Transient Actuations in Heat Exchangers

by

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A Michelle, Amelia, mis Padres y Abuela

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- 3) Antonio FAMMIGLIETTI, Berat CELIK, Antonio LECUONA, Ricardo LÓPEZ, Jose NOGUEIRA GORIBA “*Use of Parabolic Trough Collector as Direct Vapor Generator for an Absorption Machine: Experimental Study*” ISES Solar World Conference, November 04-07 2019. Santiago de Chile, Chile
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ABSTRACT

Heat exchangers are used in many industrial applications, for example, solar thermal facilities, power plants, refrigeration, and air conditioning systems to mention a few. The study and/or analysis of heat exchangers using numerical procedures provides many benefits due its flexibility and reduced cost compared with experimental procedures. This is the reason why it can be used to carry parametric study in order the design better and more efficient devices. Recently, increased attention is put on transient heat exchanger analysis, and from a numerical perspective, the use of one dimensional (1-D) models seems desirable, due to its low computational cost and high level of accuracy.

Under the distributed parameter approach, the modeling of these systems is made through a partial differential set. Due to its mathematical complexity, it is not possible to obtain an analytical or exact solution. Therefore, the solution has to be approximated numerically. To do this, the equations have to be discretized in space and time as well. In that sense, to approximate the solution many researchers tend to use the classic Euler backward or forward methods to handle the temporal terms. This thesis is focused on providing an alternative numerical methodology to cope with fast phase change processes applied to heat exchanger research. The proposed methodology is able to increase the accuracy of the solution by using high order temporal schemes. It consists in a finite volume staggered grid discretization of the governing equations. The transient terms are treated with the explicit first stage singly diagonally implicit Runge-Kutta (ESDIRK) method. The convective terms are approximated with a 1st order UPWID method. And, the coupling of velocity (mass flow) and pressure is done with the semi-implicit pressure linked equations (SIMPLE) algorithm. This methodology is suitable for dealing with the stiff equations, present in instant boiling or condensation processes. It also handles accurately typical transient effects like fluctuations around an operation point, starting and stopping operations, variations inherent to some heating sources like solar radiation, etc.

The different aspects of the numerical procedure are discussed; this work offers a complete set of verification and validation experiments using experimental and numerical

published data available in the open literature. In this way, the numerical procedure is validated under steady-state and transient-state conditions, highlighting its potential.

Additionally, a novel heat exchanger layout devised for a two-phase stratified gravity-driven regime is studied. The mathematical model consists of 1-D balance equations for mass and momentum for both fluids and energy for both fluids and the wall of the pipe that absorbs solar radiation. The model is characterized by the fact that the area (or height) of the liquid layer is treated as a dependent variable forming part of the solution. In order to couple both phases a mass-transfer based algorithm is proposed. This increases the field of applications of the high order temporal scheme already developed.

RESUMEN

Los intercambiadores de calor se emplean en muchas aplicaciones industriales, tales como instalaciones solares térmicas, plantas de energía, sistemas de refrigeración y/o aire acondicionado, solo por mencionar algunos. El estudio y/o análisis numérico de intercambiadores nos proporciona muchas ventajas debido a su flexibilidad y reducido coste asociado, en comparación con los métodos experimentales usuales. Por ello, se pueden utilizar para llevar a cabo estudios paramétricos con el fin de diseñar mejores intercambiadores, de una forma rápida y económica. Recientemente, por parte de la comunidad científica se ha prestado mayor atención al análisis transitorio de intercambiadores de calor. En este ámbito, desde un punto de vista numérico el empleo de modelos unidimensionales (1-D) parece razonable, debido a su bajo costo computacional y alto nivel de precisión.

Bajo un enfoque de parámetros distribuidos, el modelado de estos sistemas se realiza a través de un conjunto de ecuaciones diferenciales parciales. Debido a su complejidad matemática no es posible hallar una solución analítica o exacta, por lo tanto, se recurre a su aproximación numérica. Por lo tanto, las ecuaciones deben ser discretizadas tanto en espacio como en tiempo. En ese sentido, muchos investigadores tienden a usar los métodos clásicos de Euler (hacia adelante o hacia atrás) para tratar los términos temporales. Esta tesis se centra en proporcionar una metodología numérica alternativa para hacer frente a los procedimientos de cambio fase súbitos que ocurren en un intercambiador de calor. La metodología propuesta aumenta la precisión de la solución mediante el uso de esquemas temporales de alto orden. Consiste en la discretización en una malla desplazada usando el método de los volúmenes finitos. Los términos transitorios se tratan con el método explícito de primera etapa diagonalmente implícito de Runge-Kutta (ESDIRK). Los términos convectivos se aproximan con un método UPWID de primer orden. Y, el acoplamiento de la velocidad (flujo másico) y la presión se realiza con el algoritmo SIMPLE. Esta metodología es adecuada para los problemas numéricamente rígidos, presentes en procesos instantáneos de ebullición o condensación. También permite manejar con precisión los efectos transitorios típicos como fluctuaciones alrededor de un punto de operación, operaciones de inicio y parada, variaciones inherentes a algunas fuentes de calor como la radiación solar, etc.

Los distintos aspectos de este método alternativos se comentan extensamente. El trabajo ofrece una exhaustiva verificación y validation mediante un conjunto de experimentos, usando datos tanto experimentales como numéricos publicados en la literatura abierta sobre el tema. De esta manera, el procedimiento numérico se valida en condiciones de estado estacionario y transitorio, destacando su potencial.

Además, se estudia un nuevo diseño de intercambiador de calor orientado a régimen estratificado de flujo bifásico. El modelo matemático consiste en plantear el problema 1-D usando las ecuaciones de conservación de masa y de cantidad de movimiento para ambos fluidos y la ecuación de conservación de energía para ambos fluidos y la pared de la tubería, que absorbe la radiación solar. El modelo se caracteriza por el hecho de que el área (o altura) de la película de líquido se trata como una variable dependiente. Para acoplar ambas fases, se propone un algoritmo de transferencia de masa. Esto aumenta el campo de aplicación del esquema temporal de alto orden previamente desarrollado.

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Introduction

1.1 Historial Background

Since the industrial revolution back in the 19th century, heat exchangers have become an essential device in engineering applications. They exist in different types, with different geometries and topologies according to their application (Shah & Sekulic, 1999). The idea behind every heat exchanger is always the same; to transfer thermal energy (heat) by convection, conduction, and in some cases by radiation (Sunden, 2005). This transfer is typically done from one group of fluids to another, but always with a solid surface in between, excepting the direct contact types. They can be used to transfer sensible or latent heat as well, in single-phase or multi-phase heat exchangers, respectively. Therefore, they can be found in many industrial processes like heat recovery, dehydration, pasteurization, distillation, sterilization, fractioning, crystallization, and many more. This flexibility makes heat exchangers an essential device used in oil, petrochemical, food and chemical industries, power plants, solar collectors, refrigeration, air conditioning and transport applications, etc.

A considerable amount of both experimental and numerical studies have been conducted in order to obtain smaller, lighter, more efficient, and cheaper heat exchangers, not forgetting the design of control strategies. The advantages of the numerical over the experimental approach are clear; reduction in the overall cost due to reduction in experimentation time, equipment optimization, and parametrization studies before the building of a prototype.

Traditionally under numerical procedures, heat exchangers have been analyzed and designed under steady-state conditions, determining only important but basic features like required heat transfer surface area and geometrical arrangement effects but always for certain fixed (in time) operation conditions. The classical steady-state approaches are the mean temperature difference (Incropera & DeWitt, 1990; Peters & Timmerhaus, 1991), the effectiveness-NTU (ϵ -NTU) method (Kays & London, 1984;

London & Seban, 1980), P-NTU method (Shah & Mueller, 1985), or any of their multiple variants (Kurpan, 2000; Shah & Sekulic, 1999). These methods have been systematically applied for sensible and latent heat exchangers, covering the entire range of single-pass and multi-pass heat exchangers (Corberán, Fernandez de Cordoba, González, & Alias, 2001). In these simple calculation methodologies, the analysis is based on time-independent energy balance relationships in which the number of assumptions is so restrictive that much relevant physical information is lost. Therefore, a more detailed and complex mathematical description is required. More sophisticated models can be derived with the aid of continuum mechanics, not only for single-phase applications but also with phase change processes. Under this approach a full set of conservation equations for mass, linear momentum (or simply called momentum), energy and other transport variables (chemical reactions or concentration) are posed (Sunden, 2007). Under this approach it is true that the physics of the problem is captured more precisely, but also the mathematical complexity is increased. Analytical or exact solutions of these set of equations is only possible for a very few simple problems, so approximate numerical solutions are needed. To this end the use of Computational Fluid Dynamics (CFD) is mandatory.

After the first middle of the 20th century, computer processors power increased exponentially, and their cost was reduced drastically, resulting in a massive popularization of personal computers (Fuller & Millet, 2011; Runchal, 2020), therefore a high number of 2-D and 3-D CFD software's have been developed and successfully applied to heat exchanger design and research (Gosman, 1998). Among the most used commercial codes in CFD science applied to heat exchanger research, we can found Fluent (Fluent, 2006), ADINA (ADINA R & D, 2012), COMSOL Multiphysics (Comsol, 2012) among others. This kind of software is capable of handling any geometry and boundary conditions incorporating models for single and two-phase flows, turbulence, and heat transfer for both; steady-state and transient state problems. However, this approach has some drawbacks; turbulence and two-phase accurate modeling is in itself a challenge, computational cost, time-consuming, and when commercial software is used the license cost is also an issue and therefore a limitation (Kopyt & Gwarek, 2004). The number of problems behind a detailed CFD calculation is such that its use seems reasonable only on advanced design stages.

In that sense, one- dimensional (1-D) transient simulations models provide enough flexibility, reduced cost, low computing times, and reasonable accuracy. This makes it appropriate for the early to intermediate stages of design before using a more powerful computational tool and final experiment checks. Maybe the two first scientific papers devoted to that end can be attributed to (Gruber & Hyman, 1956) and (Wissler, Isbin, & Amundson, 1956). Since then, the number of papers in the open literature concerning this issue has experienced a sustained increase over time. This can be confirmed checking the number of published papers from the decade of 1950's to this day, see Figure 1. 1.

Figure 1. 1 Heat exchanger 1-D numerical modeling published papers evolution. a) 1950's profile, b) 2010's profile, c) time evolution.

Nowadays, most of the attention is put into transient simulation because as strictly speaking, heat exchangers work on transient- state all the time (Gupta, 1986). With dynamic or transient simulations the catalog of potential effects that can be analyzed in heat exchangers includes; shut-down operations, variations in inlet conditions (mass flow, pressure, temperature or vapor mass fraction) due to inherent process variations or deliberate valve operation (Gupta, 1986), scale deposit or “fouling” on heat exchange surface (Wilfried Roetzel & Xuan, 1999), safety assessment, optimization, control strategies (Wozny, 1994) and two-phase flow instabilities dynamics effects (Yüncü & Kakaç, 1988). Within this scenario, the number of possible applications for

further research on 1-D transient simulations is still open, being a promising tool for the future.

1.2 The 1-D transient modeling paradigm

Formally, the concept of modeling is referred to as how a physical system is described by a set of equations, establishing a functional relationship between the elements of another set of variables or functions. In the 1-D heat exchanger context, the idea is to found these relations to perform calculations to determine some specific behavior according to some inputs or fixed variables. Unlike steady-state modeling, in which the set of dependent variables (or functions) are uniquely related to fluid flow, thermodynamic state variables and only one space coordinate (if it is considered) as independent variables, in transient state the idea is to establish these functional relationships with time as an additional one. In this way, not only the transient path that each variable follows can be determined but also the effects over the system when one or many variables are subjected to any singular or continuously in-time disturbances.

The 1-D transient modeling can be approached in two different ways, and their level of detail and accuracy depends exclusively on the realism of the assumptions considered, deriving in more or less mathematical descriptions. According to this description, they can be classified as lumped parameter approaches and distributed parameter approaches.

1.2.1 The lumped parameter approach

In this approach, it is assumed that the fluid temperature, pressure, and density and the solid wall (if it is considered) temperature are completely homogeneous and equal to a mean average value inside the entire domain. Also, the internal conductance is considered low when is compared with internal convective resistance, ignoring this way convective transport. Therefore, under these assumptions and if the heat exchanger is treated as a single control volume see Figure 1. 2.a, applying an energy balance, the spatial coordinate can be dropped off as an independent variable. Usually, the heat flux across the control volume boundary can be modeled using a mean average heat transfer coefficient “ U ” jointly with a mean average temperature difference e.g. logarithmic mean

temperature difference (Qiao, Radermacher, & Aute, 2010). The lumped parameter approach derives in systems of ordinary or algebraic differential equations systems (Pantelides, Gritals, Morison, & Sargent, 1988) and because of its simplicity it was established like the first paradigm in dynamic process simulation.

Figure 1. 2 Modified lumped parameter approach

Strictly speaking, the lumped parameter approach is a 0-D modeling approach, but many researchers have made some modifications to transform the original approach incorporating the 1-D essence. This modification consists of dividing the entire domain into several subdomains, in which the lumped parameter assumptions still hold, see Figure 1. 2.b. After this is done, the entire domain is assembled, transforming the problem into a set of n ordinary equations. Examples of this modification can be found in the plate heat exchanger “cinematic model” solution method proposed by (Lakshmanan & Potter, 1990), shell and tube heat exchanger model proposed (Correa & Marchetti, 1987), a cross-flow heat exchanger (Xia, De Abreu- Garcia, & Hartley, 1991) and concentric counter-current evaporator (Patiño et al., 2014).

For single-phase flows, the assumptions mentioned above could be accepted in certain circumstances, but in phase-change processes like condensation or evaporation is no longer valid. Therefore, the analysis is much more complex and another approach must be taken. Formally, the way to proceed is to establish balance relations with mass, momentum, and energy balances over an infinitesimal size control volume (Aris, 1989; Batchelor, 2000). These kinds of modeling are made through a partial differential equations (PDE), which increase significantly the mathematical complexity. To overcome

this issue, the moving- boundary approach (MBA) was developed. The basic idea behind the MBA is to reformulate the problem capturing the two-phase dynamics with the mathematical simplicity of the lumped parameter approach; this means to build a model with an ordinary differential equation set description instead of the more complex partial differential modeling. The MBA can be seen as a subclass of the lumped parameter approach, and here again the entire domain is divided, but each subdomain contains only a single-phase or two-phase flow pattern individually and which can be again represented by a characteristic state inside each subdomain. For simplicity, it is useful that this characteristic state should be related somehow with some state variable average. The problem is that in the two-phase mixture regions all variables, except pressure and temperature (due to equilibrium considerations), are highly sensitive on mass quality and/or void fraction. Here is where experimentation played a crucial role in the development of the MBA, reason why some aspects should be highlighted to fully understand the approach.

In boiling flows, similar reasoning applies to condensing flows. Three zones can be distinguished: *i*) sub-cooled liquid zone (SC), *ii*) two-phase mixture zone (TP), and *iii*) superheated vapor zone (SH). See Figure 1. 3. In the pioneering work made by (Zahn, 1964), he documented rigorously the location of the separation boundary of each zone. In his experiment, Zahn observed that even when inlet mass flow was kept constant, there were oscillations (erratic behavior in his words) on the location of the boundaries that separate each zone.

Figure 1. 3 Boiling flow schematic representation

This experiment was reproduced by (Wedeking & Stoecker, 1968), but he made a step further concluding that the instantaneous position of the liquid and mixture transition point is not possible. Instead they developed a theoretical model to obtain a

mean transition point. This model was later enhanced by (Wedekind, 1971) showing that the transition point is better described by a transformed Rayleigh distribution function. Posteriorly, (Wedekind, Bhatt, & Beck, 1978) introduced the concept of mean system void fraction. This concept is useful, not only for evaporating or boiling but also for condensing flows. In his definition, he assumed that the system mean void fraction is time-invariant, taking as the starting point for the average the one determined with the statistical approach mentioned above. In this work he came to two important conclusions: *i*) a time-invariant mixture region behavior can be lumped with the mean system void fraction as the fundamental parameter, *ii*) momentum balance is unnecessary.

With these results in mind, the classic MBA was developed. Again, the whole domain is divided into sub-domains, but now each one of these subdomains contains only one phase or mode of operation. Over each sub-domain, the original differential balances (mass and energy) are applied and with the aim of the Leibniz rule (Flanders, 1973), the original PDEs are replaced by a simpler ODE set. This kind of approach has the distinctive features that the functions are expressed by average values and also the length of each sub-region form part of the unknown vector, increasing the size of the ordinary differential set in comparison with the classic lumped parameter approach.

As stated before, the MBA is formulated for each mode of operation, but a robust method may consider all the possible cases during a simulation. For example, inside an evaporator on a dry out process we can identify three modes of operation: sub-cooled liquid (SC), a two-phase mixture region (TP), and superheated vapor (SH). See Figure 1. 3. In that sense, computationally the algorithm must detect the change of the mode of operation, and therefore the number of equations to solve is different. Moreover, the combination of these modes may be different according to the process to analyze and the entire structure of the set of equations is affected. This issue is called switching and is an important aspect of MBA modeling (Bendapudi, Braun, & Groll, 2008).

Many switching algorithms have been proposed. They can be classified into two kinds of groups. The first kind is purely thermodynamic based, comparing exit enthalpy of one region with saturation enthalpy at the same pressure (Bendapudi et al., 2008). Variants of this kind can be found in by (Gräber, Strupp, & Tegethoff, 2010) but using mass quality instead. The second kind tries to avoid possible discontinues in the solution

imposing restriction over region lengths. (Willatzen, Pettit, & Ploug-Sorensen, 1998). This last kind of switching was later improved by (Zhang & Zhang, 2006) including void fraction time dependency. The number of published MBA methods is vast, but the most common are summarized in Table 1. 1.

Table 1. 1 Moving boundary approach summary

Reference	Evaporator	Condenser	Switching	Void fraction transient
(Dhar & Soedel, 1979)	TP	SH-TP	Yes	No
		TP-SC		
		SC		
(Grald & MacArthur, 1992)	TP-SH	-	-	No
(He, Liu, Asada, & Itoh, 1998)	TP-SH	SH-TP-SC	Yes	No
	TP			
(Willatzen et al., 1998)	SC-TP-SH	-	Yes	No
	TP-SH			
	SC-TP			
	TP			
(Leducq, Guilpart, & Trystram, 2003)	TP-SH	SH-TP-SC	-	No
(Zhang & Zhang, 2006)	TP-SH	-	Yes	Yes
	TP			
(Mckinley & Alleyne, 2008)	-	SH-TP-SC	Yes	No
		SH-TP		
(Li & Alleyne, 2010)	TP-SH	SH-TP-SC	Yes	Yes
		SH-TP		
		TP-SC		
	TP	TP		
		SH		
(Liang, Shao, Tian, & Yan, 2010)	TP-SH	SH-TP-SC	Yes	No
(Cecchinato & Mancini, 2012)	TP-SH	-	Yes	No
(Jensen & Tummescheit, 2013)	SC-TP-SH	-	No	No
	TP-SH			
	SC-TP			
(Esposito & Gambrotta, 2015)	SC-TP-SH	-	Yes	Yes

The review of the MBA reveals some limitations: *i)* Momentum balance is not taken into account. Therefore, pressure drop cannot be calculated, being this a fundamental variable in heat exchanger analysis. *ii)* Spatial resolution is poor because linear profiles inside each region are assumed. *iii)* Heat flux is also averaged on each volume so, simulations with variable axial heat flux are not calculated accurately. *iv)* Switching increases the complexity of the programming task. *v)* There is no universal method covering every kind of possible configuration of operation modes. *vi)* In the formulation convective terms are ignored, not being possible to simulate accurately fast input variations or two-phase flow oscillations.

However, this type of approach has also some strong points that must be highlighted: *i)* Computationally, the solution can be obtained for any of the multiple and efficient ODE solvers available in the literature (Atkinson, Han, & Stewart, 2009) or using numerical libraries (Press, Teukolsky, Vetterling, & Flannery, 2007) included in many programming languages. In both cases algorithms are very computationally efficient. *ii)* Its flexibility makes it ideal for the development of black box simulation software (Pantelides et al., 1988). *iii)* Fast computational implementation, making this approach suitable for control-oriented application (Cecchinato & Mancini, 2012) on vapor compression cycles, Rankine cycles, etc.

1.2.2 The distributed parameter approach

Unlike the lumped parameter approach that assumes a piecewise approximation of state variables, the distributed parameter approach (DPA) assumes that the functions that describe the system are continuously distributed in time and space as well, see Figure 1. 4. The modeling in this approach is made through posing a partial differential equation (PDE) set, jointly with their boundary and initial conditions, which describes the time-space evolution of all state variables. This is the type of description that the MBA tries to avoid. Before the decade of the 1970s, the complexity in finding approximate solutions for PDEs positioned the lumped parameter approach in the center of dynamical or transient modeling and simulations. After that time remarkable advances in CFD science were made; pressure field could be computed without numerical decoupling or checkboard behavior (Caretto, Gosman, Patankar, & Spalding, 1972), (S V Patankar & Spalding, 1972). From this way the Navier- Stokes equations type can be approximated numerically

as a parabolic or elliptic differential equation instead of a hyperbolic differential equation, in which case the more complicated Riemann (exacts or approximated versions) solver theory must be used (Toro, 2009), (Leveque, 2002). Later on, (S. V. Patankar & Spalding, 1974) proposed a numerical model for the transient analysis of shell and tube heat exchangers and also pointed that CFD theory was now prepared for new challenges. In that sense, heat exchangers transient analysis was an excellent candidate. After that point, many researchers started to use CFD not only for 3-D but also for 1-D simulations. Right now, the use of continuous descriptions provided by partial differential equations and solved numerically with some CFD techniques stands as the new paradigm or at least it can be seen as an extension of the existing lumped parameter paradigm.

Figure 1. 4 Distributed and lumped parameter function space and time dependency

Using this approach for single-phase heat exchangers, many researchers drop-off the momentum and mass conservation equation because propagation velocity is high enough to ensure that the associated effects are almost instantaneous. With this formulation instantaneous disturbances have been studied extensively for every possible kind of transient effect in heat exchanger research. In Table 1. 2 some remarkable models for single-phase heat exchangers are summarized.

In two-phase heat exchanger modeling, some of the assumptions taken for single-phase heat exchangers are no longer valid because two or more phases can coexist in the same stream, with different velocities and properties (density, viscosity, etc.) making the modeling more complex.

Table 1. 2 Summary of single-phase transient models

Reference	Heat exchanger type	Considered transient effect
(Sharifi & Golkar Narandji, 1995)	PHE	Inlet temperature disturbance effect
(Dwivedi & Das, 2007)	PHE	Inlet mass flow disturbance effect
(Das & Roetzel, 1995)	PHE	Phase lag effects
(Das, Spang, & Roetzel, 1995)	PHE	Phase lag effects
(Srihari, Rao, Sunden, & Das, 2005)	PHE	Maldistribution effects
(W Roetzel, Li, & Luo, 2002)	S-T P-F	Inlet temperature and mass flow disturbance effect
(Luo, Guan, Li, & Roetzel, 2003)	S-T	Inlet temperature disturbance effect
(Xu, Li, Sun, & Li, 2019)	PTC	Sun radiation transient variation effect

PHE: Plate heat exchanger, P-F: Plate and fin, S-T: shell and tube, PTC: parabolic- trough solar collector, CC: concentric circular heat exchanger

A wide range of models is available in the open literature. The simplest ones are the homogeneous flow model (HFM) (Wallis, 1969) and the quasi-homogeneous (QHFM) flow model (Hewitt, 1982). Here the flow is considered as a mixture; consequently both phases hold the same temperature and pressure. There are more sophisticated models, such as the two-fluid model (TFM) where each phase is treated separately and expressed in terms of two sets of conservation equations, one set for each phase (M Ishii, 2016). The TFM allows obtaining the differing velocity and pressure fields for each phase and the *in situ* void fraction (Mamoru Ishii & Hibiki, 2011). This approach, although being more realistic, presents some numerical stability problems due to the ill-posedness of the governing equations as an initial value problem e. g. (Song & Ishii, 2000), (Song, 2003), being this an open issue. For these reasons, the HFM and QHFM are the most used models in transient heat exchangers analysis. Some recent work devoted to two-phase flow transient heat exchanger research are summarized in Table 1.3

Intuitively, we could assure that the lumped parameter approach is computationally more efficient than the distributed parameter approach, we can reach to this conclusion analyzing the dimension of the solution vector; a couple of dozens of elements (in the case of 3 modes of operation using an MBA model) and 50 elements or

more per equation in the case of the distributed parameter approach which can part of an iteration algorithm (for implicit numerical schemes).

Table 1.3 Summary of two- phase heat exchanger research

Reference	Heat exchanger type	Model	Experiment type
(Escanes, Pérez-Segarra, & Oliva, 1995)	DPCE	HFM	Type I
(Jia, Tso, & Chia, 1995)	P-F	HFM	Type I and II
(Wang, 1997)	DPCE	TFM	Type I
(García-Valladares, Pérez-Segarra, & Rigola, 2004)	DPCE	HFM	Type I
(Hirsh, Steinmaann, & Eck, 2005)	PTSC	HFM	Type I, II and III
(García-valladares & Velázquez, 2009)	PTC	QHFM	Type I and II
(Morales-Ruiz, Rigola, Pérez-Segarra, & García-Valladares, 2009)	GCE	QHFM	Type I and II
(Serrano-Aguilera & Valenzuela, 2016)	PTC	TFM	Type II and IV

Heat exchanger type: DPCE: Double pipe condenser and evaporator. PTC: parabolic- trough solar collector. GCE: Generic pipe flow condenser and/or evaporator. P-F: Plate and fin.

Model: HFM: Homogeneous flow model. QHFM: Quasi-homogeneous flow model. .TFM: Two fluid model

Experiment type: Type I: Model proposal. Type II: numerical validation. Type III: Sinusoidal boundary heat flux disturbance. Type IV: inlet mass flow disturbance.

Some researchers had conducted some numerical experiments to answer qualitatively this question. In (Bendapudi et al., 2008), shell and tube heat exchanger computational performance was tested on an SC-TP operation mode. In this work, the measured time revealed that the MBA was 20% faster than the DPA. Similar computational performances were also reported by (Rasmussen & Shenoy, 2012), (Pangborn, Alleyne, & Wu, 2015), (Rodriguez & Rasmussen, 2016) and (Desideri et al., 2016). But in the case of (Pangborn et al., 2015) they also highlighted that the DPA is more straightforward to implement than the MBA due to the non-universality of switching criteria. Also, accuracy was greater in the DPA when the system was subjected to fast inlet disturbances. This conclusion is due to the fact that the MBA doesn't consider convective transport in their formulation. Therefore, the use of the DPA is advantageous for this kind of problem or when a more comprehensive solution is required on the entire domain.

1.3 Motivation

In a transient 1-D simulation, there is a compromise between accuracy of the results, model robustness and calculation efficiency that must be taken into account in order to select the most appropriate approach. The previous review reveals the benefits of the DPA in terms of robustness and accuracy respect to the MBA, but also shows that the DPA is computationally more expensive, especially for two-phase flow simulations.

Technically, the solution of the DPA is found replacing the continuous operator (divergence, Laplacian, etc.) to their discrete counterpart using some numerical technique (finite differences, finite volume method, finite element method, etc.). This procedure is called discretization. In that sense, time works as an additional coordinate, so that the set of equations must be discretized in time as well as in space. Unlike the behavior in space, which can be elliptic (information can travel back and forth) the time information travels only forward, acquiring a parabolic behavior (Ferziger & Peric, 2002). This means that no fixed information can be given to the solution (except at the boundaries for some particular cases) after the beginning of the computation. Therefore, the way the model advances in time is crucial, making the choice of the temporal numerical scheme to be employed of paramount importance. Regardless of the mathematical model considered (HFM, QHFM, TFM, etc.) most of the researchers prefer to use the classical backward or forward Euler method (first order of accuracy in time) for the treatment of the unsteady terms, but some other transient numerical schemes can be also used, improving the computation cost. In order to employ the most suitable temporal numerical scheme some insight on the physics involved seems necessary. For example, in typical two-phase flow problems the characteristic times can range from $10^{-5} \sim 10^{-1}$ s depending upon the nature of the propagation wave (Stewart, 1984) so that the time step in the computation must be taken with special attention. Another important aspect when choosing the temporal scheme is the expected behavior of the solution, being the so-called stiffness and important factor to consider. Therefore, to solve two-phase flows accurately under the distributed parameter approach, some specific numerical treatment seems advisable, capturing all the possible relevant physical information of the problem in a short computation time. In this way, it is reasonable to develop a numerical method that

ensures accuracy but also can reduce computational cost. This reduction of the computational cost gap can increase the DPA relevance as research and analysis tool.

1.4 Objectives of the thesis

This thesis is focused exclusively on the transient one-dimensional numerical heat exchangers analysis. Special attention is put on two-phase simulations under the distributed parameter approach. With the purpose of assessing the mentioned devices, the following specific objectives are proposed:

1.4.1 Specific objectives

- To propose a numerical method and algorithms for the homogeneous and quasi-homogeneous model in transient-state applied to heat exchangers.
- To experimentally validate and numerically verify the developed numerical method with open literature data.
- To study of boiling flow and static oscillations in evaporators.
- To extend the formulation for mass transfer processes.
- To apply the numerical methodology to other heat exchanger topologies.

1.4.2 Scope

In the present thesis, to reasonably delimitate the problem, the following limitations are made:

- Only pure water will only be considered.
- Variable time-step algorithms are not studied

1.5 Outline of the thesis

The present thesis deals with the 1-D modeling and simulation of heat exchangers in transient-state under the distributed parameter approach. More specifically, this is done for heat exchange processes with liquid-vapor phase change, covering a broad range of transient heat exchanger scopes. In that sense, two mathematical models are considered: the homogeneous flow model and the quasi-homogeneous flow model. An important aspect of this thesis consists of deriving a numerical procedure using high order

temporal schemes in order to improve the computational cost and accuracy of a simulation. A relevant effort is made to validate and verify the proposed numerical procedure. Validation is made against published experimental and numerical data, and due to lack of some data some aspects are exhaustively verified.

To achieve the objectives of this thesis, this document is organized in six (6) chapters as follows:

- In Chapter I, a state of the art about 1-D transient modeling approaches for heat exchanger analysis and simulation is provided. Additionally, the objectives and scope of the thesis are also defined.
- Chapter II offers the theoretical framework on heat exchanger modeling under the distributed parameter approach, thus condensing all the information available on that subject. Methodologically, first the problem is formulated in a general way, and then while introducing some basic concepts the 1-D transient two-phase models are posed. This is done together with their closure relationships, matter of study in this thesis. In this way, the reader can follow the ideas exposed in the following chapters, in a comprehensive way.
- Chapter III the mathematical background required to solve numerically the distinct models under the DPA is explained. Particular emphasis is put on high order time numerical schemes in order to reduce computational cost and improve the quality of the solution. These concepts are expressed in general form and could be applied to any system through appropriate differential equation sets.
- Chapter IV is divided into three main blocks. The first block offers an original numerical method based on high order temporal schemes, using the concepts explained in chapter II. The second block is devoted to validate and verify, in a steady-state and transient-state, the developed numerical method. The third block consists of evaluating the accuracy of the method for static two-phase flow instabilities phenomena and measuring the computational cost of the method.
- Chapter V addresses the problem of counter-current gravity-driven flows in parabolic trough solar collector's technology. For this type of heat exchanger, an original numerical model, based on the numerical method devised in chapter IV

is formulated. In order to allow mass transfer between both interacting phases, the inclusion of a mass transfer numerical algorithm is studied and performed in the model. It is also verified numerically and subjected to typical transient boundary problems in parabolic trough solar concentrating technologies.

- Finally, Chapter VI presents global conclusions and suggests some possibilities for future works.

Nomenclature

Acronyms

1-D	One-dimensional
2-D	Two-dimensional
3-D	Three-dimensional
CC	Concentric circular heat exchanger.
CFD	Computational fluid dynamics
DPA	Distributed parameter approach.
HFM	Homogeneous flow model.
GCE	Generic pipe flow condenser and/or evaporator
MBA	Moving boundary approach.
PDE	Partial differential equation.
PHE	Plate heat exchanger.
PTC	Parabolic trough concentrator.
P-F	Plate & Fin heat exchanger.
QHFM	Quasi-Homogeneous flow model.
SC	Sub-cooled
SH	Superheated
S-T	Shell & Tube heat exchanger.
TFM	Two- fluid model.
TP	Two-phase o mixture

References

- ADINA R & D, I. (2012). Theory and Modeling Guide Theory and Modeling Guide Volume III : ADINA CFD & FSI (Vol. III).
- Aris, R. (1989). Vectors, Tensors and the Basic Equations of Fluid Dynamics. Dover Publications Inc.
- Atkinson, K. E., Han, W., & Stewart, D. E. (2009). Numerical Solution of Ordinary Differential Equations. (J. W. & Sons, Ed.).

Batchelor, G. K. (2000). *An Introduction to Fluid Dynamics*. Cambridge University Press.

Bendapudi, S., Braun, J. E., & Groll, E. A. (2008). A Comparison of Moving-Boundary and Finite-Volume Formulations for Transients in Centrifugal Chillers. *International Journal of Refrigeration*, 31(8), 1437–1452. <https://doi.org/10.1016/j.ijrefrig.2008.03.006>

Caretto, L. S., Gosman, A. D., Patankar, S. V., & Spalding, D. B. (1972). Two Calculation Procedures for Steady, Three- Dimensional Flows with Recirculation. In *Third International Conference on Numerical Methods in Fluid Mechanics* (pp. 60–68). <https://doi.org/doi.org/10.1007/BFb0112677>

Cecchinato, L., & Mancini, F. (2012). An Intrinsically Mass Conservative Switched Evaporator Model Adopting the Moving-Boundary Method. *International Journal of Refrigeration*, 35(2), 349–364. <https://doi.org/10.1016/j.ijrefrig.2011.10.007>

Comsol, M. (2012). *Comsol Multiphysics, User’s Guide: Version 4.3*.

Corberán, J. M., Fernandez de Cordoba, P., González, J., & Alias, F. (2001). Semiexplicit Method for Wall Temperature Linked Equations (SEWTLE): A General Finite- Volume Technique for the Calculation of Heat Exchangers. *Numerical Heat Transfer, Part B*, 40(1), 37–59. <https://doi.org/10.1080/104077901300233596>

Correa, D., & Marchetti, J. (1987). Dynamic Simulation of Shell- and-Tube Heat Exchangers. *Heat Transfer Engineering*, 8(1), 50–59. <https://doi.org/10.1080/01457638708962787>

Das, S. K., & Roetzel, W. (1995). Dynamic Analysis of Plate Heat Exchangers with Dispersion in Both Fluids. *International Journal of Heat and Mass Transfer*, 38, 1127–1140. [https://doi.org/10.1016/0017-9310\(94\)00228-n](https://doi.org/10.1016/0017-9310(94)00228-n)

Das, S. K., Spang, B., & Roetzel, W. (1995). Dynamic Behavior of Plate Heat Exchangers — Experiments and Modeling. *Journal of Heat Transfer*, 117, 859–864. <https://doi.org/10.1115/1.2836302>

Desideri, A., Dechesne, B., Wronski, J., Van den Broek, M., Gusev, S., Lemort, V., & Quoilin, S. (2016). Comparison of Moving Boundary and Finite-Volume Heat Exchanger Models in the Modelica Language. *Energies*, 95(3), 1–18. <https://doi.org/10.3390/en9050339>

Dhar, M., & Soedel, W. (1979). Transient Analysis of a Vapor Compression Refrigeration System. In *Proceedings of the 25th International Congress of Refrigeration*. Venice, Italy.

Dwivedi, A. K., & Das, S. K. (2007). Dynamics of Plate Heat Exchangers Subject to Flow Variations. *International Journal of Heat and Mass Transfer*, 50, 2733–2743. <https://doi.org/10.1016/j.ijheatmasstransfer.2006.11.029>

Escanes, F., Pérez-Segarra, C. D., & Oliva, A. (1995). Thermal and fluid-dynamic behaviour of double-pipe condensers and evaporators — a numerical study. *International Journal of Numerical Methods for Heat & Fluid Flow*, 5(9), 781–795. <https://doi.org/10.1108/EUM00000000004087>

Esposito, M. C., & Gambrotta, A. (2015). A Switching Moving Boundary Model for the Simulation of ORC Plants in Automotive Applications. In 15. Internationales Stuttgarter Symposium. Springer Vieweg, Wiesbaden. <https://doi.org/10.1007/978-3-658-08844-6>

Ferziger, J. H., & Peric, M. (2002). *Computational Methods for Fluid Dynamics* (3rd Edit.). Berlin: Springer- Verlag.

Flanders, H. (1973). Differentiation Under the Integral Sign. *The American Mathematical Monthly*, 80(3), 615–627. <https://doi.org/10.2307/2319163>

Fluent. (2006). *Fluent 6.3 User's Manual*. Fluent Inc. Centerra Resource Park, 10 Cavendish Court, Lebanon, USA.: ANSYS Fluent Inc.

Fuller, S. H., & Millett, L. I. (2011). *The Future of Computing Performance: Game Over or Next Level?* (Samuel H. Fuller and Lynette I. Millett, Ed.). Washington D.C.: The National Academic Press. <https://doi.org/10.17226/12980>

García-Valladares, O., Pérez-Segarra, C. D., & Rigola, J. (2004). Numerical simulation of double-pipe condensers and evaporators. *International Journal of Refrigeration*, 27(6), 656–670. <https://doi.org/10.1016/j.ijrefrig.2004.01.006>

García-valladares, O., & Velázquez, N. (2009). Numerical Simulation of Parabolic Trough Solar Collector: Improvement Using Counter Flow Concentric Circular Heat Exchangers. *International Journal of Heat and Mass Transfer*, 52, 597–609. <https://doi.org/10.1016/j.ijheatmasstransfer.2008.08.004>

Gosman, A. D. (1998). *Developments in Industrial Computational Dynamics*. *Chemical Engineering Research and Design*, 76(2), 153–161. <https://doi.org/10.1205/026387698524721>

Gräber, M., Strupp, N. C., & Tegethoff, W. (2010). Moving Boundary Heat Exchanger Model and Validation procedure. In *EUROSIM Congress on Modelling and Simulation*. Prague. In *EUROSIM Congress on Modelling and Simulation*. Prague, Czech Republic.

Grald, E. W., & MacArthur, J. W. (1992). A Moving-Boundary Formulation for Modeling Time-Dependent Two-Phase Flows. *International Journal of Heat and Fluid Flow*, 13(3), 266–272. [https://doi.org/10.1016/0142-727X\(92\)90040-G](https://doi.org/10.1016/0142-727X(92)90040-G)

Gruber, A. R., & Hyman, S. C. (1956). Flow Distribution Among Parallel Heated Channels. *AIChE Journal*, 2(2), 199–205. <https://doi.org/10.1002/aic.690020214>

Gupta, J. P. (1986). *Fundamentals of Heat Exchangers and Pressure Vessel Technology*. New York: Hemisphere Publishing Corporation.

He, X., Liu, S., Asada, H., & Itoh, H. (1998). Multivariable Control of Vapor Compression Systems. *HVAC&R Research*, 205–230. <https://doi.org/10.1080/10789669.1998.10391401>

Hewitt, G. F. (1982). Flow Regimes. Pressure Drop. Void Fraction. In G. Hetsroni (Ed.), *Handbook of Multiphase Systems* (p. Sections 2.1-2.3). McGraw Hill.

Hirsh, T., Steinmaann, W., & Eck, M. (2005). Simulation of Transient Two-Phase Flow in Parabolic Trough Collectors using Modelica. In 4th International Modelica Conference (pp. 403–412). Hamburg, Germany.

Incropera, F., & DeWitt, D. (1990). *Fundamentals of Heat Transfer*. John Wiley & Sons Inc.

Ishii, M. (2016). Review on Two-Fluid Model for Two-Phase Flow. *Multiphase Science and Technology*, 28(6), 258–320. <https://doi.org/10.1615/MultScienTechn.v28.i3.40>

Ishii, M., & Hibiki, T. (2011). *Thermo- Fluid Dynamics of Two-Phase Flows* (Second Edi). Springer. <https://doi.org/978-1-4419-7985-8>

Jensen, J. M., & Tummescheit, H. (2013). Moving Boundary Models for Dynamic Simulations of Two-Phase Flows. In 2nd International Modelica Conference (pp. 235–244). Oberpfaffenhofen, Germany.

Jia, X., Tso, C. P., & Chia, P. K. (1995). A distributed model for prediction of the transient response of an evaporator. *International Journal of Refrigeration*, 336–342. [https://doi.org/10.1016/0140-7007\(95\)00015-4](https://doi.org/10.1016/0140-7007(95)00015-4)

Kays, W., & London, A. (1984). *Compact Heat Exchangers* (Third edition). New York: McGraw Hill.

Kopyt, P., & Gwarek, W. (2004). A Comparison of Commercial CFD Software Capable of Coupling to External Electromagnetic Software for Modeling of Microwave Heating Process. In *Proceedings of the 6th seminar in computer modeling and microwave*

power engineering (pp. 33–39). Worcester, MA: Worcester Polytechnic Institute. Austin, Texas, USA.

Kurpan, T. (2000). *Heat Exchanger Design Handbook*. New York: Marcel Dekker Inc.

Lakshmanan, C., & Potter, O. E. (1990). Dynamic Simulation of Plate Heat Exchangers. *International Journal of Heat and Mass Transfer*, 33(5), 995–1002. [https://doi.org/10.1016/0017-9310\(90\)90080-E](https://doi.org/10.1016/0017-9310(90)90080-E)

Leducq, D., Guilpart, J., & Trystram, G. (2003). Low Order Dynamic Model of a Vapor Compression Cycle for Process Control Design. *Journal of Food Process Engineering*, 26, 67–91. <https://doi.org/10.1111/j.1745-4530.2003.tb00590.x>

Leveque, R. J. (2002). *Finite Volume Methods for Hyperbolic Problems*. Cambridge University Press.

Li, B., & Alleyne, A. G. (2010). A Dynamic Model of a Vapor Compression Cycle with Shut-Down and Start-Up Operations. *International Journal of Refrigeration*, 33(3), 538–552. <https://doi.org/10.1016/j.ijrefrig.2009.09.011>

Liang, N., Shao, S., Tian, C., & Yan, Y. (2010). Dynamic Simulation of Variable Capacity Refrigeration Systems Under Abnormal Conditions. *Applied Thermal Engineering*, 30(10), 1205–1214. <https://doi.org/10.1016/j.applthermaleng.2010.01.038>

London, A. L., & Seban, R. A. (1980). A Generalization of the Methods of Heat Exchanger Analysis. *International Journal of Heat and Mass Transfer*, 23(3), 5–16. [https://doi.org/10.1016/0017-9310\(80\)90133-7](https://doi.org/10.1016/0017-9310(80)90133-7)

Luo, X., Guan, X., Li, M., & Roetzel, W. (2003). Dynamic Behaviour of One-Dimensional Flow Multistream Heat Exchangers and Their Networks. *International Journal of Heat and Mass Transfer*, 46, 705–715. [https://doi.org/10.1016/S0017-9310\(02\)00303-4](https://doi.org/10.1016/S0017-9310(02)00303-4)

Mckinley, T. L., & Alleyne, A. G. (2008). An Advanced Nonlinear Switched Heat Exchanger Model for Vapor Compression Cycles Using the Moving-Boundary Method. *International Journal of Refrigeration*, 31, 1253–1264. <https://doi.org/10.1016/j.ijrefrig.2008.01.012>

Morales-Ruiz, S., Rigola, J., Pérez-Segarra, C. D., & García-Valladares, O. (2009). Numerical Analysis of Two-Phase Flow in Condensers and Evaporators with Special Emphasis on Single-Phase/Two-Phase Transition Zones. *Applied Thermal Engineering*, 29(5–6), 1032–1042. <https://doi.org/10.1016/j.applthermaleng.2008.05.017>

Pangborn, H., Alleyne, A. G., & Wu, N. (2015). A Comparison Between Finite Volume and Switched Moving Boundary Approaches for Dynamic Vapor Compression System Modeling. *International Journal of Refrigeration*, 53, 101–114. <https://doi.org/10.1016/j.ijrefrig.2015.01.009>

Pantelides, C. C., Gritals, D., Morison, K. R., & Sargent, R. W. H. (1988). The Mathematical Modelling of Transient Systems Using Differential-Algebraic Equations. *Computers & Chemical Engineering*, 12(5), 449–454. [https://doi.org/10.1016/0098-1354\(88\)85062-2](https://doi.org/10.1016/0098-1354(88)85062-2)

Patankar, S. V., & Spalding, D. B. (1974). Calculation Procedure for Transient and Steady-State Behavior of Shell-and-Tube Heat Exchangers. In N. F. Afgan & E. U. Schlunder (Eds.), *Heat Exchanger Design and Theory Source Book*. McGraw Hill.

Patankar, S. V., & Spalding, D. B. (1972). A Calculation Procedure for Heat, Mass and Momentum Transfer in Three-Dimensional Parabolic Flows. *International Journal of Heat and Mass Transfer*, 15, 1787–1806. [https://doi.org/10.1016/0017-9310\(72\)90054-3](https://doi.org/10.1016/0017-9310(72)90054-3)

Patiño, J., Llopis, R., Sánchez, D., Sanz-kock, C., Cabello, R., & Torrella, E. (2014). International Journal of Heat and Mass Transfer A comparative analysis of a CO₂ evaporator model using experimental heat transfer correlations and a flow pattern map. *International Journal of Heat and Mass Transfer*, 71, 361–375. <https://doi.org/10.1016/j.ijheatmasstransfer.2013.12.027>

Peters, M., & Timmerhaus, K. (1991). *Plant Design and Economics for Chemical Engineers* (Fourth). McGraw Hill.

Press, W. H., Teukolsky, S. A., Vetterling, W. T., & Flannery, B. P. (2007). *Numerical Recipes: The Art of Scientific Computing* (Third edit). Cambridge University Press.

Qiao, H., Radermacher, R., & Aute, V. (2010). A Review for Numerical Simulation of Vapor Compression Systems. In *International Refrigeration and Air Conditioning Conference, 2010*, pp. 1–10. (pp. 1–10). Purdue University, West LaFayette, USA.

Rasmussen, B. P., & Shenoy, B. (2012). Dynamic Modeling for Vapor Compression Systems — Part II: Simulation Tutorial. *HVAC&R Research*, 18(5), 37–41. <https://doi.org/10.1080/10789669.2011.582917>

Rodriguez, E., & Rasmussen, B. (2016). A Comparison of Modeling Paradigms for Dynamic Evaporator Simulations with Variable Fluid Phases. *Applied Thermal Engineering*, 112, 1326–1342. <https://doi.org/10.1016/j.applthermaleng.2016.10.131>

- Roetzel, W., Li, M., & Luo, C. X. (2002). Dynamic Behaviour of Heat Exchangers.
- Roetzel, W., & Xuan, Y. (1999). Dynamic Behaviour of Heat Exchangers. Boston, Southamton: WIT Press.
- Runchal, A. (2020). 50 Years of CFD in Engineering Sciences. (A. Runchal, Ed.) (Vol. i). Springer. https://doi.org/10.1007/978-981-15-2670-1_14
- Serrano-Aguilera, J. J., & Valenzuela, L. (2016). Transient Validation of RELAP5 Model with the DISS Facility in Once-Through Operation Mode. In AIP Conference Proceedings (Vol. 1734). <https://doi.org/10.1063/1.4949097>
- Shah, R. K., & Mueller, A. C. (1985). Heat Exchanger Basic Thermal Design Methods in, 2d ed., W. M. Rohsenow, J. E Hartnett, and E. N. Gani~ (eds.), Chapter 4, Part 1, pp. 1-77, 1985. In W. M. Rohsenow, J. E. Hartnett, & E. N. Ganic (Eds.), Handbook of Heat Transfer Applications (Second ed). McGraw Hill.
- Shah, R. K., & Sekulic, D. P. (1999). Fundamentals of Heat Exchanger Design. Begell House Publication.
- Sharifi, F., & Golkar Narandji, M. R. (1995). Dynamic Simulation of Plate Heat Exchangers. International Communications in Heat and Mass Transfer, 22(2), 213–225. [https://doi.org/10.1016/0735-1933\(95\)00006-2](https://doi.org/10.1016/0735-1933(95)00006-2)
- Song, J. H. (2003). A remedy for the ill-posedness of the one-dimensional two-fluid model. Nuclear Engineering and Design, 222, 40–53. [https://doi.org/10.1016/S0029-5493\(02\)00391-6](https://doi.org/10.1016/S0029-5493(02)00391-6)
- Song, J. H., & Ishii, M. (2000). The Well-Posedness of Incompressible One-Dimensional Two-Fluid model. International Journal of Heat and Mass Transfer, 43, 2221–2231. [https://doi.org/10.1016/S0017-9310\(99\)00287-2](https://doi.org/10.1016/S0017-9310(99)00287-2)
- Srihari, N., Rao, B. P., Sunden, B., & Das, S. K. (2005). Transient Response of Plate Heat Exchangers Considering Effect of Flow Maldistribution. International Journal of Heat and Mass Transfer, 48, 3231–3243. <https://doi.org/10.1016/j.ijheatmasstransfer.2005.02.032>
- Stewart, H. B. (1984). Two- Phase Flow: Models and Methods. Journal of Computational Phy, 56(363–409). [https://doi.org/10.1016/0021-9991\(84\)90103-7](https://doi.org/10.1016/0021-9991(84)90103-7)
- Sunden, B. (2005). High Temperature Heat Exchangers (HTHE), (September), 226–238.
- Sunden, B. (2007). Computational Fluid Dynamics in Research and Design of Heat Exchangers. Heat Transfer Engineering, 28(11), 898–910. <https://doi.org/10.1080/01457630701421679>

Toro, E. F. (2009). *Riemann Solvers and Numerical Methods for Fluid Dynamics: A Practical Introduction* (3rd Edit.). Springer. <https://doi.org/10.1007/978-3-540-49834-6>

Wallis, G. B. (1969). *One-Dimensional Two-Phase Flow*. McGraw Hill.

Wang, C. (1997). A Numerical Method for Thermally Non-Equilibrium Condensing Flow in a Double-Pipe Condenser. *Applied Thermal Engineering*, 17(7), 647–660. [https://doi.org/10.1016/S1359-4311\(96\)00092-0](https://doi.org/10.1016/S1359-4311(96)00092-0)

Wedekind, G. L. (1971). An Experimental Investigation Into the Oscillatory Motion of the Mixture-Vapor Transition Point in Horizontal Evaporating Flow. *Journal of Heat Transfer*, 93(1), 47–54. <https://doi.org/10.1115/1.3449764>

Wedekind, G. L., Bhatt, B. L., & Beck, B. T. (1978). A System Mean Void Fraction Model for Predicting Various Transient Phenomena Associated with Two-Phase Evaporating and Condensing Flows. *International Journal of Multiphase Flow*, 4, 97–114. [https://doi.org/10.1016/0301-9322\(78\)90029-0](https://doi.org/10.1016/0301-9322(78)90029-0)

Wedeking, G. L., & Stoecker, W. F. (1968). Theoretical Model for Predicting the Transient Response of the Mixture- Vapor Transition Point in Evaporating Flow. *Journal of Heat Transfer*, 90(1), 165–174. <https://doi.org/10.1115/1.3597448>

Willatzen, M., Pettit, N. B. O. L., & Ploug-Sorensen, L. (1998). A General Dynamic Simulation Model for Evaporators and Condensers in Refrigeration. Part I: Moving-Boundary Formulation of Two-Phase Flows with Heat Exchange. *International Journal of Refrigeration*, 21(5), 398–403. [https://doi.org/10.1016/S0140-7007\(97\)00091-1](https://doi.org/10.1016/S0140-7007(97)00091-1)

Wissler, E. H., Isbin, H. S., & Amundson, N. R. (1956). Oscillatory Behaviour of a Two-phase Natural-circulation Loop. *AIChE Journal*, 2(2), 157–162. <https://doi.org/10.1002/aic.690020206>

Wozny, G. (1994). Dynamic Process Simulation in Industry. *International Chemical Engineering*, 34(2), 159–177.

Xia, L., De Abreu- Garcia, J. A., & Hartley, T. T. (1991). Modeling and Simulation of a Heat Exchanger. In *Proceedings of the IEEE International Conference on Systems Engineering* (pp. 453–456). Dayton, OH, USA, USA. <https://doi.org/10.1109/ICSYSE.1991.161174>

Xu, H., Li, Y., Sun, J., & Li, L. (2019). Transient Model and Characteristics of Parabolic-Trough Solar Collectors: Molten salt vs. Synthetic Oil. *Solar Energy*, 182(January), 182–193. <https://doi.org/10.1016/j.solener.2019.02.047>

Yüncü, H., & Kakaç, S. (1988). Fundamentals of Two-Phase Flow Instabilities. In S. Kakaç, A. E. Bergles, & E. O. Fernandes (Eds.), *Two-Phase Flow Heat Exchangers* (pp. 375–406). Springer. https://doi.org/10.1007/978-94-009-2790-2_11

Zahn, W. R. (1964). A Visual Study of Two-Phase Flow While Evaporating in Horizontal Tubes. *Journal of Heat Transfer*, 86(3417–429). <https://doi.org/10.1115/1.3688713>

Zhang, W., & Zhang, C. (2006). A Generalized Moving-Boundary Model for Transient Simulation of Dry-Expansion Evaporators Under Larger Disturbances. *International Journal of Refrigeration*, 29, 1119–1127. <https://doi.org/10.1016/j.ijrefrig.2006.03.002>

Heat Exchangers Physical Modelling

If we consider the matter as a continuum media, where no discontinuity is observable, the continuum hypothesis can be applied without any restriction (Batchelor, 2000). This hypothesis guarantees that all the functions (velocities, pressure, enthalpy, etc.) are continuously differentiable, and a set of equations can be derived with the aim of differential calculus. Continuum mechanics through local description of mass, momentum (forces) and energy provide the mathematical models to achieve the goal of modeling entirely a heat exchanger in reasonable detail. This chapter is devoted to defining the equations that describe mathematically the thermal-hydraulic behavior of a heat exchanger in transient state for the solid wall and the participant fluids, either for single or two-phase flows, making particular emphasis on one-dimensional simulation, which is the main topic of this thesis.

2.1 Solid Wall modeling

Solid walls play a fundamental role in heat exchangers. They not only provide structural strength but also is the media from which heat is transfer to the fluids. Assuming that the material is homogeneous, all properties (density, specific heat capacity) are constant, and heat conduction is modeled by the Fourier conduction law $q_i = -\lambda(\partial T / \partial z_i)$ the energy equation in differential and integral forms read:

$$\left(\rho C_p \frac{\partial T}{\partial t} \right)_{wall} = \lambda_{wall} \nabla^2 T_{wall} + \dot{Q}'''(z_i, t) \quad (2.1)$$

$$\rho C_p \int_V \frac{\partial T}{\partial t} dV = \lambda_{wall} \int_S \nabla T_{wall} \cdot \hat{n} dS + \int_V \dot{Q}'''(z_i, t) dt \quad (2.2)$$

2.2 Fluid flow modeling

In fluid dynamics, two different approaches are used to make a total description

of the system; Lagrangian and Eulerian. In the Lagrangian approach, the entire fluid domain is divided into a finite number of particles, and each one of them is followed in time. This tracking is made with a force balance equation, neglecting rotation, in which the particle forces include gravity, drag and lift forces. In this way we have a single equation of motion for each particle; hence a particle path can be defined at every time (t) knowing its initial position ($x_i(t_0)$). This representation, at first sight, seems very convenient, easy and even intuitive; nevertheless, the number of fluids particles that must be traced in order to obtain meaningful results is enormous and for theoretical studies and is not often used, see (Bennett, 2006) for further details.

With a Eulerian description, instead of following each particle through time, velocity is calculated in a fixed spatial domain. Under this approach velocity can be calculated as a function of space and time. This also is made for any other scalar variables (ϕ) like pressure or enthalpy for example.

$$u_i = u_i(x_j, t) \quad (2.3) \quad \phi = \phi_i(x_j, t) \quad (2.4)$$

Applying balances of mass, momentum (force), and energy using the Reynolds transport theorem, the fundamental balance relationships can be derived, (Batchelor, 2000) and (Aris, 1989). These equations for single-phase flows can be written as a system of conservation laws, in both, integral and differential form as:

Integral form

$$\frac{\partial}{\partial t} \int_V \rho \psi_i dV + \int_S \rho u_k \psi_i \cdot \hat{n}_j dS = \int_S J_i \cdot \hat{n}_j dS + \int_V \rho \phi_i dV \quad (2.5)$$

Differential form

$$\frac{\partial(\rho \psi_i)}{\partial t} + \frac{\partial(\rho u_j \psi_i)}{\partial z_j} = \frac{\partial J_i}{\partial z_i} + \rho \phi_i \quad (2.6)$$

Here ρ is the material density; ϕ any vector function per mass unit and J is the vector of surface forces, see Table 2. 1.

Table 2. 1 Summary of functions for balance equations

Balance equation	ψ	$\mathbf{J}$	ϕ
Mass Conservation	1	0	0
Momentum	u_i	$\mathbb{T}_{ij} = -p\mathbb{I}_{ij} + \tau_{ij}$	g_i
Energy	$E = e + \frac{1}{2}u_i^2$	$\dot{Q}''' - \mathbb{T}_{ij}u_i$	$gu_i + \frac{\dot{q}'''}{\rho}$

To close the system of equations, some constitutive relations for thermodynamic state (for compressible and multiphase flows) and shear stress are required. For compressible and Newtonian fluids these relations are:

$$\tau_{ij} = \frac{\mu}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (2.7)$$

$$\rho = \rho(p, h) \quad (2.8)$$

2.3 Multiphase flow modeling

The mass, momentum, and energy balances expressed in equations (2.5) and (2.6) are valid when the field of dependent functions (ψ_i) are continuous and smooth on the entire “physical” domain. This requirement holds for single-phase flows because properties and field variables don’t vary abruptly in space and/or in time. In multiphase or multicomponent flows this requirement is not fulfilled. The different phases (or components) are separated by a continuous interphase that can be considered mathematically of a surface of discontinuity. These interphases can obviously change in shape at any time t and can travel with different velocities (u_A) and even can coalesce or appear suddenly. Therefore, one can use a local instant formulation (such like single-phase flows) based on conservation laws for each phase or component k , on each subdomain (bounded by an interphase), and then model the interphase with the appropriate jump conditions relating the flow parameters on both sides of the interphase (Slattery, 1972).

According to the above discussion, the conservation laws with their respective jump conditions written in canonical form are:

$$\frac{\partial(\rho_k \psi_{i,k})}{\partial t} + \frac{\partial(\rho_k u_{j,k} \psi_{i,k})}{\partial x_j} = -\frac{\partial \mathbf{J}_{i,k}}{\partial x_i} + \rho_k \phi_k \quad (2.9)$$

With jump conditions:

$$\left[\rho_k \psi_{j,k} (u_{j,k} - u_A) + J_{j,k} \right] \cdot \hat{n}_h = \Omega_{j,k} \quad \text{Summation over } k \quad (2.10)$$

Figure 2.1 Discontinuity across an interphase

The values of ψ , J , and ϕ are the same that appear in Table 2. 1. The value of Ω are shown in Table 2. 2 and represents the interfacial source of ψ .

Table 2. 2 Jump conditions source function

Balance equation	Ω
Mass Conservation	0
Momentum	$\dot{m}$
Energy	q_i/θ

2.4 Averaging

In the previous section, formulations for single and two-phase flows were presented. It was stated that for two-phase flows one can pose the conservation laws for each phase jointly with appropriate jump conditions. The problem with this approach is that the location of the interphases is not known in advance, being enhanced by the fact that these interphases locations can be dispersed randomly all around the fluid bulk. Furthermore, from a physics point of view, the presence of an interphase has an essential effect on the full dynamics of the system (M Ishii, 2016). For example, single-phase flows share some topological similarities, the reason why they can be classified as laminar, transitional or turbulent flows. In two-phase flows, it's much more complicated. They also share some characteristic similarities but in this case the classification is due to the liquid-gas flow pattern. Much experimental work has been made to find out how many

flow patterns exists, developing stability maps for certain pipe orientations, (Hewitt, 1982) (vertical upflow and horizontal), (Hewitt & Roberts, 1969) (vertical upward), (Mandhane, Gregory, & Aziz, 1974) (horizontal flow) and (Taitel Y & Dukler A, 1976) (horizontal and nearly horizontal flows). Under this discouraging scenario, another approach must be taken. In that sense, the use of average quantities seems appropriate. The average process provides the mathematical tool to eliminate local instant fluctuations (M Ishii & Ibiki, 2011), working in this way with smooth variable fields. This averaging must be made in such way that all the relevant physics at all time and length scales are still captured. The average process can be made in several different ways. The most common average type are made in space: volume, area or length, (Nigmatulin, 1979) (Vernier & Delhay, 1968), time (M Ishii & Ibiki, 2011), combinations of time and space (Drew, 1971) and statistical averaging (Buyevich, 1971). Each one of these methods of averaging has been designed for specific applications; for example, time-averaging is useful to determine residence time of void fractions or any species concentration, statistical average have been used extensively in rheology research (Batchelor, 1974). In heat exchanger analysis it is of paramount importance to determine carefully void fraction, because it is an essential variable describing not only hydrodynamics due to the sensibility of density, and in consequence in velocity, but also in heat transfer characteristics like initiation of boiling, particularly important in safety analysis of some industrial systems like nuclear power generation. According to (Soo, 1989), volume averaging is convenient because the systems of equations can be expressed in terms of the void fraction, hence is a reasonable approach for heat exchangers, especially in 1-D modelling.

Volume average can be performed over the entire volume (total average) or over the k^{th} phase volume (intrinsic). Mathematically, volume average for any given generic function ψ is defined as:

$$\langle \psi_k \rangle = \frac{1}{V} \int_{V_k} \psi_k dV \quad (\text{Total}) \quad (2.11) \quad \tilde{\psi}_K = \frac{1}{V_k} \int_{V_k} \psi_k dV \quad (\text{Intrinsic}) \quad (2.12)$$

In a two-phase flow stream, different length scales co-exist; on the one hand, there is a geometric length scale defined by the geometry of the enclosure, the diameter or channel depth in a pipe or a parallel channel flow respectively, on the other hand, each

phase has their hydrodynamic scale: in a bubbling flow for example, the length scale is the characteristic diameter of the bubbles (or dispersed phase). This combination of scales restricts the size of the average volume in order to obtain meaningful results. Logically, the average volume must be smaller than the geometric scale (D) but the choice of the lower limit is not so intuitive.

Figure 2. 2 Volume averaging length scales

If the volume is too small, one can locally not measure any bubble; hence the volume must be greater than the characteristic length of the bubbles (Whitaker, 1969). As a rule of thumb in order to have representative measures one might restrict the averaging volume as $D < l < L$, hence, $\Delta V \sim \mathcal{O}(l^3)$.

Figure 2. 3 Volume average adjustment in 1-D modeling

In 1-D modeling only one degree of freedom is possible, the volume can be adjusted changing the axial or streamwise position due to the cross-section area is fixed. From this way we can have a decrease sequence of volumes $\Delta V_1 > \Delta V_2 > \dots > \Delta V_n$, therefore, inside that sequence we can have a volume ΔV_m with $n \leq m \leq 1$ in which the void fraction measurement is asymptotically stable. This volume must also fulfill some

other numerical requirements in order to obtain numerical stable solutions. This issue will be discussed in Chapter III.

2.5 Void fraction

The void or volume fraction can be defined simply as the total volume of a phase (or specie) contained inside an averaging volume of fluid, so that:

$$\varepsilon_k = \frac{V_k}{V} \quad (2.13)$$

With

$$\sum_k \varepsilon_k = 1 \quad (2.14)$$

In a two- phase (liquid + vapor) flow, the last equations can be simplified as:

$$\varepsilon_v = \varepsilon = \frac{V_v}{V} \quad (2.15) \quad \varepsilon_l = 1 - \varepsilon_v = 1 - \varepsilon \quad (2.16)$$

2.6 Local averaged equations

In the previous two sections, the basic conservations equations were first presented for a single-phase flow, then the mathematical difficulties in formulating the problem with macroscopic local descriptions were highlighted, introducing therefore the notion of averaging. The next step is to average the set of conservation equations for any generic k phase in order to obtain a smoothly mathematical formulation. Each equation is volume averaged using the total volume operator ($\langle \rangle$). Considering the Reynolds rules (Drew, 1971) and the derivate of averaged quantities (Slattery, 1972), (Whitaker, 1969) one yields.

$$\frac{\partial \langle \rho \psi_k \rangle}{\partial t} + \nabla \cdot \langle \rho \mathbf{u} \psi_k \rangle = \nabla \cdot \langle \mathbf{J} \rangle + \langle \rho \phi \rangle + \Gamma_k''' \quad (2.17)$$

The average balance equation functions are summarized in Table 2. 3 and a complete derivation of the equation can be found in Annex B

Table 2. 3 Summary of functions for averaged balance equations

Balance equation	ψ	$\mathbf{J}$	ϕ	Interfacial transfer (Γ_k''')
Mass Conservation	1	0	0	$\frac{1}{V} \int_{S_k} \rho(\mathbf{u}_A - \mathbf{u}) \cdot \hat{n} dS$
Momentum	$\mathbf{u}$	$\mathbb{T}$	$\mathbf{g}$	$\frac{1}{V} \int_{S_k} \rho \mathbf{u}(\mathbf{u}_A - \mathbf{u}) \cdot \hat{n} dS + \frac{1}{V} \int_{S_k} \mathbb{T} \cdot \hat{n}_k dS$
Energy	$e + \frac{1}{2} \mathbf{u} \cdot \mathbf{u}$	$\mathbb{T} \cdot \mathbf{u} + \dot{Q}'''$	$\phi \cdot \mathbf{u} + \frac{\dot{q}'''}{\rho}$	$\frac{1}{V} \int_{S_k} \rho E(\mathbf{u}_A - \mathbf{u}) \cdot \hat{n} dS + \frac{1}{V} \int_{S_k} (\mathbb{T} \cdot \mathbf{u} + \dot{\mathbf{Q}}''') \cdot \hat{n} dS$

2.7 The one- dimensional hypothesis

Strictly speaking, all physical systems are three- dimensional. This is equivalent to say that velocity, pressure, density, and any other scalar quantities (ψ) varies in a three- dimensional space, as we usually expect.

$$\mathbf{u} = u_i(x_j) \hat{e}_i \quad (2.18) \quad \psi = \psi(x_j) \quad (2.19)$$

Under this framework, Equations (2.6), (2.9) and (2.17) were derived. However, the complexity of these equations is such that it is reasonable to use some simplifications. In many engineering applications it's common to use the so-called one-dimensional approach or formulation based on the so-called one-dimensional hypothesis. This hypothesis states that all mathematical fields are constant at any cross-section normal to the main direction (streamline direction) of the flow (Hicks, Montgomery, & Wasserman, 1947), (Daneshyar, 1976). The main consequence of this assumption is that vector fields are parallel to the main direction and scalar fields can be represented by a single one independent variable function. Taking z as the main direction this assumption reads (Von Mises, 1958).

$$\mathbf{u} = u \hat{e}_z \quad (2.20) \quad \psi = \psi(z) \quad (2.21)$$

$$\frac{\partial}{\partial x_i} \equiv 0 \quad \text{for} \quad i \neq z \quad (2.22)$$

This assumption by itself is too restrictive, conferring a constant and parallel flow behavior, losing important features of the flow. For instance, the real flow varies from zero (no-slip condition) and wall temperature at the wall to a maximum value located somewhere at the bulk of the flow, see Figure 2. 4. Therefore, the one-dimensional assumption can be relaxed in order to extend the applicability with no loss of generality. The restriction can be lowered by simply assuming that the rate of change at all directions are negligible in comparison with the streamline direction.

$$\frac{\partial}{\partial x_i} \ll \frac{\partial}{\partial z} \quad \text{for } i \neq z$$

Therefore, a cross-section average value of vector fields can be obtained.

$$\bar{u}_z = \frac{1}{A} \int_A u(A) dA \quad (2.23)$$

$$\bar{\psi}_z = \frac{1}{A} \int_A \psi(A) dA \quad (2.24)$$

The resulting variables, at first sight, seem unaltered; however, the meaning of the variables is not the same. Working with area average functions gives meaningful sense of all variables. With these simplifications a one-dimensional system of conservation equations is found (Hibiki & Ishii, 2003), see Equation (2.25).

Figure 2. 4 Area averaged vector, and scalar fields for pipe flows

$$\left. \begin{aligned} \frac{\partial \langle \rho \rangle}{\partial t} + \frac{\partial \langle \rho u \rangle}{\partial z} &= \Gamma_k \\ \frac{\partial \langle \rho u \rangle}{\partial t} + \frac{\partial \langle \rho u^2 \rangle}{\partial z} &= -\frac{\partial \langle p \rangle}{\partial z} + \frac{\partial \langle p \rangle_{fr}}{\partial z} + \langle \rho \rangle g \sin \beta + M_k^\Gamma \\ \frac{\partial \langle \rho E \rangle}{\partial t} + \frac{\partial \langle \rho u E \rangle}{\partial z} &= \langle \dot{Q}'' \rangle + Q_k^\Gamma \end{aligned} \right\} \quad (2.25)$$

2.8 One dimensional two-phase flow models

Many two-phase models have been developed in the last past decades, being each one of them designed for specific applications. Among the most common models are the homogeneous flow model (HFM) (Wallis, 1969), quasi-homogeneous flow model (QHFM) (Kandlikar, 1999) and the fluid model (TFM) (M Ishii & Ibiki, 2011).

2.8.1 Homogeneous flow model

The homogeneous flow (HFM) model is the simplest possible approach in two-phase flows analysis. It is assumed that both phases are in thermal and mechanical equilibrium. This means that no momentum and energy is transfer through any interphase. Additionally, both phases have the same phase velocity, as a consequence $S_R = 1$. These assumptions are true for some particular conditions. According to (Husain, Choe, & Weisman, 1974) homogeneous to non-homogeneous transition happens at high mass fluxes ($G > 2,700 \text{ kg} \cdot \text{s}^{-1} \cdot \text{m}^{-2}$), other researchers by their side ensure that homogeneous occurs at high pressures or low densities ratios (ρ_l / ρ_v) (Meyer & Wallis, 1965). With these assumptions, only one system of equation for the mixture is needed (Hewitt, 1982), simplifying tremendously the system of equations. The basic relations in this model are:

$$u_l = u_v = u \quad (2.26) \quad \varepsilon = \frac{x}{x + (1-x) \frac{\rho_v}{\rho_l}} \quad (2.27)$$

$$\rho_{TP} = \varepsilon \rho_v + (1-\varepsilon) \rho_l \quad (2.28) \quad h_{TP} = \varepsilon h_v + (1-\varepsilon) h_l \quad \text{v}(2.29)$$

The model can be written conveniently with mass flow, density, and enthalpy as dependent variables.

$$\frac{\partial(\psi_i)}{\partial t} + \frac{\partial(K\dot{m}\psi_i)}{\partial z} = -\frac{\partial J_i}{\partial z} + \rho_{TP}\phi_i + b_i \quad (2.30)$$

Table 2. 4 Homogeneous flow model function summary

Balance equation	ψ	J	K	ϕ	b
Mass Conservation	ρ_{TP}	0	$1/\rho_{TP}$	0	0
Momentum	$\dot{m}$	pA	$1/\rho_{TP}A$	$\rho_{TP}gA \sin \beta$	$\langle \partial p / \partial z \rangle'_{fr}$
Energy	$\rho_{TP}h_{TP}A$	0	$1/\rho_{TP}A$	0	$\dot{Q}'_w$

2.8.2 Quasi-homogeneous flow model (QHM)

In the quasi-homogeneous model (QHM) the flow is still considered as a mixture in equilibrium, but in this case, both phase velocities are not assumed anymore as equal ($S_R \neq 1$), see references (Hewitt, 1982) for further details on fundamental information and (Escanes et al., 1995), (García-Valladares et al., 2004) and (Morales-Ruiz et al., 2009) for specific applications of the model. In this case, the basic relations are:

$$S_R = \frac{u_v}{u_l} \quad (2.31) \quad \varepsilon = \frac{x}{x + S_R(1-x)\frac{\rho_v}{\rho_l}} \quad (2.32)$$

$$\rho_{TP} = \varepsilon\rho_v + (1-\varepsilon)\rho_l \quad (2.33) \quad h_{TP} = \varepsilon h_v + (1-\varepsilon)h_l \quad (2.34)$$

In this model, slip velocities play a fundamental role, and the model is not restricted like HFM for low densities ratios or low pressures, covering a wider range of applications. Void fraction now depends on the slip ratio, and another equation must be coupled in order to close the problem. Maybe the first attempt to derive an expression of void fraction with slip velocities is attributed to (Lockhart & Martinelli, 1949). The basic assumption of this model is that liquid and gas phases flow simultaneously with equal local pressure between these phases. Mathematically, they derived the X^2 parameter, defined as the ratio of the single-phase liquid and gas pressure drop as:

$$X^2 = \frac{dp/dz_l}{dp/dz_v} \quad (2.35)$$

$$\phi_l^2 = \frac{dp/dz}{dp/dz_l} = 1 + \frac{C}{X} + \frac{1}{X^2} \quad \text{or} \quad \phi_v^2 = \frac{dp/dz}{dp/dz_v} = 1 + CX + X^2 \quad (2.36)$$

The values of dimensionless constant C have been found by (Chisholm, 1973) empirically to fit the model for turbulent and laminar flows, in Table 2.5, the values for C are shown.

Table 2.5 Empirical fit values for Lockhart & Martinelli curves

Liquid	Gas	C
Turbulent	Turbulent	20
Viscous	Turbulent	12
Turbulent	Viscous	10
Viscous	Viscous	5

With these definitions, the void fraction can be determined merely as:

$$\varepsilon = \frac{1 - \phi_l}{\phi_l} \quad (2.37)$$

The Lockhart & Martinelli tends to overpredict void fraction. To overcome this problem, some empirical work has been conducted. Some specific slip models correlations can be found in (Mochizuki & Ishii, 1992) and (Osmachkin & Borisov, 1970), but the most accepted correlation is the one proposed by (Premoli, Franceso, & Prina, 1971). This correlation minimized the error found in Lockhart & Martinelli equation using a vast number of experimental data, reason why is universally accepted. This correlation is:

$$S_R = 1 + E_1 \sqrt{\frac{y}{1 + yE_2}} - yE_2 \quad (2.38)$$

Where:

$$y = \frac{\beta}{1 - \beta} \quad E_1 = 1.57 Re_{lo}^{-0.19} \left(\frac{\rho_l}{\rho_v} \right)^{0.22} \quad E_2 = 0.0273 We Re_{lo}^{-0.08} \left(\frac{\rho_l}{\rho_v} \right)^{0.22} \quad \beta = \frac{Q_v}{Q_v + Q_l}$$

Re_{l0} and We are the Reynolds and Weber numbers for pure liquid, and β is the volumetric flow fraction. Using again the canonical form (2.30) the QHFM can then be summarized as.

Table 2. 6 Quasi- homogeneous flow model function summary

Balance equation	ψ	J	K	ϕ	b
Mass Conservation	ρ_{TP}	0	$1/\rho_{TP}$	0	0
Mommentum	$\dot{m}$	pA	$\frac{1}{A} \left[\frac{x^2}{\rho_g \varepsilon} + \frac{(1-x)^2}{\rho_l (1-\varepsilon)^2} \right]$	$\rho_{TP} g A \sin \beta$	$\left\langle \partial p / \partial z \right\rangle'_{fr}$
Energy	$\rho_{TP} h_{TP} A$	0	$1/\rho_{TP} A$	0	$\dot{Q}'_w$

2.9 The two-phase total pressure gradient

The total pressure gradient is caused by resistance forces applied to the fluid. These forces can be decomposed in three terms; gravitational ($\rho_{TP} g A \sin \beta$), inertial ($\partial \dot{m} / \partial t + \partial K \dot{m}^2 / \partial z$) and frictional ($\left\langle \partial p A / \partial z \right\rangle'_{fr}$), see the canonical equation (2.30). The first two terms are calculated directly from the momentum equation and the third must be calculated with an extra one. Frictional forces are caused by flow resistance at the walls of the conduits (shear stress). This force per unit length can be calculated simply as $\left\langle \partial p A / \partial z \right\rangle'_{fr} = -\tau_w S_w$. Hence, using the hydraulic diameter ($D = 4A / S_w$) and friction factor definitions, friction force can be calculated as:

$$\left. \begin{aligned} \left(\frac{\partial p A}{\partial z} \right)'_{fr} &= -\frac{4\tau_w A}{D} \\ f_F &= \frac{\tau_w}{\frac{1}{2} \rho u^2} \end{aligned} \right\} \Rightarrow \left(\frac{\partial p A}{\partial z} \right)'_{fr} = -\frac{2f_F \rho u^2 A}{D} = \frac{2f_F \dot{m}^2}{\rho D A} \quad (2.39)$$

In the above equation, f_F stands for the Fanning friction factor. Typically, the Darcy friction factor (f) is often used rather than the Fanning friction factor. Both friction factors are identically defined, except that Darcy friction factor is multiplied by a factor of four ($f = 4f_F$). The definition of friction factors will be presented in Section 2.9.1.

In the homogeneous flow model, this term is calculated using a mixture friction factor, which is defined with the two-phase mixture Reynold number.

$$\text{Re}_{TP} = \frac{\dot{m}D}{\mu_{TP}A} \quad (2.40)$$

Here μ_{TP} is the two-phase dynamic viscosity. The problem with this definition is that viscosity is not defined for mixtures, and some auxiliary models must be employed. The most common models are:

Table 2. 7 Homogeneous Two-phase viscosity definitions

Reference	Equation
(McAdams, Woods, & Bryan, 1942)	$\frac{1}{\mu_{TP}} = \frac{x}{\mu_v} + \frac{1-x}{\mu_l}$
(Cicchitti, Lombardi, Silvestri, Soldai, & Zavattarelli, 1960)	$\mu_{TP} = x\mu_v + (1-x)\mu_l$
(Owens, 1961)	$\mu_{TP} = \mu_l$
(Dukler, Wicks, & Cleveland, 1964)	$\mu_{TP} = \rho_{TP} [xv_v\mu_v + (1-x)v_l\mu_l]$
(Beattie & Whalley, 1982)	$\mu_{TP} = \omega\mu_v + (1-\omega)(1+2.5\omega)\mu_l$ $\omega = \frac{xv_v}{v_l + xv_v}$
(Lin, Kwok, Li, Chen, & Chen, 1991)	$\mu_{TP} = \frac{\mu_l\mu_v}{\mu_v + x^{1.4}(\mu_l - \mu_v)}$

As summarized in Table 2. 7 there are several ways to define two-phase viscosity, an essential parameter to calculate pressure drop. Several works had been conducted in order to establish which definition of homogeneous two-phase flow viscosity gives more accurate pressure drop predictions. In (Idsinga, Todreas, & Bowring, 1977) the comparison was made with 2,200 experimental points made for water at high pressures (250- 1,500 psia), moderate to high mass fluxes (270- 4,340 kg·s⁻¹·m²), covering the range from sub-cooled state to saturated vapor for hydraulic diameters from 2.3-33 mm. They concluded that the definitions of (Owens, 1961) and (Cicchitti et al., 1960) correlations exhibit the best performance.

By their side, the quasi-homogeneous flow model instead of assuming that the two-phase stream behaves like a homogeneous mixture, it is assumed that total force is a contribution of both phases. This concept gave birth to the concept of two-phase flow multipliers. The most extended two-phase flow multiplier model is the so-called Lockhart & Martinelli method; some basic notions of this model are mentioned in Section 2.8.2. The basic assumption of this model is that liquid and gas phases flow simultaneously with equal local pressure between these phases. This model was designed for separated flows; therefore, which is a particular case of non-homogeneous flows, it has been used for any two-phase flow pattern with excellent results. There is a consensus that this model provides good approximations. Pressure gradient terms under this scope is calculated as:

$$\left(\frac{\partial p A}{\partial z}\right)'_{fr} = -\frac{4\tau_w A}{D} = -\phi_l^2 \left(\frac{\partial p A}{\partial z}\right)'_{fr,l} = -\phi_v^2 \left(\frac{\partial p A}{\partial z}\right)'_{fr,v} \quad (2.41)$$

2.9.1 Friction factor

For pipe or closed conduit flows, the most often used equation for the Darcy friction factor is the so-called Colebrook equation (Colebrook, 1939).

$$\frac{1}{\sqrt{f}} = -2 \log_{10} \left(\frac{2,51}{\text{Re} \sqrt{f}} + \frac{R}{3,7D} \right) \quad (2.42)$$

The above equation is implicit. Hence, iterative numerical methods are needed, for example, the fixed point or Newton-Raphson method, in order to obtain solutions for f . For large scale computations, this is unacceptable due to the increase in the computational cost. In that sense, explicit formulae are attractive due to the less computational effort required. Many explicit approximations have been published. According to (Genić et al., 2011) the most accurate explicit approximations of Colebrook equation are those proposed by Zigrang & Sylvester (Chen, 1984), (Churchill, 1977) and (Haaland, 1983). Other expressions with less accuracy can be found in (Genić et al., 2011) and (Brkić, 2011).

Table 2. 8 Colebrook equation explicit approximations

Author	Equation	Range
(Churchill, 1977)	$f = \left[-2 \log_{10} \left(\frac{R}{3.7D} + \frac{7}{\text{Re}^{0.9}} \right) \right]^{-2}$	Not specified
(Zigrang & Sylvester, 1985)	$f = \left\{ -2 \log_{10} \left[\frac{R}{3.7D} - \frac{5.02}{\text{Re}} \log_{10} A \right] \right\}^{-2}$ $A = \frac{R}{3.7D} - \frac{5.02}{\text{Re}} \log_{10} \left(\frac{R}{3.7D} + \frac{13}{\text{Re}} \right)$	$\text{Re} = 4000 \sim 10^8$ $\frac{R}{D} = 4 \times 10^{-5} \sim 0.05$
(Haaland, 1983)	$f = \left\{ -1.8 \log_{10} \left[\left(\frac{R}{3.7D} \right)^{1.11} + \frac{6.9}{\text{Re}} \right] \right\}^{-2}$	$\text{Re} = 4000 \sim 10^8$ $\frac{R}{D} = 10^{-6} \sim 0.05$

The above equation is of universal use in science and engineering to calculate pressure drop. However, it is defined only for single-phase flows. Pressure drop in two-phase flow streams is much complicated, see Section 2.9.

Figure 2. 5 HFM and QHFM pressure drop comparison

2.10 Two fluid model

Other more sophisticated models for two-phase flow simulations are available in the literature. In the HFM and QHFM, the assumption of mechanical and thermal equilibrium (equal pressures and temperature) implies that interphase exchange can be neglected. Therefore the entire flow can be modeled as a mixture; hence only three differential equations are needed (mass, momentum and energy) jointly with closure relations for thermodynamic state (equation of state), friction factor and slip ratio for the QHFM. In the Two-Fluid model these assumptions are no longer valid; hence, pressures, temperatures and interphase exchange are determined individually for each

phase. For extensive information over the different models and closure relationships see references (M Ishii, 2016) and (M Ishii & Ibiki, 2011).

2.11 One dimensional transient two-phase software

Much software has been developed in the past decades for 1-D two-phase flow simulations. Each code has been designed carefully for different applications, solving different models with different numerical approaches. Among the most common 1-D software we can cite.

Table 2. 9 1-D commercial software

Software	Application	Model	Ref.
Relap 5	LWR coolant systems	Space – time-averaged 1-D TFM, 6- equation (Liquid+vapor)	(Shieh & Ransom, V. H. Krishnamurthy, 1994)
TRAC-BF1/MOD1	BWR systems	TFM, 8- equations system (Liquid+vapor+mixture)	(Borkowski & Wade, 1992)
OLGA	Two-phase flow transport in pipelines	TFM 6- equation model (Liquid+ vapor+ droplets)	(Bendiksen, Maines, Moe, & Nuland, 1991)
CATHARE	LOCA safety analysis in PWR	TFM, 6- equation (Liquid+vapor)	(Barre & Bernard, 1990)

LWR: Light water reactor, BWR: Boiling water reactors, LOCA: Lost of coolant accident, PWR: Pressure water reactors

2.12 Equations of state (EoS)

In two-phase flow simulations (either HFM, QHM, or TFM) the flow variables (pressure, mass flow, internal energy, or enthalpy and void fractions for the TFM) are determined directly with conservation laws for mass, momentum and energy. However, these equations have a strong coupling with other physical properties like density or viscosity. Therefore, a constitutive equation relating physical properties is needed to close the system of equations. This equation is the equation of state (EoS). An equation of

state is a thermodynamic equation that defines the relations between state variables (pressure, temperature, enthalpy, density, internal energy, etc.). With this equation, any state variable (φ_1) can be calculated knowing two independent state variables (φ_1, φ_2).

$$\varphi_1 = \varphi(\varphi_2, \varphi_3) \quad (2.43)$$

Many equations of state have been proposed for different fluids with different ranges of applicability. The Ideal gas equation is suitable for low pressures compared with the saturation pressure, while the Van der Waals and Redwing-Kwong EoS are suitable for higher pressures, among others. Unfortunately, these EoS are only valid for the gas phase making them not suitable for phase transition problems like boiling or condensation. Hence, more sophisticated EoS must be used to simulate liquids and vapor, especially in phase transition problems. Some examples of EoS valid for the liquid and gas phase can be mentioned, the Stiffened gas (a simple case of the Mie –Grüneisen equation of state) (Allaire, Clerc, & Kokh, 2002) and the Nobel-Abel EoS. In this thesis, two EoS are used: The Helmholtz free energy and the Nobel-Abel-Stiffened- gas equations of state.

2.12.1 The Helmholtz free energy equation of state (HFE)

As the name implies, this equation of state is based on the Helmholtz free energy. This formulation uses specific volume and temperature (or alternatively, density and temperature) as independent variables.

$$f = e(T, v) - Ts(T, v) = e(T, \rho) - Ts(T, \rho) \quad (2.44)$$

The most used version of Equation (2.44) is in dimensionless form using reduced temperature ($\tau = T_0 / T$) and specific volume ($\delta = \rho / \rho_c$) as independent variables. Additionally, the final EoS is split into two parts; ideal (0) and real parts (r).

$$\frac{a(v, T)}{RT} = \Phi(\delta, \tau) = \Phi^0(\delta, \tau) + \Phi^r(\delta, \tau) \quad (2.45)$$

After the decade of the 1970s, multi-parameter versions of Equation (2.45) are often used (Span, Wagner, Lemmon, & Jacobsen, 2001). This approach is very useful for

software development due to the ease of working with databases containing all the parameter information. The multi-parameter form of Equation (2.45) is:

$$\Phi^0(\tau, \delta) = \text{Ln } \delta + \sum_{k=1}^{k_1} c_k \tau^{m_k} + \sum_{k=k_1+1}^{k_2} c_k \text{Ln}[1 - \exp(-a_k \tau)] \quad (2.46)$$

$$\Phi^f(\tau, \delta) = \sum_{k=k_2+1}^{k_3} c_k \delta^{n_k} \tau^{m_k} + \sum_{k=k_3+1}^{k_4} c_k \delta^{n_k} \tau^{m_k} \exp -\delta^{e_k} \quad (2.47)$$

The coefficients a, c, n, m, e and $k_i (i = 1, \dots, 4)$ are determined experimentally. Some references for these coefficients and for some commons refrigerants are summarized in Table 2. 10.

Table 2. 10 Summary of references for some important refrigerants

Name	Chemical formula	Range of applicability	Reference
Water	H ₂ O	Melting line (251 K at 209.9 MPa) up to 1,273 K, 1000 MPa	(Wagner & Pruss, 2002)
R-11	CCl ₃ F	Triple point up to 600 K, 30 MPa	(Jaobsen, Penocello, & Lemmon, 1992)
R-410A	50% R32/50% R125	200 K- 450 K	(Jaobsen et al., 1992)
R-507A	50% R125/50% R143A		
R-404A	44% R125/4% R134A/52% R143A		
R-407C	23%-R32/25%-R125/52%-R134A		
Carbon dioxide	CO ₂	Triple point up to 1,100 K, 800 MPa	(Span & Wagner, 1996)
Ammonia	NH ₃	-	(Baehr & Tillner-Roth, 1995)

Using the Maxwell relations jointly with partial derivatives of (2.45) the other thermodynamic properties can be found. In Table 2. 11 some specific thermodynamic properties relations are summarized.

Table 2. 11 Summary of thermodynamic state properties

Property	Equation
Pressure	$p = \rho TR \left\{ 1 + \delta \left(\frac{\partial \Phi^r}{\partial \delta} \right)_{\tau} \right\}$
Specific internal energy	$e = TR \left\{ \tau \left[\left(\frac{\partial \Phi^0}{\partial \tau} \right)_{\delta} + \left(\frac{\partial \Phi^r}{\partial \tau} \right)_{\delta} \right] \right\}$
Specific enthalpy	$h = TR \left\{ \left[1 + \left(\frac{\partial \Phi^r}{\partial \delta} \right)_{\tau} \right] + \tau \left[\left(\frac{\partial \Phi^0}{\partial \tau} \right)_{\delta} + \left(\frac{\partial \Phi^r}{\partial \tau} \right)_{\delta} \right] \right\}$
Specific entropy	$s = R \left\{ \tau \left[\left(\frac{\partial \Phi^0}{\partial \tau} \right)_{\delta} + \left(\frac{\partial \Phi^r}{\partial \tau} \right)_{\delta} \right] - \Phi^0 + \Phi^r \right\}$

2.12.2 The Nobel- Abel Stiffened gas equation of state (NASG)

This EoS is a combination of the “Stiffened Gas” and the “Nobel- Abel” equations of state. The NASG EoS is defined as an explicit function relationship between pressure, internal energy, and specific volume (or density) as:

$$p(v, e) = (\gamma - 1) \frac{(e - q)}{v - b} - \gamma_{\infty} p_{\infty} \quad (2.48)$$

The terms b , $(\gamma - 1)(e - q)$ and $(v - b)$ represents the co-volume of the fluid, thermal agitation effects, and short distance repulsive effects respectively. The parameters p_{∞} , γ , q and b in Equation (2.48) are characteristics constants defined for each fluid and must be determined experimentally.

Table 2. 12 NASG characteristic coefficients for water

Coefficient	$T \in 300 - 500$ K		$T \in 350 - 550$ K	
	Liquid	Vapour	Liquid	Vapour
Cp [J/kgK]	4,285	1,401	4,444	903
Cv [J/kgK]	3,610	955	3,202	462
$\gamma = Cp/Cv$	1.19	1.47	1.39	1.95
p_{∞} [Pa]	$7,028 \times 10^5$	0	$8,899 \times 10^5$	0
b [m ³ /kg]	6.61×10^{-4}	0	$4,78 \times 10^{-4}$	0
q [J/kg]	-1,177,788	2,077,616	-1,244,191	2,287,484
q' [J/kg]	0	14,317	0	6,417

The values of constants for water in both liquid and vapor-phases are summarized in Table 2. 12. The values for Dodecane ($C_{12}H_{26}$) and Oxygen at different temperature ranges can be found in (Le Métayer & Saurel, 2016).

The NASG EoS has a simpler form but its range of applicability is low. In Figure 2. 6 to Figure 2. 8 the NASG and the HFE EoS are compared, showing that the great difference between them in a wide range of pressure and temperature.

Figure 2. 6 HFE and NASG saturated pressure versus temperature comparison

Figure 2. 7 Saturated densities comparison, a) liquid, b) vapor

Figure 2. 8 Saturated enthalpy comparison, a) liquid, b) vapor

Nomenclature

A	Area (m^2).
C	Constant.
C_p	Specific heat capacity at constant pressure ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
C_v	Specific heat capacity at constant volume ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
D	Diameter (m). Geometric scale.
E	Total specific internal energy ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
$\hat{e}_i$	Unitary vector.
E	Specific internal energy ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
f	Friction factor.
f_F	Fanning friction factor.
G	Mass flux ($\text{kg} \cdot \text{s}^{-1} \cdot \text{m}^{-2}$).
g	Gravity acceleration constant ($=9.81 \text{ m} \cdot \text{s}^{-2}$).
h	Specific enthalpy ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
h_l	Liquid phase-specific enthalpy ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
h_v	Vapor phase-specific enthalpy ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
h_{TP}	Two- phase flow mixture Specific enthalpy ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
$\mathbf{J}$	Surface forces vector.
L	Length (m).
l	Length (m).
M	Momentum source term.
m, n	Integer numbers.
$\dot{m}$	Mass flow ($\text{kg} \cdot \text{s}^{-1}$).
$\hat{n}_i$	Outward unitary vector.
$\mathcal{O}$	Big O notation order of magnitude function.
p	Pressure (Pa).
$\dot{Q}^r$	Energy source term.
$\dot{Q}''$	Heat flux per unit area ($\text{W} \cdot \text{m}^{-2}$).
$\dot{Q}'''$	Heat flux per unit volume ($\text{W} \cdot \text{m}^{-3}$).
R	Surface rugosity. Gas universal constant.
Re	Reynolds number.
S	Surface (m^2).
s	Specific entropy ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
S_R	Slip ratio.
t	Time (s).
T	Temperature ($^{\circ}\text{C}$).
T_c	Critic temperature ($^{\circ}\text{C}$).

$\mathbb{T}$	Total stress tensor.
U	Superficial velocity ($\text{m} \cdot \text{s}^{-1}$).
u	Velocity, phase velocity ($\text{m} \cdot \text{s}^{-1}$).
u_A	Absolute velocity ($\text{m} \cdot \text{s}^{-1}$).
$\mathbf{u}$	Velocity vector.
V	Volume (m^3).
v	Specific volume ($\text{m}^3 \cdot \text{kg}^{-1}$).
We	Weber number.
X	Lockhart- Martinelli parameter.
x	Thermodynamic Quality ($\text{kg} \cdot \text{kg}^{-1}$).
x_i	Position vector ($x_i = x_i \hat{e}_i$).
z	Axial coordinate (m).

Greek Letters

β	Tilt angle.
Γ	Mass source term.
Δ	Finite difference.
δ	Dimensionless density.
ε	Void fraction ($\text{m}^3 \cdot \text{m}^{-3}$).
λ	Thermal conductivity ($\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$).
μ	Dynamic viscosity ($\text{Pa} \cdot \text{s}^{-1}$).
ρ	Material density ($\text{kg} \cdot \text{m}^{-3}$).
ρ_l	Liquid phase material density ($\text{kg} \cdot \text{m}^{-3}$).
ρ_v	Vapor phase material density ($\text{kg} \cdot \text{m}^{-3}$).
ρ_{TP}	Two-phase flow mixture density ($\text{kg} \cdot \text{m}^{-3}$).
τ	Dimensionless temperature.
τ_{ij}	Shear stress tensor.
τ_w	Wall shear stress.
ϕ	Scalar variable field function. Lockhart and Martinelli multiplier.
ψ	Conserved quantity.
$\Phi(\delta, \tau)$	Dimensionless equation of state function.
Φ'''	Source term per unit volume.
φ	Thermodynamic state variable.
Ω	Jump conditions source function.

Subscripts

0	Initial state.
fr	Friction.
l	Liquid.

v	Vapor.
TP	Two- phase.
h,i,j,k	Index.
$wall$	Wall.

Superscripts

$'$	Per unit length.
$''$	Per unit area.
$'''$	Per unit volume.

Acronymous

BWR	Boiling water reactor.
EoS	Equation of state.
HFE	Helmholtz free energy.
HFM	Homogeneous flow model.
LWR	Light water reactor.
LOCA	Lost of coolant accident.
NASG	Nobel- Abel stiffened gas equation of state.
PWR	Power water reactor.
TFM	Two- fluid model.
QHFM	Quasi- Homogeneous flow model.

Operators

$\langle \rangle$	In Volume total average operator.
$\sim$	In Volume intrinsic average operator.
$-$	Mean area average operator.

References

Allaire, G., Clerc, S., & Kokh, S. (2002). A five-equation model for the simulation of interfaces between compressible fluids. *Journal of Computational Physics*, 181(2), 577–616. <https://doi.org/10.1006/jcph.2002.7143>

Aris, R. (1989). *Vectors, Tensors and the Basic Equations of Fluid Dynamics*. Dover Publications Inc.

Baehr, H. D., & Tillner-Roth, R. (1995). *Thermodynamic Properties of Environmentally Acceptable Refrigerants: Equations of State and Tables for Ammonia, R 22, R 134a, R 152a and R 123*. Berlin: Springer- Verlag.

Barre, F., & Bernard, M. (1990). The CATHARE code strategy and assessment. *Nuclear Engineering and Design*, 124(3), 257–284. [https://doi.org/10.1016/0029-5493\(90\)90296-A](https://doi.org/10.1016/0029-5493(90)90296-A)

Batchelor, G. K. (1974). Transport Properties of Two-Phase Materials with Random Structure. *Annual Review of Fluid Mechanics*, 6, 227–255. <https://doi.org/10.1146/annurev.fl.06.010174.001303>

Batchelor, G. K. (2000). *An Introduction to Fluid Dynamics*. Cambridge University Press.

Beattie, D. R. H., & Whalley, P. B. (1982). A Simple Two-Phase Frictional Pressure Drop Calculation Method. *International Journal of Multiphase Flow*, 8(1), 83–87.

Bendiksen, K. H., Maines, D., Moe, R., & Nuland, S. (1991). The Dynamic Two-Fluid Model OLGA: Theory and Application. *SPE Production Engineering*, 6(02), 171–180. <https://doi.org/10.2118/19451-PA>

Bennett, A. (2006). *Lagrangian Fluid Dynamics*. https://doi.org/10.1007/978-1-4614-3794-9_47

Borkowski, J. A., & Wade, N. L. (1992). TRAC-BF1/MOD1 Models and Correlations.

Brkić, D. (2011). Review of explicit approximations to the Colebrook relation for flow friction. *Journal of Petroleum Science and Engineering*, 77(1), 34–48. <https://doi.org/10.1016/j.petrol.2011.02.006>

Buyevich, Y. (1971). Statistical hydromechanics of disperse systems. Part 1. Physical background and general equations. *Journal of Fluid Mechanics*, 49(03), 489–507.

Chen, J. J. J. (1984). a Simple Explicit Formula for the Estimation of Pipe Friction Factor. *Proceedings of the Institution of Civil Engineers*, 77(1), 49–55. <https://doi.org/10.1680/iicep.1984.1272>

Chisholm, D. (1973). Pressure Gradients due to friction during the flow of evaporating two- phase mixtures in smooth tubes and channels. *International Journal of Heat and Mass Transfer*, 16, 347–358.

Churchill, S. W. (1977). Friction-factor Equation Spans all Fluid Flow Regimes. *Chemical Engineering*, 91.

Cicchitti, A., Lombardi, C., Silvestri, M., Soldai, G., & Zavattarelli, R. (1960). Two- Phase Cooling Experiments- Pressure Drop, Heat Transfer and Burnout measurements,". *Energia Nucleare*, 7(6), 407–425.

Colebrook, C. F. (1939). Turbulent Flows in Pipes, With Particular Reference to the Transition Region Between Smooth and Rough Pipe Laws. *Journal of the Institution of Civil Engineers*, 11, 133–156.

Daneshyar, H. (1976). *One-Dimensional Compressible Flow*. (W. Woods, Ed.) (1st Editio). Pergamon Press.

Drew, D. A. (1971). Averaged Field Equations for a Two Phase Media. *Studies in Applied Mathematics*, L2(2), 205–231. <https://doi.org/10.1002/sapm1971502133>

Dukler, A. E., Wicks, M., & Cleveland, R. G. (1964). Frictional Pressure Drop in Two-Phase Flow: Part A. A comparison of Existing Correlations for Pressure Loss and Holdup. *AIChE Journal*, 10(1), 38–51.

Escanes, F., Pérez-Segarra, C. D., & Oliva, A. (1995). Thermal and fluid-dynamic behaviour of double-pipe condensers and evaporators — a numerical study. *International Journal of Numerical Methods for Heat & Fluid Flow*, 5(9), 781–795. <https://doi.org/10.1108/EUM0000000004087>

García-Valladares, O., Pérez-Segarra, C. D., & Rigola, J. (2004). Numerical simulation of double-pipe condensers and evaporators. *International Journal of Refrigeration*, 27(6), 656–670. <https://doi.org/10.1016/j.ijrefrig.2004.01.006>

Genić, S., Arandjelović, I., Kolendić, P., Jarić, M., Budimir, N., & Genić, V. (2011). A review of explicit approximations of Colebrook's equation. *FME Transactions*, 39(2), 67–71. <https://doi.org/10.1016/j.petro.2011.02.006>

Haaland, S. E. (1983). Simple and Explicit Formulas for the Friction Factor in Turbulent Pipe Flow. *Journal of Fluids Engineering*, 105(1), 89. <https://doi.org/10.1115/1.3240948>

Hewitt, G. F. (1982). Flow Regimes. Pressure Drop. Void Fraction. In G. Hetsroni (Ed.), *Handbook of Multiphase Systems* (p. Sections 2.1-2.3). McGraw Hill.

Hewitt, G. F., & Roberts, D. N. (1969). *Studies of Two- Phase Flow Patterns by Simultaneous X-Ray and Flash Photography*. Harwell, Berkshire.

Hibiki, T., & Ishii, M. (2003). One-dimensional drift-flux model and constitutive equations for relative motion between phases in various two-phase flow regimes. *International Journal of Heat and Mass Transfer*, 46(25), 4935–4948. [https://doi.org/10.1016/S0017-9310\(03\)00322-3](https://doi.org/10.1016/S0017-9310(03)00322-3)

Hicks, B. L., Montgomery, D. J., & Wasserman, R. H. (1947). On the one-dimensional theory of steady compressible fluid flow in ducts with friction and heat addition. *Journal of Applied Physics*, 18(10), 891–902. <https://doi.org/10.1063/1.1697563>

Husain, A., Choe, W. G., & Weisman, J. (1974). *Applicability of the Homogeneous Flow Model to Pressure Drop in Straight Pipe and Across Area Changes*. The United States.

Idsinga, W., Todreas, N., & Bowring, R. (1977). An Assessment of Two-Phase Pressure Drop Correlations for Steam Water Systems. *International Journal of Multiphase Flow*, 3, 401–4013. [https://doi.org/10.1016/0301-9322\(77\)90019-2](https://doi.org/10.1016/0301-9322(77)90019-2)

Ishii, M. (2016). Review on Two-Fluid Model for Two-Phase Flow. *Multiphase Science and Technology*, 28(6), 258–320. <https://doi.org/10.1615/MultScienTechn.v28.i3.40>

Ishii, M., & Ibiki, T. (2011). *Thermo-Fluid Dynamics of Two-Phase Flows (Second)*. Springer.

Jaobsen, R. T., Penocello, S. G., & Lemmon, E. W. (1992). A fundamental equation for chlorodifluoromethane (R-11). *Fluid Phase Equilibria*, 80, 45–56. [https://doi.org/10.1016/0378-3812\(92\)87056-S](https://doi.org/10.1016/0378-3812(92)87056-S)

Kandlikar, S. G. (1999). *Handbook of Phase Change: Boiling and Condensation*. Taylor & Francis.

Le Métayer, O., & Saurel, R. (2016). The Noble-Abel Stiffened-Gas equation of state. *Physics of Fluids*, 28(4). <https://doi.org/10.1063/1.4945981>

Lin, S., Kwok, C. C. K., Li, R. Y., Chen, Z. H., & Chen, Z. Y. (1991). Local Frictional Pressure Drop During Vaporization of R-12 Through Capillary Tubes. *International Journal of Multiphase Flow*, 17(1), 95–102.

Lockhart, R. W., & Martinelli, R. (1949). Proposed Correlation of Data for Isothermal Two-Phase, Two-Component Flow in Pipes. *Chemical Engineering Progress*, 45, 38–48.

Mandhane, J. M., Gregory, G. A., & Aziz, K. (1974). A Flow Pattern Maps for Gas-Liquid Flow in Pipes. *International Journal of Multiphase Flow*, 1(4), 537–553. [https://doi.org/10.1016/0301-9322\(74\)90006-8](https://doi.org/10.1016/0301-9322(74)90006-8)

McAdams, W. H., Woods, W. K., & Bryan, R. L. (1942). Vaporization Inside Horizontal Tube- II- Benzene- Oil Mixtures. *Transactions of the ASME*, 64(193).

Meyer, P. E., & Wallis, G. B. (1965). Co-Current Upwards Annular-Mist Flow.

Mochizuki, Y., & Ishii, Y. (1992). Study of Thermallyhydraulics relevant to natural circulation in ATR. In Vth International Topical meeting on Reactor Thermal Hydraulics (pp. 127–134).

Morales-Ruiz, S., Rigola, J., Pérez-Segarra, C. D., & García-Valladares, O. (2009). Numerical analysis of two-phase flow in condensers and evaporators with special emphasis on single-phase/two-phase transition zones. *Applied Thermal Engineering*, 29(5–6), 1032–1042. <https://doi.org/10.1016/j.applthermaleng.2008.05.017>

Nigmatulin, R. I. (1979). Spatial averaging in the mechanics of heterogeneous and dispersed systems. *International Journal of Multiphase Flow*, 5(5), 353–385. [https://doi.org/10.1016/0301-9322\(79\)90013-2](https://doi.org/10.1016/0301-9322(79)90013-2)

Osmachkin, V. S., & Borisov, V. (1970). Pressure Drop and Heat Transfer for Flow for Boiling Water in Rod Bundles. In IVth International Heat Transfer Conference.

Owens, W. L. (1961). Two-phase Pressure Gradient. . . Int. Dev. Heat Transfer, Pt. II, ASME.

Premoli, A., Franceso, D. . D., & Prina, A. (1971). A dimensional correlation for evaluating two-phase mixture density. *La Termotecnica*, 25(1), 17–26.

Shieh, A. S., & Ransom, V. H. Krishnamurthy, R. (1994). Validation of Numerical Techniques in RELAP5/MOD3.

Slattery, J. C. (1972). *Momentum, Energy and Mass Transfer in Continua*. McGraw Hill.

Soo, S. L. (1989). *Particulates and Continuum: Multiphase Fluid Dynamics*. New York: Hemisphere Publishing Corporation.

Span, R., & Wagner, W. (1996). A New Equation of State for Carbon Dioxide Covering the Fluid Region from the Triple Point Temperature to 1100 K at Pressures up to 800 MPa. *Journal of Physical and Chemical Reference Data*, 25(6), 1509–1596. <https://doi.org/10.1063/1.555991>

Span, R., Wagner, W., Lemmon, E. W., & Jacobsen, R. T. (2001). Multiparameter equations of state - Recent trends and future challenges. *Fluid Phase Equilibria*, 183–184, 1–20. [https://doi.org/10.1016/S0378-3812\(01\)00416-2](https://doi.org/10.1016/S0378-3812(01)00416-2)

Taitel Y, & Dukler A. (1976). A model for predicting flow regime transitions in horizontal and near horizontal gas-liquid ow. *AIChE Journal*.

Vernier, P. h., & Delhayé, J. M. (1968). General Two-Phase Flow Equations Applied to the Thermodynamics of Boiling Water Nuclear Reactors. *Energie Primaire*, 4(5), 5–46.

Von Mises, R. (1958). One Dimensional Flow. In *Mathematical Theory of Compressible Fluid Flow* (pp. 135–154). Pergamon Press.

Wagner, W., & Pruss, A. (2002). Revised Release on the {IAPWS} Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use. *J. Phys. Chem. Ref. Data*, 31(2), 387–535. <https://doi.org/10.1158/0008-5472.CAN-09-0634>

Wallis, G. B. (1969). *One-Dimensional Two-Phase Flow*. McGraw Hill.

Whitaker, S. (1969). Advances in Theory of Fluid Motion in Porous Media. *Industrial & Engineering Chemistry*, 61(12), 14–28. <https://doi.org/10.1021/ie50720a004>

Zigrang, D. J., & Sylvester, N. D. (1985). Discussion of Technical note: A Simple Explicit Formula for the Estimation of Pipe Friction Factor. *Proceedings of the Institute of Civil Engineers*, 1985, 215–221

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3.1 Introduction

In the previous chapter, the distributed parameter approach based on macroscopic local descriptions for mass, momentum, and energy (fluids and walls) in transient-state are presented. With this kind of modeling one can study and analyze heat exchangers without imposing any other assumptions beyond the ones required to develop the equations, otherwise using general integral balances equations the number of assumptions is such that the range of applicability is limited, see chapter I. Thereby, the time evolution of velocity (or mass flow), pressure, enthalpy and other thermodynamic properties (with the contribution of the equation of state) of the entire system can be calculated only knowing initial and boundary conditions. Additionally, in chapter II, special attention is put on two-phase flow modeling due to phase change (boiling and condensation) phenomena that can occur in many heat exchanger equipment. Examples are: HVAC components (condensers and evaporators), boiling water reactors (BWR) and pressurized water reactors (PWR) in nuclear power plants, not forgetting direct steam generators in fueled or solar power plants, just to mention a few. This type of formulation consists of a set of non-linear partial differential equations (PDE's) which can be written in a canonical form as:

$$\frac{\partial(\rho\psi)}{\partial t} + \frac{\partial F(\psi)}{\partial z} = \Phi''' \quad (3.1)$$

Here $\psi : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}^m$ is an m dimensional vector for the specific conserved variables (mass flow or velocity, pressure, and enthalpy). $F : \mathbb{R}^m \rightarrow \mathbb{R}^m$ is the vector of convective transport due to velocity $F(\psi) = \rho u \psi$ and $\Phi''' : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}^m$ is the vector of source terms per unit volume. $\rho : \mathbb{R} \rightarrow \mathbb{R}$ is the density field function and $u : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ is the velocity vector. To close the problem (3.1) initial and boundary conditions must be included, see Equation (3.2), for simplicity the Dirichlet boundary condition is imposed at the entrance ($z = L$) of the heat exchanger, however another type of boundary conditions can also be imposed, for example, problem (3.1) could be defined in an open set $z \in (-\infty, +\infty)$ not requiring boundary conditions explicitly.

$$\left. \begin{aligned} \psi(t = 0, z) &= \psi_0(z) \\ \psi(t, z = 0) &= \tilde{\psi}(t) \end{aligned} \right\} \quad (3.2)$$

It is clear that if we know $\psi(t, z)$ one can determine the evolution of ψ at any location at any time. By the existence and uniqueness of the solution theorem (Greenspan, 1961), it can be assured that a solution for ψ exists if the problem (3.1) jointly with (3.2) is well-posed. Unfortunately, find analytical solutions for ψ is not possible, except for very simple problems. Thus, the solution must be approximated numerically. In that order of ideas this chapter is enclosed, providing the mathematical background for the numerical method developed to deal with the solutions of the transient problem (3.1), a problem of interest in this thesis.

3.2 The method of lines

The solution of (3.1) can be approximated by values of ψ on a finite number of points over the time/space domain. This solution can be defined as the set of values of ψ on each discrete point as follows.

$$\tilde{\psi} = \psi(t_1, z_1), \dots, \psi(t_1, z_n), \psi(t_2, z_1), \dots, \psi(t_m, z_1), \dots, \psi(t_m, z_n) \quad (3.3)$$

Using interpolation and the values of the set (3.3), one can construct the solution of (3.1), for example, using Lagrange interpolation polynomials, the solution would be given by:

$$\left. \begin{aligned} \psi(t^*, z^*) &= \sum_{j=0}^p \sum_{k=0}^l \psi(t_j, z_k) \alpha_j(t^*) \alpha_k(z^*) \\ \alpha_j(t^*) &= \prod_{\substack{0 \leq m \leq j \\ m \neq j}} \left(\frac{t^* - t_m}{t_j - t_m} \right) \text{ and } \alpha_k(z^*) = \prod_{\substack{0 \leq n \leq k \\ n \neq k}} \left(\frac{z^* - z_n}{z_k - z_n} \right) \end{aligned} \right\} \quad (3.4)$$

To find (3.3) some discretization technique must be applied to Eq. (3.1) in space and time as well. One popular and effective way to do it is with the so-called methods of lines (MOL) (Hyman, 1977; Schiesser, 1991) or sometimes called by other authors as a “semi-discretization method”. The MOL consist in transform the original boundary value problem BVP, using any discrete differential operator A reducing the problem (3.1) to an n continuous in time initial value problem (IVP).

$$\frac{d\psi_i}{dt} = A\psi + \Phi = \sum_{k=-h}^p A_{i,i+k} \psi_{i+k} + \Phi_i \quad \text{with } k, h \in \mathbb{Z}^+ \text{ and } i = 1, \dots, n \quad (3.5)$$

Here the index $i+k$ defines the size of the stencil used. Note that for $l = p = 1$ leads for a 3- point 1st order stencil, typically used for first-order spatial discretization schemes, and A is an $n \times n$ discrete operator.

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{pmatrix} \quad (3.6)$$

This approach has some advantages: *i*) classic stability theory for ODEs can be applied; in particular, *A-stability* theory, therefore ODEs solvers can be used, *ii*) spatial and temporal accuracy are decoupled, analyzing, therefore, the accuracy of each dimension separately, *iii*) high order methods can be designed easily (Leveque, 1992), (Hoffman, 2001), (Hundsdorfer & Verwer, 2000).

3.3 The finite volume method

As stated in the above section, space and time can be decoupled. Methods for a spatial integration of PDEs can be made in different ways. In that sense, the finite volume method (FVM) is joint with the finite element method (FEM) (Zienkiewicz, 2000) and

the finite difference method (FDM) (Ferziger & Peric, 2002) as the most common discretization methods nowadays employed. With the FVM, the discrete equations are usually derived from the integral form of the set of conservation equations (Leveque, 1992; Versteeg & Malalasekera, 1995). However, it also can be equally derived from their differential form using the Gauss or divergence theorem (Chung, 2001; Ferziger & Peric, 2002; Suhas V Patankar, 1980). Technically, the FVM consists of dividing the entire domain into a finite number of non-overlapping subdomains, finite volumes or cells, see Figure 3. 1.a. for a generic 1-D cell-centered grid. For simplicity in this work, the size of each cell is considered equal $\Delta z = l / n$, where n is the number of center nodes and l is the total length of the domain. Each volume with cell center z_i is denoted as V_i , and each volume boundaries location (Γ) are then calculated as follows:

$$z_{i\pm 1/2} = \frac{1}{2}(z_i + z_{i\pm 1}) \quad (3.7)$$

As it happens with all numerical methods to approximate ordinary and/or partial differential equations the continuity of the dependent function ψ is replaced by its discrete approximation, in this case, it is assumed that ψ is constant inside each control volume that coincides with a mean average value (in area basis), see Figure 3. 1.b.

Figure 3. 1 Generic grid. a) Cell centered control volume, b) Piecewise variable distribution

Over these sub-domains, the set of equations is integrated in space. In the process of integration, the divergence (convective) and Laplacian (diffusion) terms are transformed using the divergence theorem, calculating convection and diffusion as numerical fluxes that enter and leave each finite volume (Leveque, 1992). To put this in context, let us consider the steady-state version of (3.1) and then integrate it in space on each finite volume according to Figure 3. 1.a.

$$\int_{V_i} \frac{\partial F(\psi)}{\partial z} dV_i = \sum_{j=1}^2 \int_{\Gamma_j} F(\psi) \cdot \hat{n}_j d\Gamma_j = \int_{V_i} \Phi''' dV_i \quad (3.8)$$

$$\Rightarrow F_{i+1/2} - F_{i-1/2} = \Phi_i''' \Delta V$$

After summing over all finite volumes, the above equations is transformed into:

$$F_{n+1/2} - F_{1/2} + \underbrace{\sum_{i=2}^{n-1} F_{i+1/2} - F_{i-1/2}}_{=0, \text{ by conservation}} = \sum_{i=1}^n \Phi_i''' \Delta V_i \quad (3.9)$$

Here is where the FVM has its major strength, considering numerical fluxes instead of transforming each continuous operator directly, as happens in finite difference methods, the method is not only globally but also locally numerical conservative, see Equation (3.9). This an important feature for engineering calculations, because we require conservative quantities in order to verify mass and energy conservation principles. This method also has some useful characteristics; simple data structure and ease of programming.

3.4 The UPWIND scheme

The Equation (3.8) is still not useful; we need to express the discrete equation in terms of ψ instead of F , in order to split the original problem (3.1) in n coupled IVP, see Equation (3.5). Unfortunately, F is not linear and must be treated carefully to reproduce the underlying physics. To calculate this term accurately, we must know not only the velocity (or mass flow) at each finite volume boundary but also calculate how the physical quantity ψ is transported across Γ . The simplest, but not the least accurate, is the Upwind scheme (B. R. Courant, Isaacson, & Rees, 1952). This scheme is formulated considering the expected physical behavior of the transported quantity. This means that the direction of u defines how ψ is transported.

$$F_{i+1/2} = \begin{cases} \rho_{i+1/2} u_{i+1/2} \psi_i & \text{If } u_{i+1/2} \geq 0 \\ \rho_{i+1/2} u_{i+1/2} \psi_{i+1} & \text{If } u_{i+1/2} < 0 \end{cases} \quad (3.10)$$

The equation (3.10) can be defined in several different ways, in (Suhas V Patankar, 1980) the max function is introduced to distinguish in which direction ψ is transported.

$$F_{i+1/2}(\psi_{i+1}, \psi_i) = \max(\rho_{i+1/2} u_{i+1/2}, 0) \psi_i - \max(-\rho_{i+1/2} u_{i+1/2}, 0) \psi_{i+1} \quad (3.11)$$

In hyperbolic differential equations theory, another expression is used, writing the UPWIND scheme as a numerical flux function (Leveque, 1992).

$$\begin{aligned} F_{i+1/2} &= \frac{1}{2} u_{i+1/2} + \left| u_{i+1/2} \right| \rho_{i+1/2} \psi_i + \frac{1}{2} \left| u_{i+1/2} \right| - u_{i+1/2} \rho_{i+1/2} \psi_{i+1} \\ &= \frac{1}{2} (\rho_{i+1/2} u_{i+1/2} \psi_i + \rho_{i+1/2} u_{i+1/2} \psi_{i+1}) - \frac{1}{2} \rho_{i+1/2} \left| u_{i+1/2} \right| (\psi_{i+1} - \psi_i) \end{aligned} \quad (3.12)$$

The equation (3.12) is written for scalar problems, which is a simplification due to the Jacobian matrix is taken as a constant value u evaluated at the boundary of the finite volume. Both expressions are equivalent, however, with the UPWIND scheme formulated as Equation (3.12) it can be shown that the Upwind scheme is consistent (Leveque, 1992), (Toro, 2009); this means that

$$F(\psi_i, \psi_i) = F(\psi_i) \quad (3.13)$$

It is well known the numerical diffusivity of the first order UPWIND scheme, the reason why many researchers have developed many high-resolution schemes, e.g., CLAM (Van Leer, 1974), MUSCL (Van Leer, 1979), OSHER (Chakravarthy & Osher, 1983), SMART (Gaskell & Lau, 1988), SOUCOUP (Zhu & Rodi, 1991), STOIC (Darwish, 1993), among others. These high order schemes increase considerably the computationally cost and can suffer from numerical oscillations (Engquist & Osher, 1981), therefore they are not used in this work.

3.5 Staggered grid

The choice of the grid is not trivial as it seems; its choice determines the numerical strategy in the approximation procedure. There exist several kinds of grids, for different dimensions and topologies, nevertheless, for 1-D flows the options are logically more limited, for information over 2-D and 3-D structured and unstructured grids one can recommend to consult (Farrashkhalvat & Miles, 2003; Liseikin, 2010; Thompson, Soni, & Weatherill, 1998). In Section 3.3, the notion of grid is introduced to show the mathematical principles of the finite volume method. In 1-D flows, there are two types

of grids; collocated (non- staggered) and staggered grids. In collocated grids, all variables (scalar or vectorial) are stored at the same location, see Figure 3. 2.b. This choice seems, at first sight, appropriate, but convective terms need to evaluate fluxes at each boundary. If pressure and velocity are interpolated geometrically they can introduce the so-called checkboard pressure field behavior or pressure decoupling (Harlow & Welch, 1965), to avoid this, another interpolation strategy must be taken. The two most common ways to prevent this issue with a collocated grid are with the Rhie and Chow and Majumdar interpolation methods, see (Majumdar, 1988; Rhie & Chow, 1983). An easy remedy is to work with staggered grids arrangement (Harlow & Welch, 1965).

Figure 3. 2 Staggered grid arrangement

This arrangement consists to create two grids, in the first grid scalar quantities are stored and in the second grid is displaced $\Delta z / 2$ from the first one storing, here only velocity. This grid arrangement presents some advantages; no interpolation is needed, there is no risk of pressure decoupling, and for 1-D the data structure and memory required is not increased

3.6 Time integration schemes

Let us consider the following initial value problem.

$$\begin{aligned} \frac{d\psi_i}{dt} &= F_i(t, \psi_j) \quad \text{with } \psi_i(t=0) = \psi_{0,i} \quad t \geq 0 \\ \text{for } i, j &= 1, \dots, m \end{aligned} \tag{3.14}$$

Here $\psi : \mathbb{R} \rightarrow \mathbb{R}^m$ and $F : \mathbb{R} \times \mathbb{R}^m \rightarrow \mathbb{R}^m$ is the slope function (rate of change of ψ). If the entire time domain is divided into short segments $t^{n+1} = t^n + \Delta t$ with $\Delta t > 0$, we can integrate (3.14) between t^n and t^{n+1} , thus.

$$\psi_i^{(n+1)} = \psi_i^{(n)} + \int_{t^n}^{t^{n+1}} F_i(t, \psi_j) dt \quad (3.15)$$

If F were known explicitly, the solution of (3.15) would be straightforward, integrating F with the Riemann or Simpson rule $\psi_j^{(n+1)}$ could be calculated. Unfortunately, this is not the case because we only know the values of F evaluated at (t^n, ψ_j^n) . Therefore, the problem now moves to how accurate F can be integrated. In that sense, there are two approaches to evaluate F : explicit and implicit schemes. In explicit schemes, F is evaluated at (t^n, ψ_j^n) , and implicit schemes are referred to when F is evaluated at (t^{n+1}, ψ_j^{n+1}) , of course, the point (t^{n+1}, ψ_j^{n+1}) is not known therefore the value of ψ_j^{n+1} (via assuming F) must be iterated; in other words, defining F is part of the solution procedure.

3.6.1 The explicit Euler method (Forward)

Recalling Equation (3.14) a Taylor series of ψ_i expansion around $w = (t^n, \psi_i^n)$ can be written as:

$$\psi_i^{(n+1)} = \psi_i^{(n)} + \Delta t \left. \frac{d\psi_i}{dt} \right|_w + \frac{\Delta t^2}{2} \left. \frac{d^2\psi_i}{dt^2} \right|_w + \cdots + \frac{\Delta t^k}{k!} \left. \frac{d^k\psi_i}{dt^k} \right|_w + \mathcal{O}(\Delta t^{k+1}) \quad (3.16)$$

Here $\mathcal{O}(\Delta t^{k+1})$ is the truncation error of the series. It is said that (3.16) has a truncation error k . On the other hand, if we observe (3.14) it is noticed that $d\psi_i / dt = F$, thus (3.16) can be expressed in terms of F as:

$$\psi_i^{(n+1)} = \psi_i^{(n)} + \Delta t F_i|_w + \frac{\Delta t^2}{2} \left. \frac{dF_i}{dt} \right|_w + \cdots + \frac{\Delta t^k}{k!} \left. \frac{d^{k-1}F_i}{dt^{k-1}} \right|_w + \mathcal{O}(\Delta t^{k+1}) \quad (3.17)$$

In the Euler explicit (forward) scheme, the high order derivatives of (3.17) are dropped off ($k \geq 2$), then.

$$\psi_i^{(n+1)} \approx \psi_i^{(n)} + \Delta t F_i|_w \quad (3.18)$$

with

$$\mathcal{O}(\Delta t^2) = \frac{\Delta t^2}{2} \left. \frac{dF_i}{dt} \right|_{t_\xi} \quad (3.19)$$

The last expression shows that the Euler backward method is 1st order accurate. One can observe that comparing (3.15) with (3.18) the function F is evaluated only at (t^n, ψ_j^n) , which implies that the integration of F is made as a Riemann backward sum. The algorithm to find the solution is shown in Algorithm 3. 1:

Algorithm 3. 1 Euler Backward solver algorithm

3.6.2 The implicit Euler method (Backward)

The Euler backward scheme can be modified slightly, only assuming that F is evaluated at (t^{n+1}, ψ_j^{n+1}) .

$$\int_{t^n}^{t^{n+1}} F_i(t, \psi_j) dt \approx \Delta t F_i(t^{n+1}, \psi_j^{n+1}) \quad (3.20)$$

In this case, $F_i(t^{n+1}, \psi_j^{n+1})$ is not known; thus, it is necessary an evolution algorithm for ψ_j . This algorithm must use a linear form of F_i and iteratively determine ψ_i^{n+1} . An easy approach is using a Taylor series expansion of ψ_i around ψ_i^* , which is a guess value of ψ_i . For decoupled ODEs, the method reads:

$$F_i(t^{n+1}, \psi_i^{n+1}) \approx F_i(t^{n+1}, \psi_i^*) + (\psi_i^{n+1} - \psi_i^*) \left. \frac{\partial F_i}{\partial \psi_i} \right|_{(t^{n+1}, \psi_i^*)} \quad (3.21)$$

Combining (3.21) with (3.15) one yield:

$$\psi_i^{n+1} = \left(1 - \Delta t \left. \frac{\partial F_i}{\partial \psi_i} \right|_{(t^{n+1}, \psi_i^*)} \right)^{-1} \left(\psi_i^n + \Delta t F(t^{n+1}, \psi_i^*) - \Delta t \psi_i^* \left. \frac{\partial F_i}{\partial \psi_i} \right|_{(t^{n+1}, \psi_i^*)} \right) \quad (3.22)$$

For a system of ODEs, every component of F depends vectorially on ψ_j , therefore using multivariate Taylor series expansion again around ψ_j^* Equation (3.22) can be generalized as follows:

$$\psi_i^{n+1} = (I - \Delta t J_{ij}^*)^{-1} (\psi_i^n - \Delta t J_{ij}^* \psi_j^*) \quad \text{for } j = 1, \dots, m \quad (3.23)$$

Here J and I stand for the Jacobian and identity matrixes, respectively.

$$J_{ij}^* = \begin{pmatrix} \frac{\partial F_1}{\partial \psi_1} & \dots & \frac{\partial F_1}{\partial \psi_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_m}{\partial \psi_1} & \dots & \frac{\partial F_m}{\partial \psi_m} \end{pmatrix}_{(t^{n+1}, \psi_j^*)} \quad (3.24)$$

Algorithm 3. 2 Euler backward solver algorithm

3.7 Runge- Kutta methods

The Euler forward method is enhanced reducing the time step, this is not appropriate for long transient or unsteady problems due to highly expensive computation times. On the other hand, the Euler backward method even that the method is stable (see Section 3.8.2) is inaccurate due to the approximation of F by a simple Riemman

rule. Other approaches were proposed with improved accuracies, like the trapezoidal and midpoint rule. Therefore, a method in which high temporal accuracy (essential for high computation times) is desirable. This can be made increasing the order of truncation error of the corresponding Taylor series expansion of ψ . This approach seems convenient if we know explicitly F . However, this is not possible in many cases, especially in PDEs because F is part of the unknowns. This issue motivated the development of the so-called Runge-Kutta methods back in the late 19th and early 20th century, respectively (Butcher, 1996; Butcher & Wanner, 1996). The idea behind the R-K methods consists in advance from t^n to t^{n+1} using a numerical quadrature using a weighted sum of F , evaluated at different stages (s) inside the interval (Alexander, 1977).

$$\int_{t^n}^{t^{n+1}} F_i(t, \psi_j) dt \approx \Delta t \sum_{r=1}^q b_r F_i^{(r)} \quad (3.25)$$

Thus,

$$\psi_i^{(n+1)} = \psi_i^{(n)} + \Delta t \sum_{r=1}^q b_r F_i^{(r)} \quad (3.26)$$

Here q defines the total number of stages and the vector $F_i^{(r)}$ ($r = 1, \dots, q$) defines the value of F on each stage. On the other hand, this approximate value of F at every time stage (s) can also be approximated with another quadrature formula of the form:

$$F_i^{(r)} = F_i(t^{(r)}, \psi_j^{(r)}) = F_i \left(t^{(n)} + c_r \Delta t, \psi_j^{(r)} + \Delta t \sum_{s=1}^q a_{rs} F_j^{(s)} \right) \quad (3.27)$$

Here, the coefficients a_{rs} , b_r , and c_r are the weights of the quadrature and can be represented in the so-called Butcher Table as:

$$\begin{array}{c|c} c & a \\ \hline & b^T \end{array} = \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} \quad (3.28)$$

These coefficients have the following restrictions:

$$\left. \begin{aligned} c_r &= \sum_{s=1}^q a_{rs} = a_{rs} \delta_s \quad (\text{Row sum condition}) \\ \sum_{s=1}^q b_r &= b_r \delta_r = 1 \quad (\text{Consistency condition}) \\ 0 &\leq b_r \leq 1 \end{aligned} \right\} \quad (3.29)$$

This representation is useful because, at first sight, one can distinguish between families of Runge- Kutta methods. All Runge- Kutta methods can be classified as explicit ($a_{rs} = 0$ for $r \leq s$), semi-implicit, or diagonally implicit methods ($a_{rs} = 0$ for $r < s$) and fully implicit methods when $a_{rs} \neq 0$ for any $r > s$.

3.7.1 Derivation of Runge- Kutta methods

The number of Runge- Kutta methods is immense. In (Butcher, 2008; Hairer & Wanner, 1996; Hairer, Wanner, & Nørsett, 1993) a complete catalog of Runge- Kutta methods are reviewed. However, all of them are derived in the same way; therefore, in this section, the basics of Runge- Kutta methods are presented. The method is introduced for 3rd order methods. However, higher-order methods can be derived using the same procedure. The procedure outlined here is based on the index summation procedure used by (Gear, 1971). The method can be equally derived via graph theory (using rooted trees) and elementary differentials (Butcher, 1963), being this approach very useful for high order methods resuming the complexity in the intermediate calculations.

For convenience and to simplify the analysis, in this section, the following nomenclature is used: Three index positions are placed on every variable to specify the vector component, derivative index, and time/stage index, denoted in Equation (3.30) as ϑ , β and γ respectively.

$$\vartheta F_{\beta}^{(\gamma)} \quad (3.30)$$

With this new notation, differentiation is denoted as:

$${}^i F_{j_1} = \frac{\partial({}^i F)}{\partial x_{j_1}} \quad {}^i F_{j_1 j_2} = \frac{\partial^2({}^i F)}{\partial x_{j_1} \partial x_{j_2}} \quad {}^i F_{j_1 j_2 \dots j_m} = \frac{\partial^m({}^i F)}{\partial x_{j_1} \partial x_{j_2} \dots \partial x_{j_m}}$$

Additionally, new definitions for ψ and F are used. The new definition of ψ ($\psi = \psi({}^0\psi, {}^1\psi, \dots, {}^m\psi)$) includes the independent variable (${}^0\psi = t$) and F ($F = F({}^0F, {}^1F, \dots, {}^mF)$) includes a new component ${}^0F = 1$. These changes serve to make differentiation in a more compact way (Lambert, 1991). With these new definitions, the new problem is transformed into:

$$\frac{d({}^i\psi)}{dt} = {}^iF({}^j\psi) \quad \text{with } {}^j\psi(t=0) = {}^j\psi^{(0)} \quad \text{for } i, j = 0, 1, \dots, m \quad (3.31)$$

Transforming (3.26) and (3.27) using the new notation, the s -stage the Runge-Kutta method can be written as:

$${}^i\psi^{(n+1)} = {}^i\psi^{(n)} + \Delta t b^{(r)}({}^iF^{(r)}) \quad (3.32)$$

$${}^iF^{(r)} = {}^iF({}^j\psi^{(r)}) = {}^iF({}^j\psi^{(n)} + \Delta t a_{rs}({}^jF^{(s)})) \quad (3.33)$$

If we assume that the real solution (${}^i\psi_R$) and the numerical approximation (${}^i\psi$) of (3.31) are known, the global error can be calculated as:

$$\varepsilon = {}^i\psi_R^{(n+1)} - {}^i\psi^{(n+1)} \quad (3.34)$$

Then expanding ${}^i\psi_R^{(n+1)}$ around $t^{(0)} = {}^0\psi^{(n)}$ as a Taylor series expansion, one yields.

$${}^i\psi_R^{(n+1)} = {}^i\psi^{(n)} + \Delta t \frac{d({}^i\psi)}{dt} + \frac{\Delta t^2}{2!} \frac{d^2({}^i\psi)}{dt^2} + \frac{\Delta t^3}{3!} \frac{d^3({}^i\psi)}{dt^3} + \mathcal{O}(\Delta t^4) \quad (3.35)$$

Now, the derivatives in Equation (3.35) can be calculated using the chain rule as:

$$\left. \begin{aligned} \frac{d({}^i\psi)}{dt} &= ({}^iF) \\ \frac{d^2({}^i\psi)}{dt^2} &= ({}^iF_j)({}^jF) \\ \frac{d^3({}^i\psi)}{dt^3} &= ({}^iF_{jk})({}^kF)({}^jF) + ({}^iF_j)({}^iF_k)({}^kF) \end{aligned} \right\} \quad (3.36)$$

Hence, introducing (3.36) into (3.35), we have.

$$\begin{aligned}
 {}^i\psi_R^{(n+1)} &= {}^i\psi^{(n)} + \Delta t({}^iF) + \frac{\Delta t^2}{2!}({}^iF_j)({}^jF) + \\
 &\quad \frac{\Delta t^3}{3!}({}^iF_{jk})({}^kF)({}^jF) + ({}^iF_j)({}^iF_k)({}^kF) + \mathcal{O}(\Delta t^4)
 \end{aligned} \tag{3.37}$$

In order to calculate the global error with Equation (3.34), we must expand the numerical solution $({}^i\psi^{(n+1)})$ using a Taylor series expansion around ${}^i\psi^{(n)}$. If we look to the Equation (3.32), it is enough to expand $({}^jF^{(s)})$ around the same point.

$${}^iF^{(r)} = ({}^iF)\delta_r + \Delta t({}^iF_j)({}^jF^{(s)})a_{rs} + \frac{\Delta t^2}{2!}({}^iF_{jk})({}^jF^{(s)})({}^kF^{(p)})a_{rs}a_{rp} + \mathcal{O}(\Delta t^3) \tag{3.38}$$

The variables ${}^jF^{(s)}$ and ${}^kF^{(p)}$ are unknowns. Therefore, new Taylor series expansions are calculated as:

$$\left. \begin{aligned}
 {}^jF^{(s)} &= ({}^jF)\delta_s + \Delta t({}^jF_l)({}^lF^{(t)})a_{st} + \mathcal{O}(\Delta t^2) \\
 {}^kF^{(p)} &= ({}^kF)\delta_p + \Delta t({}^kF_m)({}^mF^{(u)})a_{pu} + \mathcal{O}(\Delta t^2)
 \end{aligned} \right\} \tag{3.39}$$

As we can observe, the problem now is recursive, hence,

$$\left. \begin{aligned}
 {}^lF^{(t)} &= ({}^lF)\delta_t + \mathcal{O}(\Delta t) \\
 {}^mF^{(u)} &= ({}^mF)\delta_u + \mathcal{O}(\Delta t)
 \end{aligned} \right\} \tag{3.40}$$

Introducing recursively Equations (3.38), (3.39), (3.40) and combining this result with (3.32), one arrives at:

$$\begin{aligned}
 {}^i\psi^{(n+1)} &= {}^i\psi^{(n)} + \Delta t({}^iF)b^{(r)}\delta_r + \frac{\Delta t^2}{2}2({}^iF_j)({}^jF)b^{(r)}a_{rs}\delta_s \\
 &\quad + \frac{\Delta t^3}{6}3({}^iF_{jk})({}^jF)({}^kF)b^{(r)}a_{rs}a_{rp}\delta_s\delta_p + 6({}^iF_j)({}^jF_l)({}^lF)b^{(r)}a_{rs}a_{st}\delta_t \\
 &\quad + \mathcal{O}(\Delta t^4)
 \end{aligned} \tag{3.41}$$

Now introducing (3.37) and (3.41) into (3.34) and after rearranging terms, we can determine the global error of the Runge- Kutta method, 3rd order in this case.

$$\begin{aligned} \varepsilon = & \Delta t ({}^i F) [1 - b^{(r)} \delta_r] + \frac{\Delta t^2}{2!} ({}^i F_j) ({}^i F) [1 - 2b^{(r)} a_{rs} \delta_s] \\ & + \frac{\Delta t^3}{3!} \left\{ ({}^i F_{jk}) ({}^k F) ({}^j F) [1 - 3b^{(r)} a_{rs} a_{rp} \delta_s \delta_p] \right. \\ & \left. + ({}^i F_j) ({}^i F_k) ({}^k F) [1 - 6b^{(r)} a_{rs} a_{st} \delta_t] \right\} + \mathcal{O}(h^4) \end{aligned} \quad (3.42)$$

The Equation (3.42) gives the order conditions that every method must fulfill. In the above derivation, no distinction is made between explicit and implicit Runge- Kutta, therefore it can be used universally.

Table 3. 1 Order conditions for Runge- Kutta method

Order		Order Condition
1	Δt	$b_r = 1$
2	Δt^2	$c_r b_r = \frac{1}{2}$
3	Δt^3	$b_r a_{rs} c_s = \frac{1}{6} \quad b_r c_r^2 = \frac{1}{3}$
4	Δt^4	$b_r c_r^3 = \frac{1}{4} \quad b_r c_r a_{rs} c_s = \frac{1}{8}$ $b_r a_{rs} a_{st} c_t = \frac{1}{24} \quad b_r a_{rs} c_s^2 = \frac{1}{12}$
5	Δt^5	$b_r c_r^4 = \frac{1}{5} \quad b_r c_r^2 a_{rs} c_s = \frac{1}{10} \quad b_r c_r a_{rs} c_s^2 = \frac{1}{15}$ $b_r a_{rs} c_s^3 = \frac{1}{20} \quad b_r a_{rs} c_s a_{rt} c_t = \frac{1}{20} \quad b_r c_r a_{rs} a_{st} c_t = \frac{1}{30}$ $b_r a_{rs} c_s a_{st} c_t = \frac{1}{40} \quad b_r a_{rs} a_{st} c_t^2 = \frac{1}{60} \quad b_r a_{rs} a_{st} a_{tu} c_u = \frac{1}{120}$

3.8 Lax equivalence theorem

When a numerical method is designed, it is necessary to know if the approximate solution is accurate. In other words, if the numerical solution reproduces the continuum solution correctly (Lambert, 1991; Strikwerda, 2004). Formally, a numerical method is said to be convergent if the approximate solution tends to the exact solution as the discretization grid (space, time, or time/space) tends to zero.

$$\lim_{\Delta t \rightarrow 0} |{}^i \psi_R - {}^i \psi| = 0 \quad (3.43)$$

Determining convergence with the last criteria is difficult, if not impossible, because the real solution is not known in advance. In practice, the way to guarantee convergence is with the Lax equivalence theorem (or the Lax-Richtmyer theorem for PDEs) (Leveque, 1992), which states that a numerical method is convergent if and only if the numerical method is consistent and stable.

$$\text{Convergence} \Leftrightarrow \text{Consistent} + \text{Stable} \quad (3.44)$$

The Lax equivalence theorem simplifies the analysis tremendously because it is enough to show that the numerical method is consistent and stable.

3.8.1 Consistency

Consistency is related to how a discretization method resembles a continuous problem. In other words, it is a metric that indicates how the discrete operators reproduce the original continuous operator as the time/grid tends to zero. This concept was introduced briefly in section 3.4 when the UPWIND scheme was presented. Additionally, in Section 3.7.1 it was shown that Runge- Kutta order of accuracy increases when more terms in the Taylor series expansion are considered; in consequence, the truncation error is lower, showing that the Runge- Kutta method is also consistent.

3.8.2 Stability

By the moment, before any formal definition, stability or instability means that the solution behaves regularly or not in time, respectively. One might think that because in numerical methods the approximation derives in algorithms to find the solution computationally, some source of error is accumulated, due to the finite number precision given by the processor internal arithmetics and subsequently deriving in instability. The truth is that round-off errors may have some impact, particularly for non-linear problems, but the main cause is another. In the classic paper by Richard Courant (R. Courant, Friedrichs, & Lewy, 1928) they establish some criteria based on mesh velocity, commonly known as the Courant number or CFL condition, ($\text{CFL} = \lambda \Delta t / \Delta z$). This pioneering work was made for hyperbolic differential equations, but its impact has been such that it has inspired generations of researchers in the study of instability based on this type of criteria. Based on this idea, the classical tools in the asses of stability are the study of

the stability regions for ODEs and Fourier transformations for the Von Neumann stability criterion in PDEs.

A stability region is defined as the region in which the corresponding stability function or stability accumulation factor $R(z) = \psi^{(n+1)} / \psi^{(n)}$ of a specific method is bounded on any non-empty region. Mathematically (Hundsdorfer & Verwer, 2000) defines a stability region as:

$$S = \{ z \in \mathbb{C} : |R(z)| \leq 1 \} \quad (3.45)$$

Depending upon the topology of the stability region, the three basic definitions of stability are, see Annex G for its mathematical definition:

- *Zero- Stability*: is referred to when the solution is bounded imposing some perturbation (Hairer et al., 1993; Lambert, 1991; Strikwerda, 2004). This definition of stability ensures that the solution will not diverge for small perturbations like round-off and errors introduced by the discretization method.
- *A- Stability*: defines if the solution is not only stable but also converges to a finite value as $t \rightarrow \infty$, (Hahn, 1967; Stetter, 1971).
- *L- stability*: when a solution is stable when large propagation velocities and/or large time steps are used and the solution is still stable (Ehle, 1969).

3.8.2.1 ODE stability

Determining the stability regions for non-linear problems is a complex task. Therefore, simplification of the problem analyzing simple linear homogeneous systems has been the way to go. With this information, one might extrapolate results to understand the behavior of more complex non-linear and/or non-homogenous cases. For autonomous ODEs solvers, the linear Dahlquist test problem (Dahlquist, 1963), is often used:

$$\left. \begin{aligned} \frac{d\psi}{dt} &= \lambda\psi \quad \text{with } \lambda \in \mathbb{C} \\ \psi(t=0) &= \psi_0 \end{aligned} \right\} \quad (3.46)$$

The problem (3.46) has an analytical solution provided by:

$$\psi = \psi_0 e^{\lambda t} \quad (3.47)$$

To illustrate the methodology for obtaining stability functions and later its corresponding stability region, the procedure for the Euler forward scheme is shown. For higher-orders the procedure is straightforward. The Euler method numerical procedure can be written as:

$$\psi^{(n+1)} = \psi^{(n)} + \Delta t F(t^{(n)}, \psi^{(n)}) \quad (3.48)$$

Therefore, for the Dahlquist test problem, (3.46) it is reduced to:

$$\begin{aligned} \psi^{(n+1)} &= \psi^{(n)} + \Delta t \lambda \\ &= (1 + \Delta t \lambda) \psi^{(n)} \end{aligned} \quad (3.49)$$

Rearranging terms the stability function can be found.

$$R(z) = \frac{\psi^{(n+1)}}{\psi^{(n)}} = (1 + z) \quad \text{with} \quad z = \Delta t \lambda \in \mathbb{C} \quad (3.50)$$

Lastly, the idea is to find the values of $|R(z)| \leq 1$. For this case, the bounded condition can be easily determined analytically:

$$|1 + z| < 1 \Leftrightarrow -2 < z < 0 \Rightarrow \Delta t < \frac{2}{\lambda} \quad (3.51)$$

This condition can be depicted graphically, one has to recall that z can be a complex number ($z = x + iy$), then the axes are the real and imaginary parts of z for the abscissa and ordinate axes respectively. In Figure 3. 3.a the stability map for the Euler Forward method is shown. Note that the condition (3.51) is fulfilled in all the points inside the unit radius circle (colored region). This means that the solution of the Dahlquist test problem is stable with values $z = \Delta t \lambda$ that lie inside the mentioned region. All the points outside that region are unstable (white region) and must be avoided.

The procedure to determine $R(z)$ for the Runge- Kutta Methods can be determined in a similar fashion used for the Euler forward method. It can be shown that for explicit methods of order p , the stability function is (Hairer & Wanner, 1996).

$$R(z) = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \dots + \frac{z^p}{p!} \quad (3.52)$$

The stability maps for the classic explicit Runge- Kutta method up to 4th order are plotted in Figure 3. 3. On these plots, the critical z values are 2, 2, 2.513, and 2.7185 from 1st up to 4th order of accuracy respectively. That is to say that we can choose bigger time steps and advance quicker in time. However, another crucial aspect is computational efficiency.

Figure 3. 3 Classic explicit Runge- Kutta stability maps

To compare the efficiency of the explicit Runge- Kutta methods, the Dahlquist test is analyzed with $\lambda = 100$ inside the interval $[0, 1]$. The number of time steps required

is simply $n = T / \Delta t$. However, the explicit Runge-Kutta methods require several evaluations inside $[t^{(n)}, t^{(n+1)}]$. This number of auxiliary evaluations (only for classical explicit methods) inside the interval coincides with the number of stages (s). This makes that the total number of evaluations is $N_{tot} = sn = s\lambda T / z_{crit}$. Therefore, the computational efficiency decreases with the increase of time accuracy, Table 3.2.

Table 3.2 Computational efficiencies for Runge- Kutta explicit methods

Order	$ z_{crit} $	Δt_{crit} (s)	n	$\varepsilon \propto \mathcal{O}(\Delta t^p)$	N_{tot}
1	2	0.02	50	0.02	50
2	2	0.02	50	4.00×10^{-4}	100
3	2.513	0.025	39.798	1.59×10^{-5}	119.393
4	2.785	0.028	35.904	6.02×10^{-7}	143.616

For implicit Runge-Kutta methods, the stability function can be calculated as in (Hairer & Wanner, 1996):

$$R(z) = 1 + zb^T(I - z\mathbf{a})^{-1}\mathbb{I} \quad (3.53)$$

Alternatively, as (Stetter 1973, Scherer 1979):

$$R(z) = \frac{\det(I - z\mathbf{a} + z\mathbb{I}b^T)}{\det(I - z\mathbf{a})} \quad (3.54)$$

here: $\mathbf{a} = \mathbf{a}_{rs}$, $b = b_r$, $\mathbf{I} = \text{diag } 1, \dots, 1$, $\mathbb{I} = 1, \dots, 1^T$

Using Equation (3.53) the stability maps for the 1st order Euler backward, 2nd order mid-point rule, 3rd order methods from Skvortsov (Skvortsov, 2006), Kennedy & Carpenter (Kennedy & Carpenter, 2003), Alexander (Alexander, 2003) and 4th order from Skvortsov (Skvortsov, 2006) are shown in Figure 3. 4. These figures show that the Euler backward, the Alexander E33a, and the Svortsov ES54 (Skvortsov, 2006) are L- Stable methods. The other cases, Mid-Point Rule, Kennedy & Carpenter, and Svortsov ES33b are only A- Stable. In Annex F their corresponding Butcher table is summarized.

 a) Euler Backward (1st order)

 b) Mid- point rule (2nd order)

 c) Skvortsov ES33b (3rd order)

 d) Kennedy & Carpenter (3rd order)

 e) Alexander ES33a (3rd order)

 f) Skvortsov ES54 (4th order)

Figure 3. 4 Implicit Runge- Kutta methods stability maps

3.8.2.2 Stability in PDEs

In the preceding section, Runge- Kutta methods stability maps are presented. That analysis was restricted for autonomous ODEs. In this Section, stability is studied for PDEs using stability maps instead of the classic Von Neumann analysis. The classic Von Neumann analysis can be consulted in any textbook of numerical methods for PDEs (Dormon, 2000; Ferziger & Peric, 2002; Leveque, 1992; Strikwerda, 2004) to mention

only a few. The approach studied here is very convenient to analyze the stability of Runge- Kutta methods due to its recursive nature and because boundary conditions are included, being this matter ignored in the classic Von Neumann Analysis, see (Hundsdorfer & Verwer, 2000; Ketcheson & Ahmadi, 2012).

To analyze linear systems of ODE's can be made extending the Dahlquist test.

$$\frac{\partial \psi_i}{\partial t} = A_{ij} \psi_i \quad (3.55)$$

Here $\psi_i(t) : \mathbb{R} \rightarrow \mathbb{R}^n$ and $A \in \mathbb{R}^n \times \mathbb{R}^n$ is a constant coefficient matrix. Again, the test case problem has an analytical solution.

$$\psi_i(t) = e^{At} \psi_{i,0} \quad (3.56)$$

In the above expression e^A stands for the exponential matrix function, defined using a power series expansion (N. J. Higham, 2008):

$$e^A = A + \frac{1}{2!} A^2 + \frac{1}{3!} A^3 + \dots + \frac{1}{n!} A^n \quad (3.57)$$

Or alternatively as:

$$e^A = \lim_{y \rightarrow \infty} \left(1 + \frac{A}{y} \right)^y \quad (3.58)$$

For systems of ODEs, any s stage (explicit or implicit) Runge- Kutta method can be written as:

$$\psi_i^{(n+1)} = R(z) \psi_i^{(n)} \quad \text{With } z = A\Delta t \quad (3.59)$$

As happened with autonomous ODEs, the method described by Equation (3.59) is A - Stable if z , now defined with constant coefficient matrix A , lies inside the stability region defined with $|R(z)| \leq 1$. Now, the solution depends on matrix A , as in Equation (3.56). Therefore definition (3.45) can now be extended to a system of ODEs (Ketcheson & Ahmadi, 2012) as:

$$\begin{aligned} \Delta t \lambda \in S \quad \text{With } \lambda \in \Lambda \\ \text{Being } \Lambda \text{ the spectrum of } A \end{aligned} \quad (3.60)$$

The definition (3.60) implies that the method (3.59) is stable if all eigenvalues of A lie inside the stability region S . From this way, knowing S and the spectrum of A one can determine the critical time step (Δt_{crit}) in order to guarantee stability.

$$\Delta t_{crit} = \max_{\Delta t \geq 0} : |R(\Delta t \lambda)| \leq 1 \quad \text{for } \lambda \in \Lambda \quad (3.61)$$

If we assume that space and time can be decoupled using the method of lines (MOL), the above result can be extended to the linear- homogeneous advection equation ($d\psi_i / dt = -v d\psi_i / dz$). In this case, matrix A is the coefficient matrix due to the space discretization. Using the UPWIND scheme (see Section 3.4) and considering that v is a positive constant, spatial grid spacing is uniform ($\Delta z_i = \Delta z = L / n$) for $i = 1, 2, \dots, n$ and imposing periodic boundary conditions $\psi_{i,1}(t) = \psi_{i,n}(t)$ matrix A has the following form.

$$A = \frac{v}{\Delta z} \begin{pmatrix} -\Delta z / v & \dots & \dots & \dots & \dots & \dots & \Delta z / v \\ 1 & -1 & 0 & \dots & \dots & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & & & \vdots \\ \vdots & & 1 & -1 & 0 & \dots & 0 \\ \vdots & & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & & 1 & -1 & 0 \\ 0 & \dots & \dots & \dots & \dots & 1 & -1 \end{pmatrix} \quad (3.62)$$

To analyze stability for the Runge- Kutta methods, the extended Dahlquist test is evaluated for $v = 1$, the unitary total length of the domain is $L = 1$. With this data, the spectrum of coefficient matrix A is plotted in Figure 3. 5. On these figures, the coefficient matrix spectrum are superimposed over the stability maps using Equations (3.52) and (3.53) for the explicit and implicit Runge- Kutta methods respectively. The results show that the explicit methods are conditionally stable. For the explicit Euler forward and 4th order classic Runge- Kutta methods, the limit Courant numbers are 1.0 and 1.39 respectively. These values were measured by (Hundsdorfer & Verwer, 2000) and also reported by (Baldauf, 2008). This experiment also shows that implicit methods are unconditionally stable, as expected. Moreover, for the implicit Runge- Kutta methods it

is observed that the solution is not only stable for large (negative) eigenvalues but also the stability function decreases while the eigenvalues are larger, see Figure 3. 4.e and Figure 3. 4.f, this behavior is significantly important to study stiff differential equations. This issue will be explained in the next section.

a) Euler Forward

b) 4th order classic explicit Runge-Kutta

c) 3rd Order Implicit Alexander ES33a

d) 4th Order Skvortsov ES54

Figure 3. 5 UPWIND scheme spectrum

3.9 Stiffness

Numerical stability analysis has been performed for linear cases, and it is concluded that a stability criterion must be fulfilled in order to avoid undesirable instabilities. However, in some cases, the required step size is significantly smaller than the step size needed to fulfill the stability criterion of the integration scheme. This difficulty gave birth to the notion or concept of “*stiffness*” of a differential equation.

In the scientific community, it is well accepted that the first influential opinion was given in (Curtiss & Hirschfelder, 1952) who pointed that “*stiff equations are equations where certain implicit methods perform better, usually tremendously better, than explicit ones.*” Later on, many other authors made contributions to this subject. For example: (Hairer & Wanner, 1996) argue that “*Stiff equations are problems for which explicit schemes don’t work*”.

In contrast, other authors establishes four different definitions of stiffness, claiming that an equation is stiff if:

- i)* the step size required for stability is much smaller than the step size required for accuracy.
- ii)* it contains some components of the solution that decay rapidly compared to other components of the solution.
- iii)* at least one eigenvalue is negative and large compared to the other eigenvalues of the system.
- iv)* the step size based on computational cost is too large to obtain an accurate solution. (Hoffman, 2001,pp 401-402)

With these intuitive definitions, it is clear that the issue with stiffness is strongly related to explicit methods, and that the step size has a major impact on the “quality” of the approximate solution. Although this intuitive notion of stiffness is quite clear, the theory for universal criteria to determine when or under which circumstances an equation is stiff is still missing, being still under debate. In that sense, (D. J. Higham & Trefethen, 1993) argued that the problem of obtaining a universal criterion is that stability is always taken into account with the modulus of the eigenvalue of the system, but the pseudo-spectra of the eigenvalue are ignored. In their work, they developed a criterion considering the pseudo-spectra of the system eigenvalues instead of their spectra, which has been the mathematical tool used by many researchers since (Curtiss & Hirschfelder, 1952). On the other hand, (Söderlind, Jay, & Calvo, 2015), in turn developed the so-called stiffness indicator functional, independent of the numerical integration scheme due to its definition in terms of the logarithmic norm. As can be seen, some researchers choose to describe stiffness with the understanding of the eigenvalues, but others prefer to work with matrix norms.

What is clear so far is that implicit numerical methods perform better for stiff differential equations than explicit methods. In that sense, implicit Runge- Kutta methods, especially diagonally implicit Runge- Kutta methods are an interesting choice due to its computational economy and flexible high order of accuracy (Ababneh, Ahmad, & Ismail, 2009; Alexander, 1977).

3.10 Concluding remarks

In the present chapter, the mathematical principles of the numerical methodology used in this thesis are presented. The usage of the Method of Lines jointly with the Finite Volume Method and implicit Runge- Kutta method ensures high quality of the solution, accurate results in a shorter computation, and time step flexibility. As part of this thesis, a computational code with these characteristics is developed in Matlab[®]. This program is codified in a very flexible way, being able to modify the temporal of accuracy changing the corresponding Butcher table. The developed numerical code has the following features:

- High temporal accuracy.
- Convergent solutions.
- The approximation can handle Stiff problems.

Nomenclature

a	Butcher table.
A	Discrete matrix operator.
b	Butcher table quadrature vector.
c	Butcher table stage location.
F	Convective transport vector. Numerical flux vector
I	Identity matrix
$\mathbb{I}$	Identity vector.
$\text{Im}(z)$	Imaginary part of complex number z .
J_{ij}	Jacobian matrix.
L	Length (m).
m, n	Integer numbers.
N_{tot}	Total number of evaluations
$\hat{n}$	Outward unitary vector.

$\mathcal{O}$	Big O notation error function.
q	Runge- Kutta method total number of stages.
$\text{Re}(z)$	Real part of complex number z .
R, s	Runge- Kutta indexes.
$R(z)$	Stability function.
S	Stability region.
t	Time (s).
T	Total time (s).
u	Velocity, phase velocity ($\text{m} \cdot \text{s}^{-1}$).
V	Volume (m^3).
w	Taylor series expansion point
z	Axial coordinate (m). Complex variable.

Greek Letters

Λ	Matrix spectrum.
α	Lagrange interpolation polynomial
β	Derivative index.
Γ	Boundary.
γ	Time/ stage index.
Δ	Finite difference.
δ	Unity vector $1, \dots, 1^T$.
ε	Error.
ϑ	Vector position index.
v	Constant
λ	Eigenvector.
ρ	Material density ($\text{kg} \cdot \text{m}^{-3}$).
ψ	Dependent variable vector.
ψ_R	Dependent variable vector exact solution.
$\tilde{\psi}(t)$	Dependent variable vector inlet boundary condition
Φ'''	Source term vector per unit volume.

Subscripts

0	Initial condition.
W, P, Ee, w, e	Cardinal system index notation.
$crit$	Critic.
v	Vapor.
h, i, j, k, p, l, u, t	Indexes
r, s	Runge- Kutta indexes.

Superscripts

'	Per unit length.
''	Per unit area.
'''	Per unit volume.
()	Time stage.
0	Initial condition.

Acronymous

BWR	Boiling water reactor.
BC	Boundary conditions.
CFL	Courant number (Courant- Friedrich- Levy).
FDM	Finite difference method.
FEM	Finite element method.
FVM	Finite volume method.
HVAC	Heating, Ventilation and Air Conditioning.
IVP	Initial value problem.
MOL	Method of lines
ODE	Ordinary differential equation.
PDE	Partial differential equation.
PWR	Power water reactor.
1-D	One dimensional

References

Ababneh, O. Y., Ahmad, R., & Ismail, E. S. (2009). Design of New Diagonally Implicit Runge – Kutta Methods for Stiff Problems. *Applied Mathematics Science*, 3(45), 2241–2253.

Alexander, R. (1977). Diagonally Implicit Runge- Kutta Methods for Stiff O.D.E.'s. *SIAM Journal of Numerical Analysis*, 14(6), 1006–1021. <https://doi.org/10.1137/0714068>

Alexander, R. (2003). Design and Implementation of DIRK Integrators for Stiff Systems. *Applied Numerical Mathematics*, 46, 1–17. [https://doi.org/10.1016/S0168-9274\(03\)00012-6](https://doi.org/10.1016/S0168-9274(03)00012-6)

Baldauf, M. (2008). Stability Analysis for linear Discretisations of the Advection Equation with Runge – Kutta Time Integration. *Journal of Computational Physics*, 227, 6638–6659. <https://doi.org/10.1016/j.jcp.2008.03.025>

Butcher, J. C. (1963). Coefficients for the Study of Runge-Kutta Integration processes. *Journal of the Australian Mathematical Society*, 3((02)), 185–201. <https://doi.org/10.1017/S1446788700027932>

Butcher, J. C. (1996). History of Runge-Kutta Methods, 20, 247–260. [https://doi.org/10.1016/0168-9274\(95\)00108-5](https://doi.org/10.1016/0168-9274(95)00108-5)

Butcher, J. C. (2008). *Numerical Methods for Ordinary Differential Equations* (2nd Edit.). John Wiley & Sons, Ltd.

Butcher, J. C., & Wanner, G. (1996). Runge-Kutta methods: some historical notes. *Applied Numerical Mathematics*, 22, 113–151. [https://doi.org/10.1016/S0168-9274\(96\)00048-7](https://doi.org/10.1016/S0168-9274(96)00048-7)

Chakravarthy, S. R., & Osher, S. (1983). High-Resolution Applications of the OSHER Upwind Scheme for the Euler Equations. In *AIAA, 6th Computational Fluid Dynamic Conference*. <https://doi.org/10.2514/6.1983-1943>

Chung, T. J. (2001). *Computational Fluid Dynamics*. Cambridge University Press.

Courant, B. R., Isaacson, E., & Rees, M. (1952). On the Solution of Nonlinear Hyperbolic Differential Equations by Finite Differences. *Communications on Pure and Applied Mathematics*, V, 243–255. <https://doi.org/10.1002/cpa.3160050303>

Courant, R., Friedrichs, K., & Lewy, H. (1928). Über die Partiellen Differenzengleichungen der Mathematischen Physik. *Mathematische Annalen*, 100, 32–74. <https://doi.org/10.1007/BF01448839>

Curtiss, C. F., & Hirschfelder, J. O. (1952). Integration of stiff equations. *Proceedings of the National Academy of Sciences*, 38(1950), 250–253. Retrieved from <http://www.ncbi.nlm.nih.gov/pmc/articles/PMC1063538/>

Dahlquist, G. G. (1963). A Special Stability Problem for Linear Multistep Methods. *BIT Numerical Mathematics*, 3(1), 27–43. <https://doi.org/10.1007/BF01963532>

Darwish, M. S. (1993). A New High- Resolution Scheme Based on the Normalized Variable Formulation. *Numerical Heat Transfer, Part B: Fundamentals: An International Journal of Computation and Methodology*, 24, 37–41. <https://doi.org/10.1080/10407799308955898>

Dormon, J. R. (2000). *Numerical Methods for Differential Equations: A Computational Approach*. CRC Press.

Ehle, B. L. (1969). On Pade Approximations to the exponential function and A-Stable Methods for the Numerical Solution of Initial Value Problems.

Engquist, B. B., & Osher, S. (1981). One-Sided Difference Approximations for Nonlinear Conservation Laws. *Mathematics of Computation*, 36(154), 321–351. <https://doi.org/10.1090/S0025-5718-1981-0606500-X>

Farrashkhalvat, M., & Miles, J. P. (2003). *Basic Structured Grid Generation: With an Introduction to Unstructured Grid Generation*. Elsevier Ltd.

Ferziger, J. H., & Peric, M. (2002). *Computational Methods for Fluid Dynamics* (3rd Edit.). Berlin: Springer- Verlag.

Gaskell, P. H., & Lau, A. K. C. (1988). Curvature- Compensated Convective Transport: SMART, A New Boundedness- Preserving Transport ALgorithm. *International Journal for Numerical Methods in Fluids*, 8, 617–641. <https://doi.org/10.1002/fld.1650080602>

Gear, C. W. (1971). *Numerical Initial Value Problems in Ordinary Differential Equations*. Prentice- Hall, Inc.

Greenspan, D. (1961). *Introduction to Partial Differential Equations*. New York: McGraw-Hill. Retrieved from file://catalog.hathitrust.org/Record/003913532

Hahn, W. (1967). *Stability of Motion*. Springer-Verlag Berlin Heidelberg. <https://doi.org/10.1007/978-3-642-50085-5>

Hairer, E., & Wanner, G. (1996). *Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems*. (Springer, Ed.) (2nd Edit.).

Hairer, E., Wanner, G., & Nørsett, S. P. (1993). *Solving Ordinary Differential Equations I: Nonstiff Problems*. (Springer, Ed.) (2nd Edit.). <https://doi.org/10.1007/978-3-540-78862-1>

Harlow, F. H., & Welch, J. E. (1965). Numerical Calculation of Time-Dependent Viscous Incompressible Flow of Fluid with Free Surface. *Physics of Fluids*, 2182–2189. <https://doi.org/10.1063/1.1761178>

Higham, D. J., & Trefethen, D. L. (1993). Stiffness of ODE's. *BIT Numerical Mathematics*, 33(August 1992), 285–303.

Higham, N. J. (2008). *Functions of Matrices: Theory and Computation*. Society for Industrial and Applied Mathematics (SIAM).

Hoffman, J. D. (2001). *Numerical Methods for Engineers and Scientists* (2nd Edit.). Marcel Dekker, Inc.

Hundsdoerfer, W., & Verwer, J. (2000). Numerical Solution of Time-Dependent Advection- Diffusion- Reaction Equations. Springer. <https://doi.org/10.1007/978-3-662-09017-6>

Hyman, J. (1977). The Methods of Lines Solutions for Partial Differential Equations. New York University.

Kennedy, C. A., & Carpenter, M. H. (2003). Additive Runge – Kutta Schemes for Convection – diffusion – Reaction Equations, 44, 139–181. [https://doi.org/10.1016/S0168-9274\(02\)00138-1](https://doi.org/10.1016/S0168-9274(02)00138-1)

Ketcheson, D. I., & Ahmadi, A. J. (2012). Optimal Stability Polynomials for Numerical Integration of Initial Value Problems. Communications in Applied Mathematics and Computational Science, 7(2), 247–271. <https://doi.org/10.2140/camcos.2012.7.247>

Lambert, J. D. (1991). Numerical Methods for Ordinary Differential Systems: The Initial Value Problem. (John Wiley & Sons Ltd, Ed.).

Leveque, R. J. (1992). Numerical Methods for Conservation Laws (2nd Edit.). Berlin: Birkhäuser.

Liseikin, V. D. (2010). Grid Generation Methods (2nd Edit.). Springer Netherlands. <https://doi.org/10.1007/978-90-481-2912-6>

Majumdar, S. (1988). Role of Underrelaxation in Momentum Interpolation for Calculation of Flow with Nonstaggered Grids. Numerical Heat Transfer, 13(1), 125–132. <https://doi.org/10.1080/10407788808913607>

Patankar, S. V. (1980). Numerical Heat Transfer and Fluid Flow. Hemisphere Publishing Corporation.

Rhie, C., & Chow, W. L. (1983). A Numerical Study of the Turbulent Flow Past An Isolated Airfoil with Trailing Edge Separation. AIAA, 21, 525–1532. <https://doi.org/10.2514/3.8284>

Schiesser, W. (1991). The Numerical Method of Lines. Elsevier academic press.

Skvortsov, L. M. (2006). Diagonally Implicit Runge – Kutta Methods for Stiff Problems. Computational Mathematics and Mathematical Physics, 46(12), 2209–2222. <https://doi.org/10.1134/S0965542506120098>

Söderlind, G., Jay, L., & Calvo, M. (2015). Stiffness 1952–2012: Sixty years in search of a definition. BIT Numerical Mathematics, 55(2), 531–558. <https://doi.org/10.1007/s10543-014-0503-3>

Stetter, H. J. (1971). Stability of Discretizations on Infinite Intervals. In Conference on Applications of Numerical Analysis: Lecture Notes in Mathematics, vol 228 (pp. 207–222). Springer, Berlin, Heidelberg.

Strikwerda, J. C. (2004). Finite Difference Schemes and Partial Differential Equations (2nd Edit.). SIAM.

Thompson, J. F., Soni, B. K., & Weatherill, N. P. (1998). Handbook of Grid Generation. (J. F. Thompson, B. K. Soni, & N. P. Weatherill, Eds.). CRC Press.

Toro, E. F. (2009). Riemann Solvers and Numerical Methods for Fluid Dynamics: A Practical Introduction (3rd Edit.). Springer. <https://doi.org/10.1007/978-3-540-49834-6>

Van Leer, B. (1974). Towards the Ultimate Conservative Difference Scheme. II. Monotonicity and Conservation Combine in a Second-Order Scheme. Journal of Computational Physics, 14, 361–370. [https://doi.org/10.1016/0021-9991\(74\)90019-9](https://doi.org/10.1016/0021-9991(74)90019-9)

Van Leer, B. (1979). Towards the Ultimate Conservative Difference Scheme. V. A Second-Order Sequel to Godunov’s Method. Journal of Computational Physics, 136, 101–136. [https://doi.org/10.1016/0021-9991\(79\)90145-1](https://doi.org/10.1016/0021-9991(79)90145-1)

Versteeg, H. K., & Malalasekera, W. (1995). Introduction to Computational Fluid Dynamics. The Finite Volume Method. Longman Group LTD.

Zhu, J., & Rodi, W. (1991). A Low Dispersion and Bounded Convection Scheme. Computer Methods in Applied Mechanics and Engineering, 92, 87–96. [https://doi.org/10.1016/0045-7825\(91\)90199-G](https://doi.org/10.1016/0045-7825(91)90199-G)

Zienkiewicz, O. C. (2000). The Finite Element Method . Volume 1 : The Basis (5th Edit., Vol. 1). Butterworth- Heinemann.

1-D Numerical Analysis of Sub – Cooled Boiling in Pipes

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4.1 Introduction

The goal in modeling 1-D two-phase flows is to determine the *in situ* phase fractions, commonly known as void fraction for the vapor phase or liquid hold-up for the liquid phase (Kandlikar, 1999), as well as both average velocities and pressure fields (or pressure gradient). However, the calculation of these flow magnitudes presents some difficulties in contrast with single-phase flows, arising from the fact that both phases differ in their velocities and densities. One of these difficulties is due to the strong relationship between quality x , void fraction ε , and density ρ . Which makes the problem to behave stiffly. This behavior is experienced in two-phase flow simulations when average mixture density changes steeply in one or several points of the domain,

like in boiling and condensing processes, see Figure 4. 1. To overcome this, some specific numerical treatment seems advisable. To capture all the possible relevant physical information of the problem in a short computation time.

Figure 4. 1 Schematic time evolution for a fixed location of a 1-D heated boiling pipe flow: a) quality and void fraction, b) mixture density.

In chapter III, it was concluded that implicit Runge- Kutta methods are a powerful and promising tool for PDEs solution. Being implicit RK methods the ideal family of methods for stiff problems. In the present chapter, the SIMPLE-ESDIRK method proposed by (Ijaz & Anand, 2007) is extended for 1-D transient two-phase flows. This extension is motivated by the high temporal order of accuracy demanded to cope with fast phase change events. This methodology is suitable for boiling heat exchangers, solar thermal receivers, etc.

4.2 Scope

Within the described scenario, the objective of this chapter is to propose a numerical algorithm based on a high order single-step numerical scheme using the RK SIMPLE-ESDIRK method to solve 1-D transient two-phase flow quasi-homogeneous model for a heated single pipe. Special emphasis is put on sub-cooled boiling, as this

process is of specific interest in highly loaded boilers. Appropriate 1-D solutions hold the advantage of presenting a high numerical efficiency that allows to easily include them in global modeling of large industrial installations and systems.

4.3 Outline

This chapter is organized as follows: Section 4.4 introduces, in mathematical terms, the physical model jointly with the respective closure relationships and boundary (BC) and initial conditions (IC). Section 4.5 is devoted to the spatial discretization for the steady-state problem, which is the starting point for the formulation of the transient algorithm, objective of this chapter. Section 4.6 develops the high order temporal scheme jointly with the resulting numerical algorithm. Section 4.7 outlines the details of the SIMPLE algorithm for two-phase problems, followed by section 4.8 where the detailed numerical algorithm is explained. In section 4.9 the experiments of (Bartolomei & Chanturiya, 1967) and (Bartolomei et al., 1982), which is used as a benchmark is described, followed by steady and transient state validation of the model. Posteriorly, in sections 4.10, 4.11 and 4.12 several numerical transient problems are studied, revealing the potential of the ESDIRK method in typical transient situations in two-phase boiling processes. Finally, in section 4.13 the conclusions of this chapter are presented.

4.4 Mathematical formulation

The assumed hypotheses are that the flow is one dimensional (1-D), thermal conduction along the longitudinal z axis is negligible, cross area section of the straight pipe is constant, liquid, and gas phases pressures are equal. With these assumptions, balances for mass, momentum, and energy are performed for each phase separately. After in-volume averaging for both phases, the quasi-homogeneous model is obtained; the details can be found in (Wallis, 1969), (Kandlikar, 1999) and chapter II as well. The model expressed per unit length is as follows:

Conservation of mass

$$\frac{\partial(\rho_{TP}A)}{\partial t} + \frac{\partial \dot{m}}{\partial z} = 0 \quad (4.1)$$

Conservation of momentum

$$\frac{\partial \dot{m}}{\partial t} + \frac{\partial(K\dot{m}^2)}{\partial z} = -\frac{\partial(pA)}{\partial z} - \left\langle \frac{\partial p}{\partial z} \right\rangle'_{fr} - \rho_{TP} g A \sin \alpha \quad (4.2)$$

Conservation of energy (Enthalpy)

$$\frac{\partial(\rho_{TP} h_{TP} A)}{\partial t} + \frac{\partial(\dot{m} h_{TP})}{\partial z} = \langle q_{wall} \rangle' \quad (4.3)$$

In the above equations $K = (1/A) \left[x^2 / \varepsilon \rho_g + (1-x)^2 / (1-\varepsilon) \rho_l \right]$. Additionally, t , z , $\dot{m}$, A , p , g , α , x , h_{TP} , ρ_{TP} and $\langle q_{wall} \rangle'$ respectively refer to time, axial coordinate, mass flow rate, cross-section area, pressure, gravity constant ($= 9.81 \text{ m} \cdot \text{s}^{-2}$), inclination angle of the pipe, void fraction (see Section 4.4.2.1, or Chapter II for its mathematical definition), thermodynamic quality, mixture density, mixture enthalpy, and wall heat flux per unit length. In the momentum balance, the shear stress at the wall τ_{wall} is built with the Darcy equation ($\tau_{wall} = f \rho u^2 / 8$) in which f represents the Churchill wall friction factor, that after integrating on the fluid element is transformed into the wall friction term $\langle \partial p / \partial z \rangle'_{fr}$.

In systems where a phase change occurs, the thermodynamic quality (x) cannot be calculated directly as the fraction of total mass that is gas, in such case, thermodynamic quality must be calculated with an energy balance as follows:

$$x = \frac{h_{TP} - h_l(p)}{h_v(p) - h_l(p)} \quad (4.4)$$

With this definition of x mixture enthalpy (h_{TP}) and density (ρ_{TP}) can also be defined as:

$$h_{TP} = \begin{cases} x h_v + (1-x) h_l & \text{if } 0 < x < 1 \\ h(T, p) & \text{elsewhere} \end{cases} \quad (4.5) \quad \rho_{TP} = \varepsilon \rho_v + (1-\varepsilon) \rho_l \quad (4.6)$$

In the above definitions sub-index l and v respectively refer to liquid and vapor saturation conditions.

4.4.1 Initial and Boundary conditions

At the initial state and in the entire domain the mass flow rate, pressure, temperature, and vapor quality must be specified.

$$\varphi(z, t = 0) = \varphi_0(z) \quad \text{with} \quad \varphi = (\dot{m} \ p \ T \ x)^T \quad (4.7)$$

The system of equations composed by Equations (4.1) to (4.3) form a hyperbolic partial differential equation system, hence, only initial conditions in Equation (4.7), are needed to well-pose the problem; therefore, the numerical approach adopted in this work requires to solve an intermediate pressure correction equation, which is elliptic (this approach is detailed in Section 4.7), the reason why it's also necessary a set of boundary conditions. These BC will be logically for mass flow and pressure, temperature and quality (if needed) in order to determine the thermodynamic state. For convenience, they will be set at the inlet of the pipe $z = 0$.

$$\varphi(z = 0, t) = \tilde{\varphi} \quad \text{with} \quad \varphi = (\dot{m} \ p \ T \ x)^T \quad (4.8)$$

4.4.2 Closure relationships

To close the problem, some empirical information is required. This section presents the empirical information required to close the mathematical model.

4.4.2.1 Void fraction

Unlike most advanced models for two-phase flows, such as the two-fluid model (Mamoru Ishii & Hibiki, 2011), in which the void fraction is calculated with its own transport equation, in the quasi-homogeneous model the void fraction is calculated by its definition (Kandlikar, 1999).

$$\varepsilon = \frac{x}{x + S_R(1 - x) \frac{\rho_v}{\rho_l}} \quad (4.9)$$

In this Chapter, in addition to the homogeneous case, in which the slip ratio is 1 ($S_R \equiv 1$), consideration is given to the possibility of slip velocities between phases

($S_R \neq 1$), determining the slip ratio by means of the Premoli correlation (Premoli et al., 1971). In Chapter II the Premoli correlation is summarized.

4.4.2.2 Friction factor

The wall friction pressure drop term in Equation (4.2) is expressed with the Churchill correlation (Churchill, 1977) combined with the Lockhart-Martinelli multiplier (Lockhart & Martinelli, 1949) (Φ) gives.

$$\left\langle \frac{\partial p}{\partial z} \right\rangle'_{fr} = \begin{cases} f_l \frac{S_{wall}}{8\rho_{TP}A^2} \frac{\dot{m}|\dot{m}|}{\Delta z} & \text{if } x < x_{NVG} \\ \Phi f_v \frac{S_{wall}}{8\rho_{TP}A^2} \frac{\dot{m}|\dot{m}|}{\Delta z} & \text{if } x_{NVG} \leq x < 1 \\ f_v \frac{S_{wall}}{8\rho_{TP}A^2} \frac{\dot{m}|\dot{m}|}{\Delta z} & \text{if } x \geq 1 \end{cases} \quad (4.10)$$

S_{wall} denotes the wetted wall surface. x_{NVG} is for the net vapor generation point, point where the void fraction effects are significant.

4.4.3 Sub-cooled model

At high heat fluxes, even if the average temperature has not reached its saturation condition boiling can occur near the heated walls. This effect is called sub-cooled boiling (Mayinger, 1978) and is a critical issue in many industrial applications. This effect must be considered in the model since it has an impact on the fluid mean density, in turn affecting the dynamics of the entire flow. In order to consider the possibility of sub-cooled boiling, the thermodynamic quality (x) is corrected with the Saha and Zuber (Saha & Zuber, 1974) profile fit model. This new absolute quality (x_a) is defined in Equation (4.11).

$$x_a = \frac{x - x_{NVG} e^{\left(\frac{x}{x_{NVG}} - 1\right)}}{1 - x_{NVG} e^{\left(\frac{x}{x_{NVG}} - 1\right)}} \quad (4.11)$$

x_{NVG} is calculated with the empirical correlation, also suggested (Saha & Zuber, 1974).

$$x_{NVG} = \begin{cases} -0.022BoRe_{lo}Pr_l & \text{if } Re_{lo}Pr_l > 70 \times 10^3 \\ -154Bo & \text{if } Re_{lo}Pr_l < 70 \times 10^3 \end{cases} \quad (4.12)$$

In the above equation Pr_l refers to the Prandtl number for pure liquid and Bo to the Boiling number. When sub-cooled boiling appears, the mixture density is redefined as follows:

$$\rho_{TP} = \begin{cases} (1 - \varepsilon)\rho_l + \varepsilon\rho_g & \text{if } x_{NVG} < x < 1 \\ \rho(h, p) & \text{elsewhere} \end{cases} \quad (4.13)$$

In this case, the void fraction is still being calculated with Equation (4.9), but the thermodynamic quality (x) is changed by the absolute quality (x_a).

4.5 Spatial discretization

For a better understanding of the ESDIRK method used for the solution of the PDE systems in Section 4.6, where the temporal scheme is presented, it is convenient at this stage to perform a preliminary discretization of the system, composed by the steady-state version of Equations (4.2) and (4.3).

$$\left. \begin{aligned} \frac{\partial(K\dot{m}^2)}{\partial z} &= -\frac{\partial(pA)}{\partial z} - \left\langle \frac{\partial p}{\partial z} \right\rangle'_{fr} - \rho_{TP}g \sin \alpha \\ \frac{\partial(\dot{m}h_{TP})}{\partial z} &= \left\langle q_w \right\rangle' \end{aligned} \right\} \quad (4.14)$$

The above equations are integrated using the finite volume method (FVM) over a staggered grid arrangement, see chapter II. The integration of the momentum equations is performed on the contrary. The nonlinear terms, due to convection in Equation (4.14), are treated with a 1st order upwind scheme. With the discretized equations written in the form, $B_e \dot{m}_e + B_w \dot{m}_w + B_{Ee} \dot{m}_{Ee} = b$ the system of Equations becomes:

Momentum

$$\left. \begin{aligned}
 B_e &= \max(-\dot{m}_w; 0)K_p + \max(\dot{m}_e; 0)K_E + S_p \\
 B_w &= -\max(\dot{m}_w; 0)K_p \\
 B_{Ee} &= -\max(-\dot{m}_e; 0)K_E \\
 b &= (p_p A_p - p_E A_E) + S_c \\
 S_p &= \Phi f_g \frac{S_w}{4\rho_{TP} A^2} \dot{m}^* \\
 S_c &= \Phi f_g \frac{S_w}{8\rho_{TP} A^2} (\dot{m}^*)^2 - \rho_{TP} g A \sin(\alpha) \Delta z
 \end{aligned} \right\} \quad (4.15)$$

Energy

$$\left. \begin{aligned}
 B_p &= \max(-\dot{m}_w; 0) + \max(\dot{m}_e; 0) \\
 B_w &= -\max(\dot{m}_w; 0) \\
 B_E &= -\max(-\dot{m}_e; 0) \\
 b &= \langle q_{wall} \rangle' \Delta z = \dot{q}_{wall}'' \frac{4D}{A} \Delta V
 \end{aligned} \right\} \quad (4.16)$$

Sub-indexes W , P , E , e , w , and Ee refer to the location of the scalar variables and mass flow rate in a cardinal coordinates system, indicated in Figure 3. 2.

4.6 ESDRK time integration scheme

As presented in Chapter III, every Runge-Kutta (RK) method has its own and unique representation in a Butcher Table, where the coefficients are calculated for a specific number of stages, numerical stability considerations, and order of accuracy. Additionally, in Chapter III, it was shown that implicit methods are not only unconditionally stable but also some of them are *L-stable*. This is an essential property to handle stiff problems (Skvortsov, 2006). Like our case of study. In this work, we consider the so-called explicit first stage diagonally implicit RK (ESDIRK) method. This family of methods has the following general Butcher table representation

$$\begin{array}{c|cccccc}
 & 0 & 0 & 0 & \cdots & 0 & 0 \\
 c & c_2 & a_{21} & \gamma & \cdots & 0 & 0 \\
 & \vdots & \vdots & \vdots & \ddots & 0 & 0 \\
 \hline
 a & c_r & a_{r1} & a_{r2} & \cdots & \gamma & 0 \\
 & 1 & b_1 & b_2 & \cdots & b_r & \gamma \\
 \hline
 b^T & & b_1 & b_2 & \cdots & b_r & \gamma
 \end{array} \quad (4.17)$$

The ESDIRK methods have the following properties:

- a) The terms $a_{1j} = 0$ for $j = 1, \dots, q$. This property makes the first step explicit.
- b) The last row satisfies $a_{qi} = b_i$. Hence, the quadrature formula to combine the intermediate solutions (inside the interval) is not necessary, see Equation (3.26) in Chapter III.
- c) The terms $a_{rs} = 0$ for $r < s$. In consequence, only s implicit calculations are needed on each r stage.

These properties have several advantages. According to properties a) and b), the calculation at the first stage (n) and quadrature formula to combine the intermediate solutions (inside the interval) are not necessary. Property c) implies that only s implicit calculations are needed on each r stage. Making this RK a compelling and computationally efficient method. The global ESDIRK algorithm can be written as:

$$\begin{aligned}
 u^n &= u^{(1)} \\
 u^{(r)} &= u^n + \Delta t \sum_{s=1}^r a_{rs} F^{(s)} \quad \text{for } r = 2, \dots, q \\
 u^{n+1} &= u^{(q)}
 \end{aligned} \quad (4.18)$$

This algorithm is generic and must be particularized for the quasi-homogeneous model to be applied to two-phase flows transient problems. To do so, a short system conformed by the momentum and energy equations, Equations (4.2), and (4.3) mass conservation equation, Equation (4.1), will be dropped aside for the moment. Latter in section 4.7, this equation is coupled with a pressure-based method, this way including pressure as the last primitive variable to be determined, closing the system of equations. This short system can be written as:

$$\frac{d\psi}{dt} = F(t, \psi) \quad (4.19)$$

In order to find the discrete form of Equation (4.19), the first step is to integrate (using the Fubini's theorem) the new system over $[t^n, t^{n+1}] \times c_i$, where $c_i = [z_i, z_i + \Delta z]$. When this procedure is applied, implicitly the Method Of Lines (MOL) is used.

$$\int_{c_i} \left(\int_{t^n}^{t^{n+1}} \frac{d\psi}{dt} dt \right) dz = \int_{t^n}^{t^{n+1}} \left(\int_{c_i} F(t, \psi) dz \right) dt = \int_{t^n}^{t^{n+1}} \tilde{F}(t, \psi) dt \quad (4.20)$$

With the above integration, the problem is reduced to m ($m = L / \Delta z$) coupled ODEs as follows.

$$\psi_i^{n+1} \Delta z = \psi_i^n \Delta z + \int_{t^n}^{t^{n+1}} \tilde{F}(t, \psi) dt \quad (4.21)$$

Here L is the length of the pipe, and the sub-index i indicates the space position and it is independent of the volume control used. In that sense $i = P$ or $i = e$ using again a cardinal position nomenclature depending upon which control volume we are working in. Hereafter, sub-indexes are referring to space discretization, and upper-indexes refer to the temporal ones. Note that $\tilde{F}$ shows that the slope function is integrated over space and it is related to the steady-state solution of the model in position i ; the discrete form of $\tilde{F}(t, \psi)$ was already calculated in section 4.5.

$$\tilde{F}(t, \psi) = \int_{c_i} F(t, \psi) dz = - \underbrace{\left(B_i \psi_i + \sum_{\substack{nb \\ nb \neq i}} B_{nb} \psi_{nb} \right)}_{\text{Steady-state discretized form}} + b_i \quad (4.22)$$

Once the integration is performed, the algorithm in Equation (4.18) can be used. Below the algorithm is developed with the final discrete form of the equations.

First stage (explicit):

$$\psi_i^n = \psi^{(1)} \quad (4.23)$$

Following stages (diagonally implicit):

$$\begin{aligned}\psi^{(r)}\Delta z &= \psi^n\Delta z + \Delta t \sum_{s=1}^r \mathbf{a}_{rs} \tilde{\mathbf{F}}^{(s)} \\ &= u^n\Delta z + \Delta t \mathbf{a}_{rr} \tilde{\mathbf{F}}^{(r)} + \Delta t \sum_{s=1}^{r-1} \mathbf{a}_{rs} \tilde{\mathbf{F}}^{(s)}\end{aligned}\quad (4.24)$$

Finally, by introducing Equation (4.22) into (4.24), developing the last term in the summation operator and finally rearranging, one gets:

$$\begin{aligned}\left(\frac{\Delta z}{\mathbf{a}_{rr}\Delta t} + \mathbf{B}_i \right) \psi_i^{(r)} + \sum_{\substack{nb \\ nb \neq i}} \mathbf{B}_{nb}^{(r)} \psi_{nb}^{(r)} &= \\ = \frac{\Delta z}{\mathbf{a}_{rr}\Delta t} \psi^n + \mathbf{b}_i^{(r)} + \frac{1}{\mathbf{a}_{rr}} \sum_{j=1}^{r-1} \mathbf{a}_{rj} \left(-\mathbf{B}_i^{(j)} \psi_i^{(j)} - \sum_{\substack{nb \\ nb \neq i}} \mathbf{B}_{nb}^{(j)} \psi_{nb}^{(j)} + \mathbf{b}_i^{(j)} \right)\end{aligned}\quad (4.25)$$

It is worth noting that the adaptation of a steady-state computational code for the study of transient problems using the ESDIRK method is straightforward; it only requires the combination of the steady-state coefficients with the Butcher Matrix coefficients, making the increase in the order of accuracy easy (Butcher, 2008), (Alexander, 1977).

4.7 Pressure correction equation

In section 4.6, the ESDIRK method was outlined to obtain approximate numerical solutions of the momentum and energy equations of the quasi-homogeneous model, dropping deliberately the mass conservation equation, having the need to determine pressure (or density) at every (r) stage by other means.

In incompressible flows, as density is constant it is impossible to determine density from the mass conservation equation (which is the only equation left) because it acts more as a restriction to the mass flow rate field rather than a dynamic equation for pressure; consequently, a pressure evolution expression must be constructed with the available information of mass flow rate. This problem gave birth to the so-called pressure-based methods, where the SIMPLE algorithm is probably the most well-known procedure for pressure-velocity coupling. Later on, further modifications were implemented, such as

the SIMPLEC (Van Doormaal & Raithby, 2007), SIMPLER (Suhas V Patankar, 1980), and the time explicit-implicit marching procedure by splitting operators, proposed by (Issa, 1981) that is called the PISO algorithm. For simplicity, the pressure-based method used in this work is the SIMPLE algorithm, but the numerical method here developed can be adapted with no additional effort for SIMPLEC and SIMPLER algorithms, taking advantage of their convergence higher rates.

To combine the SIMPLE algorithm with the ESDIRK method, the classical pressure correction method is applied on a (r) stage. Afterward, the same procedure is repeated at $r + 1$, until $r = q$.

The pressure correction equation for any (r) stage is obtained with a semi-implicit version of Equation (4.1), integrated at the scalar mesh, see Figure 3. 2.a in chapter III. Applying the same procedure as that for the momentum and energy equations, but leaving the net flow term as the unknown term.

$$\dot{m}_e^{(r)} - \dot{m}_e^{(n)} = -\frac{(\rho_{TP}^{(r)} - \rho_{TP}^{(n)})A}{a_{rr}\Delta t} - \frac{1}{a_{rr}} \sum_{s=1}^{r-1} a_{rs}(\dot{m}_e^{(s)} - \dot{m}_w^{(s)}) \quad (4.26)$$

Another option is to directly integrate Equation (4.1) again over the scalar mesh but leaving the mass accumulation term as part of the source term.

$$\dot{m}_e^{(r)} - \dot{m}_w^{(r)} = -\frac{\partial}{\partial t}(\rho_{TP}A)\Big|_p^{(r)} \Delta z \quad (4.27)$$

If we assume that the accumulation term is small, the second term in the RHS of (4.27) is negligible; therefore, the mass accumulation term ¹ can be approximated under the ESDIRK fashion at every (r) stage as:

$$\frac{\partial}{\partial t}(\rho_{TP}A)\Big|_p^{(r)} \approx \frac{(\rho_{TP}A)^{(r)} - (\rho_{TP}A)^n}{c_r\Delta t} \quad (4.28)$$

¹ For incompressible flows mass accumulation is zero.

This second option is more computationally efficient. However, for fast transients, it is not recommended.

On the other hand, pressure and mass flow rate are calculated by successive corrections, starting from guessed fields (*). These actual fields are corrected by:

$$p_p^{(r)} = p_p^* + p_p' \quad (4.29) \quad \dot{m}_e^{(r)} = \dot{m}_e^* + \dot{m}_e' \quad (4.30)$$

The preliminary set $(\dot{m}_e^*)$ is found for the guessed pressure field (p^*) , if this preliminary set is subtracted from the original mass flow field $(\dot{m}^{(r)})$ one gets the correction term $(\dot{m}_e')$.

$$\dot{m}_e^{(r)} = \dot{m}_e^* + \dot{m}_e' = \dot{m}_e^* + d_e \left(\frac{\partial p'}{\partial z} \right)_e \quad (4.31)$$

here:

$$\left(\frac{\partial p'}{\partial z} \right) \Delta z = \int_{z_w}^{z_e} \left(\frac{\partial p'}{\partial z} \right) dz \quad (4.32)$$

... is the total pressure force found by the integration over the control volume for the momentum equation in the corresponding staggered mesh. Note that it is assumed that the pressure gradient is constant inside the volume of integration and no information about the kind of spatial approximation is given. The same result is found by using the divergence theorem, but for generality and later use this way seems more convenient.

The mass flow rate correction term $\dot{m}_e'$ for 1st order interpolation functions is $\dot{m}_e' = d_e(p_p' - p_E')$, which is the common way to express it. The coefficients d_e are obtained by algebraic manipulation of the discrete momentum equation; more details can be found in (S V Patankar & Spalding, 1972) and (Suhas V Patankar, 1980). Inserting Equations (4.30) and (4.31) into Equation (4.27) the pressure correction equation is finally constructed:

$$\begin{aligned}
 (d_e + d_w)p'_P - d_e p'_E - d_w p'_W = & -(\dot{m}_e^* - \dot{m}_w^*) - \frac{(\rho_{TP}^{(r)} - \rho_{TP}^{(n)})A}{a_{rr}\Delta t} \\
 & - \frac{1}{a_{rr}} \sum_{s=1}^{r-1} a_{rs} (\dot{m}_e^{(s)} - \dot{m}_w^{(s)})
 \end{aligned} \tag{4.33}$$

Or alternatively:

$$(d_e + d_w)p'_P - d_e p'_E - d_w p'_W = -(\dot{m}_e^* - \dot{m}_w^*) - \left. \frac{\partial}{\partial t} (\rho_{TP} A) \right|_P^{(r)} \Delta z \tag{4.34}$$

4.7.1 Boundary conditions for the pressure correction equation

Boundary conditions for $\dot{m}$, h_{TP} and p were stated in section 4.4.1, these BCs are enough to well pose the problem of a single heated pipe; therefore, to apply the SIMPLE algorithm, we also need BCs for $\dot{m}^*$ and p' as well.

In the case of $\dot{m}^*$, the actual boundary conditions for $\dot{m}$ are sufficient because it is assumed that $\dot{m}^*$ is very close to $\dot{m}$, but for p' this statement is not true because p' is not actually pressure, but its correction. On the other hand, if we examine the pressure correction (Eqs. (4.33) or (4.34)), we found that it has the same form than the discrete Poisson equation, highly used in heat conduction problems, among others, needing BCs at both ends of the domain ($z = 0$ and $z = L$) due to its elliptic character. Consequently, two BCs are required such that they reproduce the hydrodynamic nature of the problem. This is one of the less obvious and more important aspects of pressure correction methods and not always is discussed in all papers. In the present chapter, the BCs will be developed without making any rigorous theoretical augmentation; for more rigorous background one can consult (Gresho, 1987). The BCs for p' are simple; when mass flow is imposed there will be no mass flow rate correction, thus $\dot{m}' = 0$, so that pressure prediction gradient must be zero, as Equation (4.31) shows. For a fixed pressure, no pressure correction is required, thus $p' = 0$. According to the above discussion, the BCs for p' are:

$$\left. \begin{aligned} \dot{m}(z = 0, t) = \dot{m}_0 & \Rightarrow \left. \frac{\partial p'}{\partial z} \right|_{z=0} = 0 \\ p(z = L, t) = p_L & \Rightarrow p'(z = L, t) = 0 \end{aligned} \right\} \tag{4.35}$$

4.7.2 Pressure translation

In the SIMPLE algorithm, an intermediate elliptic pressure correction must be solved (Equation (4.34)). To do so, BCs at both ends are needed. However, according to Equation (4.8) all BCs are placed at $z = 0$, this leading room to a contradiction. To solve this issue, at each iteration level k in the SIMPLE algorithm the real pressure that fulfills (4.8) must be calculated the available information. This is made with a pressure interpolation algorithm as follows:

$$\left. \begin{array}{l} \text{Step } i) \quad \tilde{p}^k \text{ is calculated} \\ \text{Step } ii) \quad \tilde{p}^k(z = 0) = f(z_1, z_2, \dots, z_n) \\ \text{Step } iii) \quad \Delta \tilde{p}^k = \tilde{p}^k(z = 0, t) - p(z = 0) \\ \text{Step } iv) \quad p(z, t) = \tilde{p}^k(z, t) - \Delta \tilde{p}^k \end{array} \right\} \quad (4.36)$$

In Step *ii*) any interpolation method can be used, and the stencil size must be selected according to the desired interpolation precision. In this work, a linear interpolation method was found sufficient.

$$\tilde{p}^k(z = 0, t) = - \left(\frac{\tilde{p}^k(z_2, t) - \tilde{p}^k(z_1, t)}{z_2 - z_1} \right) z_1 + \tilde{p}^k(z_1, t) \quad (4.37)$$

4.8 Overall algorithm

The algorithm for obtaining the solution of the quasi-homogeneous model is divided over one time step in two main loops: 1) inner loop where Equations (4.1), (4.2) and (4.3) are iterated until all thermodynamic and flow variables converge, 2) RK stage loop where the step 1) is repeated on all stages from $r = 2$ to the last stage q . Schematically the final procedure is indicated in Algorithm 4. 1.

4.9 Numerical Experiments and results

In the next section, several experiments are carried out to validate and show the effectiveness of the ESDIRK method in calculating two-phase flows. The validation is made in both steady and transient state with the vertical tube experiment of (Bartolomei et al., 1982) and (Bartolomei & Chanturiya, 1967) as a benchmark.

are varied according to Table 4. 1. Cases 1 to 3 taken from (Bartolomei et al., 1982), and cases 4 to 6 are taken from (Bartolomei & Chanturiya, 1967).

Table 4. 1 Simulation conditions for Bartolomei experiment

Case	p (bar)	G ($\text{kg} \cdot \text{m}^{-1} \cdot \text{s}^{-2}$)	T_{in} ($^{\circ}\text{C}$)	ΔT_{sub} ($^{\circ}\text{C}$)	$\dot{q}_w''$ ($\text{kW} \cdot \text{m}^{-2}$)	D (mm)	L (m)
1	108	966	228.85	87.85	1,130	12	1.5
2	68	998	247.85	36.02	440	12	1.5
3	147	2,014	271.85	68.69	1,720	12	1.5
4	45	900	239.85	17.59	380	15.4	2
5	30	900	214.85	19.0	380	15.4	2
6	15	900	181.85	16.44	380	15.4	2

4.9.2 Steady-state validation

The steady-state validation is performed with the ES54 method (4th order). All cases collected in Table 4. 1 are considered in order to show the reliability for different real operational conditions. All simulations start with the inlet pressure and temperature as initial conditions. Once the steady-state is reached, the void fraction and thermodynamic quality profiles are compared with the corresponding experimental results and the numerical solution of the one-dimensional semi-implicit drift flux model (DFM) and two fluid-model solutions using Relap5 software (Shieh & Ransom, V. H. Krishnamurthy, 1994), both performed by (Talebi, Kazeminejad, & Davilu, 2012). The results are shown in Figure 4. 2.

Figure 4. 2 Void fraction steady-state profile.

The results show that for all the cases considered, the ESDIRK method approximates satisfactorily the experiment values. Qualitatively, it can be assured that for medium and high-pressure levels, the developed methodology reproduces satisfactorily not only the quality and void fraction profile but also the initiation of boiling or net vapor generation point, Figure 4. 3. This is an important feature in heat exchangers with phase change fluids.

Figure 4. 3 Experimental vs. Numerical net vapor generation point.

It also can be observed that the Premoli void fraction correlation (Premoli et al., 1971) gives a better prediction than the no-slip void fraction. This happens even for high pressures, conditions in which the no-slip condition works better because the difference between saturated liquid and saturated vapor is smaller. In Table 4. 2 an error analysis is carried using the L_2 and L_∞ norms using the experimental values as reference. This

analysis demonstrates quantitatively that both correlations reproduce accurately the vertical tube experiment, but the Premoli correlation is slightly more accurate.

Table 4. 2 Void fraction prediction error analysis

Case	L_2 Norm		L_∞ Norm	
	Premoli	No- slip	Premoli	No-slip
1	0.0254	0.0724	0.0611	0.1171
2	0.0280	0.0406	0.0571	0.0989
3	0.0236	0.0174	0.0382	0.0295
4	0.0308	0.0780	0.0493	0.1401
5	0.0417	0.0888	0.0638	0.1641
6	0.0898	0.0493	0.1335	0.0897
Mean value	0.0399	0.0578	0.0672	0.1066

Figure 4. 4 shows the axial profile for case 2 at different subcooling. In this experiment, both subcooled boiling models exhibit the same accurate behavior for different subcooled inlet temperatures (ΔT_{sub}) for the numerical values extracted from (Talebi et al., 2012). Thereby, the ESDIRK method presents excellent results, reproducing accurately the flow boiling in a pipe at steady-state conditions.

Figure 4. 4 Void fraction axial profile for case 2.

4.9.3 Transient-state validation

In the previous section, the validity and accuracy of the ESDIRK method for steady-state calculations are shown; however, the validation in the transient state is also required to thoroughly analyze the reliability, capability, and accuracy of the method. This validation is essential because transients in heat exchangers occur in many

engineering applications; for example, in nuclear facilities accidents, it can occur due to pressure tank or pump failures, deriving this in a loss of coolant accident (LOCA). Another application is in cooling/heating transient response, which is of paramount importance due to unsteady behavior in cooling/heating loads, which can affect the vapor production in the evaporator, undesirable scenario for the compression stage in a refrigeration cycle. These issues make that any transient model should accurately simulate the boiling process when the system is subjected to any external disturbance. Thus, in order to guarantee the accuracy of the ESDIRK method in transient state cases 1, 2 and 3 from Table 4. 1 are validated against the numerical results provided by (Talebi et al., 2012), using the outlet void fraction ($\varepsilon(z = L)$) as tracking variable. Two experiments are carried out, on each case, different wall heat flux and inlet mass flux ($G = \dot{m} / A$) linear variations are imposed as BCs. The time steps used are 5 s, 10 s and 20 s for the EB, ES33a and ES54 ESDIRK methods respectively. The considered heat flux and mass flux variations functions are according to Equations (4.38), (4.39) and Table 4. 3.

$$Q_w''(z, t) = \begin{cases} 0.001\tilde{Q}''t & \text{if } t \leq 1000 \text{ s} \\ \tilde{Q}'' & \text{if } t > 1000 \text{ s} \end{cases} \quad (4.38)$$

$$G(z = 0, t) = \begin{cases} 0.001(\tilde{G}_2 - \tilde{G}_1)t + \tilde{G} & \text{if } t \leq 1000 \text{ s} \\ \tilde{G}_2 & \text{if } t > 1000 \text{ s} \end{cases} \quad (4.39)$$

Table 4. 3 Linear variations function constants

Case	$\tilde{Q}_w''$ (kW · m ²)	$\tilde{G}_1$ (kg · s ⁻¹ · m ²)	$\tilde{G}_2$ (kg · s ⁻¹ · m ²)
1	1,130	1,200	800
2	440	2,500	1,500
3	1,720	2,500	1,500

The results show good agreement with the numerical comparison data, in both; heat flux and mass flux linear variation experiments. For linear heat flux variations all cases exhibit zero outlet void fraction for $t < 600$ s, the moment in which vapor is being produced. After that point, vapor is produced linearly until $t = 1,000$ s and then vapor production is stable. In the case of inlet mass flux variation, vapor is produced also

linearly, but the initiation of boiling varies from case to case. This is because the heat flux is high for specific mass fluxes, see Figure 4. 6.a, producing vapor immediately after the simulation starts.

a)

a)

b)

b)

c)

c)

Figure 4. 5 Exit void fraction transient evolution for time linear variation in heat flux condition.

Figure 4. 6 Exit void fraction transient evolution for time linear variation in inlet mass flow condition.

An essential aspect of these plots is that the simulation for the three ESDIRK methods studied (EB, ES33a, and ES54) does not present any difference between them. This phenomenon is because the heat flux and mass flux function are continuous and smooth in time. Therefore, the simulation progresses in time as it where many quasi-steady states one after the other. This happens because steady-state solutions do not

depend on the ESDIRK method employed. To clarify this asseveration, Figure 4. 7.a and Figure 4. 7.b plot the relationship between ε vs. $\bar{p}$ and $\bar{h}$ vs. $\bar{p}$ for case 1 of Table 4. 1 are plotted. The upper bar means that the variable is normalized respect to the inlet condition. These relations are presented from a geometrical point of view in the phase space, similar to that used in the analysis of dynamical systems (Strogratz, 1994).

Figure 4. 7 Phase space relationships for $z = 1.125$ m, a) ε vs. p , b) h vs. p

It can be observed that the steady-state solution is the same for the three ESDIRK methods employed. This result is expected because the steady-state solution, which tends towards a stable fix point, appears when the transient effects vanish ($\partial\psi / \partial t = 0$) and stable fix points location (in the phase space) are independent of the numerical method. Thus, in quasi-steady state simulations the order of accuracy does not have any effect.

This experiment also shows that the dynamic behavior is slightly different for each ESDIRK method. For example, in Figure 4. 7.a one can see that along the trajectory in the phase space it occurs that $(\varepsilon_{\bar{p}})_{EB} \neq (\varepsilon_{\bar{p}})_{ES54} \neq (\varepsilon_{\bar{p}})_{ES33}$; even more, the same happens in Figure 4. 7.b for $\bar{h}$. This behavior can be explained by the fact that in every stage (r) and for a particular time step of the computation procedure, the corresponding coefficients in the Butcher matrix (a) act like weighting factors of the slope function. This means that the approximation of the slope function (F) may differ from one ESDIRK method to another one. This property makes the ESDIRK a powerful tool to simulate fast transients.

4.10 Transients capturing efficiency

The observation made in the above section plays an important role in transient calculations, because the result may differ according to the ESDIRK method employed. To visualize this effect, the system, after the steady-state is reached, is then subjected to a periodic square wave wall heat flux condition with an amplitude of $282.5 \text{ kW} \cdot \text{m}^{-2}$. Two frequencies are considered, $f = 0.2$ and 0.5 Hz . The first frequency is small enough to ensure that a new quasi-steady state is reached at each plateau, but this does not happen with the second higher frequency.

Figure 4. 8 a) Single-phase length for time square wave wall heat flux condition $f = 0.2 \text{ Hz}$, b) 0.5 Hz .

— ES54 ($\Delta t = 0.25 \text{ s}$) - - EB ($\Delta t = 0.1 \text{ s}$) -○- EB ($\Delta t = 0.25 \text{ s}$).

The tracking variable used is the length measured from the inlet where the fluid is still pure liquid without the gas phase L_{sp} , thus distance from inlet to the boiling starting point. Some sensitivity is noticeable, which is not surprising as this parameter is also very sensitive in reality. This test was performed for the EB scheme for two different time steps ($\Delta t = 0.25 \text{ s}$ and $\Delta t = 0.1 \text{ s}$), and for the 4th order ES54 scheme with $\Delta t = 0.1 \text{ s}$, these time steps were chosen because the solution of EB with $\Delta t = 0.25 \text{ s}$ has a similar order of accuracy than ES54 with $\Delta t = 0.25 \text{ s}$ ($\mathcal{O}(\sqrt[4]{0.1 \text{ s}}) \approx \mathcal{O}(0.25 \text{ s})$).

Figure 4. 8.b shows that both the amplitude and time rate of change are the same for the ES54 and EB schemes; however, when the time step is reduced for the EB scheme L_{sp} tends to the ES54 prediction. This outcome makes sense because, from a theoretical point of view, for smaller time steps, the solution is more accurate. A different time evolution is found in Figure 4. 8.b as not enough time is available to reach the new

steady-state condition. As a result, the amplitude of the output L_{SP} differs from one method to the other, having higher amplitude when either the order of accuracy is increased or the time step decreased. Figure 4. 8 shows that the positive effect of the higher order of accuracy is evident, supporting the effort of increasing the order. It is well-known that a reduction of the time step leads to more accurate solutions, but with the help of higher-order schemes, this refinement can be of lower effect, saving computational effort. Precise experiments on transient boiling are challenging to perform and to measure, thus almost inexistent for validating the herewith developed numerical methods. Some effort on establishing which calculation method is appropriate seems justifiable.

There exists a group of applications where an accurate determination of the amplitude of flow variables is needed. As an example, in systems that experience pulses or oscillations in pressure and/or in temperature, mechanical and thermal stresses derive into the fatigue of the materials and noise. Such a case is the direct steam generation in externally heated tubes by hot gases or by direct sun irradiation. For that, it is essential to determine amplitudes with accuracy; in those cases, the use of higher schemes can make a positive difference.

4.11 Instabilities calculation

Two-phase flows instabilities have been a vast area of research in heat exchanger analysis and design over the last century (Kakac & Bon, 2008). Its importance is because the oscillations or change of state of the operational variables can significantly affect the design point of the system. There are several kinds of instabilities; each one of them happens by their own mechanism. A comprehensive review of two-phase instabilities can be found in (Ruspini, Marcel, & Clausse, 2014).

4.11.1 Ledinegg instability description

Among all types of instabilities, the Ledinegg instabilities may be the most well-known kind. This instability happens in systems in which the flow is induced by a pump or by a pressure difference between two tanks, see Figure 4. 9. Depending upon the supplied heat flux, in steady-state conditions, the geometric place of all mass flux and

pressure drop points describes an N- shape characteristic curve like Figure 4. 10. This curve exhibits three zones

- i) All vapor zone: saturated or overheated vapor is produced because the mass flux is too small. This zone is located at the left side of the N- shape curve.
- ii) Mixture zone: liquid+vapor mixture is produced because heat flux is not enough to boil all the fluid. This zone is located at the center of the N- shape curve.
- iii) All liquid zone: heat flux is not enough to produce vapor. This zone is located at the right side of the N- shape curve.

Figure 4. 9 Schematic representation of a boiling tube system, a) pumped, b) pressure difference.

The Ledinegg instability occurs when the pumping or pressure difference system is selected (according to its external pressure characteristic curve) at some point in which any disturbance, like valve operation or any other disturbance source, to the mass flux makes that the operation point varies tremendously achieving another and not desirable stable operation point. The location of this points of instability was studied using linear bifurcation analysis by (Padki, Palmer, Kakac, & Vezirglu, 1992), concluding that a point in the N- shape curve is unstable if; i) the internal characteristic has a negative slope, ii) the internal characteristic is steeper than the external, see Equation (4.40), iii) multiple intersections between the internal and external characteristic must exist.

$$\left. \frac{\partial \Delta p_{ext}}{\partial G} \right|_{G_0} > \left. \frac{\partial \Delta p_{int}}{\partial G} \right|_{G_0} \quad (4.40)$$

Figure 4. 10 depicts an unstable system that meets the three unstable criteria described above, for pumped and pressure difference.

Figure 4. 10 Ledinegg unstable boiling system schematic representation

4.11.2 Ledinegg instability transient simulation

A variation of Case 1 from Table 4. 1 is proposed to simulate a Ledinegg instability. The only variation respect to the original data is that the orientation of the pipe is horizontal, neglecting the compressibility effects due to body forces. In this experiment, the instability due to horizontal external characteristics is studied $\Delta p_{ext} = \text{constant}$. The time step is $\Delta t = 0.1 \text{ s}$, and the grid size is $\Delta z = 0.03 \text{ m}$. First, the location of an unstable point must be located. To do so, mass flux is varied from $10 \text{ kg} \cdot \text{s}^{-1} \cdot \text{m}^{-2}$ to $3,000 \text{ kg} \cdot \text{s}^{-1} \cdot \text{m}^{-2}$ and the N- shape is drawn with the pressure drop at steady state (internal characteristic) for each mass flux input value.

Figure 4.11 N-shape curve for case 1

In Figure 4.11, the N-shape curve is shown. With this curve, the point $(\Delta p, G) = (5.5701 \text{ kPa}, 966 \text{ kg} \cdot \text{s}^{-1} \cdot \text{m}^{-2})$ is an unstable point. To simulate the Ledinegg

instability a dynamic evolution equation for the inlet mass flow rate must be included in the calculation procedure. This equation is found making a momentum balance in the whole pipe. For that balance, it is assumed that the propagation of mass flow velocity is infinite. Therefore the convective terms can be neglected due to mass conservation balance. According to these assumptions, the inlet mass flow evolution equation is as follows.

$$\begin{aligned} \int_0^L \frac{\partial \dot{m}}{\partial t} \Big|_{(z=0,t)} dz &= -(\Delta p_{ext} - \Delta p_{int})A \\ \Rightarrow \frac{\partial \dot{m}}{\partial t} \Big|_{(z=0,t)} &= -\frac{A}{L}(\Delta p_{ext} - \Delta p_{int}) \end{aligned} \quad (4.41)$$

The equation (4.41) can only be solved explicitly because we must know the time evolution of Δp_{int} , which is not possible. Therefore, the inlet mass flow boundary condition is solved explicitly, having a unique value for each time step.

$$\dot{m}_0^{(n)} = \dot{m}_0^{(n-1)} - \frac{A\Delta t}{L}(\Delta p_{ext} - \Delta p_{int}) \quad (4.42)$$

For the transient Ledinegg simulation, the EB and ES33a are considered. In both cases, the calculated unstable point is used as an initial condition. After 6 s (time enough to reach the steady-state) the inlet mass flow is perturbed ($\dot{m}_0 = \dot{m}_0 + \delta\dot{m}_0$) and then Equation (4.42) is coupled to determine the inlet mass flow rate boundary condition at the beginning of each time step. Two perturbations were studied ($\delta\dot{m}_0 = \pm 1 \times 10^{-4} \text{ kg} \cdot \text{s}$). Time step now be restricted due to the explicit nature of Equation (4.42). For the EB method time step was restricted to 0,05 s while for the ES33a method time step was settled to 0,2 s. Larger time steps were used but for both ESDIRK methods the solution was unstable. It's important to highlight that this numerical instability is because of Equation (4.42) stability restriction, not for the implicit internal calculation procedure.

The transient evolution is shown in Figure 4. 12 and Figure 4. 13 for the positive and negative inlet mass flow perturbation respectively. Such results show that the time accuracy provided by the ESDIRK method influences slightly the transient path either for inlet mass flow and pressure drop. Also, the final stable fixed point is the same independently of the ESDIRK method. These results agree with the results exposed in

sections 4.9 and 4.10. For the positive disturbance, after the perturbation, inlet mass flux increases dramatically until stability is reached ($t \approx 40$ s), also pressure drop exhibits a steep transient around 15 s. The amplitude in pressure drop transient differs from the ESDIRK method employed. In the case of negative disturbance is the opposite, mass flow decreases and pressure drop increases.

Figure 4. 12 Positive perturbation transient response, a) mass flux, b) pressure drop

Figure 4. 13 Positive perturbation transient response, a) mass flux, b) pressure drop

Finally, in Figure 4. 14, the calculated transient evolution is plotted together with the N-shape curve. This plot shows experimentally that the chosen initial condition was indeed an unstable point and that at the intersection between the external and internal characteristics locates the other two stable fix points.

Figure 4. 14 Ledinegg transient evolution

4.12 Computational performance

In practice, for a simulation to be effective there must be a favorable balance between accuracy and computational cost. In Section 4.6 it was seen that accuracy can be improved by considering high order temporal schemes; meanwhile, the computational cost depends exclusively on the number of computations required to achieve convergence on each time step, in other words depends on the algorithm employed. Recalling Algorithm 4. 1, the entire numerical procedure consists of two main loops; the outer loop is repeated from $r = 2, \dots, q$, depending the number of stages of the corresponding implicit Runge- Kutta method considered, and the inner loop is repeated until convergence, of all variables, is guaranteed in stage r . At first sight, it seems that with a lower time accuracy scheme we could expect lower computational times, because the inner loop will be repeated fewer times, e.g. for the Euler Backward method it will be repeated once. However, the computational cost may depend on many other factors, not only the time accuracy scheme but also time step and the nature of the physical problem to simulate and more precisely the convergence rate, which is intrinsically related to stiffness. To answer rigorously this question, finding out the insights of computational cost and its relationship with accuracy, a sensitivity analysis over the total simulation time (t_{CPU}) required to achieve the steady-state condition for fixed initial and boundary conditions, will be carried out in this section.

In order to make a fair comparison, the analysis will be made for constant time accuracy, taking as reference the accuracy of the Euler backward method. To do so, the metric used as a parameter in the calculations is the effective time step (Δt_{eff}), which is defined as the time step required for a specific temporal scheme (of accuracy p) in order to reproduce the accuracy of the Euler backward method.

$$\Delta t_{eff} = (\Delta t_{EB})^{1/p} \quad (4.43)$$

All the simulations were carried out in a personal computer with an Intel[®], core[™] i5 with two cores of 3.1 and 3.3 GHz, respectively, and as a benchmark we will use again the Bartolomei vertical boiling tube experiment (Bartolomei & Chanturiya, 1967), see section 4.9.1, but for two different heat flux conditions, see Table 4. 4; case 1 is with a heat flux of $1,130 \text{ kW} \cdot \text{m}^{-2}$ which ensure boiling, thus increasing the equations stiffness,

and case 2 is with $500 \text{ kW} \cdot \text{m}^{-2}$ which is low enough to guarantee that phase change will not happen, simulating a single-phase process. In this way, the performance for single-phase and two-phase flow computational response can be compared.

Table 4. 4 Computational performance experiment setups

Case	p (bar)	G ($\text{kg} \cdot \text{m}^{-1} \cdot \text{s}^{-2}$)	T_{in} ($^{\circ}\text{C}$)	ΔT_{sub} ($^{\circ}\text{C}$)	$\dot{q}_w''$ ($\text{kW} \cdot \text{m}^{-2}$)	D (mm)	L (m)
1	108	966	228.85	87.85	1,130	12	1.5
2	108	996	228.85	87.85	500	12	1.5

Measuring the total computing time since the beginning of the simulation until $t = 30 \text{ s}$, time enough to ensure that steady-state was achieved, it is observed that for $\Delta t > 0.3 \text{ s}$ in Figure 4. 15.a and for all the entire range of times steps in Figure 4. 15.b the computational cost is always lower as the order of accuracy decreases. Moreover, the computational cost in Figure 4. 15.b is almost linearly dependent on the number of stages. This indicates that the rate of convergence at each stage for different temporal schemes is similar. In the low part of Figure 4. 15.a ($\Delta t < 0.3 \text{ s}$), this “rule of thumb” doesn’t apply, and a change of behavior is observed, having a very high cost for the Euler Method. In this zone, this behavior occurs by two effects: *i*) the rate of convergence is different; *ii*) the number of time steps required to cover the transient effect also plays an important role.

Figure 4. 15 Computational time response for different time steps and temporal schemes

To visualize these two effects, we introduce the inner loop iteration velocity (V_k) as the metric to compare the rate of convergence of the temporal schemes. The inner

loop velocity is defined as the number of iterations k (in the inner loop) needed if one second is being simulated under the same conditions.

$$V_k = \frac{k}{\Delta t_{eff}} \quad (4.44)$$

Using this definition, we can observe that for values lower than $t \approx 5$ s the inner loop velocity exhibits a concave behavior. This zone is where the transient effects occur, and the discussion will be centered on this zone. For low time steps $\Delta t = 0.05$ s, Figure 4. 16.a, the inner loop velocity is higher for the Euler backward method, and for the ES33a scheme is significantly lower.

Figure 4. 16 Iteration velocity comparison, a) $\Delta t=0.05$ s, b) $\Delta t=0.05$ s.

This can be explained because for low time steps we expect higher accuracy, then for the Euler backward method (the lowest order of accuracy considered), in the inner loop as $\Delta t \rightarrow 0$ roundoff errors are more representative; therefore, the rate of convergence is smaller, increasing the iteration velocity. When time steps are greater, Figure 4. 16.b, there is a change of tendency, the Euler Backward method inner loop velocity is smaller, the reason why computational cost is lower, as shown in Figure 4. 15.a and Figure 4. 15.b. Another important aspect is due to stiffness. When using the method of lines (MOL), the entire system is reduced to an ordinary differential set. Considering the momentum and energy equations, the system of equations can be written for any (r) stage using the using the algorithm (4.24) as:

$$\left. \frac{d\psi_i}{dt} \right|^{(r)} = \frac{\Delta t a_{rr}}{\Delta z} B(\psi_i(t^{(r)}), t^{(r)}) \psi_i^{(r)} + \underbrace{\frac{\Delta t}{\Delta z} \sum_{s=1}^{r-1} a_{rs} B(\psi_i(t^{(s)}), t^{(s)}) \psi_i^{(s)}}_{\text{Source Term}} \quad (4.45)$$

Here B represents the coefficient matrix, which can be constructed as a block matrix, taking into account the momentum and energy coefficients. The spectrum of $a_{rr} B / \Delta z$ can be computed, providing information about the stability of the method, see section 3.8.2.2. Moreover, the stiff ratio can also be computed measuring how stiff are the equations (Lambert, 1991), (Söderlind et al., 2015).

$$\begin{aligned} S_r &= \frac{\lambda_{\max}}{\lambda_{\min}} \\ \lambda_{\max} &= \frac{a_{rr}}{\Delta z} \max |\lambda_i| \\ \lambda_{\min} &= \frac{a_{rr}}{\Delta z} \min |\lambda_i| \end{aligned} \quad (4.46)$$

Calculating the spectrum of B , we observe that the bumpy part of Figure 4. 16.a and Figure 4. 16.b coincide with the rising part of the transient evolution of the maximum eigenvalue of $a_{rr} B / \Delta z$, see Figure 4. 17. This indicates that when boiling occurs the system becomes stiffer, and from a computational point of view, the value of eigenvalue does not seems relevant but its transient change. Therefore, the algorithm needs more inner loop iterations to find convergence.

Figure 4. 17 Maximum eigenvalue transient behaviour for case 1

Moreover, the stiff ratio for different heat fluxes shows that for increasing heat flux the system becomes stiffer, as shown in Figure 4. 15

Figure 4. 18 Stiff ratio transient evolution for different heat fluxes.

Comparing the inner loop velocities and the spectrum of matrix B, gives us enough information providing a criterion to design numerical experiments; when a more detailed solution is required or the transient phenomena occur with higher propagation velocities is more efficient to use high order methods, using broader time steps. Additionally, the Euler backward method is suitable for large steps, but sacrificing accuracy (see Figure 4. 19), which for high sensible time step problems, like periodic inlet disturbances, see section 4.10, are not appropriate.

 Figure 4. 19 Instant density rate of change for $z=1$ m.

4.13 Conclusions

The numerical solution of the 1-D quasi-homogeneous two-phase flows equations with the ESDIRK method has been successfully implemented.

The algorithm developed provides a straightforward way to increase the temporal order of accuracy in a straightforward manner, avoiding numerical instabilities, lack of convergence, or convergence to non-physical solutions, and also offers a high degree of flexibility, i.e., the capability of diagnosing insufficient time step, or to determine the appropriate order of accuracy.

The SIMPLE-ESDIRK method shows excellent performance compared with experimental and numerical results provided by other authors on steady-state subcooled boiling flows, providing an alternative way to handle heated channels two-phase flows classical problems.

On the grounds of the results, it can be concluded that for the high orders of accuracy integration herewith proposed:

- The computational performance of the proposed scheme is advantageous, especially for high numerical stiffness events, such as boiling initiation.
- The proposed scheme is a powerful tool to simulate two-phase flow instabilities and transient external effects
- For the unsteady problem of subjecting the system to high-frequency wall heat disturbances, the use of high order schemes seems advantageous, not requiring to reduce excessively the time step, saving valuable computational time.

The proposed methodology shows the potential to predict more accurately transient thermo-fluids events in slender tubes and heated channels.

Nomenclature

a	Butcher table.
A	Area (m^2).
B	Coefficient vector or matrix.
b	Butcher table quadrature vector.
b	Source term vector
Bo	Boiling number.
c	Butcher table stage location.
D	Diameter (m).
F	Slope function.
$\tilde{F}$	Space integrated slope function
f	Friction factor, frequency (Hz)
G	Mass flux ($\text{kg} \cdot \text{s}^{-1} \cdot \text{m}^{-2}$).
g	Gravity acceleration constant ($=9.81 \text{ m} \cdot \text{s}^{-2}$).
h	Specific enthalpy ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
h_l	Liquid phase-specific enthalpy ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).

h_v	Vapor phase-specific enthalpy ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
h_{TP}	Two-phase flow mixture Specific enthalpy ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
L_{SP}	Single-phase flow pipe length (m).
L	Length (m).
L_2	Euclidean norm.
L_∞	L- infinity vector norm.
$\dot{m}$	Mass flow ($\text{kg} \cdot \text{s}^{-1}$).
$\dot{m}'$	Mass flow correction ($\text{kg} \cdot \text{s}^{-1}$).
$\dot{m}^*$	Mass flow guess ($\text{kg} \cdot \text{s}^{-1}$).
N_{SIMPLE}	Number of SIMPLE algorithm iterations.
$\mathcal{O}$	Order of accuracy.
Pr	Prandtl number.
p	Pressure (Pa).
p'	Pressure correction (Pa).
p^*	Pressure guess field (Pa).
$\dot{q}'_w$	Wall boundary heat flux per unit length ($\text{W} \cdot \text{m}^{-1}$)
$\dot{q}''_w$	Wall boundary heat flux per unit area ($\text{W} \cdot \text{m}^{-2}$)
Re	Reynolds number.
S	Surface (m^2).
S_c	Independent source term coefficient vector.
S_p	Implicit source term coefficient vector.
S_R	Slip ratio.
S_r	Stiff ratio.
t	Time (s).
t_{CPU}	Computational time cost (s)
t_{eff}	Effective time (s).
T	Temperature ($^{\circ}\text{C}$).
u	Velocity, phase velocity ($\text{m} \cdot \text{s}^{-1}$).
V_k	Inner loop iteration velocity ($\text{iterations} \cdot \text{s}^{-1}$)
x	Thermodynamic quality (kg/kg).
x_a	Absolute quality (kg/kg).
z	Axial coordinate (m).

Greek Letters

α	Pipe inclination angle
Δ	Finite difference.
Δp	Pressure drop (Pa)
Δp_{ext}	External characteristic (Pa)

Δp_{int}	Internal characteristic (Pa)
$\Delta p T_{sub}$	Sub-cooling ($^{\circ}\text{C}$).
$\delta \dot{m}_0$	Inlet mas flow perturbation.
ε	Void fraction ($\text{m}^3 \cdot \text{m}^{-3}$).
ρ	Material density ($\text{kg} \cdot \text{m}^{-3}$).
ρ_l	Liquid phase material density ($\text{kg} \cdot \text{m}^{-3}$).
ρ_v	Vapor phase material density ($\text{kg} \cdot \text{m}^{-3}$).
ρ_{TP}	Two-phase flow mixture density ($\text{kg} \cdot \text{m}^{-3}$).
τ_{wall}	Fluid wall shear stress ($\text{N} \cdot \text{m}^{-2}$).
λ	Eigenvalue
ψ	Dependent variable vector.
Φ	Lockhart and Martinelli multiplier.
φ	Boundary and initial condition state vector.

Subscripts

0	Initial state. Inlet condition.
W, P, Ee, w, e	Cardinal system index notation.
EB	Euler backward
ES33a	Alexander 3 rd order scheme.
ES54	Skvortsov 4 th order five stage scheme.
fr	Friction.
in	Inlet condition.
l	Liquid.
v	Vapor.
TP	Two-phase.
NVG	Net vapor generation.
i, j, k	Index.
$wall$	Wall.
r, s	Runge-Kutta indexes.
q	Runge- Kutta method total number of stages.

Superscripts

'	Per unit length.
"	Per unit area.
'''	Per unit volume.
*	Guess value.
N	Time step-index.
nb	Neighborhood.
()	Time stage.

Acronyms

BC	Boundary conditions.
ESDIRK	Explicit first stage diagonal implicit Runge- Kutta method
FVM	Finite volume method.
IC	Initial condition.
LOCA	Lost of coolant accident
ODE	Ordinary differential equation.
PDE	Partial differential equation.
RK	Runge- Kutta method
SIMPLE	Semi implicit pressure linked equations.
1-D	One-dimensional.

Operators

$\langle \rangle$	In Volume total average operator.
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References

Alexander, R. (1977). Diagonally Implicit Runge- Kutta Methods for Stiff O.D.E.'s. SIAM Journal of Numerical Analysis, 14(6), 1006–1021. <https://doi.org/10.1137/0714068>

Alexander, R. (2003). Design and Implementation of DIRK Integrators for Stiff Systems. Applied Numerical Mathematics, 46, 1–17. [https://doi.org/10.1016/S0168-9274\(03\)00012-6](https://doi.org/10.1016/S0168-9274(03)00012-6)

Bartolomei, G. G., Brantov, V. G., Molochikov, Y. S., Kharitonov, Y. V., Solodki, V. A., Batashova, G. N., & Mikhailov, V. N. (1982). An experimental Investigation of True Volumetric Vapour Content with Subcooled Boiling in Tubes. Thermal Engineering, 29(3).

Bartolomei, G. G., & Chanturiya, V. M. (1967). Experimental Study of True Void Fraction When Boiling Subcooled Water in Vertical Tubes. Thermal Engineering, 14, 123–128.

Butcher, J. C. (2008). Numerical Methods for Ordinary Differential Equations (Second ed). John Wiley & Sons, Ltd.

Churchill, S. W. (1977). Friction-factor Equation Spans all Fluid Flow Regimes. Chemical Engineering, 91.

Gresho, P. M. (1987). On Pressure Boundary Conditions for the Incompressible Navier- Stokes Equations. *International Journal for Numerical Methods in Fluids*, 7. <https://doi.org/10.1002/flid.1650071008>

Ijaz, M., & Anand, N. K. (2007). Simulation of Unsteady Incompressible Viscous Flow using Higher-Order Implicit Runge-Kutta Methods — Staggered Grid. *Numerical Heat Transfer, Part B: Fundamentals: An International Journal*, 52, 471–488. <https://doi.org/10.1080/10407790701563367>

Ishii, M., & Hibiki, T. (2011). *Thermo- Fluid Dynamics of Two-Phase Flows (Second Edi)*. Springer. <https://doi.org/978-1-4419-7985-8>

Issa, R. I. (1981). Solution of the Implicitly Discretised Fluid Flow Equations by Operator-Splitting. *Journal of Computational Physics*, 65, 40–65. [https://doi.org/10.1016/0021-9991\(86\)90099-9](https://doi.org/10.1016/0021-9991(86)90099-9)

Kakac, S., & Bon, B. (2008). A Review of two-phase flow dynamic instabilities in tube boiling systems. *International Journal of Heat and Mass Transfer*, 51, 399–433. <https://doi.org/10.1016/j.ijheatmasstransfer.2007.09.026>

Kandlikar, S. G. (1999). *Handbook of Phase Change: Boiling and Condensation*. Taylor & Francis.

Lambert, J. D. (1991). *Numerical Methods for Ordinary Differential Systems: The Initial Value Problem*. (John Wiley & Sons Ltd, Ed.).

Lockhart, R. W., & Martinelli, R. (1949). Proposed Correlation of Data for Isothermal Two-Phase, Two-Component Flow in Pipes. *Chemical Engineering Progress*, 45, 38–48.

Mayinger, F. (1978). Sub-Cooled Boiling. In *Two-phase flows and Heat Tranfer with Application to Nuclear Reactor Design Problems*. McGraw Hill.

Padki, M. M., Palmer, K., Kakac, S., & Vezirglu, T. N. (1992). Bifurcation Analysis of Pressure-Drop Oscillations and the Ledinegg instability. *International Journal of Energy Research*, 35(2), 525–532. [https://doi.org/10.1016/0017-9310\(92\)90287-3](https://doi.org/10.1016/0017-9310(92)90287-3)

Patankar, S. V. (1980). *Numerical Heat Transfer and Fluid Flow*. Hemisphere Publishing Corporation.

Patankar, S. V., & Spalding, D. B. (1972). A Calculation Procedure for Heat, Mass and Momentum Transfer in Three-Dimensional Parabolic Flows. *International Journal of Heat and Mass Transfer*, 15, 1787–1806. [https://doi.org/10.1016/0017-9310\(72\)90054-3](https://doi.org/10.1016/0017-9310(72)90054-3)

Premoli, A., Franceso, D. D., & Prina, A. (1971). A dimensional correlation for evaluating two-phase mixture density. *La Termotecnica*, 25(1), 17–26.

Ruspini, L. C., Marcel, C. P., & Clausse, A. (2014). Two-phase flow instabilities : A review. *International Journal of Heat and Mass Transfer*, 71, 521–548. <https://doi.org/10.1016/j.ijheatmasstransfer.2013.12.047>

Saha, P., & Zuber, N. (1974). Point of Net Vapor Generation and Vapor Void Fraction in Subcooled Boiling. In *Proceedings of the 5th international heat transfer conference*, Tokyo.

Shieh, A. S., & Ransom, V. H. Krishnamurthy, R. (1994). Validation of Numerical Techniques in RELAP5/MOD3.

Skvortsov, L. M. (2006). Diagonally Implicit Runge – Kutta Methods for Stiff Problems. *Computational Mathematics and Mathematical Physics*, 46(12), 2209–2222. <https://doi.org/10.1134/S0965542506120098>

Söderlind, G., Jay, L., & Calvo, M. (2015). Stiffness 1952–2012: Sixty years in search of a definition. *BIT Numerical Mathematics*, 55(2), 531–558. <https://doi.org/10.1007/s10543-014-0503-3>

Strogatz, S. H. (1994). *Nonlinear Dynamics and Chaos*. Perseus Books Publishing L.L.C.

Talebi, S., Kazeminejad, H., & Davilu, H. (2012). A Numerical Technique for Analysis of Transient Two-Phase Flow in a Vertical Tube Using the Drift Flux Model. *Nuclear Engineering and Design*, 242, 316–322. <https://doi.org/10.1016/j.nucengdes.2011.10.038>

Van Doormaal, J. P., & Raithby, G. D. (2007). Enhancements of the SIMPLE Method for Predicting Incompressible Flows. *Numerical Heat Transfer : An International Journal of Computation and Methodology*, 7, 37–41. <https://doi.org/10.1080/01495728408961817>

Wallis, G. B. (1969). *One-Dimensional Two-Phase Flow*. McGraw Hill.

Counter- Current Stratified Flow Modeling

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This Chapter offers a numerical model that copes with transient phenomena in countercurrent gravity-driven flows inside the receiver tube of parabolic solar collectors. The mathematical model consists of 1-D balance equations for mass and momentum for both fluids, and energy balance for both fluids and the pipe wall. The model is characterized by the fact that the area (or height) of the liquid layer is treated as an dependent variable of the solution vector. The proposed numerical method consists of a

finite volume staggered grid discretization of the governing equations. Mass flow and liquid area are calculated with a semi-implicit pressure-based method, and the transient terms are treated with the explicit first stage singly implicit Runge-Kutta (ESDIRK) method. The calculation of the mass transfer rate from liquid to vapor is calculated iteratively by a guess-and-correct mass transfer algorithm, specially developed for stratified and single interphase separated flows. The results show the applicability and benefits of this model for the not so well known counter-current stratified two-phase with evaporation/boiling. The performance of the mass transfer algorithm is discussed showing that it is monotonic decreasing and linearly convergent. Finally, a parametric study is conducted showing that the main dimensionless group that describes vapor production is the inlet boiling number.

5.1 Introduction

The growth of the world population jointly with the industrial expansion requires to provide goods and services is the primary cause of the dramatic increase in the global energy demand. It is estimated that global energy demand could increase by 50% over the next 50 years, 80% of which will come from developing countries (Gadonneix, Kim, Meyers, Ward, & Frei, 2013). In that sense, one of the challenges of modern society is to increase energy production. However, such an increase must be made through sustainable and ecological development models. This includes the reduction of fossil fuel burning, due to the certain fear of the planet's average temperature increase by the emission of greenhouse effect gases. To achieve this end, it is essential to develop technologies that use renewable energy sources. In that sense, solar energy stands out for its abundance, with the received sun radiation in the upper part of the atmosphere to be around 175 PW (Tian & Zhao, 2013). Many are the available technologies for solar thermal energy production. Among these, either parabolic trough or Fresnel type linear solar collectors are the most common for medium and high temperatures. Both technologies work on the same principle, and their layout is similar. The working principle is simple; a straight absorber (receiver) pipe is located along the focal line of one or a group of mirrors that concentrate solar radiation from below on its external surface, tracking the sun, Figure 5. 1. With this high radiation flux, a fluid stream that flows inside the straight pipe is heated.

In Parabolic trough concentrators (PTC), the technology of study in this Chapter, solar radiation concentration ratios are in the order of 15- 45, being able to raise the fluid temperature up to 400 °C (Kalogirou, 2004). This high flexibility and low specific cost make this technology an interesting choice in the years to come (Jebasingh & Herbert, 2016). Within this range of temperatures, PTCs can straightforwardly use a single-phase fluid like water or a thermal oil or even as a direct steam generator (DSG) in an attempt to simplify thermo-solar power plants (Biencinto, González, & Valenzuela, 2016; Price et al., 2002). Our aim is more advanced, to boil refrigerant mixtures like $\text{NH}_3\text{-LiNO}_3$, for power plants and absorption cooling applications.

Figure 5. 1 Schematic representation of the counter-current gravity stratified flow layout.

Nowadays, with the applications mentioned above, the liquid entirely occupies the receiver tube. This configuration has some major drawbacks; friction pressure drops increase dramatically when boiling occurs, decreasing the total efficiency of the system, or when the system is formed by two or more receiver tubes connected in a parallel configuration, uneven flow distribution or pressure drop oscillation (PDO) can appear (Stenning, 1964). These issues increase the complexity in control and operation of the entire facility, as indicated in (Murphy & May, 1983), (Natan, Barnea, & Taitel, 2003) and (Tshuva, Barnea, & Taitel, 1999).

Phenomenologically, if vapor velocity is high enough an annular stratification establishes owing to the prevalence of shear stresses over gravity force, (Rohsenow,

Harnett, & Cho, 1998), (Wallis, 1969), among others. This flowing layout has been much studied because it happens in vertical, horizontal, and inclined pipe setups, which is completely filled with liquid at its inlet side. When this configuration is subjected to intense heating, the vapor production is such that the vapor velocity increases tremendously downstream, especially at low pressures, shear driving the liquid flow. In those layouts, a complete transformation of liquid into vapor is pursued. This is not the present case, where the velocities involved are low, making gravity predominant. This type of regime is a stratified flow, which excludes vertical and quasi-vertical pipes. It happens in horizontal and/or inclined pipes, when gravity forces its stratification, making the heaviest phase to place at the bottom side, (Rohsenow et al., 1998), (Wallis, 1969) and (Taitel Y & Dukler A, 1976). Additionally, for low enough velocities, a smooth interphase is maintained separating two continuous phases, not even reaching the wavy regime. The moderate vapor production and the large inlet void fraction makes that this regime does not switch to another one, being completely stable. The flow can be co-current or counter-current depending upon the relative motion of both phases, here each fluid stream defines a phase. If both phases flow in the same direction, it is called co-current, otherwise it is counter-current, (Kandlikar, 1999), see Figure 5. 2.

Figure 5. 2 Stratified flow geometry, a) current, b) counter-current

This design offers some advantages: *i*) vapor is produced directly without intervening any intermediate heat-carrying fluid circuit, for that using pressurized water, steam or thermal oil, as customary, *ii*) uneven flow distribution and PDO appearance are avoided, *iii*) cost, weight, and bulk are reduced as well as system complexity. For many industrial processes, the temperatures involved are in the order of 120-250 °C, medium-temperature solar collection (Coccia, Di Nicola, & Hidalgo, 2016), depending upon the pressure levels. In any case, they are lower than those required by steam generation for power production, around 300-500 °C; thus, the pipe thermoelastic bending

problem is of much lesser importance, e. g. (Alguacil, Prieto, Rodriguez, & Lohr, 2014) and (Serrano-aguilera, Valenzuela, & Parras, 2014). In the particular case, when the pipe is inclined, the flow is established when the substance (pure substance liquid or multicomponent mixture for absorption cycle applications), slides continuously under the effect of gravity. This kind of pattern is called gravity-driven stratified flow, being this the layout of interest of this chapter. The inclination can be very different, up to around $\beta = 50^\circ$, see Figure 5. 1, depending on the latitude of the location and on the inclination of the roof where the solar collector is installed.

In this layout, as a result of the heat produced by the sun rays absorbed at the external surface of the receiver pipe, the liquid is heated, generating vapor, which is collected on the upper side of the pipe and then is exhausted on the upper end. No dry-out is considered in this chapter. The remaining liquid is exhausted in the lower end of the pipe. This double fluid exhaustion system can be used for several applications; for example, the vapor produced can be condensed and used as a refrigerant, as a product, or simply as steam for heat or power generation. In parallel, the exhausted liquid can be used as the hot fluid for any other thermal process required, or even it can be recirculated. This boiler configuration adds the function of liquid/vapor separation in favor of compactness. Due to its novelty, no relevant information in the open literature has been found on the topic, excepting on (Lecuona, Ventas, Vereda, & Legrand, 2016).

5.2 Motivation

As it happens with any other technological development, the ultimate goal is to build prototypes and later a pre-commercial series; therefore, numerical modeling serves as an outstanding tool to perform optimizations before materialization. This reduces drastically the overall cost of the development and of the end product (design to the minimum cost of maintenance and smooth operation, being the reduction of costs evaluated in terms of CAPEX and OPEX). In that sense 1-D numerical models offer high flexibility, capturing all the relevant physics of the problem in a reasonable computational time. Many researchers have developed 1-D numerical models for PTCs for at least two decades up to date. Good examples of overall energy balance formulations can be found in (Kalogirou, 2012), more realistic models, based on differential balances of mass, momentum, and energy, in transient-state can be found in (García-valladares &

Velázquez, 2009), (Nallusamy, Sivaram, & Suresh, 2017), (Sivaram, Nallusamy, & Suresh, 2016), (Vasquez, Demirkaya, Goswami, Stefanakos, & Rahman, 2011), among others. Unfortunately, all the models mentioned above were developed for direct steam generators in which the pipe cross-section is filled with the entering fluid, thus with an initial null void fraction. No other model was found in the open literature capable of simulating both gravity-driven and stratified internal flow in a counter-current layout with mass transfer between both phases. Hence, the description of the main phenomena occurring with this innovative solar collecting layout with a mathematical model is of high interest as it allows quantifying the effect of the design and operating variables on this rather unexplored architecture. It allows studying the sensitivity to the main parameters and also its extension to include further mechanisms, such as extended surfaces and flow retardants.

5.3 Scope

The model developed considers the pipe of a constant circular cross-section, as customary in linear solar collectors, occupying either flow cross-section a partial circular segment of a full circle. This shape, although relatively well studied for turbulent flow friction and heat transfer, has not been much described for evaporation and boiling. This work establishes a model, in a progressive way, by integrating into it the different refinements necessary to reach a correct and representative physical behavior.

The heat conduction through the pipe wall determines the pipe bending in the longitudinal z axis, (Khanna, Singh, & Kedare, 2014), which is important both for solar focusing and for structural integrity. Considering the pipe wall as an extra phase, thermally coupled with both fluid ones, allows determining its cross-section temperature distribution under a non-conventional flow regime. This study will shed light on possible structural problems. Moreover, the present study adds a more precise calculation than previously performed (Lecuona-Neumann, Rosner, & Ventas-Garzón, 2016).

Under this scenario, the present Chapter is organized as follows: In Section 5.4 the basic geometric characteristics of stratified flow are shown. Section 5.5 presents the derivation of the mathematical model is explained jointly with the empirical information needed to close the system, and the discretized equations, boundary, and initial

conditions. Sections 5.6 and 5.7 discusses the thermal and mass transfer coupling algorithms, specially developed for this work. Extensive validation of the model is made in Section 5.8, followed by a parametric study in Section 5.9. Finally, in Section 5.10 points out the conclusions of this chapter.

5.4 Countercurrent gravity-driven flow layout

Under the assumptions described in the introduction, Section 5.1, one can assume that in the pipe cross-section, a plane and horizontal interphase is located between liquid and vapor, but the height of the liquid vein δ_l can change downstream. According to Figure 5. 3, some geometric relations can be found.

$$A_l = \frac{1}{8} 2\varphi - \sin 2\varphi D_i^2 \quad (5.1) \quad A_{total} = \frac{1}{4} \pi D_i^2 = A_l + A_v \quad (5.2)$$

$$\varphi = \pi - \cos^{-1} \left[\left(\delta_l - \frac{D_i}{2} \right) / D_i / 2 \right] \quad (5.3) \quad A_v = D_i \sin \varphi \quad (5.4)$$

5.5 Mathematical formulation

In this section, the mathematical formulation is presented. For this purpose, the entire domain is separated into three independent zones (phases) that interact with each other, Figure 5. 1. These three zones are *i*) The liquid zone, located at the bottom side of the pipe. Here the dense phase is located, which can be sub-cooled or saturated liquid, *ii*) The vapor zone, located on the upper side of the pipe; this zone is where all the vapor generated in the liquid zone is collected and finally flows away from the upper end of the pipe, *iii*) The solid wall, a zone that will receive the net heating of the radiation heat flux, transmitting this heat to both flows.

The assumptions for the flows are: both fluids are Newtonian, the flow is 1-D in the pipe axis direction (z), the flows are completely stratified and separated by a continuous smooth interphase; each substance is perfectly mixed in their respective zone, and mass transfer from the liquid to the vapor zone happens under saturated conditions. The fluid velocities and the respective velocity between them are small enough ($\sim 1 \text{ m} \cdot \text{s}^{-1}$) to guarantee that no significant ripples or waves are present in the interphase (Andreussi & Persen, 1987) and (Taitel Y & Dukler A, 1976). The inner pipe

diameter D_i is in the order of some centimeters, so that surface tension is affecting only a tiny region near the wall. The vertical hydrostatic pressure can be neglected in front of the main pressure imposed by the vapor-liquid equilibrium; thus, both streams share the same pressure. For the solid wall, the assumptions are that the axial heat conduction (z direction) is negligible in front of circumferential one, all properties are constant, and finally, the heat flux by convection inside the outer surface is taken into account by a net solar radiation flux.

Figure 5.3 a) Control volume, b) cross-section.

The mathematical formulation relies on balances for mass and momentum for both flows and energy balance for them and the solid wall. The equations are applied to an initially differential element of length dz , according to Figure 5.3. For such balances, 1st order Taylor series expansions are used, neglecting the higher-order terms. The mass

and momentum for both fluids ($k = l, v$) and the energy balance for both fluids and the solid wall can be written in integral form as:

Conservation of mass

$$\int_V \frac{\partial}{\partial t} (\rho_k A_k) dV + \int_A \dot{m}_k \cdot \hat{n} dA + \varepsilon_k \dot{m}'_{ip} = 0 \quad (5.5)$$

Conservation of momentum

$$\begin{aligned} \int_V \frac{\partial \dot{m}_k}{\partial t} dV + \int_A \left(\frac{1}{\rho_k A_k} \right) \dot{m}_k^2 \cdot \hat{n} dA = & - \int_A p A_k \hat{n} dA - \int_{S_k} \tau_{w,k} \cdot \hat{n}_k dS_k \\ & - \varepsilon_k \int_{S_k} \tau_{ip} \cdot \hat{n}_{ip} dS_{ip} - \int_V \rho_k g \sin \beta dV \end{aligned} \quad (5.6)$$

Conservation of energy (Fluids)

$$\int_V \frac{\partial (\rho_k A_k h_k)}{\partial t} dV + \int_A \dot{m}_k h_k \cdot \hat{n} dA + \varepsilon_k \dot{m}'_{ip} h_{ig} = Q''_{wall,k} + \varepsilon_k Q''_{ip,k} \quad (5.7)$$

Conservation of energy (solid wall)

$$(\rho C p)_{wall} \int_V \frac{\partial T}{\partial t} dV = Q''_{rad} - Q''_{wall} - Q''_{wall,k} + \int_{S_\theta} \frac{\lambda_{wall}}{r} \frac{\partial T_{wall}}{\partial \theta} dA \quad (5.8)$$

The balance equations for both flows are similar; the only difference is in the direction in which mass, momentum, and energy are transferred from one zone to the other; hence the fluid zone integer function (ε_k) is introduced. This function defines the normal vector direction at the interphase, being oriented in the direction of the liquid to the vapor zone. This function is defined mathematically as:

$$\varepsilon_k = \begin{cases} 1 & \text{if } k = l \\ -1 & \text{if } k = v \end{cases} \quad (5.9)$$

Since the model is 1-D, heat fluxes are approximated by means of the Newton cooling law, using average temperatures:

$$Q''_{wall,k} = \alpha_{wall,k} \bar{T}_{wall,k} - T_k \quad (5.10) \qquad Q''_{ip,k} = \alpha_{ip} \bar{T}_{ip} - T_k \quad (5.11)$$

Here α is the convective heat transfer coefficient, T is for absolute temperature and the superscript $(-)$ refers to its surface mean value for the wall:

$$\bar{T}_{wall,k} = \frac{\int_{\varphi_{k,i}}^{\varphi_{k,f}} r T_{wall}(\varphi) d\theta}{r_i \int_{\varphi_{k,i}}^{\varphi_{k,f}} d\theta} \quad (5.12)$$

On the other hand, the interphase heat flux can be calculated as $Q''_{ip} = \alpha_{ip,l}(T_l - \bar{T}_{ip})$ or $Q''_{ip} = \alpha_{ip,v}(\bar{T}_{ip} - T_v)$, depending upon which zone is considered. In order to guarantee: temperature continuity between the liquid zone and the vapor zone, and heat flux continuity in the interphase $\bar{T}_{ip}$ is defined as:

$$\bar{T}_{ip} = \frac{\alpha_{ip,l} T_l + \alpha_{ip,v} T_v}{\alpha_{ip,l} + \alpha_{ip,v}} \quad (5.13)$$

5.5.1 Empirical information

The model formed by Equations (5.5) to (5.8) requires some empirical information. For the momentum equations, the shear stresses are calculated using the Darcy formula.

$$\tau_{w,k} = \frac{1}{2} f_k \rho_k U_k^2 \quad (5.14) \qquad \tau_{ip} = \frac{1}{2} f_{ip} \rho_{ip} U_{ip}^2 \quad (5.15)$$

Here f is the friction factor and U_{ip} is the average (bulk) velocity difference between both phases in contact.

Many correlations to calculate the friction factors f have been developed, Chapter II summarizes some common friction factor correlations. Unfortunately, all of them are for stratified co-current flows, therefore if we assume that the total amount of vapor generated in the liquid zone is small compared to the liquid mass flow, we can infer with a high level of certainty that the behavior of the counter-current stratified flow under this condition is similar than the co-current stratified smooth pattern. In that

sense, according to (Andreussi & Persen, 1987), the shear stress at the wall interphases can be calculated as it were a single-phase flow, with the hydraulic diameter ($D_{h,k} = 4A_k / P_k$) as the characteristic length. For the liquid/vapor interphase, the shear stress is highly important when relative motion between two phases is high, being responsible for the interfacial wave generation mechanism and liquid holdup. Anyhow, the value of f_{ip} is again calculated by the criterion of (Andreussi & Persen, 1987). This criterion is based on their observations, later confirmed independently by (Hanratty & Andritsos, 1984), in which they concluded that for a stratified smooth pattern the interfacial friction factor is approximately equal to the one of the gas flow ($f_{ip} \cong f_v$). Some corrections can be added because of the effusion velocity by vapor transfer, but it seems to be quite low so that it has been neglected.

For the local heat transfer coefficients (both fluids/wall and liquid/solid interphase), the Gnielinski correlation (Gnielinski, 1976) is used for the calculation of the fully developed turbulent flow Nusselt number, Equation (5.16). It is modified by the entrance correction of Al-Arabi (Al-Arabi, 1982), Equation (5.17). Both correlation and correction correlations can also be found in Sigalés (Sigalés, 2003). The heat flux is a maximum in the order of $10 \text{ kW} \cdot \text{m}^{-2}$, a low value for fired boilers. Consequently, in the present study, we neglected the enhancement by bubbles formation at the wall, this way being conservative.

$$Nu_{\infty} = \frac{\alpha D_h}{\lambda} = \frac{\frac{f}{8}(Re - 1,000)Pr}{1 + 12.7(f/8)^{1/2}(Pr^{2/3} - 1)} \quad (5.16)$$

$$\frac{Nu(z)}{Nu_{\infty}} = 1 + 0.56 \left(\frac{D_h}{z} \right)^{0.8} \Rightarrow Nu(z) = \left[1 + 0.56 \left(\frac{D_h}{z} \right)^{0.8} \right] \frac{\frac{f}{8}(Re - 1,000)Pr}{1 + 12.7(f/8)^{1/2}(Pr^{2/3} - 1)} \quad (5.17)$$

5.5.2 Discretised equations

The system of balance equations is solved numerically using the method of lines (MOL) jointly with the finite volume method and the Explicit First Stage Diagonally implicit Runge-Kutta method (ESDIRK), as space and time integration techniques respectively. In Chapter III these concepts are studied extensively, and in Chapter IV

the numerical method used is explained in detail. For space integration, four coupled meshes are used to transform the continuum model into a discrete algebraic system. The first two meshes (flows) consist of a staggered grid arrangement; here scalar variables ϕ (pressure, enthalpy, area, vapor quality, etc.) are collocated at the center of the volume and the mass flow rate at the boundaries, Figure 5. 4.a. The integration of the momentum equations is performed in the opposite way, Figure 5. 4.b. The third mesh consists of a collocated grid for the wet surface average wall temperature, Figure 5. 4.a to Figure 5. 4.c. This temperature is collocated at the center of the volume and in the same axis of the scalar variables in the fluid main mesh. Finally, an auxiliary mesh is also used for the collocation of the wall temperatures in order to calculate angular wall heat conduction. This temperature is also at the center of each volume Figure 5. 4.d.

The dependent variable vector is $\psi = (\dot{m}_l \ \dot{m}_v \ h_l \ h_v \ T_{wall} \ p \ A)^T$. The first five variables are determined with the momentum and energy equations of each fluid and the wall, respectively. The other two variables (pressure and liquid zone area) are calculated with a pressure correction method.

d)

Figure 5. 4 Meshes: a) staggered grid fluid main mesh (scalar variable $\emptyset$), b) staggered grid fluid mass flow mesh, c) auxiliary wet surface average grid, d) auxiliary angular wall temperature grid.

For $\psi = (\dot{m}_l \ \dot{m}_v \ h_l \ h_v \ T_{wall})^T$ the balance equations are integrated (space and time) over the staggered grid flow mesh for $\dot{m}_k$, the staggered grid main mesh for h_k and the auxiliary angular wall temperature mesh for T_{wall} . With these simplifications, the model written in the discrete form $B_{e/P} \psi_{e/P} + B_{w/W} \psi_{w/W} + B_{Ee/E} \psi_{Ee/E} = b$ is:

Conservation of Momentum

$$\left. \begin{aligned} B_{e,k} &= (\rho_k A_k)_{P,k}^{-1} \max(-\dot{m}_{w,k}; 0) + (\rho_k A_k)_{E,k}^{-1} \max(\dot{m}_{e,k}; 0) + S_p \\ B_{e,k} &= -(\rho_k A_k)_{P,k}^{-1} \max(\dot{m}_{w,k}; 0) \\ B_{Ee,k} &= -(\rho_k A_k)_{E,k}^{-1} \max(-\dot{m}_{e,k}; 0) \\ b_k &= (p_P A_P - p_E A_E)_k + \frac{1}{a_{rr}} \sum_{j=1}^{r-1} a_{rj} \tilde{F}_k^{(j)} + S_c^{(r)} + S_c^f \\ S_p &= \frac{\Delta z}{a_{rr} \Delta t} + f_k \frac{S_{wall,k}}{4 \rho_k A_k^2} \text{sign}(\dot{m}_{e,k}^*) \dot{m}_{e,k}^* \\ S_c &= \frac{\Delta z}{a_{rr} \Delta t} \dot{m}_{e,k}^{(r)} \\ S_c^f &= f_k \frac{S_{w,k}}{8 \rho_k A_k^2} \text{sign}(\dot{m}_{e,k}^*) (\dot{m}_{e,k}^*)^2 - \rho_k g A_k \sin(\beta) \Delta z \\ \tilde{F}_k^{(j)} &= -B_{i,k}^{(j)} \dot{m}_{i,k}^{(j)} - \sum_{\substack{nb \\ nb \neq i}} B_{nb,k}^{(j)} \dot{m}_{nb,k}^{(j)} + b_{i,k}^{(j)} \end{aligned} \right\} \quad (5.18)$$

Conservation of energy (Flows)

$$\left. \begin{aligned}
 B_{P,k} &= \max(-\dot{m}_{w,k}; 0) + \max(\dot{m}_{e,k}; 0) + S_P \\
 B_{W,k} &= -\max(\dot{m}_{w,k}; 0) \\
 B_{E,k} &= -\max(-\dot{m}_{e,k}; 0) \\
 b_k &= \frac{1}{a_{rr}} \sum_{j=1}^{r-1} a_{rj} \tilde{F}_k^{(j)} - \varepsilon_k \dot{m}_{ip} h_v^{sat} + S_c^0 + S_c^Q \\
 S_P &= \frac{\Delta z}{a_{rr} \Delta t} \rho_k^{(r)} A_k^{(r)} \\
 S_c^0 &= \frac{\Delta z}{a_{rr} \Delta t} \rho_k^{(r)} A_k^{(r)} h_k^{(r)} \\
 S_c^Q &= \alpha_{wall,k}^{(n)} A_{P,k}^{(n)} \bar{T}_{wall,k}^{(r)} - T_{P,k}^{(r)} + \varepsilon_k \alpha_{ip}^{(n)} A_{ip}^{(n)} (\bar{T}_{ip}^{(r)} - T_{k,P}^{(r)}) \\
 \tilde{F}_k^{(j)} &= -B_{i,k}^{(j)} h_{i,k}^{(j)} - \sum_{\substack{nb \\ nb \neq i}} B_{nb,k}^{(j)} h_{nb,k}^{(j)} + b_{i,k}^{(j)}
 \end{aligned} \right\} \quad (5.19)$$

Conservation of energy (solid wall)

$$\left. \begin{aligned}
 B_{P,k} &= (\rho C p)_{wall} \frac{\Delta V}{a_{rr} \Delta t} + 2 \frac{\lambda_{wall} \Delta r}{\bar{r} \Delta \theta} \\
 B_{W,k} &= -\frac{\lambda_{wall} \Delta r}{\bar{r} \Delta \theta} \\
 B_{E,k} &= -\frac{\lambda_{wall} \Delta r}{\bar{r} \Delta \theta} \\
 b_k &= S_c^0 + S_c^Q + \frac{1}{a_{rr}} \sum_{j=1}^{r-1} a_{rj} \tilde{F}_k^{(j)} \\
 S_c^0 &= \frac{\Delta V}{a_{rr} \Delta t} (\rho C p)_{wall} T_i^{(n)} \\
 S_c^Q &= \pi D_o \Delta z Q_{rad}'' - \alpha_{l,w}^{(n)} A_{l,P}^{(n)} \bar{T}_{l,z} - T_{l,p} - \alpha_{v,w}^{(n)} A_{v,P}^{(n)} \bar{T}_{v,z} - T_{v,p} \\
 \tilde{F}_P^{(j)} &= -B_P^{(j)} T_{P,wall}^{(j)} - \sum_{\substack{nb \\ nb \neq i}} B_{nb,k}^{(j)} T_{nb,wall}^{(j)} + b_{i,k}^{(j)} \\
 \Delta V &= \bar{r} \Delta r \Delta \theta \Delta z
 \end{aligned} \right\} \quad (5.20)$$

The two equations left are for mass conservation of both fluids, which integrated over the staggered main mesh, result in semi-implicit form as follows:

$$\dot{m}_{e,k} - \dot{m}_{w,k} = -\frac{\partial}{\partial t} (\rho_k A_k) \Delta z - \varepsilon_k \dot{m}_{P,ip} \quad (5.21)$$

Here the mass accumulation term can be approximated under the ESDIRK fashion at every (r) stage as:

$$\left. \frac{\partial(\rho_k A_k)}{\partial t} \right|_P^{(r)} \approx \frac{\rho_k A_k^{(r)} - \rho_k A_k^{(n)}}{c_r \Delta t} \quad (5.22)$$

This equation acts more of a restriction to the mass flow field than as a dynamic equation for pressure and liquid area. Therefore a pressure/liquid cross-area evolution equation must be constructed. Focusing on both; liquid and vapor zones momentum equations, the driving force is given by (pA_k) , so the same procedure to build this evolution equation applies for pressure (p) in the vapor zone and for the liquid area (A_l) in the liquid zone. This is an old issue in incompressible flows giving birth to the so-called semi-implicit-pressure-linked-equation (SIMPLE) algorithm, (S V Patankar & Spalding, 1972). The pressure/liquid area correction method starts with a guessed mass flow field $(\dot{m}_k^*)$, and both mass flow fields are corrected on each iteration as $\dot{m}_k = \dot{m}_k^* + \dot{m}_k'$. The mass flow guess field is calculated with a guessed pressure/liquid area field $p = p^* + p'$ and $A_l = A_l^* + A_l'$. With these correction equations combined with the discrete Equation (5.18) and mass conservation Equation (5.21) the pressure/liquid area correction on each (r) level can be built.

$$(d_{v,e} + d_{v,w})p'_P - d_{v,e}p'_E - d_{v,w}p'_W = -(\dot{m}_{v,e}^* - \dot{m}_{v,w}^*) - \left. \frac{\partial(\rho_v A_v)}{\partial t} \right|_P^{(r)} \Delta z - \dot{m}_{P,ip} \quad (5.23)$$

$$(d_{l,e} + d_{l,w})A'_{l,P} - d_{l,e}A'_{l,E} - d_{l,w}A'_{l,W} = -(\dot{m}_{l,e}^* - \dot{m}_{l,w}^*) - \left. \frac{\partial(\rho_l A_{l,P}^*)}{\partial t} \right|_P^{(r)} \Delta z + \dot{m}_{P,ip} \quad (5.24)$$

In the above equations, the coefficients $d_{k,e}$ are obtained by algebraic manipulation of the discrete momentum equation. More details can be found in (S V Patankar & Spalding, 1972) and (Suhas V Patankar, 1980).

5.5.3 Initial and boundary conditions

For an inlet thermodynamic state (enthalpy and pressure), mass flow and area (or height) are needed as boundary conditions (BCs). The thermodynamic state can be imposed independently. However, the hydrodynamic BCs are coupled (i.e. the liquid flow

velocity and its cross-section area). According to the assumption of gravity-driven flow, after the fluid enters the pipe, a terminal velocity is reached. This velocity is due to the balance between body forces and the shear stress at the wall. The transition zone can be assumed to be very small, and the terminal velocity conditions can be used at the inlet as a boundary condition. Therefore, simplifying Equation (5.18) for steady-state conditions a cross-sectional area can be found for any liquid mass flow, Equation (5.25). This equation is implicit and must be solved before starting the numerical procedure for the entire model. The solution of this equation is depicted in Figure 5. 5 showing its dependency on the tilt angle; here, $\beta < 0$ for falling flow.

$$gA_{l,z=0} \sin \beta = \frac{1}{2} f(U_{l,z=0}) S_{w,l} A_{l,z=0} U_{l,z=0}^2 = \frac{1}{2} f(U_{l,z=0}) S_{w,l} (A_{l,z=0}) \left(\frac{\dot{m}_l}{\rho_l A_l} \right)_{z=0}^2 \quad (5.25)$$

Figure 5. 5 Inlet terminal hydraulic conditions, a) mass flow vs. liquid area, b) mass flow vs. terminal velocity

5.6 Flow and thermal algorithms

The 1-D transient discrete flow model consists of momentum and energy Equations (5.18), (5.19) and (5.20), plus the pressure/liquid area correction, Equations (5.23) and (5.24). The system of discrete equations is solved with the TDMA algorithm (Press, Teukolsky, Vetterling, & Flannery, 2007) taking advantage of the form of the coefficient matrices.

The numerical methodology consists in solving the corresponding system of equations for each zone sequentially in the following order: liquid, vapor, and wall. Because all variables are highly coupled, the entire system of balance equations must be solved iteratively on each (r) ESDIRK stage inside the interval $t + \Delta t$. To ensure

convergence a tolerance value must be settled, and this convergence criterion is applied to the mean average wall and flows interphase temperatures. Algorithm 5. 1 shows the details of the algorithm.

5.7 The mass transfer correction algorithm

At this point, the discrete conservation and pressure/liquid area correction equations are solved with the mass transfer rate at the interphase ($\dot{m}_{ip}$) as a parameter. Mass transfer through the interphase is controlled by many factors such as the shape of the interphase, interphase surface tension, molecular diffusion, turbulent mixing, plus convection and concentration gradient in multicomponent mixtures. All this information is modeled through the so-called mass transfer coefficient (K); hence, if we assume that all the vapor is generated by the addition of latent heat and all this vapor is transferred instantly to the vapor phase ($K = 1$), the mass transfer rate can be modeled as $\dot{m}_{ip} = \dot{m}x$. Particularized in discrete form in our integration stencil, the mass transfer rate finally becomes.

$$\dot{m}_{P,ip} = \begin{cases} 0 & \text{if } x_{P,l} \leq 0 \text{ (sub-cooled state)} \\ \dot{m}_{w,l} x_{P,l} & \text{if } x_{P,l} > 0 \text{ (liquid+vapor mixture)} \end{cases} \quad (5.26)$$

Application of Equation (5.26) to calculate $\dot{m}_{P,ip}$ requires to know $\dot{m}_{w,l}$, h_l and p on each (r) stage, however, the mass transfer rate is strongly coupled with the mass flow, enthalpy and pressure, therefore Equations (5.18), (5.19), (5.20), (5.23), (5.24) and (5.26) must be solved sequentially in an iterative fashion. Unfortunately, Equation (5.26) is not a dynamic equation for $\dot{m}_{P,ip}$, so the way to fulfill the correct mass transfer rate is by correcting the numerical procedure, using Equation (5.27).

$$\dot{m}_{ip} = \dot{m}_{ip}^{**} + \Delta \dot{m}_{ip} \quad (5.27)$$

Here $\dot{m}_{ip}^{**}$ stands for the guess mass flow through the interphase field and $\Delta \dot{m}_{ip}$ stands for its correction, which is calculated after every iteration level with Equation (5.26) using logically the value of quality calculated with enthalpies of the same iteration level.

The idea behind this correction procedure is that by successive iterations, the mass transfer rate is adjusted, such that the generated vapor is instantly transferred and the liquid stream is always in saturation conditions. Algorithm 5. 2 shows the mass transfer correction algorithm for the transient regime under the ESDIRK method.

Algorithm 5. 1 Flowchart of thermal fluid for (r) stage ESDIRK algorithm.

5.8 Validation test case

Verification and validation form the essential procedure to determine the reliability and accuracy of CFD codes and models (Oberkampf & Trucano, 2002). The way to proceed is simple, with the aim of test cases as benchmark comparative simulations are performed. Unfortunately, there is a lack of experimental data or analytical solution to be used as a benchmark for the counter-current flows with mass transfer between phases, whose layout is of interest in this work. In that sense, a simple conceptual test case as a benchmark is proposed hoping that in the near future

experiments can be carried out and serve as a basis for the required comparison. The proposed test case consists of a simple startup operation of the collector when a sub-cooled water stream partially fills ($\delta_l = 7.5$ mm) a 6 m long tube. The pipe of the collector is made of commercial steel ($\lambda_{wall} = 15 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$, $\rho_{wall} = 7,900 \text{ kg} \cdot \text{m}^{-3}$ and $Cp_{wall} = 500 \text{ J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$) with an inner diameter $D_i = 3$ cm and 5 mm wall thickness and an inclination angle of the pipe $\beta = -30^\circ$. The inlet temperatures of the liquid and vapor streams are respectively 118.21°C , 125°C , and 20°C for the wall. Pressure for the liquid and vapor is equal to 200 kPa. The initial mass flow rates for the liquid and vapor are $0.01 \text{ kg} \cdot \text{s}^{-1}$ and $0 \text{ kg} \cdot \text{s}^{-1}$ respectively. Solar net irradiance is a function of the angle of the pipe, Equation (5.28). This function would be the same for any z position at any time.

$$Q''_{rad} = \begin{cases} 500 \text{ W} \cdot \text{m}^{-2} & \text{for } 330^\circ \leq \theta < 210^\circ \\ 800 \text{ W} \cdot \text{m}^{-2} & \text{for } 210^\circ \leq \theta < 330^\circ \end{cases} \quad (5.28)$$

This solar irradiance is concentrated with a parabolic device, such that the total net heat flux at the outside diameter is, including losses to ambient:

$$Q''_{rad} = \begin{cases} 500 \text{ W} \cdot \text{m}^{-2} & \text{for } 330^\circ \leq \theta < 210^\circ \\ 7,680 \text{ W} \cdot \text{m}^{-2} & \text{for } 210^\circ \leq \theta < 330^\circ \end{cases} \quad (5.29)$$

5.8.1 Numerical parameters

According to our test case, the initial ($t = 0$) conditions are: $p_l(0, z) = p_v(0, z) = 200 \text{ kPa}$, $T_l(z, \theta, t = 0) = 20^\circ\text{C}$, $T_l(0, z) = 118.21^\circ\text{C}$, $T_v(0, z) = 125^\circ\text{C}$. The solution method requires to solve an intermediate pressure/ liquid area Poisson equation; therefore, the boundary conditions are:

Liquid	Vapor
$\dot{m}_l(z = 0, t) = 0.01 \text{ kg} \cdot \text{s}^{-1}$ $A_l(z = 0, t) = A_{l,z=0}$	$\dot{m}_v(z = L, t) = 0 \text{ kg} \cdot \text{s}^{-1}$ $p_v(z = 0, t) = 200 \text{ kPa}$
(5.30)	(5.31)

Note that for the liquid, both BC's are specified at the inlet. Because of the elliptic character of the pressure Poisson equation, BC's must be specified at both ends. To

transform the actual BC's at the inlet to BC's at both ends a translation and guess and correct procedure is required. Chapter III explains this produce.

Algorithm 5. 2 Flows interphase mass transfer algorithm

Besides, some numerical parameters are required. In this work, the temporal integration is performed with the 3rd order of accuracy ESDIRK method developed by Alexander (Alexander, 2003), in Annex F its corresponding Butcher table can be consulted. This temporal numerical scheme is implicit, making the numerical method to be unconditionally stable, not requiring any restriction on the time step. Also, there is no rapid variation in the boundary conditions so that no rapid transient phenomena will occur, hence the time step was set to $\Delta t = 0.25$ s. The total simulation time is 120 s, a

time long enough to reach the steady-state condition. The relaxation factor for pressure is constant and set to 0.5. On the other hand, the relaxation factor for liquid area correction equation is inversely proportional to the number of volumes employed; in our numerical experiments, it was varied from 0.05 for $N = 150$ and to 0.25 for $N = 20$. The selection of the liquid area relaxation factor is an important issue in this numerical model. The reason behind this unusual value for the area correction equation is because the liquid area must always be a positive quantity and the use of the area correction equation makes that the solution oscillates around the solution point at any iteration level, bringing the risk of negative liquid areas, leading to unphysical solutions.

5.8.2 Grid sensitivity analysis

In order to guarantee the consistency of the numerical model proposed in this paper, with the initial and boundary conditions explained in Section 5.8.1 a grid sensitivity analysis is carried out before the correct simulation results are presented in Section 5.8.3. As three different grids are used, the analysis is made out in two ways. First, the number of volumes in the wall is fixed ($N_w = 90$ volumes) varying the volumes of both flows (N) and finally, the same procedure is repeated oppositely, fixing the number of flows volumes and varying the wall ones. The selected tracking variables are the vapor enthalpy and mass flow; both measured at the vapor outlet ($z = 0$). Figure 5. 6 shows the temporal evolution of these variables. It can be observed that the grid refinement makes that the solution tends asymptotically to a stable solution while $N \rightarrow \infty$ or $\Delta z \rightarrow 0$. This behavior evidences the consistency of the numerical schemes; in other words, the numerical fluxes that cross the volume boundaries tend to the real numerical flux as $\Delta z \rightarrow 0$. This result is not surprising due to the fact that the employed 1st order UPWIND scheme is consistent. On the other hand, in the case of vapor mass flow of Figure 5. 6.a, it can also be observed that the solutions for $N = 50$ and $N = 100$ volumes are very close with error respect to the solution with $N = 50$ of -0.067% and -0.051% respectively. A similar result is observed for the enthalpy evolution, Figure 5. 6.b. From an asymptotic point of view, both solutions are acceptable. When the number of volumes is increased the computational effort required increases. This behavior is explained not only because the dimension of the linear systems to solve is larger, but also because of the relaxation factors for the liquid area correction Equation (5.24) must be

lower for a larger number of volumes, see Section 5.8 for the definition of the relaxation factors.

Figure 5. 6 Grid sensitivity for N_w fixed and varying N for two tracking variables, a) vapor mass flow rate, b) vapor enthalpy.

For the next sensitivity experiment proposed, the number of flow volumes is settled to $N = 50$ and the influence of the number of wall volumes (N_w) is analyzed. These results are shown in Figure 5. 7. It shows that for a low number of volumes $N_w < 20$ a spurious high vapor enthalpy appears for long times; this occurs because for a low number of volumes the mean wall temperatures calculated with Equation (5.13) are not well approximated, so that in this case the vapor mean wall temperature is higher, transferring more heat to the vapor zone. With the grid refinement, the solution tends asymptotically to a stable solution, but again the computational cost increases, in this case, when $N_w > 48$. It also can be observed that for $50 \text{ s} < t < 100 \text{ s}$ and $t > 100 \text{ s}$ a decrease and later increase in vapor enthalpy is found, this effect is because initially, the wall temperature distribution is lower than the initial vapor temperature (see Section 5.8). Therefore heat is transferred from the vapor zone to the wall ($t < 100 \text{ s}$) and later on the heat flux is reversed when the mean vapor wall equals the vapor zone temperature.

Figure 5. 7 Grid sensitivity for N fixed varying N_w , a) vapor mass flow rate, b) vapor enthalpy.

According to this analysis, 50 volumes ($\Delta z = 0.03$ m) for the liquid and vapor zones and 48 volumes ($\Delta\theta = 0.1308$ rad) for the wall at each z location are enough to ensure an asymptotically convergent solution.

5.8.3 Transient numerical solution

Once the number of volumes is settled, the temperature spatial distribution is shown. It corresponds to the same test case proposed in Section 5.8.2. The results for liquid temperature are shown in Figure 5. 8. The results show that for $t < 90$ s there is the washout of the cold entering liquid with a thermal wave traveling downstream. This phenomenon is caused by the initial wall temperature that was set at a lower than the initial liquid temperature, hence heat is transferred from the liquid to the wall and therefore the wall is heated not only by sun radiation but by the liquid heat as well until its large heat capacity allows it to gain temperature. This is coherent with the results shown in Figure 5. 9, which shows that for $t = 40$ s, well downstream the pipe wall is still cold. This kind of behavior is an important aspect to take into account if an analysis of the startup or shutdown of the installation has to be carried out. Later on, for example at $t > 50$ s, in some sections of the pipe near the liquid inlet, the wall temperature is recovered, switching the direction of heat flux. Once the heat flux is towards the liquid, it begins to increase its temperature until the saturation condition is reached at the inlet pressure of 200 kPa. It is important to highlight that as part of the numerical algorithm the pressure inside the pipe is maintained constant until vapor is generated, this is because pressure is determined by the coupling of the momentum and mass equations in the vapor zone; hence this coupling is not performed until there is no vapor inside the top zone; this is to avoid having zeros in the main diagonals of the matrices involved in the SIMPLE algorithm for the vapor zone. The exact subcooled pressure downstream gradient would be slightly positive owing to the counter-current vapor flow. The subcooled region corresponds to the almost linear temperature increase with z near the liquid inlet, shown in Figure 5. 8.b, as only sensible heating is produced.

Once the saturation condition is locally reached, vapor begins to be generated, and instantly it is transferred to the upper vapor zone. Even that initial conditions for temperature were constant for both liquid and wall, the way in which they evolve thermally downstream is not uniform. The reason for this is that the convective

coefficient is not constant along the pipe, as Figure 5. 9.b shows, mainly due to the entrance correction in Nusselt number, Equation (5.17). This non-uniformity affects the vapor generation and can be clearly observed in Figure 5. 9.a as a bulge shaped curve for $\dot{m}_{ip}$, especially for $50 \text{ s} < t < 120 \text{ s}$.

Figure 5. 8 a) Liquid temperature transient evolution, b) close-up of a).

Figure 5. 9 Transient evolution, a) mass transfer through the flows interphase $\dot{m}_{ip}$, b) wall/liquid convective coefficient.

One of the novelties incorporated in the model is the simultaneous calculation of the wall temperature dynamics. Figure 5. 10 shows the wall temperature distribution at four different locations for $t = 40 \text{ s}$. It can be observed how the lower part of the pipe is hotter than the upper part, mainly near the inlet of the pipe despite the increased entrance effect. Also, it shows the heating of the upper part by thermal diffusion, affecting this way the efficiency of the solar system and eventually superheating the vapor. The full angular description of wall temperature allows studying problems with a non-symmetric solar angular concentration that happens when tracking the sun along the day. Relevant information can be extracted for extended analysis like the determination of the pipe thermal fatigue and the evaluation of pipe longitudinal bending.

Figure 5. 10 Angular wall temperature distribution, $t=40$ s.

5.8.4 Performance of the mass transfer algorithm

The mass transfer algorithm developed for this work is a crucial part of the numerical procedure. It allows logically determining the mass transfer rate and also to fulfill the saturation conditions of the liquid stream. This is the reason why some attention must be paid to its performance. Figure 5. 11 shows the mass transfer correction ($\Delta \dot{m}_{ip}$) for different locations at $t = 54$ s, the instant at which vapor generation has already started, coherently with Figure 5. 8 and Figure 5. 9. Inside the interval $0.5 \text{ m} < z < 1.8 \text{ m}$ is where saturation is reached and the mass transfer algorithm operates: Outside that interval, the fluid is still sub-cooled and no mass correction is needed because $x < 0$. It can be observed from Figure 5. 11.a how the mass transfer correction is larger in the first iteration levels; after the iteration level advances, this mass correction monotonically decreases toward zero. This means that the energy transfer through the interphase source term $\varepsilon_k \dot{m}_{ip} h_v^{sat}$ is being recalculated for accuracy. In other words, the algorithm is transferring the correct energy flux so that the liquid stream remains saturated. It could be observed that at all locations, the mass transfer correction exhibits the same convergence performance. Figure 5. 11.b shows a sample, again for $t = 54$ s. It can be observed that the convergence rate is almost the same for all z points and moreover, $\Delta \dot{m}_{ip}$ approaches zero monotonically decreasing. Hence, it can be argued

that the algorithm is always convergent; furthermore, if one calculates the convergence sequence as $\Delta\dot{m}_{ip}^{k+1} / \Delta\dot{m}_{ip}^k$, where k is the iteration level, we found that this sequence converges to 0.921, 0.904 and 0.909 for $z = 0.54$ m, $z = 0.78$ m and $z = 1.5$ m respectively. This means that the mass transfer algorithms are linearly convergent with a mean order of convergence of 0.901. These results evidence the potential of using this algorithm for the determination of transient mass transfer rates in stratified evaporation/boiling flows.

Figure 5. 11 Mass transfer algorithm performance, a) mass transfer correction performance, b) convergence historical.

5.9 Parametric study

The vapor produced in the PTC with this layout can feed a machine using an absorption heat pump cycle or a Rankine power cycle. Therefore the determination of the vapor production rate is of paramount importance. The variables that control the production are many; heat radiation, the tilt angle of the receiver tube, inlet mass flow, and inlet degree of saturation. The effect of total radiation heat over the receiver tube seems to be obvious, more heat implies more vapor production. However, the effect of the spatial radiation distribution is not that obvious. Unveiling this issue is particularly important because the irradiance profile on the receiver pipe is not uniform due to many factors such as errors in the mirror shape manufacturing, error in the tracking system positioning or due to the tube own shadow over the mirror. Also, as the flow inside the receiver pipe is gravity stratified; the liquid is always placed in the bottom of the pipe, so depending on the sun position the radiation heat flux will be concentrated at some region at the outer surface of the pipe that will not always correspond to the one wet by the flowing liquid. On the other hand, tilt angle and inlet mass flow conditions determine

the mean liquid velocity and void fraction, having a direct effect on convective heat transfer. Because of the novelty of the counter-current gravity-driven flow in a PTC, this section explores the dependency of the above-mentioned variables.

5.9.1 Numerical experiments

Two numerical experiments were carried out. In both experiments, the geometric and physical characteristics of the receiver tube are the same. The receiver tube is 6 m long with an inner diameter of 3 cm and a wall thickness of 3 mm, which is initially at 30 °C. This pipe material is commercial steel with $\lambda_{wall} = 15 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$, $Cp_{wall} = 500 \text{ J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$ and $\rho_{wall} = 7,900 \text{ kg} \cdot \text{m}^{-3}$. The additional data for the first experiment are an inlet mass flow $\dot{m}_{l,z=0} = 100 \text{ g} \cdot \text{s}^{-1}$ of sub-cooled water ($T_{l,z=0} = 118.21 \text{ °C}$ and $p_{z=0} = 2 \text{ bar}$) flowing in a $\beta = -30^\circ$ tilted pipe in which three different irradiation profiles are tested, keeping constant the total irradiation heat ($Q_{irr,tot} = 1,745.21 \text{ W}$). The three considered irradiation profiles are depicted in Figure 5.12.

Figure 5.12 Heat irradiation profiles for experiment #1.

The second experiment consists in varying the inlet mass flow rate, keeping fixed the inlet thermal condition (the same as the first experiment) using Q_1'' . This experiment was repeated for different tilting angles β .

5.9.2 Results and discussion

The results for both experiments are shown in Figure 5. 13 and. In these graphs, it is worth to highlight that:

5.9.2.1 Experiment #1 (variations of the irradiation profile).

- Independently of the radiation profile, the heat from the wall to the vapor is much smaller than the heat from the wall to the liquid. It means that azimuthal heat conduction is much larger than convective heat transfer in the vapor, and the vapor temperature varies easily to maintain this condition. This occurs because the vapor heat capacity, thermal conductivity, and convection coefficient are much lower than that for the liquid, thus getting lower heat transfer rates

Figure 5. 13 Results for experiment #1, a) Liquid temperature and mass transfer axial profile, b) Vapour production, and heat ratio transient behavior.

- As a consequence, the increase in temperature of the liquid is linear until saturation temperature is reached at any axial location, starting boiling.
- The saturation temperature is reached inside the tube at $t \approx 50$ s, for larger times, the location of the vapor generation initial point moves towards the inlet, Figure 5. 13.
- As the liquid absorbs almost all the heat, the vapor production follows the same transient behavior for all cases, having a very small delay in the case of Q_2'' . In this case, the extreme bad distribution of the radiation heat increases the heat transferred to the vapor enough to produce this effect that, nevertheless, keeps being small.
- Figure 5. 13.b shows the wall total heat ratio ($Q_{w,v,tot} / Q_{w,l,tot}$) confirming that the heat quantity transferred to the vapor is negligible compared to the one to the liquid. This indicates that no matter how irregular the radiation distribution is, Figure 5. 12, the behavior of the liquid phase is almost the same. Thus, the vapor production is almost insensitive to the transversal radiation distribution.

5.9.2.2 Experiment # 2 (variations of liquid flow mass and tilt angle)

- It can be observed that while the liquid flow absorbs most of the heat, the vapor generation is inversely proportional to the liquid mass flow. This is so because the heat received by the liquid is used for two phenomena: *i*) raising the inlet temperature up to saturation conditions and *ii*) generating vapor. The larger the liquid mass flow is, the larger the amount of total heat that has to be used for the first phenomenon. Consequently, the saturation temperature is reached later downstream in the tube and there is less tube length for vapor generation. This emphasizes the need for reducing the inlet subcooling, especially for large liquids loads.
- For a given liquid mass-flow, the tilt angle varies the ratio between velocity and liquid cross-section, or equivalently, the void fraction $\varepsilon = A_v / A$.
- Although most of the wall heat is received by the liquid, for a given liquid mass flow rate, the small part received by the vapor increases for larger tilt angles. This indicates that the reduction of the liquid wet wall is more relevant than the increase in velocity.

Figure 5. 14 Steady-state solutions for experiment #2. a) The ratio between liquid and vapor mass flow rates at the upper end of the tube. b) Vapor production and heat ratio transient behavior.

According to these results, the amount of vapor production depends mainly on the liquid behavior (through the inlet conditions, its heating, and the saturation temperature) and on the total heat absorbed ($Q_{rad,tot} = Q_{wall}'' A_{wall}$) by the receiver. Therefore a functional relationship can be obtained using only these parameters.

$$\dot{m}_{v,z=0} = F(\dot{m}_{l,z=0}, T_{l,z=0}^{sat} - T_{l,z=0}, \dot{Q}_{rad,tot}, h_v^{sat} - h_l^{sat}, Cp_{l,z=0}) \quad (5.32)$$

Performing a dimensional analysis, Equation (5.32) can be reduced and expressed with dimensionless parameters, as Equation (5.33).

$$SR = \varphi(Bo, \Delta T^*) \quad (5.33)$$

Where the dimensionless groups are defined as:

$$SR = 100 \frac{|\dot{m}_{v,z=0}|}{|\dot{m}_{l,z=0}|} \quad \Delta T_{sat}^* = \frac{Cp_{l,z=0}(T_{sat}^p - T_{l,z=0})}{h_v^{sat} - h_l^{sat}} \quad Bo = \frac{\dot{Q}_{rad,tot}}{\dot{m}_{l,z=0}(h_v^{sat} - h_l^{sat})}$$

The functional relationship (5.33) is fitted with a bilinear regression model. The coefficients of the regression model are obtained with 496 simulations in which tilt angles, inlet pressures, liquid mass flows, and sub-coolings are varied. The correlation and its coefficients are:

$$SR = a_1 + a_2 \Delta T_{sat}^* + a_3 Bo \quad \text{Where} \quad \begin{cases} a_1 = 0.00291 \\ a_2 = -96.8849 \\ a_3 = 95.3345 \end{cases} \quad (5.34)$$

Figure 5. 15 Correlation verification.

This correlation was tested for different boiling numbers at different inlet sub coolings and pressure levels, having a maximum error of $\pm 5\%$, see Figure 5. 15.

5.9.2.3 Range of validity

The validity of this result is limited by the fact that heat has to reach the liquid with preference to be absorbed by the vapor; this means that the following parameters have to be small and have been checked above with the numeric value indicated:

- $Bo \leq 0.4$.
- $\bar{\alpha}_v / \alpha_l \leq 0.0188$
- $Cp_{v,z=0} \dot{m}_{v,z=0} / Cp_{l,z=0} \dot{m}_{l,z=0} \leq 0.281$

5.10 Conclusions

A 1-D numerical model has been developed for the transient simulation of heat and mass transfer in counter-current gravity-driven and gravity stratified liquid and vapor flows inside the receiver pipe of concentration linear solar collector, aiming at direct vapor production and separation. It has been performed using well-known methodologies and implementing further advances over current thermal 1-D modeling.

The method of solution allows in the entire domain the calculation of pressure, liquid cross-area (or height), mass flow rates and temperature for both streams (liquid and vapor). Additionally, this method determines axial and traverse distributions of the pipe wall temperature as well as mass transfer between both phases. With this model, the transient performance of solar linear receivers can be modeled with only a reduced set of input data. This tool can be of help to perform even more realistic analysis for the design and optimization of this kind of devices.

The test cases used for checking the algorithms show all the phenomena involved in the correct way and are coherent, demonstrating good performance.

The parametric analysis is performed using a transient numerical method in which the transversal heat irradiation profiles and inlet flow conditions were varied. According to the results, it can be concluded that:

- For realistic conditions, neither, angular irradiance profile or tilt angle affects the vapor production rate for a given inlet mass flow rate, being the heat transfer to the liquid the mechanism that controls the production.
- Under the framework analyzed, both the low heat capacities and thermal conductivities in the vapor, linked to the high transversal conduction inside the solid metal wall, make it possible for the solar heat to effectively reach the liquid flow, independently of the irradiation profile on the tube.
- Liquid inlet conditions, its specific heat, saturation temperature, and total radiation heat are sufficient to determine the vapor production rate, and the dimensionless group that describes the production rate is the Boiling number corrected

by a non-dimensional subcooling degree parameter. The developed correlation has a maximum error of $\pm 5\%$ for the conditions evaluated.

Nomenclature

a	Butcher table.
A	Area (m^2).
A_l	Liquid zone area (m^2).
A_{lv}	Liquid-vapor interphase area (m^2).
A_v	Vapour zone area (m^2).
A'	Area correction.
A^*	Area guess field.
B	Coefficient vector.
b	Butcher table quadrature vector.
B	Source term coefficient vector.
Bo	Boiling number.
Cp	Specific heat capacity ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
c	Butcher table stage location.
D	Diameter (m).
D_i	Pipe inner diameter (m).
D_o	Pipe outer diameter (m).
$\tilde{F}$	Space integrated slope function.
F	Friction factor.
G	Mass flux ($\text{kg} \cdot \text{s}^{-1} \cdot \text{m}^{-2}$).
g	Gravity acceleration constant ($= 9.81 \text{ m} \cdot \text{s}^{-1}$).
h	Specific enthalpy ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
h_l	Liquid phase specific enthalpy ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
h_v	Vapor phase phase specific enthalpy ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$).
K	Mass transfer coefficient.
L	Length (m).
$\dot{m}$	Mass flow ($\text{kg} \cdot \text{s}^{-1}$).
$\dot{m}'$	Mass flow correction.
$\dot{m}^*$	Mass flow guess.
$\dot{m}_{ip}$	Mass transfer through the interphase ($\text{kg} \cdot \text{s}^{-1}$).
$\dot{m}_{ip}'$	Mass transfer through the interphase per unit length ($\text{kg} \cdot \text{s}^{-1} \cdot \text{m}^{-1}$).
$\dot{m}_{ip}^{**}$	Mass transfer guess field.

N	Number of finite volumes.
Nu	Nusselt number.
$\hat{n}_i$	Outward unitary vector.
P	Wet perimeter (m).
p	Pressure (Pa).
p'	Pressure correction.
p^*	Pressure guess field.
$\dot{Q}''$	Heat flux per unit area ($\text{W} \cdot \text{m}^{-2}$).
$\dot{Q}_{rad}''$	Solar radiation mass flux per unite area ($\text{W} \cdot \text{m}^{-2}$).
r	Radius (m).
S	Surface (m^2).
S_c	Independent source term coefficient vector.
S_p	Implicit source term coefficient vector.
S_R	Slip ratio.
t	Time (s).
T	Temperature ($^{\circ}\text{C}$).
U	Superficial velocity ($\text{m} \cdot \text{s}^{-1}$).
u	Velocity, phase velocity ($\text{m} \cdot \text{s}^{-1}$).
V	Volume (m^3) ($\text{m}^3 \cdot \text{kg}^{-1}$).
x	Thermodynamic Quality ($\text{kg} \cdot \text{kg}^{-1}$).
z	Axial coordinate (m).

Greek Letters

α	Convective coefficient ($\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$).
β	Inclination angle.
Δ	Finite difference.
$\Delta \dot{m}_{ip}$	Mass transfer correction.
δ_l	Liquid film height (m).
ε	Fluid zone integer function.
θ	Angular coordinate.
λ	Thermal conductivity ($\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$).
ρ	Material density ($\text{kg} \cdot \text{m}^{-3}$).
τ	Shear stress.
ψ	Dependent variable vector.
φ	Liquid film angle.

Subscripts

0	Initial state. Inlet condition.
W, P, Ee, w, e	Cardinal system index notation.

l	Liquid.
v	Vapor.
H	Hydraulic.
i,j	Indexes.
k	Fluid phase index.
ip	Interphase.
w	Wall location.
$wall$	Wall.
r,s	Runge-Kutta indexes.
sat	Saturation.

Superscripts

$'$	Per unit length.
$''$	Per unit area.
$()$	Time stage.
$*$	Guess value.

Acronymous

BWR	Boiling water reactor.
BC	Boundary conditions.
CAPEX	Capital expense
DSG	Direct steam generator
ESDIRK	Explicit first stage diagonal implicit Runge-Kutta method.
MOL	Method of lines
OPEX	Operational expenditures.
PDO	Pressure drop oscillation.
PTC	Parabolic trough concentrator
1-D	One dimensional

References

- Al-Arabi, M. (1982). Turbulent Heat Transfer in the Entrance Region of a Tube. *Heat Transfer Engineering*, 3, 76–83. <https://doi.org/10.1080/01457638108939586>
- Alexander, R. (2003). Design and Implementation of DIRK Integrators for Stiff Systems. *Applied Numerical Mathematics*, 46, 1–17. [https://doi.org/10.1016/S0168-9274\(03\)00012-6](https://doi.org/10.1016/S0168-9274(03)00012-6)

Alguacil, M., Prieto, C., Rodriguez, A., & Lohr, J. (2014). Direct Steam Generation in Parabolic Trough Collectors. *Energy Procedia*, 49, 21–29. <https://doi.org/10.1016/j.egypro.2014.03.003>

Andreussi, P., & Persen, L. N. (1987). Stratified Gas-Liquid Flow in Downwardly inclined Pipes. *International Journal of Multiphase Flow*, 13(4), 565–575. [https://doi.org/10.1016/0301-9322\(87\)90022-X](https://doi.org/10.1016/0301-9322(87)90022-X)

Biencinto, M., González, L., & Valenzuela, L. (2016). A Quasi-Dynamic Simulation Model for Direct Steam Generation in Parabolic Troughs Using TRNSYS. *Applied Energy*, 161, 133–142. <https://doi.org/10.1016/j.apenergy.2015.10.001>

Coccia, G., Di Nicola, G., & Hidalgo, A. (2016). Parabolic Trough collector for Prototypes for Low- Temperature Process Heat. Springer. <https://doi.org/10.1007/978-3-319-27084-5>

Gadonneix, P., Kim, Y. D., Meyers, K., Ward, G., & Frei, C. (2013). World Energy Resources: 2013 Survey.

García-valladares, O., & Velázquez, N. (2009). Numerical Simulation of Parabolic Trough Solar Collector : Improvement Using Counter Flow Concentric Circular Heat Exchangers. *International Journal of Heat and Mass Transfer*, 52, 597–609. <https://doi.org/10.1016/j.ijheatmasstransfer.2008.08.004>

Gnielinski, V. (1976). New Equations for Heat and Mass Transfer in Turbulent Pipe and Channel Flow. *Int. Chem. Eng.*, 16(2), 359–368.

Hanratty, T. J., & Andritsos, N. (1984). Effect of Pipe Diameter on Stratified Flow in Horizontal Pipes.

Jebasingh, V. K., & Herbert, G. M. J. (2016). A Review of Solar Parabolic Trough Collector. *Renewable and Sustainable Energy Reviews*, 54, 1085–1091. <https://doi.org/10.1016/j.rser.2015.10.043>

Kalogirou, S. A. (2004). Solar Thermal Collectors and Applications. *Progress in Energy and Combustion Science*, 30, 231–295. <https://doi.org/10.1016/j.pecs.2004.02.001>

Kalogirou, S. A. (2012). A Detailed Thermal Model of a Parabolic Trough Collector Receiver. *Energy*, 48(1), 298–306. <https://doi.org/10.1016/j.energy.2012.06.023>

Kandlikar, S. G. (1999). Handbook of Phase Change: Boiling and Condensation. Taylor & Francis.

Khanna, S., Singh, S., & Kedare, S. B. (2014). Effect of Angle of Incidence of Sun Rays on the Bending of Absorber Tube of Solar Parabolic Trough Concentrator. *Energy Procedia*, 48, 123–129. <https://doi.org/10.1016/j.egypro.2014.02.015>

Lecuona-Neumann, A., Rosner, M., & Ventas-Garzón, R. (2016). Transversal Temperature Profiles of Two-Phase Stratified Flow in the Receiver Tube of a Solar Linear Concentrator. Simplified Analysis. In International Solar Energy Society (ISES). EuroSun 2016. Palma de Mallorca, Spain. <https://doi.org/10.18086/eurosun.2016.04.17>

Lecuona, A., Ventas, R., Vereda, C., & Legrand, M. (2016). Linear Tube Solar Receiver as Stratified Flow Vapor Generator/Separator for Absorption Machines using NH₃/LiNO₃. In 11th EUROSUN 2016 ISES conference proceedings. Palma (Mallorca). Spain.

Murphy, L. M., & May, E. K. (1983). Performance Benefits of the Direct Generation of Steam in Line-Focus Solar Collectors. *Journal of Solar Energy Engineering, Transactions of the ASME*, 105, 126–133. <https://doi.org/10.1115/1.3266355>

Nallusamy, N., Sivaram, P. M., & Suresh, M. (2017). Numerical Modelling of Solar Parabolic Trough Receiver Employed for Thermal Energy Storage System. *Journal of Clean Energy Technologies*, 5(2), 107–113. <https://doi.org/10.18178/jocet.2017.5.2.353>

Natan, S., Barnea, D., & Taitel, Y. (2003). Direct Steam Generation in Parallel Pipes. *International Journal of Multiphase Flow*, 29, 1669–1683. <https://doi.org/10.1016/j.ijmultiphaseflow.2003.07.002>

Oberkampf, W. L., & Trucano, T. G. (2002). Verification and Validation in Computational Fluid Dynamics. *Progress in Aerospace Sciences*, 38, 209–272. [https://doi.org/10.1016/S0376-0421\(02\)00005-2](https://doi.org/10.1016/S0376-0421(02)00005-2)

Patankar, S. V. (1980). *Numerical Heat Transfer and Fluid Flow*. Hemisphere Publishing Corporation.

Patankar, S. V., & Spalding, D. B. (1972). A Calculation Procedure for Heat, Mass and Momentum Transfer in Three-Dimensional Parabolic Flows. *International Journal of Heat and Mass Transfer*, 15, 1787–1806. [https://doi.org/10.1016/0017-9310\(72\)90054-3](https://doi.org/10.1016/0017-9310(72)90054-3)

Press, W. H., Teukolsky, S. A., Vetterling, W. T., & Flannery, B. P. (2007). *Numerical Recipes: The Art of Scientific Computing* (Third Ed). Cambridge University Press.

Price, H., Lüpfert, E., Kearney, D., Zarza, E., Cohen, G., Gee, R., & Mahoney, R. (2002). Advances in Parabolic Trough Solar Power Technology. *Journal of Solar Engineering*, 124(May), 109–125. <https://doi.org/10.1115/1.1467922>

Rohsenow, W. M., Harnett, J. P., & Cho, Y. I. (1998). *Handbook of Heat Transfer*, Third Edition ed., New York (Third Edit). New York: McGraw Hill.

Serrano-aguilera, J. J., Valenzuela, L., & Parras, L. (2014). Thermal 3D Model for Direct Solar Steam Generation Under Superheated Conditions. *Applied Energy*, 132, 370–382. <https://doi.org/10.1016/j.apenergy.2014.07.035>

Sigalés, B. (2003). *Transferencia de Calor Técnica*. Barcelona: Editorial Reverté.

Sivaram, P. M., Nallusamy, N., & Suresh, M. (2016). Experimental and numerical investigation on solar parabolic trough collector integrated with thermal energy storage unit. *International Journal of Energy Research*, 40(11), 1564–1575. <https://doi.org/10.1002/er.3544>

Stenning, A. H. (1964). Instabilities in the Flow of a Boiling Liquid. *Journal of Basic Engineering*, 86(2), 213–217. <https://doi.org/10.1115/1.3653038>

Taitel Y., & Dukler A. (1976). A model for predicting flow regime transitions in horizontal and near horizontal gas-liquid ow. *AIChE Journal*.

Tian, Y., & Zhao, C. Y. (2013). A Review of Solar Collectors and Thermal Energy Storage in Solar Thermal Applications. *Applied Energy*, 104, 538–553. <https://doi.org/10.1016/j.apenergy.2012.11.051>

Tshuva, M., Barnea, D., & Taitel, Y. (1999). Two-phase Flow in Inclined Parallel Pipes. *International Journal of Multiphase Flow*, 25, 1491–1503. [https://doi.org/10.1016/S0301-9322\(99\)00048-8](https://doi.org/10.1016/S0301-9322(99)00048-8)

Vasquez, R., Demirkaya, G., Goswami, D. Y., Stefanakos, E., & Rahman, M. M. (2011). Heat Transfer Analysis of Parabolic Trough Solar Receiver. *Applied Energy*, 88(12), 5097–5110. <https://doi.org/10.1016/j.apenergy.2011.07.012>

Wallis, G. B. (1969). *One-Dimensional Two-Phase Flow*. McGraw Hill.

Conclusions and Future Work

6.1 Conclusions

The research presented in this thesis aims at increasing the knowledge on 1-D transient numerical simulation in heat exchangers under the distributed parameter approach. Particular emphasis has been put on two-phase flow applications, and for that purpose, two models were used, the homogeneous flow model and quasi-homogeneous flow model.

In the first part of the thesis, this work offers a comprehensive review of 1-D transient modeling on heat exchangers. Models for single-phase and more specifically for two-phase flows, jointly with their closure relationships are offered. In this way, the available information over this subject can be easily consulted and the reader can revisit some important concepts used throughout the thesis.

The central part of this thesis develops an original numerical method capable of coping with fast phase change events. Therefore, an exhaustive discussion of numerical background is offered. We show that a combination of the method of lines with the finite volume method, jointly with the implicit Runge-Kutta method, are suitable to cope with fast transients. More specifically, we demonstrate that the Euler Backward (EB) method, the Alexander (ES33a) and Svortsov (ES54) method, are L-Stable methods, ideals for stiff differential equations, present in instant boiling or condensation processes. With this, the work increases the catalog of numerical methods used in 1-D transient simulations applied to heat exchangers.

With these ideas, the thesis develops the original numerical procedure based on the explicit first stage diagonally implicit Runge- Kutta (ESDIRK) method. This is combined with the first order UPWIND method to deal with the non-linear terms in the equations and the semi-implicit pressure linked equations (SIMPLE) algorithm to calculate pressure fields. This numerical procedure has been subjected to many validations and verification

tests. Both, steady-state and transient-state conditions are implemented, using experimental and numerical published data. In all cases, the tests show good agreement, revealing that the methodology satisfactorily reproduces the physics in boiling processes. It also indicates, that the usage of high order schemes is suitable for fast transients, like input periodic square disturbances inputs, specifically for high frequencies. Moreover, from a computational point of view, the high order schemes present some advantages with respect to the classic Euler backward method: low computational cost and high order of accuracy.

The novel numerical method has been applied for two different topologies: single pipes heat exchangers and parabolic trough solar collectors with receiving tubes. In the first case, the method reproduces satisfactorily a two-phase flow static instability, opening a new field for its application. For the second case, the methods allows for developing model for stratified gravity-driven stratified two-phase flow of industrial interest for developing new absorption machines of direct solar vapor generation. This model has been applied for relatively thin liquid film layouts applied in parabolic trough solar collectors. One relevant feature of this modeling methodology comes from a numerical point of view: the mass transfer algorithm presents an outstanding performance; the correction to be applied is monotonically decreasing when iterating and it is lower bounded. This makes the algorithm linearly convergent with a calculated mean order of convergence of 0.901 for the proposed problem. The effect of the collector tilt angle, irradiation profile variation and inlet liquid mass flow was also studied. The results show that the main parameter that controls the vapor production is the inlet mass flow rate. Finally, a correlation that is based on these results is offered, showing a mean error of $\pm 5\%$.

6.2 Further works

Future research work could include:

- Enhancing the convergence speed, including a multistep algorithm, with detection of fast transient.
- To apply the numerical methodology to more complex substances.

- To combine the theory of approximate Riemann solvers with implicit numerical methods, to study faster transients.
- To apply the developed methodology to a whole absorption machine of chapter V, and impose operation transients and verify its applicability in terms of accuracy and computational cost.
- Design experiments for gravity-driven flows, and validate the model with experimental data, complementing the numerical verification.

Scalars, Vectors and, Tensors

A.1 Preliminaries

A scalar is a physical quantity that can be represented by a single magnitude or dimension number. Examples of scalars are pressure, temperature, enthalpy, among others. Mathematically, a scalar can vary in space, hence for any arbitrary space $\bar{r} = x_1, x_2, x_3$ it can be written as:

$$\phi = \phi(x_1, x_2, x_3) = \phi(\bar{r}) \quad (\text{A.1})$$

A vector is a mathematical tool that lets tracking two pieces of information (magnitude and direction) for any physical quantity like velocity or force for example. In a 3 dimensional space (like in scalar quantities) a vector is defined with three magnitudes and their respective direction defined by unitary vectors.

$$\bar{u} = u_1 \hat{e}_1 + u_2 \hat{e}_2 + u_3 \hat{e}_3 = \sum_{i=1}^3 u_i \hat{e}_i \quad (\text{A.2})$$

Generally, every component can vary in space and time.

$$\bar{u} = \sum_{i=1}^3 u_i(t, x_j) \hat{e}_i \quad \text{for } j = 1, 2, 3 \quad (\text{A.3})$$

The unitary vectors are defined as:

$$\hat{e}_i = \frac{1}{\|\bar{r}\|} \frac{\partial \bar{r}}{\partial x_j} = \begin{bmatrix} \hat{e}_1 \\ \hat{e}_2 \\ \hat{e}_3 \end{bmatrix} = \frac{1}{\sqrt{x_1^2 + x_2^2 + x_3^2}} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad (\text{A.4})$$

Figure A. 1) 1 Position ($\bar{r}$) and velocity ($\bar{u}$) vector in a Cartesian coordinate system.

The notion of a vector can be extended to a more general mathematical definition called tensor. In that sense a scalar is tensor of rank 0 and vectors are tensors of rank 1. Following the rules of number of directions according to their rank, a second-order tensor must have two directions for every magnitude. This means that with a second-order tensor we have information not only and magnitude and direction of the vector but also the plane in which that vector acts. An example of second-order tensors is stress and deformations of any material.

Figure A. 2 Stress components in a Cartesian coordinates system

$$T = \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{pmatrix} = \sum_{i=1}^3 \sum_{j=1}^3 T_{ij} \hat{e}_i \hat{e}_j \quad (\text{A.5})$$

A.2 Einstein notation (indexing)

$$\bar{u} = u_1 \hat{e}_1 + u_2 \hat{e}_2 + u_3 \hat{e}_3 + \cdots + u_n \hat{e}_n \quad (\text{A.6})$$

The same can be expressed by a finite sum as:

$$\bar{u} = \sum_{i=1}^n u_i \hat{e}_i \quad (\text{A.7})$$

In Einstein notation, the summation operator is omitted, hence:

$$\bar{u} = u_i \hat{e}_i \quad (\text{A.8})$$

For tensorial quantities the summation is made over the repeated index in the form:

$$A_{ij} b_j = A_{i1} b_1 + A_{i2} b_2 + A_{i3} b_3 + \cdots + A_{in} b_n \quad (\text{A.9})$$

A.3 Symbolic notation

Either way, Einstein notation can be further simplified, omitting the use of sub-index that indicates the direction of any quantity. In this way, the vector or tensor quantity can be written in a more general and compact form not being restricted to any specific coordinate system. For this notation the quantity is written in bold letters, for example:

$$\mathbf{u} = u_i \hat{e}_i \quad (\text{A.10})$$

$$\mathbf{T} = T_{ij} \hat{e}_i \hat{e}_j \quad (\text{A.11})$$

In Table A. 1 some common differential operators written in vectorial, indexing, and symbolic are summarized.

Table A. 1 Summary of notations for tensors and most frequently used differential operators

		Regular notation	Indicial notation	Symbolic notation
Vector		$u_1 \hat{e}_1 + u_2 \hat{e}_2 + u_3 \hat{e}_3$	u_i	$\mathbf{u}$
Tensor		$T_{11} \hat{e}_1 \hat{e}_1 + T_{12} \hat{e}_1 \hat{e}_2 + T_{13} \hat{e}_1 \hat{e}_3 +$ $T_{21} \hat{e}_2 \hat{e}_1 + T_{22} \hat{e}_2 \hat{e}_2 + T_{23} \hat{e}_2 \hat{e}_3 +$ $T_{31} \hat{e}_3 \hat{e}_1 + T_{32} \hat{e}_3 \hat{e}_2 + T_{33} \hat{e}_3 \hat{e}_3$	T_{ij}	$\mathbb{T}$
Scalar	Gradient	$\frac{\partial \phi}{\partial x_1} \hat{e}_1 + \frac{\partial \phi}{\partial x_2} \hat{e}_2 + \frac{\partial \phi}{\partial x_3} \hat{e}_3$	$\frac{\partial \phi}{\partial x_i}$	$\nabla \phi$
	Laplacian	$\frac{\partial^2 \phi}{\partial x_1^2} \hat{e}_1 + \frac{\partial^2 \phi}{\partial x_2^2} \hat{e}_2 + \frac{\partial^2 \phi}{\partial x_3^2} \hat{e}_3$	$\frac{\partial^2 \phi}{\partial x_i^2}$	$\nabla^2 \phi$ or $\nabla \cdot \nabla \phi$
Vector	Gradient	$\frac{\partial u_1}{\partial x_1} \hat{e}_1 \hat{e}_1 + \frac{\partial u_2}{\partial x_1} \hat{e}_1 \hat{e}_2 + \frac{\partial u_3}{\partial x_1} \hat{e}_1 \hat{e}_3 +$ $\frac{\partial u_1}{\partial x_2} \hat{e}_2 \hat{e}_1 + \frac{\partial u_2}{\partial x_2} \hat{e}_2 \hat{e}_2 + \frac{\partial u_3}{\partial x_2} \hat{e}_2 \hat{e}_3 +$ $\frac{\partial u_1}{\partial x_3} \hat{e}_3 \hat{e}_1 + \frac{\partial u_2}{\partial x_3} \hat{e}_3 \hat{e}_2 + \frac{\partial u_3}{\partial x_3} \hat{e}_3 \hat{e}_3$	$\frac{\partial u_i}{\partial x_j}$	$\nabla \mathbf{u}$
	Divergence	$\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}$	$\frac{\partial u_i}{\partial x_i}$	$\nabla \cdot \mathbf{u}$
	Laplacian	$\left(\frac{\partial^2 u_1}{\partial x_1^2} + \frac{\partial^2 u_1}{\partial x_2^2} + \frac{\partial^2 u_1}{\partial x_3^2} \right) \hat{e}_1 +$ $\left(\frac{\partial^2 u_2}{\partial x_1^2} + \frac{\partial^2 u_2}{\partial x_2^2} + \frac{\partial^2 u_2}{\partial x_3^2} \right) \hat{e}_2 +$ $\left(\frac{\partial^2 u_3}{\partial x_1^2} + \frac{\partial^2 u_3}{\partial x_2^2} + \frac{\partial^2 u_3}{\partial x_3^2} \right) \hat{e}_3$	$\frac{\partial^2 u_i}{\partial x_j^2}$	$\nabla^2 \mathbf{u}$ or $\nabla \cdot \nabla \mathbf{u}$
2nd Order Tensor	Divergence	$\left(\frac{\partial T_{11}}{\partial x_1} + \frac{\partial T_{21}}{\partial x_2} + \frac{\partial T_{31}}{\partial x_3} \right) \hat{e}_1 +$ $\left(\frac{\partial T_{12}}{\partial x_1} + \frac{\partial T_{22}}{\partial x_2} + \frac{\partial T_{32}}{\partial x_3} \right) \hat{e}_2 +$ $\left(\frac{\partial T_{13}}{\partial x_1} + \frac{\partial T_{23}}{\partial x_2} + \frac{\partial T_{33}}{\partial x_3} \right) \hat{e}_3$	$\frac{\partial T_{ij}}{\partial x_i}$	$\nabla \cdot \mathbb{T}$

References

Aris, R. (1989). *Vectors, Tensors and the Basic Equations of Fluid Dynamics*. Dover Publications Inc.

Cox, W. (1998). *Vector Calculus*. Elsevier.

Two-Phase Flows

B.1 Preliminaries

In a liquid- gas stream, the liquid (dense) phases can be denoted with subscript l , and v will be used to denote vapor (gas or light phase) The total mass flow is $\dot{m}_t$, hence making a mass balance and assuming steady-state conditions $\dot{m}_t$ is:

$$\dot{m}_t = \dot{m}_l + \dot{m}_v \quad (\text{B.1})$$

$$\dot{m}_l = \rho_l u_l A_l \quad (\text{B.2})$$

$$\dot{m}_v = \rho_v u_v A_v \quad (\text{B.3})$$

Here A_l and A_v are the total areas occupied by each phase on a specific cross-section, see Fig B.1.

Figure B. 1 Cross-section of a two-phase flow stream

Knowing both areas and mass flows, Equations (B.2) and (B.3) can be turned around defining phase “real” mean velocities, as:

$$u_l = \frac{\dot{m}_l}{\rho_l A_l} \quad (\text{B.4})$$

$$u_v = \frac{\dot{m}_v}{\rho_v A_v} \quad (\text{B.5})$$

These last definitions represent the real mean velocity; however, in a two-phase flow stream it is difficult to determine the total area occupied by each phase. Hence, a new velocity known as superficial velocity (U) is introduced. This velocity defines the velocity that each phase would have if the entire volume is occupied for each phase.

$$U_l = \frac{\dot{m}_l}{\rho_l A} \quad (\text{B.6})$$

$$U_v = \frac{\dot{m}_v}{\rho_v A} \quad (\text{B.7})$$

Both definitions of velocity are also related. Dividing the corresponding definitions for each phase one will obtain:

$$U_l = \varepsilon_l u_l \quad (\text{B.8})$$

$$U_v = \varepsilon_v u_v \quad (\text{B.9})$$

In the above equations, the void fraction (ε) is introduced. Void fraction is the proportion of gas in a specific volume (cross area section or length) respect to the total sample length, see Annex C for its formal definition. On another order of ideas, the mass fraction or quality is defined as the fraction of gas contained in a specific volume of fluid. From these definitions, it follows that:

$$x = \frac{\dot{m}_v}{\dot{m}_v + \dot{m}_l} = \frac{\dot{m}_v}{\dot{m}_t} \quad (\text{B.10})$$

And as a consequence:

$$\dot{m}_v = x \dot{m}_t \quad (\text{B.11})$$

$$\dot{m}_l = (1 - x) \dot{m}_t \quad (\text{B.12})$$

Another useful quantity is the relation of the gas and liquid phase velocities, known as the slip ratio (S_R).

$$S_R = \frac{u_v}{u_l} \quad (\text{B.13})$$

It had already be shown that each phase mass flow can be calculated knowing the quality and total mass flow (Equations (B.11) and (B.12)) and this, in turn, had be equated with the respective velocity. Then, if we combine (B.6) to (B.9) with (B.11) and (B.12) recalling the slip ratio definition (Equation (B.13)), we find an equation relating the void fraction, saturated densities, and phase velocity:

$$\varepsilon = \frac{x}{x + (1 - x) S_R \frac{\rho_v}{\rho_l}} \quad (\text{B.14})$$

When $S_R = 1$, the flow is called homogeneous and the resulting void fraction is called homogeneous void fraction (ε_H). Note, that the last definition of the void fraction depends not only on thermodynamic properties but also on velocities; therefore, the void fraction is not a thermodynamic property.

Following the definitions of total mass flow, void fraction, and quality, we can find an equation for a two-phase mixture (apparent) density. This mixture density is not a mass-weighted density, as happens inside the two-phase region but a mean average density that obviously takes into account each phase density but also its velocity; therefore, it can be seen as a local instant density.

$$\rho_{TP} = \varepsilon \rho_g + (1 - \varepsilon) \rho_l \quad (\text{B.15})$$

Finally, if we assume that both phases (for single component flows) are in thermodynamic equilibrium, one can relate quality with specific thermodynamic variables at the saturated state at constant pressure or temperature. From this way two-phase enthalpy is:

$$h_{TP} = x h_v + (1 - x) h_l \quad (\text{B.16})$$

B.2 Volumetric averaging, rules and theorems

Let's consider Figure B.2 in which inside a fixed control volume Ω (of volume V) is filled by phases l and part of phase k . The part of phase k that is included in Ω has a volume V_k (where $V_k = \Omega \cap \Omega_k$), both volumes are separated by a continuous interphase of area S_k with outward unitary vector $\hat{n}_k$ (pointing from k to l). The volume V_k contains any scalar, vectorial, or tensorial quantity ψ_k . If ψ_k is continuous and smooth inside V_k , ψ_k can be averaged inside V or V_k like:

$$\tilde{\psi}_k = \frac{1}{V_k} \int_{V_k} \psi_k dV \quad (\text{Intrinsic}) \quad (\text{B.17}) \quad \langle \psi_k \rangle = \frac{1}{V} \int_{V_k} \psi_k dV \quad (\text{Total}) \quad (\text{B.18})$$

Figure B. 2 Volume averaging schematic representation

These two averages are connected with the volume or void fraction ($\varepsilon_k = V_k/V$)

like:

$$\tilde{\psi}_k = \frac{1}{V_k} \int_{V_k} \psi dV = \frac{V}{V} \frac{1}{V_k} \int_{V_k} \psi dV = \frac{\frac{1}{V} \int_{V_k} \psi dV}{\frac{V}{V_k}}$$

$$\Rightarrow \langle \psi_k \rangle = \varepsilon_k \tilde{\psi}_k \quad (\text{B.19})$$

The averaging process took place around an arbitrary point x_i inside the flowing bulk, and n different phases can be contained in V . Therefore, the sum of the individual phases volumes must be equal to V .

$$V = \sum_{k=1}^n V_k \quad (\text{B.20})$$

And as a consequence.

$$\sum_{k=1}^n \varepsilon_k = 1 \quad (\text{B.21})$$

B.3 Averaging rules

The averaging procedure satisfies the following rules (Drew, 1983).

$$\text{Reynold's rule} \left| \begin{array}{l} \langle f + g \rangle = \langle f \rangle + \langle g \rangle \\ \langle cf \rangle = c \langle f \rangle \quad c \in \mathbb{R} \\ \langle \langle f \rangle g \rangle = \langle f \rangle \langle g \rangle \end{array} \right.$$

Additionally, for f be any scalar, vectorial or tensorial quantity, (Whitaker, 1969) and (Slattery, 1972) developed theorems for averaged derivatives.

$$\langle \nabla f \rangle = \nabla \langle f \rangle + \frac{1}{V} \int_{S_k} f \cdot \hat{n}_j dS \quad (\text{B.22})$$

$$\langle \nabla \cdot f \rangle = \nabla \cdot \langle f \rangle + \frac{1}{V} \int_{S_k} f \cdot \hat{n}_j dS \quad (\text{B.23})$$

$$\left\langle \frac{\partial f}{\partial t} \right\rangle = \frac{\partial}{\partial t} \langle f \rangle - \frac{1}{V} \int_{S_k} f U_A \cdot \hat{n}_j dS \quad (\text{B.24})$$

B.4 Volume Average equations and interfacial balance

For a single-phase flow, the equations of mass, momentum are:

$$\left. \begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\ \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= \nabla \cdot \mathbb{T} + \rho \phi \\ \frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho \mathbf{u} E) &= \nabla \cdot (\mathbb{T} \cdot \mathbf{u} + \dot{\mathbf{Q}}''') + \rho \left(\phi \cdot \mathbf{u} + \frac{\dot{q}'''}{\rho} \right) \end{aligned} \right\} \quad (\text{B.25})$$

Averaging equations (B.25) using volumetric average reads:

$$\left. \begin{aligned} \left\langle \frac{\partial \rho}{\partial t} \right\rangle + \langle \nabla \cdot (\rho \mathbf{u}) \rangle &= 0 \\ \left\langle \frac{\partial \rho \mathbf{u}}{\partial t} \right\rangle + \langle \nabla \cdot (\rho \mathbf{u} \mathbf{u}) \rangle &= \langle \nabla \cdot \mathbb{T} \rangle + \langle \rho \phi \rangle \\ \left\langle \frac{\partial \rho E}{\partial t} \right\rangle + \langle \nabla \cdot (\rho \mathbf{u} E) \rangle &= \langle \nabla \cdot (\mathbb{T} \cdot \mathbf{u} + \dot{\mathbf{Q}}''') \rangle + \left\langle \rho \left(\phi \cdot \mathbf{u} + \frac{\dot{q}'''}{\rho} \right) \right\rangle \end{aligned} \right\} \quad (\text{B.26})$$

and keeping in mind the averaging theorems (B.22) to (B.25)

$$\left. \begin{aligned}
& \frac{\partial \langle \rho \rangle}{\partial t} + \nabla \cdot \langle \rho \mathbf{u} \rangle - \frac{1}{V} \int_{S_k} \rho \mathbf{U}_A \cdot \hat{n} dS + \frac{1}{V} \int_{S_k} \rho \mathbf{u} \cdot \hat{n} dS = 0 \\
& \frac{\partial \langle \rho \mathbf{u} \rangle}{\partial t} + \nabla \cdot \langle \rho \mathbf{u} \mathbf{u} \rangle - \frac{1}{V} \int_{S_k} \rho \mathbf{U}_A \cdot \hat{n} dS + \frac{1}{V} \int_{S_k} \rho \mathbf{u} \mathbf{u} \cdot \hat{n} dS = \\
& \quad \nabla \cdot \langle \mathbb{T} \rangle + \langle \rho \phi \rangle + \frac{1}{V} \int_{S_k} \mathbb{T} \cdot \hat{n} dS \\
& \frac{\partial \langle \rho E \rangle}{\partial t} + \nabla \cdot \langle \rho \mathbf{u} E \rangle - \frac{1}{V} \int_{S_k} \rho E \mathbf{U}_A \cdot \hat{n} dS + \frac{1}{V} \int_{S_k} \rho E \mathbf{u} \cdot \hat{n} dS = \\
& \quad \nabla \cdot \langle \mathbb{T} \cdot \mathbf{u} + \dot{\mathbf{Q}}''' \rangle + \frac{1}{V} \int_{S_k} (\mathbb{T} \cdot \mathbf{u} + \dot{\mathbf{Q}}''') \cdot \hat{n} dS + \left\langle \rho \left(\phi \cdot \mathbf{u} + \frac{\dot{q}'''}{\rho} \right) \right\rangle
\end{aligned} \right\} \quad (\text{B.27})$$

Rearranging terms and after some algebra equations (B.27) one yields:

$$\left. \begin{aligned}
& \frac{\partial \langle \rho \rangle}{\partial t} + \nabla \cdot \langle \rho \mathbf{u} \rangle = \Gamma_k \\
& \frac{\partial \langle \rho \mathbf{u} \rangle}{\partial t} + \nabla \cdot \langle \rho \mathbf{u} \mathbf{u} \rangle = \nabla \cdot \langle \mathbb{T} \rangle + \langle \rho \phi \rangle + \mathbf{M}_k^\Gamma \\
& \frac{\partial \langle \rho E \rangle}{\partial t} + \nabla \cdot \langle \rho \mathbf{u} E \rangle = \nabla \cdot \langle \mathbb{T} \cdot \mathbf{u} + \dot{\mathbf{Q}}''' \rangle + \left\langle \rho \left(\phi \cdot \mathbf{u} + \frac{\dot{q}'''}{\rho} \right) \right\rangle + \mathbf{Q}_k^\Gamma
\end{aligned} \right\} \quad (\text{B.28})$$

Where,

Figure B. 3 Table Interfacial balances and transfer terms

Equation	Interfacial Transfer $\Gamma_{k,i}$	Interfacial Balance
Mass	$\Gamma_k = \underbrace{\frac{1}{V} \int_{S_k} \rho (\mathbf{u}_A - \mathbf{u}) \cdot \hat{n} dS}_{\text{Interphacial Mass transfer}}$	$\sum_k \Gamma_k = 0$
Mommentum	$\mathbf{M}_k^\Gamma = \underbrace{\frac{1}{V} \int_{S_k} \rho \mathbf{u} (\mathbf{u}_A - \mathbf{u}) \cdot \hat{n} dS}_{\text{Interfacial Momentum Transfer}} + \underbrace{\frac{1}{V} \int_{S_k} \mathbb{T} \cdot \hat{n}_k dS}_{\text{Interfacial Stress}}$	$\sum_k \mathbf{M}_k^\Gamma = 0$
Energy	$\mathbf{Q}_k^\Gamma = \underbrace{\frac{1}{V} \int_{S_k} \rho E (\mathbf{u}_A - \mathbf{u}) \cdot \hat{n} dS}_{\text{Interfacial Energy Transfer}} + \underbrace{\frac{1}{V} \int_{S_k} (\mathbb{T} \cdot \mathbf{u} + \dot{\mathbf{Q}}''') \cdot \hat{n} dS}_{\text{Interfacial Heat}}$	$\sum_k \mathbf{Q}_k^\Gamma = 0$

Here $\mathbb{T}_{ij}$ and $\mathbb{I}$ stands for the total stress and identity tensors ($\mathbb{T}_{ij} = -p\mathbb{I} + \sigma_{ij}$).

B.5 One dimensional homogeneous flow model (HFM)

The homogeneous flow model is based on the assumption that both phase velocities are equal.

B.5.1 Mass conservation

To obtain the mass conservation equation, first, a mass balance is made for each phase separately on V and then are volume averaged.

$$\begin{aligned}\frac{\partial \langle \rho_v \rangle}{\partial t} + \frac{\partial}{\partial z} \langle \rho_v u_v \rangle &= \Gamma_v \\ \frac{\partial \langle \rho_l \rangle}{\partial t} + \frac{\partial}{\partial z} \langle \rho_l u_l \rangle &= \Gamma_l\end{aligned}\tag{B.29}$$

Adding both equations and keeping in mind that interfacial mass balance must be fulfilled ($\Gamma_l = -\Gamma_v$) we have.

$$\begin{aligned}\frac{\partial}{\partial t} \langle \rho_v \rangle + \langle \rho_l \rangle + \frac{\partial}{\partial z} \langle \rho_v u_v \rangle + \langle \rho_l u_l \rangle &= 0 \\ \Rightarrow \frac{\partial}{\partial t} (\varepsilon \tilde{\rho}_v + (1 - \varepsilon) \tilde{\rho}_l) + \frac{\partial}{\partial z} (\varepsilon \tilde{\rho}_v \tilde{u}_v + (1 - \varepsilon) \tilde{\rho}_l \tilde{u}_l) &= 0\end{aligned}\tag{B.30}$$

By the assumption of homogeneous flow, both velocities are equal and mixture density can be calculated as $\rho_{TP} = \varepsilon \rho_v + (1 - \varepsilon) \rho_l$; therefore, multiplying the last equation by the cross-section area (A) equation (B.30) can be reduced to:

$$A \frac{\partial \rho_{TP}}{\partial t} + \frac{\partial \dot{m}}{\partial z} = 0\tag{B.31}$$

Dividing (B.31) by the cross-section area A , one obtains the equation in per volume unit.

$$\frac{\partial \rho_{TP}}{\partial t} + \frac{\partial G}{\partial z} = 0\tag{B.32}$$

B.5.2 Momentum conservation

Similarly, the momentum equation can be obtained as:

$$\begin{aligned} \frac{\partial \langle \rho_v u_v \rangle}{\partial t} + \frac{\partial}{\partial z} \langle \rho_v u_v u_v \rangle &= -\frac{\partial p_v}{\partial z} + \left\langle \frac{\partial p_v}{\partial z} \right\rangle_{fr}''' + \langle \rho_v g \rangle + M_v \\ \frac{\partial \langle \rho_l u_l \rangle}{\partial t} + \frac{\partial}{\partial z} \langle \rho_l u_l u_l \rangle &= -\frac{\partial p_l}{\partial z} + \left\langle \frac{\partial p_l}{\partial z} \right\rangle_{fr}''' + \langle \rho_l g \rangle + M_l \end{aligned} \quad (B.33)$$

$$\begin{aligned} \frac{\partial \langle \rho_v u_v \rangle + \langle \rho_l u_l \rangle}{\partial t} + \frac{\partial}{\partial z} \langle \rho_v u_v u_v \rangle + \langle \rho_v u_v u_v \rangle &= \\ -\frac{\partial \langle p_v \rangle + \langle p_l \rangle}{\partial z} + \left\langle \frac{\partial p_v}{\partial z} + \frac{\partial p_l}{\partial z} \right\rangle + \langle \rho_v + \rho_l \rangle g \\ \Rightarrow \frac{\partial}{\partial t} [(\varepsilon \rho_v + (1-\varepsilon) \rho_l) u] + \frac{\partial}{\partial z} [(\varepsilon \rho_v + (1-\varepsilon) \rho_l) u^2] &= -\frac{\partial [(\varepsilon \rho_v + (1-\varepsilon) \rho_l)]}{\partial z} + \\ &+ \left\langle \frac{\partial p_v}{\partial z} + \frac{\partial p_l}{\partial z} \right\rangle + (\varepsilon \rho_v + (1-\varepsilon) \rho_l) g \\ \Rightarrow \frac{\partial}{\partial t} (\rho_{TP} u) + \frac{\partial}{\partial z} (\rho_{TP} u^2) &= -\frac{\partial p}{\partial z} + \left\langle \frac{\partial p}{\partial z} \right\rangle + \rho_{TP} g \end{aligned} \quad (B.34)$$

References

- Drew, D. A. (1983). Mathematical Modeling of Two-Phase Flow. Annual Review of Fluid Mechanics, 15, 261–291. <https://doi.org/10.1146/annurev.fl.15.010183.001401>
- Hetsroni, G. (1982). Handbook of Multiphase Systems. Hemisphere Publishing Corporation.
- Kandlikar, S. G. (1999). Handbook of Phase Change: Boiling and Condensation. Taylor & Francis.
- Prosperetti, A., & Tryggvason, G. (2007). Computational Methods for Multiphase Flow. Cambridge University Press.
- Slattery, J. C. (1972). Momentum, Energy and Mass Transfer in Continua. McGraw Hill.
- Wallis, G. B. (1969). One-Dimensional Two-Phase Flow. McGraw Hill.
- Whitaker, S. (1969). Advances in Theory of Fluid Motion in Porous Media. Industrial & Engineering Chemistry, 61(12), 14–28. <https://doi.org/10.1021/ie50720a004>

Equations of State

C.1 Helmholtz free energy equation of state

All thermodynamic properties can be determined with a canonical equation known as the equation of state (EoS). One possibility is to use the Helmholtz free energy as the fundamental property.

$$f = e - Ts \quad (\text{C.1})$$

Helmholtz free energy equation can also be written with temperature (T) and either specific volume (v) or density (ρ) as independent variables. On the other hand, Equation (C.1) can be transformed into a two-part split functional with the ideal-gas (a^0) and residual part (a^r) contribution.

$$a(v, T) = a(\rho, T) = a^0(v, T) + a^r(v, T) \quad (\text{C.2})$$

... or in dimensionless form.

$$\frac{a(v, T)}{RT} = \Phi(\delta, \tau) = \Phi^0(\delta, \tau) + \Phi^r(\delta, \tau) \quad (\text{C.3})$$

Here R , Φ , δ and τ stand for the specific gas constant, dimensionless Helmholtz free energy function, reduced volume (or density), and reduced temperature.

$$\tau = \frac{T_c}{T} \quad \text{and} \quad \delta = \frac{\rho}{\rho_c} = \frac{v_c}{v} \quad (\text{C.4})$$

The Equation (C.3) is also split into two parts, ideal and real (Φ^0 and Φ^r). The ideal part considers the ideal part of the fluid ($\delta \rightarrow 0$)

$$\Phi(\tau, \delta) = \Phi^0(\tau, \delta) + \Phi^r(\tau, \delta) \quad (\text{C.5})$$

$$\Phi^0(\tau, \delta) = a_1^0 + a_2^0 \tau + \text{Ln } \delta + \Phi^*(\tau) \quad (\text{C.6})$$

There, the ideal and real parts can be written in functional form as:

$$\Phi^0(\tau, \delta) = \text{Ln } \delta + \sum_{k=1}^{k_1} c_k \tau^{m_k} + \sum_{k=k_1+1}^{k_2} c_k \text{Ln} [1 - \exp(-a_k \tau)]$$

$$\Phi^r(\tau, \delta) = \sum_{k=k_2+1}^{k_3} c_k \delta^{n_k} \tau^{m_k} + \sum_{k=k_3+1}^{k_4} c_k \delta^{n_k} \tau^{m_k} \exp(-\delta^{e_k})$$

$$\alpha^0(\tau, \delta) = \text{Ln } \delta + c_1 \text{Ln } \tau + \sum_{i=2}^{i_1} c_i \tau^{m_i} + \sum_{i=i_1+1}^{i_2} c_i \text{Ln} [1 - e^{(-a_i \tau)}]$$

C.2 Nobel-Abel Stiffened Gas equation of state

By definition, the NASG equation of state is:

$$p(v, e) = (\gamma - 1) \frac{(e - q)}{v - b} - \gamma_\infty p_\infty \quad (\text{C.7})$$

Where, p , v , and e stand for pressure specific volume and specific internal energy, respectively. On the other hand γ , q , p_∞ and b are characteristic constants for each fluid. The terms $(\gamma - 1)(e - q)$, $(v - b)$ and $\gamma_\infty p_\infty$ represents thermal agitation, repulsive short distance effects, and attractive effects to matter cohesion in condensed states respectively.

C.2.1 Calculation of $e(p, T)$

The Maxwell relation reads:

$$\left(\frac{\partial e}{\partial v} \right)_T = T \left(\frac{\partial p}{\partial T} \right)_v - p \quad (\text{C.8})$$

Using Equation (C.7), one can find that:

$$\left. \begin{aligned} \left(\frac{\partial e}{\partial T} \right)_v &= \frac{(v-b)}{\gamma-1} \left(\frac{\partial p}{\partial T} \right)_v \\ \left(\frac{\partial e}{\partial v} \right)_T &= \frac{(v-b)}{\gamma-1} \left(\frac{\partial p}{\partial v} \right)_T + \frac{p + \gamma p_\infty}{\gamma-1} \end{aligned} \right\} \quad (\text{C.9})$$

Introducing derivatives (C.9) into (C.8) we find that:

$$\left(\frac{\partial p}{\partial v} \right)_T = \frac{(\gamma-1)T}{v-b} \left(\frac{\partial p}{\partial T} \right)_v + \frac{p + \gamma p_\infty}{\gamma-1} \quad (\text{C.10})$$

On the other hand, if we assume that heat capacity on constant volume is constant and equal to $Cv = (\partial e / \partial T)_v$ using the relation of $(\partial e / \partial T)_v$ calculated in Eq. (C.9) it yields:

$$\left(\frac{\partial p}{\partial T} \right)_v = \frac{(\gamma-1)}{(v-b)} Cv \quad (\text{C.11})$$

Integrating the last equation over an isothermal line:

$$p(v, T) = \frac{(\gamma-1)}{v-b} CvT + \phi(v) \quad (\text{C.12})$$

This last expression can be differenced over v at constant T and introducing Eq. (C.11) and (C.12) into (C.10) one find the following system of equations:

$$\left. \begin{aligned} \left(\frac{\partial p}{\partial v} \right)_T &= -\frac{(\gamma-1)CvT}{(v-b)^2} - \frac{\gamma}{v-b} (\phi(v) + p_\infty) \\ \left(\frac{\partial p}{\partial v} \right)_T &= -\frac{(\gamma-1)}{(v-b)^2} CvT + \frac{d\phi(v)}{dv} \end{aligned} \right\} \quad (\text{C.13})$$

Equating both expressions one find the following 1st order differential equation:

$$\frac{d\phi}{dv} + \frac{\gamma}{v-b} (\phi + p_\infty) = 0 \quad (\text{C.14})$$

Which has the following solution:

$$\phi(v) = \frac{C}{(v-b)^\gamma} - p_\infty \quad \text{with } C \in \mathbb{R} \quad (\text{C.15})$$

Constant C can be calculated using any reference state $(v_{ref}, p_{ref}, T_{ref})$ or imposing $C = 0$, hence:

$$\left. \begin{aligned} p(v, T) &= \frac{(\gamma - 1)}{v - b} CvT - p_{\infty} \\ e(v, T) &= \frac{p + \gamma p_{\infty}}{p + p_{\infty}} CvT + q \\ h(v, T) &= e + pv = \gamma CvT + bp + q \end{aligned} \right\} \quad (C.16)$$

C.3 Gibbs function

The Gibbs function reads:

$$g(p, T) = h(p, T) - Ts(p, T) \quad (C.17)$$

And another Maxwell is:

$$\left(\frac{\partial s}{\partial p} \right)_T = - \left(\frac{\partial v}{\partial T} \right)_p \quad (C.18)$$

The procedure is similar that the one used to obtain $p(v, T)$. 1) First, it is to calculate $(\partial v / \partial T)_p$ and it is introduced into the new Maxwell relation. 2) That equation is integrated over p at constant T . 3) The result is introduced in the definition of Gibbs function. Finding:

$$g(p, T) = (\gamma Cv - q')T - CvT \operatorname{Ln} \left[\frac{T^{\gamma}}{(p + p_{\infty})^{\gamma-1}} \right] + bp + q \quad (C.19)$$

C.4 Pressure and temperature at saturated state

The above equations were obtained for liquid and vapor phases; the only difference is with the constants γ , q , p_{∞} , b and q' , that must be derived experimentally for each phase. In the saturation line, p and T must be related, but also the Gibbs function is also the same. Hence:

$$g_l(p, T) = g_v(p, T) \quad (C.20)$$

$$\Rightarrow \quad \text{Ln}(p + p_{\infty,v}) = A + \frac{B + Ep}{T} + C \text{Ln}(T) + D \text{Ln } p + p_{\infty,l}$$

Where

$$\begin{aligned} A &= \frac{Cp_l - Cp_v + q'_v - q'_l}{Cp_v - Cv_v} & B &= \frac{q_l - q_v}{Cp_v - Cv_v} \\ C &= \frac{Cp_l - Cp_v}{Cp_v - Cv_v} & D &= \frac{Cp_l - Cp_v}{Cp_v - Cv_v} \\ E &= \frac{b_l - b_v}{Cp_v - Cv_v} \end{aligned} \quad (\text{C.21})$$

References

- Le Métayer, O., Massoni, J., & Saurel, R. (2004). Elaborating Equations of State of a Liquid and its Vapor for Two-Phase Flow Models. *International Journal of Thermal Sciences*, 43, 265–276. <https://doi.org/10.1016/j.ijthermalsci.2003.09.002>
- Le Métayer, O., & Saurel, R. (2016). The Noble-Abel Stiffened-Gas equation of state. *Physics of Fluids*, 28(4). <https://doi.org/10.1063/1.4945981>
- Lemmon, E. W., & Tillner-Roth, R. (1999). A Helmholtz Energy Equation of State for Calculating the Thermodynamic Properties of Fluid Mixtures. *Fluid Phase Equilibria Phase*, 165, 1–21. [https://doi.org/10.1016/S0378-3812\(99\)00262-9](https://doi.org/10.1016/S0378-3812(99)00262-9)
- Span, R., Wagner, W., Lemmon, E. W., & Jacobsen, R. T. (2001). Multiparameter equations of state - Recent trends and future challenges. *Fluid Phase Equilibria*, 183–184, 1–20. [https://doi.org/10.1016/S0378-3812\(01\)00416-2](https://doi.org/10.1016/S0378-3812(01)00416-2)

Differential Equations

D.1 Partial differential classification

An equation is said to be a differential equation when it contains one or more derivatives of the dependant variables respect to the independent variables. For one dependant (u) and two independent (x and y) variables, the above definition can be written as:

$$A \frac{\partial^2 u}{\partial^2 x} + B \frac{\partial^2 u}{\partial x \partial y} + C \frac{\partial^2 u}{\partial^2 y} + D \frac{\partial u}{\partial x} + E \frac{\partial u}{\partial y} + Fu = G \quad (\text{D.1})$$

From a physical point of view, PDEs can be classified as Elliptic (steady-state or equilibrium processes), Parabolic (evolutionary problems that lead to a steady-state configuration), and Hyperbolic (transport phenomena or wave propagation problems).

At a point, (x_0, y_0) the type (as described above) can be calculated using the sign of the discriminant as:

$$\Delta(x_0, y_0) \equiv \begin{vmatrix} B & 2A \\ 2C & B \end{vmatrix} = B^2 - 4AC \quad (\text{D.2})$$

Hence,

$$\begin{aligned} \text{If } \Delta > 0 & \text{ The equation is Hyperbolic} \\ \text{If } \Delta < 0 & \text{ The equation is Elliptic} \\ \text{If } \Delta = 0 & \text{ The equation is Parabolic} \end{aligned} \quad (\text{D.3})$$

References

Lapidus, L., & Pinder, G. F. (1999). Numerical Solution of Partial Differential Equations in Science and Engineering. John Wiley & Sons Inc.

Taylor Series Expansions

E.1 Taylor theorem of functions of one variable

If a function $y = f(x)$ is continuously differentiable $n - 1$ times on the interval $[a, a + h]$, and if also the n^{th} derivative exists in the interior of the interval, then the Taylor formula or Taylor expansion is.

$$f(a + h) = f(a) + \frac{h}{1!} f'(a) + \frac{h}{2!} f''(a) + \cdots + \frac{h^{n-1}}{(n-1)!} f^{(n-1)}(a) + \frac{h^{(n)}}{n!} f'(a + \Theta h) \quad (\text{E.1})$$

With $0 < \Theta < 1$

E.2 Taylor theorem for several variables

The analogous representation using differential operators:

$$f(x_1 + \Delta x_1, x_2 + \Delta x_2, \dots, x_m + \Delta x_m) = f(x_1, x_2, \dots, x_m) + \frac{1}{1!} \sum_{i=1}^m \Delta x_i \frac{\partial f}{\partial x_i} \Big|_{x_0} + \frac{1}{2!} \sum_{i=1}^m \sum_{j=1}^m \Delta x_i \Delta x_j \frac{\partial^2 f}{\partial x_i \partial x_j} \Big|_{x_0} + \cdots + \frac{1}{n!} \sum_{i=1}^m \sum_{j=1}^m \cdots \sum_{k=1}^m \Delta x_i \Delta x_j \cdots \Delta x_k \frac{\partial^{(n)} f}{\partial x_i \partial x_j \cdots \partial x_k} \Big|_{x_0} \quad (\text{E.2})$$

References

Bronshstein, N., Semendyayev, A., Musiol, G., & Muehlig, H. (2007). Handbook of Mathematics (Fifth Edit). Springer.

Runge- Kutta Methods

All Runge- Kutta families can be classified into three ones, according to their Butcher table representation.

$ \begin{array}{c cccc} c_1 & 0 & \cdots & \cdots & 0 \\ c_2 & a_{2,1} & 0 & \cdots & 0 \\ c_3 & a_{3,1} & a_{3,2} & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s,1} & a_{s,2} & \cdots & a_{s,s-1} & 0 \\ \hline & b_1 & b_2 & \cdots & b_{s-1} & b_s \end{array} $	$ \begin{array}{c cccc} c_1 & a_{1,1} & \cdots & \cdots & \cdots & 0 \\ c_2 & a_{2,1} & a_{2,2} & \cdots & \cdots & 0 \\ c_3 & a_{3,1} & a_{3,2} & a_{3,3} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s,1} & a_{s,2} & \cdots & a_{s,s-1} & a_{s,s} \\ \hline & b_1 & b_2 & \cdots & b_{s-1} & b_s \end{array} $	$ \begin{array}{c ccc} c_1 & a_{1,1} & \cdots & a_{1,s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s,1} & \cdots & a_{s,s} \\ \hline & b_1 & \cdots & b_s \end{array} $
Explicit	Diagonally implicit	Fully implicit

F.1 Explicit methods

The Butcher tables for the classic explicit Runge-Kutta methods from 1st to 4th order are summarized below.

F.1.1 Euler forward

$$\begin{array}{c|c}
 0 & 0 \\
 \hline
 & 1
 \end{array} \tag{F.1}$$

F.1.2 Classic explicit 2nd order Runge-Kutta

$$\begin{array}{c|cc}
 0 & 0 & 0 \\
 1/2 & 1/2 & 0 \\
 \hline
 & 0 & 1
 \end{array} \tag{F.2}$$

F.1.3 Classic 3rd order Runge-Kutta

$$\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
1/2 & 1/2 & 0 & 0 \\
1 & -1 & 2 & 0 \\
\hline
& 1/6 & 2/3 & 1/6
\end{array} \tag{F.3}$$

F.1.4 Classic 4th order Runge-Kutta

$$\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
1/2 & 1/2 & 0 & 0 & 0 \\
1/2 & 0 & 1/2 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 \\
\hline
& 1/6 & 1/3 & 1/3 & 1/6
\end{array} \tag{F.4}$$

F.2 Implicit methods**F.2.1 Euler backward**

$$\begin{array}{c|c}
1 & 1 \\
\hline
& 1
\end{array} \tag{F.5}$$

F.2.2 Midpoint rule

$$\begin{array}{c|c}
1/2 & 1/2 \\
\hline
& 1
\end{array} \tag{F.6}$$

F.2.3 Alexander (ES33a)

$$\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
0.87173304 & 0.43586652 & 0.43586652 & 0 & 0 \\
0.60896663 & 0.26488049 & -0.0917038 & 0.43586652 & 0 \\
1 & 0.19210136 & -0.61812188 & 0.99015401 & 0.43586652 \\
\hline
& 0.19210136 & -0.61812188 & 0.99015401 & 0.43586652
\end{array} \tag{F.7}$$

F.2.4 Skvortsov (ES33b)

0	0	0	0	0	
0.31796	0.15898	0.15898	0	0	
0.539745	0.19190584	0.19190584	0.15898	0	(F.8)
1	0.15046472	0.15036875	0.54018653	0.15898	
	0.15046472	0.15036875	0.54018653	0.15898	

F.2.5 Skvortsov (ES54)

0	0	0	0	0	0	0	
1 / 3	1 / 6	1 / 6	0	0	0	0	
2 / 3	1 / 6	1 / 3	1 / 6	0	0	0	
1	11 / 24	-1 / 4	5 / 8	1 / 6	0	0	(F.9)
1	11 / 36	-1 / 6	11 / 12	-2 / 9	1 / 6	0	
1	1 / 8	3 / 8	3 / 8	-2 / 9	1 / 24	1 / 6	
	1 / 8	3 / 8	3 / 8	-2 / 9	1 / 24	1 / 6	

References

Alexander, R. (2003). Design and Implementation of DIRK Integrators for Stiff Systems. *Applied Numerical Mathematics*, 46, 1–17. [https://doi.org/10.1016/S0168-9274\(03\)00012-6](https://doi.org/10.1016/S0168-9274(03)00012-6)

Butcher, J. C. (2008). *Numerical Methods for Ordinary Differential Equations* (2nd Edit.). John Wiley & Sons, Ltd.

Hairer, E., & Wanner, G. (1996). *Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems*. (Springer, Ed.) (2nd Edit.).

Hairer, E., Wanner, G., & Nørsett, S. P. (1993). *Solving Ordinary Differential Equations I: Nonstiff Problems*. (Springer, Ed.) (2nd Edit.). <https://doi.org/10.1007/978-3-540-78862-1>

Kennedy, C. A., & Carpenter, M. H. (2003). Additive Runge – Kutta Schemes for Convection - diffusion - Reaction Equations, 44, 139–181. [https://doi.org/10.1016/S0168-9274\(02\)00138-1](https://doi.org/10.1016/S0168-9274(02)00138-1)

Skvortsov, L. M. (2006). Diagonally Implicit Runge – Kutta Methods for Stiff Problems. *Computational Mathematics and Mathematical Physics*, 46(12), 2209–2222. <https://doi.org/10.1134/S0965542506120098>

Stability

G.1 Zero stability

Definition G.1: Let $(\delta(x), \delta)$ and $(\delta^*(x), \delta^*)$ be any two perturbations of an IVP and let $(u(x), u)$ and $(u^*(x), u^*)$ be the resulting perturbations. Then if there exists a positive constant S such that, for all $x \in [a, b]$,

$$\begin{aligned} \|z(x) - z^*(x)\| &\leq S\varepsilon \quad \text{whenever} \\ \|\delta(x) - \delta^*(x)\| &\leq S\varepsilon \quad \text{and} \quad \|\delta - \delta^*\| \leq S\varepsilon \end{aligned} \tag{G.1}$$

Then the initial value problem is said to be stable (Hairer et al., 1993), (Lambert, 1991) and (Strikwerda, 2004).

G.2 A-Stability

Definition G.2: A method whose stability domain satisfies:

$$S \supset \mathbb{C}^- = \{z; \operatorname{Re}(z) \leq 0\} \tag{G.2}$$

...is called stable (Hundsdorfer & Verwer, 2000). As a consequence, a Runge-Kutta method is *A-stable* if (Hahn, 1967), (Stetter, 1971).

$$|R(iy)| \leq 1 \quad \text{with} \quad y \in \mathbb{R} \tag{G.3}$$

The above definition restricts the value of z to be in the left half-plane; in this way, the solution not only will converge to a finite value as $t \rightarrow \infty$, but also the solution is stable. To verify this statement recall that the solution for the test IVP is:

$$u(t) = u_0 e^{\lambda t} \tag{G.4}$$

G.3 L-Stability

Definition G.3: A method is called *L-stable* if a method is stable and in addition (Ehle, 1969),

$$\lim_{z \rightarrow \infty} R(z) = 0 \quad (\text{G.5})$$

References

Ehle, B. L. (1969). On Pade Approximations to the exponential function and A-Stable Methods for the Numerical Solution of Initial Value Problems.

Hahn, W. (1967). Stability of Motion. Springer-Verlag Berlin Heidelberg. <https://doi.org/10.1007/978-3-642-50085-5>

Hairer, E., Wanner, G., & Nørsett, S. P. (1993). Solving Ordinary Differential Equations I: Nonstiff Problems. (Springer, Ed.) (2nd Edit.). <https://doi.org/10.1007/978-3-540-78862-1>

Hundsdorfer, W., & Verwer, J. (2000). Numerical Solution of Time-Dependent Advection- Diffusion- Reaction Equations. Springer. <https://doi.org/10.1007/978-3-662-09017-6>

Lambert, J. D. (1991). Numerical Methods for Ordinary Differential Systems: The Initial Value Problem. (John Wiley & Sons Ltd, Ed.).

Stetter, H. J. (1971). Stability of Discretizations on Infinite Intervals. In Conference on Applications of Numerical Analysis: Lecture Notes in Mathematics, vol 228 (pp. 207–222). Springer, Berlin, Heidelberg.

Strikwerda, J. C. (2004). Finite Difference Schemes and Partial Differential Equations (2nd Edit.). SIAM.