with dimensions taken from the field example of Martin et al. [30] represented using a 10x10x1 cartesian grid, with hot-water injection at a constant rate from one corner and production at the diagonally opposite corner. The well blocks are treated fully implicitly. The initial water saturation in the reservoir is 0.2, and the API gravity of the oil is 20. The end-point mobility-ratio is 30, and the corresponding fractional flow curve is similar to that shown in Figure 6.1.

Case (i): Analysis of thermal conduction and convection

The study of thermal conduction versus heat convection is more evident in a 2-D simulation as compared to 1-D systems, where distinguishing between the effects of conduction and convection is nontrivial, because heat transfer due to conduction and the saturation front are both in the same direction. In 2-D scenarios, it is straightforward to locate the saturation front and distinguish that from regions not invaded by the water. However, due to conduction, heat transfer occurs everywhere in the reservoir, leading to pockets, where conduction is comparable to convection that cannot be observed in 1-D. The CFLT magnitude directly depends on the value of the thermal conductivity ($\kappa$) (described by Eq. (3.36)). The heat conduction value used in this simulation is high (1000 BTU/ft-day-F), such that the magnitude of the conduction term in the CFLT expression of Eq. (3.36) becomes comparable, or larger, than the convection term.

The water saturation and temperature maps in the reservoir at 0.2 PVI are shown in Figures 6.6(a) and 6.6(c), respectively. The temperature front lags behind the saturation front due to heat contained in the rock. Figures 6.6(d) and 6.6(b) show the governing CFL maps for the two cases when temperature is treated explicitly and implicitly, respectively. As the figures indicate, when temperature is implicit, the time step sizes are governed by the stability of the explicit saturation variable. However, when temperature is explicit, the time step sizes are governed by the stability of both explicit saturation and temperature. The CFLS expression given by Eq. (3.49) corresponds to the saturation front as shown in Figures 6.6(a) and 6.6(b).

With a large heat conductivity of 1000 BTU/ft-day-F, the CFLT numbers become higher than the CFLS numbers. The CFLS numbers take their largest values near wells and saturation fronts. On the other hand, the CFLT numbers take their largest values near wells due to heat convection by fluids and in regions away from fronts due to heat conduction. The
Figure 6.6: Injection well is at the lower left corner, and the producer is at the upper right corner. CFLS corresponds to the saturation profile. Injection is at 400 F, and the initial temperature is 100 F. The temperature front lags behind the saturation front due to heat contained in the rock.
The time step is calculated using the largest of the CFLS or CFLT values in the reservoir. The CFLT number that controls the time step is near the injection well, and both convection and conduction contribute to the CFLT in the near-well region. This can be seen from the conduction and convection contribution maps for the explicit-temperature case shown in Figures 6.6(e) and 6.6(f). It is evident that in parts of the reservoir, where the water front has not yet arrived, the CFLT number is larger than the CFLS number. The value of the thermal conductivity used in this case is artificially high (1000 BTU/ft-day-F) and is not found in practical cases of interest. If very high conductivities exist in parts of the reservoir, and they are treated explicitly, they will create stability related problems when a large time step is used. In a percentage-based TAIM scheme, the percentage break up needs to be honored and could lead to tiny time steps, if regions dominated by conduction are present. With a variable-based switching algorithm, we can label temperature implicit only in the regions where the CFLT number is violated due to high conduction. The example illustrating the variable-based TAIM in the next test case will further clarify the details.

The time step size is sensitive to the level of conduction, as described earlier in Eq. (3.36). In the IMPEST mode, the time steps are about half the size of that allowed in the IMPTES mode. Figure 6.7 shows a comparison between the time steps when temperature is taken
explicit and implicit. It can be observed that much larger time steps are allowed when conduction is high, if temperature is implicit. The drop in the time step sizes at 0.6 PVI happens because of water breakthrough at the producer.

Case (ii): Influence of Rock Heat Capacity and Conduction

We studied the effect of changing the rock heat capacity on the saturation and temperature profiles. Rock heat capacity appears in the accumulation term of the energy equation and directly influences the temperature CFL. When the rock heat capacity is large, the heat available to fluids for convection is reduced. This results in the fluid front advancing faster than the heat front. In order to study the balance between conduction and convection using the temperature equation (Eq. (3.35)), we define the term $\chi$, which is the ratio of the amount of heat conduction to heat convection in a gridblock. This is a local number that indicates which mechanism is stronger in a gridblock at a particular time and is defined as:

$$\chi = \frac{2\kappa}{\gamma f}.$$  \hspace{1cm} (6.2)

Note that $\chi$ depends on the fluid heat capacities and the heat conduction coefficient $\kappa$. $\chi$ has a direct influence on the CFLS and CFLT values. For high heat conduction, we observe large values of $\chi$, and the CFLT controls the time step. For very low values of $\chi$, the CFLS number controls the time-step size. For values of $\chi$ close to unity, we observed that sometimes CFLS and sometimes CFLT is the governing CFL for time step selection.

The test results consist of three scenarios: (i) FIM: all variables ($P$, $T$, $S_o$) implicit; (ii) IMPEST: only $P$ implicit; and (iii) IMPTES: only $S_o$ explicit, for various values of rock heat capacity ranging from extremely low to the standard values found in references on thermal oil recovery [37]. We considered two different heat conduction coefficients to study the stability and time step behavior.

Figure 6.8 shows the water saturation profiles at 0.2 PVI for different values of rock heat capacity and heat conduction. From this figure, we find that the water saturation distribution does not depend on the value of the rock heat capacity, or conduction. This is expected because the saturation transport equations given by Eqs. 3.20 and 3.21 do not depend on either of these two parameters. Figure 6.9 shows the temperature distribution for the FIM simulation. The profiles for the IMPEST and IMPTES simulations are similar. As
Figure 6.8: Water saturation profiles at time 0.2 PVI for different rock heat capacities and conduction. Injection well is at the lower left corner; water front moves towards the producer at the upper right corner.

Figure 6.9: Temperature profiles at time 0.2 PVI for different rock heat capacities and conduction.
observed, when the conduction coefficient is low ($\kappa = 25$ BTU/ft-day-F), the effect of rock heat capacity on the temperature profile is obvious. For extremely low heat capacities, the temperature and water saturation fronts move together. Physically this means that no heat is being retained by the rock, and all the heat content moves with the fluids. However, when the heat capacity is relatively large, the rock retains significant amounts of heat, and we observe that the temperature front lags behind the water saturation front. The second order diffusion term accounts for the thermal heat conductivity in the energy transport equation given by Eq. 3.22. From Figure 6.9 we observe that when we have high heat conduction, the temperature profile is more dispersed compared to the low heat conductivity case.

In order to draw conclusions from this experiment, we first recap the expression for CFLT. From Eq. 3.36, we have

$$CFLT = \Delta t \left( \frac{A\gamma_f}{\phi V \gamma_s} + \frac{2T_H}{\phi V \gamma_s} \right),$$

where, $T_H$ is the heat conduction transmissibility, given by

$$T_H = \frac{A\kappa}{\Delta x}.$$

The expressions for $\gamma_f$ and $\gamma_s$ were given earlier (see Eq. (3.35)). We observe that the CFLT value is inversely proportional to the rock heat capacity and directly proportional to the heat conductivity coefficient. This implies that when the rock heat capacity is small, or $\kappa$ is large, the CFLT values are large. A higher CFLT translates into a smaller allowable time step size due to the maximum CFL limit.

Next, we compare the relative effects of rock heat capacity and thermal conduction on the time step size. This is illustrated in Figure 6.10, which shows the time step history for four different combinations of rock heat capacity and thermal conductivity, namely, (i) low rock heat capacity, low heat conductivity; (ii) low rock heat capacity, high heat conductivity; (iii) high rock heat capacity, low heat conductivity; and (iv) high rock heat capacity, high heat conductivity. As observed from the figure, the thermal conductivity, $\kappa$, has a larger influence on the time step size compared with the rock heat capacity. When the heat conductivity is low, the effect of varying the rock heat capacity on the time step size is small. When heat conduction is kept constant, with a smaller rock heat capacity, the time step profile shows slightly smaller time steps than the profile for the higher heat capacity.
Figure 6.10: Time step history for the explicit saturation and temperature case for different rock heat capacities and conduction.

case. However, with a larger heat conductivity, time step sizes are reduced to half their magnitudes due to the very large CFLT values. When heat conductivity is large and heat capacity is small, the time steps are extremely tiny. Thus, we conclude that the influence of heat conduction on the CFLT values and time step sizes is more significant than the influence of the rock heat capacity. We observe a drop in the time step sizes at 0.6 PVI because of water breakthrough at the producer well. The water breakthrough brings about strong gradients in the vicinity of the well. The stability criteria make sure that saturations and temperatures do not oscillate by forcing a lower time step at this time.

Case (iii): Variable-based TAIM

This test case represents a realistic scenario of tertiary hot-water flooding in a heavy-oil reservoir using our variable-based TAIM switching algorithm. The results are also compared with the percentage-based TAIM approach. The setup is the same as in the 2-D test case described earlier for Case (i). We use a standard value of 25 BTU/ft-day-F and a high value of 100 BTU/ft-day-F; the high value could occur due to local variations in heat conductivity caused by sudden temperature changes or fluid saturation distributions. Due to the high
oil viscosity, water breaks through at the producer in a very short time. Therefore, we plot
the water saturation map and the corresponding CFLS map just before breakthrough at 0.1
PVI. These are shown in Figures 6.11(a) and 6.11(b). As observed, the correspondence of
the two is similar to that in the 1-D case described earlier. However, when water moves in
every part of the reservoir due to the spreading caused by the high mobility ratio, there is
two-phase flow everywhere. The leading saturations advance with the highest speeds in the
vicinity of the producer; as a result, the highest CFLS numbers occur near the well. The

![Figure 6.11: Injection well is at the lower left corner, and the producer is at the upper right corner. Observe the correspondence between Figures 6.11(a) and 6.11(b). At later times after breakthrough, time-step is controlled by large velocities as opposed to large saturation gradients.](image-url)
saturation and CFLS maps after breakthrough are shown in Figures 6.11(c) and 6.11(d). The time step is now controlled by large velocities as opposed to large saturation gradients.

For the lower heat conductivity value of 25 BTU/ft-day-F, the CFLT number is never the governing CFL. We observe that the highest CFLT values are due to convection rather than conduction as illustrated by Figures 6.12(a) and 6.12(b), which show the conduction and convection contribution to the CFLT value, respectively. Figure 6.13 is the CFLT profile at 0.1 PVI, and we observe that convection is the main contributing mechanism to
CHAPTER 6. VALIDATION USING GPRS

Figure 6.14: Implicit level structure at 0.1 PVI. 1 implicit variable means only Pressure (P) implicit, 2 implicit variables mean both Pressure and Saturation (S) implicit, and 3 implicit variables mean Pressure, Saturation and Temperature (T) implicit. Observe that convection makes both variables, P and S, implicit in the region invaded by water. Even with a higher thermal conduction, the implicit level structures looks similar. T is implicit only near the well region.

In order to compare the percentage and variable-based TAIM schemes, the same simulation was performed using a predefined percentage breakdown of IMPEST (80%) and FIM (20%). We observe that the time steps are much smaller in the percentage-based TAIM, as compared to the variable-based TAIM. This is shown in Figure 6.15. The time steps in the percentage-based TAIM depend on a user-defined breakdown of implicit level schemes.

The maximum time step size used for the FIM and the variable-based TAIM in this case is
Figure 6.15: Time steps for various schemes. Note that the variable based TAIM uses large time steps and gives an optimized implicit level structure as shown in Figure 6.14(a).

Figure 6.16: Implicit level structure at 0.5 PVI. Observe that a larger time step size of 8.25 CPVI forces more FIM blocks compared to the smaller time step size of 5.5 CPVI.

5.5 CPVI (cell pore volumes injected). 1 CPVI is the dimensionless time during which the injected fluid invades 1 gridblock of the reservoir. It is given as $CPVI = \frac{Q_{inj} t}{\phi V_{cell}}$. However, if we take an even more aggressive time step size for the variable-based TAIM, we observe that the implicit level structure contains more FIM blocks. This is shown in the implicit level
distribution shown in Figures 6.16(a) and 6.16(b). This happens because some of the blocks with CFL numbers less than unity for the smaller time steps become greater than unity for the larger time step. Thus, variable-based TAIM labels the implicit level distribution based on any given time step size. If the time step size is extremely large, variable-based TAIM would treat everything fully implicitly.

6.3 Phase Changes

For the phase change test case, single-phase gas is injected into single-phase oil. The gas injection is done in an isothermal setting to study the phase behavior effects, specifically the appearance and disappearance of the phases, and the effectiveness of the stability criteria and switching algorithms for the AIM method. The physical set-up for this test case is a 1-D reservoir 15000 ft in length divided into 50 gridblocks. A mixture of methane and carbon dioxide in a 1:9 proportion is injected into single-phase oil with four components, namely, \( CH_4, CO_2, C_4H_{10} \) and \( C_{10}H_{22} \). The injector and producer are BHP controlled and are located in gridblocks 1 and 50, respectively. The system is homogeneous with an absolute permeability of 1 darcy and 30 percent porosity. Relative permeabilities of the oil and gas phases are quadratic functions. Each of the components can exist in either of the two phases based on their phase behavior. The primary variables for this simulation are the pressure \( P \), \( n_p - 1 \) phase saturations \( S_p \), and \( n_c - n_p \) mole fractions \( y_c \), where \( n_p \) is the total number of phases, and \( n_c \) is the total number of components in the system. The implicitness in a gridblock can be defined by either having only pressure implicit, both pressure and saturations implicit with mole fractions explicit, or all the variables implicit.

The current version of GPRS is designed such that when a phase disappears, the primary variables become \( P \), and \( n_c - 1 \) mole fractions \( y_c \) or \( x_c \) depending on whether the oil or the gas phase disappeared, respectively. However, when the phase changes in the middle of solving for a time step, the implicit level that was decided based on the stability criteria at the beginning of the time step may not be adequate to handle the nonlinear evolution. AIM in GPRS is designed to treat both the mole fractions and the saturations as explicit (IMPES-AIM mode), or the mole fractions explicit and the saturations implicit (IMPSAT-AIM mode). If saturations are treated implicitly and the mole fractions are explicit, the time step size would be such that it honors the explicit mole fraction treatment. In that
case, treating the $n_p - 1$ mole fractions implicitly is a conservative strategy that does not affect the stability of the simulation.

The derived stability criteria are based on the linear von Neumann method, so they may not be able to capture the nonlinear behavior of the system during the time step, and hence not be able to always predict if a phase would reappear during the nonlinear solver iterations. This means that a single-phase gridblock with primary variables $P$, and $n_c - 1$ mole fractions ($y_c$ or $x_c$) will now have the original set of variables consisting of phase saturations $S_p$. For such cases, the implicit level with respect to saturation is defined by calculating the single-phase saturation CFL. It has been observed in the test cases that this method is able to specify the saturation implicit level correctly without any loss of monotonicity in the saturation profile.

A more conservative approach, however, would be to treat saturation implicitly in all the single-phase gridblocks, or to use heuristics to have implicit saturations in single-phase gridblocks in the vicinity of multi-phase gridblocks, or be able to assign new implicit levels in the middle of the time step when a phase reappears. The current version of GPRS is not designed for changing the implicit levels during a time step.

With the above mentioned implicit level assignment logic, in order to study phase-change
Figure 6.18: Time step profile for FIM, variable-based AIM and percentage-based AIM.

Figure 6.19: CFL profile at different times for percentage-based AIM. The number of gridblocks going unstable increases with time, and therefore time step size reduces with the fixed percentage breakup.
Figure 6.20: CFLS profile at different times for variable-based AIM. CFLS is greater than unity at later times for many gridblocks.

Figure 6.21: CFLX profile at different times for variable-based AIM. CFLX is lesser than CFLS.
behavior and whether the derived stability criteria and the switching algorithms explained in the previous chapters are functioning as desired, we designed a test case with both reappearance and disappearance of phases. We evaluate the performance of the variable-based and the percentage-based AIM schemes against the fully implicit method. Figure 6.17 shows the gas saturation profile in the reservoir at different times using the variable-based AIM. We observe that as time increases, gas invades the reservoir from left to right. The gas phase appearance and disappearance occurs in different parts of the reservoir.

The time step profiles for the FIM, variable-based AIM, and percentage-based AIM with 70 percent IMPES and 30 percent FIM are shown in Figure 6.18. We observe that the variable-based AIM takes time steps as large as the FIM simulation; however, the percentage-based AIM takes time steps which are smaller in size due to stability restrictions. Figure 6.19 shows the CFL profile for the percentage-based AIM. As time increases, more blocks violate the CFL criteria. Thus, keeping the percentage of IMPES blocks fixed, we are forced to use smaller and smaller time steps. This is avoided by using the variable-based AIM, where initially we operate with almost 95 percent IMPES and 5 percent FIM, and later on in the simulation, the percentage of FIM blocks progressively increases, while we continue to use the same time step size.

Figures 6.20 and 6.21 show the saturation CFL (CFLS) and the composition CFL (CFLX) profiles at different times. We observe that CFLS is always larger than CFLX during the simulation. With the choice of time step size for the variable-based AIM, we observe that both CFLS and CFLX are greater than unity for blocks in the vicinity of the gas front and the well blocks. The correspondence between the gas front and CFLS can be observed from Figures 6.17 and 6.20. Thus, only those few blocks had to be treated implicitly, and everywhere else, only pressure was implicit. This can be seen from the implicit level structure shown in Figure 6.22. At later times, the time step size for variable-based AIM is quite large, such that we need fully implicit treatment in most of the reservoir model. Additionally, when we reduce the time step size used for the variable-based switching to half the size used in the above experiment, we observed that only the saturation CFL was violated. Thus, the implicit level structure at different times shows that only saturation requires implicit treatment, which tracks the moving gas front; the mole fractions stayed explicit throughout the simulation. This is the major benefit of the variable-based algorithm, as it allows selective treatment of variables based on their stability for a desired time step.
The second test case is a three-phase thermal-compositional case studied in a 1-D setting with 50 gridblocks. We inject hot water in the first gridblock and produce from the last gridblock. The initial composition consists of a mixture of oil and gas with four hydrocarbon components, namely, $CH_4$, $CO_2$, $C_4H_{10}$ and $C_{10}H_{22}$, and water. Water is immiscible with both the gas and the oil phases. We study the performance of the TAIM method and we compare it to the FIM method using two different relative permeability models. In the first model, we use quadratic exponent values with the Honarpour [24] relative permeability empirical relations. The relative permeability for the intermediate wettability oil phase is calculated using Stone’s method II [39]. The relative permeability for the oil phase as a function of the gas and the water saturations is shown in Figure 6.23. The corresponding fractional flow curves for the water and the gas phases are shown in Figures 6.24(a) and 6.24(b), respectively. Recall that the assumptions made in determining the CFL numbers for saturation are that the eigenvalues obtained using Eq. 3.52 are bounded and that the two-by-two matrices are very close to normality. The normality of a matrix $A$ is determined by evaluating the norm of $AA' - A'A$. If the norm is on the order of $10^{-2}$, the matrix $A$ is
Figure 6.23: Oil relative permeability as a function of the water and the gas phases for Honarpour exponent values equal to 2.

Figure 6.24: Fractional flow curves for water and gas for quadratic relative permeabilities corresponding to Figure 6.23.
Figure 6.25: Oil relative permeability as a function of the water and the gas phases for Honarpour exponent values equal to five.

Figure 6.26: Fractional flow curves for water and gas for quadratic relative permeabilities corresponding to Figure 6.25.
Figure 6.27: Water saturation and the governing saturation CFL profile at time = 160 days for the quadratic relative permeabilities. Note that CFLS corresponds to the water saturation profile shown in Figure 6.27(a).

Figure 6.28: Time step profile for the FIM, the variable-based and the percentage-based TAIM schemes for the quadratic relative permeabilities.
considered to be close to normal. For the quadratic relative permeability model, the matrices are very close to normality. However, for highly nonlinear systems, such that the exponent value used with the Honarpour relative permeability empirical relations is as large as five, the two-by-two matrices have bounded eigenvalues, but the matrices far from normal. The norms are then of order one. The oil-relative permeability is given in Figure 6.25 for this case. We observe that the relative permeability gradients are sharper for this large exponent of five compared with the quadratic relative permeabilities shown in Figure 6.23. The corresponding fractional flow curves for the water and the gas phases in this case are shown in Figures 6.26(a) and 6.26(b), respectively.

Figure 6.27(a) shows the water saturation profile for the FIM, variable-based TAIM, and the percentage-based TAIM schemes when we use the fractional flow curves of Figures 6.24(a) and 6.24(b). We observe that the percentage-based TAIM has the least amount of numerical dispersion in the water saturation profile. The governing CFL number is the saturation CFL. Both the temperature and the composition CFL numbers are much smaller than unity. The corresponding CFLS profile is shown in Figure 6.27(b). The maximum CFL number is obtained near the front. Note that we only show the first 10 gridblocks on the figures in order to highlight the solution behavior in the critical regions at the given time. The time step history is shown in Figure 6.28. We observe that when we increase the percentage
of the fully implicit scheme in the TAIM method, the time steps are comparable to those used in the FIM simulation. For an 80 percent IMPEST fraction in the TAIM method, we obtained time steps that are the same as the FIM method for this particular test case. The results are similar to those given above when we used the fractional flow curves with the more nonlinear relative permeabilities. Figure 6.29 shows the water saturation profile for the FIM, variable-based TAIM, and the percentage-based TAIM schemes when we use the fractional flow curves of Figures 6.26(a) and 6.26(b). We observe that the variable-based and the percentage-based TAIM profiles are identical. This implies that at the given time step size, the variable-based TAIM uses the same number of implicit variables as in the percentage-based TAIM. Clearly, there is more numerical dispersion in the FIM profile compared to the TAIM profiles. The saturation CFL number governs the time step for this case. Thus, even for a more nonlinear system with eigenvalue matrices far from normality, the CFL numbers obtained using our stability analysis allow for choosing the time step without compromising the stability or accuracy of the TAIM formulation.

### 6.4 Gravity

In the previous examples, we covered horizontal test cases that were either one or two-dimensional. That allowed testing physical mechanisms such as fluid and heat convection, thermal conduction, and phase change behavior. In this section, we focus on gravity effects. We compare the analytical solution of the gravity segregation problem with GPRS simulations in 1-D. We then study the effects of gravity segregation in an isothermal immiscible oil-water system with a low rate of injection. Following that, we analyze the performance of TAIM for a miscible thermal gas-injection problem with gravity and complex phase-change behavior. The objective is to evaluate whether the TAIM algorithm is able to calculate CFL numbers and assign the implicit levels when complex nonlinear behaviors due to gravity and phase change take place in the reservoir model.

We begin with comparing the analytical solution of vertical segregation for a simplified one-dimensional immiscible problem with numerical simulations using GPRS. Subsequently, we show the results for both the immiscible and miscible cases for a 2-D vertical setting. Finally, we conclude this chapter with the results for a 3-D case, in which we compare the time step sizes and number of implicit variables taken at each time step using FIM,
variable-based and percentage-based TAIM.

The test case is designed for a one-dimensional vertical plane 30 ft by 100 ft divided into 100 blocks in the vertical dimension, with the top half layers fully saturated with oil, and the bottom half layers saturated with gas at residual oil saturation of 0.22. Thus, we expect the heavier oil to flow down due to gravity and the lighter gas to move upward. The following derivation explains the mathematical equations that describe the terms relating to viscous and gravitational effects and the relevant physical factors.

![Figure 6.30: Set-up for derivation of gravity to viscous ratio.](image)

For the set-up shown in Figure 6.30, for two phases, with phase 1 overlying on phase 2, with densities \( \rho_1 \) greater than \( \rho_2 \) and viscosities \( \mu_1 \) and \( \mu_2 \), the darcy equations are given as follows:

\[
v_1 = -\frac{k k_{r1}}{\mu_1} \left( \frac{\partial P_1}{\partial z} + \rho_1 g \right), \quad (6.3)
\]

and

\[
v_2 = -\frac{k k_{r2}}{\mu_2} \left( \frac{\partial P_2}{\partial z} + \rho_2 g \right). \quad (6.4)
\]

Conservation of mass for each of the two phases gives the following equations:

\[
\phi \frac{\partial S_1}{\partial t} + \frac{\partial v_1}{\partial z} = 0,
\]

(6.5)
and

\[ \phi \frac{\partial S_2}{\partial t} + \frac{\partial v_2}{\partial z} = 0. \]  

(6.6)

Also, we have \( S_1 + S_2 = 1 \). Adding Eqns. 6.5 and 6.6, we obtain the following relation between the phase velocities:

\[ \phi \frac{\partial (S_1 + S_2)}{\partial t} + \frac{\partial (v_1 + v_2)}{\partial z} = 0, \]

\[ \Rightarrow v_1 + v_2 = \text{constant} = 0, \]  

(6.7)

\[ \Rightarrow v_1 = -v_2. \]  

(6.8)

We eliminate the pressure terms in Eqns. 6.3 and 6.4 ignoring the effects of capillary pressure and obtain the following relation between the velocity \( v_2 \) and the physical properties:

\[ \frac{\partial (P_2 - P_1)}{\partial z} = \frac{\mu_1 v_1}{k k_{r1}} - \frac{\mu_2 v_2}{k k_{r2}} + g (\rho_1 - \rho_2) = 0, \]

\[ \Rightarrow v_2 = \frac{g (\rho_1 - \rho_2) k}{\frac{\mu_1}{k_{r1}} + \frac{\mu_2}{k_{r2}}}. \]  

(6.9)

We can write Eq. 6.9 in the following form, replacing the subscript 1 with \( o \) for the oil phase, and 2 with \( g \) for the gas phase:

\[ v_g = \frac{g (\rho_o - \rho_g) k}{\mu_g} F(S_g), \]  

(6.10)

where,

\[ F(S_g) = \frac{k_{rg}}{1 + \frac{k_{rg}}{k_{ro} \mu_g}}. \]  

(6.11)

Hence, from Eq. 6.6:

\[ \phi \frac{\partial S_g}{\partial t} + \frac{\partial v_g}{\partial z} = \phi \frac{\partial S_g}{\partial t} + \frac{g (\rho_o - \rho_g) k}{\mu_g} \frac{\partial F}{\partial S_g} \frac{\partial S_g}{\partial z} = 0, \]  

(6.12)
\[ \frac{\partial S_g}{\partial t} + \frac{g(\rho_o - \rho_g)}{\phi \mu_g} F'(S_g) \frac{\partial S_g}{\partial z} = 0. \] (6.13)

Introducing the dimensionless time \( t_D \), and distance \( z_D \), as given by the following definitions:

\[ t_D = t \frac{g(\rho_o - \rho_g)}{\phi \mu_g H}, \] (6.14)

where, \( H \) is defined as the total thickness of half of the layers; in this case \( H \) is equal to 50 ft, and

\[ z_D = \frac{z}{H}. \] (6.15)

We can write the governing equation in dimensionless form as:

\[ \frac{\partial S_g}{\partial t_D} + F'(S_g) \frac{\partial S_g}{\partial z_D} = 0. \] (6.16)

Figure 6.31: \( F(S_g) \) function for Honarpour relative permeability curves, and the tangents showing the Buckley-Leverett shocks. Saturation at point \( C \) is static.

The \( F(S_g) \) function is a bell shaped function when Honarpour [24] relative permeability functions are used with the parameters \( n_g = n_o = 2, S_{oi} = 0.22, S_{gr} = 0, k_{ro}^o = 0.9 \) and \( k_{rg}^o = 1 \). We use \( \mu_o = 1.2 \) and \( \mu_g = 0.96 \). Figure 6.31 shows the \( F(S_g) \) function plotted against the gas saturation. The saturations to the right of point \( C \) will move with a positive velocity, and those to the left will move with a negative velocity. The saturation at point \( C \) will not move. There are two shocks, the gas shock propagating upward, and the oil
Figure 6.32: Gas saturation profiles as a function of the dimensionless distance $z_D$. The shocks reverse direction at $t_D = 3.1$ and $3.5$ for the gas and oil respectively.

shock moving downward. We observe from the tangent construction on Figure 6.31 that the gas shock moves with a velocity of 0.325, and the oil shock with a velocity of 0.287. The stationery gas saturation at point $C$ is 0.37. Gas saturations between 0.28 and 0.46 travel as a spreading wave. After $t_D = 3.1$, the faster gas shock reaches the top boundary, which creates a new discontinuity in saturation at the boundary, and the shock reflects back and moves in the opposite direction. Similarly, after $t_D = 3.5$, the oil shock reaches the lower boundary, and the reflected shock travels in the upward direction. This can be observed from the saturation profiles from the GPRS simulation shown in Figure 6.32. The saturation profiles from the simulation are different from what is expected for the analytical solution due to the shocks being smeared due to numerical dispersion. However, we get an accurate estimate of the shock velocities and times required for their reversals. We also note that after the shocks reach the respective boundaries and reverse their directions, the segregation of the gas and oil takes place very slowly, and even after $t_D = 15$, complete separation had not yet occurred.

We simulated the above test case using the variable-based switching algorithm. The implicit-level structure in the domain for this case at various times is shown in Figure 6.33. We observe that initially when the shocks start moving, the implicit blocks correspond to the leading edges of both the faster moving gas shock and the slower moving oil shock.
Figure 6.33: Implicit level structure for the variable-based AIM showing the implicit variables taken by the simulator at different times. Saturation is explicit everywhere except green blocks that indicate implicit saturation.

More gridblocks are required to be implicit around the faster moving shock compared to the slower shock. Later, when the shocks reflect back, the implicit blocks exist both near the top and the bottom boundaries. For very late times, when the saturation gradients are no longer sharp, the CFL numbers are small and large time steps can be taken. So, the simulation runs in explicit saturation mode. Thus, the CFL numbers for saturation are quite accurate, and the AIM scheme labeled the variables implicitly in a consistent and correct manner.

We show results for a case that is similar to the one described above, but that additionally includes fluid injection such that we can compare the relative effects of viscous and gravitational forces. Assuming the viscous flow rate is $q_2$ into the system, using Eq. 6.9 the ratio between the viscous and gravitational flow is given by...
\[
\frac{q_2}{A v_2} = \frac{q_2 \left( \frac{\mu_1}{k_{r1}} + \frac{\mu_2}{k_{r2}} \right)}{k A (\rho_1 - \rho_2) g}.
\]

(6.17)

From Eq. 6.17, we observe that higher the density difference between the two fluids, the higher is the ratio of gravitational and viscous force. Similarly, gravity effects increase as the vertical permeability \((k)\) of the medium increases. The following numerical experiment was conducted with the flow rate such that dimensionless ratio of viscous to gravity forces defined by the above equation is of the order of \(10^{-3}\). In this test case, we have a vertical domain with 10 gridblocks in each direction. The top half layers are water saturated at zero residual oil saturation, and the bottom half layers are oil saturated at a residual water saturation of 0.22. The bottom left of the reservoir has an injection well with a very low oil injection rate, such that gravity is dominant compared with convection. The top right of the reservoir has a producer in order to avoid pressure build-up in the domain.

Figure 6.34: Water saturation distribution at the start of the simulation. Heavier water will flow down and replace the lighter oil.

Figure 6.34 shows the water saturation distribution at the start of the simulation. After initializing the reservoir as described above, we observe that saturation changes start to occur near the middle, as that is the location with largest density difference across the
Figure 6.35: Oil injection well is at the lower left corner, and the producer at the upper right corner. CFLS map corresponds with the $S_w$ map. The variables are treated implicitly in regions with gravitational flow.
Figure 6.36: Water saturation, CFLS and Implicit level structures at later times for the case shown in Figures 6.35(a)-6.35(f). Observe that water saturation changes are small after 0.4 PVI.
gridblocks. As the simulation proceeds, the water saturation decreases in the layers above the middle of the reservoir and increases in the bottom half. After about 0.3 PVI, water saturation in the bottom layers becomes larger than the water saturation in the top layers, indicating that gravity played its role and redistributed the fluids according to their densities. From Figures 6.35(a) - 6.36(f), we observe that the CFLS number corresponds to the saturation change map. The CFLS numbers are largest in regions with the highest density differences, leading to flow due to gravity. When we increased the density difference, the CFLS numbers increase in magnitude, and the saturations change at a faster rate. At 0.4 PVI, the water saturation does not change significantly in the bottom layers. Thus, the CFLS numbers are lower in the bottom layers but continue to be high in the top layers, where the water saturation is still changing due to redistribution of the fluids.

The implicit level structure looks like a band in the beginning, when the fluids just start to flow, and later depending upon the CFL numbers, the structure changes to accommodate the stability of the saturation variable. This simulation was also run using the percentage-based AIM with different percentage distributions of IMPES and FIM. The time step profiles for the various schemes are shown in Figure 6.37. We observe that initially when the fluids start to segregate, the stability criteria restrict the time step sizes. However, after a time of 0.4 PVI, the system is more stable and the percentage-based AIM can take time steps as large as FIM, or variable-based AIM. The 90 percent AIM still struggles to reach the larger
Figure 6.38: Gas saturation, CFLS and CFLX maps at time = 35 days and 170 days. Observe that CFLX is much smaller than CFLS at late time during the simulation.
(a) Implicit level at time = 35 days.  
(b) Implicit level at time = 170 days.

Figure 6.39: Gas injection well is at the lower left corner, and the producer at the upper right corner. Early in the simulation, both compositions and saturations are treated implicitly, whereas later only saturations are implicit. Temperature is treated explicitly everywhere, except the well blocks.

Figure 6.40: Time step profile for FIM, variable-based TAIM and percentage-based TAIM.

time step sizes, however.

The second test case is an application of the combined effects of fluid convection, gravity and phase change. We inject hot gas into a four-component oil and gas miscible system. The flow rates for the injection and production wells are such that both viscous and gravitational forces contribute to flow, as the density difference between the oil and the gas phases is very high, and we use a $\frac{k_v}{k_h}$ ratio of 0.1. We inject single phase gas through an injection well
located in the lower left corner of the domain and produce from the well located in the upper right corner of the reservoir. This test case is difficult to solve numerically because of the highly nonlinear phase behavior in the system. The Appleyard Chop algorithm described in the implementation helps to converge the Newton iterations.

We conducted the simulations for this test case using the fully implicit method, and the thermal adaptive implicit method using both the percentage-based and the variable-based switching algorithms. Figures 6.38(a) and 6.38(b) show the gas saturation maps at two different times obtained using the variable-based TAIM simulation. We observe that as the simulation proceeds, the less dense gas phase flows toward the top of the reservoir displacing the more dense oil phase, and the reservoir becomes saturated with gas in the top portion. Both oil and gas are produced at the producer well. Figures 6.38(c) and 6.38(d) show the saturation CFL (CFLS) maps, which correspond to the gas saturation maps at their respective times. The composition CFL (CFLX) maps are shown in Figures 6.38(e) and 6.38(f). We observe that initially with component transfer between the oil and the gas phases, the CFLX is larger than unity, and compositions need to be treated implicitly. Later in the simulation, the rate of mole fraction flux is much lower as compared to the saturation gradients leading to an implicit treatment of the saturations in these regions. Temperature is always treated explicitly as the temperature CFL (CFLT) values are much less than unity throughout the reservoir. The implicit level structures for the two times are shown in Figures 6.39(a) and 6.39(b), respectively.

We compare the time step sizes taken by the different simulation modes, namely FIM and TAIM in Figure 6.40. We observe that as the percentage of FIM increases in the TAIM method, larger time steps are used. When temperature, saturation and mole fractions are treated explicitly, as shown in the IMPEST profile, extremely tiny time steps are necessary. The variable-based TAIM performs significantly better than IMPEST and the percentage-based algorithm, with time step sizes comparable to that of FIM simulation.

The third 3-D test problem is performed in order to show the significant gains that can potentially be achieved using the adaptive implicit method in reservoir simulation. We conducted this test on a 30x30x5 grid and inject hot gas into a four-component oil and gas miscible system with the same physical properties as in the previous test case. The injector and producer wells are completed in the top layer in a quarter of a five-spot pattern. There are five independent primary variables, namely, pressure, saturation, temperature and two
Figure 6.41: Time step profile for FIM, variable-based TAIM and percentage-based TAIM for the 3-D test case.

Figure 6.42: Number of implicit variables taken at each time step for FIM, variable-based TAIM and percentage-based TAIM for the 3-D test case. Observe that the number of implicit variables treated at each step is significantly lesser in the TAIM methods compared to FIM.
mole fractions for each gridblock. We compare the time step sizes used for FIM and TAIM simulations using both the variable-based and the percentage-based (90 percent IMPEST, 10 percent FIM) strategies. Figures 6.41 and 6.42 show the time step profile and the implicit variables, respectively. We note that the variable-based TAIM uses time steps that are comparable to FIM. The percentage-based TAIM time steps in the early period are smaller due to stability restrictions; however, later the time steps catch up with the FIM, and variable-based TAIM time steps. From the implicit variables plot in Figure 6.42, we observe that the number of implicit variables solved using the FIM method is 22500 at each time step, whereas this number is significantly reduced when we use the TAIM method. The first time step in TAIM is an FIM solve. Subsequent time steps employ a much smaller percentage of implicit variables depending upon the stability criteria. For the variable-based TAIM case, the governing saturation CFL ranges between values of five and nine in the early period. We also note that the variable-based TAIM is more flexible compared to the percentage-based TAIM. In the early period, the variable-based TAIM solves for a larger number of implicit variables compared to the percentage-based algorithm, but later in the simulation the number of implicit variables goes down quite significantly.

Several limitations must be kept in mind. First, the criteria and the switching algorithms have not been tested with steam injection. Steam injection involves highly nonlinear behavior with simultaneous phase change and gravitational effects in addition to fluid convection and heat conduction. The current stability analysis is expected to work for steam simulations and has been tested for hot water injection problems involving all of the major physical complex behaviors. Second, we have not tested cases where capillary forces in heterogeneous stratified reservoirs are present, which may lead to difficulties in gravity segregation experiments.

Thermal EOR processes with steam can be broadly classified into three major categories [37], [10], namely, (i) steam drives, (ii) cyclic steam injection, and (iii) steam assisted gravity drainage (SAGD). We provide an overview regarding the applicability of the TAIM method for steam stimulation processes. Steam drives are different from hot-water drives due to the presence and effects of the condensing vapor. The light hydrocarbon components in the crude are distilled to the gas phase. If we perform the numerical simulation for a steam drive experiment using the TAIM method, we should observe implicit treatment of
saturation and mole fraction variables in the vicinity of the steam front. The condensation front is preceded by a hot-water front. The oil viscosity is considerably reduced due to high temperatures leading to an improvement in the mobility ratio. At the hot water front, saturation variables would require an implicit treatment. It is likely that in steam drives, temperature may not require implicit treatment in regions with large temperature gradients.

Cyclic steam injection, also known as the Huff and Puff method, consists of three stages: injection, soaking and production. Steam is first injected into a well for a certain amount of time to heat the oil in the surrounding reservoir to a temperature at which it flows. After it is decided enough steam has been injected, the steam is usually left to soak for some time. Then oil is produced out of the same well. The mechanisms involved during cyclic steam injection are quite complex. During the injection phase, the TAIM method would essentially behave as that for the steam drive case mentioned above. Thus, implicit treatment would be required for saturations and mole fractions, whereas temperatures could be explicit in much of the model. During the soak phase, when fluids are not convecting, thermal conduction becomes significant owing to the heat added to the reservoir by steam. Thus, implicit treatment of temperature is likely to be necessary. Finally, in the production phase, the driving forces are mainly gravity drainage and solution-gas drive. The flow direction is now reversed, and TAIM would label the saturations at the shock fronts as implicit, and treat the other variables explicitly. Heat losses from the reservoir will affect the oil viscosity as a function of time. The rate of change of oil viscosity will influence the temperature CFL numbers.

Steam assisted gravity drainage (SAGD) is an EOR technology for producing heavy crude oil and bitumen. It is an advanced form of steam stimulation in which a pair of horizontal wells is drilled into the oil reservoir, one a few feet above the other. Low pressure steam is continuously injected into the upper wellbore to heat the oil and reduce its viscosity, causing the heated oil to drain into the lower wellbore, where it is pumped out. The basis of the process is that the injected steam forms a steam chamber that grows vertically and horizontally in the formation. Countercurrent flow of oil and water exists in the reservoir, and the main driving mechanism is gravity. The variable-based TAIM method would be particularly useful in a SAGD operation. The different mechanisms of transport, namely,
fluid and heat convection, thermal conduction, phase change and gravity exist simultaneously in the reservoir. TAIM would be able to classify the primary variables as implicit or explicit depending upon their stability numbers. Thus, implicit saturations would be found at the two countercurrent oil and water shocks. In regions where conduction would dominate over convection, temperature would be treated implicitly.
Chapter 7

Conclusions and Recommendations

Compositional and thermal-compositional reservoir simulations are increasingly required for reservoir performance predictions of Enhanced Oil Recovery processes. Thermal-compositional reservoir simulation is complex involving a large number of components and complex nonlinear behaviors. Solving the governing coupled nonlinear equations in a fully implicit manner is computationally inefficient and infeasible for large reservoirs. The adaptive implicit method provides an accurate and efficient numerical simulation technique and is key to our ability to model large-scale problems in high-resolution reservoir models with large numbers of components. This Chapter summarizes the major findings in developing Thermal Adaptive Implicit Method (TAIM) followed by recommendations for future research.

7.1 Conclusions

We developed an efficient TAIM method capable of solving the nonlinear system of equations of thermal-compositional displacement processes while treating as many variables as possible explicitly. The TAIM method takes into account the key physical phenomena found in reservoirs, namely, fluid and heat convection, thermal conduction, phase change and gravity. TAIM was implemented in GPRS and validated using various one and two-dimensional test cases. The key contributions and results are as follows:

1. **Formulation of a Thermal Adaptive Implicit method:**
   - Stability Criteria – We derived comprehensive thermal-compositional stability
criteria for saturation, temperature, and compositions of one-dimensional systems using the von Neumann method, which is a linear stability analysis technique. The criteria are easily extensible to multiple dimensions.

- Switching Algorithm – We developed a variable-based switching algorithm that uses a pre-specified time step size with stability criteria responsible for deciding if a variable needs to be explicit or implicit in a gridblock. The percentages of gridblocks with different implicit-level schemes vary in space and time.

2. Implementation in GPRS:

- Stability Criteria – We implemented the thermal stability criteria in GPRS. Pressure is always considered implicit, whereas temperature, saturation(s) and compositions could be implicit or explicit.

- Switching Algorithm – We implemented both percentage-based and variable-based switching algorithms. The percentage-based algorithm computes the maximum allowable time step size given a user-specified implicit level break-up. The variable-based algorithm decides on the implicitness of the variables depending on their CFL numbers.

3. Validation of the Criteria:

- Convection dominated flows – We designed test cases where fluid and heat convection are more dominant compared with heat conduction in a one-dimensional setting for both black-oil and compositional scenario. We studied a two-phase hot water injection in a cold oil reservoir problem with no phase disappearance or reappearance. We observed that saturations control the time step size.

- Conduction dominated flows – It is easier to study the effect of conduction in a two-dimensional test case, because there are regions far away from fluid fronts, where fluid and heat convection are small and conduction effects can be dominant. We conducted numerical experiments with the conduction transmissibility varying from low to very high values. We also studied the influence of changing the rock heat capacity. We observed that high conduction leads to stringent restrictions on the time step size, and it is computationally more efficient to solve for temperature implicitly in such cases.
• Phase change behavior – Phase change is a highly complex phenomenon in reservoir simulation. Theoretically, it involves removal or addition of variables dynamically due to phases appearing and disappearing. However, the physics of vapor-liquid equilibrium is quite complex, as variables become interdependent and variable-substitution algorithms are required. Thus, keeping track of, and quantifying, phase change is quite challenging. We studied test cases involving phase appearance and disappearance using a gas injection problem. We observed that mole fractions dominate the governing CFL at the start of the simulation, while later on saturations control the time step. In the case of steam, more rigorous analysis and validation are required.

• Gravity – We compared the analytical solution to the one-dimensional gravity segregation problem with TAIM simulation. We found that the stability criteria and the variable-based switching algorithm captured the difficult countercurrent flows and the shock reflections quite accurately. We concluded with a thermal-compositional test case that involves all of the above mentioned physical aspects simultaneously in a two-dimensional vertical domain. We observed that TAIM requires a very small percentage of the gridblocks to be treated implicitly.

7.2 Recommendations

There are three aspects to further extend and improve TAIM, in terms of formulation as well as implementation.

GPRS Enhancements for TAIM

Adaptive Timestep Control: In the variable-based TAIM strategy, we currently use a pre-specified time step that allocates the variables implicit or explicit based on their CFL numbers. Deciding the time step is nontrivial, requiring trial-and-error. A large time step would lead to a significant percentage of the gridblocks to be treated implicitly, while a small time step would be computationally inefficient. An adaptive timestep control in GPRS could leverage the time step history from previous simulations correlated with the physical reservoir description. This would further simplify the selection of the time steps not requiring guesswork from the user.
Evaluation of CFL on Selective Timesteps: CFL numbers are calculated at each time step in GPRS. We have observed that the implicit level structure in the reservoir does not change significantly between successive time steps. In other words, we can further improve the computational efficiency of the TAIM method by evaluating the CFL numbers for selective intervals instead of at each time step. This algorithm would require information about the CFL structure and the time step history. Using the CFL change history along with the time step size, it would be possible to determine intervals where CFL calculation can be avoided. An additional optimization is to evaluate the CFL numbers only in certain regions with the maximum saturation changes. However, the complexity involved in order to track the fronts may render it infeasible.

Rigorous Treatment of Phase Change During a Timestep: We evaluate the CFL numbers at the beginning of a time step assuming that the obtained time step size would give a stable solution at convergence. A more effective method is to do a nonlinear stability analysis that ensures stability even in the most difficult cases. However, a compromise to using impractical nonlinear stability analysis is to define the implicit level structure in between the Newton iterations. In highly nonlinear cases, this strategy would be particularly useful as the implicit level of a variable during the middle of Newtons might be very different from that at the start.

Linear Solvers for TAIM: Modern reservoir simulation faces increasingly complex physical models and highly resolved unstructured grids. Compositional models for heterogeneous, or fractured, reservoirs provide a considerable challenge to solver robustness and efficiency. The coupling between the mass and the energy balance equations in the Jacobian is complex and requires the development of efficient multi-stage linear solvers.

Criteria Improvements

No Heat Loss Assumption: In thermal operations, there is heat loss through the overburden and the underburden. This might affect the energy balance significantly as some of the heat would be conducted through the rock. The current formulation of the criteria assumes there is no heat loss to the surroundings.

Use of Type B variables: Currently the thermal stability criteria have been derived for the natural variable set [34]. Adjacent gridblocks may have different sets of primary variables, and we need to switch variables when a hydrocarbon phase disappears or reappears.
The variable selection (pressure, temperature, saturations and component mole fractions) in the model currently used in GPRS is called the natural variable set, or Type A variables, since the mass balance equations can be directly expressed in terms of these variables and calculation of derivatives of the Jacobian matrix is relatively straightforward. For AIM formulations, additional work is required to track the variables used in each gridblock to check the existence of individual hydrocarbon phases and perform the switch accordingly. On the other hand, Type B variables use overall compositions as the primary variables, and the same primary variables can be used for all gridblocks throughout the simulation. Even though we have to use the chain rule to calculate the derivatives for the Jacobian matrix, AIM formulation would not require additional tracking to deal with phase changes.

Additional Physical Phenomena

**Steam:** Phase changes are a highly complex phenomena in reservoir simulation. When the natural-variable set is used, they involve removal or addition of variables dynamically. Vapor-liquid equilibrium physics is complex, and variables may become interdependent, especially in processes involving steam. The choice of the primary variables in a gridblock depends on the phase state in that block. Thus, quantifying phase changes is highly complex. We have to study steam injection and SAGD problems. We currently face the limitation that we cannot run tests in GPRS with steam. This work is currently in progress by other members of the research group. We need rigorous analysis in order to be able to state any conclusion for steam-based experiments.

**Chemical Reaction Modeling:** Chemical reactions take place in many EOR processes, such as chemical flooding and in-situ combustion. It is of practical interest to be able to model these physical phenomena using adaptive implicit techniques. This requires including molecular dispersion terms and reaction rates into the governing mass-balance equations and deriving the stability criteria.
Bibliography


Appendix A

Expressions of the Stability Criteria

In order to derive the stability criteria for IMPEST systems, the saturation equation must be derived from Eq. (3.20) and Eq. (3.21), and temperature equation from Eq. (3.20) and Eq. (3.22). Thus Eq. (3.20) becomes

\[ - \rho_w u_t \frac{\partial f_w}{\partial S_w} \frac{\partial S_w}{\partial x} - \rho_w k \lambda P_c \frac{\partial^2 S_w}{\partial x^2} - \left( u_w \frac{\partial \rho_w}{\partial T} + \rho_w u_t \frac{\partial f_w}{\partial T} \right) \frac{\partial T}{\partial x} = \phi \left( \rho_w \frac{\partial S_w}{\partial t} + S_w \frac{\partial \rho_w}{\partial T} \frac{\partial T}{\partial t} \right) + \phi \left( S_w \frac{\partial \rho_w}{\partial P_w} \frac{\partial P_w}{\partial t} \right), \]  

(A.1)
and Eq. (3.21) can be expressed as

\[
\begin{align*}
\rho_o u_t \frac{\partial f_w}{\partial S_w} \frac{\partial S_w}{\partial x} + \rho_o k \bar{\lambda} P'_c \frac{\partial^2 S_w}{\partial x^2} \\
- \left( u_o \frac{\partial \rho_o}{\partial T} - \rho_o u_t \frac{\partial f_w}{\partial T} \right) \frac{\partial T}{\partial x} \\
= \phi \left( -\rho_o \frac{\partial S_w}{\partial t} + S_o \frac{\partial \rho_o}{\partial T} \frac{\partial T}{\partial t} \right) \\
+ \phi \left( S_o \frac{\partial \rho_o}{\partial P_o} \frac{\partial P_o}{\partial t} \right),
\end{align*}
\]  

(A.2)

We can eliminate the \( \frac{\partial P_n}{\partial t} \) terms from the above two equations and using Eq. (3.19) to obtain the following equation in \( S_w \) and \( T \):

\[
\begin{align*}
A \frac{\partial S_w}{\partial t} + B \frac{\partial T}{\partial t} &= -C \frac{\partial S_w}{\partial x} + D \frac{\partial^2 S_w}{\partial x^2} \\
&- E \frac{\partial T}{\partial x},
\end{align*}
\]  

(A.3)

where

\[
A = \frac{\rho_o}{S_o \frac{\partial \rho_o}{\partial P_o}} + \frac{\rho_w}{S_w \frac{\partial \rho_w}{\partial P_w}} - P'_c,
\]  

(A.4)

\[
B = \frac{\frac{\partial \rho_w}{\partial T}}{\frac{\partial \rho_w}{\partial P_w}},
\]  

(A.5)

\[
C = \frac{u_t}{\phi} \frac{\partial f_w}{\partial S_w} \left( \frac{\rho_o}{S_o \frac{\partial \rho_o}{\partial P_o}} + \frac{\rho_w}{S_w \frac{\partial \rho_w}{\partial P_w}} \right),
\]  

(A.6)

\[
D = -\frac{k \bar{\lambda} P'_c}{\phi} \left( \frac{\rho_o}{S_o \frac{\partial \rho_o}{\partial P_o}} + \frac{\rho_w}{S_w \frac{\partial \rho_w}{\partial P_w}} \right),
\]  

(A.7)

and

\[
E = \frac{u_t}{\phi} \frac{\partial f_w}{\partial T} \left( \frac{\rho_o}{S_o \frac{\partial \rho_o}{\partial P_o}} + \frac{\rho_w}{S_w \frac{\partial \rho_w}{\partial P_w}} \right) \\
- \frac{1}{\phi} \left( \frac{u_o}{S_o \frac{\partial \rho_o}{\partial P_o}} - \frac{u_w}{S_w \frac{\partial \rho_w}{\partial P_w}} \right),
\]  

(A.8)

A similar expansion of the derivative terms in Eq. (3.22) provides the second equation in terms of \( S_w \) and \( T \). Assuming the conduction transmissibility coefficient, \( \Upsilon_c \), to be constant,
the energy equation takes the form:

\[
\begin{align*}
Q \frac{\partial S_w}{\partial x} + R \frac{\partial^2 S_w}{\partial x^2} + V \frac{\partial T}{\partial x} + W \frac{\partial^2 T}{\partial x^2} &= L \frac{\partial S_w}{\partial t} + M \frac{\partial P_o}{\partial t} + N \frac{\partial T}{\partial t}.
\end{align*}
\]  

(A.9)

where

- \( Q = u_t \frac{\partial f_w}{\partial S_w} (\rho_o H_o - \rho_w H_w), \)
- \( R = k \bar{\lambda} P'_c (\rho_o H_o - \rho_w H_w), \)
- \( V = u_t \frac{\partial f'_w}{\partial T} (\rho_o H_o - \rho_w H_w) - u_o \frac{\partial (\rho_o H_o)}{\partial T} \)
  - \( - u_w \frac{\partial (\rho_w H_w)}{\partial T} \)
- \( W = T_c, \)
- \( L = \phi \left( -\rho_o U_o + \rho_w U_w - U_w S_w \frac{\partial \rho_w}{\partial P_w} \right), \)
- \( M = \phi \left( S_o \frac{\partial (\rho_o U_o)}{\partial P_o} + S_w \frac{\partial (\rho_w U_w)}{\partial P_w} \right), \)
- \( N = \phi \left( S_o \frac{\partial (\rho_o U_o)}{\partial T} + S_w \frac{\partial (\rho_w U_w)}{\partial T} \right) \)
  \( + (1 - \phi) \frac{\partial U_R}{\partial T}. \)

We can see that the energy equation is very similar in form to the mass conservation equations. The conduction transmissibility term appearing in the coefficient \( K \) of the energy equation is analogous to the capillary pressure term in the saturation equation, Eq. (A.3). We can eliminate \( \frac{\partial P_o}{\partial t} \) terms by subtracting modified Eq. (3.20) from Eq. (A.9) to obtain the following second equation in \( S_w \) and \( T \), the first being Eq. (A.3):

\[
\begin{align*}
F \frac{\partial S_w}{\partial t} + G \frac{\partial T}{\partial t} &= -H \frac{\partial S_w}{\partial x} + I \frac{\partial^2 S_w}{\partial x^2} \)
  \( - J \frac{\partial T}{\partial x} + K \frac{\partial^2 T}{\partial x^2}, \)
\end{align*}
\]  

(A.10)
APPENDIX A. EXPRESSIONS OF THE STABILITY CRITERIA

where

\[
F = -\rho_o U_o + \rho_w U_w - U_w S_w P'_c \frac{\partial \rho_w}{\partial P_w} + \frac{\rho_o}{S_o} \frac{\partial \rho_o}{\partial P_o} + \rho_w \frac{\partial \rho_w}{\partial P_w}
\]

(A.11)

\[
G = \frac{S_o \frac{\partial (\rho_o U_o)}{\partial T}}{S_o \frac{\partial (\rho_o U_o)}{\partial P_o} + S_w \frac{\partial (\rho_w U_w)}{\partial P_w}} + \frac{1}{\rho_o} \frac{\partial H_o}{\partial T} \frac{\partial \rho_o}{\partial P_o} + \frac{\partial \rho_o}{\partial P_o}
\]

(A.12)

\[
H = \frac{u_t \frac{\partial f w}{\partial S_w}}{\phi} \left( \frac{\rho_o}{S_o} \frac{\partial \rho_o}{\partial P_o} - \frac{\rho_o H_o - \rho_w H_w}{S_o \frac{\partial (\rho_o U_o)}{\partial P_o} + S_w \frac{\partial (\rho_w U_w)}{\partial P_w}} \right)
\]

(A.13)

\[
I = \frac{k \bar{\lambda} P'_c}{\phi} \left( \frac{\rho_o}{S_o} \frac{\partial \rho_o}{\partial P_o} - \frac{\rho_o H_o - \rho_w H_w}{S_o \frac{\partial (\rho_o U_o)}{\partial P_o} + S_w \frac{\partial (\rho_w U_w)}{\partial P_w}} \right)
\]

(A.14)

\[
J = -\frac{u_t \frac{\partial f w}{\partial T}}{\phi} \left( \rho_o H_o - \rho_w H_w \right) - u_o \frac{\partial (\rho_w H_w)}{\partial T} - u_w \frac{\partial (\rho_w H_w)}{\partial T} + \frac{\rho_o u_t \frac{\partial f w}{\partial T}}{\phi S_o} - \frac{\rho_o u_t \frac{\partial f w}{\partial T}}{\phi S_o}
\]

(A.15)

\[
K = \frac{\Upsilon_c}{\phi} \left[ S_o \frac{\partial (\rho_o U_o)}{\partial P_o} + S_w \frac{\partial (\rho_w U_w)}{\partial P_w} \right]
\]

(A.16)

In expressing the results, we use the same coefficients as obtained in the final derived form of the conservation equations given by Eq. (A.3) and Eq. (A.10). It will then be shown how the comprehensive stability criteria reduce to the more widely known isothermal criteria when temperature terms are dropped.
A.1 Comprehensive Stability Criteria

The comprehensive stability criteria for two explicit variables, here $S_w$ and $T$, as derived by Eq. (3.34) in section 3.2 are obtained from the following relation:

$$A + D \pm \sqrt{(A - D)^2 + 4BC} < 4,$$

(A.17)

where

$$A = 2 \left( \frac{A_1 \Delta t}{\Delta x} + \frac{2A_2 \Delta t}{(\Delta x)^2} \right),$$

(A.18)

$$B = 2 \left( \frac{B_1 \Delta t}{\Delta x} + \frac{2B_2 \Delta t}{(\Delta x)^2} \right),$$

(A.19)

$$C = 2 \left( \frac{C_1 \Delta t}{\Delta x} + \frac{2C_2 \Delta t}{(\Delta x)^2} \right),$$

(A.20)

$$D = 2 \left( \frac{D_1 \Delta t}{\Delta x} + \frac{2D_2 \Delta t}{(\Delta x)^2} \right),$$

(A.21)

and

$$\begin{pmatrix}
-A_1 & A_2 & -B_1 & B_2 \\
-C_1 & C_2 & -D_1 & D_2
\end{pmatrix} = \begin{pmatrix}
A' & B' \\
F' & G'
\end{pmatrix}^{-1} \begin{pmatrix}
-C' & D' & -E' & 0 \\
-H' & I' & -J' & K'
\end{pmatrix}. \quad (A.22)$$

On expanding the inverse of the matrix, we get the following form:

$$\begin{pmatrix}
-A_1 & A_2 & -B_1 & B_2 \\
-C_1 & C_2 & -D_1 & D_2
\end{pmatrix} = \frac{1}{\text{Det}} \begin{pmatrix}
G' & -B' \\
-F' & A'
\end{pmatrix} \begin{pmatrix}
-C' & D' & -E' & 0 \\
-H' & I' & -J' & K'
\end{pmatrix}, \quad (A.23)$$

where $\text{Det} = A'G' - B'F'$ and this leads to the following expressions:
APPENDIX A. EXPRESSIONS OF THE STABILITY CRITERIA

\[ A_1 = \frac{G'C' - B'H'}{\text{Det}}, \]
\[ A_2 = \frac{G'D' - B'I'}{\text{Det}}, \]
\[ B_1 = \frac{G'E' - B'J'}{\text{Det}}, \]
\[ B_2 = \frac{-B'K'}{\text{Det}}, \]
\[ C_1 = \frac{-F'C' - A'H'}{\text{Det}}, \]
\[ C_2 = \frac{-F'D' - A'I'}{\text{Det}}, \]
\[ D_1 = \frac{-F'E' - A'J'}{\text{Det}}, \]

and \[ D_2 = \frac{A'K'}{\text{Det}}. \]

The coefficients \( A' - K' \) are summarized below as:

\[ A' = \frac{\rho_o}{S_o \frac{\partial \rho_o}{\partial P_o}} + \frac{\rho_w}{S_w \frac{\partial \rho_w}{\partial P_w}} - P'_c, \]
\[ B' = \frac{\partial \rho_w}{\partial T} - \frac{\partial \rho_o}{\partial T}, \]
\[ C' = \frac{u_t}{S_w \frac{\partial \rho_w}{\partial T_w}} \left( \frac{\rho_o}{S_o \frac{\partial \rho_o}{\partial P_o}} + \frac{\rho_w}{S_w \frac{\partial \rho_w}{\partial P_w}} \right), \]
\[ D' = -\frac{k \lambda P'_c}{\phi} \left( \frac{\rho_o}{S_o \frac{\partial \rho_o}{\partial P_o}} + \frac{\rho_w}{S_w \frac{\partial \rho_w}{\partial P_w}} \right), \]

\[ E' = \frac{u_t}{\phi} \left( \frac{\rho_o}{S_o \frac{\partial \rho_o}{\partial P_o}} + \frac{\rho_w}{S_w \frac{\partial \rho_w}{\partial P_w}} \right) - \frac{1}{\phi} \left( \frac{u_o}{S_o \frac{\partial \rho_o}{\partial P_o}} - \frac{u_w}{\frac{\partial \rho_w}{\partial P_w}} \right), \]
\[ F' = \frac{\rho_o}{S_o \frac{\partial \rho_o}{\partial P_o}} + \frac{-\rho_o U_o + \rho_w U_w - U_w S_w P'_c \frac{\partial \rho_w}{\partial P_w}}{U_o S_o \frac{\partial \rho_o}{\partial P_o} + U_w S_w \frac{\partial \rho_w}{\partial P_w} + \frac{1 - \phi}{\phi} C_{PR} (T - T_i) \frac{\partial \rho_R}{\partial T}}, \]

\[ G' = \frac{U_o S_o \frac{\partial \rho_o}{\partial P_o} + \rho_o S_o \frac{\partial U_o}{\partial P_o} + U_w S_w \frac{\partial \rho_w}{\partial P_w} + \rho_w S_w \frac{\partial U_w}{\partial P_w} + \frac{1 - \phi}{\phi} C_{PR} (T - T_i) \frac{\partial \rho_R}{\partial T}}{U_o S_o \frac{\partial \rho_o}{\partial P_o} + U_w S_w \frac{\partial \rho_w}{\partial P_w} + \frac{1 - \phi}{\phi} C_{PR} (T - T_i) \frac{\partial \rho_R}{\partial P_o} - \frac{\partial \rho_R}{\partial P_o}}. \]
\[ H' = \frac{u_t}{\phi} \frac{\partial f}{\partial S_w} \left( \frac{\rho_o}{S_o} \frac{\partial \rho_o}{\partial P_o} - \frac{\rho_o H_o - \rho_w H_w}{U_o S_o \frac{\partial \rho_o}{\partial P_o} + U_w S_w \frac{\partial \rho_w}{\partial P_w} + \frac{1-\phi}{\phi} C_{PR} (T - T_i) \frac{\partial P_R}{\partial P_o}} \right), \]

\[ I' = k \frac{\bar{\lambda} P'_c}{\phi} \left( \frac{\rho_o}{S_o} \frac{\partial \rho_o}{\partial P_o} - \frac{\rho_o H_o - \rho_w H_w}{U_o S_o \frac{\partial \rho_o}{\partial P_o} + U_w S_w \frac{\partial \rho_w}{\partial P_w} + \frac{1-\phi}{\phi} C_{PR} (T - T_i) \frac{\partial P_R}{\partial P_o}} \right), \]

\[ J' = -\frac{u_t}{\phi} \frac{\partial f}{\partial T} \left( \rho_o H_o - \rho_w H_w \right) - u_o \left( H_o \frac{\partial \rho_o}{\partial T} + \rho_o \frac{\partial H_o}{\partial T} \right) - u_w \left( H_w \frac{\partial \rho_w}{\partial T} + \rho_w \frac{\partial H_w}{\partial T} \right) \]

\[ + \frac{\rho_o u_t}{\phi} \frac{\partial f}{\partial T} - u_o \frac{\partial \rho_o}{\partial T}, \]

\[ K' = \gamma_c \left( \frac{U_o S_o \frac{\partial \rho_o}{\partial P_o} + U_w S_w \frac{\partial \rho_w}{\partial P_w} + \frac{1-\phi}{\phi} C_{PR} (T - T_i) \frac{\partial P_R}{\partial P_o}} \right). \]

The stability numbers can be calculated from the above expressions and used in the simulator when both \( S_w \) and \( T \) are explicit.

### A.2 Isothermal Stability Criteria

From the final result of Section A.1 we can obtain the isothermal stability criteria and verify that they match with the general two-phase isothermal stability criteria as derived by Coats. [15], [16]

Substituting zero for temperature derivative terms, the various expressions become as follows:
APPENDIX A. EXPRESSIONS OF THE STABILITY CRITERIA

\[ A' = \frac{\rho_o}{S_o} \frac{\partial \rho_o}{\partial P_o} + \frac{\rho_w}{S_w} \frac{\partial \rho_w}{\partial P_w} - P_c', \]
\[ B' = 0, \]
\[ C' = \frac{u_t}{\phi} \frac{\partial f_w}{\partial S_w} \left( \frac{\rho_o}{S_o} \frac{\partial \rho_o}{\partial P_o} + \frac{\rho_w}{S_w} \frac{\partial \rho_w}{\partial P_w} \right), \]
\[ D' = -\frac{k}{\lambda} P_c' \frac{\rho_o}{\phi} \left( \frac{\rho_o}{S_o} \frac{\partial \rho_o}{\partial P_o} + \frac{\rho_w}{S_w} \frac{\partial \rho_w}{\partial P_w} \right), \]
\[ E' = 0, \]
\[ F' = \frac{\rho_o}{S_o} \frac{\partial \rho_o}{\partial P_o}, \]
\[ G' = 0, \]
\[ H' = u_t \frac{\partial f_w}{\partial S_w} \left( \frac{\rho_o}{\phi} \right), \]
\[ I' = k \frac{\lambda}{\phi} P_c' \left( \frac{\rho_o}{S_o} \frac{\partial \rho_o}{\partial P_o} \right), \]
\[ J' = 0, \]
\[ \text{and } K' = 0. \]

Thus Eq. (A.3) and Eq. (A.10) can be summarized as follows:

\[ A' \frac{\partial S_w}{\partial t} = -C' \frac{\partial S_w}{\partial x} + D' \frac{\partial^2 S_w}{\partial x^2}, \quad (A.24) \]
\[ F' \frac{\partial S_w}{\partial t} = -H' \frac{\partial S_w}{\partial x} + I' \frac{\partial^2 S_w}{\partial x^2}. \quad (A.25) \]

Each of the two equations above is of the same form as Eq. (3.38) and can be used to determine the stability criteria. We should note that we need only one equation for stability analysis because we just have one explicit variable, and that is \( S_w \) here. Thus from Eq. (A.24) we obtain the stability criteria given by Eq. (3.48) obtained in section 3.4. Therefore, we conclude that the isothermal stability criteria are a special form of the more comprehensive thermal stability criteria.
A.3 Stability Criteria in Matrix Form

The stability criteria shown in A.1 can be written in matrix form for the ease of reading them in simulation codes as follows:

\[
\begin{pmatrix}
S_w \left( \frac{\partial \rho_w}{\partial P_w} + \frac{\rho_w}{\phi} \frac{\partial \phi}{\partial P_w} \right) & \rho_w - S_w P'_c \frac{\partial \rho_w}{\partial P_w} & S_w \left( \frac{\partial \rho_w}{\partial T} + \frac{\rho_w}{\phi} \frac{\partial \phi}{\partial T} \right) \\
S_o \left( \frac{\partial \rho_o}{\partial P_o} + \frac{\rho_o}{\phi} \frac{\partial \phi}{\partial P_o} \right) & -\rho_o & S_o \left( \frac{\partial \rho_o}{\partial T} + \frac{\rho_o}{\phi} \frac{\partial \phi}{\partial T} \right)
\end{pmatrix} \begin{pmatrix} P_w \\ T' \end{pmatrix} = \begin{pmatrix} -\rho_o U_o + \rho_w U_w - U_w S_w P'_c \frac{\partial \rho_w}{\partial P_w} \\ 0 \end{pmatrix}
\]

\[-\Delta x \frac{q_v}{P'V} \begin{pmatrix} 0 & \rho_w \frac{\partial f_w}{\partial S_w} & f_w \frac{\partial \rho_w}{\partial T} + \rho_o \frac{\partial \phi}{\partial T} & \frac{\partial P_o}{\partial \phi} \\
0 & -\rho_o \frac{\partial f_w}{\partial S_w} & f_o \frac{\partial \rho_o}{\partial T} - \rho_o \frac{\partial \phi}{\partial T} & \frac{\partial S_o}{\partial \phi} \\
0 & -\frac{\partial f_w}{\partial S_w} (\rho_o H_o - \rho_w H_w) & 0 & \frac{\partial^2 T}{\partial \phi^2} \end{pmatrix}
\]

\[+\Delta x^2 \begin{pmatrix} 0 & -\frac{T}{P'V} \rho_w \tilde{\lambda} P'_c \\
0 & \frac{T}{P'V} \rho_o \tilde{\lambda} P'_c \\
0 & \frac{T}{P'V} \tilde{\lambda} P'_c (\rho_o H_o - \rho_w H_w) \frac{H T}{P'V} & 0
\end{pmatrix} \begin{pmatrix} \frac{\partial^2 P_w}{\partial \phi^2} \\
\frac{\partial^2 S_o}{\partial \phi^2} \\
\frac{\partial^2 T}{\partial \phi^2}
\end{pmatrix}
\]

where

\[A = S_o \frac{\partial (\rho_o U_o)}{\partial P_o} + S_w \frac{\partial (\rho_w U_w)}{\partial P_w} + \frac{1 - \phi}{\phi} \frac{\partial (\rho_R U_R)}{\partial P_o} + \frac{\partial (S_w \rho_w U_w + S_o \rho_o U_o - \rho_R U_R)}{\partial \phi} \frac{\partial \phi}{\partial P_o},\]

\[B = S_o \frac{\partial (\rho_o U_o)}{\partial T} + S_w \frac{\partial (\rho_w U_w)}{\partial T} + \frac{1 - \phi}{\phi} \frac{\partial (\rho_R U_R)}{\partial T} + \frac{\partial (S_w \rho_w U_w + S_o \rho_o U_o - \rho_R U_R)}{\partial \phi} \frac{\partial \phi}{\partial T},\]

\[C = -\left( \frac{\partial f_w}{\partial S_w} (\rho_o H_o - \rho_w H_w) - f_o \frac{\partial (\rho_o H_o)}{\partial T} - f_w \frac{\partial (\rho_o H_w)}{\partial T} \right).\]

We can premultiply each of the above matrices by the following matrix:

\[
\begin{pmatrix}
1 & 0 & 0 \\
-S_o \left( \frac{\partial \rho_o}{\partial \phi} + \frac{\rho_o}{\phi} \frac{\partial \phi}{\partial \phi} \right) & S_w \left( \frac{\partial \rho_w}{\partial \phi} + \frac{\rho_w}{\phi} \frac{\partial \phi}{\partial \phi} \right) & 0 \\
-A & 0 & S_w \left( \frac{\partial \rho_w}{\partial \phi} + \frac{\rho_w}{\phi} \frac{\partial \phi}{\partial \phi} \right)
\end{pmatrix}
\]

This decouples the pressure terms, and we get the system in \( S_w \) and \( T \), on which we can do the linear stability analysis.
Appendix B

Physical properties

B.1 Relative Permeability

The relative permeability functions can be expressed as:

\[ k_{ro} = k_{ro}^o (1 - S_w)^2, \quad \text{(B.1)} \]

and

\[ k_{rw} = k_{rw}^o S_w^2, \quad \text{(B.2)} \]

where the end point relative permeabilities are \( k_{ro}^o = 1 \) and \( k_{rw}^o = 0.6 \).

B.2 Capillary Pressure

The capillary pressure curve is taken from [37]. Capillary pressure is inversely related to water saturation. The function is given as:

\[ P_c = \frac{1}{0.1 + S_w}. \quad \text{(B.3)} \]

B.3 Viscosity

The water viscosity is assumed to be dependent on temperature only. The following function mapped from the data in [37] was used:
The oil viscosity is a function of both pressure and temperature. The combined dependence is evaluated by:

\[ \mu_o = \mu_o(P) \mu_o(T), \]  

where the functions \( \mu_o(P) \) and \( \mu_o(T) \) are given as:

\[ \mu_o(P) = 6 \times 10^{-7} P^2 - 0.0046 P + 11.179, \]  
\[ \mu_o(T) = -4.8611 \ln(T) + 29.775. \]

For the higher mobility ratio case, we multiply the viscosity function given by Eq. (B.5) with a factor of 10.

### B.4 Density

The density of both oil and water is a function of pressure and temperature. The density is evaluated as follows:

\[ \rho_n = \frac{\rho_n^o}{B_n(P) B_n(T)}. \]

For water \( \rho_w^o = 62 \text{ lb/ft}^3 \), and for oil \( \rho_o^o = 45 \text{ lb/ft}^3 \). The formation volume factors are given as follows:

\[ B_o(P) = 1 - 5 \times 10^{-6} (P - 14.7), \]  
\[ B_o(T) = 1 + 3.8 \times 10^{-4} (T - 293), \]  
\[ B_w(P) = 1 - 2.66 \times 10^{-6} (P - 14.7), \]  
\[ B_w(T) = 1 + 3 \times 10^{-4} (T - 293) + 3 \times 10^{-6} (T - 293)^2. \]
B.5 Rock Properties

The density of the rock is a function of pressure, given by the following equation:

$$\rho_R = \frac{\rho_R^0}{B_R(P)},$$

(B.13)

where $\rho_R^0 = 156 \text{ lb/ft}^3$, and $B_R(P) = 1 + 4 \times 10^{-6} (P - 3600) + 8 \times 10^{-12} (P - 3600)^2$. The specific heat of the rock $C_{pR} = 0.7 \text{ BTU/lb-F}$, and the rock conduction transmissibility $\Upsilon_c = 1000 \text{ BTU/day-ft-F}$. 
Appendix C

Maximum Eigenvalue Derivation

This section uses the error analysis approach introduced by von Neumann to arrive at the required stability criteria for non-oscillatory stability, and shows why $\beta = n \pi$ gives the maximum eigenvalues. This can be explained by taking an example of the following single-phase saturation equation:

$$\frac{\partial S_w}{\partial t} = -C \frac{\partial S_w}{\partial x} + D \frac{\partial^2 S_w}{\partial x^2}$$

can be discretized explicitly as follows:

$$\frac{S_{w_j}^{n+1} - S_{w_j}^{n}}{\Delta t} = -C \left[ \frac{S_{w_j}^{n} - S_{w_j}^{n-1}}{\Delta x} \right] + D \left[ \frac{S_{w_{j+1}}^{n} - 2 S_{w_j}^{n} + S_{w_{j-1}}^{n}}{(\Delta x)^2} \right]. \quad (C.1)$$

In the above equation, the first term on the RHS is phase-based upwind discretization, and the second term on the RHS is central discretization. The discrete value in the difference equation, Eq.(C.1) is replaced by its generalized Fourier component:

$$S_{w_j}^{n} = \xi^n e^{i \beta j}, \quad (C.2)$$

which along with the expansion identity $e^{i \beta j} = \cos \beta j + i \sin \beta j$ results in the following equation:

$$\frac{\xi^{n+1}}{\xi^n} = 1 - \left( \frac{C \Delta t}{\Delta x} + \frac{2 D \Delta t}{(\Delta x)^2} \right) (1 - \cos \beta) - i \frac{C \Delta t}{\Delta x} \sin \beta. \quad (C.3)$$

For non-oscillatory stability, the sufficient condition is:
APPENDIX C. MAXIMUM EIGENVALUE DERIVATION

\[ \left| \frac{\xi_{n+1}}{\xi_n} \right| < 1. \quad (C.4) \]

From Eq. (C.3), this error propagation factor is derived as:

\[ |\lambda|^2 = \left| \frac{\xi_{n+1}}{\xi_n} \right|^2 = \left[ 1 - \left( \frac{C \Delta t}{\Delta x} + \frac{2 D \Delta t}{(\Delta x)^2} \right) (1 - \cos \beta) \right]^2 + \left[ \frac{C \Delta t}{\Delta x} \sin \beta \right]^2. \quad (C.5) \]

The maximum value of this factor is obtained by using the following criterion:

\[ \frac{d}{d\beta} (|\lambda|^2) = 0, \]

\[ \Rightarrow \frac{d}{d\beta} (|\lambda|^2) = -2[1 - A(1 - \cos \beta)]A \sin \beta + 2B \sin \beta \cos \beta = 0, \]

where

\[ A = \frac{C \Delta t}{\Delta x} + \frac{2 D \Delta t}{(\Delta x)^2}, \]

and \[ B = \frac{C \Delta t}{\Delta x}. \]

From the above inequality, we get \( \beta = n \pi \), which can be substituted in the second derivative \( \frac{d^2}{d\beta^2} (|\lambda|^2) \) to get a negative number, thereby confirming that \( \beta = n \pi \) is a maximum value!