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Application of the rate form of the equation of state for the dynamic simulation of thermal-hydraulic systems

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Abstract

The modelling of multi-phase water flow is an important modern-day design tool used by engineers to develop practical systems which are beneficial to society. Multi-phase water flow can be found in many important industrial applications such as large scale conventional and nuclear power systems, heat transfer machinery, chemical process plants, and other important examples.

Because of many inherent complexities in physical two-phase flow processes, no generalised system of equations has been formulated that can accurately describe the two-phase flow of water at all flow conditions and system geometries. This has led to the development of many different models for the simulation of two-phase flow at specific conditions. These models vary greatly in complexity.

The simplest model that can be used to simulate two-phase flow is termed the homogeneous equilibrium (HEM) two-phase flow model. This model has been found useful in investigations of choking and flashing flows, and as an initial investigative model used before the formulation of more complex models for specific applications. This flow model is fully defined by three conservation equations, one each for mass, momentum and energy. To close the model, an equation of state (EOS) is required to deliver system pressure values. When solving the HEM, a general practice is to employ an equation of state that is derived from a fundamental expression of the second law of thermodynamics. This methodology has been proven to deliver accurate results for two-phase system simulations.

This study focused on an alternative formulation of the equation of state which was previously developed for the time dependent modelling of HEM two-phase flow systems, termed the rate form of the equation of state (RFES). The goal of the study was not to develop a new formulation of the EOS, but rather to implement the RFES in a transient simulation model and to verify that this implementation delivers appropriate results when compared to the conventional implementation methodology. This was done by formulating a transient pipe and reservoir network model with the HEM, and closing the model using both the RFES and a benchmark EOS known to deliver accurate system property values. The results of the transient model simulations were then compared to determine whether the RFES delivered the expected results.

It was found that the RFES delivered sufficiently accurate results for a variety of system transients, pressure conditions and numerical integration factors.

Keywords: Equation of state; Rate form; Two-phase flow; Thermal-hydraulic system; Transient simulation.

Declaration

I, Lambert Hendrik Fick (Identity Number: 890215 569 1081), hereby declare the work contained in this dissertation to be my own. All information which has been gained from various journal articles, text books or other sources has been referenced accordingly.

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Nomenclature

General

A	Area [m^2]
A/f	Helmholtz free-energy [J]
B	Body force [$kg - m/s^2$]
D	Diameter [m]
f	Dimensionless friction factor $[-]$
g	Gravitational acceleration [m/s^2]
h	Specific enthalpy [J/kg]
K	Temperature [K]
K_L	Pressure loss coefficient $[-]$
L	Length [m]
$\dot{m}$	Mass flow [kg/s]
p	Pressure [Pa]
$\dot{Q}$	Total heat transfer rate [W]
$\dot{q}$	Heat per unit volume [J/m^3]
R	Specific gas constant [$J/kg \cdot K$]
S	Entropy [J/K]
T	Temperature [$^{\circ}C$]
t	Time [s]
u	Specific internal energy [J/kg]
U	Secondary loss coefficient $[-]$
V	Velocity [m/s]
$\forall$	Volume [m^3]
$\dot{W}$	Total work rate [W]
$\dot{w}$	Work per unit volume [J/m^3]
x	Quality $[-]$
z	Elevation [m]

Greek Letters

Δp	Pressure drop [Pa]
Δt	Integration time step length [s]
δ	Dimensionless density ratio $[-]$
ν	Specific volume [m^3/kg]
ρ	Density [kg/m^3]
τ	Surface force [$kg - m/s^2$]
ϕ	Dimensionless Helmholtz function $[-]$

Subscripts

c	Continuity
e	Energy
f	Saturated liquid
g	Saturated vapour
m	Momentum
o	Total/stagnation
s	Saturation

Superscripts

o	Value at previous time step
p	Ideal gas part
r	residual part

Metric prefixes

k	kilo-
M	mega-

Acronyms and abbreviations

AF	Approximation Function
BC	Boundary Conditions
CFD	Computation Fluid Dynamics
EES	Engineering Equation Solver
EOS	Equation of state
HEM	Homogeneous Equilibrium Model
HNEM	Homogeneous non-Equilibrium Model
IAPWS	International Association for the Properties of Water and Steam
IC	Initial Conditions
IFC	International Formulations Committee
IUPAC	International Union of Pure and Applied Chemistry
LOCA	Loss of Coolant Accident
NIST	National Institute of Standards and Technology
NBS	National Bureau of Standards
NRC	Nuclear Regulatory Commission
RFES	Rate form of the equation of state
SCFD	System Computation Fluid Dynamics
TRACE	TRAC/RELAP Advanced Computational Engine
T-F	Thermal-Fluid

Chapter 1

Introduction

1.1 Background

The formulation of two-phase flow models for the simulation of physical two-phase systems has been an area of substantial interest for a number of decades ([Todreas and Kazimi, 1990](#)). The fundamental difficulty associated with two-phase flow description arises from the numerous flow configurations that must be accounted for when solving simulations that model these flow conditions. Because of this inherent complexity, no two-phase flow model has yet been formulated that can accurately account for two-phase flow at all conditions. Fortunately, a number of simplified models have been developed that model two-phase flow systems based on specific simplifying assumptions. One of the most important of these simplified two-phase flow models, which has been used in engineering design calculations in a number of diverse applications, is the homogeneous equilibrium two-phase flow model ([Collier, 1972](#)).

The one-dimensional homogeneous equilibrium model (HEM) is fully determined by three conservation equations, one each for mass, momentum and energy ([Stadtke, 2006](#)). The mathematical set of equations that results for this two-phase flow model is a set of three equations, with four unknowns. The three values determined by the conservation equations are density, velocity, and enthalpy. The fourth value that is required to solve these three equations is pressure. Therefore, a fourth equation is required to close the homogeneous equilibrium model. This final equation that is required to close the model must be able to use the system property value information provided by the conservation equations to calculate the pressure in the system. Such an equation, which relates system thermodynamic property values, is termed an equation of state. The equation of state describes the relationship between any three thermodynamic properties of a substance, two of which are independent. If any two of the properties are known, the third can be determined in a system by the equation of state.

Modern T-F simulation software such as EES (Engineering Equation Solver), RELAP5-3D and TRACE (TRAC/RELAP Advanced Computational Engine) have built-in functions for the equation of state of various substances. In the case of light water, EES can for example determine the needed thermodynamic properties using either the 1984 NBS/NRC (National Bureau of Standards/Nuclear Regulatory Commission), or the 1995 IAPWS (International Association for the Properties of Water and Steam) formulations for the equation of state ([Klein, 2012](#)). The latter of these formulations is endorsed by the IAPWS as the most accurate representa-

tion of the thermodynamic properties of ordinary water over a wide range of conditions and is recommended for general and scientific use (Wagner and Pruss, 2002). These formulations have been extensively developed, tested and improved upon since being accepted for use and are therefore deemed sufficiently accurate. Any of these equation of state formulations may therefore be implemented as the fourth equation required to solve the HEM for a two-phase flow system simulation model.

Based on certain limitations identified in the equations of state mentioned above, Garland and Sollychin (1987) suggested an alternative formulation methodology for the equation of state for the HEM based on a derivation of specific relations which is defined for homogeneous equilibrium two-phase systems. The resultant formulation solves for the rate of change of pressure in a system as a function of the rates of change of density and enthalpy in the system. This equation was termed the rate form of the equation of state. It was combined with a set of thermodynamic property approximation functions - initially developed by Garland and Hoskins (1988), and expanded subsequently - to form a complete alternate EOS formulation (termed the rate formulation or method in this study) that could be used to replace the conventional EOS formulations discussed in the preceding paragraph. The motivations for the development of this alternative EOS formulation were primarily based on limitations of contemporary computer resources that were used to solve these system simulation models. The developers of the method sought to formulate an equation of state methodology that was more numerically efficient (requiring less processing time) and required less computational resources in terms of computer memory. Today, these limitations have been mitigated to a large extent by the advances in computer systems and computational technology.

Even though this primary reason for the implementation of a method such as the rate formulation has been somewhat diminished, the method remains relevant and of interest today because it forms the basis for the formulation that is required in the simulation of two-phase flow which is not at thermal equilibrium.

The HEM represents the biggest mathematical simplification of a physical two-phase flow system. The assumptions driving this simplification have been proven to be valid in many applications where the HEM continues to deliver accurate system model results. However, some physical systems are more aptly described by models that do not make a simplifying assumption of equilibrium between phases. Therefore, in addition to developing the rate method for equilibrium two-phase systems, Garland (1998) also derived a rate form of the equation of state for non-equilibrium two-phase flow systems. Unfortunately, no specific investigation of this non-equilibrium application of the RFES can be found in literature. Thus, no implementation of the rate form of the equation of state for non-equilibrium two-phase flow conditions as developed by Garland (1998) has been found.

The aim of this study was therefore to be a starting point for a possible investigation of the non-equilibrium formulation of the RFES, by serving as an initial work on the implementation of the RFES and its constitutive components for the simpler equilibrium case.

1.2 Problem statement

The application of a rate form implementation methodology of the equation of state when modelling two-phase flow systems at non-equilibrium conditions is of interest to T-F system modellers and may warrant further investigation. However, little or no investigative work regarding the implementation of such a method for non-equilibrium two-phase flow has been found. A homogeneous equilibrium two-phase simulation model which incorporates the RFES needs to be developed and verified in terms of solution validity as an initial model. This model may then be expanded to account for non-equilibrium conditions in subsequent studies.

1.3 Objectives

Based on the problem statement, the objectives of this study are:

- Perform a thorough literature survey with regards to the following items:
 - A general overview with regards to the derivation of two-phase flow models of varying complexity.
 - The rate formulation for the equation of state, including all information regarding its formulation and application.
 - An appropriate equation of state which may serve as verification benchmark and it's formulation.
- Correctly incorporate the rate formulation for the equation of state into a suitable T-F simulation model.
- Verify the appropriateness of the solution delivered by the RFES by comparing the transient model results with those delivered by a model solved using a benchmark EOS that is known to deliver acceptable results.

By completing these objectives, the correctness of the solution values delivered by the model incorporating the RFES may be ensured. If required, the model may then be expanded to account for non-equilibrium conditions in subsequent studies.

1.4 Methodology

The primary aim of this work was to incorporate the rate form implementation methodology of the equation of state as a method to calculate system thermodynamic property values in a transient homogeneous equilibrium two-phase flow simulation model.

To accomplish this task, the relevant literature pertaining to two-phase flow simulation, and the rate method was reviewed to determine how it could be successfully implemented. Once the necessary understanding was developed, the HEM incorporating the rate method was implemented in a computer simulation model using the EES software package.

EES allows for the formulation of complex steady-state and transient T-F simulation models, while also providing a library of equation of state formulations which can be used to determine thermodynamic properties of many fluids, including steam. The program was therefore ideal for use as a test bed in which to implement the model and evaluate the validity of the model results.

To implement the rate method, a transient HEM pipe and reservoir network model was developed. The chosen simulation model was programmed in EES using the built-in correlations for the equation of state. Once the program was completed and verified, a set of test scenarios were developed that could be used to test the correctness of the implementation. These test scenarios were then simulated by using both the correlations for the equation of state built into EES, as well as the rate method. The data generated by these approaches was then compared with regards to chosen criteria. Based upon this comparison, the validity of the rate method results and the effects of certain solution parameters on the delivered results could be determined.

1.5 Overview of document

This document comprises of six chapters and four appendix sections.

Chapter 1 serves as an introduction to the study. The relevant background is given, after which the problem statement is formulated. The objectives of the study are given and the methodology followed to achieve these objectives is briefly discussed. Chapter 2 is dedicated to the literature survey. Scientific literature relevant to the study is discussed here. The mathematical modelling theory relevant to the study is discussed in Chapter 3. The conservation equations for mass, momentum, and energy, as well as the equations of state that were used in this study are given. Only the final equations relevant to the study are given in this chapter, with the detail derivations given in the appendices. The derivation of the rate form of the equation of state for homogeneous equilibrium two-phase flow is derived in detail in Appendix A, while the conservation equations are derived in detail in Appendix B. Chapter 4 is dedicated to detailing the methodology employed to achieve the goals of the study stipulated in Section 1.3. Attention is given to determining the accuracy of the constitutive parts of the rate form of the equation of state, the formulation of the relevant simulation models, and the verification of these models. The code for the transient pipe and reservoir network simulation models that was developed in EES to evaluate the rate form of the equation of state is given in Appendix C. The code is given for the model that is solved using the IAPWS 1995 algebraic equation of state, as well as the model that is solved using the rate form of the equation of state. The results of the transient simulation models used to evaluate the rate form of the equation of state is given and discussed in Chapter 5. The conclusions drawn from the study are given in Chapter 6. Recommendations based on the findings of this study are also given in this chapter.

Chapter 2

Literature Survey

An understanding of the background, as well as the formulations and theory relevant to two-phase flow modelling was required to accomplish the stipulated goals of the study. The literature survey served to facilitate this understanding. The literature survey further served to identify an appropriate equation of state formulation that could be used as a benchmark/reference equation of state when verifying the results of the HEM when incorporating the rate method.

This study focused on a formulation of the equation of state; however, the broader goal to which this work pertained was the accurate modelling of two-phase flow. To facilitate the understanding of the relevance of the rate form of the equation of state in the field of two-phase flow modelling, the literature survey addressed the broader scope of two-phase flow modelling and gives a qualitative description of the various approaches used to model two-phase flow.

Attention was firstly given to developing a high-level understanding of the complexity of two-phase flow and how this influences the formulation of the fully complex, two-fluid models that have been developed to most accurately model the physical reality. Note that these complex flow models were not the focus of the study, and therefore only a perfunctory introduction is given which describes the models in a qualitative manner. An introduction to the concepts of equilibrium and homogeneity is given. These concepts are then investigated in more detail, specifically in terms of how equilibrium and homogeneity can be employed as simplifying assumptions, to allow for the formulation of simpler two-phase flow models. Examples of these simplified flow models are the drift-flux, homogeneous non-equilibrium and homogeneous equilibrium models, which are discussed.

The homogeneous equilibrium model was investigated in detail, as the rate form of the equation of state which is the focus of this study, was developed for application in this model. To ensure that the implementation of the rate method was valid, a benchmark equation of state was needed that is known to deliver appropriate thermodynamic property values. Therefore, the survey reviewed literature pertaining to relevant T-F simulation codes to determine which equations of state these codes employ. Based on these findings, a suitable equation of state formulation was chosen as a benchmark formulation against which to evaluate the correctness of the implementation of the rate formulation.

The basis for and reasoning behind this study is given after the review of the literature pertain-

ing to the reference equation of state. The literature regarding the rate form of the equation of state was then reviewed to develop an understanding of the method.

The application of the rate form of the equation of state, or rate method, requires several elements. These include approximation functions for the relevant thermodynamic properties of water, derivatives of these approximation functions and the rate formulation of the equation of state itself. The literature survey focused on elaborating on the rate method and all its constitutive parts.

2.1 Two-phase flow modelling

Two-phase flow is generally understood as being a simultaneous flow of two different immiscible phases separated by an infinitesimally thin interface ([Morales-Ruiz et al., 2012](#)). Two-phase flow is relevant in many scientific and technical disciplines, ranging from environmental research to the modelling of normal operation or accident conditions in nuclear, chemical or process engineering installations ([Flatten and Lund, 2011](#); [Stadtke, 2006](#)). Much work has been done in the field of analysis of two-phase flow systems and the development of related numerical simulation methods. This development has been largely driven by the specific requirements for the safety analysis of nuclear pressurised water reactors ([Wulff, 2011](#)), which relies largely on the prediction capability of computer codes for complex two-phase flow and heat transfer processes.

Works that will be cited regularly in this section will include those of ([Ishii and Hibiki, 2011](#); [Stadtke, 2006](#); [Levy, 1999](#); [Todreas and Kazimi, 1990](#); [Collier, 1972](#)). These texts give overarching qualitative descriptions of two-phase flow modelling and its importance in various industries. They also describe in detail the mathematical theory of two-phase flow modelling and the various two-phase flow models that have been formulated. As these texts are freely available, a complete summary of the works will not be given, and will only be referenced where relevant. The reader is encouraged to investigate these works if a fuller understanding of two-phase flow modelling is desired.

This section focuses on the various two-phase flow models that have been developed and are discussed in literature. A top-down approach is used, beginning with the fully complex separated two-fluid models and ending with the fully simplified homogeneous equilibrium model. The simplifying assumptions made in the derivation of the various two-phase flow models are investigated to develop an understanding of their impact on the accuracy and applicability of the resulting models. Assumptions such as thermal equilibrium, mechanical equilibrium, and equal phase velocity (or homogeneous flow) are specifically investigated.

2.1.1 Two-fluid two-phase flow model

The two-fluid model is the most complex model for two-phase flow simulation, using separate mass, momentum and energy equations for the two phases ([Stadtke, 2006](#)). This means that these models incorporate different gas- and liquid-velocities, dissimilar gas- and liquid-temperatures and consider the effects of co- and counter-current flow ([Rousseau, 2012a](#)). Many

advanced thermal-hydraulic system simulation codes such as the United States NRC's TRAC, RELAP5 and TRACE codes incorporate this full two-fluid (six-equation) model ([NRC, 2007](#); [INL, 2005](#); [NRC, 2001](#))

[Wulff \(2011\)](#) illustrated the complexity of the two-fluid model by tabulating all the equations required to close the model. Additional to the six conservation equations, the two-fluid model requires intrinsic constitutive relations describing material properties of the fluid phases and properties of solid structures contacting the fluid, extrinsic constitutive relations for the transfer of mass, momentum and energy between the two phases and boundary conditions for fluid-solid exchange of momentum and energy between structural walls and each contacting phase. These equations constitute the closure relations for the model. All included, the two-fluid model requires the solution of 29 conservation and constitutive equations.

The closure relations in the two-fluid model continues to present a problem even when implemented in modern state-of-the-art two-phase flow models. Because of the complexity of the rapidly changing geometry and areas of the contact interfaces between the two phases, equations describing the transfer of mass, momentum and energy are difficult to formulate([Levy, 1999](#)). [Wulff \(2007\)](#) stated that at least four of the important closure laws for the transfer between phases in a mixture and their flow conduits are still lacking. The closure equations must usually be obtained from empirical data, and they are a major source of error ([Stewart and Wendroff, 1984](#)). [Attou and Seynhaeve \(1999\)](#) also stated that the complete formulation of the general two-fluid model remains only quasi-feasible due to the limited practical knowledge of the transfer processes in multiphase systems. Closing the model therefore remains an open problem.

Ideally, the equations describing a system should be solved at each point in space in a specific system. For two-phase flow, the above mentioned conservation and closure relations represent the complete local description of the flow, and the solution of these equations for each point in the system under consideration would constitute the ideal of a complete solution. Unfortunately, because of the complexity of two-phase flow, this fully localised solution is impossible. It is therefore necessary to resort to models which suppress some of the detail of the flow, but which are solvable ([Stewart and Wendroff, 1984](#)). A way to achieve this is to derive models that are based on the averaging of the complete local description of the flow ([Levy, 1999](#)). There are various averaging methods that can be employed to obtain a practically solvable model. Averaging methods can be broadly divided into time-, spatially-, or statistical averaging. The work of [Ishii and Hibiki \(2011\)](#) provides a detailed source of averaging techniques that is applicable in two-phase flow modelling.

The literature further reveals that there is little consensus as yet to the correct formulation of the two-fluid model. [Stadtke \(2006\)](#), for example, mentioned that much controversy remains when the correct formulation of the basic two-fluid equations and the appropriate form of the closure laws are discussed, with a commonly accepted approach yet to be found. Therefore, it is seen that the complexity of the two-fluid model is still presently detracting somewhat from its acceptance as the simulation model of choice for modelling two-phase flow in complex systems.

2.1.2 Simplifying assumptions

With an understanding of the complexity of the two-fluid model achieved, attention is now given to the various simplifying assumptions that can be made to reduce the complexity of two-phase flow modelling. Introduced are the various definitions of equilibrium, and how these concepts are used to decrease the level of model complexity by decreasing the number of conservation equations that need to be solved in different two-phase flow models.

Thermodynamic equilibrium is defined as follows: When a system is in equilibrium regarding all possible changes of state, that system is said to be in thermodynamic equilibrium ([Borgnakke and Sonntag, 2009](#)). Within this definition of thermodynamic equilibrium, there are several sub-definitions of equilibrium. Thermal equilibrium is defined as when the entire control mass that composes a system is at a uniform temperature, meaning that there will be no tendency for the temperature at a certain point to change with time, assuming that the system is isolated from its surroundings. Mechanical equilibrium can be defined in a similar way, only with it being related to pressure.

By assuming equilibrium between phases in a two-phase system, models can be developed which are simplified in terms of the number of equations that need to be solved ([Aursand et al., 2013](#); [Yoon et al., 2006](#)). This is because an assumption of equilibrium removes the need for additional closure relations that describe mass and energy transport between the phases. Simplification of two-phase flow models by assuming equilibrium is justified by the fact that any general two-phase flow model must also be valid for the equilibrium states ([Flatten and Morin, 2012](#)).

Another simplifying assumption that can be made is flow homogeneity. Homogeneous flow is defined as a two-phase flow system whose constitutive phases have equal average local flow velocities ([Rousseau, 2012b](#)). As in the case of equilibrium, this assumption can also be used to reduce the number of equations that need to be solved in a two-phase flow model, thereby reducing its complexity ([Levy, 1999](#)).

These simplifying assumptions can be combined in various manners to develop two-phase flow models of differing complexity. The next subsections will briefly introduce some of these simplified flow models and the assumptions used to derive them.

2.1.3 Drift-flux model

As mentioned previously, the general two-fluid model is formulated using two sets of conservation equations governing the balance of mass, momentum and energy for each phase. The introduction of two momentum equations, as in the two-fluid model, presents considerable difficulties due to mathematical complications and uncertainties in specifying interfacial interaction terms between two phases ([Ishii and Hibiki, 2011](#)). Some of the difficulties associated with the two-fluid model can be mitigated by simulating two-phase flow systems with the drift-flux model.

The drift-flux model is derived from the full two-fluid model making the assumption of mechanical equilibrium ([Aursand et al., 2013](#)). If the pressures in both phases are assumed to be equal, the momentum conservation equations can be combined into a single equation. The model is not homogeneous however, since the liquid and vapour velocities need not be equal. A constitutive slip relation is used in combination with the assumption of mechanical equilibrium. This slip relation relates the velocities of the phases in the system, thereby allowing for a single momentum conservation equation, even though the phase velocities differ.

The drift-flux model is known as a mixture model, and it is best used to describe two-phase flow in which the phases are tightly coupled. Tight coupling implies that the relative velocity of the phases with regards to one another is small. It is argued that mixture models can be superior to the general two-fluid model in situations where the flow is tightly coupled with chaotically deforming interfaces, as in industrial systems with complex geometries ([Wulff, 2007](#)).

Thermal equilibrium may or may not also be assumed in the drift-flux model ([Martinez Ferrer et al., 2012](#)). If not assumed, the drift-flux model reduces to a system of five equations plus the slip relationship. By assuming thermal equilibrium, i.e. equal phase temperatures, the energy conservation equations can also be combined into a single equation. This reduces the number of conservation equations from six to four. In the thermal equilibrium case the drift-flux model is therefore defined by a mixture energy conservation equation, two mass conservation equations and a mixture momentum equation combined with a constitutive slip relation which expresses the relative velocity of the phases. The mass conservation equations are cast for the mixture mass conservation as well as the dispersed phase mass conservation. This is required because the mass conservation equations are functions of phase velocity. Because the phase velocities differ, two mass conservation equations are required. This means that the model also requires less constitutive equations and boundary values that need to be solved, thereby greatly decreasing its complexity.

2.1.4 Homogeneous non-equilibrium model

The homogeneous non-equilibrium model (HNEM) differs from the drift-flux model in the sense that in the HNEM model, the phase velocities are assumed to be equal ([Yoon et al., 2006](#)), whereas the phase velocities in the drift-flux model may differ ([Aursand et al., 2013](#)). Thermal non-equilibrium is assumed in the HNEM model, allowing for different phase temperatures. By assuming homogeneity, the momentum equations for the phases can be combined to create a mixture momentum equation. This leads to a system of five conservation equations, with separate mass and energy equations for the liquid and gas phases and a single mixture equation for momentum conservation ([Stadtke, 2006](#)).

Various research works in literature employ homogeneous non-equilibrium models in the modelling of two-phase critical and choking flow. Choking flow takes place in accident situations such as a LOCA (Loss of Coolant Accident) in nuclear reactors or breaks in high pressure pipelines, and the accurate modelling of this phenomenon is therefore important in the safety design of these systems ([Yoon et al., 2006](#); [Lenzing et al., 1998](#)). Proponents of this model argue that the fully simplified homogeneous equilibrium model may not model the physical

reality entirely accurately. [Yoon et al. \(2006\)](#) stated that the homogeneous equilibrium method assumes a constant adherence of fluid properties to the saturation line, where in reality the bulk upstream fluid may be at saturation conditions, but fluid at the choking point is at a superheated condition, leading to thermal non-equilibrium in the two-phase fluid that must be accounted for. According to [Downar-Zapolski et al. \(1996\)](#), the non-equilibrium vapour generation is an important feature in flashing liquid flows. Because the homogeneous equilibrium model assumes equilibrium vapour generation, it fails to reproduce experimentally observed distributions of flow parameters.

Various other papers discuss homogeneous non-equilibrium models as they are used to model critical two-phase flow, such as [Levy and Abdollahian \(1982\)](#) for light water and [Travis et al. \(2012\)](#) for other fluids.

2.1.5 Homogeneous equilibrium model

The homogeneous equilibrium model (HEM) is the final two-phase flow model under investigation. It is the simplest model used for two-phase flow modelling, or alternately, it represents the model with the highest number of simplifying assumptions ([Wulff, 2007](#)).

The homogeneous equilibrium model assumes no slip between phases (equal phase velocity) and thermal equilibrium ([Valero and Parra, 2002](#)). It is also assumed that both phases are subject to the same local pressure, i.e. the phases are in mechanical equilibrium ([Rousseau, 2012b](#)). The model is based on the assumption of infinite rate of transfer processes between the phases for mass, momentum and energy, allowing the description of the two-phase mixture as a single, pseudo fluid. This means that there is no need for any description of interfacial coupling conditions since all transfer processes are implicitly determined by the assumption of mechanical and thermal equilibrium between the phases ([Stadtke, 2006](#)). This model can be seen as a further simplification of the four-equation drift flux model, with the additional assumption of no-slip between phases. By using these simplifying assumptions of equilibrium and homogeneity, the homogeneous equilibrium model is fully determined by three mixture conservation equations for mass, momentum and energy respectively.

The homogeneous equilibrium model has been specifically relevant in early investigations of choking flow. Even though this model has been largely replaced as the model of choice for simulating choking flow, [Webber \(2011\)](#) states that the assumption of homogeneous equilibrium is qualitatively justified in certain circumstances for modelling two-phase conditions in accident scenarios. Generalised correlations for the modelling of homogeneous equilibrium flashing choked flow have been developed, e.g. [Lenzing et al. \(1998\)](#), and the homogeneous equilibrium model is used in many sources in literature as a benchmark in the development of more complex non-equilibrium models. Examples include the papers by [Attou and Seynhaeve \(1999\)](#) and [Downar-Zapolski et al. \(1996\)](#). The coupling of the homogeneous equilibrium model with other two-phase flow models has also been attempted ([Ambroso et al., 2009](#)).

[Levy \(1999\)](#) stated that this model is an important tool as computer codes based on this model are simple to implement and do not take long to run. They are also the only tool available when closure laws for more complex two-fluid models still need to be developed for a system under

consideration. From the literature it is therefore seen that the HEM is especially important as an initial investigative tool, which can later be substituted by more complex models as they are formulated and applied. It can be used to generate initial data in two-phase flow systems and allows for the development of intuition regarding two-phase flow phenomena in these systems.

The rate form of the equation of state under investigation in this study was formulated for use in homogeneous equilibrium two-phase flow modelling. Therefore, the HEM was employed as the chosen two-phase flow model in this study.

The three conservation equations that define a homogeneous equilibrium two-phase flow system solve for the enthalpy, mass flow and density in the system. However, these equations require the value of an additional variable, namely pressure. An equation of state is used to close the model by solving for pressure in the system as a function of density and enthalpy. The different equations of state found in literature are discussed in the following section.

2.2 Equation of state

When solving the three conservation equations for mass, momentum and energy in the homogeneous equilibrium model, there are three equations with four unknowns, namely:

- Density (ρ),
- Velocity (V)/Mass Flow ($\dot{m}$),
- Enthalpy (h), and
- Pressure (p).

The fourth equation that is needed for closure is the equation of state ([Garland, 1998](#)). The equation of state of a substance describes the relationship between any three thermodynamic properties of the substance, two of which are independent. If any two of the three properties are fixed, the third is determined. The equation of state therefore allows for the expression of the pressure as a function of property values determined from the conservation equations, for example density and enthalpy:

$$p = f(\rho, h) \tag{2.1}$$

A brief overview of the solution of the conservation equations and equation of state is given in [Fig. 2.1](#). These equations are all also subject to the correct initial and boundary conditions (IC and BC). The closed system of four equations are related to one-another in the following manner:

The momentum equation provides flow (or velocity) information from one point to another, based on a given pressure, flow, mass and energy distribution in the system. This flow information is used by the mass and energy equations to update the mass and energy contents at

each point (node) in the system. The new mass and energy values at each location is given to the equation of state, which updates the pressure distribution. The new pressure, along with the new densities and energies are then once again used by the momentum equation, and so on. This allows for the development of a time history of fluid evolution. Only the main variables are noted here, with the assumption that the various empirical correlations and constitutive relations are solved as needed to update the main variables.

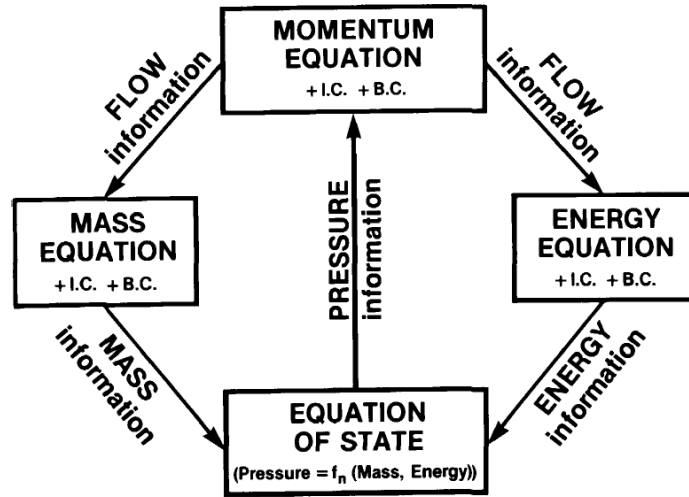


Figure 2.1: The conservation equations, equation of state and the information links between them. (Garland, 1998)

The importance of the equation of state as a closing equation which is used to calculate system pressure (or any other required property) values means that any formulation of the EOS (Equation of State) must deliver accurate thermodynamic property values across a large range of possible conditions to be practically applicable in T-F system modelling.

In the subsections that follow, two separate forms of the equation of state will be discussed. The first form, referred to as an algebraic form, delivers any required thermodynamic property value, e.g. pressure, density, enthalpy, as a function of two known property values based on time independent equation of state formulations. The second method, referred to as a rate method, solves for pressure values using a time dependent equation, while other properties are calculated using algebraic thermodynamic property approximation functions.

The following subsection will elaborate on various algebraic equations of state used to determine the thermodynamic property values of water. Specific attention is given to equations of state that are used in major T-F simulation codes. This was done to determine which equation of state could be used as an acceptable benchmark EOS to evaluate the implementation of the rate method.

2.2.1 Equation of state formulations

This subsection will discuss equations of state in general, rather than focusing only on how pressure is determined. These equations of state may be used to determine all relevant thermodynamic property values, including the pressure value, using time independent correlations for the equation of state.

The literature pertaining to equations of state for fluids is voluminous. This is because equations of state are widely applied in science, engineering and industry for the modelling of many different kinds of physical systems ([Sengers et al., 2000](#)). This study however, is interested in a very specific application for equations of state, namely the modelling of two-phase systems with water as the working fluid. Therefore, to ensure that the literature survey remains focused in addressing the goals stipulated for this study, an appropriate equation of state for use in the aforementioned application will firstly be identified. After this EOS has been identified, the formulation will be discussed in more detail.

Because the equation of state is a required closure equation when developing T-F simulation models, all commercial T-F simulation codes employ selected EOS formulations. Therefore, to facilitate the identification of an appropriate equation of state for the modelling of homogeneous equilibrium two-phase flow, the literature pertaining to various thermal-fluid system modelling codes such as RELAP5-3D, TRACE, Flownex SE and EES was investigated to determine which equations of state these codes employ when modelling water at two-phase conditions. Based on these findings, an appropriate equation of state could be selected to serve as benchmark against which to evaluate the correctness of a model solved using the rate method.

Large T-F simulation codes such as RELAP5-3D and TRACE, which are used by the U.S. NRC to model the T-F conditions in nuclear reactors, employ various formulations of the EOS. RELAP5-3D is able to use thermodynamic property data from steam tables generated by the 1967 IFC (International Formulation Committee) formulation of the EOS for industrial use. RELAP5-3D can also use steam tables based on the 1984 NBS/NRC formulation of the EOS ([INL, 2005](#)). RELAP5-3D also uses a formulation analogous to the rate methodology discussed in the following subsections when solving semi-implicit finite difference equations. It is used to calculate the phasic density in the system as a function of the rates of change of different system properties, including pressure. This is similar to the rate method, which uses the rates of change of energy and mass in the system to calculate the rate of change of pressure.

TRACE, which is the successor code to RELAP5-3D, is able to deliver thermodynamic property values via interpolation of steam table data based on the IAPWS 1995 formulation of the equation of state ([NRC, 2007](#)). TRACE is also able to deliver thermodynamic property data by using polynomial fits of steam table data. This is the same approach used in the formulation of thermodynamic property approximation functions which form part of the rate methodology investigated in this study. The approximation functions are described in Section [2.2.4](#).

Flownex SE uses steam table data from the NIST (National Institute of Standards and Technology) steam tables, which are in turn derived from the IAPWS-95 EOS formulation. EES allows for the calculation of thermodynamic property values with either the 1984 NBS/NRC formulation of the EOS, or the 1995 IAPWS formulation of the EOS ([Klein, 2012](#)).

From the literature it is therefore determined that these codes, some of which are used to model nuclear systems and therefore rigorously verified and validated, use equations of state based on the following formulations:

- IFC-67 EOS.
- 1984 NBS/NRC EOS.
- IAPWS-1995 EOS.

These EOS formulations may be employed in the respective codes as subroutines that can be called by the main program to deliver the required fluid property based on specified input data, as in the case of EES. In this approach, any two known thermodynamic property values may be supplied as the independent parameters to determine the third, unknown parameter in real-time. Alternatively, the code may make use of pre-generated steam tables where the required property values are tabulated as functions of other thermodynamic properties. TRACE, RELAP5-3D and Flownex SE make use of the latter approach. For example, the NIST steam tables based in the IAPWS-1995 EOS tabulate the fluid properties along the vapour-liquid saturation curve as a function of pressure and temperature ([Harvey, 1998](#)). Tabulating thermodynamic property data as a function of pressure and temperature is the generally used approach.

Having determined that the equation of state formulations listed above represent the preferred method for determining the thermodynamic property values of water in T-F simulation codes, a brief history of the development of these equations of state is given to illustrate which code is the most applicable today to serve as a reference equation of state when evaluating the correctness of a model that utilises the rate method

The papers by [Wagner and Pruss \(2002\)](#), and [IAPWS \(2009\)](#), detail the evolution of the listed equations of state and the subsequent development of the IAPWS-1995 formulation in detail. Since these papers are the source documents for the formulation, they can be considered the definitive sources of information regarding the IAPWS-1995 formulation of the equation of state. The following paragraphs provide a summary of the most pertinent information (for the purpose of this study) regarding the listed IFC-67 and 1984 NBS/NRC equations of state and specifically the IAPWS-1995 EOS formulation, as detailed in these two papers.

According to [Wagner and Pruss \(2002\)](#), numerous correlations for the thermodynamic properties of water exist in literature, but most of them cover only small parts of the fluid region and do not meet present demands on accuracy. The paper tabulates the characteristic features of the best equations of state that have been published since 1968. The first four columns of this table is given in table [2.1](#).

Table 2.1: Information on selected equations of state for water (Recreated from [Wagner and Pruss \(2002\)](#))

Authors	Year	Standard name	Temp range [K]	Pressure range [MPa]
IFC	1968	IFC-68	273-1073	0-100
Keenan et al.	1969		273-1673	0-100
Pollak	1974		273-1200	0-300
Haar et al.	1984	IAPS-1984	273-1273	0-1000
Saul and Wagner	1989		273-1273	0-25000
Hill	1990		273-1273	0-1000

The two EOS packages used by the discussed T-F simulation packages were both considered the state of the art for determining the thermodynamic properties of water over large ranges of applicability in their respective time periods. Both of these codes remain accurate and relevant, as is attested to by the fact that they are still currently employed in major T-F simulation packages.

The IFC-68 equation package was the first formulation of the equation of state to be accepted as the international standard for the equation of state of water and steam for scientific and general use. This equation of state was based on a further development of the IFC-67 EOS formulation for industrial use. This was replaced as the international standard in 1984 by the Helmholtz free-energy formulations of Haar et al. This formulation, known as the IAPS-84 standard, is the basis for the 1984 NBS/NRC steam tables used in RELAP5-3D. This formulation represents the thermodynamic properties of water very well, but exhibits certain weaknesses near the critical point of water. In response to these weaknesses, the IAPWS accepted the EOS formulation of [Wagner and Pruss \(2002\)](#) as the new international standard for determining the thermodynamic properties of water in 1995. This means that the IAPWS-1995 serves as the current international standard equation of state for determining the thermodynamic properties of water.

Because the IAPWS-1995 EOS represents the state of the art in terms of accurately delivering thermodynamic property values for water for the conditions simulated in this study, this formulation can serve as a viable benchmark formulation against which to evaluate the correctness of the solutions delivered by the of the rate form of the equation of state and its associated thermodynamic property approximation functions. The mathematical basis for this formulation is discussed in more detail in Subsection [3.3.1](#).

The next subsection will discuss the reasoning behind the investigation of an alternative form of the equation of state.

2.2.2 Need for an alternative implementation of the EOS in transient process modelling

The rate method, which will be discussed in the subsection below, was formulated because the developers of the method felt that algebraic EOS formulations had certain limitations when

solving for pressure in T-F simulation models. Some of these limitations have been diminished by advances in computational technology that have occurred since the rate method was developed. The limitations as set out by the developers of the rate method will be summarised, after which the historical context is explained to illustrate why these limitations may have become less relevant and are specifically not relevant to this study.

A first limitation of the algebraic method is the fact that temperature and pressure are the independent variables used in the tabulation of thermodynamic property data, i.e. in the steam tables. As discussed in Subsection 2.2.1, many T-F simulation models determine thermodynamic property values from steam tables where pressure and temperature are the independent variables. This can be seen as a drawback since temperature and pressure are seldom the independent variables when simulating dynamic T-F systems (Garland and Sollychin, 1987). In general, the independent variables in transient system simulations are density and enthalpy, which are solved for by the mass and energy conservation equations as a function of time. This means that when density and enthalpy are the independent variables, the steam tables must be interpolated using the density and enthalpy values to determine the corresponding pressure data. Because the pressure data is not calculated directly from the available property values delivered by the conservation equations, but must instead be calculated through iteration until consistent with the density and enthalpy values, calculation time is increased. This is exacerbated by the fact that searching algorithms must also be employed when using steam table data to look up the relevant data.

When the rate method was developed by Garland and Sollychin (1987), the computer resources available to T-F system modellers were a fraction of what is available today from even a modest desktop computer. Because of the limitations in computer memory, large data files (from a historical perspective), such as thermodynamic property tables were troublesome to work with. Also, because of the low processing power of the computers of the time, additional searching and interpolation algorithms coupled with iterative pressure solution schemes could account for a significant increase in computational time. Because of these factors, system modellers such as Garland and Sollychin proceeded with the development of the non-iterative, rate form pressure solution scheme using approximation functions which could be programmed with little memory cost relative to bulky thermodynamic property table files or EOS subroutines that contained large amounts of variables that had to be stored for solving the EOS in real time.

Because of the exponential increase in overall computing power since the time when the rate method was developed, the factors mentioned above have largely been mitigated. Steam table data files are easily stored, while interpolation algorithms and real-time subroutine calculations for property values have a negligible impact on calculation speed in most circumstances. Therefore, though the increased efficiency offered by directly calculating the pressure using the rate form of the equation of state may account for an absolute increase in calculation speed, in measurable terms it may be negligible. This investigation is therefore not directly concerned with increase in computational efficiency possibly provided by this method.

A second possible limitation is the fact that an algebraic equation of state makes an implicit assumption of thermodynamic equilibrium when calculating fluid properties (Garland, 1998). The reason for this is examined in the section pertaining to the IAPWS-1995 equation of

state in Subsection 3.3.1. In other words, an algebraic equation of state is cast as a pure function of the local state of the fluid, meaning it does not consider the change of properties over time. An algebraic EOS can therefore not track changes in the system, which may be of a non-equilibrium nature, over time and simply solves each time step in a transient simulation as if the system as at an equilibrium, steady-state conditions at that moment in time. In physical systems that incorporate two-phase flow, e.g. pressurised water reactors, the phases present in the system are not always in equilibrium. These non-equilibrium conditions may arise in transient/accident scenarios such as LOCA (Yoon et al., 2006), as well as in normal operating conditions, e.g. nucleate boiling, where the bulk fluid temperature is sub-cooled, but boiling occurs in the superheated thermal boundary layer of the system (Rousseau, 2012b). Therefore, when employing an algebraic equation of state, equations that were derived at equilibrium conditions are used to model non-equilibrium systems, leading to a possible inconsistency in the formulation.

This possible limitation is not well documented. The work of Garland (1998) was the only work found in literature to explicitly make note of this possible limitation of an algebraic form of the equation of state. This possible limitation does not detract from the accuracy of the solutions that algebraic formulations provide, but may be inconsistent when taking the physics of the process into account. The rate formulation, which is discussed in the following subsection, may provide the basis for an alternative formulation of the EOS which may prove to more accurately represent the non-equilibrium physics in two-phase flow systems. This deduction is based solely on the intuition of the author and the study leaders for this project. The reasoning behind this study is to serve as an initial implementation of the rate method for homogeneous systems, after which a more detailed analysis of the non-equilibrium considerations of the rate methodology may be done. Thus, this study will not address the non-equilibrium facet of the rate methodology.

Based on the preceding paragraphs, it may seem difficult to quantify a definite or specific reason to investigate an alternative formulation of the equation of state. That may be because the nature of the study is somewhat esoteric in the fact that it marries investigation of equations of state, which falls in the domain of fundamental and experimental thermodynamics, with engineering application in T-F system modelling. The goal of this study is not to develop or propose an alternate equation of state for use in T-F simulation models, or to examine the fundamental physical differences between different equation of state formulations, but rather to properly implement the rate method in a chosen T-F simulation model after which it may be expanded to investigate the non-equilibrium aspects of the method in subsequent studies.

The rest of this study focuses solely on implementing and ensuring the appropriateness of the results of the rate form of the equation of state compared with results from a state of the art equation of state when solving for thermodynamic property values in a T-F simulation model. The rate method method is discussed in the following subsection.

2.2.3 Rate form implementation of the equation of state

The rate, or time derivative, form of the equation of state used to solve pressure in a system was initially developed and investigated by [Garland and Sollychin \(1987\)](#). This methodology was subsequently implemented in papers such as those of [Gaboury and Garland \(1993\)](#). Generally, the equation of state is cast as an algebraic equation, meaning that it is only dependent on the local state of the fluid. In contrast to this, the equations governing the conservation of mass, momentum and energy are all cast in rate form and must be solved or traced as a function of both space and time. In the article, [Garland and Sollychin \(1987\)](#) presented an approach where the equation of state was also cast as a rate equation, thereby giving it the same form as the time dependent conservation equations. This formulation specifically solves for pressure using a rate equation, as pressure is the fourth unknown variable needed to close a homogeneous equilibrium two-phase flow model. The difference between a fundamental EOS such as IAPWS-95 and rate formulations is shown in Table 2.2. When employing the rate method, the conservation equations keep their form, but the equation of state which closes the system of equations changes from an algebraic equation to a rate equation.

Table 2.2: Basic form of the conservation equations and form of the algebraic and rate formulation of the equation of state

Conservation equations and equation of state		
Equation	Algebraic formulation	Rate formulation
Mass conservation	$\frac{d\rho}{dt} = f(\dots)$	$\frac{d\rho}{dt} = f(\dots)$
Momentum conservation	$\frac{dm}{dt} = f(\dots)$	$\frac{dm}{dt} = f(\dots)$
Energy conservation	$\frac{dh}{dt} = f(\dots)$	$\frac{dh}{dt} = f(\dots)$
Equation of state	$p = f(\rho, h)$	$\frac{dp}{dt} = f\left(\frac{d\rho}{dt}, \frac{dh}{dt}\right)$

When the rate form of the equation of state is employed, the authors of the rate form of the equation of state cite that the resultant equation set has two distinct advantages over the mixed form equation set obtained when combining the conservation rate equations with an algebraic equation of state. The first advantage is that the equation set consists of four rate equations: the mass and energy conservation equations and the equation of state for every node, or point in space; and the momentum conservation equation for each element, or nodal interface. Because of this consistent formulation, the system characteristics, or eigenvalues can be extracted without having to solve the equations numerically. The second advantage is that the rate form allows for the numerical calculation of pressure without the need for interpolation of the steam tables. This drastically reduces the calculation time needed to determine pressure. Additionally, because the pressure is explicitly expressed in terms of slowly varying system parameters, an implicit numerical scheme can easily be formulated.

From their findings, [Garland and Sollychin \(1987\)](#) state that the rate method offers many advantages:

- The form of the RFES (Rate Form of the Equation of State) makes it appropriate for eigenvalue extraction as well as numerical simulation.
- Programs are easier to implement.
- Time step control and detection of rapid changes, such as phase change, is improved.
- The method is faster than the algebraic method in delivering pressure and temperature data.
- The method is at least as accurate as the algebraic method (or more accurate than).

The objectives of this study correspond with the final advantages cited above. Its purpose was to implement the RFES in a specific T-F simulation model and ensure that an appropriate solution was obtained. Based on the stated properties of the method, a correct implementation of the RFES would deliver simulation results consistent with those delivered by a fundamental EOS formulation of the same model. More detailed studies may be done in future to investigate the numerical implication of the RFES compared to the fundamental EOS approach, as well as to investigate its possible applicability in non-equilibrium two-phase flow modelling.

The solution of the rate form of the equation of state for two-phase flow requires saturation property values for enthalpy and density in the system under consideration. Also required are derivatives of these properties with regards to pressure. To make provision for this requirement of the rate formulation of the equation of state, the developers of the rate method also developed a set of simple approximation functions for the required thermodynamic properties of light water, which is discussed in the following subsection.

2.2.4 Thermodynamic property approximation functions

As mentioned in Section 2.2.2, the developers of the rate method wanted to decrease the amount of computer memory required to calculate thermodynamic property values. To do this, the developers derived a set of thermodynamic property approximation functions which could be used to calculate required thermodynamic property values without the need for steam tables. The reference steam tables used to formulate the approximation functions are the 1984 NBS/NRC steam tables ([Garland and Hoskins, 1988](#)). These steam tables are based on the Helmholtz EOS formulation of Haar, Gallagher and Kell, which is also known as IAPS-84.

The approximation functions for the thermodynamic properties of water at saturation were initially developed by [Garland and Hoskins \(1988\)](#), using a least squares method to accurately fit simple functions to the reference steam tables. At saturation conditions, temperature can be expressed as a function of pressure and vice versa. In other words, saturation property values of water can be calculated from only one independent variable. Therefore, thermodynamic properties can be represented by a number of simple functions containing only one independent

variable, namely pressure. These functions provide accurate values for thermodynamic properties such as density(or specific volume), specific enthalpy, saturation pressure and temperature, etc. for a pressure range from below one atmosphere to just below the critical point. In this range, the maximum deviation from the reference values for any property was not more than 0.22%.

The range of applicability of the thermodynamic property approximation functions was expanded in a subsequent paper to include the sub-cooled and superheated regionsc(Garland and Hand, 1989). This made the approximation functions applicable anywhere in the temperature range between 90° C and 450° C, and a pressure range between 0.085 MPa and 21.3 MPa. The error for the values of entropy, enthalpy and specific volume were found to be less than 1% in the sub-cooled and superheated regions.

A final extension of the range of applicability of the approximation functions at saturation conditions was made by Garland et al. (1992) to include very low pressure and temperature conditions. The upper limit of the applicable pressure range was also consistently limited to 21.5 MPa. The final form of the approximation functions are valid in the temperature range between 18° C and 450° C, and a pressure range between 0.002 MPa and 21.5 MPa.

These expansions of the approximation function ranges of validity are not directly relevant in this study, as the T-F simulation model that was developed in this study only models conditions in the saturated two-phase region. A summary of the expanded ranges are given only to illustrate the applicability of the approximation functions in the sub-cooled and superheated regions.

2.2.5 Derivatives of approximation functions

Apart from accurate saturation thermodynamic property values, the RFES requires derivatives of these values with regards to pressure. Because the approximation functions are expressed only as a function of pressure at saturation conditions, they are simply differentiated with respect to pressure (Garland and Hoskins, 1988) to deliver the required saturation property derivative values.

2.2.6 Validity of rate method based on theoretical considerations

Before initiating an in-depth review of all the modelling theory relevant to this study, it is important to reiterate the validity of the RFES by explaining why it is expected that the RFES will provide valid solutions for a homogeneous equilibrium two-phase system model. This is done in this subsection by briefly synthesising the theoretical knowledge regarding the two-phase flow models and different equation of state formulations reviewed in this chapter.

As discussed in Subsection 2.2.1, the IAPWS-95 formulation of the equation of state is the internationally accepted standard for determining the thermodynamic properties of ordinary water. Before being replaced by IAPWS-95, the equation of state for water by Haar, Gallagher and Kell (IAPS-84) was the internationally accepted standard (Jacobsen et al., 2000). This formulation was also based on Helmholtz-free energy, and provided accurate values for thermo-

dynamic properties of water over a large range of conditions ([Wagner and Pruss, 2002](#)). It was replaced primarily because of an identified weakness in calculating certain properties as the critical point for water was approached. This property of IAPS-84 is not relevant in the context of this study. This is because the conditions simulated in this study do not approach the critical point. Therefore, we will assume that the IAPS-84 and IAPWS-95 EOS formulations are both valid and deliver the same (to a high level of accuracy) property values at the conditions that are under consideration in this study. The relevance of this assumption is explained.

The IAPS-84 formulation was the basis of the thermodynamic property approximation functions developed by [Garland et al. \(1992\)](#), [Garland and Hand \(1989\)](#), and [Garland and Hoskins \(1988\)](#). These approximation functions were formulated by using least-squares methods to curve fit property functions to property data given by steam tables based on the EOS of Haar, Gallagher and Kell. Therefore, because it was proven in the above mentioned papers that the thermodynamic property approximation functions provided accurate thermodynamic property values compared with the values given by the EOS on which it was based, it can be accepted that these approximation functions are valid. Because it is expected that the IAPS-84 and IAPWS-95 EOS formulations will provide similar values for thermodynamic properties under consideration, it can by extension be expected that the approximation functions will deliver property values that compares well with the property values delivered by IAPWS-95. Thus, based on theoretical considerations, the first component (approximation functions) of the rate methodology is expected to deliver results consistent with those of IAPWS-95.

The second component of the rate methodology, the rate equation used to calculate the system pressure, is also expected to deliver accurate results based on theoretical considerations. This is because it is a derivation based on a valid fundamental definition of fluid property values at saturated, equilibrium two-phase conditions. It uses data from the conservation equations (which is valid when correctly derived for the situation under consideration), and property values delivered by the above mentioned valid and accurate approximation functions to calculate the pressure in the system using the derived expression. The form in which the pressure data is delivered differs from that of IAPWS-95 in the fact that the pressure data is given as a time dependent parameter. To find the pressure value itself at a specific time step, it must be integrated with respect to time. Therefore, time dependence is an added factor which must be considered when using the rate method to calculate pressure. The implication of the time dependent nature of the RFES is discussed further in subsequent chapters. Because it is based on theoretically valid methods and assumptions, it is expected that the pressure rate equation will deliver pressure values that is consistent with those delivered by a benchmark EOS, such as the IAPWS-95 fundamental EOS formulation.

2.3 Summary

The literature survey served as a means of developing the necessary understanding of two-phase flow simulation methodology, as well as the role of the equation of state in this methodology. A general qualitative investigation of the various two-phase flow models was done to develop an understanding of where homogeneous equilibrium two-phase flow modelling, which is employed in this study, is applicable. The role of the equation of state as a closure equation in

homogeneous equilibrium two-phase flow modelling was then investigated. The fundamental formulations of the equation of state, which are used in many T-F simulation codes were identified. Based on the review of this information, a suitable equation of state formulation was identified which could serve as a benchmark against which to evaluate results delivered by the rate method. Certain drawbacks of these algebraic formulations of the EOS were summarised. The historical basis for these drawbacks were discussed. The basis and motivation behind this study was also stated. The rate method, as well as its constitutive parts were researched to develop an understanding of how the method solves for pressure values in a T-F simulation model.

In conclusion, the literature survey served to complete the first goal of this study, namely to develop an understanding of the relevant two-phase models, the rate form of the equation of state and the benchmark IAPWS-95 EOS formulation. With this completed, the subsequent goals of the study could be addressed. The next chapter details the mathematical formulation of a homogeneous equilibrium two-phase flow model which could serve as a suitable model in which to implement the RFES. The mathematical basis of the IAPWS-1995 equation of state, which was determined from literature to be the current state of the art in terms of thermodynamic property value accuracy, is also investigated. Finally, the mathematical formulation of the rate form of the equation of state and its constitutive parts is discussed.

Chapter 3

Modelling Theory

The rate form implementation of the equation of state evaluated in this study was developed to determine pressure values in homogeneous equilibrium two-phase flow models. This chapter will focus on developing an understanding of the relevant mathematical approaches and formulae used to create a transient simulation model based on homogeneous equilibrium two-phase flow.

The modelling approach used in this study is based on a SCFD (System Computational Fluid Dynamics) methodology. A brief introduction on one-dimensional SCFD modelling is given. The mass, momentum and energy conservation equations for one-dimensional homogeneous equilibrium flow are then discussed. The formulations for the IAPWS-95 and rate forms of the equations of state are also given. The detailed derivations of the rate form of the equation of state, as well as the conservation equations are given in Appendices [A](#) and [B](#). Finally, the derivation of the thermodynamic property approximation functions used in this study is given.

3.1 Nodalisation

A SCFD simulation methodology is employed in this study, whereby a thermal-fluid system is represented by a collection of nodes that are connected by one-dimensional elements. The elements represent any type of thermal-fluid component ([Du Toit et al., 2006](#)), whereas the function of the nodes is to connect these components to one-another ([Greyvenstein and Rousseau, 2003](#)). The nodes may either function simply as links between the elements with no physical significance, or may have an associated volume in which case the node represents a reservoir or tank.

The nodalisation approach used in this study is analogous to the staggered grid approach employed in conventional CFD (Computational Fluid Dynamics). The nodes represent all of the mass and energy in the system, while the elements, which serve as the interfaces between the nodes, account for the momentum changes in the flow between the nodes. The fluid properties in each node are represented by a single average value. An example of other codes that use this method is the RELAP5-3D T-F code, which utilises the same nodalisation methodology when simulating transient, one-dimensional two-phase flow ([INL, 2005](#)). The detailed discretisation of the mass, momentum and energy conservation control volumes as they were implemented in

this study is discussed in Chapter 4.

3.2 Conservation equations

The conservation equations for mass, momentum and energy that define the HEM are given in the following sections. Fig. 3.1 illustrates the generic infinitely small control volume used for the derivation of the one-dimensional mixture conservation equations used in homogeneous equilibrium two-phase flow modelling. The integral form of each conservation equation is initially given. To apply the conservation equations in the transient network model developed in this study, the differential form of the conservation equations was required. This is given subsequently to the integral form of each conservation equation. The detail derivations to transform the integral equations into differential equations can be found in Appendix B.

All conservation equations used in this study are based on those derived by Rousseau (2012b). Therefore, the equations that follow are not original work by the author, but rather a summary of equations derived by a source in literature. These equations are given here so that the reader may have access to these simplified two-phase flow conservation equations, as the form of the equations used specifically in this study may not be easily obtainable from literature.

Several textbooks pertaining to thermal-fluid and two-phase flow modelling also list or derive the equations for homogeneous two-phase flow conditions. These include the books by Ishii and Hibiki (2011), Stadtke (2006), Todreas and Kazimi (1990), and Collier (1972). The notation used by these texts vary, but they provide formulations of the homogeneous model that are consistent with the model derived and used in this study.

The mass, momentum and energy conservation equations are derived using the infinitesimally small control volume defined in Fig. 3.1. The flow is one-dimensional, meaning that the property value under consideration is considered homogeneous (averaged) over the cross-sectional area of the control volume, with the averaged property values changing only in the direction of fluid flow. The direction of fluid flow through the control volume is defined by the arrows. The length of the control volume is given as $d\ell$. The geometric properties of the control volume may change over its length, e.g. the cross-sectional area (A) may change from an initial value, A , to a new value based upon the increase in area per length, $\frac{\partial A}{\partial \ell}$. This is also true for fluid properties, e.g. pressure and velocity, which may change over the length of the control volume. Final consideration must be given to the component forces that does work on the fluid. Forces such as friction works on the fluid in the opposite direction to the fluid flow direction, while gravity forces does work perpendicular to the flow direction when considering a control volume with zero inlet and outlet elevations.

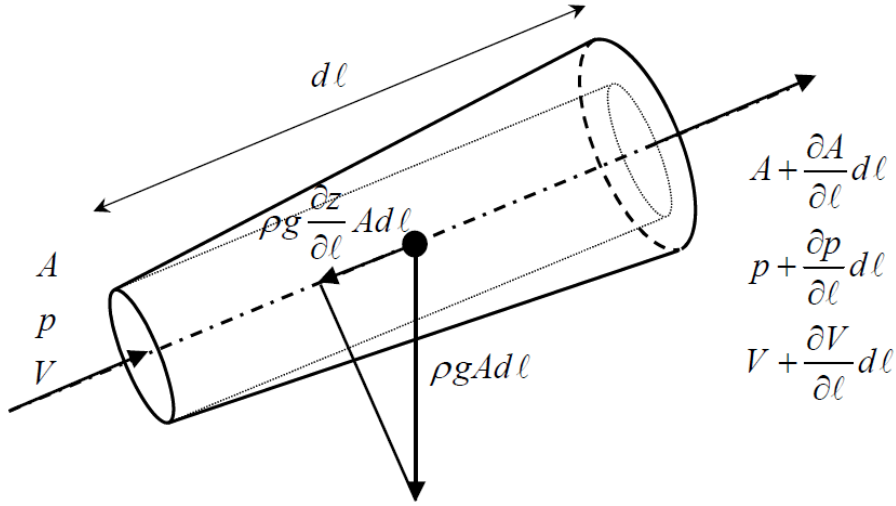


Figure 3.1: Infinitesimal control volume used for derivation of conservation equations. (Rousseau, 2012a)

3.2.1 Conservation of mass

The integral form of the mass conservation equation for a finite control volume is given as:

$$\frac{\partial}{\partial t} \left(\iiint \rho d\mathcal{V} \right) + \oint \rho \bar{V} \cdot \bar{dA} = 0 \quad (3.1)$$

with $\mathcal{V}$ the volume, ρ the average density in the control volume and V the velocity relative to the control volume. The unit for time is given as t . All units with a bar notation indicates averaged units. By using the appropriate derivation, discussed in detail in Appendix B.1, the differential form of the mass conservation equation can be written as follows:

$$\mathcal{V} \frac{\partial \rho}{\partial t} + \dot{m}_e - \dot{m}_i = 0 \quad (3.2)$$

3.2.2 Conservation of momentum

The integral form of the linear momentum conservation equation for an inertial control volume is given as:

$$\oint \tau \bar{dA} + \iiint \bar{B} \rho d\mathcal{V} = \frac{\partial}{\partial t} \left(\iiint \bar{V} \rho d\mathcal{V} \right) + \oint \bar{V} (\rho \bar{V} \cdot \bar{dA}) \quad (3.3)$$

The first term in eq. (3.3) represents the surface forces working on the control volume, and the second term represents the body forces in the control volume. By implementing the proper

derivation, discussed in Appendix B.2, the integral form of the momentum conservation equation can be rewritten in the following differential form:

$$\rho L \frac{\partial V}{\partial t} + (p_{0e} - p_{0i}) - \frac{1}{2} V_i V_e (\rho_e - \rho_i) + \rho g (z_e - z_i) + \Delta p_{0L} = 0 \quad (3.4)$$

where z denotes elevation, g the gravitational acceleration and Δp_{0L} represents the pressure loss.

A note must be made in terms of the densities defined in the conservation equations used in this study. Some texts in literature, e.g. (Levy, 1999), define different density values such as kinetic density and momentum density. These different definitions of density are incorporated in the conservation equations. These densities become relevant in flow with differing phasic velocities and where equilibrium conditions are not assumed. In the case of homogeneous equilibrium flow, which is employed in this study, these densities collapse into a single density value. This means that the homogeneous equilibrium conservation equations employed in this study are consistent with those derived by texts that make use of different density definitions for more complex flow models.

3.2.3 Conservation of energy

The integral form of the energy conservation equation for a finite control volume is given as:

$$\begin{aligned} \dot{Q} + \dot{W} = \frac{\partial}{\partial t} \left(\iiint \left(u + \frac{1}{2} V^2 + gz \right) \rho dV \right) \\ + \oint \left(h + \frac{1}{2} V^2 + gz \right) \rho \bar{V} \cdot \bar{dA} \end{aligned} \quad (3.5)$$

$\dot{Q}$ and $\dot{W}$ represent the total heat and work loads in the control volume respectively, while u denotes specific internal energy.

By applying the derivation discussed in detail in Appendix B.3, the integral form of the energy conservation equation can be written in the following differential form:

$$\dot{Q} + \dot{W} = \dot{V} \frac{\partial}{\partial t} (\rho h_0 - p) + \dot{m}_e h_{0e} - \dot{m}_i h_{0i} + \dot{m}_e g z_e - \dot{m}_i g z_i \quad (3.6)$$

3.3 Equation of state

The equation of state is used to calculate the pressure when solving the three mixture conservation equations (Garland, 1998). The reference equation of state for this study is the IAPWS

1995 formulation based on the Helmholtz free-energy equation. The alternative equation of state investigated in this study is the rate form of the equation of state developed by [Garland and Sollychin \(1987\)](#). These formulations of the equations of state are described in Subsections 3.3.1 and 3.3.2. The IAPWS 1995 formulation is discussed only briefly, as the method is complex and derived fully in the papers discussed in Subsection 2.2.1 of the literature survey.

3.3.1 IAPWS-95 equation of state

The IAPWS-95 formulation is a fundamental equation of the specific Helmholtz free-energy, f . In other publications, especially those endorsed by IUPAC (International Union of Pure and Applied Chemistry), Helmholtz free-energy is given by the symbol a . Helmholtz free-energy is an example of a thermodynamic potential, where a thermodynamic potential is a quantity used to describe the thermodynamic state of a system. This potential is derived directly from the second law of thermodynamics, which may be written for a phase in the absence of a external field as follows,

$$dU = TdS - pdV \quad (3.7)$$

where dU represents the change in internal energy of the system and it is solved as a function of the simultaneous changes dS in the entropy S and dV in the volume V . This expression is the most fundamental expression of the second law of thermodynamics ([Sengers et al., 2000](#)). However, entropy is not a convenient experimental variable. Because of this, alternate forms to eq. (3.7) were derived to remove the dependence of the relation on entropy. One of these fundamental derivations was the Helmholtz free-energy, a . For pure systems in equilibrium with their environment, this fundamental relation may be written in the following form:

$$a = a(v, T) \quad (3.8)$$

where v is the specific volume and T the temperature. Although other forms of the fundamental equation such as the internal energy, enthalpy, and Gibbs energy may be derived from the fundamental equation for the second law of thermodynamics, the Helmholtz energy is the only fundamental relation that is suitable for the development of equations of state which describe the whole fluid region ([Jacobsen et al., 2000](#)). Eq. 3.8 is equivalent to the definition for Helmholtz free-energy given by [Wagner and Pruss \(2002\)](#):

$$a = a(v, T) = f(\rho, T) \quad (3.9)$$

This relation may be expressed in a dimensionless form,

$$\phi = \frac{f(\delta, \tau)}{RT} \quad (3.10)$$

with R the specific gas constant, T the temperature. The dependent variable δ is dimensionless and defined as $\delta = \frac{\rho}{\rho_c}$, where ρ_c is a specified reference density. The variable τ gives the same relation, only for the temperature instead of the density. The IAPWS-95 formulation of the equation of state is an empirical description of this Helmholtz free-energy function. The function is separated into two parts, an ideal gas part, ϕ^p and a residual part ϕ^r . This gives the form:

$$\frac{f(\rho, T)}{RT} = \phi(\delta, \tau) = \phi^p(\delta, \tau) + \phi^r(\delta, \tau) \quad (3.11)$$

The ideal gas part of this equation may be written in expanded form as,

$$\phi^p(\delta, \tau) = \ln \delta + n_1^o + n_2^o + n_3^o \ln \tau + \sum_{i=4}^8 n_i^o \ln[1 - e^{-\gamma_i^o \tau}] \quad (3.12)$$

and the residual part is given as,

$$\begin{aligned} \phi^r(\delta, \tau) = & \sum_{i=1}^7 n_i \delta^{d_i} \tau^{t_i} + \sum_{i=8}^{51} n_i \delta^{d_i} \tau^{t_i} e^{-\delta_i^c} \\ & + \sum_{i=52}^{54} n_i \delta^{d_i} \tau^{t_i} e^{-\alpha_i (\delta - \epsilon_i)^2 - \beta_i (\tau - \gamma_i)^2} \\ & + \sum_{i=55}^{56} n_i \Delta^{b_i} \delta \Phi \end{aligned} \quad (3.13)$$

From the above equations it can be seen that there is a substantial amount of information required to solve these equations. The coefficients shown in eqs. (3.12) and (3.13) requires a large amount empirical data as well as theoretical considerations to be determined. Any more specific details pertaining to the determination of these coefficients in the formulation of the IAPWS-95 formulation is beyond the scope of this study. These equations are given here to

show that the formulation of a fundamental EOS is not a trivial matter. Should the reader require more information regarding the complete formulation of the IAPWS-95 EOS, the paper by [Wagner and Pruss \(2002\)](#) is the definitive source of information regarding the formulation.

Any relevant thermodynamic property can be accurately calculated by using the appropriate combinations of the ideal gas part ϕ^p and the residual part ϕ^r of the dimensionless Helmholtz free-energy equation given in eq. (3.11) and their derivatives. For example, pressure may be solved using the following equation derived from eq. (3.11),

$$p = \rho RT \left(1 + \delta \frac{\partial \phi^r}{\partial \delta} \right) \quad (3.14)$$

and enthalpy may be expressed as,

$$\frac{h}{RT} = \tau \left(\frac{\partial \phi^0}{\partial \tau} + \frac{\partial \phi^r}{\partial \tau} \right) + \delta \frac{\partial \phi^r}{\partial \delta} + 1 \quad (3.15)$$

This formulation is therefore capable of solving for all the thermodynamic properties of water, including pressure which is required by the conservation equations. The EES simulation code employed in this study allows for the use of this formulation of the equation of state to determine fluid properties of water.

Because this equation of state is in turn based on a fundamental thermodynamic potential which describes the state of a fluid, the pressure is taken to be a pure function of the local state of the fluid under consideration. This means the calculation of pressure is time independent, or in other words the value for pressure is determined directly from the state variable values supplied to the equation of state, without taking the rate of change of these property values with respect to time into consideration.

3.3.2 Rate form of the equation of state

In contrast to the fundamental formulation of the equation of state, the rate form of the equation of state relates the rate of change of pressure to the rates of change of density and enthalpy in the system. It therefore describes pressure as a function of both space and time. As in the case of the conservation equations, it allows for the development of a time history of system pressure, which can then be integrated for specific time steps to yield the pressure value at discrete moments in time. The RFES is defined by the following equation:

$$\frac{dp}{dt} = G_1(p, x) \frac{d\rho}{dt} + G_2(p, x) \frac{dh}{dt} \quad (3.16)$$

with $G_1(p, x)$:

$$G_1(P, x) = \frac{(h_g - h_f)[x\nu_g + (1 - x)\nu_f]^2}{\left[x\frac{\partial h_g}{\partial p} + (1 - x)\frac{\partial h_f}{\partial p}\right](\nu_g - \nu_f) - \left[x\frac{\partial \nu_g}{\partial p} + (1 - x)\frac{\partial \nu_f}{\partial p}\right](h_g - h_f)} \quad (3.17)$$

and $G_2(p, x)$:

$$G_2(P, x) = \frac{(v_g - v_f)}{\left[x\frac{\partial h_g}{\partial p} + (1 - x)\frac{\partial h_f}{\partial p}\right](\nu_g - \nu_f) - \left[x\frac{\partial \nu_g}{\partial p} + (1 - x)\frac{\partial \nu_f}{\partial p}\right](h_g - h_f)} \quad (3.18)$$

The full derivation of the rate form of the equation of state for homogeneous equilibrium two-phase fluid is given in Appendix A.

3.4 Approximation functions

The thermodynamic property approximation functions discussed here were developed specifically to deliver the thermodynamic property values required to solve the RFES discussed in Subsection 3.3.2. They form a part of the rate methodology, where the RFES, which solves for the system pressure is combined with these approximation function, which deliver the required density and enthalpy values to the equation. Therefore, when these two components are combined, the form a complete and alternate EOS methodology which can be used as a substitute for EOS formulations such as IAPWS-95.

The approximation functions developed by [Garland and Hoskins \(1988\)](#) were obtained by fitting functions to the reference steam tables by means of a least squares method. To ensure accuracy while maintaining a continuous first derivative over the entire pressure range, the approximation functions were segmented to cover specific pressure ranges. This means that there are several discrete equations describing the property over the entirety of the defined pressure range for each thermodynamic property.

The approximation functions were initially formulated to deliver values for thermodynamic properties only at saturation conditions. These functions were subsequently expanded to be able to deliver values for properties in the sub-cooled and superheated regions as well. The derivation of the final form which is able to determine saturation properties, as well as sub-cooled and superheated properties is done as follows.

Consider an arbitrary thermodynamic property $F = F(p, T)$. The first two terms of the Taylor expansion of property F in pressure, about the point at saturation conditions corresponding to

the temperature T , are:

$$F(p, T) = F_f(T) + \left. \frac{\partial F}{\partial p} \right|_T (p - p_s(T)) \quad (3.19)$$

The first term in the Taylor expansion represents the thermodynamic property value at saturation conditions. This is true because at saturation conditions the pressure p is equal to the saturation pressure p_s , giving:

$$\begin{aligned} F(p, T) &= F_f(T) + \left. \frac{\partial F}{\partial p} \right|_T (p_s(T) - p_s(T)) \\ &= F_f(T) + \left. \frac{\partial F}{\partial p} \right|_T (0) \\ &= F_f(T) \end{aligned} \quad (3.20)$$

The saturation formulae were however developed as a function of pressure. At saturation conditions, pressure can be expressed as a function of temperature and vice-versa. These correlations are simply written as:

$$p_s = p_s(T) \quad (3.21)$$

$$T_s = T_s(P) \quad (3.22)$$

This allows the first term in eq. (3.19) to be rewritten in terms of the saturation pressure p_s , which is a function of T :

$$F(p, T) = F_f(p_s(T)) + \left. \frac{\partial F}{\partial p} \right|_T (p - p_s(T)) \quad (3.23)$$

For sub-cooled conditions, properties are a strong function of temperature, but only a weak function of pressure. Thus the derivative of the function with respect to pressure gives a slowly varying, almost constant function. By rearranging eq. (3.23) the following is obtained:

$$\left. \frac{\partial F}{\partial p} \right|_T = \frac{F(p, T) - F_f(p_s(T))}{(p - p_s(T))} \quad (3.24)$$

Garland and Hand (1989) calculated these derivatives at given temperatures across a pressure range (0.07 MPa to 20 MPa), after which it was averaged. This was done for temperatures between 90 °C and 350 °C. The resulting averages were fitted with simple, non-linear functions of temperature. The derivative can therefore be rewritten as a function of T :

$$\left. \frac{\partial F}{\partial P} \right|_T = R(T) \quad (3.25)$$

This allows eq. (3.24) to be rewritten in the following form:

$$F(p, T) = F_f(p_s(T)) + R(T)(p - p_s(T)) \quad (3.26)$$

which is the final form to determine the saturated and sub-cooled fluid properties of steam in the defined pressure and temperature ranges.

The approximation functions for the superheated properties can not be derived in the same manner as for the sub-cooled properties. This is because the properties are strong functions of both pressure and temperature in the superheated region. Consider again an arbitrary thermodynamic property $F = F(p, T)$. The first two terms of the Taylor expansion of F in temperature, around a point of saturation corresponding to pressure p , are:

$$F(p, T) = F_g(p) + \left. \frac{\partial F}{\partial T} \right|_p (T - T_s(p)) \quad (3.27)$$

The first term of the Taylor expansion again represents the property at saturated vapour conditions because at this condition the temperature T is equal to the saturation temperature T_s so that:

$$F(p, T) = F_g(p) \quad (3.28)$$

The derivative of the property is rewritten as follows:

$$R(p, T) = \left. \frac{\partial F}{\partial T} \right|_p \quad (3.29)$$

Because the derivative is a strong function of both temperature and pressure, it is more difficult to fit than the $R(p, T)$ function in the sub-cooled equation. The approach followed by [Garland and Hand \(1989\)](#) was to plot R as function of pressure for several constant temperatures. A set of curves resembling those of $R(p, T)$ were then chosen. The approximation functions chosen to generate $R(p, T)$ are simple and non-linear in nature.

The generic form of the approximation functions for thermodynamic properties in the super-heated region is therefore given by:

$$F(p, T) = F_g(p) + R(p, T)(T - T_s(p)) \quad (3.30)$$

In the case of this study, only saturated liquid and saturated vapour property values were required. Therefore the second term in both eqs. (3.26) and (3.30) become zero, reducing the equations to:

$$F_f(p, T) = F_f(p_s(T)) \quad (3.31)$$

and:

$$F_g(p, T) = F_g(p) \quad (3.32)$$

which are the forms employed in this study.

3.5 Numerical integration for time dependent systems

The rate form of the equation of state under investigation in this study was formulated as a time dependent equation. The conservation equations that were derived in the previous sections are also written as time dependent equations. Therefore, to formulate a model that uses the rate method, a transient simulation model had to be developed. This meant that an appropriate time-wise integration scheme had to be chosen. The purpose of this time-wise scheme is to allow for the simulation of the conditions in the system as time is progressed. To avoid extraneous complication of the transient pipe and network model developed in EES, the literature was reviewed to identify a simple numerical time-wise integration scheme that could provide acceptable results for the chosen time step resolutions.

3.5.1 Euler's Method

From literature, it was seen that one of the simplest methods for integrating differential equations with respect to time is the Euler method (Butcher, 2008; Hirsch, 2007). To ensure the model remained as simple as possible, the Euler method was therefore chosen for use as the numerical integration method for the model developed in EES. The method can be described by considering an example. In the case of this study, the solution of values of pressure as a function of density and enthalpy is considered. This differential equation is written in a simplified form as:

$$\frac{dp}{dt} = f(\rho, h, x) \quad (3.33)$$

This equation simply states that the change in the pressure values from the current time to a next specified time is given by a function that is dependent on the density, enthalpy and quality of the system. The time from the current time to the next time considered is called the time step and is defined as,

$$\Delta t = t^1 - t^0 \quad (3.34)$$

The change in pressure across one time step is defined as the pressure value at the subsequent time minus the pressure value at the initial time,

$$\Delta p = p^1 - p^0 \quad (3.35)$$

where p^0 is the pressure value and p^1 is the pressure value at the subsequent time-step. Eq. 3.33 may therefore be rewritten in the following manner:

$$\frac{dp}{dt} = \frac{\Delta p}{\Delta t} = \frac{p^1 - p^0}{t^1 - t^0} = f(\rho, h, x) \quad (3.36)$$

This form is termed the finite difference form of the differential equation. The equation in this form may be implemented in a numerical simulation model to solve for pressure as a function of changing time. Rewriting this equation:

$$p^1 = p^0 + \Delta t[f(\rho, h, x)] \quad (3.37)$$

This equation shows that a new value of pressure may be obtained using the old pressure value and adding the value of the function which describes the rate of change of the pressure multiplied by the time step length. If the function delivers a negative value, the new pressure will be lower than the initial pressure, while it will be higher if the function returns a positive change value. This process is illustrated graphically in Fig. 3.2

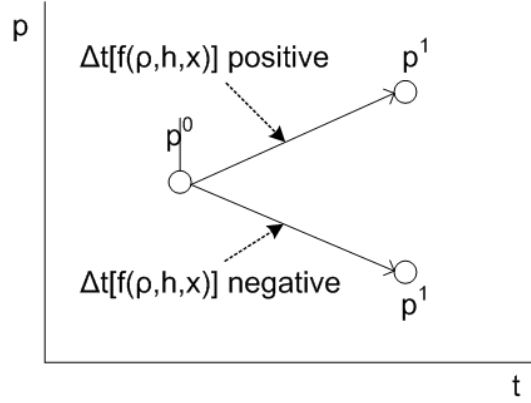


Figure 3.2: Change in pressure from initial value to new value based on change function information. P^0 represents the initial time step, while P^1 represents the subsequent time step.

The next aspect of this integration methodology is to consider where the information required to solve the change function ($f(\rho, h, x)$) is obtained from. The amount by which the pressure will change over a given time step is dependent on the pressure change value delivered by the change function. The change function is in turn dependent on values of density, enthalpy, and mass quality. The simplest way to determine the change function is to use the values for density, enthalpy, and mass quality that were already solved at the initial time step. In other words, the change function is solved using values at the previous time step, so that

$$p^1 = p^0 + \Delta t[f(\rho^0, h^0, x^0)] \quad (3.38)$$

From eq. 3.38 it can be seen that this solution, where the property values required to calculate the change function are calculated using their values at the previous time step, leads to an explicit numerical solution. This is because the value of p^1 can be explicitly calculated from known values at the previous time step. This type of solution method is known as the forward Euler method, and was the initial method developed by Leonhard Euler in 1913 (Hirsch, 2007).

A variant of the general, or forward Euler method, is known as the backward Euler method. This integration method has the same form as the general Euler equation, but instead of using property values at the previous time step to calculate the change function, this method uses

the property values calculated at the next time step to calculate the change function value. This is given by the following equation:

$$p^1 = p^0 + \Delta t[f(\rho^1, h^1, x^1)] \quad (3.39)$$

The backward Euler method is therefore implicit in time, which means that property values are required from the initial time step as well as the new time step to be able to calculate the required new property value. Therefore, when using the implicit Euler approach iteration of the equations will be necessary to obtain a solution.

A final variant of the Euler method involves combining both the forward and backward Euler approaches. When this is done, a solution method known as the Crank-Nicolson method results. This method is given mathematically as follows:

$$p^1 = p^0 + \Delta t[\frac{1}{2}f(\rho^0, h^0, x^0) + \frac{1}{2}f(\rho^1, h^1, x^1)] \quad (3.40)$$

Because eq. 3.40 also requires property values at the new time step, it is also an implicit method. This statement may be generalised by stating that only the forward Euler method is an explicit method in time. Any solution that requires the values of properties at the new time step is therefore an implicit method.

3.5.2 Stability and order of accuracy

The forward and backward Euler, and Crank-Nicolson integration schemes have different properties in terms of stability and accuracy. Stability refers to the ability of the a numerical method to converge to the exact solution as time step size is increased. If a numerical method is unconditionally stable, it will converge to the correct solution independent of integration step size. If a method is not numerically stable, it may fail to converge to the correct solution if the integration step length becomes too large.

The accuracy of a numerical method is generally given quantified by the order of accuracy. The order of accuracy of the method is defined as the power of c with which the error tends to zero (Hirsch, 2007). Therefore, higher order accuracy methods will be more accurate than lower order methods. Table 3.1 summarizes the stability and accuracy characteristics of forward and backward Euler, and the Crank-Nicolson solution schemes.

Table 3.1: Stability and accuracy characteristics of the different numerical integration schemes.

Numerical Scheme	Order of accuracy	Stability
Forward Euler	First order	Unstable (large integration steps)
Backward Euler	First order	Unconditionally stable
Crank-Nicolson	Second order	Unstable (large integration steps)

The numerical integration of the transient pipe and reservoir network that was programmed in EES utilised a generalisation of the approaches discussed above. Instead of specifically implementing each method separately to solve the model, an integration weighting factor α was assigned so that the transient integration solution method could be switched between all three of the the methods described above, as well as arbitrary weightings of implicit/explicit integration preference. When this generalisation is applied, the general Euler equation defined in eq. (3.41) becomes the following:

$$p^1 = p^0 + c[\alpha f(\rho^1, h^1, x^1) + (1 - \alpha)f(\rho^0, h^0, x^0)] \quad (3.41)$$

where $0 \leq \alpha \leq 1$. In this manner, the solution can be weighted between the fully explicit forward Euler solution at $\alpha = 0$ or the fully implicit backward Euler solution at $\alpha = 1$. The Crank-Nicolson solution is achieved at $\alpha = 0.5$. This numerical scheme is used to integrate all of the conservation equations in the transient pipe and reservoir network developed in EES, as well as the rate form of the equation of state which is used here as an example.

3.5.3 Integration time step length

The integration time step length value used in the model developed in this study is defined as the time step length. The time step length therefore dictates the time that elapses between the solution of the model at a previous time step and the solution of the model at a following time step. It is important to ensure that the time step length used for the numerical does not become so large as to introduce numerical integration errors when solving for a transient system.

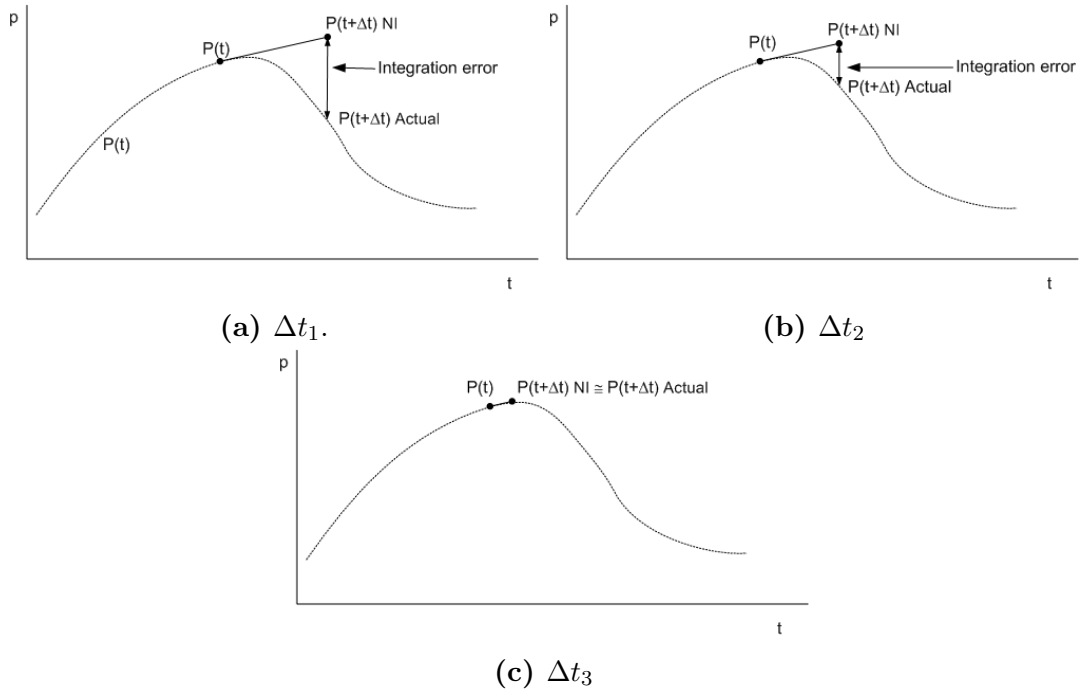


Figure 3.3: Example of transient integration errors when solving a model with different integration time step lengths. In this case $\Delta t_1 > \Delta t_2 > \Delta t_3$

Figure 3.3 provides an example of integration error. Here the change of pressure at a point of interest is expressed as a function of time. The continuous line represents the actual change in pressure values in a system as a function of time. It can be seen that the pressure changes in an arbitrary manner. At a certain point in time, the increase in pressure value stops and the pressure begins to decrease. If the integration time step length is too long, a situation as depicted in Fig. 3.3a will result, where the $P(t + \Delta t)$ NI value represents the numerical approximation value of the pressure. The change function, which is a gradient function that gives the rate of change in pressure as over a specific time period, is multiplied by a time step value that is too long relative to the rate at which the pressure in the physical system changes. This leads to an overshoot or overestimation of the pressure value at the next time step. This error will propagate as additional time steps are taken in the simulation and build until either the model simulating the physical phenomenon fails or a solution is obtained that does not reflect the physical phenomenon at all. As the time step length is shortened, the integration error becomes smaller, as in Fig. 3.3b, until the numerical value reflects the actual pressure value to an acceptable accuracy in Fig. 3.3c.

While the improved accuracy shown in Fig. 3.3c is obviously the desired outcome, the improvement in accuracy because of shorter time steps is offset by an additional computational burden. Because the time steps are roughly 4-5 times shorter in Fig. 3.3c when compared with those in Fig. 3.3a it means that instead of the system of equations that constitute the model being solved only once, the equation set must be solved 4-5 times to arrive at the same $t + \Delta t$ point as in the first figure. This means that the model will take 4-5 times (all other factors considered equal) as long to solve in the case of this example. There is therefore a practical limit to how small the time step sizes can be made before a point of diminishing returns is encountered in

terms of solution accuracy versus computational time.

The possibility of numerical errors and their impact on the accurate modelling of transient T-F systems is specifically important to this study. The rate methodology which is evaluated in this study adds an additional time dependent equation to the standard model of the pipe and reservoir network which is formulated in this study. Instead of only integrating the three time dependent conservation equations, the rate form of the equation of state is now also integrated over time. This increases the possibility of time wise integration based errors. Therefore, to evaluate the impact of the addition of the rate form of the equation of state on the transient integration error of the system, the model was solved at different time step lengths using the RFES. These results were then compared to a solution of the model that used an equation of state that is solved independent of time (IAPWS), thereby enabling a quantitative evaluation of the impact the RFES has on the transient integration accuracy of the pipe and network model. This quantitative comparison is discussed in Chapter 5.

Chapter 4

Methodology

This chapter outlines the methodology employed in the implementation of the rate method in a transient T-F simulation model.

The methodology followed a systematic approach whereby the constitutive parts of the rate formulation were firstly coded/implemented and evaluated for correct solutions in isolation to ensure that they were properly implemented. The RFES for homogeneous equilibrium two-phase flow requires accurate values of state properties to determine the rate of change of pressure in the system under consideration. The RFES further requires derivatives of the state properties with regards to pressure. These constitutive parts were implemented by coding them as procedure files in EES. To ensure that the approximation and derivative functions were properly coded and would deliver the accurate property values and derivatives that were required, these functions were coded and then compared directly with property values generated by the IAPWS-95 formulation of the equation of state. Because the IAPWS-95 EOS is the accepted standard for calculating thermodynamic property values, and the approximation functions were proven to be accurate by their developers, a good agreement between the IAPWS-95 values and approximation function values would mean that the functions were incorporated correctly in EES.

The rate form of the equation of state was then implemented in a transient simulation model of an unstructured pipe and reservoir flow network in EES. The RFES was used to solve for the system pressure during various transients in the pipe and reservoir network in parallel with the IAPWS-95 EOS. This allowed for a direct comparison of the RFES with the fundamental EOS approach. The results of the transient simulations and discussions thereof are given in Chapter 5.

4.1 Approximation function implementation

From the equation of the RFES given in Subsection 3.3.2, it is seen that saturation values for density and enthalpy are required to solve this equation of state. The thermodynamic property approximation functions developed by [Garland and Hoskins \(1988\)](#) were specifically formulated to deliver these saturation density and enthalpy values. To facilitate the solving of pressure values in the EES model developed in this study via the RFES, these approximation functions were written as EES procedure files that could be called when simulating the transient net-

work model. Because the approximation functions had already been proven to be accurate by the developers of the functions, it remained to ensure that no errors were made when coding the approximation functions as procedure files in EES. Therefore, the saturation property values delivered by the approximation functions EES procedures were compared with saturation property values delivered by the IAPWS-95 EOS to ensure that the expected good correlation between property values was achieved.

To test the implementation of the approximation functions, a parametric table was created dividing a pressure range of 0.05 MPa to 21 MPa into one thousand (1000) increments. This range was chosen as it falls within of the range of validity of the approximation functions. The range also includes the operating pressures of pressurised light water reactors and boiling water reactors. This is relevant as the rate form of the equation of state was developed for use in nuclear reactor system simulations (Garland, 1998).

Table 4.1: Parametric accuracy evaluation of saturated fluid enthalpy values.

Accuracy: Saturated fluid enthalpy			
Run	Pressure [MPa]	Saturation temperature [$^{\circ}C$]	Error [%]
1	0.05	81.35	0.02024
$\vdots$	$\vdots$	$\vdots$	$\vdots$
1000	21	369.9	-0.04594

Table 4.1 illustrates the form of the parametric table generated in EES, with the example given for the saturated fluid enthalpy, h_f . The saturation temperature was determined from the pressure value using eq. (3.22). The deviation of the approximation function value from the value generated by the IAPWS-95 EOS was termed the error value. The error value was determined by the following equation:

$$Error = \left(\frac{F_{AF} - F_{IAPWS}}{F_{IAPWS}} \right) \times 100 \quad (4.1)$$

where F_{AF} is the thermodynamic property value delivered by the relevant approximation function and F_{IAPWS} the thermodynamic property value delivered by the IAPWS 1995 formulation of the EOS. This equation therefore calculated the percentage difference between values delivered by the two methods. After the parametric tables were generated, the percentage error for each thermodynamic property was plotted over the chosen pressure range.

4.1.1 Saturation properties

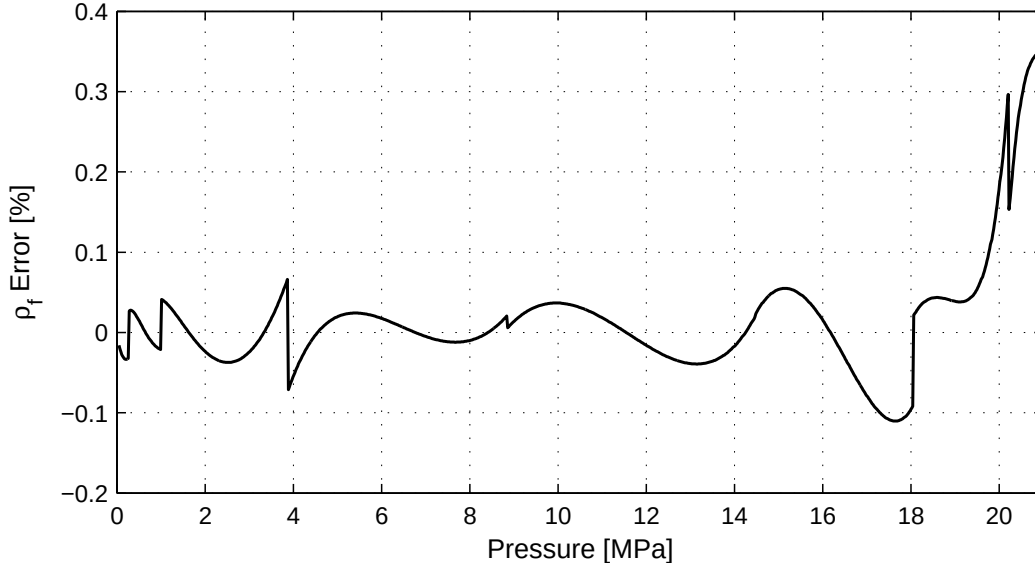


Figure 4.1: Percentage error for liquid density over designated pressure range.

The accuracy of the approximation function for density at liquid saturation is illustrated in Fig. 4.1. The error when compared to the IAPWS 1995 formulation is not more than 0.1% for $0 < p < 17$ MPa. For $p > 17$ MPa the error is slightly higher up to 0.36%, which is high relative to the rest of the range, but remains small in absolute terms. This increase in error as the critical pressure is approached may be expected based on the fact that the approximation functions are based on data from the IAPS-84 EOS formulation, which was known to exhibit some weakness for certain properties as the critical pressure was approached. The IAPWS-95 EOS formulation replaced the IAPS-84 EOS because of this. Thus the larger difference seen in Fig. 4.1 might be as a result of the more accurate IAPWS-95 density value differing more from the IAPS-84 density value as the critical point is approached.

Table 4.2: Discrete pressure ranges for approximation for density at saturated liquid conditions.

Pressure ranges: Saturated fluid enthalpy	
Equation Number	Range of Validity [MPa]
1	$0.020 \leq P < 0.01468$
2	$0.01468 \leq P < 0.275$
3	$0.275 \leq P \leq 1.000$
4	$1.000 < P \leq 3.880$
5	$3.880 < P \leq 8.840$
6	$8.840 < P \leq 14.463$
7	$14.463 < P < 18.052$
8	$18.052 \leq P < 20.204$
9	$20.204 \leq P \leq 21.500$

Fig. 4.1 shows sharp discontinuities at certain points in the pressure range. These points of discontinuity coincide with the beginning and end of the pressure ranges where each discrete approximation equation is valid for the given thermodynamic property (See Section 3.4). The pressure ranges for the nine discrete equations used to determine the saturated fluid density over the entire pressure range are given in Table 4.2. The table is given to describe the nature of these curve discontinuities. These discontinuities are also present in the error plots of the other fluid properties under consideration, but for the sake of brevity the pressure domains of these functions are not listed here. The reader is referred to the literature discussed in Section 2.2.4 if further information is required.

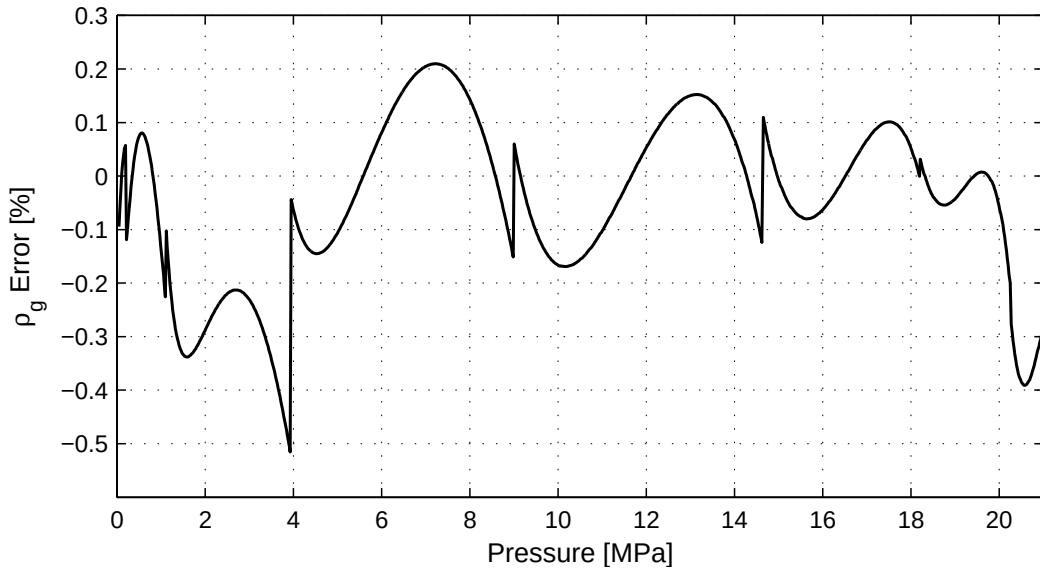


Figure 4.2: Percentage error for vapour density over designated pressure range.

Fig. 4.2 shows the error in the values for saturated vapour density. The error is somewhat higher than for the saturated fluid density, with a maximum of roughly 0.5%.

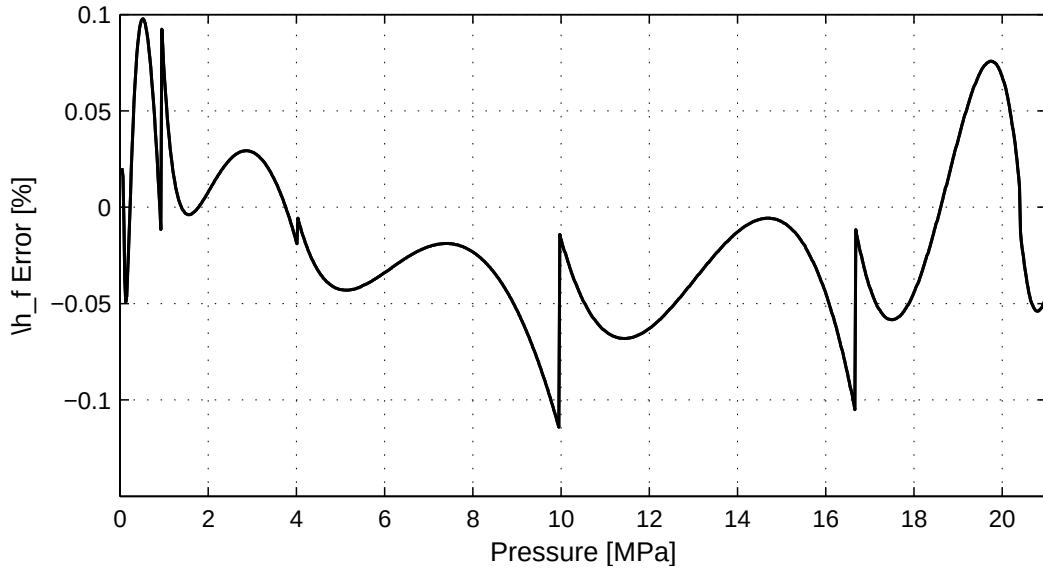


Figure 4.3: Percentage error for liquid enthalpy over designated pressure range.

Figs. 4.3 and 4.4 show the error for the saturation values of enthalpy for the liquid and vapour respectively. The error for saturated liquid enthalpy is not larger than 0.1%, while for saturated vapour enthalpy the error has a maximum value of 0.25% at high pressure.

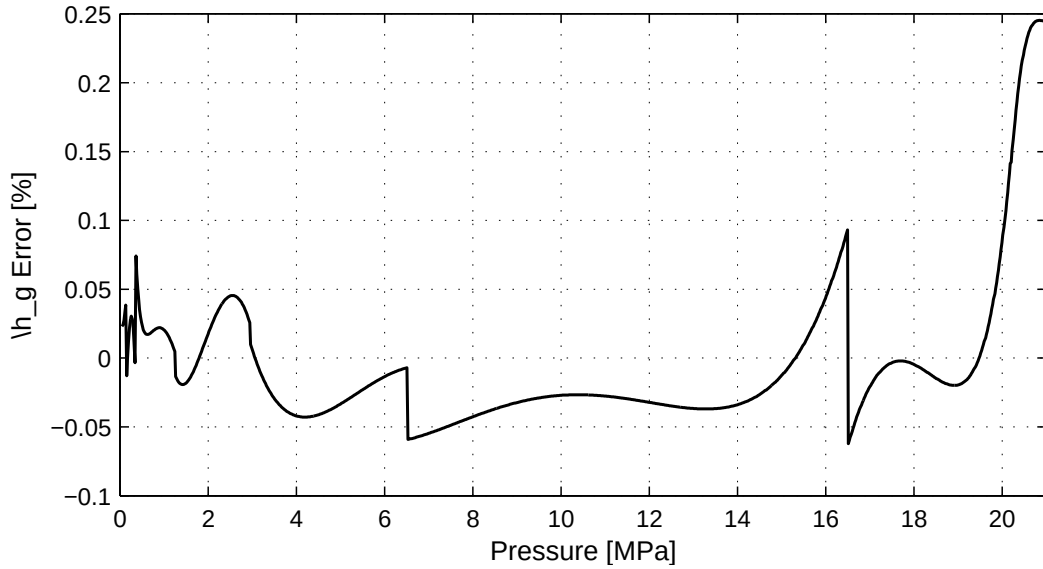


Figure 4.4: Percentage error for vapour enthalpy over designated pressure range.

4.1.2 Saturation property derivatives

To solve the RFES, derivatives of saturation density and enthalpy with regards to pressure are also required. Because the approximation functions at saturation conditions are written only as functions of pressure, these functions are simply differentiated with respect to pressure to generate the required derivative functions. The authors of the approximation functions did

not explicitly give the equations for the derivatives of the approximation functions in their works, nor do they explicitly evaluate their accuracy when compared with derivatives from another approximation function. They simply state that the required derivative functions may be obtained by differentiating the given approximation functions with regards to pressure. Therefore, to implement the rate formulation in this study, the approximation functions had to be differentiated and then written as procedure files implemented in EES. To ensure that no error was generated when implementing the derivative EES procedures in the network model developed in this study, the gradient values delivered by the approximation function derivatives were compared with gradient values generated using perturbations of the IAPWS-95 EOS.

To test the accuracy of the derivatives of the approximation functions, the same pressure range was again defined from 0.05 MPa to 21 MPa and discretized into 1000 increments.

The IAPWS 1995 EOS does not allow for the direct calculation of derivatives. Therefore, derivatives were generated by perturbation calculations using the following formula:

$$\begin{aligned}\frac{dF}{dp} &= \frac{\Delta F}{\Delta p} \\ &= \lim_{\Delta p \rightarrow 0} \frac{F(p, x)_{+\Delta p} - F(p, x)_{-\Delta p}}{p_{+\Delta p} - p_{-\Delta p}}\end{aligned}\quad (4.2)$$

where $F(p, x)$ is an arbitrary thermodynamic property. Δp is defined as the length of the perturbation step used to generate the gradient value at the discrete pressure value under consideration.

The IAPWS 1995 EOS requires two independent variables to be able to determine the needed property value. The pressure is defined as the discretized values across the chosen pressure range. At saturation conditions, the quality of the fluid and vapour phases are defined as $x = 0$ and $x = 1$ respectively. These values were therefore used as the second independent variable to determine the saturated fluid and saturated vapour gradients for density and enthalpy. The percentage difference between gradient values generated with the RFES and the IAPWS 1995 EOS, termed the error, is given by the following:

$$Error = \left(\frac{DF_{AF} - DF_{IAPWS}}{DF_{IAPWS}} \right) \times 100 \quad (4.3)$$

where DF_{AF} is the derivative value delivered by the approximation function derivatives and DF_{IAPWS} the derivative values delivered by the perturbation calculations using the IAPWS 1995 EOS.

The error for the saturated liquid density is illustrated in Fig. 4.5. For $0 < p < 3$ MPa, the error is less than 2%. For the $p > 3$ MPa the error generally remains below 4%, only peaking

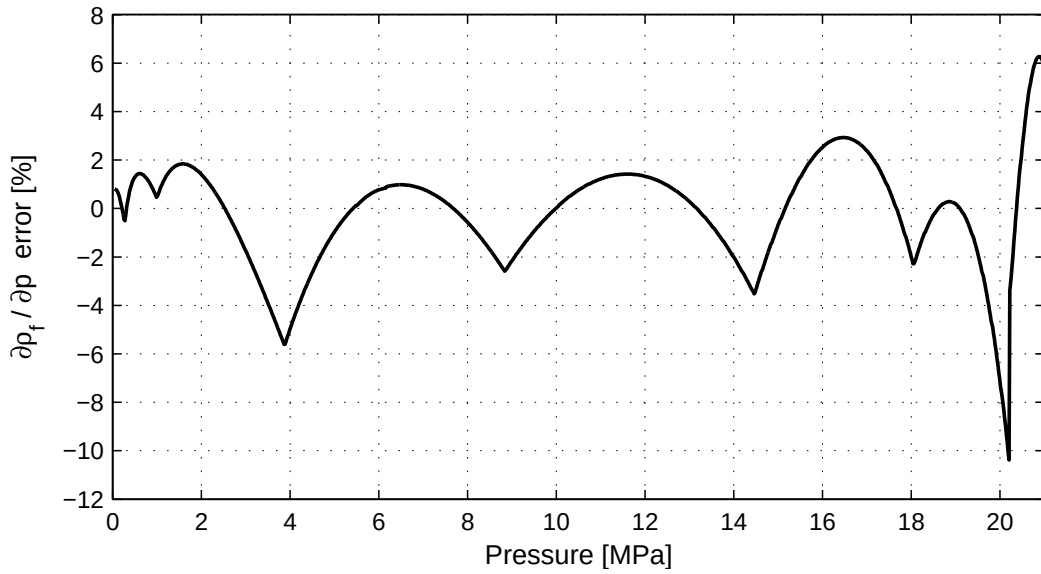


Figure 4.5: Percentage error for liquid density derivative over the designated pressure range.

above this value above 20 MPa. Once again, the increase in error values for these derivatives at the higher pressure ranges may be attributed to the fact that the IAPWS-95 EOS formulation delivers property values that differ somewhat from those delivered by IAPS-84, on which the approximation functions and their derivatives are based.

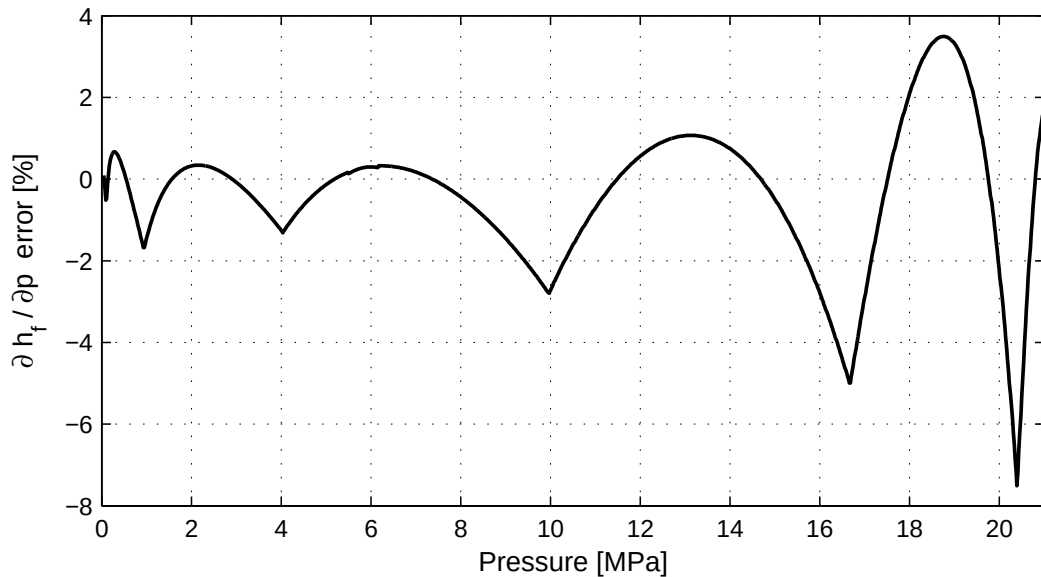


Figure 4.6: Percentage error for liquid enthalpy derivative over the designated pressure range.

For the saturated liquid enthalpy shown in Fig. 4.6, the error increases in an almost oscillatory manner as the pressure increases, peaking at a maximum of roughly 8%.

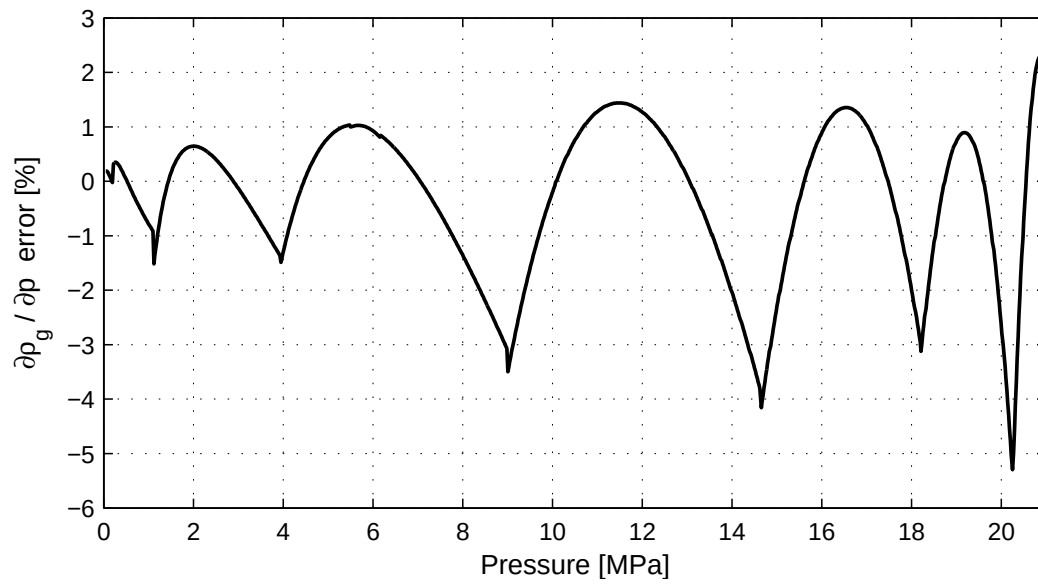


Figure 4.7: Percentage error for vapour density derivative over the designated pressure range.

The error for the saturated vapour density also increases in an almost oscillatory manner as the pressure value increases, peaking at a maximum value of roughly 5% as seen in Fig. 4.7.

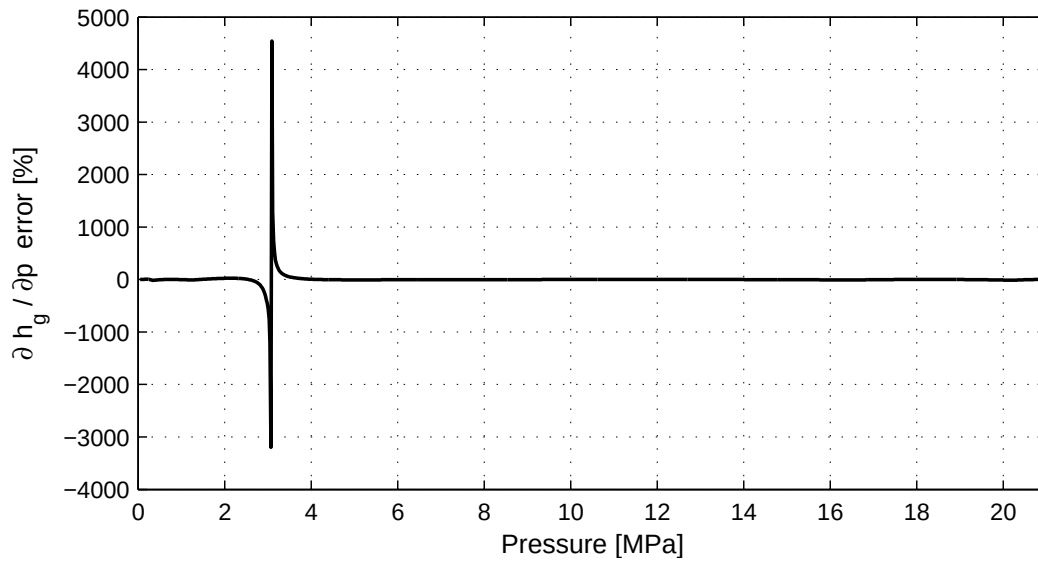


Figure 4.8: Percentage error for vapour enthalpy derivative over the designated pressure range.

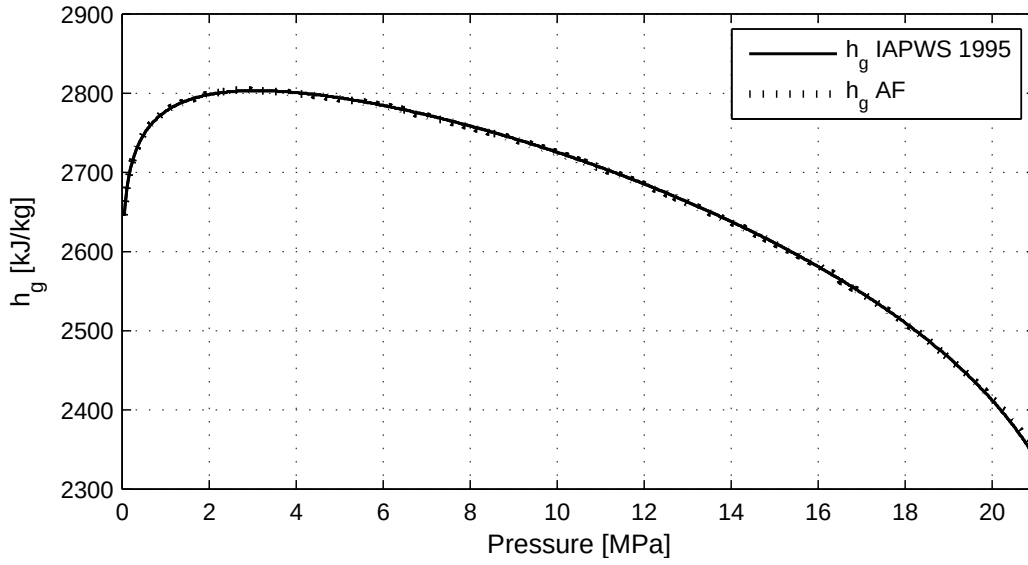


Figure 4.9: Values for saturated vapour enthalpy generated by the approximation functions and IAPWS 1995 EOS.

The error for the saturated vapour enthalpy derivative value is given in Fig. 4.8. It can be seen that the gradient error becomes exceedingly large at roughly 3 MPa. This large error is attributable to the fact that the vapour enthalpy gradient value changes from positive to negative at this point, coupled with the manner in which the percentage error of the gradient is calculated (see eq. (4.3)). From Fig. 4.9 it can be seen that the gradient of the saturated vapour enthalpy passes through zero at roughly 3 MPa. Because of the manner in which the percentage error is calculated, where the gradient value delivered by the IAPWS 1995 formulation is used as the denominator in the error fraction, even a small absolute deviation by the approximation function derivative will lead to a very large error value as the denominator value approaches zero. A singularity therefore occurs at the point where the saturated vapour enthalpy derivative value passes through zero, leading to a very large returned error value.

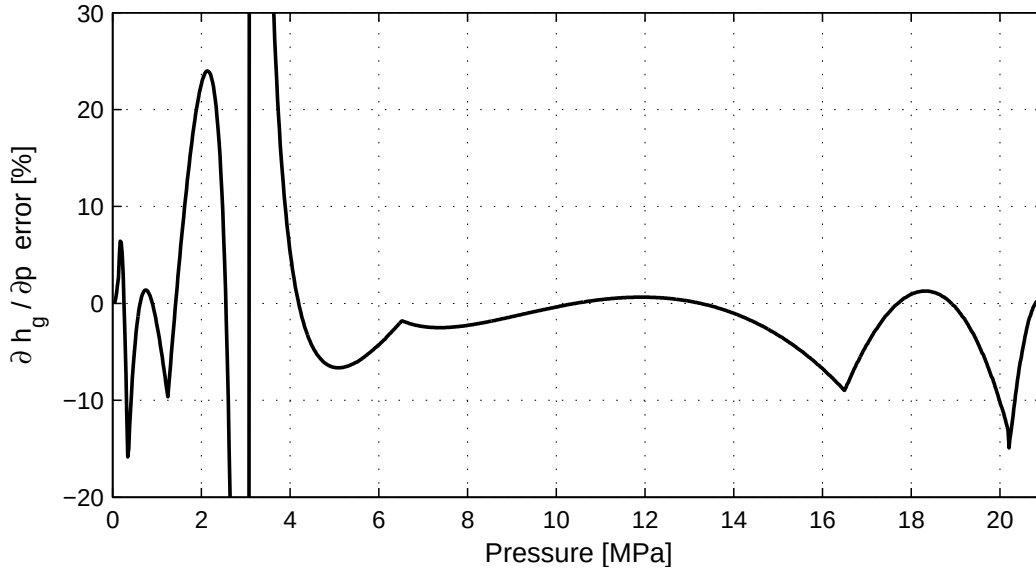


Figure 4.10: Zoom plot for percentage error for vapour enthalpy derivative over the designated pressure range.

Fig. 4.10 again shows the error for the saturated vapour enthalpy. However, the vertical axis in this plot has been defined to exclude the maximum error values surrounding the singularity point. This was done to better illustrate the general error values across the entire defined pressure range for the saturated vapour density derivative. From the plot it can be seen that the error for this derivative when compared with the values generated by the IAPWS 1995 EOS is high, peaking at roughly 24% when not taking the area immediately surrounding the singularity point into account.

Concluding in general for the error of the thermodynamic property approximation function derivative values, it was seen that the error for the gradient values were much higher than for the specific values of the properties under consideration. The influence of this lower degree of accuracy on the final accuracy of the rate form of the equation of state was evaluated by employing the RFES in a thermal-hydraulic simulation model and directly comparing results with those generated by the IAPWS 1995 EOS when simulating different transients in EES.

4.2 Transient network simulation model

The chosen transient simulation model represents an unstructured pipe and reservoir network. The methodology applied in the development of the pipe and reservoir network follows that of [Rousseau \(2012a\)](#). The nodes are given volumes to represent reservoirs, while the elements connecting the nodes represent pipes linking the reservoirs. The nodalisation approach used solved for the mass and energy in the system at the nodes, while the momentum was solved at the interfaces between the nodes, i.e. the elements.

This network was chosen as it is relatively simple, but is analogous to an unstructured T-F network with the necessary degrees of freedom to serve as a adequate test bed for the RFES.

The chosen network model also provides certain advantages over a model that only incorporates a single volume with a basic pipe in and outflow. The elements in the network may be changed from simple pipes to more complex components such as pumps, turbines or heat sources, while the element connectivity may also be trivially rearranged and/or expanded to provide new flow configurations within the network. These features of the chosen model are advantageous when considering an eventual expansion of the model to a more complex model which may also take non-equilibrium conditions into account in subsequent studies.

The EES programs for the model solved using the IAPWS-95 EOS and RFES respectively are given in Appendix C.

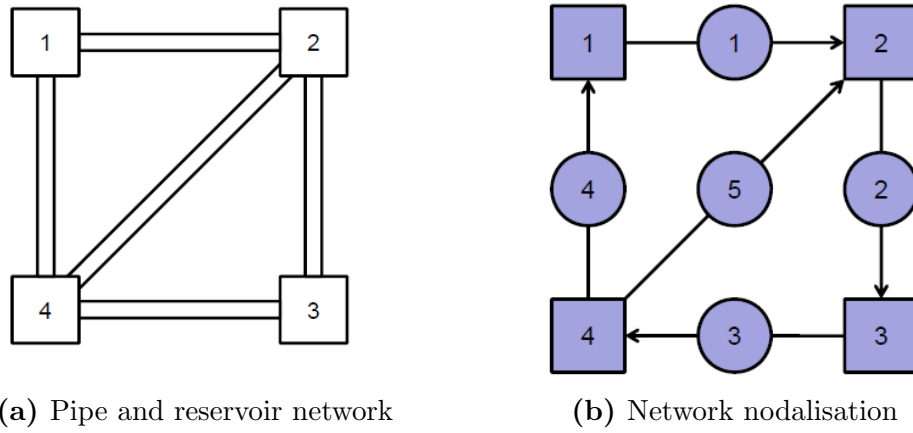


Figure 4.11: Pipe and reservoir network layout and the nodalisation of the network.
(Rousseau, 2012a)

The layout of the pipe and reservoir network that was modelled one-dimensionally in EES is illustrated in Fig. 4.11a. The network comprises of four nodes, numbered 1-4, connected by five pipes in the manner illustrated in the figure. The formulation of the network model allows for different physical volumes to be attributed to the nodes, while the pipes can be modelled with different cross-sections and lengths. Fig. 4.11b illustrates the nodalisation of the network, with the elements represented by the circles and the nodes represented by the squares. For each pipe an arbitrary positive flow direction was assigned. This flow direction is defined by the direction of the arrows. This means that when the network is solved, a positive mass flow result will indicate flow in the direction of the arrows, whereas a negative mass flow value will mean flow in the opposite direction. The discretisation for each conservation equation is described in the following subsections.

4.2.1 Conservation of mass

The energy and mass present in the system is represented in the nodes, whereas the momentum conservation is accounted for in the elements. The elements have zero volume, implying that there can be no accumulation of mass or energy within elements, only within nodes.

The mass conservation control volumes of the pipe and reservoir network is given in Fig. 4.12. These control volumes consist of the actual volume of the node, as well as half of the volume

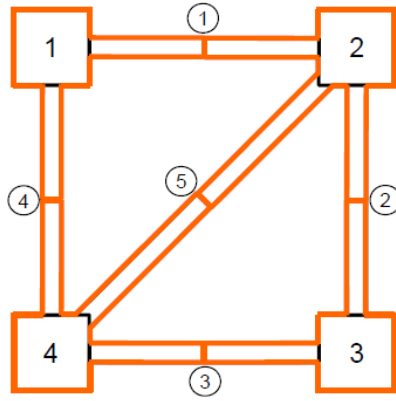


Figure 4.12: Control volumes defined for mass conservation.

of the pipes connected to the node. This results in the inclusion of all the mass present in the system in the four nodes that represent the reservoirs in the system. Each node in the network includes a mass source, where mass can be added or removed from the system. This adds an extra term to eq. (3.2), giving:

$$\frac{\partial \rho}{\partial t} = \frac{1}{V} \left(\sum \dot{m}_i - \sum \dot{m}_e + \dot{m}_s \right) \quad (4.4)$$

where ρ is the homogeneous average density in the mass control volume, $\sum \dot{m}_i$ represents all the mass flows into the node, $\sum \dot{m}_e$ represents all the mass flow out of the nodes and $\dot{m}_s$ the rate of mass addition via the mass source, which may be positive or negative. The number of mass conservation equations that must be solved in the network model is equal to the number of nodes in the network.

4.2.2 Conservation of momentum

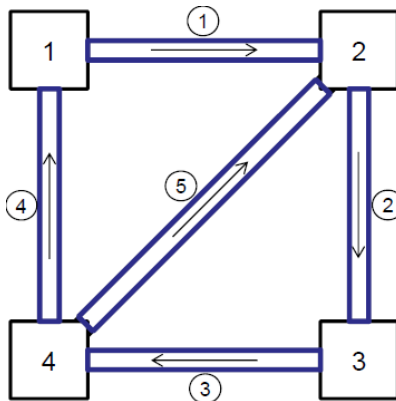


Figure 4.13: Control volumes defined for momentum conservation.

Fig. 4.13 illustrates the momentum conservation control volumes defined for the flow network. The momentum conservation is solved at the interfaces between the nodes, i.e. the elements.

As mentioned, the elements have no volume, implying that there can be no mass storage in the elements. This means that any mass flowing into the element will also flow out of the element. Furthermore, no energy can be accumulated in the element. The fluid flowing through the element may however experience a change in properties between the inlet and outlet. If, for example, heat is added or removed from the fluid in the element, the total energy content of the fluid flowing out of the element will differ from the energy content of the fluid flowing into the element. Because the momentum conservation is solved in the elements, the total number of momentum conservation equations in the model equals the number of elements in the network.

The conservation of momentum is given by eq. (3.4) as the following:

$$\rho L \frac{\partial V}{\partial t} + (p_{0e} - p_{0i}) - \frac{1}{2} V_i V_e (\rho_e - \rho_i) + \rho g (z_e - z_i) + \Delta p_{0L} = 0 \quad (4.5)$$

The use of the mass flow rate is preferred over using the velocity as given above. Using the definition of mass flow ($\dot{m} = \rho V A$):

$$\rho L \frac{\partial V}{\partial t} = \frac{L}{A} \frac{\partial \dot{m}}{\partial t} - LV \frac{\partial \rho}{\partial t} \quad (4.6)$$

eq. (4.5) can be rewritten as:

$$\frac{\partial \dot{m}}{\partial t} = \frac{A}{L} \left(\frac{1}{2} V_i V_e (\rho_e - \rho_i) - (p_{0e} - p_{0i}) - \rho g (z_e - z_i) - \Delta p_{0L} + LV \frac{\partial \rho}{\partial t} \right) \quad (4.7)$$

The Δp_{0L} term describes the pressure loss in the element as a result of frictional- and geometry-related losses. The term is defined as follows:

$$\Delta p_{0L} = \left(\frac{fL}{D_H} + \sum U \right) \frac{|\dot{m}| \dot{m}}{2\rho A^2} \quad (4.8)$$

where f is the dimensionless friction factor, L the length of the pipe, D_H the pipe hydraulic diameter and $\sum U$ the sum of the dimensionless secondary loss coefficients in the system. Because this study focused on determining the accuracy of the rate form of the equation of state rather than accurately simulating pressure losses, the pressure loss term was simplified to decrease the complexity of the transient simulation model. To achieve this simplification, the friction factor was fixed as a constant. No secondary losses were also assumed. These assumptions are analogous to combining the dependencies into a single constant so that the final pressure loss equation becomes:

$$\begin{aligned}
 \Delta p_{0L} &= \left(\frac{fL}{D_H} + \sum U \right) \frac{|\dot{m}|\dot{m}}{2\rho A^2} \\
 &= (K + 0) \frac{|\dot{m}|\dot{m}}{2\rho A^2} \\
 &= (K_L) \frac{|\dot{m}|\dot{m}}{2\rho A^2}
 \end{aligned} \tag{4.9}$$

where K_L represents the constant pressure loss coefficient in each pipe. The pressure drop was therefore only a function of the average fluid density and the mass flow in the pipe under consideration. The $|\dot{m}|\dot{m}$ form for the square of the mass flow rate is used to ensure that the sign of the mass flow rate is conserved in each element.

4.2.3 Conservation of energy

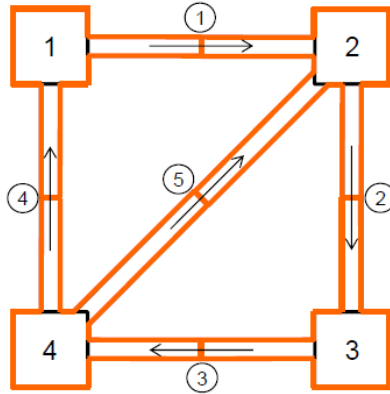


Figure 4.14: Mass control volumes with assumed mass flow directions illustrated.

Considering multiple inlets and outlets, as well as the mass sources present in each node, eq. (3.6) for the conservation of energy can be rewritten as follows:

$$\forall \frac{\partial}{\partial t} (\rho h_0 - p) = \sum \dot{m}_i (h_{0i} + gz_i) - \sum \dot{m}_e (h_{0e} + gz_e) + \dot{m}_s h_{0s} + \dot{Q} + \dot{W} \tag{4.10}$$

The properly account for the effects of heat ($\dot{Q}$) and work ($\dot{W}$) addition in the elements in the energy conservation control volumes, the element outflow conditions are written as a function of the element inflow conditions:

$$\dot{m} (h_{0e} + gz_e) = \dot{m} (h_{0i} + gz_i) + \dot{Q} + \dot{W} \tag{4.11}$$

The node to which the inlet of the element is linked defines the energy content at the element inflow. Heat addition to an element whose inlet is connected to a specific node, and whose mass flow is in the defined positive flow direction, will not influence the upstream node. Heat addition in an element only influences the downstream (with regards to flow direction) node. Eq. 4.11 accounts for the change in energy content of the fluid in the elements by heat addition and work. The node connected to the outlet of the element is therefore affected by the change in energy in the fluid in the element.

It is preferred to write the energy conservation in terms of the rate of change of enthalpy in each node. Rewriting:

$$V \frac{\partial}{\partial t} (\rho h_0 - p) = V \left(\rho \frac{\partial h_0}{\partial t} + h_0 \frac{\partial \rho}{\partial t} - \frac{\partial p}{\partial t} \right) \quad (4.12)$$

Substituting eq. (4.12) in to eq. (4.10), the energy conservation for each node is rewritten as:

$$\begin{aligned} \frac{\partial h_0}{\partial t} = \frac{1}{\rho V} & \left(\sum \dot{m}_i (h_{0i} + gz_i) \right. \\ & - \sum \dot{m}_e (h_{0e} + gz_e) \\ & + \dot{m}_s h_{0s} + \dot{Q} + \dot{W} \\ & \left. + V \left(\frac{\partial p}{\partial t} - h_0 \frac{\partial \rho}{\partial t} \right) \right) \end{aligned} \quad (4.13)$$

As with mass conservation, the conservation of energy is solved at each node in the system. Therefore the number of energy conservation equations solved equals the number of nodes in the model.

4.2.4 Time-wise integration

EES does not have a built-in time-wise integration functionality, therefore a time-wise integration scheme based on Euler integration, which is discussed in Section 3.5, was implemented in the model code to allow for transient simulations.

EES uses a variation of Newton's method to solve all the equations constituting the model under consideration simultaneously to a specified tolerance. In the case of transient simulations this means that EES solves all the equations in the model to the desired tolerance for each discrete time step before moving on to the next time step.

To allow for transient time stepping, the parametric table functionality of EES was used. Each row in the parametric table represented a time step in the transient simulation. EES was programmed to solve each row, i.e. time step, before beginning calculation of the next time step, allowing for a time history of the simulation to be developed in the parametric table. The purpose of the time-wise integration scheme discussed here was therefore to provide the required property values at the initiation of the next time step in the transient simulation based on the property values calculated at the previous time step. Based on this methodology, the rate of change of a system property value, e.g. density, could therefore be rewritten from the analytical mass conservation equation given by eq (4.4) in the following manner:

$$\frac{\rho - \rho^o}{\Delta t} = \frac{1}{V} \left(\sum \dot{m}_i - \sum \dot{m}_e + \dot{m}_s \right) \quad (4.14)$$

where ρ represents the density value at the new time step, ρ^o is the density at the previous time step and Δt is the time step length. The term on the right hand side of the equation is termed the source term, as this term calculates the density change in the system based on the mass flow in the system. Thus the source term can be written as:

$$S_c = \frac{1}{V} \left(\sum \dot{m}_i - \sum \dot{m}_e + \dot{m}_s \right) \quad (4.15)$$

Substituting eq. (4.15) into eq. (4.14) and rewriting the equation gives the following form:

$$\rho = \rho^o + S_c \Delta t \quad (4.16)$$

From this equation it is seen that the density value at the new time step is equal to the density value at the old time step plus the change in density delivered by the source term (change term described in Section 3.5). This change may be positive or negative.

For the implementation of the RFES, it was necessary to see the effect that different time-wise integration schemes had on the accuracy of the method. A weighting factor, α , was therefore employed to allow for the selection of an integration scheme. Using the weighting factor, eq. (4.16) is rewritten as:

$$\rho = \rho^o + (\alpha S_c + (1 - \alpha) S_c^o) \Delta t \quad (4.17)$$

where S_c^o is the source term value at the previous time step and S_c the source term value at the new time step. An α -value of zero will imply a fully explicit solution, where the source

term is kept constant at its old value for the duration of the time step and only changes to its new value at the end of the time step. An α -value of one will imply a fully implicit solution, where the source term value changes to its new value at the beginning of the time step. Any α -value between zero and one represents a weighted integration scheme. In the general scientific literature, an alpha value of between zero and one is termed a semi-implicit integration factor. In this study, an integration scheme will be termed semi-explicit if any weighting factor value below 0.5 is used. An integration scheme with α equal to 0.5 will be termed the Crank-Nicolson solution. Finally any solution using an α -value above 0.5 will be termed a semi-implicit solution.

A similar approach is taken in defining the source terms for momentum and energy conservation, leading to the following solution for momentum conservation:

$$\dot{m} = \dot{m}^o + (\alpha S_m + (1 - \alpha) S_m^o) \Delta t \quad (4.18)$$

and the the following solution for the energy conservation:

$$h_0 = h_0^o + (\alpha S_e + (1 - \alpha) S_e^o) \Delta t \quad (4.19)$$

where the subscripts m and e define the momentum and energy conservation source terms respectively. The discussed formulation of the conservation equations and transient source term solution method allowed for the transient simulation of various case studies using the pipe and reservoir network model. These studies aimed to illustrate the applicability and accuracy of the rate method. They are discussed in detail in the next chapter.

4.2.5 Geometry and boundary conditions

The pipe and reservoir network comprises of four reservoirs connected in an arbitrary manner by five pipes. The system is insulated from its surroundings so that no energy transfer can take place between the system and the environment. The geometry of each component in the network is listed in Table 4.3 below.

In the context of this study a grid independent solution, whereby the solution is independent of the discretisation of the network, was not required. In a study where the emphasis was on the accurate simulation of a physical system, each pipe in the network would have needed to be discretised further to ensure a grid independent solution. In this study the emphasis was on capturing all of the flow phenomena and then making direct comparisons between the solutions of the algebraic and rate form of the equation of state. Therefore, while the results of the model may not be correct in the sense of being grid independent, they were valid in terms of the direct comparison.

Table 4.3: Network pipe lengths and reservoir volumes.

Component geometry.			
Reservoir	Volume [m^3]	Pipe	Length [m]
1	0.5	1	5
2	0.05	2	10
3	0.1	3	1
4	0.3	4	15
		5	10

The friction factor defined in Section 4.2.2 is independent of the length of the pipes in the network, therefore the different pipe lengths would not impact the frictional losses in each pipe. The different pipe lengths therefore only impacted the total volume of each node in the system, as this value was calculated as the volume of the node itself along with half the volume of the pipes connected to the node. This ensures that all the mass in the system was accounted for. The cross-sectional area for all the pipes was constant at 0.025 m^2 . All elevations are set as zero and the averaged velocities in all the reservoirs and mass sources and sinks were assumed to be zero at all time. No secondary inlet or outlet losses were present in the system.

4.2.6 Initial conditions

The solution of the model as it was programmed in EES required an initial steady state solution at time zero. After this initial solution was obtained, the transient simulation could then be commenced. System properties were specified in a manner that allowed for the network to solve to the initial conditions desired. The same combination of input system properties were used to generate initial conditions for all the simulations done in this study. The property inputs used to generate the desired initial system states are listed below:

- Node mass sources/sinks,
- node density, and
- node enthalpy.

This choice of defined input properties allowed for the network to be set to the desired initial state. The mass sources/sinks were set to zero to ensure no mass flow in the pipes between the reservoirs at the initiation of the transient. Specified initial nodal enthalpy and density values allowed for setting initial nodal pressures and temperatures to the desired condition, while also allowing the quality in each node to be defined as desired. To ensure that the entire system remained at a two-phase condition throughout the transient, the quality in each node was initially set at a point exactly between saturated fluid and saturated vapour, i.e. 0.5.

4.3 EES model formulation

The previous section dealt with the theoretical basis of the formulation of the simulation model as it was developed in EES. This section will serve to explain the methodology used to program the model in EES. Thus, this section will elaborate on the process used to set up the model. This model was chosen as a preliminary test bed for the RFES because it allowed for the dynamic simulation of transient mass and energy effects in a pipe network system.

This section will be structured so as to provide information on each section of the EES program codes that are supplied in Appendix C. This will assist the reader in developing an understanding of how the model was developed in EES.

Transient modelling in EES can be explained best as a two-step process. The first step is to complete the model for steady state conditions, so that the model is closed and all the required steady state solution values are obtained. After this initial steady state solution, the model is switched to deliver time dependent results. Therefore, to ensure the reader understands this methodology, the initial explanation of the structure of the model will be given with regards to the algebraic steady state solution given in Appendix C.1. After this, the methodology for converting to a transient solution by means of the EES parametric table functionality will be explained.

4.3.1 EES model qualitative sectional description

The sections described here correspond to the sections of the EES model code found in Appendix C.1.

Section 1

This section provides constants necessary for the model and defines the working fluid and equation of state to be used by EES.

Section 2

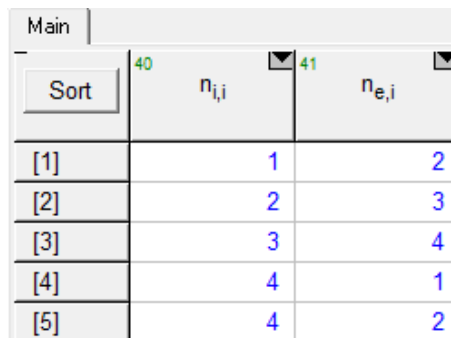
This section establishes the connectivity of the pipes to the reservoirs in the system, i.e. the connectivity of the elements to the nodes.

Connectivity					
	1	2	3	4	5
Paste Special	Column1	Column2	Column3	Column4	Column5
Row 1	-1	0	0	1	0
Row 2	1	-1	0	0	1
Row 3	0	1	-1	0	0
Row 4	0	0	1	-1	-1

Figure 4.15: Definition of element inlet and outlets supplied to the EES code.

The connectivity data is supplied to EES in lookup table format. Fig. 4.15 shows the lookup table as it is generated in EES. In this table, the rows represent the nodes, while the Columns represent the elements. Each element has an inlet and outlet, hence each column has two values. The -1 value represents the pipe outlet, while the value 1 represents the pipe inlet. For example it can be seen from the lookup table that element 1 (Column 1) has an outlet connected to node 1 (Row 1), and an inlet connected to node 2 (row 2). Comparing this with Figure 4.11a, it is seen that this holds for the pipe network under consideration. The rest of the network connectivity may then also be discerned in this manner.

The next part of the code in this section uses the data in the connectivity lookup table to establish the connectivity of the network which is subsequently used to solve the model. The data is interpreted by using an in line "IF" function to deliver the following column values in the EES solution array table.



	$n_{i,i}$	$n_{e,i}$
[1]	1	2
[2]	2	3
[3]	3	4
[4]	4	1
[5]	4	2

Figure 4.16: Element connectivity solution in EES solution array table.

These tabulated values are found in the EES solution array, where all the solution values are tabulated by EES when the model is solved. The column $n_{i,i}$ represents the element inlet values, while the column $n_{e,i}$ represents the element outlet values. These values range from 1 – 4 and correspond to the node to which the inlet or outlet of each of the elements are connected.

Section 3

The node and element geometry conditions are given in this section. The volumes and elevations of the nodes are given. Referring back to Subsection 4.2.1, when solving the mass conservation equations for the network, it is important to include all the mass in the system, i.e. in the nodes as well as the elements. To account for this, the mass conservation control volumes were discretised as in Fig. 4.12 by the node volume calculation equation in this section.

Section 4

This section defines the mass source enthalpy values used by the energy conservation equation based in the nodal mass quality value. A "CALL" function is used in this section to deliver saturated liquid and gas enthalpy values as a function of pressure and temperature. The pressure referenced is the nodal pressure. Because the phases are in equilibrium saturation conditions, the temperature is simply the saturation temperature corresponding to the pressure in the node. The functions that are called are the thermodynamic property approximation functions discussed in Section 2.2.4, and in this case specifically those for enthalpy. The thermodynamic property approximation functions used in this study are included, as they are written in EES procedure form, in Appendix D. These approximation functions were developed to deliver thermodynamic property values for saturation, as well as sub-cooled and superheated conditions. It can be seen from the procedures in Appendix D that the approximation functions are written in the following form,

$$h = h_g + [f(p, T)] * (T - T_s) \quad (4.20)$$

where vapour enthalpy is used as an example in this instance. The first term in this expression represents the saturated vapour enthalpy, while the second term accounts for the additional enthalpy of the fluid at superheated conditions. If the working fluid in the system is at saturation conditions, the temperature T is equal to the saturation temperature T_s , meaning that the second term is multiplied by zero and falls away. This is the case in the model under consideration in this study. The saturated vapour enthalpy therefore becomes a pure function of pressure, as can be seen in the appendix. This is discussed in detail in Section 3.4. It can be seen that the pressure value supplied to all the approximation functions in the study are divided by a factor of a thousand. This is because the EES model was written with the pressure units expressed in kPa, while the approximation functions were developed for input values to be given in MPa. Therefore it was required to convert the pressure input values from kPa to MPa when calling the approximation functions.

Section 5

The transient integration factors are listed in this section. They are not applicable in the initial steady state solution, but remain defined for when the transients are simulated. In this case the alpha value is defined as 1, meaning an implicit backward Euler solution will be delivered for integration time step lengths of 0.05 seconds.

Section 6

The property values required for the solution of the momentum conservation equations are calculated in this section. As discussed in Section 4.2.2, the momentum conservations

are solved in the elements.

Section 7

This section solves the momentum conservation equations for each of the elements. When the system is solved for steady state conditions, the mass conservation source term, defined as $S_m[e]$, is given as zero. This is because for steady state conditions there is no momentum being added or removed from the system. When the system is being solved for time dependent conditions, the changes in mass and energy in the nodes of the system will result in momentum variations in the elements which is expressed by the momentum source term.

"!Section 7: Momentum conservation calculations"

"Calculate momentum conservation source term"

$S_m[e] = (A_bar[e] / L[e]) * (0.5 * V_bar[e]^2 * (rho_e[e] - rho_i[e]) - 1e3 * (p_0e[e] - p_0i[e]) \&$
 $- rho_bar[e] * g * (z_e[e] - z_i[e]) - k_L[e] * (ABS(m_dot[e]) * m_dot[e]) / rho_bar[e] + L[e] * A_e[e] * drhodt_bar[e])$

"Steady state"

$S_m[e] = 0$

$drhodt_bar[e] = 0$

"Transient integration for element mass flow rate"

$\{S_m_old[e] = tablevalue(Row-1, 43+e)$

$m_dot_old[e] = tablevalue(Row-1, 25+e)$

$rho_bar_old[e] = tablevalue(Row-1, 30+e)$

$drhodt_bar[e] = (rho_bar[e] - rho_bar_old[e]) / deltatime$

$dmdotdt[e] = alpha_m * S_m[e] + (1 - alpha_m) * S_m_old[e]$

$m_dot[e] = m_dot_old[e] + dmdotdt[e] * deltatime\}$

End

Figure 4.17: Section 7 of the EES model for a steady state solution.

Figs. 4.17 and 4.18 illustrate the difference between the EES model when solving for steady state conditions and transient conditions respectively. The sections of codes included in parenthesis and colored blue are sections of code which is excluded from the simulation. It can be seen that for the steady state case the transient terms are excluded with the source term, $S_m[e]$ as well as the average density time derivative, $\frac{\delta \rho}{\delta t}$, set to zero. For the transient case, the two above mentioned values are excluded and the model solves for the required transient parameters.

"!Section 7: Momentum conservation calculations"

"Calculate momentum conservation source term"

```
S_m[e]=(A_bar[e] / L[e]) * (0.5 * V_bar[e] ^ 2 * (rho_e[e] - rho_i[e]) - 1e3 * (p_0e[e] - p_0i[e]), &  
|- rho_bar[e] * g * (z_e[e] - z_i[e]) - k_L[e] * (ABS(m_dot[e]) * m_dot[e]) / rho_bar[e] + L[e] * A_e[e] * drhodt_bar[e])
```

"Steady state"

```
{S_m[e]=0  
drhodt_bar[e]=0}
```

"Transient integration for element mass flow rate"

```
S_m_old[e]=tablevalue(Row-1,43+e)  
m_dot_old[e]=tablevalue(Row-1,25+e)  
rho_bar_old[e]=tablevalue(Row-1,30+e)  
drhodt_bar[e]=(rho_bar[e]-rho_bar_old[e])/deltatime  
dmdotdt[e]=alpha_m*S_m[e]+(1-alpha_m)*S_m_old[e]  
m_dot[e]=m_dot_old[e]+dmdotdt[e]*deltatime
```

End

Figure 4.18: Section 7 of the EES model for a transient solution.

Section 8

This section calculates the mass and energy conservation source terms based on the nodal properties and momentum information supplied by the momentum conservation equations for the elements. As in the case of the momentum conservation, for steady state conditions the mass and energy source terms, $S_e[n]$ and $S_e[n]$, are zero as there are no sources for steady state conditions.

Fig. 4.19 gives an example of how the conservation source terms are specified for each component in the network. As mentioned previously, the momentum conservation equations are solved in the elements (E: 1) in the figure, while the mass and energy conservation equations are solved in the nodes. The model therefore solves five momentum equations and 4 equations each for the mass and energy conservation respectively in the simulation model. For the steady state solution all the discussed source term values are zero.

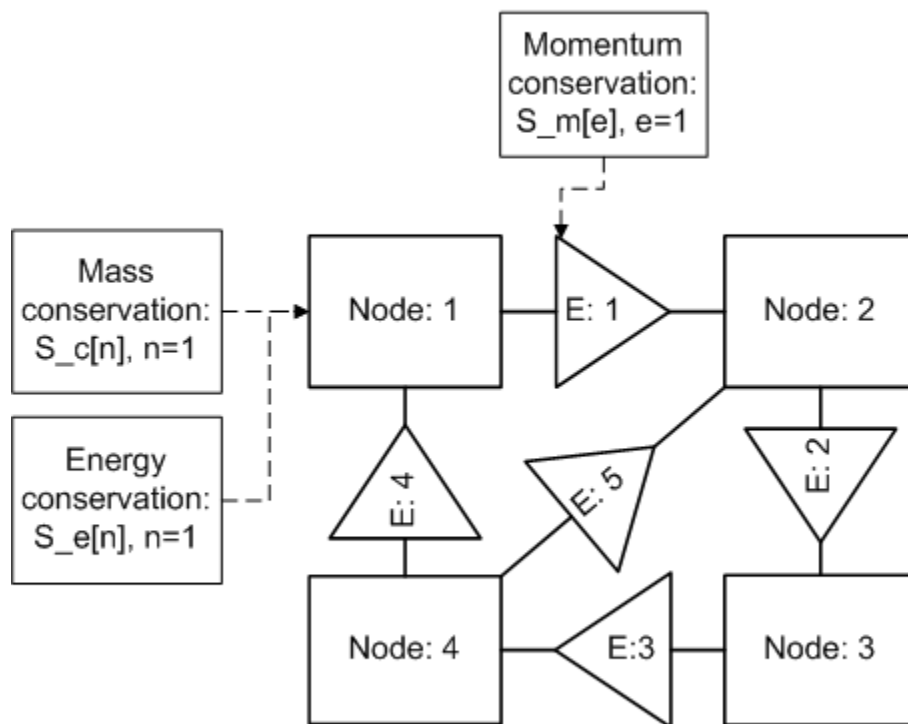


Figure 4.19: Illustration of source term solutions relating to the pipe and reservoir network coded in EES.

Section 9

Section 9 solves for nodal pressure and temperature when using the rate form of the equation of state. Because this method is based on the rate of change of system properties and is therefore time dependent, it is not used to solve for pressure at steady state conditions.

The functions called in Section 9 of the EES model code are for the saturated liquid and vapour derivative functions for specific volume and enthalpy respectively. As mentioned in Subsection, the rate form of the equation of state requires derivatives of density (or specific volume) and enthalpy to be solved. Because the approximation functions are only a function of pressure at saturation conditions, the derivatives could be obtained by simply differentiating the required approximation functions with regards to pressure.

Section 10

This section solves for nodal pressure and temperature using the IAPWS equation of state.

The qualitative overview given above gives a brief summary and explanation of each section of the simulation model that was developed in EES for the pipe and reservoir network. Much of the intricacy of the model can be attributed to ensuring the correct connectivity between the pipes and reservoirs in the network. When these equations are properly formulated, the model can be solved for steady state conditions based on the initial and boundary conditions stipulated in Sections 4.2.5 and 4.2.6 for the specified system geometry.

4.3.2 EES model transient integration technique

The previous subsection qualitatively outlined the model that was developed in EES to simulate a pipe and reservoir network for homogeneous two-phase flow conditions. This model, as it is given in Appendix C.1, delivers the initial steady state solution to the network. To initiate the transient simulation of the pipe network, the parametric table functionality built in to EES is employed.

Table 1									
1.1	time [s]	$\dot{m}_{s1}$ [kg/s]	$\dot{m}_{s2}$ [kg/s]	$\dot{m}_{s3}$ [kg/s]	$\dot{m}_{s4}$ [kg/s]	P_1 [kg/m ³]	P_2 [kg/m ³]	P_3 [kg/m ³]	P_4 [kg/m ³]
Run 1	0.000	-0.000	0.000	0.000	0.000	174	174	174	174
Run 2	0.050	0.000	0.000	0.000	0.000				
Run 3	0.100	0.000	0.000	0.000	0.000				
Run 4	0.150	0.000	0.000	0.000	0.000				

Figure 4.20: Section of the parametric table generated in EES when the model is solved at steady state conditions.

A section of the parametric table, where the solution values are generated, is shown in Fig. 4.20. The 1..1 under the green solve icon indicates that the model is only solved for the first run or in other words the steady state solution at time zero. The section of the parametric table shown shows the solution values for the mass source flow rates, as well as the nodal density values for node 1-4. The numbers in blue represent values that were solved by the model, while the numbers in black represent the initial values supplied to the model. The initial values supplied to the model are discussed in Subsection 4.2.6.

Table 1									
2.101	time [s]	$\dot{m}_{s1}$ [kg/s]	$\dot{m}_{s2}$ [kg/s]	$\dot{m}_{s3}$ [kg/s]	$\dot{m}_{s4}$ [kg/s]	P_1 [kg/m ³]	P_2 [kg/m ³]	P_3 [kg/m ³]	P_4 [kg/m ³]
Run 1	0.000	-0.000	0.000	0.000	0.000	174	174	174	174
Run 2	0.050	0.000	0.000	0.000	0.000	174	174	174	174
Run 3	0.100	0.000	0.000	0.000	0.000	174	174	174	174
Run 4	0.150	0.000	0.000	0.000	0.000	174	174	174	174

Figure 4.21: Section of the parametric table generated in EES when the model is solved at transient conditions.

After the steady state solution is obtained, the model is switched to a transient solution method. The same section that was presented in Fig. 4.20 for the steady state solution is now shown in Fig. 4.21. The mass conservation equation, which is used to solve for the nodal densities, is shown in Fig. 4.22. From this figure it can be seen that several values are referenced when solving the mass conservation equation of a new time step. The old source term value $S_c[e]$ is

referenced first. In the case of the first transient time step at $t = 0.05s$, the value of $S_c[e]$ will be zero, as there is no source terms at steady state condition (illustrated in Fig. 4.17. The old density values, seen in Fig. 4.21 is also referenced. These values are then used, along with the source term equation value and the integration weighting equation to deliver the value of $\frac{\partial \rho}{\partial t}$ and subsequently the density value at the new time step.

```
"Calculate mass conservation source term value"
S_c[n]=1/Vol[n]*(SUM(c[n,e]*m_dot[e],e=1,elements)+m_dot_s[n])

"Steady state"
{S_c[n]=0
drhodt[n]=0}

"Transient integration for node density"
S_c_old[n]=tablevalue(Row-1,35+n)
rho_old[n]=tablevalue(Row-1,5+n)
drhodt[n]=alpha_c*S_c[n]+(1-alpha_c)*S_c_old[n]
rho[n]=rho_old[n]+drhodt[n]*deltatime
```

Figure 4.22: Section of the EES model used in the transient integration of the mass conservation equation.

It can be seen from Figs. 4.20 and 4.21 that the mass source values are specified for every time step in the parametric table. These mass flow values, as well as energy values which are not shown in the figures, are boundary condition values which are used to control the transients in the system. The transients which are discussed in the following chapters are initiated by altering these source term values at the times where transients are desired. Which values are altered depends on what type of transient, as well as in which node the transient is desired.

Run 10	0.450	0.000	0.000	0.000	0.000	174	174	174	174
Run 11	0.500	0.000	0.000	-40.000	0.000	173.9	172.7	159.7	173.4
Run 12	0.550	0.000	0.000	-40.000	0.000	173.7	171.1	146.7	172.5
Run 13	0.600	0.000	0.000	-40.000	0.000	173.4	169.5	134.7	171.5
Run 14	0.650	0.000	0.000	-40.000	0.000	173	167.8	123.2	170.4
Run 15	0.700	0.000	0.000	-40.000	0.000	172.6	166.1	112.3	169.2
Run 16	0.750	0.000	0.000	-40.000	0.000	172.1	164.3	101.8	168
Run 17	0.800	0.000	0.000	-40.000	0.000	171.5	162.5	91.66	166.7
Run 18	0.850	0.000	0.000	-40.000	0.000	171	160.8	81.8	165.4
Run 19	0.900	0.000	0.000	-40.000	0.000	170.4	159	72.18	164.1
Run 20	0.950	0.000	0.000	-40.000	0.000	169.7	157.3	62.75	162.7
Run 21	1.000	0.000	0.000	0.000	0.000	169.1	155.9	70.58	161.4

Figure 4.23: $-40 \frac{kg}{s}$ Mass transient initiated in node 3 at $0.5s < t < 1s$. The rapid change in nodal density values can be observed when a large mass of working fluid is removed from the system.

Fig. 4.23 illustrates how a mass transient was initiated in the system. The figure shows a mass sink being activated at $t = 0.5s$ (time t , first column in the figure) and deactivated at $t = 0.95s$ in node 3 of the system. This means the mass sink is active for $0.5s$ in the system. The mass and energy transients modeled in the system are discussed in Section 5.2.

The two-step time nature of solving for transient systems of the EES can be attributed to how the EES solver functions. Inherently, EES is an equation solver that solves systems of non-linear algebraic equations using a specific numerical solution scheme. This numerical scheme is a variant of Newton's method and the EES solution methodology also uses additional techniques to increase the efficiency of the solver. The details regarding the solver used by EES can be found in Klein (2012) and is not discussed further here. What this implies is that when a

model is coded in EES and solved, the solver simply solves the entire set of equations at once to a specified general error tolerance. There are no inner and outer iteration loops where for example pressure needs to be solved to tolerance first before being given to the conservation equations which are then solved, etc. Therefore, to be able to solve a time dependent problem in EES, the parametric table functionality is used to simulate transient integration via the Euler method. Each row in the parametric table is considered a time step. EES will therefore solve the entire set of equations for each time step based on the input values referenced from the previous time step. The manner in which the previous time step values are used to calculate the new time step values is dependent on the chosen integration weighting factor defined for the Euler time step integration method. In effect, EES simply solves the same set of equations for different input values to a specified tolerance before repeating the procedure. This time history of the system as it was solved for each time step then illustrates the system behavior over time. The solution of the steady state problem is therefore required to initiate the process and deliver an initial set of solution values for the system which can be referenced by the model when the transient simulation is initiated.

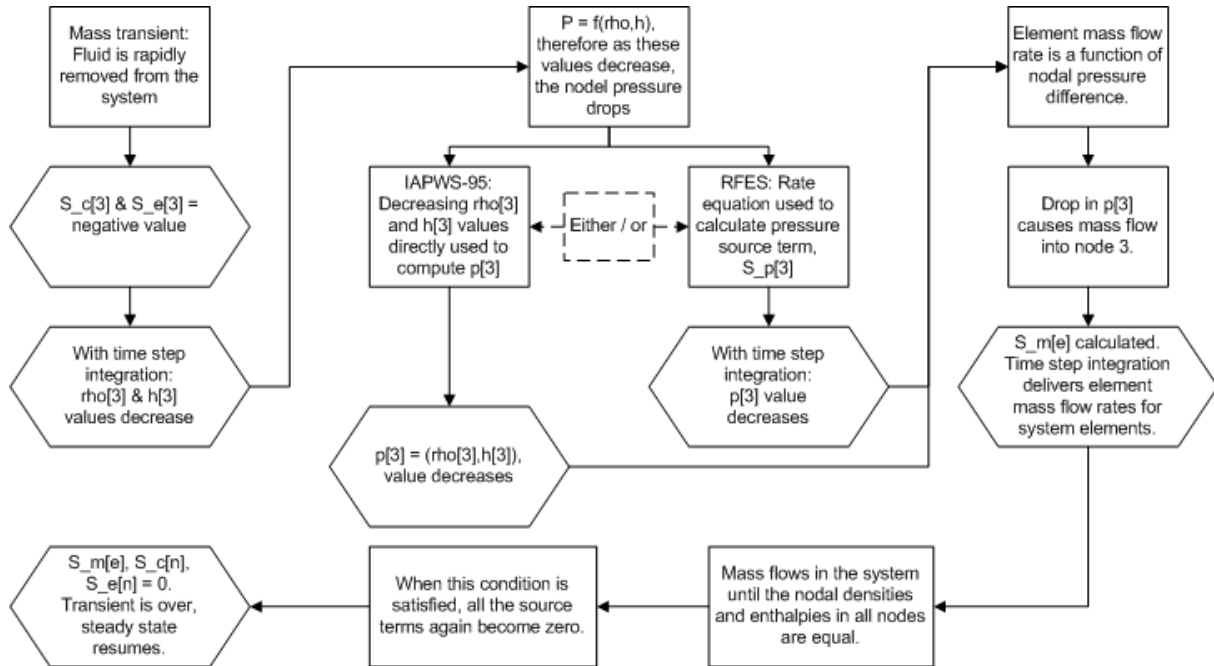


Figure 4.24: Conceptual information flow path for node 3 mass transient example.

Even though EES does not distinguish between different types of equations when solving a simulation model, it necessarily remains important for the modeller to conceptually understand how the equations that define the fluid flow in the model are interacting to propagate the changes in the state of the system. Using the mass transient shown in Fig. 4.23 as an example, the flow of information can be visualised as shown in Fig. 4.24. A perturbation in the system at steady state conditions results in a change in system state parameters over time. As parameter values change in certain parts of the system, the parameters in other parts of the system will react to these changes by changing as well. In this manner, the conditions in the whole system changes as a result of this perturbation, in this case a loss of mass from node 3. When all external forces are removed, i.e. the mass sink is deactivated, the property values throughout

the system will fluctuate until a new steady state condition is attained where all the forces in the system are once again balanced or, in other words, there are no system property gradients that can drive changes in the properties throughout the system.

4.3.3 EES model equation of state switching

The goal of the EES simulation model explained in the previous subsections was to serve as a model in which to incorporate the rate formulation and ensure its correct implementation by comparing the results delivered by the rate formulation with results delivered a reference equation of state when simulating transient equilibrium two-phase flow in a flow network. Therefore, both these equations of state had to be implemented in the model. The model could then be solved separately using both equations of state, after which the model solutions could be compared. The rate form of the equation of state and IAPWS-95 are included in sections 9 and 10 of the EES model respectively. As mentioned previously, the rate form of the equation of state is time dependent and is therefore not used to generate the steady state solution for time zero. Once the steady state solution has been established, either the RFES or algebraic equation of state may be used to solve the model by deactivating (by putting the EOS in parenthesis) the other equation of state in the model.

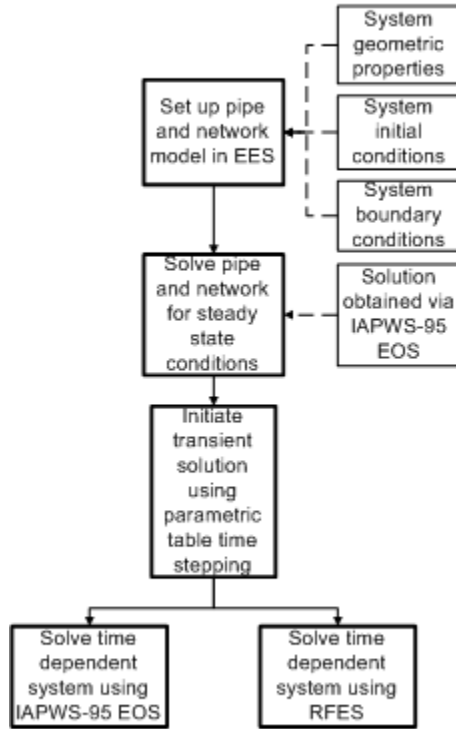


Figure 4.25: Methodology for the programming and solution of the transient pipe and network model in EES.

The EES model programming and transient solution methodology that was followed during this study was discussed in the previous subsections. Fig. 4.25 summarises the discussed solution methodology in flow chart form. It illustrates the steps followed to obtain a transient model solution after the model was initially formulated in EES. The comparison of the results delivered by the IAPWS-95 and rate form equations of state are discussed in detail in Chapter 5.

4.4 Flownex verification

To ensure that the transient network simulation model that was developed in EES in which the rate method was to be implemented delivered meaningful results within the context of the assumptions that were made, it was necessary to verify the model. Flownex SE, a proprietary T-F simulation package, was therefore chosen as a verification platform (M-Tech Industrial, 2013). Flownex SE is a one-dimensional SCFD package that is able to solve complex T-F models for single- and multi-phase flow. It uses the same node-link methodology for solving T-F models as was used in this study, and was therefore an applicable verification platform.

4.5 Flownex theoretical formulation

4.5.1 Conservation equations

To ensure that a meaningful verification of the EES model could be done using Flownex, it was necessary to review the theoretical model used by Flownex to model two-phase flow systems. The relevant theory employed in Flownex was found in the Flownex SE theory manual (?).

Flownex employs the homogeneous equilibrium model for the modelling of two-phase flow systems. This meant that the results delivered by the Flownex model was expected to deliver results consistent with those of the HEM two-phase flow model developed in EES. The conservation equations derived in the Flownex manual for two-phase flow yield the following three conservation equations:

- Mass:

$$\frac{\partial}{\partial t} (\rho A) + \frac{\partial}{\partial x} (\rho V A) = 0 \quad (4.21)$$

- Momentum:

$$\begin{aligned} \frac{\partial V}{\partial t} = \frac{1}{\rho \Delta x} \left(- (p_{0e} - p_{0i}) + \frac{\rho^2 V^2 A^2 (\rho_e - \rho_i)}{2 \rho_i \rho_e A_i A_e} - \rho g (z_e - z_i) \right. \\ \left. - \frac{\bar{\tau}_w P \Delta s}{A} + (p_{0i} - \tilde{p}_{0i}) + (p_{0e} - \tilde{p}_{0e}) \right) \end{aligned} \quad (4.22)$$

- Energy:

$$q''' + \frac{P_h q''}{A} = (\dot{m}_e h_{0e} - \dot{m}_i h_{0i}) + V \frac{\partial}{\partial t} (\rho h_0 - p) + g (\dot{m}_e z_e - \dot{m}_i z_i) \quad (4.23)$$

When these conservation equations are compared with the conservation equations derived for the HEM in this study (given in Section 4.2), it is seen that the conservation equations are of a similar form. For the mass conservation, the equations are basically identical, while for the energy conservation it is also observed that the equations are similar if the difference in form of the heat and work rate terms are taken into account.

The momentum equations differ somewhat, but by making certain assumptions the momentum equation used by Flownex may also be simplified to be consistent with the momentum equation derived in this study. It is stated in the Flownex theory manual that for two-phase flow at low speeds, the pseudo-total pressures given in the Flownex equation as $\tilde{p}_0$ may be set equal to the total pressure p_0 . This reduces the momentum equation to,

$$\frac{\partial V}{\partial t} = \frac{1}{\rho \Delta x} \left((p_{0e} - p_{0i}) + \frac{\rho^2 V^2 A^2 (\rho_e - \rho_i)}{2 \rho_i \rho_e A_i A_e} + \rho g (z_e - z_i) - \frac{\bar{\tau}_w P \Delta s}{A} \right) \quad (4.24)$$

The last term is simply the pressure drop term and may be rewritten to be consistent with the notation used in this study. Finally, if it is known that the flow areas of the pipes used in the model will not differ and that there will be no large changes in the density of flows through the pipes as a result of energy addition or removal, the second term on the right side of the equation may be simplified in the following manner:

$$\frac{\partial V}{\partial t} = \frac{1}{\rho \Delta x} \left(- (p_{0e} - p_{0i}) + \frac{\rho^2 V^2 A^2 (\rho_e - \rho_i)}{2 \rho^2 A^2} - \rho g (z_e - z_i) - \Delta p \right) \quad (4.25)$$

which becomes,

$$\frac{\partial V}{\partial t} = \frac{1}{\rho \Delta x} \left(- (p_{0e} - p_{0i}) + \frac{1}{2} V^2 (\rho_e - \rho_i) - \rho g (z_e - z_i) - \Delta p \right) \quad (4.26)$$

which has the same form as the momentum conservation equation derived in Section 4.2. Based on this investigation, it was seen that the Flownex model used the same conservation equations that were used to develop the EES model. Therefore, consistent results could be expected between the two models.

4.5.2 Simulation code solvers

Based on a review of the solvers used by Flownex and EES, it was seen that the solvers differ for the two codes. While EES uses Newton's method with certain added optimisation parameters to solve the entire system of programmed equations simultaneously, Flownex uses a solution methodology termed the Implicit Pressure Correction Method. This method employs a segregated solution algorithm in which different equations that define the model are solved sequentially. It therefore differs from the EES solver in the fact that it does not solve the equations simultaneously, but rather sequentially.

A full investigation of the effects that the difference in solvers between the two models has on the solution values of the EES and Flownex models is beyond the scope of this study. For the purpose of this verification, it was assumed that the solvers would deliver the same solution values for the models if the other aspects of the models were formulated consistently for both models.

4.5.3 Pressure drop correlation

Because of the theoretical nature of the model that was developed, it was decided not to use one of the many empirical two-phase pressure drop correlations available in literature. These cor-

relations include the Homogeneous pressure drop correlation, Lockhart-Martinelli, Martinelli-Nelson, Baroszy, and Friedel correlations (Collier, 1972). Instead, the friction factor defined in eq. (4.9) was fixed as a constant so that the manner in which mass flowed in the system could be controlled. The magnitude of this constant value was decided based on how the system was desired to evolve during a transient.

In the case of this study, the pressure drop term may be viewed as a function that retards the flow through the pipes in the network. If a mass sink is initiated in a node in the system, the amount of fluid in the node volume would decrease, leading to a pressure differential between the node where the mass is removed and the other nodes. Mass would then flow from the other nodes to the node where the mass is removed until the pressure differential once again becomes zero. If the flow through the pipes is retarded, it will take a longer time for the flows from the other nodes to neutralise the pressure differential. Therefore, the pressure in the node will continue to decrease if the transient is kept active, because the flow from the other nodes can not compensate quickly enough for the loss in pressure as a result of a loss in mass. When the transient is then deactivated, the flows from the other nodes will then increase the mass in the transient node, thereby increasing its pressure until the pressure differential between the nodes is removed. At that point, the system would again be at a steady state condition.

On the other hand, if the flow is not retarded, mass would freely flow from the other nodes in the system to the node where the transient takes place. When the loss of mass stops, the node pressures stabilise to a new steady state pressure consistent with the amount of mass in the system.

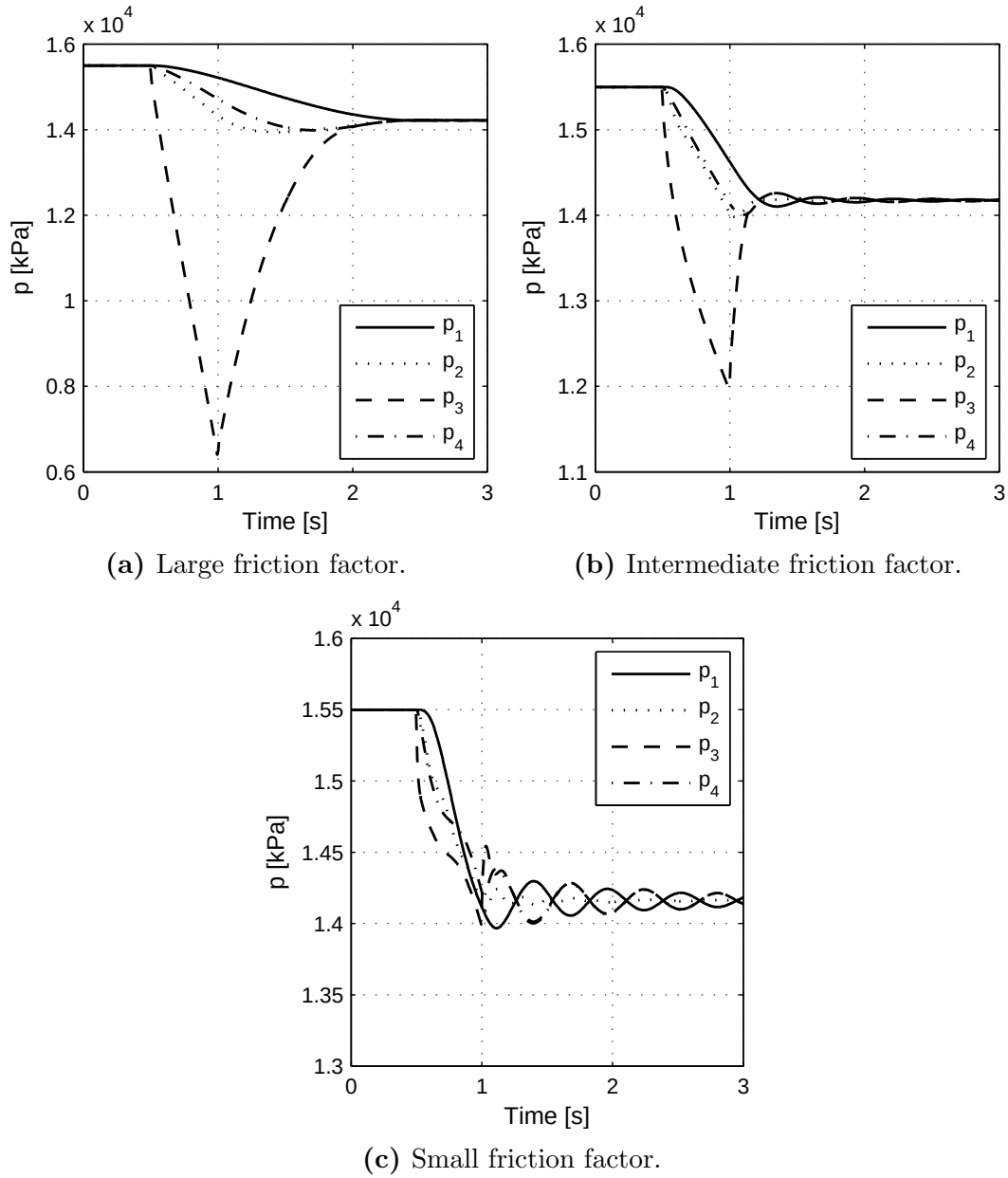


Figure 4.26: Pressure solution as a function of different magnitudes of friction factor obtained for a large mass sink transient in node 3.

The influence of the friction factor is illustrated in Fig. 4.26. It can be seen that for a large friction factor, as is used in Fig. 4.26a, the pressure in the node where the mass source is active (node 3) drops quickly as the flow from the other nodes is retarded and cannot compensate for the loss of pressure due to the loss of mass. For the intermediate case, shown in Fig. 4.26b, the loss of pressure in node 3 is less severe because the flow is not retarded that greatly. For the case where only a small friction factor is used, as in Fig. 4.26c, mass flows freely from the other nodes to node three, so the pressure for all the nodes drops approximately at the same rate. It is important to note that the model solves to the same new steady state condition independent of the magnitude of the friction factor. This is because the system is isolated from the environment and the same amount of mass is removed from the system in each case. The oscil-

lations visible in Fig. 4.26c are a result of the low retardation of the flow between the nodes. It can be seen from the figure that they show decreasing magnitude and will eventually damp out.

Because the study focused on correctly implementing a rate formulation for determining pressure in a transient system, it was desired to generate large pressure gradients in the system. If the rate formulation accurately simulated the situations where large pressure gradients existed, it would also correctly simulate transients where smaller gradients resulted. Therefore the solutions of the EES model discussed in Chapter 5 were generated using a large friction factor.

Flownex does not offer the functionality to specify a fixed friction factor in combination with a pressure drop term equal to the one defined for the EES model. The pressure drop term for the EES model is defined as,

$$\Delta p = \frac{1}{2A^2} k_L \frac{\dot{m}|\dot{m}|}{\rho} \quad (4.27)$$

where A is the flow area, k_L is the dimensionless friction factor, $\dot{m}$ the mass flow rate and ρ the average density of the fluid. Because retardation of the flow was desired in this study to generate large pressure gradients, an analogous approach was used in the Flownex model to generate the required retardation. A flow restrictor component with a fixed pressure loss coefficient was implemented instead of using the two-phase pressure drop correlation implemented as standard in Flownex (Lockhart-Martinelli pressure drop correlation). The pressure drop term associated with this component in Flownex is defined as,

$$\Delta p = C_l p_{ol} \left(1 - \frac{p_s}{p_{ol}} \right) \quad (4.28)$$

with C_l the loss coefficient, p_{ol} , the total pressure, and p_s the static pressure. Because these pressure drop terms use different parameters to calculate the Δp term in their respective models, it needed to be ensured that the terms in Flownex and EES models delivered similar pressure drop values when they were compared in the verification. This could be done by varying the C_l loss coefficient in the Flownex model until it generated the same pressure drop as that delivered by the pressure drop correlation used in EES.

An initial starting value for the loss coefficient C_l was obtained by implementing both forms of the pressure drop term in the formulated EES model. The value of the k_L factor was set at a constant value that generated the desired gradients in the flow model. The value of C_l factor was varied until the pressure drop given by the Flownex pressure loss correlation matched the pressure drop given by the EES pressure loss correlation. This was found to be at $C_l = 4k_L$.

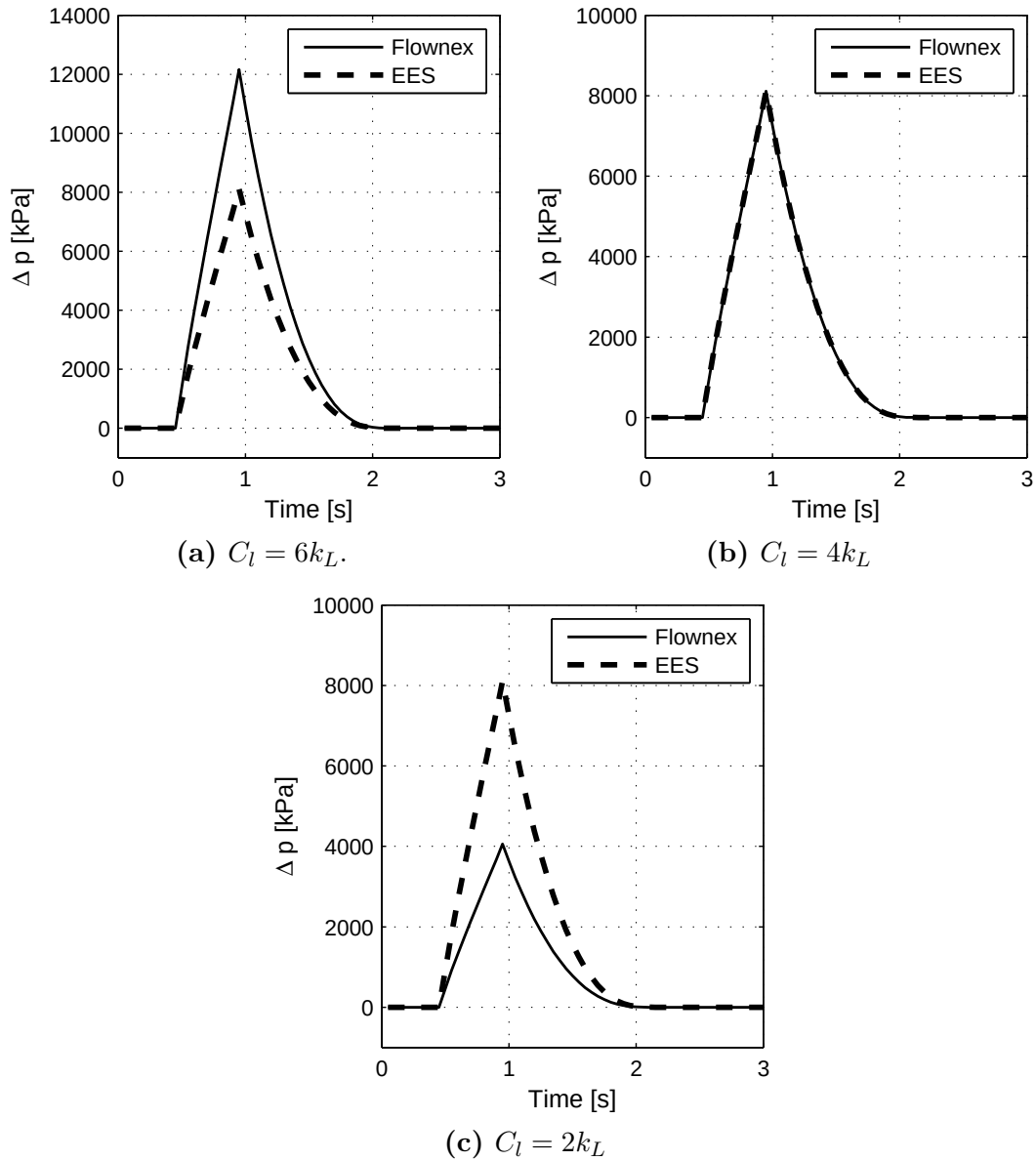


Figure 4.27: Pressure drop as a function of time in element 3 for different sizes of the loss coefficient C_l .

The correlation between the pressure drop calculated using the EES pressure drop equation when compared with the correlation used by Flownex can be seen in Fig. 4.27. Pipe 3 in the pipe and reservoir model is used in this illustration. The results shown for this pipe is consistent for all the pipes in the network. It can be from Fig. 4.27b that for a value of $C_L = 4k_L$, the pressure drop given by both correlations are the same.

Based on the fact that the models were shown to use similar formulations of the conservation equations and that the pressure loss terms were investigated and equated, it was expected that the EES model and Flownex model would evolve in the same manner when a transient scenario was simulated.

4.6 Verification process

The verification was done by constructing the same T-F network model in Flownex that was developed in EES. All geometries and boundary conditions used in Flownex were set to their corresponding values in the EES model. The transients were set up and solved in the same manner as in EES, therefore allowing for a direct comparison of the EES transient results with the Flownex transient results. The integration time step length was chosen as 0.005 seconds and a Crank-Nicolson integration factor was used as this is also employed in Flownex. The small time step length was chosen to ensure that any time step integration related errors were kept to a minimum. Because the model incorporating the IAPWS-95 equation of state was used as the benchmark case in this study, the Flownex transient results were used to verify only the model developed with the IAPWS-95 EOS, after which the EES model incorporating the RFES could be meaningfully compared with the verified model.

The following subsections will show the plots of the property values produced by the Flownex transient simulation model superimposed over those produced by the EES transient model using the algebraic EOS. The properties included are the nodal densities and enthalpies, along with their corresponding nodal saturation pressures and temperatures. The verification was done for both the mass sink simulation, as well as the energy sink simulation discussed in Chapter 5.

The goal of the plots in the following subsections are only to show the correlation between the Flownex and EES models. All discussions of said plots therefore only pertain to this aspect. Only a brief outline of the transient simulations that were done is given here for general information. A detailed discussion regarding the changes in fluid property values as a result of the transient simulations is given in Chapter 5.

In the case of the mass sink simulation, a large mass sink was activated in node 3 of the T-F network model, leading to a rapid loss of mass from the system. This resulted in a rapid transient in the system. The change in fluid property values resulting from this transient is illustrated as a function of time in the following subsections. Once the mass sink was deactivated, the fluid property values converged to a new steady state-condition. The new steady-state condition differed from the initial steady-state conditions as a result of the mass that was lost from the system during the transient. The energy sink case was done using the same methodology as the mass sink case, only with energy being extracted from the system instead of mass.

4.6.1 Mass transient verification

From Fig. 4.28 it can be seen that the results generated in EES show good agreement with those generated by Flownex. The property values for both cases converge to the same new steady state value after the transient, which shows that the conservation equations used in the EES model were correctly formulated and implemented. A difference between the enthalpy values for the EES and Flownex models is observed in Fig. 4.28d. The difference between these values is on the order of 0.5% and therefore still within acceptable accuracy.

The property values generated in EES during the transient closely resemble those generated in Flownex. The largest deviation of the EES values from those of Flownex is seen during the transient, at time $0.5 < s < 2.5$, in the node where the transient takes place. For the other nodes in the system all the properties correlate well, with little apparent differences observed between the property value solutions of the two models.

In the case of the rapid mass transient simulated in this study, it can be seen that the form of the solutions in the node where the transient takes place differs somewhat between the Flownex and EES models. EES predicts a sharper drop in system properties in the node where the transient takes place compared with the change in properties in the Flownex model. The scale of the transient, or in other words the magnitude of the rate of change of properties in the system as a result of a perturbation may play a role in how well the simplified EES model solution correlates to that of the Flownex model. This may be deduced from the fact that for the energy transient shown in Fig. 4.30, which results in a slower rate of change of the system properties, the EES and Flownex models show a high degree of correlation throughout the transient in all the nodes of the system.

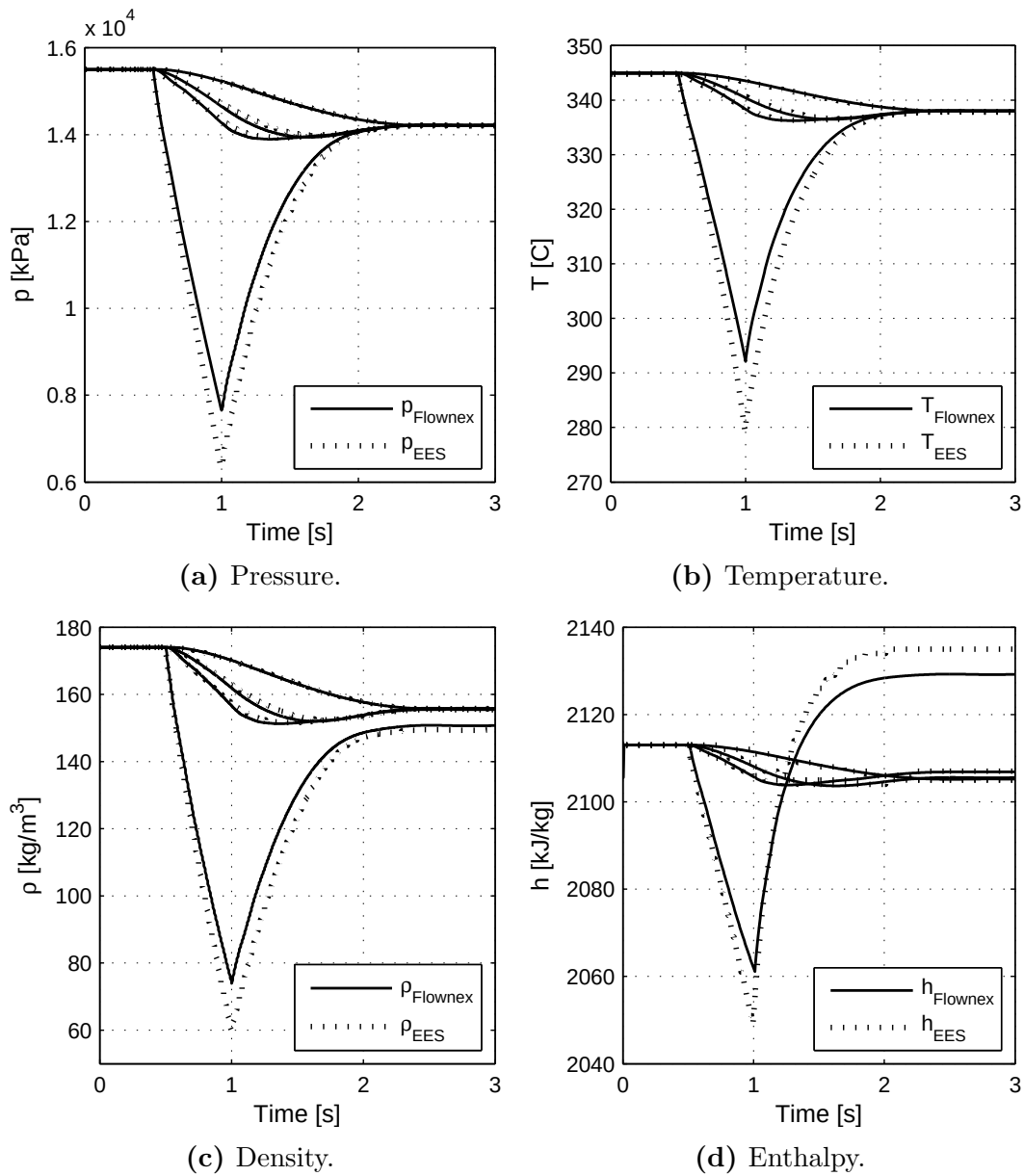


Figure 4.28: Comparison of nodal property values delivered by the EES and Flownex models for the mass transient case.

Based on this observation, the Flownex model was run again. This time, the pressure drop loss coefficient in the Flownex model was set somewhat higher, as this was expected to lead to a greater correlation between the results of the Flownex and EES models. This was found to be the case. Fig. 4.29 shows the correlation between the Flownex and EES model solutions for a loss coefficient value of approximately $C_l = 5.75k_L$. A direct relation of the pressure drop terms for the two models by using a constant value was seen to require some adjustment of the loss coefficient values. However, based on the in depth study of the sensitivity of the pressure loss terms and their effects on the evolution of the system, it was felt with enough confidence that the EES model could be deemed verified for the mass sink case.

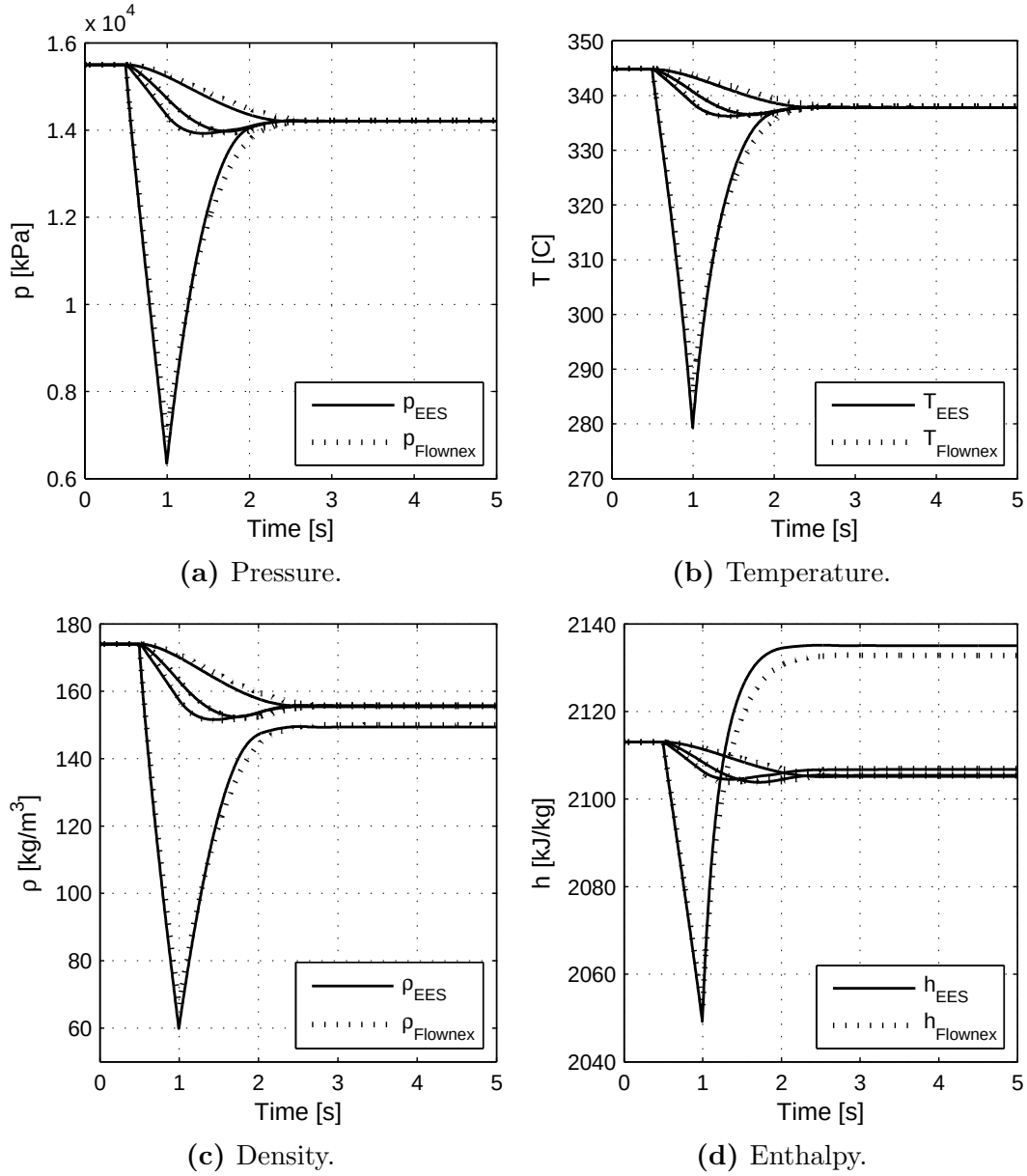


Figure 4.29: Comparison of nodal property values delivered by the EES and Flownex models for the mass transient case with a higher pressure loss coefficient C_l value.

If follow on studies are desired based on this study, the verification of the EES model by using the Flownex model may be updated and improved by employing the same pressure loss correlations in both models to create a 1:1 comparison, which can then again be verified. The objective of the verification of the EES model in this study was to ensure that the EES model delivered meaningful results taking the assumptions made in developing the model into account. Based on the fact that a good understanding was achieved with regards to the impact of the different pressure loss correlations used in the models, as well as the fact that the conservation equation formulations were theoretically consistent and converged to the same steady state solutions, the EES model was deemed verified with good confidence.

4.6.2 Energy transient verification

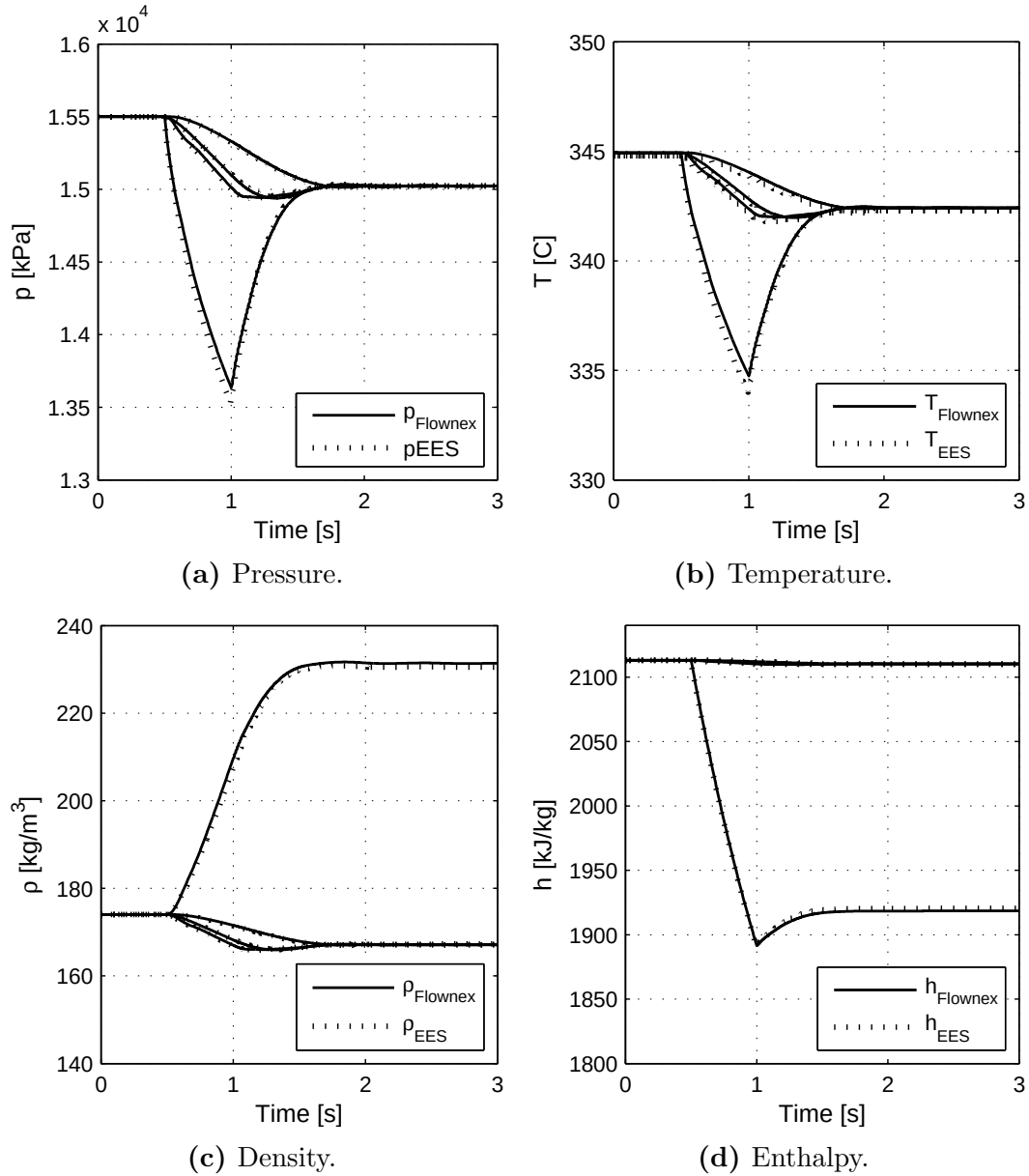


Figure 4.30: Comparison of nodal property values delivered by the EES and Flownex models for the energy transient case.

The comparison plots for the difference between property values delivered by the EES and Flownex transient models for the energy sink case are given in Fig. 4.30. As in the mass case, the property values under consideration show good agreement between the models. Based on this agreement, the EES transient network model was considered verified for the energy sink case.

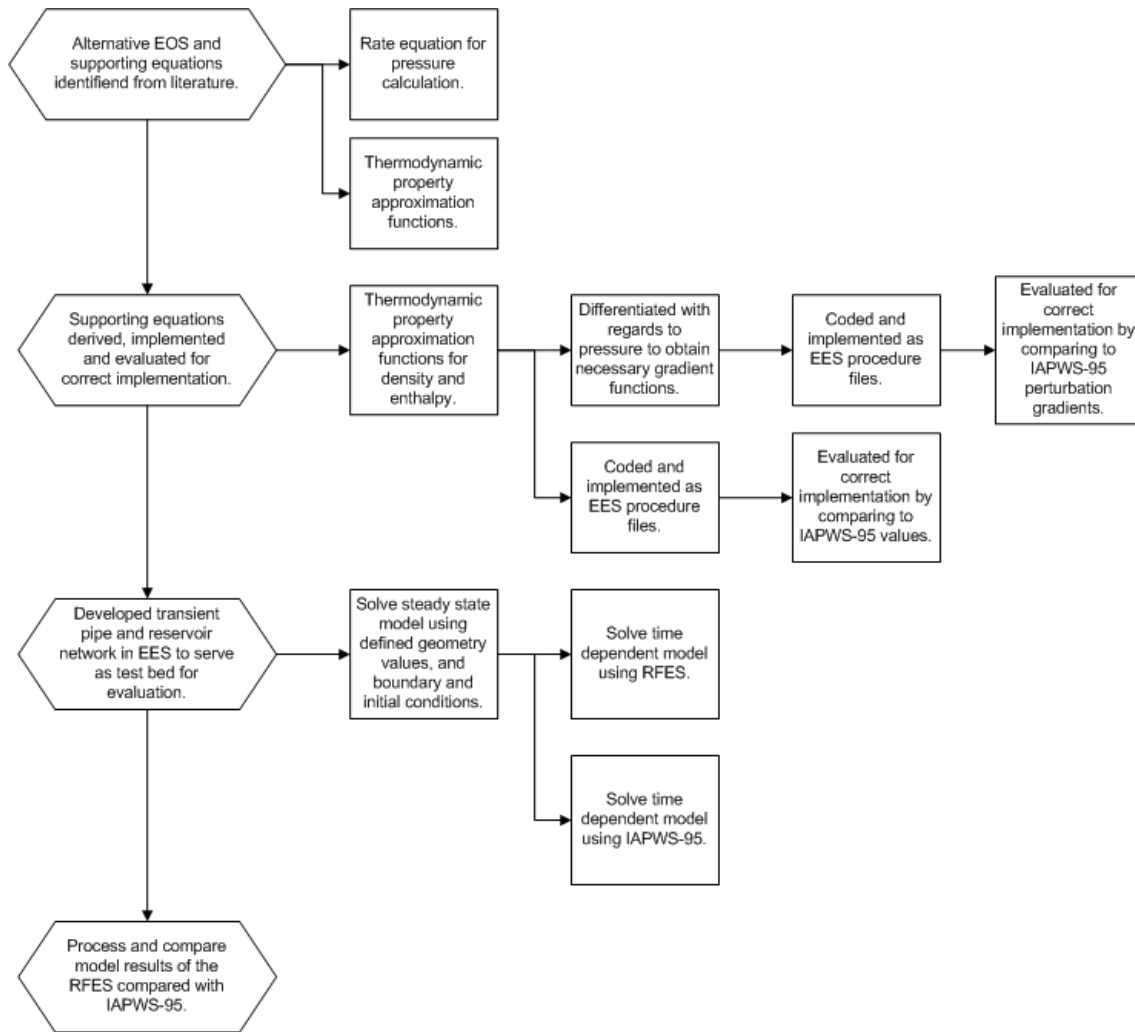


Figure 4.31: Summary of methodology followed in the evaluation of the rate method and it's supporting equations.

4.7 Summary

This chapter outlined the methodology followed in implementing the various components of the rate methodology in EES and developing a T-F network simulation model which could be used to solve a homogeneous equilibrium two-phase flow model using the rate methodology. The first component that was implemented was the thermodynamic property approximation functions and their derivatives. These functions and derivatives were written as EES procedure files that could be called when solving the formulated transient network model. Their correct implementation was verified by comparing the property values they delivered with those delivered by the benchmark IAPWS-95 EOS over the pressure range for which they are defined. The transient pipe and reservoir network model that was developed in EES to serve a T-F simulation model which incorporates the rate formulation was verified by developing an equivalent model in the Flownex SE proprietary T-F simulation code. This code employs the same SCFD approach and homogeneous equilibrium two-phase flow model to T-F systems as was used for the EES model, and was therefore deemed to be a sufficient benchmarking tool. The EES and Flownex models showed good agreement for both the mass and energy transient cases that will be discussed in

detail in the following chapter. A summary of the methodology is presentend in Fig. [4.31](#)

The goal of this project was to evaluate a rate form of the equation of state as an alternative to the algebraic equation of state in terms of the applicability and accuracy. This meant that both methods had to be employed in a suitable test simulation to evaluate the accuracy of the rate method. The simulation model discussed in this chapter was chosen as a theoretical test model as it allows for the simulation of various transient phenomena in a thermal-hydraulic system. It does however not represent an actual physical system, and was formulated only to enable the simulation of all the relevant physical processes. An accurate solution of the model with regards to a physical system, which can be validated, was therefore not required. The inclusion of simplified loss factors and coarse discretisation was therefore justified in the context of this study.

The following chapter will discuss in detail the transient cases that were simulated to determine the correctness of the results results delivered by the network model that solved with the rate method. These cases were solved using both the IAPWS-95 and rate forms of the EOS, after which the property values delivered by the two methods could be compared directly and evaluated.

Chapter 5

Transient Model Comparison

The previous chapter dealt with the implementation of the constituent components of the rate formulation, as well as the formulation and verification of the transient pipe and reservoir network that was chosen as a test bed in which to implement the method.

This chapter will serve to evaluate the level of agreement between solutions of the model using IAPWS-95 and the rate method respectively. It was expected that the rate formulation would deliver results that correlated well with those delivered via the verified IAPWS-95 model. As stated in Section 3.5, the rate form of the equation of state for determining pressure in the system adds an additional time dependent equation to the set of equations used to model the system. It was therefore important to quantify the impact of this additional time dependent equation on the level of agreement between the two models. Also, by evaluating the error of the rate method by comparing its results to those of the IAPWS-95 solution, an understanding could be developed as to which integration scheme and time step lengths delivered acceptable model solutions.

5.1 Comparison strategy

The three conservation equations that represented the pipe and reservoir network model that was developed could be closed and solved in three separate manners:

1. By using the IAPWS-95 EOS formulation in combination with the derived conservation equations to solve the model for the chosen transients. This method was verified by comparing the results delivered with those obtained via Flownex. It was therefore the reference case used for comparison.
2. By using the rate method. This included the rate equation for determining pressure, as well as the thermodynamic property approximation functions for the saturation density and enthalpy values and their gradients.
3. The developers of the rate method did not derive an explicit approximation function for determining pressure as a function of other property values. However, because EES simply solves the entire system of equations it is given to a specified tolerance, if the number of equations equals the number of unknown variables, EES can still solve the

model. This meant that pressure could be made to be implicitly solved in the system of equations by using only the approximation functions and a valid extra relation to provide the final equation in the EES model, instead of providing an equation that explicitly solved for pressure. The reasoning behind this method was that it would allow a direct comparison between the solution of the EES model using only the algebraic approximation functions and a solution using the rate equation for determining pressure combined with the approximation functions.

5.1.1 Implicit pressure solution method

The first and second methods of solving the transient model has been discussed in detail. This subsection briefly discusses the reasoning and methodology for the final solution option.

The third option stated above would allow for the direct comparison between a model based on an algebraic solution using the derived approximation functions and one that used the rate equation for determining pressure. Because a small, yet quantifiable difference exists between the solution of the model using the approximation functions and the model using the IAPWS-95 solution, these differences might contribute to the error in a comparison between the IAPWS-95 solution and a solution based on the rate method. This is illustrated in Fig. 5.1.

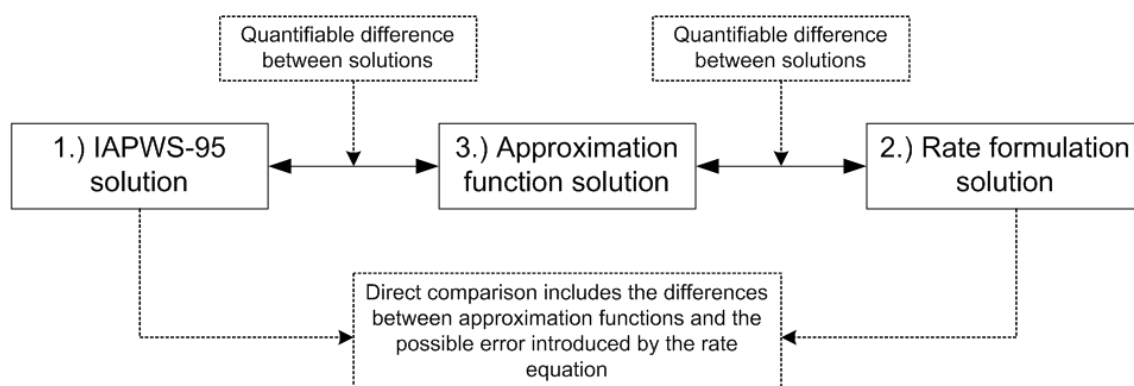


Figure 5.1: Possible errors included when comparing different solutions of the EES models.

Because the approximation functions were shown to be correctly implemented and delivered property values that correlated well with the IAPWS-95 property values in Subsection 4.1.1, it was expected that the solution of a model that used only the approximation functions would also correlate well with the solution of the model using the IAPWS-95 EOS. Therefore, to isolate the difference in solution values generated by the pressure rate equation, the solution based on this method could be compared directly with the approximation function only solution to remove the possibility of an additional error in the comparison. This is illustrated in Fig. 5.2.

For both the IAPWS-95 and rate equation model solutions, there is an explicit equation that is used to solve for the pressure in the system. For the case where the model is closed to solve the pressure implicitly with the use of only the approximation functions, another defined relation is used as a substitute for a explicit pressure equation. Because the fluid in the EES model is at saturation conditions, the saturation temperature and saturated fluid and vapour density

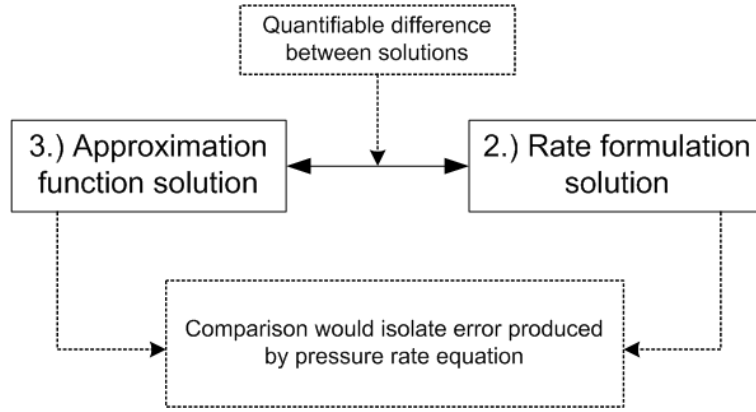


Figure 5.2: Removal of a possible additional error in the comparison provides a method for directly quantifying error produced by pressure rate equation.

and enthalpy values are a function of the pressure of the system. Once the pressure value is known, these values can be fixed. This is shown in Fig. 5.3. For the density and enthalpy, the saturation values only give property values at saturated liquid (h_f, v_f) and saturated vapour (h_g, v_g) . To fix the specific property values (h, v) at the point in the saturated region where the system is functioning, the definition of static quality or thermodynamic quality may be used, where the static and thermodynamic qualities are defined as,

$$x = \frac{v - v_f}{v_g - v_f} \quad (5.1)$$

and,

$$x = \frac{h - h_f}{h_g - h_f} \quad (5.2)$$

respectively. Either of these relations may be used in the EES model to calculate the nodal quality value and determine the point within the saturation region that is consistent with the density and enthalpy values delivered by the conservation equations for the specific pressure condition. For cases one and two, where the EES model solves the pressure using an explicit function, the static quality is used to determine the quality value. When the model is solved using only the approximation functions, another equation is required to close the model. In this case, both the static and thermodynamic quality equations are used in EES. This closes the model and allows for the implicit calculation of the pressure within the system of equations.

In theory, the approximation function only solution could now be compared to the solution using the approximation functions, as well as the pressure rate equation. This would allow for the specific impact of the pressure rate equation to be quantified. However, when this solution

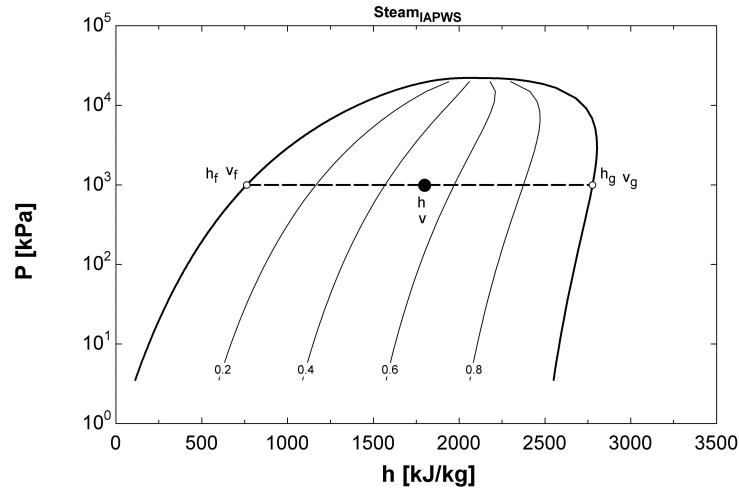


Figure 5.3: Graphical representation of saturation fluid properties and relation to quality factor.

method was implemented in EES, it was found that it was very difficult to obtain solutions for the transient model. The model proved highly unstable and would not converge once a very fast transient was initiated in the system. A number of different time step lengths and integration factors were attempted to try and remedy the problem, with little success. The model solved correctly for conditions where no transients were taking place, but attempts to solve the model when transients were simulated failed in almost all cases. Only for one case, where a 0.05s time step length and integration weighting factor of 0.6 – 0.8 was used, could a solution be obtained.

As expected, the solution of the IAPWS-95 model correlated well with the solution of the approximation function only model for the one solution that could be obtained. This is illustrated in Fig 5.4. A good correlation is shown for all property values when comparing the approximation function (AF) solution with the IAPWS-95 solution. The solution incorporating the pressure rate equation can be seen to differ somewhat from the other two solutions. Based on the following considerations, it was decided that a direct comparison of the AF-RFES solution to the IAPWS-95 solution could be justified for the rest of this study:

- The difficulty of obtaining solutions for the implicit pressure solution method for comparative purposes.
- For the case where an implicit solution could be obtained, it was seen that there was no practically significant difference between the solution values for the IAPWS-95 and AF models.
- The implicit pressure solution was obtained for a relatively large time step size. It was assumed that for smaller time step sizes, the difference between the IAPWS-95 solution and AF solution would remain small. This would be true in general, as both these EOS methods are time independent.

The rest of the comparisons discussed in this chapter will therefore compare the IAPWS-95 solution directly with the solution using the full rate method. Even though a direct quantifica-

tion of the integration error introduced by the pressure rate equation based will not be possible as a result of this, the goal of correctly implementing the rate method can still be achieved. If the difference in solutions delivered by the two models becomes small, it means that both the quantifiable differences shown in Fig. 5.1 are minimised, which contributes to achieving the goal of correctly implementing the rate method, i.e. delivering solutions that are consistent with those delivered by IAPWS-95.

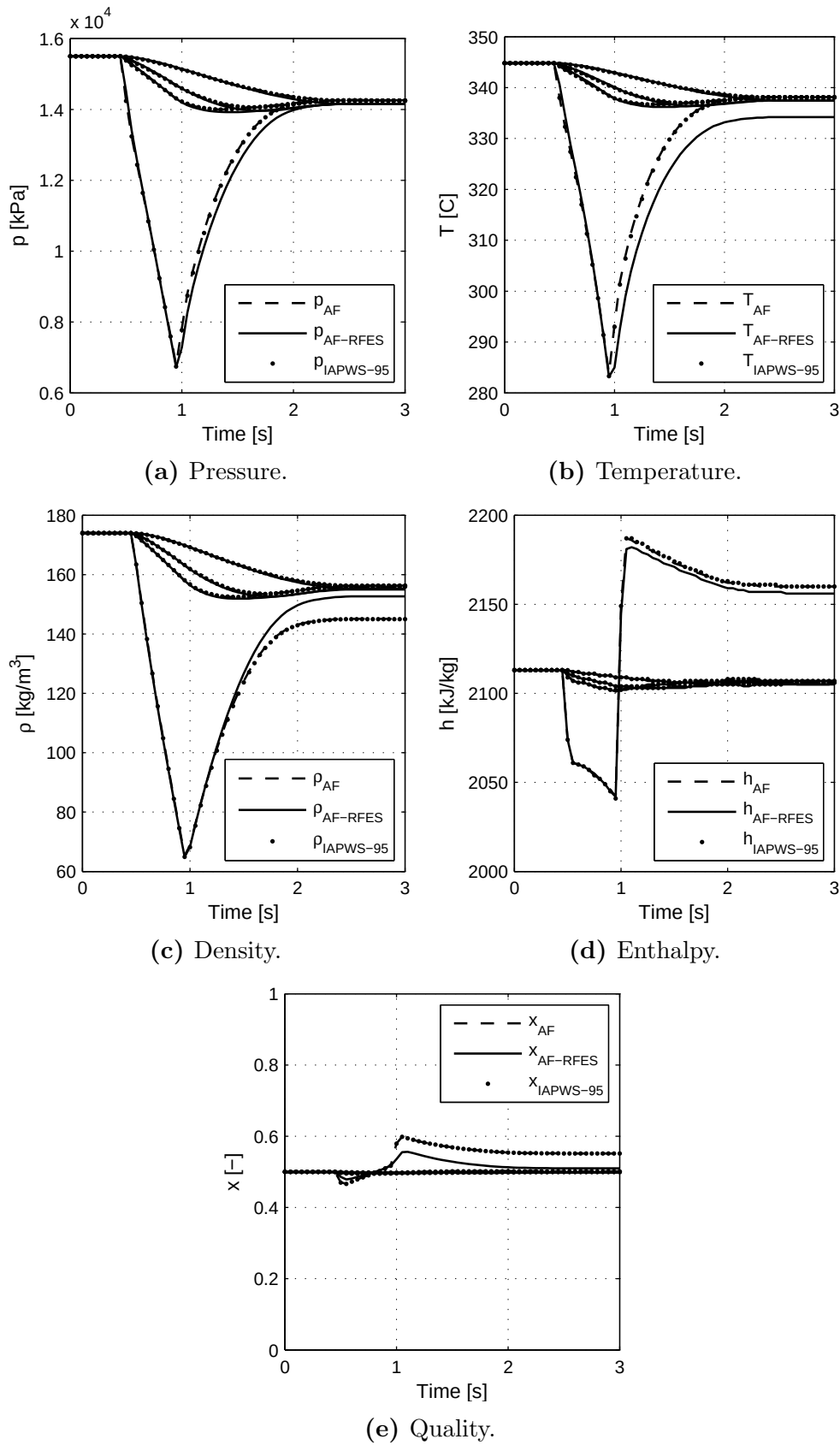


Figure 5.4: Plot of nodal property values versus time for the mass sink case solved using the IAPWS-95, AF, and AF-RFES method. Solution obtained for a $0.05s$ time step length and integration weighting factor of 0.75.

5.2 Mass sink transient simulation

The simulation was set up with the boundary conditions defined in Subsection 4.2.5. The nodal pressures for node 1-4 was set at 15.5 MPa and the temperature at the corresponding saturation temperature. The system was initially run at steady state conditions for 0.5 seconds. At 0.5 seconds, a large mass sink was activated in node 3 for 0.5 seconds, leading to a rapid pressure blow-down as mass was lost from the system. The system was then left to stabilise at a new steady state condition before the simulation was terminated at 5 seconds. The nodal property values for each node is plotted as a function of time in Fig. 5.5. The property plots were obtained by solving the model with a 0.005s integration time step length using a fully implicit integration weighting factor.

The loss of pressure as a result of the mass sink in node 3 is seen in Fig. 5.5a. The change in temperature during the transient directly mirrors the pressure change. This is true because the system is operating at saturation conditions, where the temperature is a pure function of pressure. The drop in density in node 3 is a result of the rapid loss of mass from the node. Once the mass sink is deactivated, the density increases as mass from the other nodes flows into node 3. The enthalpy in node 3 shows the same trend, with the enthalpy in node 3 decreasing as mass is lost from the system. Once the mass sink is deactivated, the enthalpy increases as a result of the flow of steam into node 3.

It is seen from Figs. 5.5c and 5.5d that the density and enthalpy values do not converge to the same steady state values as those of the other nodes. This is due to the fact that the vapour quality in node 3 increases (i.e. steam is produced via evaporation) during the transient. When the mass sink is deactivated, the system stabilises at a new steady state condition where the temperatures and pressures are equal for all the nodes. In other words, the system converges to a new equilibrium condition where there are no pressure or temperature differences between the nodes. Because of the increase in vapour quality in node 3, the steady state density corresponding to the new nodal pressure and temperature conditions is lower. The increase in vapour quality will also result in a higher enthalpy value for the node at the new steady state conditions.

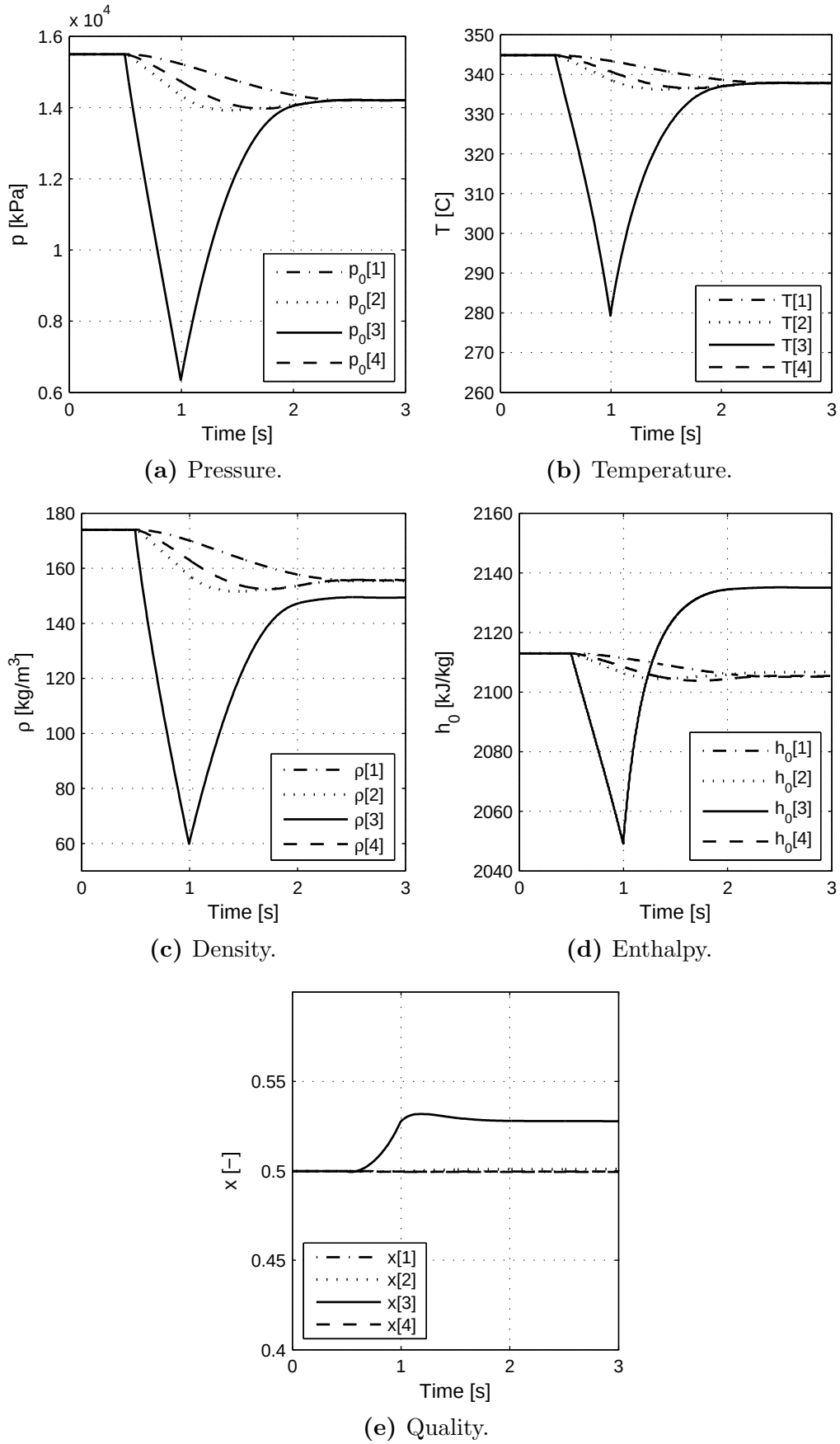


Figure 5.5: Plot of nodal property values versus time for the mass sink reference case. Plot generated using the algebraic EOS with a fully implicit integration scheme for 0.005 second time steps.

To quantify the level of agreement the rate method solution showed with the IAPWS-95 solution, the model was solved using both EOS formulations for a range of time step lengths and integration weighting factors. For the purpose of this study, an arbitrary solution error value of less than one percent was deemed a threshold value. Model solution values that showed an agreement of less than one percent difference therefore indicated that the solution values calculated using the rate method could be considered to show an appropriate level of agreement (correctness).

Table 5.1: Time step lengths and integration weighting factors used to solve the mass sink and energy sink cases.

Time step lengths and integration factors.					
Time step length [s]	Weighting factor [α]				
	0.1	0.25	0.5	0.75	1
0.0005	✓	✓	✓	✓	✓
0.001	✗	✓	✓	✓	✓
0.005	✗	✗	✓	✓	✓
0.01	✗	✗	✓	✓	✓
0.025	✗	✗	✓	✓	✓
0.05	✗	✗	✓	✓	✓
0.1	✗	✗	✓	✓	✓

The weighting factors employed for each time step length are illustrated in Table 5.1. Initial simulations were only done for time steps of 0.005 and larger, with weighting factors of 0.5, 0.75 and 1. This was because any weighting factor lower than 0.5 proved to be too unstable due to the explicit characteristics of the solution and therefore unable to solve for these larger time step lengths. The shorter time step lengths were later included in the study to test the accuracy of the RFES when using more explicitly weighted integration factors. It was not possible to test a fully explicit integration scheme as this proved unstable even at very small time steps.

The following subsections elaborate on the percentage difference, termed the error, between the property values of the IAPWS-95 solution of the model and the rate solution of the model. Two error metrics were considered.

The first is the maximum deviation of the rate simulation property values from those of the IAPWS-95 simulation property values during the transient. The importance of this metric is apparent when considering simulation models that are developed to test rapid single transients, such as depressurisation in the case of pipe breaks or similar phenomena, where over- or under-prediction of property values and flow conditions can lead to errors in the safety system design.

The second metric considered is the final error. This is the percentage difference between the rate simulation property values and those of the IAPWS-95 simulation at the conclusion of the transient once steady-state is again achieved. This error becomes significant if models are developed to simulate systems where multiple successive transients occur within the time for which the system is simulated. In this case the error from the previous transient is carried forward and contributes to the error in the following transient. Determining the final error was

therefore important to measure to what extent the rate method would be accurate in situations where multiple successive transients were simulated in a given system.

In each of the cases that follows, the EES simulations employing the respective equations of state were run for the same time step lengths and integration factors, so that the only difference in each case was the equation of state formulation used. Therefore, the integration errors produced in the time-wise integration of the conservation equations were the same when solving both the IAPWS-95 and rate EOS models.

5.2.1 Pressure

Because the network comprised of four nodes, the data set generated contained four discrete sets of property values with one set for each node under consideration. This data was cumbersome to process in its entirety. The data was therefore reduced to include only the node where the maximum deviation of the RFES property values were found. In the case of the mass sink simulation, the large mass sink was activated in node 3. Consequently, this was where the rate of change of nodal property values was expected to be the most significant and where the largest error was expected to occur when employing a rate based method. This proved to be true. The largest deviation of the rate property values from the IAPWS-95 solution values were consistently found to be in node 3. The figures below therefore include the maximum and final errors for the properties of node 3.

A log-scale was used for the horizontal-axes of all the error graphs. A log-scale was also used where needed for the vertical-axes of the error graphs. This is noted in the sub-captions of relevant graphs.

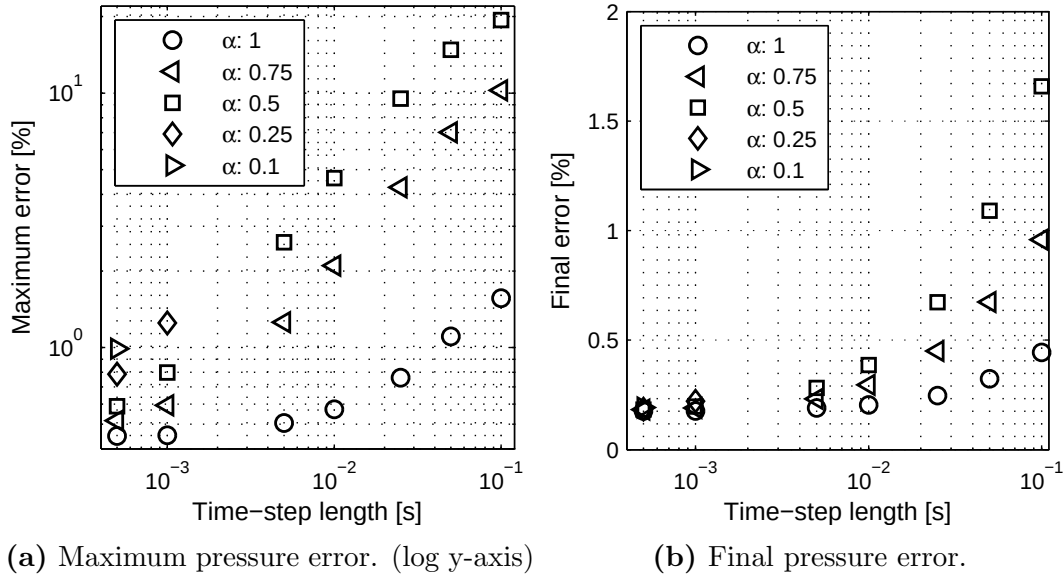


Figure 5.6: The maximum and final pressure errors for different combinations of integration weighting factor and time step length.

Fig. 5.6a shows the maximum pressure error generated when solving the reference transient. The effect of integration time step size can be seen. As it increases, the maximum pressure error becomes significantly larger compared to that for smaller time steps. The Crank-Nicolson solution ($\alpha = 0.5$) shows the largest time step sensitivity and the error generated by this scheme quickly becomes large. Inversely, the fully implicit solution shows the smallest degree of time step length sensitivity. All the weighting factors considered delivered an error of less than 1% when the smallest time step was used.

This trend holds for the final error illustrated in Fig. 5.6b. The fully implicit solution yielded the best accuracy when considering all the time step lengths, with the error never being more than 0.5%.

It can be seen that the Crank-Nicolson solution is not the most accurate integration weighting factor. This is interesting, as one would expect that the Crank-Nicolson solution, which is second order accurate, would become more accurate than the other integration weighting factors which are only first order accurate. Because the error remains very small in absolute terms for all the integration weighting factors at sufficiently small time step lengths, this aspect was not investigated in more detail.

5.2.2 Temperature

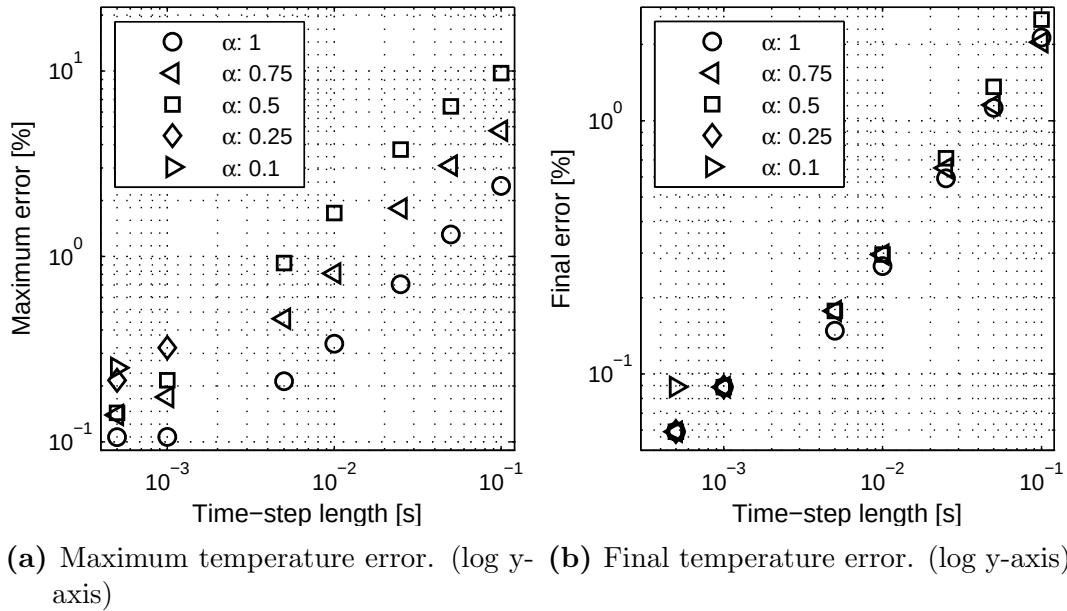


Figure 5.7: The maximum and final temperature errors for different combinations of integration weighting factor and time step length.

The plots for temperature error show a pattern similar to those for the pressure. Fig. 5.7a shows that the maximum temperature error is not as large as that for the pressure. The final error values converge to a similar value for all the weighting schemes at the smaller time step

lengths, as shown in 5.7b. The final temperature error drops below 0.1% for all the integration schemes at the two smallest time step lengths.

5.2.3 Density

The RFES is not directly responsible for generating errors in the density and enthalpy values in the network nodes because density and enthalpy are solved via the mass and energy conservation equations respectively. However, the pressure values delivered by the RFES are provided to the momentum conservation equation to calculate the mass flow in each pipe in the network. This mass flow information is then used by the mass and energy conservation equations to update the nodal densities and enthalpies in the system. Any error in the pressure will therefore induce a feedback effect, so that density and enthalpy values may also become inconsistent with those obtained when solving the system with the algebraic EOS. It was therefore important to assess the level of disagreement imparted on the density and enthalpy values in the system when solving the network with the rate method.

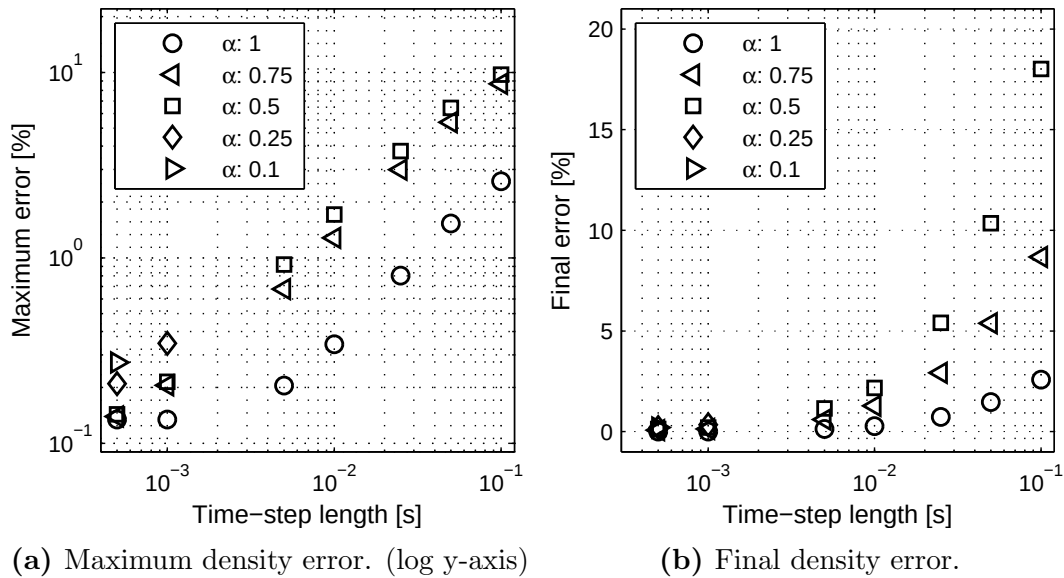


Figure 5.8: The maximum and final density errors for different combinations of integration weighting factor and time step length.

The maximum and final density errors follow the same trend as those for the pressure and temperature. For larger time step lengths significant errors were produced in terms of the maximum and final errors. The fully implicit solution scheme once again proved to be the least sensitive to an increase in time step length.

5.2.4 Enthalpy

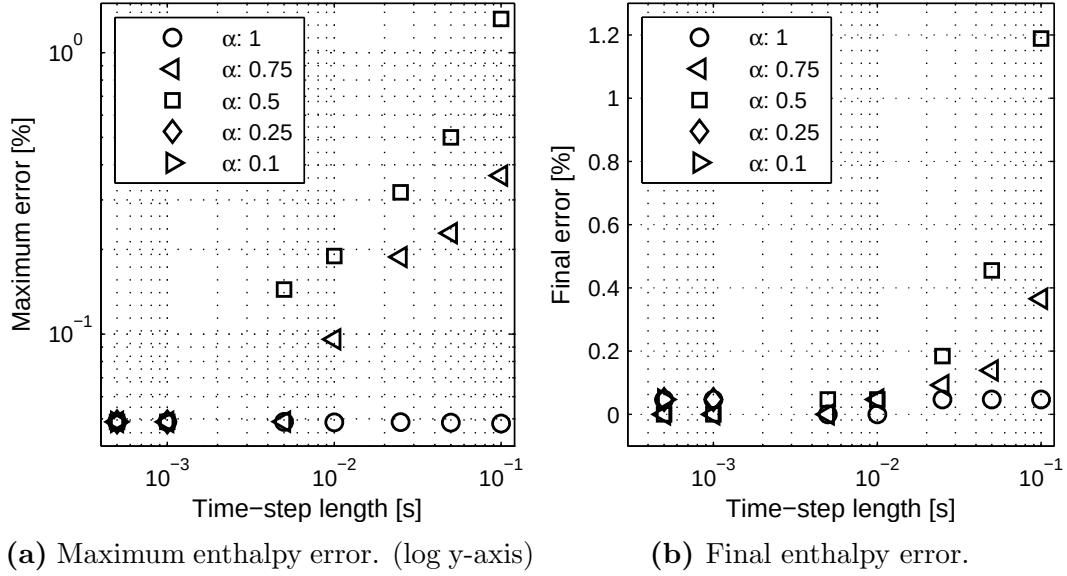


Figure 5.9: The maximum and final enthalpy errors for different combinations of integration weighting factor and time step length.

The enthalpy error plots in Fig. 5.9 show that this property is solved more accurately for all time step lengths than the other property values. Only the Crank-Nicolson solution at the largest time step returned an error larger than 1%. The difference between the error of the enthalpy when compared with that of the density is attributable to the fact that the rate of change of density in the two-phase system under consideration was larger than the rate of change of the enthalpy. Larger time steps will contribute more significantly to the error if the rate of change of the property under consideration is large. They will not contribute the same degree of error to slowly varying properties.

5.3 Energy sink simulation

The reference simulation in the previous section dealt with the accuracy of the RFES when simulating a rapid mass transient in the network. The accuracy of the RFES also had to be considered in the case of rapid energy transients. To evaluate the accuracy of the RFES when solving energy transients, the exact same reference simulation was used, but instead of a mass sink as in the previous case, a large energy sink was used to generate the transient in node 3. The change of system properties over time is shown in Fig. 5.10.

During the energy transient, a large energy sink was activated in node 3. The system behaved in a similar manner as in the mass transient case when considering pressure and temperature. When the energy sink is activated, the pressure and temperature in node 3 drop significantly. When the sink is deactivated, the pressure and temperature again converge to a new steady state pressure and temperature, along with the other nodes. The changes in enthalpy and density differ from the mass sink case. Because of the rapid loss of energy from the system, the

vapour quality in node 3 drops as the steam condenses, leading to a large increase in density. This condensation along the saturation line also leads to a decrease in enthalpy in node 3.

Figs. 5.11 - 5.14 show the maximum and final errors for the properties under investigation. The errors produced for the energy transient were smaller than in the case of the mass transient. This is because the mechanism triggering the transient differs from the mass transient case. In the energy case no mass is lost from the system, so the overall effect of the transient on the pressure drop is smaller, leading to smaller error values. In general, there is a measure of increase in error as the time step length increases, especially in the case of the Crank-Nicolson solution, but overall the errors appear more random for the energy case. This may be attributable to the small absolute error between the property values returned by both methods, which allows for numerical solution errors in EES and the differences between the approximation function property values and IAWPS-95 property values to contribute somewhat to the error. The main observation, however, was that the rate method proved to be quite accurate compared to the algebraic method for the energy transient case. Only the Crank-Nicolson solution combined with the largest time step could produce an error larger than 1% in any of the properties under consideration.

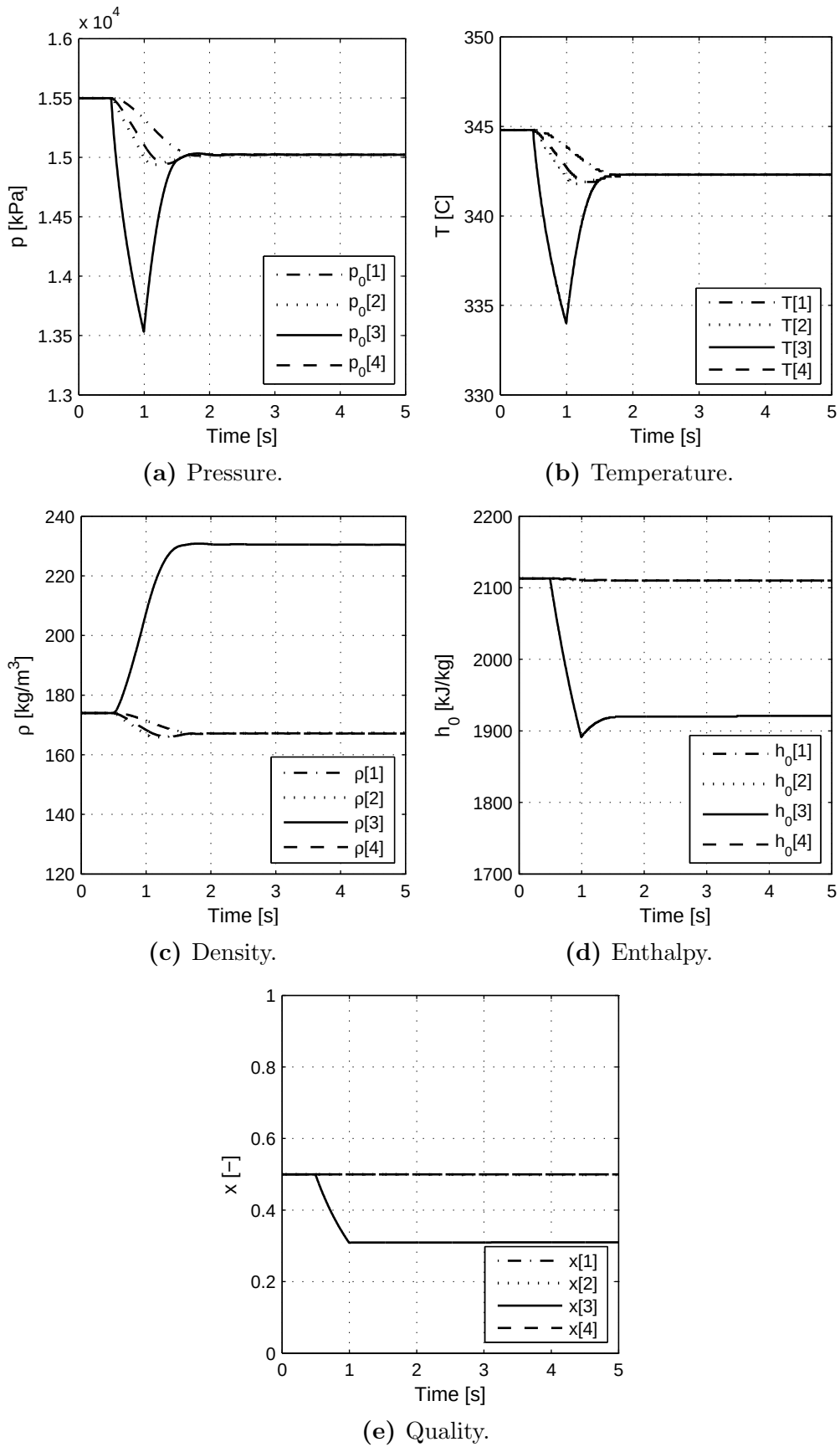


Figure 5.10: Plot of nodal property values versus time for the energy sink case. Plot generated using the algebraic EOS with a fully implicit integration scheme for 0.005 second time steps.

5.3.1 Pressure

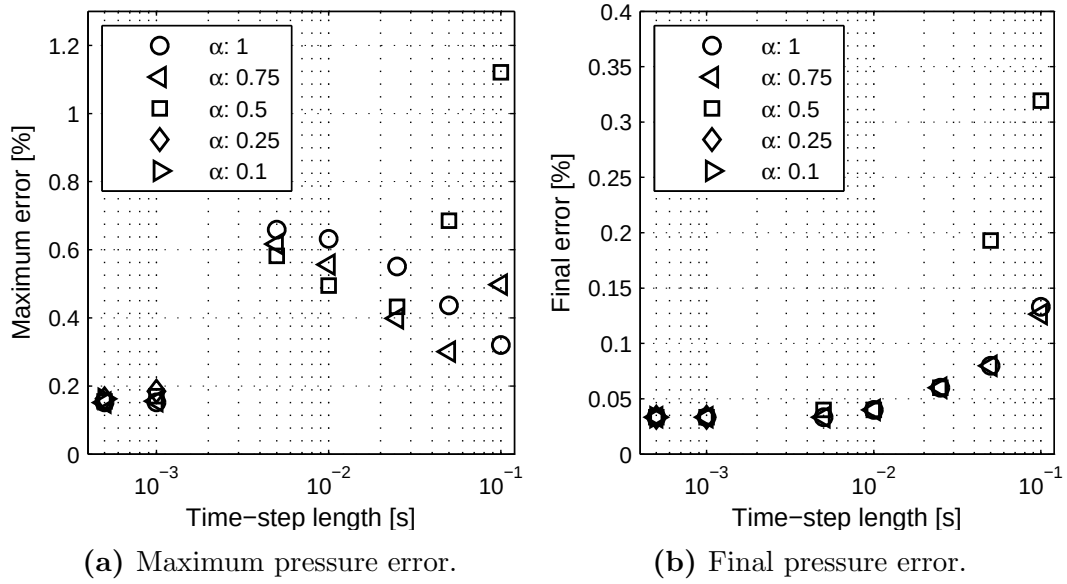


Figure 5.11: The maximum and final pressure errors for different combinations of integration weighting factor and time step length. (Energy case)

The maximum errors shown in Fig. 5.11 do not follow a decreasing trend as the time step length decreases. The trend is hard to quantify directly, but the error remains below 1% for all combinations of time step length and integration factor, except for the C-N solution at the largest time step length.

5.3.2 Temperature

As in the case of the nodal pressures, the nodal temperature errors observed in Fig. 5.12 do not show a definite trend. Both the maximum and final errors for the nodal temperature are well below 1% in all cases.

5.3.3 Density

The maximum and final density errors, shown in Fig. 5.13, exhibit a generally decreasing trend in error values as the time step length decreases. The maximum error is largest for the C-N solution at the largest time step, falling just below 2%. The final error for all the cases are below 1%.

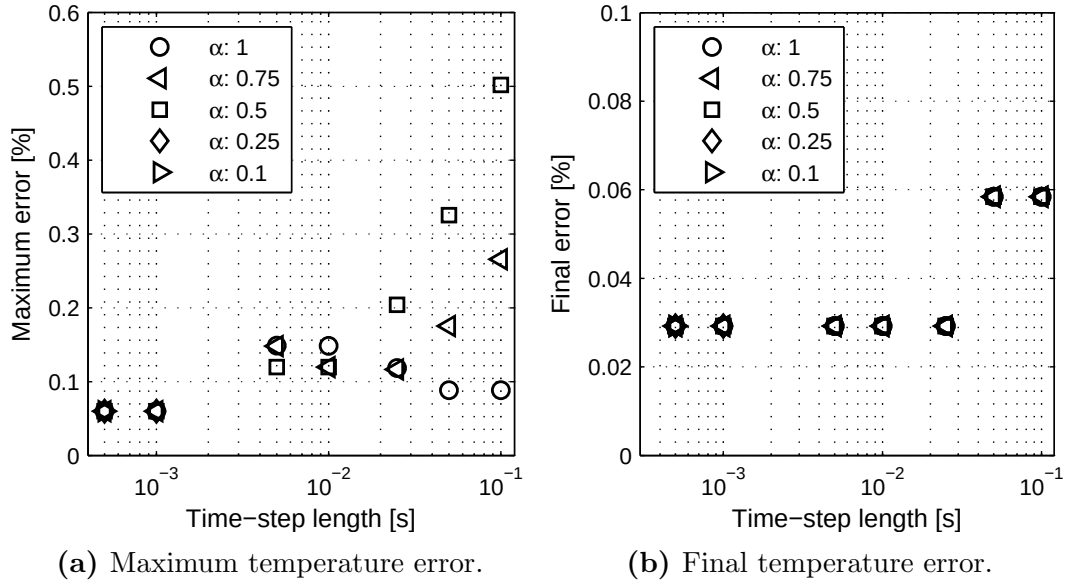


Figure 5.12: The maximum and final temperature errors for different combinations of integration weighting factor and time step length. (Energy case)

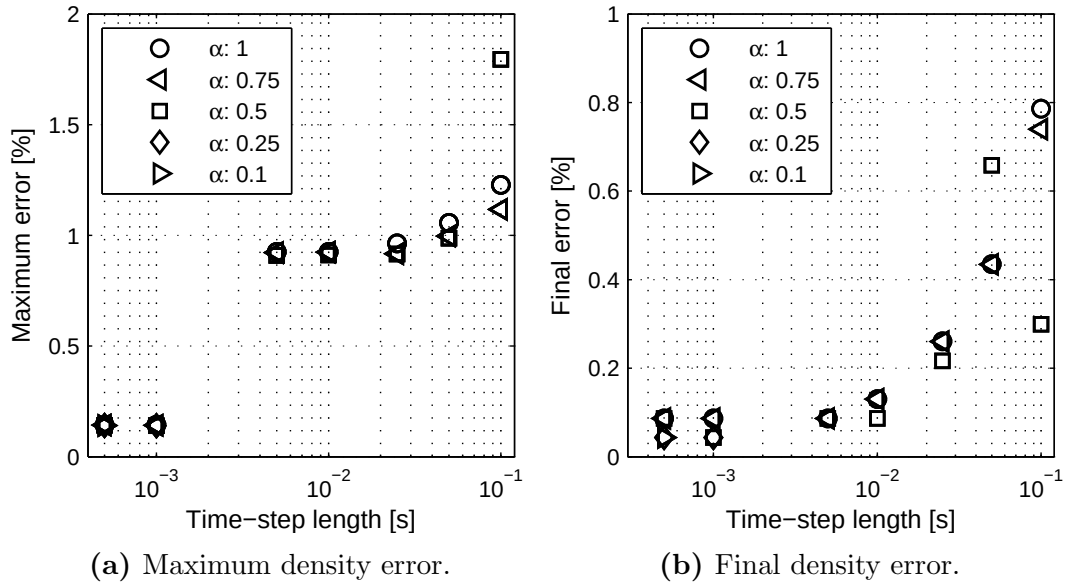


Figure 5.13: The maximum and final density errors for different combinations of integration weighting factor and time step length. (Energy case)

5.3.4 Enthalpy

The maximum and final errors for the nodal enthalpies, given in Fig. 5.14, show the smallest error of the properties under consideration. The error value for both metrics generally fall below 0.2%, except in the case of the C-N solution at the two longest time step lengths.

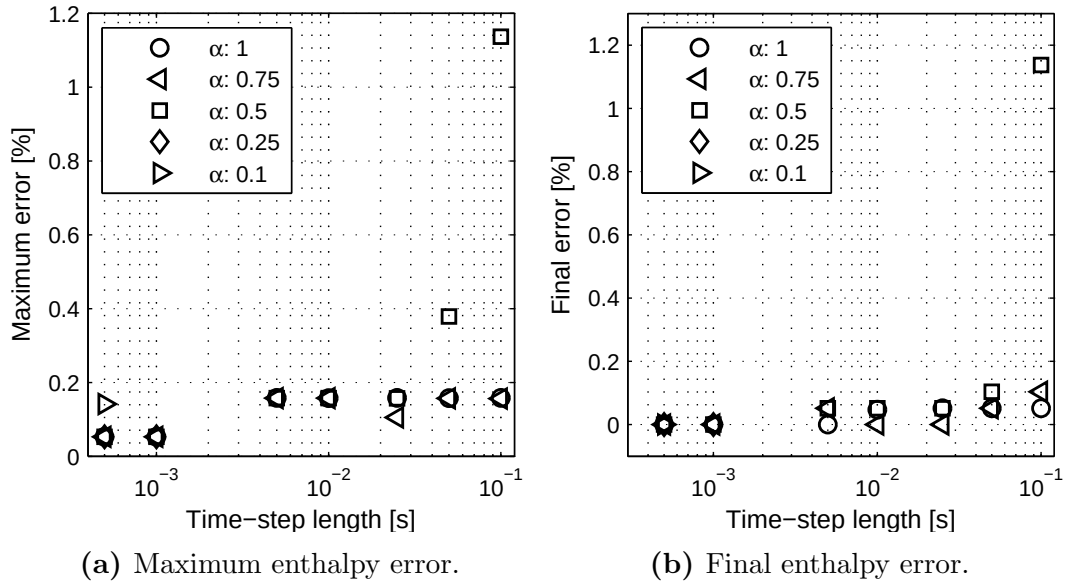


Figure 5.14: The maximum and final enthalpy errors for different combinations of integration weighting factor and time step length. (Energy case)

5.4 Low and intermediate pressure cases

After determining the effects of the time step length and integration scheme have on the accuracy of the rate method, the method was also evaluated with the network initial conditions set to two additional pressure levels. This was done to evaluate the accuracy of the RFES at different points in the range of pressures where the method is valid. An intermediate pressure was chosen at 3.1 MPa and a low pressure was chosen at 0.1 MPa. The intermediate pressure was chosen to correspond with the pressure point where the maximum error was observed for the vapour enthalpy derivative in Fig. 4.8. It also corresponds somewhat with the pressure typically observed at the inlet of the intermediate pressure turbine in a typical three-stage Rankine cycle power plant. This was done to determine the effect of a large gradient error on the accuracy of the RFES.

A mass sink transient was done in both the intermediate and low pressure cases. The simulation was set up in the same manner as for the reference case. A mass sink was activated in node 3 at 0.5 seconds and shut off at 1 second. The size of the mass sink was chosen so that the pressure in node 3 dropped by at least 50-60% of the original node pressure by the time the transient terminated at 1 second.

Based on the findings regarding the error for different time step lengths and integration schemes considered in Sections 5.2 and 5.3, a combination of a fully implicit integration scheme and 0.05 second time step length was chosen for the intermediate and low pressure simulations. These input variables were chosen as they allowed for reasonable accuracy and fast solution time. As with the previous cases, only the error values for node 3 is given as these represent the largest error values in the network.

Table 5.2: Maximum and final errors for the properties under consideration at 3.1 MPa.

Error	Pressure [%]	Temperature [%]	Density [%]	Enthalpy [%]
Maximum	0.19	1.22	0.15	0.053
Final	0.07	1.18	0.15	0.01

Table 5.3: Maximum and final errors for the properties under consideration at 0.1 MPa.

Error	Pressure [%]	Temperature [%]	Density [%]	Enthalpy [%]
Maximum	0.52	1.35	0.70	0.07
Final	0.09	1.24	0.70	0.01

The results shown in Tables 5.2 and 5.3 show good agreement with the temperature in both cases representing the largest error of slightly larger than 1%. The rate method was therefore also shown to be accurate at intermediate and low pressures. This was generally expected, as the constitutive parts of the rate method exhibited good accuracy over the entire pressure range over which it was defined. The effect of the large error in the gradient of the vapour enthalpy derivative also proved to be insignificant in the case of 3.1 MPa.

5.5 Summary

This chapter discussed the level of agreement achieved between the two EOS methods implemented in the transient network model developed in EES. The network model was solved with the IAPWS-95 and rate formulations of the equation of state respectively for each case under consideration. The agreement of the solutions delivered by the rate method compared with the IAPWS-95 equation of state solutions was evaluated at various integration time step lengths, integration weighting factors and for different types of transient phenomena. The rate method was also evaluated at different pressure points to evaluate the level of agreement of the solution methods over a range of pressures.

For all the cases simulated in this chapter, the rate method solutions could be made to deliver an agreement of less than one percent difference for the property values under consideration. Based on this, the second and third goals defined in Chapter 1 was considered achieved.

The following chapter will draw overarching conclusions regarding all the findings of this study, and provides certain recommendations for further work with regards to the RFES based on the mentioned conclusions.

Chapter 6

Conclusions and recommendations

The goal of this study was to implement the rate formulation of the equation of state for the homogeneous equilibrium model in a T-F system simulation model. This meant that the pressure rate equation itself, as well as the additional components that constitute the rate approach had to be correctly implemented. This implementation was done according to the methodology described in the preceding chapters. This final chapter will draw general conclusions from the results generated during the study, and also briefly highlight how the work done for this study may be used as a starting point for subsequent studies involving more complex problems.

6.1 Conclusions

The following general conclusions may be highlighted from the study:

1. The thermodynamic property approximation functions that were implemented in EES proved to be accurate for the saturation conditions simulated in this study. Additional testing will however be required to evaluate its accuracy when simulating systems at sub-cooled or superheated conditions, as this was not included in the scope of this study. The functions were simple to implement in EES (not quantified) and provided sufficiently accurate values for all saturation thermodynamic properties required.
2. The pressure derivatives of the saturation thermodynamic property values were seen to be less accurate than the approximation functions themselves. Some large outliers were observed in terms of the accuracy, but these were investigated and the reason for the larger than average errors could be quantified. Furthermore, the larger degree of inaccuracy did not significantly contribute to inaccuracy of the rate method when implemented in the transient network simulation. The accuracy of the rate method at very small time steps showed that when integration related errors are minimised, the solutions converge to the IAPWS-95 solution. If the gradients were not accurate, this would not have been the case.
3. The rate formulation of the equation of state for the HEM, which combines the functions mentioned above with a rate equation to determine system pressure, was implemented in EES. The formulation was incorporated in a transient pipe and reservoir network simulation model and used to solve the model for a variety of transients and initial conditions.

The solutions of the model using the rate method were compared with solutions for the model generated by the IAPWS-95 EOS, which represents the currently accepted standard for EOS formulations. Because a sufficient level of agreement was obtained between the two solution methods, the implementation of the rate formulation of the equation of state was deemed successful.

6.2 Recommendations

The recommendations based on the findings of this study are the following:

- The rate method has been shown to show acceptable agreement with accepted EOS formulations when incorporated in simplified theoretical two-phase flow simulation mode. Subsequent studies may be based on this theoretical work by implementing the rate method in a transient model that simulates a real world process such as a loss of coolant or pipe break accident where rapid transients occur. These types of physical processes are experimentally realisable and may therefore be used to generate empirical data with which to validate models based on the RFES.
- The evaluation of the numerical efficiency, e.g. calculation time, of the rate method when compared with an algebraic EOS was not in the scope of this study. EES uses a variant of Newton's method to solve the system of equations that represents the model under consideration. This solver simply solves the entire the system of equations simultaneously for each time step before moving on to the next time step. This means that as long as the equations are correctly formulated, the EES solver will solve the system of equations to a specified tolerance. Because of this, EES was not suited to evaluate the numerical efficiency implications of using the rate method versus the algebraic method. A model with an alternate numerical solver, perhaps based on a Runge-Kutta type solver, may therefore be programmed in a different code to evaluate the numerical efficiency of the RFES.
- The RFES was implemented in this study in the development of a homogeneous equilibrium two-phase flow model. This model represents the largest mathematical simplification of actual two-phase flow processes. As the rate method was successfully implemented for this simplified equilibrium two-phase flow model, a next step may be to expand the model to account for non-equilibrium conditions. The non-equilibrium rate equations that were identified in literature may then be used to solve for system pressure, allowing for the investigation of chosen non-equilibrium considerations.

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Appendix A

Rate form derivation (HEM)

The rate form of the equation of state for homogeneous equilibrium two-phase fluid is derived in the following manner for intensive properties.

For a two-phase homogeneous mixture the following is defined:

$$\nu = x\nu_g + (1 - x)\nu_f \quad (\text{A.1})$$

$$h = xh_g + (1 - x)h_f \quad (\text{A.2})$$

where h is the specific enthalpy, and ν the specific volume. The rate of change of pressure is related to the rates of change in density and enthalpy by the following:

$$\frac{dp}{dt} = G_1(p, x) \frac{d\rho}{dt} + G_2(p, x) \frac{dh}{dt} \quad (\text{A.3})$$

The values of $\frac{d\rho}{dt}$ and $\frac{dh}{dt}$ are available from the mass and energy conservation equations. To obtain $G_2(p, x)$, ρ (or ν) is kept constant. Differentiating eq. (A.2):

$$\begin{aligned} \frac{dh}{dt} &= \left(\frac{\partial h}{\partial p} \right)_\rho \frac{dp}{dt} = \left[x \frac{\partial h_g}{\partial p} + h_g \frac{\partial x}{\partial p} + \frac{\partial h_f}{\partial p} - x \frac{\partial h_f}{\partial p} - h_f \frac{\partial x}{\partial p} \right] \frac{dp}{dt} \\ &= \left[x \frac{\partial h_g}{\partial p} + (1 - x) \frac{\partial h_f}{\partial p} + \frac{\partial x}{\partial p} (h_g - h_f) \right] \frac{dp}{dt} \end{aligned} \quad (\text{A.4})$$

When ρ is held constant, there is no change of density with changing pressure. Therefore the derivative of eq. (A.1) is zero when ρ is held constant:

$$\frac{\partial \nu}{\partial p} = \left[x \frac{\partial \nu_g}{\partial p} + \nu_g \frac{\partial x}{\partial p} + \frac{\partial \nu_f}{\partial p} - x \frac{\partial \nu_f}{\partial p} - \nu_f \frac{\partial x}{\partial p} \right] = 0$$

Rewriting in terms of $\frac{\partial x}{\partial p}$:

$$\frac{\partial x}{\partial p} = -\frac{1}{(\nu_g - \nu_f)} \left[x \frac{\partial \nu_g}{\partial p} + (1 - x) \frac{\partial \nu_f}{\partial p} \right] \quad (\text{A.5})$$

Substituting eq. (A.5) in eq. (A.4):

$$\frac{dh}{dt} = \left[\left(x \frac{\partial h_g}{\partial p} + (1 - x) \frac{\partial h_f}{\partial p} \right) - \frac{(h_g - h_f)}{(\nu_g - \nu_f)} \left(x \frac{\partial \nu_g}{\partial p} + (1 - x) \frac{\partial \nu_f}{\partial p} \right) \right] \frac{dp}{dt} \quad (\text{A.6})$$

Multiplying by $(\nu_g - \nu_f)$:

$$(\nu_g - \nu_f) \frac{dh}{dt} = \left[(\nu_g - \nu_f) \left(x \frac{\partial h_g}{\partial p} + (1 - x) \frac{\partial h_f}{\partial p} \right) - (h_g - h_f) \left(x \frac{\partial \nu_g}{\partial p} + (1 - x) \frac{\partial \nu_f}{\partial p} \right) \right] \frac{dp}{dt} \quad (\text{A.7})$$

Rewriting in terms of $\frac{dp}{dt}$:

$$\begin{aligned} \frac{dp}{dt} &= \frac{(\nu_g - \nu_f)}{\left[x \frac{\partial h_g}{\partial p} + (1 - x) \frac{\partial h_f}{\partial p} \right] (\nu_g - \nu_f) - \left[x \frac{\partial \nu_g}{\partial p} + (1 - x) \frac{\partial \nu_f}{\partial p} \right] (h_g - h_f)} \frac{dh}{dt} \\ &= G_2(P, x) \frac{dh}{dt} \end{aligned} \quad (\text{A.8})$$

This gives the pressure rate response due to an enthalpy change, holding ρ constant. To determine $G_1(p, x)$, the above is repeated with h held constant. This gives:

$$\frac{dp}{dt} = \frac{-(h_g - h_f)}{\left[x \frac{\partial h_g}{\partial p} + (1 - x) \frac{\partial h_f}{\partial p} \right] (\nu_g - \nu_f) - \left[x \frac{\partial \nu_g}{\partial p} + (1 - x) \frac{\partial \nu_f}{\partial p} \right] (h_g - h_f)} \frac{d\nu}{dt} \quad (\text{A.9})$$

Using the following:

$$\begin{aligned}\frac{d\nu}{dt} &= -\frac{1}{\rho^2} \frac{d\rho}{dt} \\ &= -[x\nu_g + (1-x)\nu_f]^2 \frac{d\rho}{dt}\end{aligned}\tag{A.10}$$

eq. (A.9) can be rewritten as

$$\begin{aligned}\frac{dp}{dt} &= \frac{(h_g - h_f)[x\nu_g + (1-x)\nu_f]^2}{\left[x\frac{\partial h_g}{\partial p} + (1-x)\frac{\partial h_f}{\partial p}\right](\nu_g - \nu_f) - \left[x\frac{\partial \nu_g}{\partial p} + (1-x)\frac{\partial \nu_f}{\partial p}\right](h_g - h_f)} \frac{d\rho}{dt} \\ &= G_1(P, x) \frac{d\rho}{dt}\end{aligned}\tag{A.11}$$

The functions $G_1(p, x)$ and $G_2(p, x)$ depend only on the local saturation fluid properties and their slopes at the local pressure. By combining eq. (A.8) and eq. (A.11), the total pressure rate response for varying ρ and h is determined.

Appendix B

Conservation equations (HEM)

The full derivation for the conservation equations governing mass, momentum and energy is given as applicable to homogeneous equilibrium two-phase flow. All conservation equations used in this study are based on those derived by [Rousseau \(2012b\)](#).

B.1 Conservation of Mass

The integral form of the mass conservation equation for a finite control volume is given by:

$$\frac{\partial}{\partial t} \left(\iiint \rho dV \right) + \oiint \rho \bar{V} \cdot \bar{dA} = 0 \quad (\text{B.1})$$

with V the volume and V the velocity relative to the control volume. If applied to the infinitely small one-dimensional control volume given in Fig. 3.1, the rate of change of mass inside the control volume can be written as:

$$\begin{aligned} \frac{\partial}{\partial t} \left(\iiint \rho dV \right) &= \frac{\partial}{\partial t} (\rho A d\ell) \\ &= \frac{\partial \rho}{\partial t} A d\ell \end{aligned} \quad (\text{B.2})$$

and the nett mass flow rate out of the the control volume can be written as:

$$\begin{aligned} \oiint \rho \bar{V} \cdot \bar{dA} &= \left(\rho V A + \frac{\partial}{\partial \ell} (\rho V A) d\ell \right) - \rho V A \\ &= \frac{\partial}{\partial \ell} (\rho V A) d\ell \end{aligned} \quad (\text{B.3})$$

Substituting eqs. (B.2) and (B.3) in to eq. (B.1):

$$\frac{\partial \rho}{\partial t} + \frac{1}{A} \frac{\partial}{\partial \ell} (\rho V A) = 0 \quad (\text{B.4})$$

Integrating with respect to $d\ell$ for a control volume with finite length L , average cross-section A , and average density

$$\begin{aligned} A \frac{\partial \rho}{\partial t} \int_i^e d\ell + \int_i^e \frac{\partial}{\partial \ell} (\rho V A) d\ell &= 0 \\ A(\ell_e - \ell_i) \frac{\partial \rho}{\partial t} + (\rho_e V_e A_e - \rho_i V_i A_i) &= 0 \end{aligned} \quad (\text{B.5})$$

Appropriate substitution and integration leads to the following equation for mass conservation:

$$AL \frac{\partial \rho}{\partial t} + (\rho_e V_e A_e - \rho_i V_i A_i) = 0 \quad (\text{B.6})$$

where the symbols without subscripts refer to values that have been averaged over the control volume, and e and i refer to the outlet and inlet of the control volume respectively. By using the definition of mass flow rate ($\dot{m} = \rho V A$), eq. (B.6) can be rewritten as:

$$V \frac{\partial \rho}{\partial t} + \dot{m}_e - \dot{m}_i = 0 \quad (\text{B.7})$$

which is the desired differential form of the mass conservation equation.

B.2 Conservation of Momentum

The integral form of the linear momentum conservation equation for an inertial control volume is given by:

$$\oint \tau d\bar{A} + \iiint \bar{B} \rho dV = \frac{\partial}{\partial t} \left(\iiint \bar{V} \rho dV \right) + \oint \bar{V} (\rho \bar{V} \cdot d\bar{A}) \quad (\text{B.8})$$

For the infinitesimal control volume in Fig. 3.1, the surface force term acting in the flow direction may be written as:

$$\begin{aligned}
 \sum \tau \overline{dA} &= \left(pA - \left(p + \frac{\partial p}{\partial \ell} d\ell \right) \left(A + \frac{\partial A}{\partial \ell} d\ell \right) \right) \\
 &+ \left(\frac{1}{2} \left(p + \left(p + \frac{\partial p}{\partial \ell} d\ell \right) \right) \left(\left(A + \frac{\partial A}{\partial \ell} \right) - A \right) \right) \\
 &- \left(\frac{\Delta P_{0L}}{L} A d\ell \right) = - \left(\frac{\partial p}{\partial \ell} + \frac{\Delta P_{0L}}{L} \right) A d\ell
 \end{aligned} \tag{B.9}$$

where $\frac{\Delta P_{0L}}{L}$ represents the total pressure drop due to frictional and other losses per unit length and per unit volume. The body force term may be written as:

$$B \rho dV = -\rho g \frac{\partial z}{\partial L} A d\ell \tag{B.10}$$

The rate of change of momentum in the control volume is:

$$\frac{\partial}{\partial t} (V \rho dV) = \frac{\partial}{\partial t} (\rho V) A d\ell \tag{B.11}$$

The net outflow of momentum from the control volume is:

$$\begin{aligned}
 \sum \bar{V} (\rho \bar{V} \cdot \bar{dA}) &= \left(V + \frac{\partial V}{\partial \ell} d\ell \right) \left(\rho V A + \frac{\partial}{\partial \ell} (\rho V A) d\ell \right) - V (\rho V A) \\
 &= \frac{\partial}{\partial \ell} (V (\rho V A)) d\ell
 \end{aligned} \tag{B.12}$$

Substituting eqs. (B.9) - (B.9) in to eq. (B.8), the differential form may be written as:

$$\frac{\partial}{\partial t} (\rho V) + \frac{1}{A} \frac{\partial}{\partial \ell} (\rho V^2 A) + \frac{\partial p}{\partial \ell} + \rho g \frac{\partial z}{\partial \ell} + \frac{\Delta P_{0L}}{L} = 0 \tag{B.13}$$

Appropriate substitution, simplification and integration leads to the final form of the momentum conservation equation:

The first two terms may be rewritten in the following manner:

$$\begin{aligned}
 \frac{\partial}{\partial t}(\rho V) + \frac{1}{A} \frac{\partial}{\partial \ell}(\rho V^2 A) &= \rho \frac{\partial V}{\partial t} + \rho V \frac{\partial V}{\partial \ell} + V \left(\frac{\partial \rho}{\partial t} + \frac{1}{A} \frac{\partial}{\partial \ell}(\rho V A) \right) \\
 &= \rho \frac{\partial V}{\partial t} + \rho V \frac{\partial V}{\partial \ell}
 \end{aligned} \tag{B.14}$$

This substituting back in to eq. (B.13):

$$\rho \frac{\partial V}{\partial t} + \rho V \frac{\partial V}{\partial \ell} + \frac{\partial p}{\partial \ell} + \rho g \frac{\partial z}{\partial \ell} + \frac{\Delta P_{0L}}{L} = 0 \tag{B.15}$$

Manipulating eq. (B.15) as follows:

$$\rho \frac{\partial V}{\partial t} + \rho V \frac{\partial V}{\partial \ell} + \frac{\partial}{\partial \ell} \left(p + \frac{1}{2} \rho V^2 \right) - \frac{\partial}{\partial \ell} \left(\frac{1}{2} \rho V^2 \right) + \rho g \frac{\partial z}{\partial \ell} + \frac{\Delta P_{0L}}{L} = 0 \tag{B.16}$$

Defining total pressure as:

$$p_0 = p + \frac{1}{2} \rho V^2 \tag{B.17}$$

eq. (B.17) becomes:

$$\rho \frac{\partial V}{\partial t} + \rho V \frac{\partial V}{\partial \ell} + \frac{\partial p_0}{\partial \ell} - \frac{\partial}{\partial \ell} \left(\frac{1}{2} \rho V^2 \right) + \rho g \frac{\partial z}{\partial \ell} + \frac{\Delta P_{0L}}{L} = 0 \tag{B.18}$$

Integrating over a control volume with a finite length, L:

$$\begin{aligned}
 \rho L \frac{\partial V}{\partial t} + (p_{0e} - p_{0i}) + \frac{1}{2} (\rho_e V_e + \rho_i V_i) (V_e - V_i) \\
 - \frac{1}{2} (\rho_e V_e^2 - \rho_i V_i^2) + \rho g (z_e - z_i) + \Delta p_{0L} = 0
 \end{aligned} \tag{B.19}$$

This equation can be simplified by the following:

$$(\rho_e V_e + \rho_i V_i)(V_e - V_i) - (\rho_e V_e^2 - \rho_i V_i^2) = -V_i V_e (\rho_e - \rho_i) \quad (\text{B.20})$$

Finally, eq. (B.19) becomes:

$$\rho L \frac{\partial V}{\partial t} + (p_{0e} - p_{0i}) - \frac{1}{2} V_i V_e (\rho_e - \rho_i) + \rho g (z_e - z_i) + \Delta p_{0L} = 0 \quad (\text{B.21})$$

which is the desired differential form of the momentum conservation equation.

B.3 Conservation of Energy

The integral form of the energy conservation equation for a finite control volume is given by:

$$\begin{aligned} \dot{Q} + \dot{W} = & \frac{\partial}{\partial t} \left(\iiint \left(u + \frac{1}{2} V^2 + gz \right) \rho dV \right) \\ & + \oint \left(h + \frac{1}{2} V^2 + gz \right) \rho \bar{V} \cdot \bar{dA} \end{aligned} \quad (\text{B.22})$$

The variable $\dot{Q}$ denotes the total rate of heat transfer to the fluid and $\dot{W}$ the total rate of work done on the fluid. The rate of change of energy within the control volume may be written as:

$$\begin{aligned} & \frac{\partial}{\partial t} \left(\iiint \left(u + \frac{1}{2} V^2 + gz \right) \rho dV \right) \\ & = \frac{\partial}{\partial t} \left(\rho \left(u + \frac{1}{2} V^2 + gz \right) A d\ell \right) \end{aligned} \quad (\text{B.23})$$

The net outflow of energy from the control volume is:

$$\begin{aligned} \oint \left(h + \frac{1}{2} V^2 + gz \right) \rho \bar{V} \cdot \bar{dA} & = E_1 \left(A + \frac{\partial A}{\partial \ell} \partial \ell \right) - \left(\left(h + \frac{1}{2} V^2 + gz \right) \rho V \right) (A) \\ & = \frac{\partial}{\partial \ell} \left(\left(h + \frac{1}{2} V^2 + gz \right) \rho V A \right) d\ell \end{aligned} \quad (\text{B.24})$$

with:

$$E_1 = \left(\left(h + \frac{1}{2}V^2 + gz \right) \rho V + \frac{\partial}{\partial \ell} \left(\left(h + \frac{1}{2}V^2 + gz \right) \rho V \right) d\ell \right)$$

By substituting eqs. (B.23) and (B.24) in eq. (B.22), and by dividing by $A d\ell$ to cast the energy conservation on a per unit volume basis the following is obtained:

$$\delta \dot{q} + \delta \dot{w} = \frac{\partial}{\partial t} \left(\rho \left(u + \frac{1}{2}V^2 + gz \right) \right) + \frac{1}{A} \frac{\partial}{\partial \ell} \left(\rho V A \left(h + \frac{1}{2}V^2 + gz \right) \right) \quad (\text{B.25})$$

with $\dot{q}$ the heat added to the flow per unit volume and $\dot{w}$ the work done on the flow per unit volume. The fundamental definition for specific internal energy is given as:

$$u = h - \frac{p}{\rho} \quad (\text{B.26})$$

By using this definition, the first term in the right hand side of eq. (B.25) can be rewritten as:

$$\frac{\partial}{\partial t} \left(\rho \left(u + \frac{1}{2}V^2 + gz \right) \right) = \frac{\partial}{\partial t} \left(\rho \left(h - \frac{p}{\rho} + \frac{1}{2}V^2 + gz \right) \right) \quad (\text{B.27})$$

Substituting eq. (B.27) back in to eq. (B.25):

$$\delta \dot{q} + \delta \dot{w} = \frac{\partial}{\partial t} \left(\rho \left(h + \frac{1}{2}V^2 - \frac{p}{\rho} + gz \right) \right) + \frac{1}{A} \frac{\partial}{\partial \ell} \left(\rho V A \left(h + \frac{1}{2}V^2 + gz \right) \right) \quad (\text{B.28})$$

Since $\frac{\partial}{\partial t}(gz) = 0$ for a stationary control volume, and by definition total enthalpy is given as $h_0 = h + \frac{1}{2}V^2$, eq. (B.28) can be rewritten as:

$$\delta \dot{q} + \delta \dot{w} = \frac{\partial}{\partial t} \left(\rho h_0 - p \right) + \frac{1}{A} \frac{\partial}{\partial \ell} \left(\rho V A \left(h_0 + gz \right) \right) \quad (\text{B.29})$$

Integrating for a control volume with finite length, L and average cross-sectional area, A gives the following equation:

$$\dot{Q} + \dot{W} = \mathcal{V} \frac{\partial}{\partial t} (\rho h_0 - p) + \dot{m}_e h_{0e} - \dot{m}_i h_{0i} + \dot{m}_e g z_e - \dot{m}_i g z_i \quad (\text{B.30})$$

which is the desired differential form of the energy conservation equation.

Appendix C

EES Programs

The EES models used to solve the transient pipe and reservoir network are given in this appendix. EES makes it somewhat difficult to export the input file in a user friendly manner. To ensure no information is distorted when converting the EES code to another format, the EES model code is given in this appendix as a series of images. These images were taken from EES exactly as they were coded and therefore provide the reader with a source of reference when the EES model is discussed in [Section 4.3](#).

C.1 Steady state network model: Algebraic EOS

```
"!Transient network simulation"

"!Section 1: Constants"

F$ = 'Steam_IAPWS'                                "Working fluid Equation of state selection"
g=9.81 [m/s^2]                                     "Gravitational acceleration"
x_f = 0                                             "Saturated liquid quality"
x_g = 1                                             "Saturated vapour quality"

"!Section 2: Connectivity"

nodes=4                                             "Number of nodes in network"
elements=5                                         "Number of elements in network"

Duplicate n=1,nodes
  Duplicate e=1,elements
    c[n,e]=lookup('Connectivity',n,e)             "Pipe connectivity lookup from lookup table"
  End
End

Duplicate e=1,elements
  n_i[e]=sum(IF(c[n,e],0,n,0,0),n=1,nodes) "Element inlet connection"
  n_e[e]=sum(IF(c[n,e],0,0,0,n),n=1,nodes) "Element outlet connection"
End

"!Section 3: Geometry"

"!Nodes: Node volumes and elevations defined"

Vol_n[1]=0.5
z[1]=0

Vol_n[2]=0.05
z[2]=0

Vol_n[3]=0.1
z[3]=0

Vol_n[4]=0.3
z[4]=0

V_n=0 "Velocity in all nodes assumed to be zero"

Duplicate n=1,nodes
  Vol[n]=Vol_n[n]+0.5*(sum(abs(c[n,e])*Vol_e[e],e=1,elements)) "Node volume calculation based on elements connected"
End

"!Elements: Inlet areas, outlet areas and pipe lengths defined"

A_i[1]=0.0025
A_e[1]=0.0025
L[1]=5.0

A_i[2]=0.0025
A_e[2]=0.0025
L[2]=10.0

A_i[3]=0.0025
```

```

A_e[3]=0.0025
L[3]=1.0

A_i[4]=0.0025
A_e[4]=0.0025
L[4]=15.0

A_i[5]=0.0025
A_e[5]=0.0025
L[5]=10.0

Duplicate e=1,elements
  A_bar[e]=0.5*(A_i[e]+A_e[e])           "Average pipe area"
  Vol_e[e]=A_bar[e]*L[e]                 "Pipe volume"
  z_i[e]=z[n_i[e]]                       "Pipe inlet elevation"
  z_e[e]=z[n_e[e]]                       "Pipe outlet elevation"
  k_L[e]=1e7                             "Pipe friction factor"
End

"Section 4: Boundary values for mass source terms"

duplicate n=1,nodes

CALL ENTHALPY_LIQ(T[n], P[n]/1e3, P[n]/1e3: h_0sf1[n], h_0sf[n])
CALL ENTHALPY_VAP(T[n], T[n], P[n]/1e3: h_0sg1[n], h_0sg[n])

h_0s[n] = x[n] * h_0sg[n] + (1 - x[n]) * h_0sf[n] "Mass source enthalpy based on node mass quality"

end

{h_0s[1]=ENTHALPY(F$,x=x[1],P=p[1])
h_0s[2]=ENTHALPY(F$,x=x[2],P=p[2])
h_0s[3]=ENTHALPY(F$,x=x[3],P=p[3])
h_0s[4]=ENTHALPY(F$,x=x[4],P=p[4])}

"Section 5: Timewise integration factors"
deltatime=0.05           "Time step length"
alpha=1                  "Integration factor"
alpha_c=alpha            "Integration factor for continuity equation"
alpha_m=alpha            "Integration factor for momentum equation"
alpha_e=alpha            "Integration factor for energy equation"
Row=1+time/deltatime     "Row number in parametric table"

"Section 6: Element calculations"

Duplicate e=1,elements

  "Assign values at inlet and outlet"
  p_0i[e]=p_0[n_i[e]]
  p_0e[e]=p_0[n_e[e]]
  h_0i[e]=IF(m_dot[e],0.0,h_0e[e]+g*z_e[e]-1/m_dot[e]*Q_e[e]-g*z_i[e],h_0[n_i[e]],h_0[n_i[e]])
  h_0e[e]=IF(m_dot[e],0.0,h_0[n_e[e]],h_0[n_e[e]],h_0i[e]+g*z_i[e]+1/m_dot[e]*Q_e[e]-g*z_e[e])

  CALL SATTEMP(p_0i[e]/1e3:T_i[e])
  CALL ENTHALPY_LIQ(T_i[e], p_0i[e]/1e3, p_0i[e]/1e3: h_0if1[e], h_0if[e])
  CALL ENTHALPY_VAP(T_i[e], T_i[e], p_0i[e]/1e3: h_0ig1[e], h_0ig[e])
  h_0i[e] = x_i[e] * h_0ig[e] + (1 - x_i[e]) * h_0if[e]

```

```

CALL DENSITY_LIQ(T_i[e], p_0i[e]/1e3, p_0i[e]/1e3: rho_fi1[e], rho_fi[e])
CALL DENSITY_VAP(T_i[e], T_i[e], p_0i[e]/1e3: rho_gi1[e], rho_gi[e])
v_fi[e] = 1 / rho_fi[e]
v_gi[e] = 1 / rho_gi[e]

1 / rho_i[e] = x_i[e] * v_gi[e] + (1 - x_i[e]) * v_fi[e]

CALL SATTEMP(p_0e[e]/1e3: T_e[e])
CALL ENTHALPY_LIQ(T_e[e], p_0e[e]/1e3, p_0e[e]/1e3: h_0efl[e], h_0eff[e])
CALL ENTHALPY_VAP(T_e[e], T_e[e], p_0e[e]/1e3: h_0eg1[e], h_0eg[e])
h_0e[e] = x_e[e] * h_0eg[e] + (1 - x_e[e]) * h_0efl[e]
CALL DENSITY_LIQ(T_e[e], p_0e[e]/1e3, p_0e[e]/1e3: rho_fe1[e], rho_fe[e])
CALL DENSITY_VAP(T_e[e], T_e[e], p_0e[e]/1e3: rho_ge1[e], rho_ge[e])
v_fe[e] = 1 / rho_fe[e]
v_ge[e] = 1 / rho_ge[e]

1 / rho_e[e] = x_e[e] * v_ge[e] + (1 - x_e[e]) * v_fe[e]

```

```

{rho_i[e]=DENSITY(F$,H=h_0i[e],P=p_0i[e])}
{rho_e[e]=DENSITY(F$,H=h_0e[e],P=p_0e[e])}

```

"Calculate average values"

```

p_bar_0[e]=Average(p_0i[e],p_0e[e])
h_bar_0[e]=Average(h_0i[e],h_0e[e])
h_bar[e]=h_bar_0[e]-1e-3*0.5*V_bar[e]^2
rho_bar[e]=Average(rho_i[e],rho_e[e])
V_bar[e]=ABS(m_dot[e])/(rho_bar[e]*A_bar[e])

```

"Element heat load"

Q_e[e]=0.0

"No heat energy is added or removed in the elements"

"!Section 7: Momentum conservation calculations"

"Calculate momentum conservation source term"

```

S_m[e]= (A_bar[e] / L[e]) * (0.5 * V_bar[e] ^ 2 * (rho_e[e] - rho_i[e]) - 1e3 * (p_0e[e] - p_0i[e]) - rho_bar[e] * g * (z_e[e] - z_i[e]) - k_L[e] * (ABS(m_dot[e]) * m_dot[e]) / rho_bar[e] + L[e] * A_e[e] * drhodt_bar[e])

```

"Steady state"

S_m[e]=0

drhodt_bar[e]=0

"Transient integration for element mass flow rate"

```

{S_m_old[e]=tablevalue(Row-1,43+e)}
{m_dot_old[e]=tablevalue(Row-1,25+e)}
{rho_bar_old[e]=tablevalue(Row-1,30+e)}
drhodt_bar[e]=(rho_bar[e]-rho_bar_old[e])/deltatime
dmdotdt[e]=alpha_m*S_m[e]+(1-alpha_m)*S_m_old[e]
m_dot[e]=m_dot_old[e]+dmdotdt[e]*deltatime}

```

End

"!Section 8: Node calculations"

Duplicate n=1,nodes

"Calculate mass conservation source term value"

```

S_c[n]=1/Vol[n]*(SUM(c[n,e]*m_dot[e],e=1,elements)+m_dot_s[n])

```

```
"Steady state"
S_c[n]=0
drhodt[n]=0
```

```
"Transient integration for node density"
{S_c_old[n]=tablevalue(Row-1,35+n)
rho_old[n]=tablevalue(Row-1,5+n)
drhodt[n]=alpha_c*S_c[n]+(1-alpha_c)*S_c_old[n]
rho[n]=rho_old[n]+drhodt[n]*deltatime}
```

```
"Calculate energy conservation source term value"
S_e[n]=1/(rho[n]*Vol[n])*(SUM(IF(c[n,e],0,0,0,0,m_dot[e]*(h_0e[e]+1e-3*g*z_e[e])),e=1,elements)-SUM(IF(c[n,e],0,m_dot[e]*(h_0[e]+1e-3*g*z_e[e]),0,0,0,0),e=1, elements)+IF(m_dot_s[n],0,0,m_dot_s[n]*h_0[n],0,0,m_dot_s[n]*h_0s[n])+Q_n[n]+Vol[n]*(dpdt[n]-h_0[n]*drhodt[n]))
```

```
"Steady state"
S_e[n]=0
dpdt[n]=0
```

```
"Transient integration for node total enthalpy"
{S_e_old[n]=tablevalue(Row-1,39+n)
p_old[n]=tablevalue(Row-1,13+n)
h_0_old[n]=tablevalue(Row-1,21+n)
dpdt[n]=(p[n]-p_old[n])/deltatime
dh0dt[n]=alpha_e*S_e[n]+(1-alpha_e)*S_e_old[n]
h_0[n]=h_0_old[n]+dh0dt[n]*deltatime}
```

```
"Calculate node parameters"
h[n]=h_0[n]-0.5*V_n^2
p[n]=p_0[n]
```

```
{v_f[n]=Volume(F$,P=P[n],x=x_f)
v_g[n]=Volume(F$,P=P[n],x=x_g)
h_f[n]=Enthalpy(F$,P=P[n],x=x_f)
h_g[n]=Enthalpy(F$,P=P[n],x=x_g)}
```

```
CALL DENSITY_LIQ(T[n], P[n]/1e3, P[n]/1e3: rho_f1[n], rho_f[n])
CALL DENSITY_VAP(T[n], T[n], P[n]/1e3: rho_g1[n], rho_g[n])
CALL ENTHALPY_LIQ(T[n], P[n]/1e3, P[n]/1e3: h_f1[n], h_f[n])
CALL ENTHALPY_VAP(T[n], T[n], P[n]/1e3: h_g1[n], h_g[n])
```

```
v_f[n] = 1 / rho_f[n]
v_g[n] = 1 / rho_g[n]
rho[n] = 1 / v[n]
v[n] = x[n]*v_g[n] + (1 - x[n])*v_f[n]
```

```
"Steady state p and T"
p[n]=p_APWS[n]
T[n]=T_sat[n]
```

```
"Section 9: Rate form of the equation of state"
```

```
{CALL DELTAH_LIQ(P[n]/1e3: deltah_f[n])
CALL DELTAH_VAP(P[n]/1e3: deltah_g[n])
CALL DELTAV_LIQ(P[n]/1e3: deltavu_f[n])
CALL DELTAV_VAP(P[n]/1e3: deltavu_g[n])
```

```
G_1[n] = ((h_g[n] - h_f[n]) * (x[n] * v_g[n] + (1 - x[n]) * v_f[n])^2) / ((x[n] * deltah_g[n] + (1 - x[n]) * deltah_f[n]) * (v_g[n] - v_f[n]) - (x[n] * deltavu_g[n] + (1 - x[n]) * deltavu_f[n]) * (h_g[n] - h_f[n]))
G_2[n] = (v_g[n] - v_f[n]) / ((x[n] * deltah_g[n] + (1 - x[n]) * deltah_f[n]) * (v_g[n] - v_f[n]) - (x[n] * deltavu_g[n] + (1 - x[n]) * deltavu_f[n]) * (h_g[n] - h_f[n]))
```

```
"Steady state"
{S_g[n] = 0}

"Transient integration for node pressure"
S_g_old[n] = tablevalue(Row-1,52+n)
S_g[n] = (G_1[n] * drhodt[n]) + (G_2[n] * dh0dt[n])
dPgdt[n] = alpha_m * S_g[n] + (1 - alpha_m) * S_g_old[n]
P[n] = p_old[n] + (deltatime * dPgdt[n]) * 1e3

"Non-Equilibrium temperature tracking"
CALL DELTAT_SAT(P[n]/1e3:deltaT_s[n])

"Steady state"
{S_g_T[n] = 0}

"Transient integration for node temperature"
T_old[n]=tablevalue(Row-1,9+n)
S_g_old_T[n] = tablevalue(Row-1,56+n)
S_g_T[n] = dPgdt[n] * deltaT_s[n]
dTgdt[n] = alpha_m * S_g_T[n] + (1 - alpha_m) * S_g_old_T[n]
T[n] = T_old[n] + (deltatime * dTgdt[n])}

"!—Algebraic pressure and temperature—"

P_IAPWS[n] = Pressure(F$, h=h[n],v=v[n])
error_P[n] = ((P[n] - P_IAPWS[n]) / P_IAPWS[n]) * 100

T_sat[n]=T_sat(Steam_IAPWS,P=P[n])
error_T[n] = ((T[n] - T_sat[n]) / T_sat[n]) * 100

End
```

C.2 Transient network model: Algebraic EOS

```
"!Transient network simulation"

"!Section 1: Constants"

F$ = 'Steam_IAPWS'                                "Working fluid Equation of state selection"
g=9.81 [m/s^2]                                     "Gravitational acceleration"
x_f = 0                                             "Saturated liquid quality"
x_g = 1                                             "Saturated vapour quality"

"!Section 2: Connectivity"

nodes=4                                             "Number of nodes in network"
elements=5                                         "Number of elements in network"

Duplicate n=1,nodes
  Duplicate e=1,elements
    c[n,e]=lookup('Connectivity',n,e)             "Pipe connectivity lookup from lookup table"
  End
End

Duplicate e=1,elements
  n_i[e]=sum(IF(c[n,e],0,n,0,0),n=1,nodes) "Element inlet connection"
  n_e[e]=sum(IF(c[n,e],0,0,0,n),n=1,nodes) "Element outlet connection"
End

"!Section 3: Geometry"

"!Nodes: Node volumes and elevations defined"

Vol_n[1]=0.5
z[1]=0

Vol_n[2]=0.05
z[2]=0

Vol_n[3]=0.1
z[3]=0

Vol_n[4]=0.3
z[4]=0

V_n=0 "Velocity in all nodes assumed to be zero"

Duplicate n=1,nodes
  Vol[n]=Vol_n[n]+0.5*(sum(abs(c[n,e])*Vol_e[e],e=1,elements)) "Node volume calculation based on elements connected"
End

"!Elements: Inlet areas, outlet areas and pipe lengths defined"

A_i[1]=0.0025
A_e[1]=0.0025
L[1]=5.0

A_i[2]=0.0025
A_e[2]=0.0025
L[2]=10.0

A_i[3]=0.0025
```

```

A_e[3]=0.0025
L[3]=1.0

A_i[4]=0.0025
A_e[4]=0.0025
L[4]=15.0

A_i[5]=0.0025
A_e[5]=0.0025
L[5]=10.0

Duplicate e=1,elements
  A_bar[e]=0.5*(A_i[e]+A_e[e])           "Average pipe area"
  Vol_e[e]=A_bar[e]*L[e]                 "Pipe volume"
  z_i[e]=z[n_i[e]]                       "Pipe inlet elevation"
  z_e[e]=z[n_e[e]]                       "Pipe outlet elevation"
  k_L[e]=1e7                             "Pipe friction factor"
End

"!Section 4: Boundary values for mass source terms"

duplicate n=1,nodes

CALL ENTHALPY_LIQ(T[n], P[n]/1e3, P[n]/1e3: h_0sf1[n], h_0sf[n])
CALL ENTHALPY_VAP(T[n], T[n], P[n]/1e3: h_0sg1[n], h_0sg[n])

h_0s[n] = x[n] * h_0sg[n] + (1 - x[n]) * h_0sf[n] "Mass source enthalpy based on node mass quality"

end

{h_0s[1]=ENTHALPY(F$,x=x[1],P=p[1])
h_0s[2]=ENTHALPY(F$,x=x[2],P=p[2])
h_0s[3]=ENTHALPY(F$,x=x[3],P=p[3])
h_0s[4]=ENTHALPY(F$,x=x[4],P=p[4])}

"!Section 5: Timewise integration factors"
deltatime=0.05           "Time step length"
alpha=1                  "Integration factor"
alpha_c=alpha            "Integration factor for continuity equation"
alpha_m=alpha            "Integration factor for momentum equation"
alpha_e=alpha            "Integration factor for energy equation"
Row=1+time/deltatime     "Row number in parametric table"

"!Section 6: Element calculations"

Duplicate e=1,elements

  "Assign values at inlet and outlet"
  p_0i[e]=p_0[n_i[e]]
  p_0e[e]=p_0[n_e[e]]
  h_0i[e]=IF(m_dot[e],0.0,h_0e[e]+g*z_e[e]-1/m_dot[e]*Q_e[e]-g*z_i[e],h_0[n_i[e]],h_0[n_i[e]])
  h_0e[e]=IF(m_dot[e],0.0,h_0[n_e[e]],h_0[n_e[e]],h_0i[e]+g*z_i[e]+1/m_dot[e]*Q_e[e]-g*z_e[e])

  CALL SATTEMP(p_0i[e]/1e3:T_i[e])
  CALL ENTHALPY_LIQ(T_i[e], p_0i[e]/1e3, p_0i[e]/1e3: h_0if1[e], h_0if[e])
  CALL ENTHALPY_VAP(T_i[e], T_i[e], p_0i[e]/1e3: h_0ig1[e], h_0ig[e])
  h_0i[e] = x_i[e] * h_0ig[e] + (1 - x_i[e]) * h_0if[e]

```

```

CALL DENSITY_LIQ(T_i[e], p_0i[e]/1e3, p_0i[e]/1e3: rho_fi1[e], rho_fi[e])
CALL DENSITY_VAP(T_i[e], T_i[e], p_0i[e]/1e3: rho_gi1[e], rho_gi[e])
v_fi[e] = 1 / rho_fi[e]
v_gi[e] = 1 / rho_gi[e]

1 / rho_i[e] = x_i[e] * v_gi[e] + (1 - x_i[e]) * v_fi[e]

CALL SATTEMP(p_0e[e]/1e3: T_e[e])
CALL ENTHALPY_LIQ(T_e[e], p_0e[e]/1e3, p_0e[e]/1e3: h_0ef1[e], h_0ef[e])
CALL ENTHALPY_VAP(T_e[e], T_e[e], p_0e[e]/1e3: h_0eg1[e], h_0eg[e])
h_0e[e] = x_e[e] * h_0eg[e] + (1 - x_e[e]) * h_0ef[e]
CALL DENSITY_LIQ(T_e[e], p_0e[e]/1e3, p_0e[e]/1e3: rho_fe1[e], rho_fe[e])
CALL DENSITY_VAP(T_e[e], T_e[e], p_0e[e]/1e3: rho_ge1[e], rho_ge[e])
v_fe[e] = 1 / rho_fe[e]
v_ge[e] = 1 / rho_ge[e]

1 / rho_e[e] = x_e[e] * v_ge[e] + (1 - x_e[e]) * v_fe[e]

```

```

{rho_i[e]=DENSITY(F$,H=h_0i[e],P=p_0i[e])}
{rho_e[e]=DENSITY(F$,H=h_0e[e],P=p_0e[e])}

```

"Calculate average values"

```

p_bar_0[e]=Average(p_0i[e],p_0e[e])
h_bar_0[e]=Average(h_0i[e],h_0e[e])
h_bar[e]=h_bar_0[e]-1e-3*0.5*V_bar[e]^2
rho_bar[e]=Average(rho_i[e],rho_e[e])
V_bar[e]=ABS(m_dot[e])/(rho_bar[e]*A_bar[e])

```

"Element heat load"

Q_e[e]=0.0

"No heat energy is added or removed in the elements"

"!Section 7: Momentum conservation calculations"

"Calculate momentum conservation source term"

```

S_m[e]= (A_bar[e] / L[e]) * (0.5 * V_bar[e] ^ 2 * (rho_e[e] - rho_i[e]) - 1e3 * (p_0e[e] - p_0i[e]) - rho_bar[e] * g * (z_e[e] - z_i[e]) - k_L[e] * (ABS(m_dot[e]) * m_dot[e]) / rho_bar[e] + L[e] * A_e[e] * drhodt_bar[e])

```

"Steady state"

```

{S_m[e]=0
drhodt_bar[e]=0}

```

"Transient integration for element mass flow rate"

```

S_m_old[e]=tablevalue(Row-1,43+e)
m_dot_old[e]=tablevalue(Row-1,25+e)
rho_bar_old[e]=tablevalue(Row-1,30+e)
drhodt_bar[e]=(rho_bar[e]-rho_bar_old[e])/deltatime
dmdotdt[e]=alpha_m*S_m[e]+(1-alpha_m)*S_m_old[e]
m_dot[e]=m_dot_old[e]+dmdotdt[e]*deltatime

```

End

"!Section 8: Node calculations"

Duplicate n=1,nodes

"Calculate mass conservation source term value"

```

S_c[n]=1/Vol[n]*(SUM(c[n,e]*m_dot[e],e=1,elements)+m_dot_s[n])

```

```
"Steady state"
{S_c[n]=0
drhod[n]=0}
```

```
"Transient integration for node density"
S_c_old[n]=tablevalue(Row-1,35+n)
rho_old[n]=tablevalue(Row-1,5+n)
drhod[n]=alpha_c*S_c[n]+(1-alpha_c)*S_c_old[n]
rho[n]=rho_old[n]+drhod[n]*deltatime
```

```
"Calculate energy conservation source term value"
S_e[n]=1/(rho[n]*Vol[n])*(SUM((F(c[n,e],0.0,0.0,0.0,m_dot[e]*(h_0e[e]+1e-3*g*z_e[e])),e=1,elements)-SUM((F(c[n,e],0,m_dot[e]*(h_0[e]+1e-3*g*z_e[e]),0.0,0.0),e=1, elements)+IF(m_dot_s[n],0.0,m_dot_s[n]*h_0[n],0.0,m_dot_s[n]*h_0s[n])+Q_n[n]+Vol[n]*(dpdt[n]-h_0[n]*drhod[n]))
```

```
"Steady state"
{S_e[n]=0
dpdt[n]=0}
```

```
"Transient integration for node total enthalpy"
S_e_old[n]=tablevalue(Row-1,39+n)
p_old[n]=tablevalue(Row-1,13+n)
h_0_old[n]=tablevalue(Row-1,21+n)
dpdt[n]=(p[n]-p_old[n])/deltatime
dh0dt[n]=alpha_e*S_e[n]+(1-alpha_e)*S_e_old[n]
h_0[n]=h_0_old[n]+dh0dt[n]*deltatime
```

```
"Calculate node parameters"
h[n]=h_0[n]-0.5*V_n^2
p[n]=p_0[n]
```

```
{v_f[n]=Volume(F$,P=P[n],x=x_f)
v_g[n]=Volume(F$,P=P[n],x=x_g)
h_f[n]=Enthalpy(F$,P=P[n],x=x_f)
h_g[n]=Enthalpy(F$,P=P[n],x=x_g)}
```

```
CALL DENSITY_LIQ(T[n], P[n]/1e3, P[n]/1e3: rho_f1[n], rho_f[n])
CALL DENSITY_VAP(T[n], T[n], P[n]/1e3: rho_g1[n], rho_g[n])
CALL ENTHALPY_LIQ(T[n], P[n]/1e3, P[n]/1e3: h_f1[n], h_f[n])
CALL ENTHALPY_VAP(T[n], T[n], P[n]/1e3: h_g1[n], h_g[n])
```

```
v_f[n] = 1 / rho_f[n]
v_g[n] = 1 / rho_g[n]
rho[n] = 1 / v[n]
v[n] = x[n] * v_g[n] + (1 - x[n]) * v_f[n]
```

```
"Steady state p and T"
p[n]=p_IAPWS[n]
T[n]=T_sat[n]
```

```
"!Section 9: Rate form of the equation of state"
```

```
CALL DELTAH_LIQ(P[n]/1e3: deltah_f[n])
CALL DELTAH_VAP(P[n]/1e3: deltah_g[n])
CALL DELTAV_LIQ(P[n]/1e3: deltanu_f[n])
CALL DELTAV_VAP(P[n]/1e3: deltanu_g[n])
```

```
{G_1[n] = ((h_g[n] - h_f[n]) * (x[n] * v_g[n] + (1 - x[n]) * v_f[n])^2) / ((x[n] * deltah_g[n] + (1 - x[n]) * deltah_f[n]) * (v_g[n] - v_f[n]) - (x[n] * deltanu_g[n] + (1 - x[n]) * deltanu_f[n]) * (h_g[n] - h_f[n]))
G_2[n] = (v_g[n] - v_f[n]) / ((x[n] * deltah_g[n] + (1 - x[n]) * deltah_f[n]) * (v_g[n] - v_f[n]) - (x[n] * deltanu_g[n] + (1 - x[n]) * deltanu_f[n]) * (h_g[n] - h_f[n]))
```

```
"Steady state"
{S_g[n] = 0}

"Transient integration for node pressure"
S_g_old[n] = tablevalue(Row-1,52+n)
S_g[n] = (G_1[n] * drhodt[n]) + (G_2[n] * dh0dt[n])
dPgdt[n] = alpha_m * S_g[n] + (1 - alpha_m) * S_g_old[n]
P[n] = p_old[n] + (deltatime * dPgdt[n]) * 1e3

"Non-Equilibrium temperature tracking"
CALL DELTAT_SAT(P[n]/1e3:deltaT_s[n])

"Steady state"
{S_g_T[n] = 0}

"Transient integration for node temperature"
T_old[n]=tablevalue(Row-1,9+n)
S_g_old_T[n] = tablevalue(Row-1,56+n)
S_g_T[n] = dPgdt[n] * deltaT_s[n]
dTgdt[n] = alpha_m * S_g_T[n] + (1 - alpha_m) * S_g_old_T[n]
T[n] = T_old[n] + (deltatime * dTgdt[n])}

"!—Algebraic pressure and temperature—"

P_IAPWS[n] = Pressure(F$, h=h[n],v=v[n])
error_P[n] = ((P[n] - P_IAPWS[n]) / P_IAPWS[n]) * 100

T_sat[n]=T_sat(Steam_IAPWS,P=P[n])
error_T[n] = ((T[n] - T_sat[n]) / T_sat[n]) * 100

End
```

C.3 Transient network model: RFES

```
"!Transient network simulation"

"!Section 1: Constants"

F$ = 'Steam_IAPWS'                                "Working fluid Equation of state selection"
g=9.81 [m/s^2]                                     "Gravitational acceleration"
x_f = 0                                              "Saturated liquid quality"
x_g = 1                                              "Saturated vapour quality"

"!Section 2: Connectivity"

nodes=4                                              "Number of nodes in network"
elements=5                                           "Number of elements in network"

Duplicate n=1,nodes
  Duplicate e=1,elements
    c[n,e]=lookup('Connectivity',n,e)              "Pipe connectivity lookup from lookup table"
  End
End

Duplicate e=1,elements
  n_i[e]=sum(IF(c[n,e],0,n,0,0),n=1,nodes) "Element inlet connection"
  n_e[e]=sum(IF(c[n,e],0,0,0,n),n=1,nodes) "Element outlet connection"
End

"!Section 3: Geometry"

"!Nodes: Node volumes and elevations defined"

Vol_n[1]=0.5
z[1]=0

Vol_n[2]=0.05
z[2]=0

Vol_n[3]=0.1
z[3]=0

Vol_n[4]=0.3
z[4]=0

V_n=0 "Velocity in all nodes assumed to be zero"

Duplicate n=1,nodes
  Vol[n]=Vol_n[n]+0.5*(sum(abs(c[n,e])*Vol_e[e],e=1,elements)) "Node volume calculation based on elements connected"
End

"!Elements: Inlet areas, outlet areas and pipe lengths defined"

A_i[1]=0.0025
A_e[1]=0.0025
L[1]=5.0

A_i[2]=0.0025
A_e[2]=0.0025
L[2]=10.0

A_i[3]=0.0025
```

```

A_e[3]=0.0025
L[3]=1.0

A_i[4]=0.0025
A_e[4]=0.0025
L[4]=15.0

A_i[5]=0.0025
A_e[5]=0.0025
L[5]=10.0

Duplicate e=1,elements
  A_bar[e]=0.5*(A_i[e]+A_e[e])           "Average pipe area"
  Vol_e[e]=A_bar[e]*L[e]                 "Pipe volume"
  z_i[e]=z[n_i[e]]                       "Pipe inlet elevation"
  z_e[e]=z[n_e[e]]                       "Pipe outlet elevation"
  k_L[e]=1e7                             "Pipe friction factor"
End

"Section 4: Boundary values for mass source terms"

duplicate n=1,nodes

CALL ENTHALPY_LIQ(T[n], P[n]/1e3, P[n]/1e3: h_0sf1[n], h_0sf[n])
CALL ENTHALPY_VAP(T[n], T[n], P[n]/1e3: h_0sg1[n], h_0sg[n])

h_0s[n] = x[n] * h_0sg[n] + (1 - x[n]) * h_0sf[n] "Mass source enthalpy based on node mass quality"

end

{h_0s[1]=ENTHALPY(F$,x=x[1],P=p[1])
h_0s[2]=ENTHALPY(F$,x=x[2],P=p[2])
h_0s[3]=ENTHALPY(F$,x=x[3],P=p[3])
h_0s[4]=ENTHALPY(F$,x=x[4],P=p[4])}

"Section 5: Timewise integration factors"
deltatime=0.05           "Time step length"
alpha=1                  "Integration factor"
alpha_c=alpha            "Integration factor for continuity equation"
alpha_m=alpha            "Integration factor for momentum equation"
alpha_e=alpha            "Integration factor for energy equation"
Row=1+time/deltatime     "Row number in parametric table"

"Section 6: Element calculations"

Duplicate e=1,elements

  "Assign values at inlet and outlet"
  p_0i[e]=p_0[n_i[e]]
  p_0e[e]=p_0[n_e[e]]
  h_0i[e]=IF(m_dot[e],0.0,h_0e[e]+g*z_e[e]-1/m_dot[e]*Q_e[e]-g*z_i[e],h_0[n_i[e]],h_0[n_i[e]])
  h_0e[e]=IF(m_dot[e],0.0,h_0[n_e[e]],h_0[n_e[e]],h_0i[e]+g*z_i[e]+1/m_dot[e]*Q_e[e]-g*z_e[e])

  CALL SATTEMP(p_0i[e]/1e3:T_i[e])
  CALL ENTHALPY_LIQ(T_i[e], p_0i[e]/1e3, p_0i[e]/1e3: h_0if1[e], h_0if[e])
  CALL ENTHALPY_VAP(T_i[e], T_i[e], p_0i[e]/1e3: h_0ig1[e], h_0ig[e])
  h_0i[e] = x_i[e] * h_0ig[e] + (1 - x_i[e]) * h_0if[e]

```

```

CALL DENSITY_LIQ(T_i[e], p_0i[e]/1e3, p_0i[e]/1e3: rho_fi1[e], rho_fi[e])
CALL DENSITY_VAP(T_i[e], T_i[e], p_0i[e]/1e3: rho_gi1[e], rho_gi[e])
v_fi[e] = 1 / rho_fi[e]
v_gi[e] = 1 / rho_gi[e]

1 / rho_i[e] = x_i[e] * v_gi[e] + (1 - x_i[e]) * v_fi[e]

CALL SATTEMP(p_0e[e]/1e3: T_e[e])
CALL ENTHALPY_LIQ(T_e[e], p_0e[e]/1e3, p_0e[e]/1e3: h_0ef1[e], h_0eff[e])
CALL ENTHALPY_VAP(T_e[e], T_e[e], p_0e[e]/1e3: h_0eg1[e], h_0eg[e])
h_0e[e] = x_e[e] * h_0eg[e] + (1 - x_e[e]) * h_0eff[e]
CALL DENSITY_LIQ(T_e[e], p_0e[e]/1e3, p_0e[e]/1e3: rho_fe1[e], rho_fe[e])
CALL DENSITY_VAP(T_e[e], T_e[e], p_0e[e]/1e3: rho_ge1[e], rho_ge[e])
v_fe[e] = 1 / rho_fe[e]
v_ge[e] = 1 / rho_ge[e]

1 / rho_e[e] = x_e[e] * v_ge[e] + (1 - x_e[e]) * v_fe[e]

```

```

{rho_i[e]=DENSITY(F$,H=h_0i[e],P=p_0i[e])}
{rho_e[e]=DENSITY(F$,H=h_0e[e],P=p_0e[e])}

```

"Calculate average values"

```

p_bar_0[e]=Average(p_0i[e],p_0e[e])
h_bar_0[e]=Average(h_0i[e],h_0e[e])
h_bar[e]=h_bar_0[e]-1e-3*0.5*V_bar[e]^2
rho_bar[e]=Average(rho_i[e],rho_e[e])
V_bar[e]=ABS(m_dot[e])/(rho_bar[e]*A_bar[e])

```

"Element heat load"

Q_e[e]=0.0

"No heat energy is added or removed in the elements"

"!Section 7: Momentum conservation calculations"

"Calculate momentum conservation source term"

```

S_m[e]= (A_bar[e] / L[e]) * (0.5 * V_bar[e] ^ 2 * (rho_e[e] - rho_i[e]) - 1e3 * (p_0e[e] - p_0i[e]) - rho_bar[e] * g * (z_e[e] - z_i[e]) - k_L[e] * (ABS(m_dot[e]) * m_dot[e])/rho_bar[e] + L[e] * A_e[e] * drhodt_bar[e])

```

"Steady state"

```

{S_m[e]=0
drhodt_bar[e]=0}

```

"Transient integration for element mass flow rate"

```

S_m_old[e]=tablevalue(Row-1,43+e)
m_dot_old[e]=tablevalue(Row-1,25+e)
rho_bar_old[e]=tablevalue(Row-1,30+e)
drhodt_bar[e]=(rho_bar[e]-rho_bar_old[e])/deltatime
dmdotdt[e]=alpha_m*S_m[e]+(1-alpha_m)*S_m_old[e]
m_dot[e]=m_dot_old[e]+dmdotdt[e]*deltatime

```

End

"!Section 8: Node calculations"

Duplicate n=1,nodes

"Calculate mass conservation source term value"

```

S_c[n]=1/Vol[n]*(SUM(c[n,e]*m_dot[e],e=1,elements)+m_dot_s[n])

```

```
"Steady state"
{S_c[n]=0
drhod[n]=0}
```

```
"Transient integration for node density"
```

```
S_c_old[n]=tablevalue(Row-1,35+n)
rho_old[n]=tablevalue(Row-1,5+n)
drhod[n]=alpha_c*S_c[n]+(1-alpha_c)*S_c_old[n]
rho[n]=rho_old[n]+drhod[n]*deltatime
```

```
"Calculate energy conservation source term value"
```

```
S_e[n]=1/(rho[n]*Vol[n])*(SUM(IF(c[n,e],0.0,0.0,0,m_dot[e]*(h_0e[e]+1e-3*g*z_i[e]),e=1,elements)-SUM((F(c[n,e],0,m_dot[e]*(h_0[e]+1e-3*g*z_i[e]),0.0,0.0),e=1, elements)+F(m_dot_s[n],0.0,m_dot_s[n]*h_0[n],0.0,m_dot_s[n]*h_0s[n])+Q_n[n]+Vol[n]*(dpdt[n]-h_0[n]*drhod[n]))
```

```
"Steady state"
```

```
{S_e[n]=0
dpdt[n]=0}
```

```
"Transient integration for node total enthalpy"
```

```
S_e_old[n]=tablevalue(Row-1,39+n)
p_old[n]=tablevalue(Row-1,13+n)
h_0_old[n]=tablevalue(Row-1,21+n)
dpdt[n]=(p[n]-p_old[n])/deltatime
dh0dt[n]=alpha_e*S_e[n]+(1-alpha_e)*S_e_old[n]
h_0[n]=h_0_old[n]+dh0dt[n]*deltatime
```

```
"Calculate node parameters"
```

```
h[n]=h_0[n]-0.5*v_n^2
p[n]=p_0[n]
```

```
{v_f[n]=Volume(F$,P=P[n],x=x_f)
v_g[n]=Volume(F$,P=P[n],x=x_g)
h_f[n]=Enthalpy(F$,P=P[n],x=x_f)
h_g[n]=Enthalpy(F$,P=P[n],x=x_g)}
```

```
CALL DENSITY_LIQ(T[n], P[n]/1e3, rho_f1[n], rho_f[n])
CALL DENSITY_VAP(T[n], T[n], P[n]/1e3, rho_g1[n], rho_g[n])
CALL ENTHALPY_LIQ(T[n], P[n]/1e3, P[n]/1e3, h_f1[n], h_f[n])
CALL ENTHALPY_VAP(T[n], T[n], P[n]/1e3, h_g1[n], h_g[n])
```

```
v_f[n] = 1 / rho_f[n]
v_g[n] = 1 / rho_g[n]
rho[n] = 1 / v[n]
v[n] = x[n] * v_g[n] + (1 - x[n]) * v_f[n]
```

```
"Steady state p and T"
```

```
{p[n]=p_IAPWS[n]
T[n]=T_sat[n]}
```

```
"Section 9: Rate form of the equation of state"
```

```
CALL DELTAH_LIQ(P[n]/1e3, deltax_f[n])
CALL DELTAH_VAP(P[n]/1e3, deltax_g[n])
CALL DELTAV_LIQ(P[n]/1e3, deltanu_f[n])
CALL DELTAV_VAP(P[n]/1e3, deltanu_g[n])
```

```
G_1[n] = ((h_g[n] - h_f[n]) * (x[n] * v_g[n] + (1 - x[n]) * v_f[n])^2) / ((x[n] * deltax_g[n] + (1 - x[n]) * deltax_f[n]) * (v_g[n] - v_f[n]) - (x[n] * deltanu_g[n] + (1 - x[n]) * deltanu_f[n]) * (h_g[n] - h_f[n]))
G_2[n] = (v_g[n] - v_f[n]) / ((x[n] * deltax_g[n] + (1 - x[n]) * deltax_f[n]) * (v_g[n] - v_f[n]) - (x[n] * deltanu_g[n] + (1 - x[n]) * deltanu_f[n]) * (h_g[n] - h_f[n]))
```

```
"Steady state"
{S_g[n] = 0}

"Transient integration for node pressure"
S_g_old[n] = tablevalue(Row-1,52+n)
S_g[n] = (G_1[n] * drhodt[n]) + (G_2[n] * dh0dt[n])
dPgdt[n] = alpha_m * S_g[n] + (1 - alpha_m) * S_g_old[n]
P[n] = p_old[n] + (deltatime * dPgdt[n]) * 1e3

"Non-Equilibrium temperature tracking"
CALL DELTAT_SAT(P[n]/1e3:deltaT_s[n])

"Steady state"
{S_g_T[n] = 0}

"Transient integration for node temperature"
T_old[n]=tablevalue(Row-1,9+n)
S_g_old_T[n] = tablevalue(Row-1,56+n)
S_g_T[n] = dPgdt[n] * deltaT_s[n]
dTgdt[n] = alpha_m * S_g_T[n] + (1 - alpha_m) * S_g_old_T[n]
T[n] = T_old[n] + (deltatime * dTgdt[n])

"!—Algebraic pressure and temperature—"

{P_IAPWS[n] = Pressure(F$, h=h[n],v=v[n])
error_P[n] = ((P[n] - P_IAPWS[n]) / P_IAPWS[n]) * 100

T_sat[n]=T_sat(Steam_IAPWS,P=P[n])
error_T[n] = ((T[n] - T_sat[n]) / T_sat[n]) * 100}
```

End

Appendix D

Thermodynamic property approximation functions

D.1 Saturation temperature

```
PROCEDURE SATTEMP(P:T_s)

  IF (P>=0.002) and (P<0.01672) THEN GOTO 1
  IF (P>=0.01672) and (P<0.07250) THEN GOTO 2
  IF (P>=0.07250) and (P<0.359) THEN GOTO 3
  IF (P>=0.359) and (P<=1.676) THEN GOTO 4
  IF (P>1.676) and (P<=8.511) THEN GOTO 5
  IF (P>8.511) and (P<17.690) THEN GOTO 6
  IF (P>=17.690) and (P<=21.850) THEN GOTO 7

  1: T_s=270.1210*P^0.135019-99.2
  RETURN

  2: T_s=254.6831*P^0.156108-78.2
  RETURN

  3: T_s=236.2315*P^0.1784767-57
  RETURN

  4: T_s=207.9248*P^0.2092705-28
  RETURN

  5: T_s=185.0779*P^0.2323217-5
  RETURN

  6: T_s=195.1819*P^0.2241729-16
  RETURN

  7: T_s=227.2963*P^0.201581-50
  RETURN

END
```

D.2 Saturated liquid density

```
PROCEDURE DENSITY_LIQ(T,P_s,P:rho_f,rho)

IF (P>=0.02) and (P<=0.01468) THEN GOTO 1
IF (P>=0.01468) and (P<=0.275) THEN GOTO 2
IF (P>=0.275) and (P<=1) THEN GOTO 3
IF (P>1) and (P<=3.88) THEN GOTO 4
IF (P>3.88) and (P<=8.840) THEN GOTO 5
IF (P>8.84) and (P<=14.463) THEN GOTO 6
IF (P>14.463) and (P<18.052) THEN GOTO 7
IF (P>=18.052) and (P<20.204) THEN GOTO 8
IF (P>=20.204) and (P<=21.5) THEN GOTO 9

1: rho_f=(1.9118*104)*P_s0.546472+0.0009947(-1)
rho=rho_f+((170/(375-T))-0.2)*(P-P_s)
RETURN

2: rho_f=(1.380934*104)*P_s0.388715+0.000987(-1)
rho=rho_f+((170/(375-T))-0.2)*(P-P_s)
RETURN

3: rho_f=(1.2746977*104)*P_s0.4644339+0.001(-1)
rho=rho_f+((170/(375-T))-0.2)*(P-P_s)
RETURN

4: rho_f=(1.0476071*104)*P_s0.5651090+0.001022(-1)
rho=rho_f+((170/(375-T))-0.2)*(P-P_s)
RETURN

5: rho_f=(3.2836717*105)*P_s+1.12174735*103(-1)
rho=rho_f+((170/(375-T))-0.2)*(P-P_s)
RETURN

6: rho_f=(3.3551046*104)*exp(5.8403566*10-2*P_s+0.00085)(-1)
rho=rho_f+((170/(375-T))-0.2)*(P-P_s)
RETURN

7: rho_f=(3.1014626*108)*P_s3.284754+0.001430(-1)
rho=rho_f+((170/(375-T))-0.2)*(P-P_s)
RETURN

8: rho_f=(1.5490787*1011)*P_s5.7205+0.001605(-1)
rho=rho_f+((170/(375-T))-0.2)*(P-P_s)
RETURN

9: rho_f=(4.1035988*1024)*P_s15.03329+0.00189(-1)
rho=rho_f+((170/(375-T))-0.2)*(P-P_s)
RETURN

END
```

D.3 Saturated vapour density

```
PROCEDURE DENSITY_VAP(T,T_s,P:rho_g,rho)

IF (P>0.002) and (P<0.2139) THEN GOTO 1
IF (P>=0.2139) and (P<1.112) THEN GOTO 2
IF (P>=1.112) and (P<3.932) THEN GOTO 3
IF (P>=3.932) and (P<8.996) THEN GOTO 4
IF (P>=8.996) and (P<14.628) THEN GOTO 5
IF (P>=14.628) and (P<=18.210) THEN GOTO 6
IF (P>18.210) and (P<=20.253) THEN GOTO 7
IF (P>20.253) and (P<=21.5) THEN GOTO 8

1: rho_g=(5.0981616*P^0.936226-0.00025)
rho=(rho_g*(0.000466/P-(((0.12/(T+100))-0.00106)*P^0.1)/sqrt(1.96*10^(-8)*(T+8)^4-P^2))^(T-T_s))^(-1)
RETURN

2: rho_g=(5.126076*P^0.9475862+0.012)
rho=(rho_g*(0.000466/P-(((0.12/(T+100))-0.00106)*P^0.1)/sqrt(1.96*10^(-8)*(T+8)^4-P^2))^(T-T_s))^(-1)
RETURN

3: rho_g=(4.630832*P^1.035519+0.520)
rho=(rho_g*(0.000466/P-(((0.12/(T+100))-0.00106)*P^0.1)/sqrt(1.96*10^(-8)*(T+8)^4-P^2))^(T-T_s))^(-1)
RETURN

4: rho_g=(2.868721*P^1.252148+3.8)
rho=(rho_g*(0.000466/P-(((0.12/(T+100))-0.00106)*P^0.1)/sqrt(1.96*10^(-8)*(T+8)^4-P^2))^(T-T_s))^(-1)
RETURN

5: rho_g=(0.5497653*P^1.8311282+18.111)
rho=(rho_g*(0.000466/P-(((0.12/(T+100))-0.00106)*P^0.1)/sqrt(1.96*10^(-8)*(T+8)^4-P^2))^(T-T_s))^(-1)
RETURN

6: rho_g=(8.5791582*10^(-3)*P^3.176484+50)
rho=(rho_g*(0.000466/P-(((0.12/(T+100))-0.00106)*P^0.1)/sqrt(1.96*10^(-8)*(T+8)^4-P^2))^(T-T_s))^(-1)
RETURN

7: rho_g=(3.5587113*10^(-6)*P^5.660939+88)
rho=(rho_g*(0.000466/P-(((0.12/(T+100))-0.00106)*P^0.1)/sqrt(abs(1.96*10^(-8)*(T+8)^4-P^2))))^(T-T_s))^(-1)
RETURN

8: rho_g=(3.558734*10^(-16)*P^13.03774+138)
rho=(rho_g*(0.000466/P-(((0.12/(T+100))-0.00106)*P^0.1)/sqrt(abs(1.96*10^(-8)*(T+8)^4-P^2))))^(T-T_s))^(-1)
RETURN

END
```

D.4 Saturated liquid enthalpy

```
PROCEDURE ENTHALPY_LIQ(T,P_s,P:h_f,h)
```

```
IF (P>0.002) and (P<0.0173) THEN GOTO 1  
IF (P>0.0173) and (P<0.1028) THEN GOTO 2  
IF (P>0.1028) and (P<0.942) THEN GOTO 3  
IF (P>=0.942) and (P<4.020) THEN GOTO 4  
IF (P>=4.020) and (P<9.964) THEN GOTO 5  
IF (P>=9.964) and (P<16.673) THEN GOTO 6  
IF (P>=16.673) and (P<20.396) THEN GOTO 7  
IF (P>=20.396) and (P<=21.5) THEN GOTO 8
```

```
1: h_f=1128.777*P_s^0.1351960-413.72  
h=h_f+(1.4*(169/(369-T)))*(P-P_s)  
RETURN
```

```
2: h_f=1050.7085*P_s^0.1617970-306.50  
h=h_f+(1.4*(169/(369-T)))*(P-P_s)  
RETURN
```

```
3: h_f=912.1779*P_s^0.2061637-150  
h=h_f+(1.4*(169/(369-T)))*(P-P_s)  
RETURN
```

```
4: h_f=638.0621*P_s^0.2963192+125  
h=h_f+(1.4*(169/(369-T)))*(P-P_s)  
RETURN
```

```
5: h_f=373.7665*P_s^0.4235532+415  
h=h_f+(1.4*(169/(369-T)))*(P-P_s)  
RETURN
```

```
6: h_f=75.38673*P_s^0.8282384+900  
h=h_f+(1.4*(169/(369-T)))*(P-P_s)  
RETURN
```

```
7: h_f=0.1150827*P_s^2.711412+1440  
h=h_f+(1.4*(169/(369-T)))*(P-P_s)  
RETURN
```

```
8: h_f=9.1417257*10^(-14)*P_s^11.47287+1752  
h=h_f+(1.4*(169/(369-T)))*(P-P_s)  
RETURN
```

```
END
```

D.5 Saturated vapour enthalpy

```
PROCEDURE ENTHALPY_VAP(T,T_s,P:h_g,h)

IF (P>=0.002) and (P<0.1379) THEN GOTO 1
IF (P>=0.1379) and (P<=0.348) THEN GOTO 2
IF (P>0.348) and (P<=1.248) THEN GOTO 3
IF (P>1.248) and (P<2.955) THEN GOTO 4
IF (P>=2.955) and (P<=6.522) THEN GOTO 5
IF (P>6.522) and (P<=16.497) THEN GOTO 6
IF (P>=16.497) and (P<20.193) THEN GOTO 7
IF (P>=20.193) and (P<=21.5) THEN GOTO 8

1: h_g=529.44008*P^0.108652+2263.5
h=h_g+(((4.5*P)/sqrt(7.4529*10^(-0.6)*T^3-P^2))+0.28*exp(-0.008*(T-162))-100/T-2.225)*(T-T_s)
RETURN

2: h_g=-4.0381938*10^(-6)*(3.0-P)^15.72364+2750
h=h_g+(((4.5*P)/sqrt(7.4529*10^(-0.6)*T^3-P^2))+0.28*exp(-0.008*(T-162))-100/T-2.225)*(T-T_s)
RETURN

3: h_g=-0.5767304*exp(-1.66153*(P-3.2))+2800
h=h_g+(((4.5*P)/sqrt(7.4529*10^(-0.6)*T^3-P^2))+0.28*exp(-0.008*(T-162))-100/T-2.225)*(T-T_s)
RETURN

4: h_g=-7.835986*(P-3.001)^2-2.934312*(P-3.001)+2803.71
h=h_g+(((4.5*P)/sqrt(7.4529*10^(-0.6)*T^3-P^2))+0.28*exp(-0.008*(T-162))-100/T-2.225)*(T-T_s)
RETURN

5: h_g=-1.347244*(P-2.999)^2-2.326913*(P-2.999)+2803.35
h=h_g+(((4.5*P)/sqrt(7.4529*10^(-0.6)*T^3-P^2))+0.28*exp(-0.008*(T-162))-100/T-2.225)*(T-T_s)
RETURN

6: h_g=-0.9219176*(P-9)^2-16.38835*(P-9)+2742.03
h=h_g+(((4.5*P)/sqrt(7.4529*10^(-0.6)*T^3-P^2))+0.28*exp(-0.008*(T-162))-100/T-2.225)*(T-T_s)
RETURN

7: h_g=-3.532177*(P-8)^2+29.81305*(P-8)+2565
h=h_g+(((4.5*P)/sqrt(7.4529*10^(-0.6)*T^3-P^2))+0.28*exp(-0.008*(T-162))-100/T-2.225)*(T-T_s)
RETURN

8: h_g=-22.62521*(P-18)^2+44.23671*(P-18)+2415.01
h=h_g+(((4.5*P)/sqrt(7.4529*10^(-0.6)*T^3-P^2))+0.28*exp(-0.008*(T-162))-100/T-2.225)*(T-T_s)
RETURN

END
```

D.6 Liquid density derivative

```
PROCEDURE DELTAV_LIQ(P:deltanu_f)

  IF (P>=0.02) and (P<=0.01468) THEN GOTO 1
  IF (P>=0.01468) and (P<=0.275) THEN GOTO 2
  IF (P>=0.275) and (P<=1) THEN GOTO 3
  IF (P>1) and (P<=3.88) THEN GOTO 4
  IF (P>3.88) and (P<=8.840) THEN GOTO 5
  IF (P>8.84) and (P<=14.463) THEN GOTO 6
  IF (P>14.463) and (P<=18.052) THEN GOTO 7
  IF (P>=18.052) and (P<=20.204) THEN GOTO 8
  IF (P>=20.204) and (P<=21.5) THEN GOTO 9

  1: deltanu_f = 0.000104475 / P^0.453528
  RETURN

  2: deltanu_f = 0.000053679 / P^0.611285
  RETURN

  3: deltanu_f = 0.0000592013 / P^0.535566
  RETURN

  4: deltanu_f = 0.0000592012 / P^0.434891
  RETURN

  5: deltanu_f = 0.0000328367
  RETURN

  6: deltanu_f = 0.000019595 * exp(0.0584036 * P)
  RETURN

  7: deltanu_f = 1.01875e-7 * P^2.28475
  RETURN

  8: deltanu_f = 8.8615e-11 * P^4.7205
  RETURN

  9: deltanu_f = 6.616906e-23 * P^14.0333
  RETURN

END
```

D.7 Vapour density derivative

```
PROCEDURE DELTAV_VAP(P:deltanu_g)

IF (P>0.002) and (P<0.2139) THEN GOTO 1
IF (P>=0.2139) and (P<1.112) THEN GOTO 2
IF (P>=1.112) and (P<3.932) THEN GOTO 3
IF (P>=3.932) and (P<8.996) THEN GOTO 4
IF (P>=8.996) and (P<14.628) THEN GOTO 5
IF (P>=14.628) and (P<=18.210) THEN GOTO 6
IF (P>18.210) and (P<=20.253) THEN GOTO 7
IF (P>20.253) and (P<=21.5) THEN GOTO 8

1: deltanu_g = -4.77303 / (P^0.063774 * (0.00025 - 5.09816 * P^0.936226)^2)
RETURN

2: deltanu_g = -4.8574 / ((5.12608 * P^0.947586 + 0.012)^2 * P^0.0524138)
RETURN

3: deltanu_g = -(4.79531 * P^0.035519) / (4.63083 * P^1.03552 + 0.52)^2
RETURN

4: deltanu_g = -(3.59206 * P^0.252148) / (2.86872 * P^1.25215 + 3.8)^2
RETURN

5: deltanu_g = -(1.00669 * P^0.831128) / (0.549765 * P^1.83113 + 18.111)^2
RETURN

6: deltanu_g = -(0.0272516 * P^2.17648) / (0.00857916 * P^3.17648 + 50)^2
RETURN

7: deltanu_g = -(0.0000201456 * P^4.66094) / (3.55871e-6 * P^5.66094 + 88)^2
RETURN

8: deltanu_g = -(4.63978e-15 * P^12.0377) / (3.55873e-16 * P^13.0377 + 138)^2
RETURN

END
```

D.8 Liquid enthalpy derivative

Procedure DELTAH_LIQ(P:deltah_f)

IF (P>0.002) and (P<0.0173) THEN GOTO 1
IF (P>0.0173) and (P<0.1028) THEN GOTO 2
IF (P>0.1028) and (P<0.942) THEN GOTO 3
IF (P>=0.942) and (P<4.020) THEN GOTO 4
IF (P>=4.020) and (P<9.964) THEN GOTO 5
IF (P>=9.964) and (P<16.673) THEN GOTO 6
IF (P>=16.673) and (P<20.396) THEN GOTO 7
IF (P>=20.396) and (P<=21.5) THEN GOTO 8

1: deltah_f = 152.606 / P^{0.864804}
RETURN

2: deltah_f = 170.001 / P^{0.838203}
RETURN

3: deltah_f = 188.058 / P^{0.793836}
RETURN

4: deltah_f = 189.08 / P^{0.703681}
RETURN

5: deltah_f = 158.31 / P^{0.576447}
RETURN

6: deltah_f = 62.4382 / P^{0.171762}
RETURN

7: deltah_f = 0.312037 * P^{1.71141}
RETURN

8: deltah_f = 1.04882e-12 * P^{10.4729}
RETURN

D.9 Vapour enthalpy derivative

```
PROCEDURE DELTAH_VAP(P:deltah_g)

  IF (P>=0.002) and (P<0.1379) THEN GOTO 1
  IF (P>=0.1379) and (P<=0.348) THEN GOTO 2
  IF (P>0.348) and (P<=1.248) THEN GOTO 3
  IF (P>1.248) and (P<2.955) THEN GOTO 4
  IF (P>=2.955) and (P<=6.522) THEN GOTO 5
  IF (P>6.522) and (P<=16.497) THEN GOTO 6
  IF (P>=16.497) and (P<20.193) THEN GOTO 7
  IF (P>=20.193) and (P<=21.5) THEN GOTO 8

  1: deltah_g = 57.5247 / P^0.891348
  RETURN

  2: deltah_g = 0.0000634951 * (3 - P) ^ 14.7236
  RETURN

  3: deltah_g = 195.245 * exp(-1.66153 * P)
  RETURN

  4: deltah_g = 44.0973 - 15.672 * P
  RETURN

  5: deltah_g = 5.75386 - 2.69449 * P
  RETURN

  6: deltah_g = 0.206167 - 1.84384 * P
  RETURN

  7: deltah_g = 86.3279 - 7.06435 * P
  RETURN

  8: deltah_g = 858.744 - 45.2504 * P
  RETURN

END
```