Numerical stability analysis of natural circulation driven supercritical water reactors

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Abstract

The SuperCritical Water cooled Reactor (SCWR) is one of the six Generation IV nuclear reactors, a selection of some of the more sustainable, safer and financially attractive reactors of the future. The SCWR is operated at high coolant temperatures (500°C) by which thermodynamic efficiencies up to 45% are achieved, making the SCWR suitable for economic energy production. In addition to the European SCWR design, the High Performance Light Water Reactor (HPLWR), it is suggested to drive the coolant flow by natural circulation, thereby further increasing the inherent safety of the reactor (Rohde et al., 2011). Natural circulation introduces extra sources of flow instability, as is also observed in analogous boiling water reactors, such as the Economic Simplified Boiling Water Reactor (ESBWR, Marcel, 2007). To assess the flow stability of natural circulation SCWRs, a scaled coolant loop, named DeLight (Delft Light water reactor), was built in the PNR group (Rohde et al., 2011). This facility contains a single channel three pass core (following the HPLWR design) that is cooled by Freon R23. Thermal hydraulic- neutronic coupling due to the moderating effect of the coolant is artificially introduced in the core by means of a reactor physics model.

The objective of this thesis is to assess whether relatively simple numerical models are sufficiently accurate to capture the physics of flow instability in real systems, such as the experimental DeLight facility. To this end, the stability of DeLight is predicted with an in-house developed 1D, transient, non-linear model (Kam, 2011). Several additions are made to this model, including the implementation of a scaled heat exchanger geometry and a more extensive representation of local pressure losses. Also, the buffer vessel model is replaced and heat losses to the environment are taken into account.

Before simulating the DeLight facility, the model is benchmarked with the numerical stability studies of Jain and Rizwan-Uddin (2008) and T’Joen et al. (2012). Both show good agreement for steady state mass flow rate and stability, validating the thermal hydraulics model. Distinct resonance frequencies are observed in the transient analysis of both cases; their presence is related to the location of the reservoir in the downcomer, nevertheless, no definite physical origin could be identified. Replacing the NIST REFPROP fluid property database by enthalpy dependent spline evaluations reduced the computational time by 60%.

Steady state mass flow rates of DeLight are predicted within 8% of relative error, indicating that the friction distribution is represented well by the model. The thermal hydraulic model predicts unstable working points, whereas no instabilities were observed during experiments. As expected, the neutronic coupling destabilizes the system, but the stability boundary does not match the measured values accurately. At last, the fuel time constant of the numerical model is found to have little impact on stability. A possible reason for the discrepancy is the simplified modelling of heat transfer in the core and heat exchangers, e.g. by assuming uniform heat flux and zero wall heat capacity. Others may be the implementation of isothermal friction models or the integral modelling of heat losses. It is concluded that more comprehensive modelling is required to accurately predict the stability of real systems.
# Contents

Abstract

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Chapter 1

Introduction

1.1 SCWR and HPLWR design

The SuperCritical Water cooled Reactor (SCWR) is one of the six reactors considered in the Generation IV International Forum. This program bundles efforts of industrial and academic partners to develop a new generation of economical, inherently safe, sustainable and proliferation resistant reactors. The SCWR is a Light Water Reactor (LWR) operated at coolant pressures above the supercritical point of water ($T_c = 373.9^\circ C$, $p_c = 22.06MPa$) and is primarily designed for economic energy production (OECD, 2012).

Economic profits are directly related to the reactor efficiency, i.e. of the conversion from fission heat generated in the core to electrical energy. The thermal efficiency of such a Rankine cycle is determined by the temperature difference between the hot and cold reservoirs, i.e. the reactor core and condenser outlet temperature. Typical heat sinks are open water and ambient air, which have temperatures in the range of $10 - 20^\circ C$. Hence, substantial efficiency improvements in this kind of cycles are mainly achieved by increasing the core outlet temperature.

The first type of LWR, the Boiling Water Reactor (BWR), is operated at the boiling point of water. It cannot go beyond this point and is therefore limited in core outlet temperature. The boiling point shifts to higher temperatures with increasing pressure, as is seen in the phase diagram of water (Figure 1.2). Pressurized Water Reactors (PWR) extend the operating window to higher temperatures by increasing the system pressure. In the supercritical regime, the core outlet temperature is not limited by the vapour-liquid equilibrium but rather by the much higher material temperature limits; e.g. of the fuel cladding, which has a maximum allowable temperature of $620^\circ C$. Steady operating temperatures up to $500^\circ C$ are feasible, resulting in projected thermal efficiencies of 45% for the SCWR with respect to 33% for BWRs. Phase separation equipment as found in BWRs is no longer required, allowing for simpler plant designs. Also, the boiling crisis, in which a vapour film strongly reduces heat transfer from fuel to coolant, cannot occur in SCWR systems. Downside of the design is that high pressures (above 22MPa) are required to reach supercritical conditions. Supercritical operation has however some more advantages, for instance: supercritical water can directly drive the turbine (see Figure 1.1) as a result of the strong density reduction at $500^\circ C$, whereas PWRs require a secondary cycle for steam generation. In addition, the heat capacity of water increases with pressure, resulting in smaller flow rate and corresponding equipment capacity requirements under supercritical conditions.
Several SCWR designs are proposed by the partners of the Generation IV International Forum, such as the Japanese (SCLWR), American (US-SCWR) and Canadian (CANDU-SC). The European consortium contributes with the High Performance Light Water Reactor (HPLWR) design. This particular SCWR is primarily designed for a thermal neutron spectrum and is fuelled with conventional uranium oxide or MOX fuel. The fuel elements are developed by Hofmeister et al. (2007) and are grouped in assembly boxes, which in turn form clusters (see Figure 1.3a). Coolant water flows in the voids, named channels, between the fuel rods and is heated from 280°C to 500°C at a pressure of 25MPa. Flow rates may deviate per channel due to manufacturing uncertainties, with the corresponding risk of hot streaks that exceed cladding limits. To reduce the impact of flow reductions, Schulenberg et al. (2008)
propose to split the HPLWR core into three passes with in-between channel mixing (see Figure 1.3b,c). This configuration homogenizes the water temperature before it can reach critical material values and safe operation is assured. All three passes, i.e. evaporator, super heater 1 and 2, consist of 52 fuel clusters. The core sections are named according to their application in fossil fired power plants, where supercritical cooling is already considered proven technology.

![Diagram of HPLWR core design](image)

**Figure 1.3:** Zoom-in on a cluster of nine fuel assemblies (a) and the HPLWR three pass core design with indicated coolant flow (b,c) (source: Hofmeister et al. (2007); Ortega Gómez (2009); Schulenberg et al. (2008)).

The coolant water has two functions in the HPLWR; besides transport of fission energy it also acts as neutron moderator. Moderation takes place as fast neutrons loose kinetic energy in collisions with the hydrogen atoms of water; the degree of moderation therefore depends on the water density. Fluid properties undergo severe changes near the critical point (Figure 1.4); for instance, the density of water changes from 780kg/m$^3$ to 90kg/m$^3$ in the HPLWR core. To compensate for the corresponding loss of moderation, part of the high density feedwater is directed through the square channel at the center of the fuel assembly (Figure 1.3a). The flow in this so called moderator box is directed from top to bottom and mixes with the remaining feedwater at the evaporator entrance (Figure 1.3b).

The large density difference between riser and downcomer can also be beneficial; it can be used to drive the coolant flow by natural circulation. Pumps can be omitted by designing the height of this loop such that the natural mass flow rate is sufficient to cool the core, thereby increasing both the plant economics and inherent safety. Natural circulation is not part of the general HPLWR project objectives but is considered in the current work in combination with the HPLWR three pass core design.

### 1.2 Flow instability

Flow instabilities, i.e. mass flow resonance oscillations with unbounded amplitude growth in time, can occur in forced and natural circulating systems (Ambrosini, 2007; Ortega Gómez, 2009; Van Bragt, 1998). Natural circulation is considered more innovative and is already
applied successfully in for instance the Dodewaard BWR, Dodewaard, The Netherlands. Its successor, the Economic Simplified Boiling Water Reactor (ESBWR), is developed by General Electrics. Several studies on the ESBWR show that the large density change associated with boiling may lead to flow instabilities; these can deteriorate heat transfer in the core and should be avoided at all times (Marcel, 2007; Rohde et al., 2010).

The transition from high to low density in supercritical water is more gradual and over a wider range of enthalpies compared to subcritical water (see Figure 1.4). The transition for supercritical pressures occurs at the so called pseudo critical point and is defined at the maximum in heat capacity. Although two-phase boiling systems and single-phase supercritical systems are physically different, density changes as function of enthalpy show great similarity (Ortega Gómez, 2009). Analogous instability mechanisms are expected to exist in SCWRs and have to be understood well before full scale reactors can be licensed.

Several types of flow instability can occur in channel flows. Boure et al. (1973) made a classification of static and dynamic instabilities. Ledinegg is one example of static instability and refers to systems with multiple steady state solutions in between which the flow may oscillate in a non-periodic way. Unstable working points can be predicted by analysis of steady state channel characteristics. Dynamic instabilities, on the other hand, are the system response to flow perturbations and occur due to the presence of feedback mechanisms. These instabilities require transient analysis for their prediction.

Density Wave Oscillations (DWO) are dynamic instabilities commonly encountered in BWRs and have been studied quite extensively in literature (for example March-Leuba and Rey (1993) were one of the first). DWOs are created as mass flow fluctuations (e.g. induced by turbulence) are heated in the reactor core; fluid packages of reduced flow rate will have a lower density at the core outlet than high flow rate packages. The result is a sinusoidal DWO travelling through the system, affecting the other variables as well.

In case the core exit temperature lies close to the boiling point (or pseudo critical point for SCW), large amplitude DWOs are created due to the sensitive dependency of density on temperature. In turn, these DWOs cause a corresponding oscillation in the gravitational...
1.2. FLOW INSTABILITY

Figure 1.5: Density wave oscillations in the reactor core. In this example inlet flow and total pressure drop are $180^\circ$ out of phase, resulting in type II instability (source: Ortega Gómez (2009)).

Pressure drop over the riser and hence in the driving force for natural circulation. Positive feedback exists in the system if the core inlet mass flow and riser pressure drop oscillations are $180^\circ$ out of phase; e.g., when an increase in flow rate at the core inlet results in a decrease in riser pressure drop. This type of instability, related to the gravitational pressure drop oscillations in the riser, is referred to as type I instability (Fukuda and Kobori, 1979). The frequency of this oscillation directly relates to the transit time in the vertical core and riser sections.

Type II instabilities are created due to positive feedback between core inlet flow and frictional pressure drop over the core, as illustrated in Figure 1.5. Whereas type I instabilities are found only in natural circulation systems, type II instabilities can occur in forced system as well. While travelling along the heated core, the amplitude of the incoming DWOs increases (mid Figure 1.5). The local pressure drop oscillates correspondingly. The total core pressure drop, again a sinusoidal (top Figure 1.5), is found by integrating over the local pressure drops, where the largest contribution is made by the DWO pressure drop at the core outlet. The latter are delayed with respect to the inlet oscillation due to the finite transit time in the core and, similar to type I instabilities, the resulting phase shift can cause self-sustained instabilities. Type II instabilities occur at high core power and are characterized by higher frequencies than type I instabilities due to the short transit time of the core.

In nuclear reactors, another type of feedback is present due to coupling between the coolant flow and core neutronics. As discussed in the previous section, water has the dual function of coolant and moderator in the HLPWR. DWOs present in the coolant channel therefore cause fluctuations in the degree of moderation and in turn in core power via the neutron population. The water density however depends again on the core power. This feedback loop is different in the sense that it is not instantaneous; fission energy is released in the interior of the fuel rods and requires time to transport to the coolant. This coupled neutronic-thermal hydraulic feedback mechanism is an additional source of DWO instability in nuclear reactors that has to be considered.

If positive feedback exists in the system, oscillations will grow in amplitude and the system is said to be unstable (decay ratio $> 1$). Decaying oscillations indicate a stable system (decay
ratio < 1); an example of a stable and unstable system is given in Figure 1.6. At the transition between stable and unstable oscillations, the system is said to be neutrally stable (decay ratio = 1). Oscillations in this point will not grow or decay in time. The Neutral Stability Boundary (NSB) is commonly used to distinguish stable and unstable regimes for a range of operating conditions.

![Figure 1.6](image)

**Figure 1.6**: Examples of stable (a) and unstable (b) core outflow oscillations.

1.3 Literature survey

Several reports of supercritical loops driven by natural circulation are found in literature. Chatoorgoon et al. (2005) were one of the first to study flow instabilities of supercritical CO\(_2\) in a loop geometry using a non-linear code (see also Chatoorgoon, 2001). Jain and Rizwan-Uddin (2008) repeated the case including grid independency tests and presented low power stability data. Lomperski et al. (2004) obtained experimental thermal hydraulic data from the SNAC loop at Argonne National Institute. No instabilities were found for the powers considered, even though both linear and non-linear codes of Jain and Corradini (2006) predicted system instability under the same conditions. Recently, T’Joen et al. (2012) benchmarked his linear code with the stability data of Jain and Rizwan-Uddin (2008) and found good agreement. T’Joen expanded the NSB to higher powers and observed distinct, high frequency, DWO instabilities. Static instabilities were found at high powers in the analysis of core characteristics, similar to the observations of Ambrosini (2007). The static instabilities of T’Joen et al. (2012) appeared to be located in the unstable DWO region.

Some models incorporating coupled neutronic-thermal hydraulic feedback are found in literature; Yi et al. (2004) presented stability data for a forced convection SCWR loop and Ortega Gómez (2009) studied the stability of the HPLWR core. In the latter study no negative slopes were found in the core characteristics, thereby excluding Ledinegg instabilities in the HPLWR core within realistic operating conditions.

The section Physics of Nuclear Reactors (PNR) at Delft University of Technology has built an experimental natural circulation driven cooling loop, with the incentive to generate a set of stability benchmark data (T’Joen and Rohde, 2012). The facility is named Delft Light water reactor (DeLight) and is a scaled version of the HPLWR. It is built according to the scaling rules derived by Rohde et al. (2011) and is operated at 5.7MPa with Freon R23 coolant. Freon R23 is selected as it reduces the operating pressure while behaving similar to
water over a wide range of conditions. The core sections are electrically heated and artificial neutronic-thermal hydraulic coupling is introduced by adjusting the core power according to the measured coolant density variation. To this end, a reactor physics model including a density reactivity term was implemented in Labview. The presence of density reactivity destabilized the system, as was found by Yi et al. (2004). Decreasing the fuel transfer time constant led to a more stable system under all conditions. Without density reactivity feedback this loop is found to be stable within the experimental range allowed by electrical power and heat exchanger capacities.

Within the same section, Kam (2011) adjusted the 1D non-linear transient model of Koopman (2008) to include the same reactor physics model as implemented in DeLight. Kam benchmarked the steady state of DeLight at a single core inlet temperature. In his model the wall friction in the heat exchanger is adjusted to account for unknown friction. Kam found that DeLight is predicted to be more unstable at high powers than was measured. The implemented mass buffer model, however, is suspected of affecting the system stability. No extended parameter studies were performed due to the large computational time required by the code.

1.4 Thesis objectives and outline

The objective of this thesis is to assess whether relatively simple numerical models, such as those found in literature, are sufficiently accurate to capture the physics of experimental facilities, such as DeLight. The starting point of this work is the numerical model of Kam (2011). First, an attempt will be made to reduce the computational costs of this model by replacing the external fluid property database (NIST REFPROP 7.0) with enthalpy dependent spline evaluations. Also, a semi-implicit scheme will be implemented in order to obtain a higher numerical accuracy. The influence of the mass buffer model on flow stability will be investigated by observing the time signals of buffer in- and out flow rate as function of the model parameter.

In addition, an effort will be made to improve the physical model representation of the DeLight facility. To this end, the local pressure losses due to several loop components (such as valves, junctions and bends) are implemented extensively. The heat exchanger is modelled such that the pressure drop and residence time are maintained equal. Furthermore, heat losses to the environment in the core and downcomer sections are taken into account by using the data from thermocouple measurements.

Before evaluating the DeLight facility, the implementation of the thermal hydraulics model will be tested by performing steady state and stability benchmarks with the numerical cases of Jain and Rizwan-Uddin (2008) and T'Joen et al. (2012). With the renewed model a steady state analysis of DeLight will be made for multiple core inlet temperatures. Pure thermal hydraulic and coupled neutronic-thermal hydraulic stability benchmarks will be performed to assess the quality of the DeLight model. Finally, the influence of the fuel time constant is considered in a parameter study.

The outline of the thesis is as follows. After this introduction chapter, the benchmark cases are introduced in Chapter 2. The analytical thermal hydraulic and reactor physics models are derived in Chapter 3, followed by their discretization in Chapter 4. Chapter 4 elaborates on the solution algorithm as well. The numerical considerations made to improve the modelling of the DeLight facility, as discussed in this section, are given in Chapter 5.
Chapter 6 describes how the model is utilized to analyse the loop stability. The results of the literature and DeLight benchmarks are presented in Chapter 7, followed by conclusions and recommendations in Chapter 8.
Chapter 2

Description of the benchmark cases

In the subsequent chapters (3 and 4) a numerical model is derived to describe the physics of natural circulation supercritical loops. This model has to be compared to reference cases in order to validate the model; these so called benchmark cases are introduced in this chapter. First, benchmarks with the numerical cases of T’Joen et al. (2012) and Jain and Rizwan-Uddin (2008) are made to validate the implementation of the thermal hydraulics model. These cases concern simple, rectangular loop geometries and are described in Section 2.1. Secondly, a benchmark is made with the experimental data obtained from the DeLight facility to assess whether such numerical models are capable of accurately simulating non-theoretical, physical, systems. Section 2.2 introduces the geometry and components of DeLight and mentions the performed measurements.

2.1 Literature benchmarks

2.1.1 R23 loop

T’Joen et al. (2012) have introduced a simple, rectangular, loop (as shown in Figure 2.1a) to study the stability behaviour of natural circulating supercritical flows. Freon R23 was selected as cooling fluid. The loop is equipped with a core section in the bottom and a heat exchanger in the top. The model implementation is such that the quantity of heat supplied to the core is removed by a negative, uniform flux in the heat exchanger. The enthalpy of the heat exchanger outflow is therefore not necessarily constant under transient conditions. To assure a constant core inlet temperature, the downcomer flow is mixed with the contents of a large coolant reservoir, which is kept at the set point temperature. The reservoir is also maintained at constant pressure to stabilize the loop pressure at 5.7MPa.

T’Joen et al. (2012) have analysed the steady state and stability of the R23 loop with a linear, frequency domain COMSOL model. Frictional losses in the flow are modelled by the Haaland friction relation for pipe flow (Equation 3.7d) with an absolute wall roughness of $\epsilon = 4 \cdot 10^{-7}$m. The pressure drop in the bends, located at the riser and downcomer in- and outlets, is modelled by means of a local friction factor ($K = 0.5$, see Equation 3.9). No gravity and wall friction are included in the bend sections. Neutronic- thermal hydraulic coupling, as simulated in DeLight, is not considered in this work.
2. DESCRIPTION OF THE BENCHMARK CASES

2.1.2 CO₂ loop

The loop proposed by Chatoorgoon et al. (2005) and later adopted by Jain and Rizwan-Uddin (2008) has a similar geometry as the R23 loop of T’Joen et al. (2012), see Figure 2.1b. This loop is operated at a pressure of 8MPa with CO₂ as the coolant. The Blasius and McAdams friction relations for smooth pipes are implemented to model friction losses (Equations 3.7b,c; the transition between the Blasius and McAdams relations is made at $Re = 30,000$). Local frictions $K_i$ are present at the reservoir inlet and outlet, as shown in Figure 2.1b. The local friction factor $R_i$, as defined by Jain and Rizwan-Uddin, relates to the factor used in this work as $K_i = 2R_i = 1.0$. Jain and Rizwan-Uddin (2008) have analysed the steady state and stability of the CO₂ loop with a non-linear transient model. They report stability data for a narrow range of operating conditions. T’Joen (2012) has analysed the same loop with the linear COMSOL model and has provided stability data over a wider range of conditions.

2.2 DeLight facility

2.2.1 Geometry and components

The stability of a natural circulation driven SCWR is studied experimentally by means of the scaled test facility DeLight (T’Joen and Rohde, 2012). The scaling is performed by matching the non-dimensional numbers that arise from the relevant transport equations (conservation of mass, momentum and energy plus the equation of state) of the HLPWR and the facility. This analysis, resulting in a set of scaling rules that determine the measures and operating conditions of the facility, is presented in the work of Rohde et al. (2011). The same authors
2.2. DELIGHT FACILITY

have selected Freon R23 as scaling fluid, which allows for a strong reduction in operating pressure with respect to water cooled loops (5.7MPa versus 25MPa). The operating temperatures are reduced from 280°C and 500°C to -30°C and 100°C at the core in- and outlet respectively, making the system more suitable for lab scale application.

The DeLight facility is equipped with a single channel three pass core, following the HPLWR design (Schulenberg et al., 2008), and is depicted schematically in Figure 2.2. The stainless steel tubing has an internal diameter of 6mm in the core and 10mm in the riser and downcomer. Transitions in tube diameter are made over a length of 3cm by a gradual contraction / expansion. The loop height is 10.6m and is selected such that the core section can be cooled by natural circulation under all operating conditions. More detailed measures can be found in Appendix A or online (ref.: DeLight website).

Heat is supplied in the core section by sending an electrical current through the tube wall. This results in a uniform heat flux over the length of the tube. The power provided by the Delta SM15-200 power units is divided over the three core sections (evaporator, superheater 1 and 2) and the preheater. The power delivered to each section can be set independently and is controlled by adjusting the voltage. This allows for non-uniform power distributions over the core sections, such as the 53/30/17% distribution (evaporator / superheater 1 / 2) of the HPLWR (Fischer et al., 2009). The maximum, total, power that can be supplied to the system is 18kW. The temperature gradient over the core section can lead to significant thermal stresses in the tubing; the tubing is therefore mounted to the wall by movable spacers.
Table 2.1: DeLight heat exchanger properties.

<table>
<thead>
<tr>
<th></th>
<th>SWEP</th>
<th>Vahterus</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>B16DWX14/1P-5C-UHP</td>
<td>PSHE 2HA-86/4/2</td>
</tr>
<tr>
<td>Primary side</td>
<td>Freon R23</td>
<td>Freon R23</td>
</tr>
<tr>
<td>Secondary side</td>
<td>Building supply water</td>
<td>Freon R235</td>
</tr>
<tr>
<td>Primary volume (L)</td>
<td>0.75</td>
<td>7.9</td>
</tr>
<tr>
<td># plates</td>
<td>28</td>
<td>86</td>
</tr>
<tr>
<td>Hydraulic channel diameter (mm)</td>
<td>2.76</td>
<td></td>
</tr>
<tr>
<td>Channel length (mm)</td>
<td>320</td>
<td></td>
</tr>
</tbody>
</table>

with pre-stressed springs that allow for some relaxation. In addition, the core section contains two corrugated hoses that can buffer deformations.

The heat sink of the HPLWR (i.e. the turbine and condenser) is taken into account by two heat exchangers placed in series (see Table 2.1 for their specifications). The first, the SWEP heat exchanger, is fed on the secondary side by the building water supply. The secondary side flow rate is over-designed for the application, resulting in a constant R23 outlet temperature of 17°C. Hence, the transition from super- to subcritical R23, with corresponding large density changes, always occurs in the SWEP heat exchanger. During experiments, the Vahterus heat exchanger is used to set the core inlet temperature. In some cases the fourth heated section, the preheater, is used to regulate the core inlet temperature more accurately. To minimize heat losses in the system, the tubing is isolated with a 25mm thick layer of Armacell. The heated sections, i.e. core and preheater, are not isolated.

The coolant can expand during transient operation (e.g. reactor start-up), by which the system pressure increases. The loop is therefore connected to a buffer vessel, containing a movable piston (Parker Series 5000 Piston Accumulator) that can in- or decrease the volume of the loop. The position of the piston is controlled by modifying the nitrogen pressure on the exterior side of the piston. This is done such that a constant system pressure of 5.7MPa is maintained.

DeLight is equipped with a range of sensors to monitor the thermal hydraulics. A coriolis flow meter (ABB CoriolisMaster FCM2000, ±0.25%, indicated with symbol F in Figure 2.2) is installed to measure the mass flow rate. The coolant temperature in the core is monitored with 5 thermocouples in each section (type K thermocouples, ±0.1K, symbol T in Figure 2.2). Several other thermocouples are placed near the core and heat exchangers. All thermocouples are calibrated with three reference thermocouples. The measured temperatures are also passed to a safety system that shuts off the power supply in case pre-described values are exceeded. Absolute pressure sensors are present in top and bottom of the loop (Symbol P, ±0.15%). Relative pressure drops are measured over the valves (Symbol ΔP, ±0.5%, ±200/500mbar) to determine the friction. The valves can be used to increase the local frictions, which are known to affect system stability (Ambrosini and Sharabi, 2008; Ortega Gómez, 2009). For data storage limitations, only part of the sensors are logged during experiment. These are: absolute pressure at the riser exit, mass flow rate, power, average core density and core in- and outlet and heat exchanger outlet temperatures.
Table 2.2: Neutronic constants for the HPLWR (Ortega Gómez, 2009) and the scaled values for DeLight.

<table>
<thead>
<tr>
<th>Group</th>
<th>Fractions $\beta_i$ ($-$)</th>
<th>Decay constants $\lambda_i$ (1/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.038</td>
<td>HPLWR 0.0127 DeLight 0.0290</td>
</tr>
<tr>
<td>2</td>
<td>0.213</td>
<td>HPLWR 0.0317 DeLight 0.0724</td>
</tr>
<tr>
<td>3</td>
<td>0.188</td>
<td>HPLWR 0.115 DeLight 0.263</td>
</tr>
<tr>
<td>4</td>
<td>0.407</td>
<td>HPLWR 0.311 DeLight 0.710</td>
</tr>
<tr>
<td>5</td>
<td>0.128</td>
<td>HPLWR 1.40 DeLight 3.20</td>
</tr>
<tr>
<td>6</td>
<td>0.026</td>
<td>HPLWR 3.87 DeLight 8.84</td>
</tr>
</tbody>
</table>

| $\beta$ | $(-)$ | HPLWR 0.0065 | DeLight 0.0065 |
| $\Lambda$ | $(\mu s)$ | 50 | 22 |
| $\rho_{\text{reactivity}}$ | $(m^3/kg)$ | $3.5 \cdot 10^{-5}$ | $2.1 \cdot 10^{-5}$ |
| $\tau$ | $(s)$ | 6 | 2.63 |

2.2.2 Reactor physics

Coupled neutronic-thermal hydraulic feedback is simulated in DeLight by means of a reactor physics model. This model is based on the six-group point kinetics equations and contains a density reactivity term to predict the response of the core power to variations in the coolant density. The density reactivity depends on the average coolant density in the core, which is obtained from the 15 thermocouple measurements made in the core sections and the equation of state. Furthermore, the response is artificially delayed by the heat transfer through the fuel pin, this effect is taken into account by a fuel transfer function.

The constants in the point kinetics equations are reported by Ortega Gómez (2009) for the HPLWR, see Table 2.2. For implementation in DeLight, the precursor decay times and mean generation time are scaled by the time scaling factor $X_t = \frac{t_p}{t_{\text{DeLight}}} = 0.438$, derived by Rohde et al. (2011). The HPLWR reactivity constant is scaled with $X_{\rho} = \frac{\rho_p}{\rho_{\text{DeLight}}} = 1.69$.

This reactor physics model is evaluated in a LabVIEW code and is used to perturb the nominal core power. The same model is implemented in the numerical model considered in this thesis and is discussed more elaborately in Section 3.2.

2.2.3 Measurements

The coolant flow in DeLight is started with the electrical pump placed in the bottom of the loop. When a flow is initiated, the heat exchangers are activated and the core power is increased to reach steady state in the desired working point. During this operation, the piston in the buffer vessel is moved to maintain a constant system pressure of 5.7MPa. At steady state, the average core density is measured for two minutes. The time average of this series ($\rho_{\text{coolant,0}}$) is used as input for the reactor physics model (Equation 3.15). The stability analysis is started by turning on the reactor physics model.

Oscillations in the mass flow rate will dampen or grow in time, depending whether the working point is stable or unstable. The oscillation can be observed in all flow variables (flow rate, enthalpy, density and pressure). The temperature measured at the core outlet is selected...
to retrieve the decay ratio of the oscillation. This is done by fitting the function:

\[ y = a_0 + (1 - a_0 - a_1) e^{b_1 \tau} + a_1 e^{b_2 \tau} \cos (\omega \tau) \]  

(2.1)

to the first two periods of the auto correlation function (Marcel, 2007; T’Joen and Rohde, 2012). The decay ratio is then found from:

\[ DR = e^{\frac{2 \pi b_2}{|\omega|}} \]  

(2.2)

The facility is used to measure the influence of several parameters on stability, e.g.: density reactivity- and fuel time constants, system pressure and the effect of local frictions applied by closing valves at the core in- and outlet. For data storage limitations, only part of the sensors are logged during experiment. These are: absolute pressure at the riser exit, mass flow rate, power, average core density and core in- and outlet and heat exchanger outlet temperatures.
Chapter 3

Model equations

The thermal hydraulics of the coolant flow are governed by the conservation of mass, momentum and energy. An additional Equation Of State (EOS) is required to close the model of the four system variables, being: mass flow rate (\(M\)), pressure (\(p\)), enthalpy (\(h\)) and density (\(\rho\)). For DeLight, where neutronic-thermal hydraulic coupling is considered, the core power is variable as well. Its value is obtained from the point kinetics equations combined with a fuel rod heat transfer model. The first section of this chapter provides the thermal hydraulic model equations, the second considers the reactor physics.

3.1 Thermal hydraulics

For the geometries under consideration, the axial length scale is two orders of magnitude larger than the channel diameter. Hence, a one dimensional approach with a wall friction model is adopted. Below the set of 1D transport equations derived by Koopman (2008) and Kam (2011) is presented with all additional assumptions and considerations.

3.1.1 Conservation of mass

The continuity equation in its general three dimensional form,

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0
\]  

consists of the rate of change and the convective term. The 1D model equation is derived by integrating over the control volume \(dV\). The volume integral over the convective term is rewritten using Gauss’ theorem:

\[
\int_V \frac{\partial \rho}{\partial t} dV + \int_S \rho \vec{v} \cdot \hat{n} dA = 0
\]  

Contributions to the resulting surface integral are only made by flow through the cross sectional planes. Assuming constant properties in the control volume and evaluating the integrals leads to:

\[
A \frac{\partial \rho}{\partial t} + \frac{\partial M}{\partial x} = 0
\]  

in the limit of \(\Delta x \to 0\). Here the density and mass flow rate are averaged over the channel cross section. Average bars and direction subscript are omitted by defining \(\rho\) as the cross-section...
sectional average density and $M$ as the cross sectional average mass flow rate in the axial-, or $x$-direction.

### 3.1.2 Conservation of momentum

As for the continuity equation, the general momentum balance,

$$\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot \vec{\tau} + \rho g$$  \hspace{1cm} (3.4)

is integrated over the control volume to result in the following 1D relation:

$$\frac{\partial M}{\partial t} + \frac{\partial}{\partial x} \left( M^2 \frac{\rho A}{\rho} \right) = -A \frac{dp}{dx} - \bar{\tau}_w P_w + A \rho g$$  \hspace{1cm} (3.5)

$\bar{\tau}_w$ is defined as the average wall shear stress and is modelled using Darcy’s definition (Todreas and Kazimi, 1989):

$$\bar{\tau}_w = f \frac{M^2}{8 \rho A^2}$$  \hspace{1cm} (3.6)

$f$ is the Darcy-Weisbach friction factor, its value is obtained from either of the following models, depending on the benchmark case:

- **Poisseuille**
  
  $$f = \frac{64}{Re} \hspace{1cm} Re < 2.000$$  \hspace{1cm} (3.7a)

- **Blasius**
  
  $$f = 0.316 Re^{-0.25} \hspace{1cm} Re < 30.000$$  \hspace{1cm} (3.7b)

- **McAdams**
  
  $$f = 0.184 Re^{-0.20} \hspace{1cm} 30.000 < Re < 10^6$$  \hspace{1cm} (3.7c)

- **Haaland**
  
  $$f = \left( -1.8 \log_{10} \left[ \left( \frac{\epsilon}{3.7D} \right)^{10/9} + \frac{6.9}{Re} \right] \right)^{-2} \hspace{1cm} 4.000 < Re < 10^8$$  \hspace{1cm} (3.7d)

Pressure losses due to local obstacles, such as bends, joints and contractions, are taken into account by means of additional pressure drops;

$$\frac{\partial M}{\partial t} + \frac{\partial}{\partial x} \left( M^2 \frac{\rho A}{\rho} \right) = -A \frac{dp}{dx} - \sum_i \Delta p_i H_{step}(x_i) - \bar{\tau}_w P_w + A \rho g$$  \hspace{1cm} (3.8)

The local friction factor $K_i$ is introduced to describe the local pressure drop in terms of the mass flow rate (Todreas and Kazimi, 1989),

$$\Delta p_i = K_i \frac{M^2}{2 \rho A^2}$$  \hspace{1cm} (3.9)

Substitution leads to the final form of the 1D momentum balance under consideration:

$$\frac{\partial M}{\partial t} + \frac{\partial}{\partial x} \left( M^2 \frac{\rho A}{\rho} \right) = -A \frac{dp}{dx} \sum_i K_i \frac{M^2}{2 \rho A} \delta(x - x_i) - \frac{P_w M^2}{8 \rho A^2} + A \rho g$$  \hspace{1cm} (3.10)

Note that differentiation of the step function produces the delta function (with units 1/m) that defines the local friction $K_i$ in control volume $i$. 
3.1.3 Conservation of energy

Starting point is the enthalpy balance for fluid flow,

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot \rho h \vec{v} = -\nabla \cdot q'' + q''' + \frac{Dp}{Dt} + \phi$$ (3.11)

Here $\phi$ is the heat production term due to shear. This term is small for systems with only moderate velocity gradients in low viscosity fluids, such as water and Freon. The system has no internal heat production and the work done by pressure is neglected. Turbulent diffusivity in the DeLight system is estimated using Reichardt’s model for developed turbulent pipe flow (Todreas and Kazimi, 1989); the corresponding penetration length scale within one loop transit time is $\sim 1\text{cm}$ (for $\epsilon = 6.9 \cdot 10^{-7} \text{m}^2/\text{s}$, $t = 40\text{s}$), which is relatively small with respect to the wavelength of typical oscillations in the dynamic system (half the oscillation wavelength is estimated to be $> 0.20\text{m}$ for DeLight). Axial turbulent diffusivity is therefore not expected to significantly affect the decay ratio and is not incorporated in the current model. For the high Reynolds number flows under consideration, axial dispersion is dominated by turbulent rather than molecular transport; therefore heat conduction is not considered either.

Integration over the control volume then leads to:

$$A \frac{\partial \rho h}{\partial t} + \frac{\partial Mh}{\partial x} = q'$$ (3.12)

Where $q'$ is the wall perimeter averaged, or linear, heating rate in W/m. $q'$ entails all in- and outflows in the core and heat exchanger sections of the loop. The linear heat flux is obtained from the power by dividing by the heated length; for instance, the core heat flux is defined as:

$$q'_{\text{core}} = \frac{P_{\text{core}}}{L_{\text{core}}}$$ (3.13)

3.2 Reactor physics

Heat is generated in the HPLWR core due to fission of the uranium oxide or MOX fuel. The rate of fission depends on the concentration (or flux) of thermal neutrons, i.e. neutrons that have lost kinetic energy in the moderator. For the HPLWR, water serves as the moderator, thereby coupling the neutron concentration to the density of the water. However, the response is not instantaneous due to the finite thermal conductivity in the fuel rod. This delayed coupling can lead to a neutronic feedback that affects the stability.

The DeLight core is electrically heated, i.e. no neutronics take place in DeLight. To simulate the neutronic-thermal hydraulic coupling, the core power is perturbed according to a reactor physics model. This model is implemented in Delight by means of a LabVIEW code, as mentioned briefly in Section 2.2.2. The same reactor physics model is included in the numerical model considered in this thesis.
3.2.1 Point kinetics

The neutron population in the core is modelled using a six-group point kinetics equation:

\[
\frac{dn(t)}{dt} = \rho_{\text{reactivity}}(t) - \beta \Lambda n(t) + \sum_{i=1}^{6} \lambda_i c_i(t)
\]

\[
\frac{dc_i(t)}{dt} = \frac{\beta_i}{\Lambda} n(t) - \lambda_i c_i(t), \quad \text{for } i = 1...6
\]

Where \(\beta\) is the delayed neutron fraction, \(\lambda_i\) the precursor decay constant and \(\Lambda\) the mean generation time. The neutron balance contains a density reactivity term (\(\rho_{\text{reactivity}}\), where reactivity is the relative deviation from reactor criticality) that accounts for the neutronic-thermal hydraulic coupling. The density reactivity is proportional to the deviation from the steady state core density:

\[
\rho_{\text{reactivity}} = \alpha_{\text{reactivity}} (\rho_{\text{coolant}}(t) - \rho_{\text{coolant},0})
\]

With \(\rho_{\text{coolant}}\) the average core density. The density reactivity constant is defined as \(\alpha_{\text{reactivity}} = \frac{\partial \rho_{\text{reactivity}}}{\partial \rho_{\text{coolant}}}\) and has to be positive to assure negative feedback. For the HPLWR, a relation for the reactivity constant can be found in the work of Schlagenhaufer et al. (2007):

\[
\alpha_{\text{reactivity}} = -1.424 \times 10^{-8} \rho_{\text{coolant}}(t) + 4.236 \times 10^{-5}
\]

During the experiments performed in DeLight, the value for the density in Equation 3.16 was kept fixed at 500kg/m\(^3\). This was done to keep the density reactivity constant under all operating conditions, thereby decoupling the effect of variable density reactivity constant from other variables, such as the fuel time constant introduced in Section 3.2.2. This allowed for a more clear interpretation of the results.

The relation between fluctuations in neutron concentration and core power is derived in the following. Rewriting the neutron and precursor concentrations in terms of steady state and fluctuating components,

\[
n(t) = n_0 + n'(t)
\]

\[
c_i(t) = c_{i,0} + c_i'(t)
\]

\[
\rho_{\text{reactivity}}(t) = \rho_{\text{reactivity}}'(t)
\]

and subtracting the steady state (zero transients and reactivity) results in the point kinetics equations for the fluctuating concentrations. Dividing by the steady state neutron concentration gives relative fluctuating concentrations,

\[
n'_i(t) = \frac{n'_i(t)}{n_0}
\]

\[
c'_i(t) = \frac{c'_i(t)}{n_0}
\]

in the point kinetics relations:

\[
\frac{dn'_i(t)}{dt} = \frac{\rho_{\text{reactivity}}'(t)}{\Lambda} + \frac{\rho_{\text{reactivity}}'(t) - \beta}{\Lambda} n'_i(t) + \sum_{i=1}^{6} \lambda_i c'_i(t)
\]

\[
\frac{dc'_i(t)}{dt} = \frac{\beta_i}{\Lambda} n'_i(t) - \lambda_i c'_i(t), \quad \text{for } i = 1...6
\]
Since the variables are defined as relative quantities, the power fluctuation is now directly related to the neutron fluctuation:

\[ n'(t) = \frac{n'(t)}{n_0} = \frac{P'(t)}{P_0} = P'(t) \]  (3.18)

### 3.2.2 Fuel transfer model

Fluctuations in core power as described by Equation 3.18 do not result in an instantaneous response in the coolant temperature, as the thermal conductivity in the fuel rod is finite. The fuel rod consists of the fuel pellet, a gap region and the cladding and the heat transfer through the material is described by three diffusion equations, resulting in a complex heat transfer function. Van Bragt (1998) assumed that the transfer function is essentially dominated by one time constant. The response of the channel wall heat flux to a power fluctuation is therefore modelled via a first order process with fuel time constant \( \tau \), as used by Van Bragt (1998):

\[ \tau \frac{\partial q'_w}{\partial t} + q'_w = P' \]  (3.19)

The power fluctuation \( P' \) can be interpreted as the driving force for heat flux variations \( q'_w \). The HPLWR fuel time constant is approximated by \( \tau = 2 - 6 \)s, as found by Van der Hagen (1988) for BWRs. These time constants are scaled and used in the reactor physics model of DeLight.
Chapter 4

Numerical model

The model equations (derived in Chapter 3) are discretized for numerical evaluation by using a finite volume method with first order upwinding. First order upwind schemes are relatively easy to implement, at the price of being diffusive. Numerical diffusion has an artificial stabilizing effect on flow resonances that is proportional to the resonance frequency and amplitude. It is therefore important to select a sufficiently small discretization step for the system under consideration. Physically, the choice for the upwind scheme makes sense as information in convective flows is only received from the ‘upwind’ stream direction.

In time, the model is discretized using the backward Euler scheme. This fully implicit scheme is unconditionally stable, even for large time steps, but is computationally demanding as the resulting system of equations is coupled. The fully explicit alternative, forward Euler time stepping, is accurate and computationally cheap per time step. It requires however sufficiently small time steps to assure numerical stability, thereby greatly increasing the computational cost. A semi-implicit scheme (combining implicit and explicit terms) is considered in addition to the fully implicit scheme.

The discretization of the implicit model equations is made in the first two sections of this chapter. The derivation of the semi-implicit model is similar, and is left to Appendix E. The third section elaborates on the solution algorithm and relates the model equations to the corresponding Fortran functions in the numerical code.

4.1 Thermal hydraulics model

The thermal hydraulic transport equations are discretized on a staggered grid (see Figure 4.1a) to avoid odd-even decoupling of the pressure field (Patankar, 1980). In the following the model is discretized assuming flow in positive direction. The spatial indices of the staggered grid \((i, j)\) are defined in Figure 4.1. Negative flows (encountered in case of severe start-up oscillations or long time unstable operation) reverse the index of upwinded terms, i.e. the convective terms of momentum and energy balances. The indices corresponding to negative flows are indicated within round brackets in the variable subscript. Time discretization index \(n\) is denoted in the variable superscript. The to be evaluated time step has index \(n + 1\).
4. NUMERICAL MODEL

**Figure 4.1:** Control volume definitions for the staggered grid (a). The enthalpy balance and continuity equation are integrated over the solid control volume with index \( j \) (b), the momentum balance over the dashed control volume with index \( i \) (c).

### 4.1.1 Continuity equation

The mass balance (Equation 3.3) is integrated over the control volume indicated in Figure 4.1b to discretize the convective term:

\[
A \frac{\partial \rho}{\partial t} + \frac{M|_{x+\Delta x} - M|_x}{\Delta x} = 0 \quad (4.1)
\]

In terms of the grid indices defined in Figure 4.1a, the discretized continuity equation reads:

\[
A_j \frac{\rho^{n+1}_j - \rho^n_j}{\Delta t} + \frac{M^{n+1}_i - M^{n+1}_{i-1}}{\Delta x_j} = 0 \quad (4.2)
\]

### 4.1.2 Momentum balance

Starting point for discretization of the momentum balance is Equation 3.10. Integration is carried out over the control volume in the staggered grid, indicated in Figure 4.1c.

\[
\frac{\partial M}{\partial t} + \frac{M^2|_{x+\Delta x} - M^2|_x}{\Delta x} = -A \frac{p|_{x+\Delta x} - p|_x}{\Delta x} - K \frac{M^2}{2\rho A} - f \frac{p_{w,\text{in}} M^2}{8\rho A^2} + \rho Ag \quad (4.3)
\]

Using the upwind approximation for the mass flow rates in the convective term:

\[
\frac{M_i^{n+1} - M_i^n}{\Delta t} + \frac{M_{i+1}^{n+1} - M_{i-1}^{n+1}}{A_j + A_{j+1}} \frac{\Delta x_i}{\Delta x_j} = -A_i \frac{p_j^{n+1} - p_j^n}{\Delta x_i} - K_i \frac{M_i^{n+1} |M_i^{n+1}|}{2\Delta x_i A_j \rho^{n+1}_i} - f_i^{n+1} P_{w,\text{in}} \frac{M_i^{n+1} |M_i^{n+1}|}{8A_i^2 \rho^{n+1}_i} + \rho_i^{n+1} A_i g_i \quad (4.4)
\]

\( K_i \) is only non-zero at the location of the local frictions and \( \Delta x_i \) is by definition of the staggered grid equal to the average of \( \Delta x_j \) and \( \Delta x_{j+1} \). The friction and gravity forces on the right hand side of Equation 4.4 are defined in the centre of the momentum control volume \( i \); fluid properties other than flow rate are not defined here and are obtained by linear interpolation or by taking the upwind value. Simulations show that the choice of approximation does not influence the solution. In order to assure that the friction forces are always counter-directional
4.1. THERMAL HYDRAULICS MODEL

To the flow, the absolute value of one of the flow rates is taken in these terms. Note that no upwind approximation had to be made for the pressure gradient as result of the staggered grid definition.

4.1.3 Energy balance

The energy balance (Equation 3.12) is integrated over the control volume in Figure 4.1b,

\[ A \frac{\partial \rho h}{\partial t} + \frac{Mh|_{x+\Delta x} - Mh|_x}{\Delta x} = q' \] (4.5)

and discretized along the same lines as for the mass and momentum balances:

\[ A_j \rho_j^{n+1} h_j^{n+1} - \rho_j^n h_j^n \frac{\Delta t}{\Delta x_j} + \frac{M_i^{n+1} h_{j(i+1)}^{n+1} - M_{i-1}^{n+1} h_{j(i-1)}^{n+1}}{\Delta x_j} = q_j^{n+1} - A_j \rho_j^n \left( h_j^{n+1} - h_{HX} \right) C_{t,i} \] (4.6)

Here the upwind values are taken for enthalpy carried across the node faces with flow rate \( M \).

During the performed simulations, the heat exchanger power is set equal to the core power (as done by Jain and Rizwan-Uddin (2008) and T’Joen et al. (2012)). The model contains a forcing function at the heat exchanger outlet to impose a predefined, constant, outlet enthalpy under transient conditions. This fixes the core inlet enthalpy and the working point of the system (in combination with the selected core power). The heat flux of the forcing function is made proportional to the deviation from the desired heat exchanger outlet enthalpy, making it an explicit function of fluid enthalpy. It is therefore expressed separately from the \( q' \) term in Equation 4.6. \( C_{t,i} \) is a constant with units 1/s and is non-zero only in the control volume in which the forcing function is defined. \( C_{t,i} \) can be interpreted as the inverse of the time constant of the forcing function. Its magnitude was chosen to be \( 1/\Delta t \), as in the model of Kam (2011). Alternatively, a time constant independent of the time step can be adapted. It is found that the magnitude of this constant does not influence the steady state solution or the decay ratio and frequency of system resonances. However in high power working points the selection of a larger constant improved the rate of convergence to steady state.

Finally, the transient and convective terms are simplified somewhat by subtracting the continuity equation (Equation 4.2) multiplied with \( h_j^{n+1} \):

\[ A_j \rho_j^{n+1} h_j^{n+1} - h_j^n \frac{\Delta t}{\Delta x_j} + M_{i-1(i)}^{n+1} \frac{h_{j(i+1)}^{n+1} - h_{j-1(i)}^{n+1}}{\Delta x_j} = q_j^{n+1} - A_j \rho_j^{n+1} \left( h_j^{n+1} - h_{HX} \right) C_{t,i} \] (4.7)

4.1.4 Equation of state

Splines for density, temperature and viscosity as function of enthalpy are derived from the NIST REFPROP 7.0 database at the loop operating pressure. The assumption of constant pressure is reasonable as pressure drops in the system are small with respect to the absolute system pressure, thereby having only minor influence on fluid properties (Ortega Gómez, 2009). To construct the splines, the enthalpy range of the fluid properties is divided into subdomains, or bins. In these bins a third order polynomial fit is made to the NIST data. The splines are build up of this series of polynomials, forming an accurate and continuous fit to the original property function.
The number of bins is minimized by coupling the bin width to the gradient of the data. In this case, larger bins can be used to accurately describe low gradient regions. However, a series of time consuming if-statements is required to find the bin corresponding to a certain enthalpy. Uniform bin sizes are therefore adapted to allow for a quick bin number look-up via a linear function of enthalpy. The bin width is chosen such that the largest gradients are still captured adequately. The maximum relative error with the NIST density data is $10^{-2}\%$ for R23 and CO$_2$ property splines.

### 4.1.5 Pressure correction scheme

The conservation equations describing the unknowns $M^{n+1}$, $p^{n+1}$, $h^{n+1}$ and $\rho^{n+1}$ are coupled and non-linear, therefore, an iterative method is required to obtain the solution (Patankar, 1980). The method adapted here is the pressure correction scheme for compressible fluids presented by Bijl (1999). First, the unknown quantities in the discretized conservation equations are expressed in terms of iteration index $k$:

\[
\begin{align*}
\text{Mass:} & \quad A_j\frac{\rho_j^{k+1} - \rho_j^n}{\Delta t} + \frac{M_i^{k+1} - M_i^{k+1}}{\Delta x_j} = 0 \quad (4.8a) \\
\text{Momentum:} & \quad \frac{M_i^{k+1} - M_i^n}{\Delta t} + \frac{M_{i+1}^{k+1} - M_{i+1}^{k+1}}{A_{i+1}^\rho^{k+1}} \frac{\rho_j^{k+1}}{\Delta x_j} = -A_i \frac{\rho_j^{k+1} - \rho_j^{k+1}}{\Delta x_i} - K_i \frac{h_i^{k+1}}{2\Delta x_i A_i} \rho_i^{k+1} P_{w,i} - f_i^{k+1} P_{w,i} M_i^{k+1} M_i^{k+1} + 8A_i^2 \rho_i^{k+1} + \rho_i^{k+1} A_i g_i \quad (4.8b) \\
\text{Energy:} & \quad A_j\rho_j^n \frac{h_j^{k+1} - h_j^n}{\Delta t} + M_{i-1}^{k+1} \frac{h_{j+1}^{k+1} - h_{j-1}^{k+1}}{\Delta x_j} = q_j^{n+1} - A_j \rho_j^{k+1} \left( h_j^{k+1} - h_{HX} \right) C_{t,i} \quad (4.8c)
\end{align*}
\]

The iteration is started by estimating $h_j^{k+1}$ from the enthalpy balance. To this end, values of the previous iteration $k$ are used to approximate $M^{k+1}$ and $\rho^{k+1}$:

\[
A_j\rho_j^n \frac{h_j^{k+1} - h_j^n}{\Delta t} + M_{i-1}^{k+1} \frac{h_{j+1}^{k+1} - h_{j-1}^{k+1}}{\Delta x_j} = q_j^{n+1} - A_j \rho_j^{k+1} \left( h_j^{k+1} - h_{HX} \right) C_{t,i} \quad (4.9)
\]

The heat flux $q'$ depends on the core neutronics and is updated at the beginning of every time step $n+1$ using the previous time step density. Core neutronics are not included in the pressure correction iteration, therefore $q'$ is constant throughout each time step.

Then, using the same approach, $M^{k+1}$ is estimated from the momentum balance using the old pressure $p^k$, i.e. $M^{k+1} \left( p^{k+1} \right) \approx M^{k+1} \left( p^k \right) \equiv M^*$:

\[
\begin{align*}
\frac{M_i^* - M_i^n}{\Delta t} + \frac{M_{i+1}^{k+1} - M_{i+1}^{k+1}}{A_{i+1}^\rho^{k+1}} \frac{\rho_j^{k+1}}{\Delta x_j} = -A_i \frac{\rho_j^{k+1} - \rho_j^{k+1}}{\Delta x_i} - K_i \frac{h_i^{k+1}}{2\Delta x_i A_i} \rho_i^{k+1} + f_i^{k+1} P_{w,i} \frac{M_i^* |M_i^k|}{8A_i^2 \rho_i^{k+1}} + \rho_i^{k+1} A_i g_i \quad (4.10)
\end{align*}
\]
Here the quadratic $M^*$ terms are linearised to $M^* M^k$ to allow for matrix notation in the form of Equation 4.26. The friction factor $f^{k+1} (M^{k+1})$ is a non-linear function of the unknown flow rate and is evaluated with the flow rate from the previous iteration $k$ for the same reason.

The error made in the estimation for the flow rate, $M^{k+1} \approx M^*$, is defined as the mass flow rate correction. Similarly, the deviation of pressure from the previous iteration is defined as the pressure correction:

$$M'_i = M^{k+1}_i - M^*_i \quad (4.11)$$
$$p'_j = p^{k+1}_j - p^*_j \quad (4.12)$$

The relation between the two corrections, sometimes referred to as the flow rate or velocity correction equation, is found by subtracting the momentum balances for $M^{k+1} (p^{k+1})$ and $M^*$ while neglecting differences in acceleration and friction terms:

$$M'_i = \frac{\Delta t}{\Delta x_i} A_i (p'_j - p'_{j+1}) \quad (4.13)$$

Finally, the relation between $p'$ and $M^*$ is found from the pressure correction equation, which is obtained by taking the continuity equation and eliminating $M^{k+1}$ using the mass flow correction (Equations 4.11 and 4.13):

$$\frac{\Delta t}{\Delta x_j} \left( A_i \frac{p_j^{k+1} - p_j'}{\Delta x_i} - A_{i-1} \frac{p'_j - p'_{j-1}}{\Delta x_{i-1}} \right) = A_j \frac{p_j^{k+1} - p^n_j}{\Delta t} + \frac{M^*_i - M^*_{i-1}}{\Delta x_j} \quad (4.14)$$

Here, by employing the continuity equation, mass conservation is enforced while correcting the pressure. Solving Equation 4.14 for $p'$ gives $M'$ from Equation 4.13 and subsequently $M^{k+1}$ from Equation 4.11. $p^{k+1}$ is found directly from the pressure correction definition (Equation 4.12). This pressure correction scheme is iterated until convergence is reached. Note that $p' \to 0$ and $M^* \to M^{k+1}$ upon iteration and that Equation 4.14 reduces to the continuity equation 4.8a. The residual of the continuity equation will converge to zero and can be used to check the degree of convergence. Another criterion would be to demand the pressure correction $p'$ to be smaller than some threshold value.

The derivation of the mass flow correction equation (Equation 4.13) is typical for the pressure correction method at hand. The method of Bijl, for instance, neglects the complete acceleration terms while the often applied SIMPLE scheme includes the central contribution to the convective term. Other schemes, such as SIMPLER, SIMPLEC and PISO take more elaborate approximations into account (Ferziger and Peric, 2002). However, neglecting terms in the pressure correction equation does not influence the solution once convergence is reached. Upon convergence, the mass flow satisfies the continuity equation in all control volumes, irrespective of the pressure correction method applied. The more advanced methods can however increase the rate of convergence (Patankar, 1980). In the current work, using the method of Bijl, the implicit code is found to converge typically with one iteration per time step.

### 4.1.6 Notes with respect to the original code

The original version of the code employed the following pressure dependent EOS:

$$p^{k+1}_j = p^k_j + \frac{\partial p}{\partial T} \bigg| _j \left( T^{k+1}_j - T^k_j \right) + \frac{\partial p}{\partial p} \bigg| _j \left( p'_j - p'_{j-1} \right) \quad (4.15)$$
The properties in this model are obtained from the external NIST database. The first project objective is to define the fluid properties at constant system pressure in order to replace the computationally slow NIST calls by splines evaluations (i.e. replacing the above EOS with an enthalpy dependent spline evaluation). Removing the dependency on pressure has some consequences for the modelling approach. To start with, it makes the absolute system pressure a free variable; hence $p'$ depends only on relative pressure differences. This introduces a singularity in the system of pressure correction equations (Equations 4.14), i.e. in the matrix $A$ in $A \cdot p' = b$, an issue also addressed by Patankar (1980). It is solved by specifying a constant $p'$ value in one of the control volumes.

Then, the magnitude and location of the constant pressure correction $p'$ have to be selected. Assigning zero pressure correction has physical meaning; namely that pressure is maintained constant in the specific control volume. The natural location of this assignment would be near the buffer vessel (or reservoir) where pressure is kept close to the desired system pressure. Pressure is kept constant in the model of Kam (2011) by including a mass outflow term proportional to the deviation from set point pressure:

$$M_{buffer,i} = F(p_i - p_{set})$$  \hspace{1cm} (4.16)

Depending on the choice of the constant $F$, this buffer model affects system stability, as is further discussed in Appendix C. The advantage of the $p' = 0$ specification is that the buffer model is made obsolete, removing the related stability issues and the selection of an appropriate constant $F$. The combination of the enthalpy forcing function and the $p' = 0$ definition is equivalent to having a large reservoir connected to the loop (such as applied in the cases considered by T’Joen et al. (2012) and Jain and Rizwan-Uddin (2008)) that damps any incoming enthalpy and pressure oscillations.

Absolute pressure independency is further checked by setting the system pressure to 0MPa. Indeed the same solutions are obtained. The absolute system pressure is of course still present in the definition of the fluid property splines, assuring the correct physical solution.

The model of Kam (2011) preserves the $\frac{\partial p}{\partial t}$ term in the enthalpy balance. This leads to convergence problems for small time steps in the pressure independent model. In the original code $\frac{\partial p}{\partial t}$ is found to be small and does not significantly affect steady state mass flow rates nor resonance decay ratio and frequency. The term is neglected by several other authors, e.g. Ambrosini (2007), Yi et al. (2004), Jain and Rizwan-Uddin (2008). The $\frac{\partial p}{\partial t}$ term is omitted in this work as well to assure proper convergence at smaller time steps.

### 4.2 Reactor physics model

The point kinetics equations (Equation 3.17) are discretized using implicit time stepping:

$$\frac{n^{m+1} - n^m}{\Delta t} = \frac{\rho_{\text{reactivity}}}{\Lambda} + \frac{\rho_{m+1} - \beta}{\rho^{n+1} - \beta} n^{m+1} + \sum_{i=1}^{6} \lambda_i \xi_i^{m+1}$$  \hspace{1cm} (4.17a)

$$\frac{c_i^{m+1} - c_i^m}{\Delta t} = \frac{\beta_i n^{m+1} - \lambda_i \xi_i^{m+1}}{\Lambda}, \text{ for } i = 1...6$$  \hspace{1cm} (4.17b)

The precursor concentrations at the new time step, $\xi_i^{m+1}$, can be eliminated from the point kinetics equations in favour of the known values from the previous step, $\xi_i^m$. This results in
the following equation for the relative amount of fluctuating neutrons at time $n + 1$:

$$\left( \frac{1}{\Delta t} - \frac{\rho_{\text{reactivity}}^m n}{\Lambda} + \sum_{i=1}^{6} \frac{\lambda_i \Delta t}{1 + \lambda_i \Delta t \Lambda} \right) \tilde{n}^{m+1} = \frac{\rho_{\text{reactivity}}^m n}{\Delta t} + \sum_{i=1}^{6} \frac{\lambda_i}{1 + \lambda_i \Delta t} \tilde{q}_i^m$$  \hspace{1cm} (4.18)

Note that the reactivity is evaluated using the previous time step coolant density $\rho_i^n$, as $\rho_i^{n+1}$ is not yet obtained. After solving Equation 4.18 for $\tilde{n}^{m+1}$, the neutron fluctuation is adjusted to account for heat transfer delay (as discussed in Section 3.2.2).

The fuel rod transfer function is obtained by discretizing the time derivative in the first order model (Equation 3.19) and $z$-transforming it to the Laplace domain (Kam, 2011),

$$G_F(z) = \frac{q_p'(z)}{P'(z)} = \frac{1}{b_1 + b_2 z^{-1}}$$  \hspace{1cm} (4.19)

With:

$$b_1 = 1 + \frac{\tau}{\Delta t}$$
$$b_2 = -\frac{\tau}{\Delta t}$$  \hspace{1cm} (4.20)

Where $\Delta t$ is the time step made in the discretization of Equation 3.19.

The delayed response of coolant temperature to fluctuations in the neutron population is physically caused by the heat transfer in the fuel rod. Mathematically, it is equivalent to delay the fluctuations in the neutron population according to the fuel dynamics (while having instantaneous heat transfer from fuel to coolant) instead of delaying the heat transfer itself (Kam, 2011). Hence, Equation 4.19 can be used to define the 'effective' neutron concentration $\tilde{n}_{eff}'(z)$ contributing to the instantaneous wall heat flux:

$$G_F(z) = \frac{n_{eff}'(z)}{n'(z)} = \frac{1}{b_1 + b_2 z^{-1}}$$  \hspace{1cm} (4.21)

Taking the inverse $z$-transform gives the discrete time domain relation,

$$n_{eff}'(t) = \frac{1}{b_1} (n'(t) + b_2 n_{eff}'(t - \Delta t))$$  \hspace{1cm} (4.22)

or in terms of the time stepping index $n$:

$$\tilde{n}_{eff}^{m+1} = \frac{1}{b_1} \left( \tilde{n}_{eff}^{m+1} + b_2 n_{eff}^m \right)$$  \hspace{1cm} (4.23)

The effective power fluctuation is then easily found from Equation 3.18:

$$P_{eff}'(t) = n_{eff}'(t) P_0$$  \hspace{1cm} (4.24)

The effective power, $P_{eff}(t) = P_0 + P_{eff}'(t)$, is divided by the core length and provided to the linear flux source term of the enthalpy balance, thereby closing the coupled neutronics-thermal hydraulic set of equations.

$$q_{core}^m = \frac{P_0 + P_{eff}^m}{L_{core}} = \frac{P_0 \left( 1 + \tilde{n}_{eff}^{m+1} \right)}{L_{core}}$$  \hspace{1cm} (4.25)
4.3 Solution Algorithm

The 1D domain is divided into \( N \) equally sized control volumes. The flow in each control volume is described by the discretized enthalpy and momentum balances, in combination with the momentum and pressure correction equations, as derived in Section 4.1.5 (or the semi-implicit equations in Appendix E). The flow field along the length of the coolant channel is obtained by solving all \( N \) equations for each variable. In generic matrix notation:

\[
\mathbf{A} \mathbf{\phi} = \mathbf{s}
\]

Where \( \mathbf{\phi} \) is the vector containing the \( h^{k+1}, M^*, p' \) or \( M' \) for all control volumes. \( \mathbf{\phi} \)-independent terms are gathered in the solution vector \( \mathbf{s} \). The coefficient matrix \( \mathbf{A} \) is sparse and has specific properties for the system under consideration. First, due to the choice for first order upwinding, the diagonal elements are only related to their left and right neighbours, making the matrix tri-diagonal. Secondly, \( \mathbf{A} \) is cyclic due to the periodic nature of the loop geometry.

Cyclic tri-diagonal matrices can be solved directly, i.e. without requiring iteration, by the Sherwood-Morrison (SM) method (Press et al., 1986; Koopman, 2008). The SM method describes \( \mathbf{A} \) in terms of a non-cycle matrix \( \mathbf{A}' \) and a perturbation: \( \mathbf{A} \mathbf{\phi} = (\mathbf{A}' + \mathbf{u} \otimes \mathbf{v}) \mathbf{\phi} = \mathbf{s} \). If \( \mathbf{A} \) is defined as,

\[
\mathbf{A} = \begin{bmatrix}
a_1 & c_1 & \beta \\
b_2 & a_2 & \ddots \\
& \ddots & \ddots \\
\alpha & \cdots & a_{N-1} & c_{N-1} & b_N & a_N
\end{bmatrix}
\]

(4.27)

then \( \mathbf{A}' \), \( \mathbf{u} \) and \( \mathbf{v} \) are defined as

\[
\mathbf{A}' = \begin{bmatrix}
a_1 - \gamma & c_1 & 0 \\
b_2 & a_2 & \ddots \\
& \ddots & \ddots \\
0 & \cdots & a_{N-1} & c_{N-1} & b_N & a_N - \frac{\alpha \beta}{\gamma}
\end{bmatrix}, \quad \mathbf{u} = \begin{bmatrix}
\gamma \\
0 \\
\vdots \\
0 \\
\alpha
\end{bmatrix}, \quad \mathbf{v} = \begin{bmatrix}
1 \\
0 \\
\vdots \\
0 \\
\beta
\end{bmatrix}
\]

(4.28)

The parameter \( \gamma \) is independent and can be set to any value. If for the vectors \( \mathbf{y} \) and \( \mathbf{z} \) the following holds:

\[
\mathbf{A}' \mathbf{y} = \mathbf{s}, \quad \text{and} \quad \mathbf{A}' \mathbf{z} = \mathbf{u}
\]

(4.29)

then the solution to system 4.26 is given by:

\[
\mathbf{\phi} = \mathbf{y} - \left[ \frac{\mathbf{v} \cdot \mathbf{y}}{1 + \mathbf{v} \cdot \mathbf{z}} \right] \mathbf{z}
\]

(4.30)

The SM method reduces the problem to solving the non-cyclic systems of equations 4.29. In this work the Holmes algorithm, as described in Koopman (2008), is adopted to solve the non-cyclic systems.

The set of discretized equations is solved iteratively in each time step according to the pressure correction scheme, using the Sherwood-Morrison algorithm to solve the systems of
4.3. SOLUTION ALGORITHM

Figure 4.2 displays a flowchart of the solution algorithm of the numerical model. The pressure correction procedure is indicated by the red box. Density reactivity feedback is taken into account at the beginning of each time step using the previous time step density, $\rho^n$. At this point, the linear heating rate $q^{n+1}$ is determined. The loop for time stepping, indicated in blue in Figure 4.2, is run until the desired simulation time is reached. Also indicated in the flowchart are the initialization steps such as the loading of simulation details from the input file, allocation of variables, defining the geometry and control volumes.
30 4. NUMERICAL MODEL

Figure 4.2: Flowchart of the numerical model. The boxes indicate the two major loops in the code: time stepping (blue) and pressure correction iteration (red).
Chapter 5

The DeLight benchmark: numerical considerations

The numerical model considered in this work is benchmarked with the experimental results from the DeLight facility. For a correct representation by the model, several physical aspects of DeLight have to be identified and modelled appropriately. These include the modelling of the geometry, frictions, heat exchangers and heat losses, and are addressed separately in the following sections.

5.1 Geometry

The dimensions of the DeLight loop are implemented according to the technical drawing in the Appendix A. Only the complex geometry of the tubing to, in-between and from the heat exchangers is simplified in the current model (see Figure 5.1). This is done while preserving the length of the riser in order to maintain an equal driving force for natural circulation.

5.2 Loop friction

Wall friction is implemented by the set of friction relations in Equation 3.7. In practice, the supercritical flow in the heated sections is complex, especially near the pseudo critical point, and is not captured accurately by friction factors based on the bulk properties of isothermal, subcritical, developed flows. For instance, Yamashita et al. (2003) show that deteriorated heat transfer can occur near the pseudo critical point, resulting in increased wall temperatures and reduced wall friction.

In principle these effects can be incorporated into the model by using one of the several correlations available from experiments, see for example Fang et al. (2012) for a review. The available models introduce corrections to the single phase, isothermal, friction factor in the form of ratios of bulk and wall properties such as density, viscosity, Prandtl number or combinations of those. In the current 1D model, no information regarding wall properties is directly available. Yoon et al. (2003) recognized this issue for engineering applications and introduced a Nusselt correlation depending only on bulk and pseudo critical properties. Unfortunately, no engineering model was presented for wall friction, although its accuracy would be debatable in the first place. T’Joen et al. (2011) describe an iterative method to
Figure 5.1: DeLight model geometry. Note that not all junctions are represented in the figure and that the effective heating length in the core sections is 80cm due to the placement of the power connectors. For detailed measures see Figure A.1.

determine the wall temperature and friction using the Kirillov friction factor in combination with the Bishop Nusselt relation. This method introduces however two additional iteration steps to determine the wall temperature and velocity.

As no definite friction model for supercritical, heated flow is obtained from literature, the isothermal models provided in Equations 3.7 are implemented (the transitions between the Blasius-McAdams and McAdams-Haaland relations are set at $Re = 30,000$ and $40,000$ respectively). The absolute wall roughness of $\epsilon = 4 \cdot 10^{-7} \text{m}$ was provided by the manufacturer of the tubing (note that the same value was used by T'Joen et al. for the R23 loop).

The DeLight geometry contains several elements that cause a local loss of pressure, namely: bends, expansion/contraction, valves and the T- or cross-junctions at the sensor locations. Also included in the loop are two corrugated hoses with significant pressure drops (the hoses are installed to absorb thermal deformations of the tubing). These pressure losses are modelled as local frictions with the loss factors obtained from empirical relations (Janssen and Warmoeskerken (1997), Schmitz (2012)). The locations of the elements are indicated in Figure 5.1 and the corresponding loss factors are listed in Table 5.1.

5.3 Heat exchangers

DeLight contains two heat exchangers connected in series, as was described in Section 2.2.1. The SWEP heat exchanger is modelled such that both pressure drop and residence time are preserved. The resulting hydraulic diameter and tube length are 8.2 and 509mm, their
Table 5.1: Overview of local friction loss factors in the DeLight geometry.

<table>
<thead>
<tr>
<th>ID (mm)</th>
<th>Friction Factor $K_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sharp bends</td>
<td>6 and 10</td>
</tr>
<tr>
<td>Expansions (3cm)</td>
<td>6 $\rightarrow$ 10</td>
</tr>
<tr>
<td></td>
<td>10 $\rightarrow$ 6</td>
</tr>
<tr>
<td>T-junction</td>
<td>all</td>
</tr>
<tr>
<td>Open valves</td>
<td>all</td>
</tr>
<tr>
<td>Looking glass</td>
<td>26</td>
</tr>
<tr>
<td>Corrugated hose core inlet (50cm)</td>
<td>9.7</td>
</tr>
<tr>
<td>Corrugated hose core (23cm)</td>
<td>6.4</td>
</tr>
</tbody>
</table>

derivation can be found in Appendix B. The loss factor $K$ of the SWEP heat exchanger is measured experimentally under isothermal conditions and is found to be 5.77, with reference to a 1cm internal diameter tube. This result allows to check whether the derived model predicts the correct amount of wall friction in the SWEP. The local friction is obtained from Equation 3.9:

$$K_{\text{model}} = \frac{2\rho_{\text{avg}} \Delta p A^2}{M^2} \quad (5.1)$$

The local friction $K_{\text{model}}$ of the SWEP is found to be 2.61 (averaged over all points in the power flow map, Figure 7.14, with a standard deviation of 0.15). The wall friction in the SWEP heat exchanger model is therefore scaled with a factor of 2.21 to match the experimental value. The quantity of heat supplied to the core is removed by a negative, uniform flux in the SWEP heat exchanger, similar to the approach in the R23 and CO$_2$ loops (see Section 2.1).

The Vahterus plate shell heat exchanger is used to cool the R23 phase to the desired core inlet temperature. The large volume of this heat exchanger (in fact four times the total tubing volume) results in residence times of $\sim$2min for typical mass flow rates. The period of system oscillations is in the order of seconds, which is relatively small compared to the residence time. The heat exchanger therefore acts as a dampener to enthalpy oscillations, forcing all incoming enthalpies to the core inlet enthalpy. The Vahterus is therefore essentially modelled by the enthalpy forcing function described in Section 4.1.3. Furthermore, the R23 density at the Vahterus inlet is high (945kg/m$^3$ at 17°C, 5.7MPa) which, in combination with the large volume, results in small velocities and corresponding wall friction. Therefore the pressure drop can be neglected. The $p' = 0$ control volume is placed at the location of the buffer piston in the DeLight loop. Note that the combination of the Vahterus heat exchanger and the buffer piston is in fact taken into account by using the reservoir model used in the R23 and CO$_2$ loops (as suggested in Figure A.1).

5.4 Heat losses

The mass flow rate will be established according to the balance of friction forces and the gravitational force. Both of these need to be modelled adequately to obtain correct predictions. Friction forces were covered in Section 5.2. The gravitational driving force is invoked by density differences between riser and down comer due to core heating. However, as the
system is not ideally adiabatic, heat (or cold) losses to the environment need to be considered as they affect the magnitude of the driving force. The mechanisms of heat loss are:

- Heat conduction in the isolated sections,
- Transport by radiation and natural convection of air in non-isolated sections, i.e. core and preheater.

Conductive losses in the isolated sections can be implemented by considering a simple heat transfer model taking only the resistance in the isolating layer of Armacell into account,

\[ q'' = -\lambda \frac{T_{\text{coolant}} - T_{\text{air}}}{\ln \left( \frac{R_{\text{tube}}}{R_{\text{isolation}}} \right)} \]

The effect of including this term in the enthalpy balance is small; for a test case with riser and downcomer coolant temperatures of 70°C and -34°C respectively, the mass flow rate was reduced by 0.6%. This result can be understood by considering the R23 density as function of temperature. The fluid density is most sensitive to temperature changes around the pseudo critical point (see Figure 1.4), which is 33°C for R23 at 5.7MPa. Temperature changes of 1-2°C around the mentioned temperatures have only little effect on fluid density, explaining the minor effect on mass flow rate. Heat losses near the pseudo critical point are expected to be small as well, as the temperature difference with the environment is small. Hence, in this work it is assumed that the isolated sections are adiabatic under all conditions.

The energy supplied to the preheater is not logged during experiments and is therefore derived from the temperatures measured at the heat exchanger outlet and core inlet (see Figure A.1 for the location of the sensors). This heat flux is inserted into the model as the preheater power, automatically including conductive losses in the downcomer plus the radiative and convective losses in the preheater. Similarly, the heat loss in the core section is estimated from the measured core in- and outlet temperatures and the power applied. The loss is taken into account by a core efficiency factor (typically 1-10% of the core power).

5.5 Reactor physics

The same reactor physics model as found in the Labview code of DeLight is implemented in the numerical model. The core density is obtained by averaging over all control volumes in the core, similar to the averaging of 15 thermocouple measurements in the facility. The constants used in the point kinetics equations are directly adopted from DeLight as well and can be found in Table 2.2.
Chapter 6

Experimental procedure

This chapter will describe how the system steady state and stability are determined using the numerical model.

6.1 Acquiring steady state

Steady state is obtained by solving the time dependent transport equations while gradually increasing the reactor power to the desired level. Implicit time stepping is used (i.e. $\theta = 1$) for steady state calculations. Prior to performing simulations, grid and time step independency tests are made for each benchmark case to estimate the discretization error. These tests are made by running a series of simulations in a fixed working point for several temporal- and spatial step sizes. Different heating curves (linear, exponential and s-shaped) are proposed and their influence on the steady state solution is tested as well.

The two geometries adopted from literature (see Section 2.1) are symmetrical in the vertical axis, as both core and heat exchanger are centrally located in the horizontal sections of the loop. Starting the reactor from zero power, the coolant will have no preference for flow in either positive or negative direction. To assure positive flow, an initial flow rate of the order of 10% of the steady state flow rate is given to the fluid.

Steady states are represented by plotting mass flow rate as function of core power at fixed core inlet temperature. These curves are referred to as power flow maps.

6.2 Stability analysis

Steady state can be obtained using large time steps, which is allowed by the implicit time discretization. Stability analysis requires much smaller time steps, especially if high frequency resonances are present. To keep computational costs to a minimum, the steady state is evaluated separately from stability calculations. Steady state profiles along the loop (mass flow rate, enthalpy, pressure and density) are taken as initial condition for the small time step stability analysis. Prior to performing stability analyses, grid and time step independency tests are performed for each benchmark case. Steady state profiles are interpolated in case finer grids are required for the subsequent stability analysis. For stability analysis, the semi-implicit parameter $\theta$ is decreased to increase numerical accuracy. A value of 0.6 is chosen as
values closer to 0.5 led to model instabilities (see Appendix E for the model equations with $\theta \leq 1$).

The system stability is determined by observing the growth or decay of oscillations in any of the system variables. Oscillations can be created by perturbing one of the variables (order 1%) but are in general already induced in the first time step by the transition from the coarse steady state grid to a finer grid.

The degree of system stability is made quantitative by analysing the autocorrelation of the time signal. A mathematical representation of growing or decaying waves is fitted to the autocorrelation function, revealing both the decay ratio and the frequency of the oscillations. The fitting function used for the analysis of DeLight measurements (see Section 2.2.3) is extended with extra terms for resonances containing multiple frequencies. In case of three frequencies:

$$y = a_0 + \left(1 - a_0 - \sum_{i=2}^{4} a_i \right) e^{b_i \tau} + \sum_{i=2}^{4} a_i e^{b_i \tau} \cos(\omega_i \tau) \quad (6.1)$$

Note that the amplitude of the exponential is defined such that the amplitude at $\tau = 0$ is unity. The resonance decay ratios ($DR_i$) and frequencies ($f_i$) are then determined from the fitting parameters:

$$DR_i = e^{\frac{2\pi b_i}{|\omega_i|}} \quad (6.2)$$
$$f_i = \frac{|\omega_i|}{2\pi} \quad (6.3)$$

The non-linear fit is made using the *nlinfit.m* function from the Matlab function database. The power spectral density (PSD) is obtained by Fourier transforming the signal with *fft.m* to give additional insight into the frequency distribution.

Fitting errors of the parameters are obtained by processing the *nlinfit.m* output with the *nlparci.m* function. Absolute errors of compound properties such as the decay ratio are obtained by applying the error propagation rules, i.e.:

$$\left(\Delta DR_{i,fit}\right)^2 = \left[\frac{\partial DR_i}{\partial b_i}\right]^2 \left(\Delta b_i\right)^2 + \left[\frac{\partial DR_i}{\partial \omega_i}\right]^2 \left(\Delta \omega_i\right)^2 \quad (6.4)$$

to derive the absolute and relative errors in the decay ratio:

$$\left(\Delta DR_{i,fit}\right)^2 = \left(2\pi \frac{DR_i}{|\omega_i|}\right)^2 \left(\Delta b_i\right)^2 + \left(2\pi b_i \frac{DR_i}{|\omega_i|^2}\right)^2 \left(\Delta \omega_i\right)^2 \quad (6.5)$$
$$\epsilon_{DR,fit} = \frac{\Delta DR_{i,fit}}{DR_i} 100\% \quad (6.6)$$

Results of system stability analyses are represented by the Neutral Stability Boundary (NSB, i.e. $DR = 1$, obtained by interpolation between stable and unstable points) in the non-dimensional plane of pseudo-subcooling and pseudo-phase change numbers, as found in Ortega Gómez (2009) and T’Joen and Rohde (2012).

$$N_{PCH} = \frac{P_{core}}{Mh_{pc}} \quad (6.7)$$
$$N_{SUB} = \frac{h_{pc} - h_{in}}{h_{pc}} \quad (6.8)$$
Table 6.1: Fluid properties at the pseudo critical point (Source: NIST REFPROP 7.0).

<table>
<thead>
<tr>
<th></th>
<th>Freon R23</th>
<th>CO₂</th>
<th>H₂O</th>
</tr>
</thead>
<tbody>
<tr>
<td>Critical pressure (MPa)</td>
<td>4.83</td>
<td>7.38</td>
<td>22.06</td>
</tr>
<tr>
<td>Critical temperature (°C)</td>
<td>26.14</td>
<td>30.98</td>
<td>373.95</td>
</tr>
<tr>
<td>Operating pressure (MPa)</td>
<td>5.70</td>
<td>8.00</td>
<td>25.00</td>
</tr>
<tr>
<td>(T_{pc}) (°C)</td>
<td>33.22</td>
<td>34.67</td>
<td>384.90</td>
</tr>
<tr>
<td>(h_{pc}) (kJ/kg)</td>
<td>288.33</td>
<td>341.33</td>
<td>2152.90</td>
</tr>
</tbody>
</table>

See Table 6.1 for the enthalpies at the pseudo critical point for some coolants. The label 'phase change' originates from boiling reactors where phase change occurs. Supercritical systems do not undergo phase changes, however, similar dimensionless numbers are used because of the strong analogy with boiling systems. This is stressed by the addition of 'pseudo' to 'phase change' (Ortega Gómez, 2009). The representation in the \(N_{PCH}, N_{SUB}\) plane includes all operating points and allows for easy comparison with other scaled systems.
Chapter 7

Results

In this chapter the performance of the numerical model, as derived in Chapter 3, is assessed. The first evaluation is made according to the achieved computational savings and is given in Section 7.1.

The physical performance of the model is evaluated by comparison with the results of three reference cases, that were introduced in Chapter 2. Steady state benchmarks are made by comparing steady state mass flow rates in the plane of power versus mass flow rate. This so called power flow map is made for a range of core inlet temperatures, thereby covering most working points of the loop. System stability is represented by the Neutral Stability Boundary (NSB, separating stable and unstable regions) in the stability plane, i.e. the plane of the dimensionless pseudo phase change and sub cooling numbers ($N_{PCH}$ and $N_{SUB}$ respectively, see Section 6.2 for their definition).

The results from the two numerical literature benchmarks, i.e. the R23 and CO$_2$ loops of T’Joen et al. (2012) and Jain and Rizwan-Uddin (2008), are discussed together in Section 7.2. The comparison of the model predictions with the experimental data obtained from the DeLight facility is treated separately in Section 7.3. The steady state and stability analyses in Sections 7.2 and 7.3 are addressed in the subsections.

7.1 Computational time savings

The first objective of this work is to reduce the required computational time. To this end, the NIST REFPROP database, that was used to evaluate the equation of state (of density, temperature and viscosity), is replaced by property splines. The splines evaluate the fluid property using a series of polynomials, that are defined in separate bins (see Section 4.1.4). Two types of splines were tested; the first with a minimal number of bins (variable bin size), the second with a minimal number of if-statements (uniform bin size). A reduction of 60% computational time is achieved by introducing splines in favour of the NIST REFPROP database, see Figure 7.1. No differences in computational time were found between the two types of splines, however the uniform bin spline simplified the coding.

In general, steady states are obtained within 15 minutes whereas stability analysis requires typically 3 hours. Obviously, these times depend on the maximum allowed discretization error and the number of simulated resonance periods.
7. RESULTS

Figure 7.1: Illustration of the computational time saving achieved by replacing the NIST REFPROP database calls by spline evaluations. The data is based on 7 simulations, ran on several hours of the day.

7.2 Literature benchmarks

7.2.1 Steady state

Grid and time step independency test
For the grid independency test, the steady state mass flow rate is calculated for a range of spatial discretization steps. The corresponding trend is normalized by the mass flow rate of the finest grid, to result in the plot displayed in Figure 7.2. Note that the solution does not show a converging trend, however, the change in flow rate with step size is small. The discretization error is estimated by extrapolating the trend to infinitely small discretization steps, in this particular case resulting in an error of less than one promille. The grid independency test is performed for two core powers. The high power case requires a finer grid to acquire the same accuracy; this is explained by the fact that the enthalpy gradient in the heated sections is larger. A similar analysis is made to examine the sensitivity of the solution to the selected time step. Figure 7.2 shows that the relative difference between the mass flow rates is of the order of $10^{-5}$, indicating that the solution is relatively insensitive to the temporal step size, as may be expected for steady state calculations. In fact, the reactor start-up time was maintained equal for all cases; the reduced accuracy at larger steps may therefore be caused by the smaller amount of steps, rather than by the step size itself.

Grid independency test of the CO$_2$ and DeLight loops show similar trends and are left to Appendix D.1. It is concluded from these graphs that steady state can be calculated on coarse grids without significant loss of accuracy, i.e. the discretization error for steady state calculations is negligible. A summary of the selected grids is given in Table 7.1.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>$\Delta t$ (s)</th>
<th>$\Delta x$ (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R23 loop</td>
<td>1</td>
<td>0.5</td>
</tr>
<tr>
<td>CO$_2$ loop</td>
<td>1</td>
<td>5</td>
</tr>
<tr>
<td>DeLight</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 7.1: Spatial- and temporal discretization step sizes selected for steady state calculations.
Steady state benchmark

The steady state behaviour of the model is benchmarked with the reference data of T’Joen et al. (2012) and Jain and Rizwan-Uddin (2008). This is done by comparing the power flow maps, see Figures 7.3 and 7.4. The maximum relative errors are below 1% for both cases, indicating a close match of the two results.

The power flow maps show a particular trend: increasing flow rate at low power and decreasing flow rate at high power. The flow rate of natural circulating loops is determined by the balance of buoyancy and frictional forces. At low power, velocity and corresponding friction is small, resulting in the flow rate to increase with core power due to the decreasing density (that generates buoyancy). Velocity increases with power in the whole power range while the density decrease flattens at enthalpies above the pseudo critical point (see Figure 1.4). Hence, at high power, friction starts to dominate buoyancy, resulting in a decrease of flow rate with power. Reduction of the core inlet temperature shifts the maximum as more power is required to acquire the same core outlet enthalpy.

Note that the CO$_2$ loop has a large tube diameter (7.5 vs. 0.6cm) and riser length (10 vs. 2m) compared to the R23 loop. The tube diameter determines the wall friction and, together with the riser length, the weight of the coolant column. The CO$_2$ loop therefore has more driving force and less wall friction, resulting in considerably higher flow rates, as is observed in Figures 7.3 and 7.4.

7.2.2 Stability

Obtaining the oscillation decay ratio and frequency

Perturbations are made to the steady state solution to induce flow rate oscillations in the loop. The decay ratio and frequency of this oscillation indicate the stability of the flow (stable if DR<1) and may reveal the origin of the instability (as the inverse of the frequency compares to the transit time of the relevant loop component). Their values are obtained from the time signal of the core outlet temperature, using the non-linear fit described in Section 6.2. An
Figure 7.3: The predicted power flow maps of the R23 loop for several core inlet temperatures. The results of T'Joen et al. (2012) are matched within 1% of relative error.

Figure 7.4: The predicted power flow map of the CO₂ loop at a core inlet temperature of 25°C. The map is compared to the result reported by Jain and Rizwan-Uddin (2008), showing good agreement (with relative errors below 1%).
containing three frequencies. In general, for the analyses made in this thesis, the fitting error of the decay ratio is found to be well below 1%, with few outliers of 2 to 3% in case of multiple frequency fits. The error in frequency is below 0.5%. At last, the stability is independent of the type of perturbation made to the system. For instance, the perturbation can be made to any of the system variables, e.g.: the core power, core inlet mass flow rate or enthalpy. In the simulations performed in this work, the system was perturbed naturally by using the coarse grid steady state solution as the initial condition for the fine grid calculations.

Figure 7.5: Time series of an unstable resonance (a), the Power Spectral Density revealing three distinct frequencies (b) and the autocorrelation function with the frequencies and decay ratios obtained from the non-linear fit (c) (1/5 of the fitted data points are shown). This example is taken from the analysis of the R23 loop, in the working point \( N_{PCH} = 0.616, N_{SUB} = 0.119 \).
7. RESULTS

Figure 7.6: Grid and time step independency test for stability analysis of the CO$_2$ loop in the working point $N_{PCH} = 1.67, N_{SUB} = 0.117$. The system contains oscillations of three frequencies in this working point; the decay ratios are plotted for each frequency component. The semi-implicit time stepping parameter, $\theta$, is set to 0.6 in these simulations.

Figure 7.7: Grid and time step independency test for stability analysis of the R23 loop ($N_{PCH} = 0.809, N_{SUB} = 0.085$). A semi-implicit time stepping parameter, $\theta$, of 0.6 is used, except for the two implicit cases (i.e. $\theta = 1$) indicated in the legend.

gradients, that are more susceptible to numerical diffusion. Note that the data is sampled at least every 10ms, excluding the possibility of under sampling. Based on these findings, smaller spatial steps are selected for the working points containing higher frequencies.

The frequencies found in the three benchmark cases differ and are roughly categorized as low frequency (<1Hz) or high frequency (>1Hz). For instance, to capture the high frequency oscillations in the R23 loop a grid of 0.25cm and 1ms semi-implicit time stepping is selected. A summary of the selected grids for all benchmark cases is given in Table 7.2. The relative discretization errors estimated from the grid and time step independency tests are provided here as well. Note that the step sizes are considerably smaller than those selected by Kam
7.2. LITERATURE BENCHMARKS

Table 7.2: Selected grids for stability analysis. The semi-implicit parameter $\theta$ is chosen 0.6 in all cases. The relative discretization errors are estimated from the grid and time step independency tests. The errors for high frequencies are further specified for two groups of frequencies.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>$\Delta t$ (ms)</th>
<th>$\Delta x$ (cm)</th>
<th>Errors (%) $\Delta t/\Delta x$</th>
<th>$\Delta t$ (ms)</th>
<th>$\Delta x$ (cm)</th>
<th>Errors (%) $\sim 2Hz$</th>
<th>$\sim 3Hz$</th>
</tr>
</thead>
<tbody>
<tr>
<td>R23 loop</td>
<td>1</td>
<td>0.5</td>
<td>1 / 3</td>
<td>1</td>
<td>0.25</td>
<td>1 / 5</td>
<td>1 / 6</td>
</tr>
<tr>
<td>CO$_2$ loop</td>
<td>1</td>
<td>5</td>
<td>1 / 2</td>
<td>1</td>
<td>2.5</td>
<td>1 / 5</td>
<td>2 / 10</td>
</tr>
<tr>
<td>DeLight</td>
<td>2.5</td>
<td>1</td>
<td>1 / 4</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

(2011), who used a grid of 1cm and 25ms time step.

Stability benchmark

Shown in Figures 7.8 and 7.9 are the NSB benchmarks. In general, the simulated NSBs correspond well to the respective literature references. Figure 7.9 shows that the location of the reservoir greatly affects the system NSB. The reservoir dampens enthalpy fluctuations in the downcomer; its position therefore determines the amount of density fluctuations in the downcomer. These fluctuations enhance gravitationally driven instabilities, possibly explaining the decreased system stability if the reservoir is placed at the core inlet.

![Stability benchmark with results of the CO$_2$ loop. Also included in the figure is the stability data provided by T’Joen for the same loop.](image-url)
Remarkable is the occurrence of distinct frequency regions (separated by the kinks in the NSB, see also Figure 7.10) if the reservoir is placed in the bottom of the downcomer. The sharp frequency transitions might, at first sight, be related to numerical effects, however, this peculiar behaviour is predicted by a very different model as well (i.e. the linear frequency domain code of T’Joen et al.). Only one single group of low frequencies is observed when the reservoir is placed in the top of the downcomer (see Figure 7.11). The reason for this interesting effect of the reservoir location was not found in the course of this work.

According to BWR stability analysis, the resonance frequency is related to the transit time of the section in which the physical feedback mechanism drives the instability (see Section 1.2). A plot of the resonance frequencies along the NSB of the R23 loop are given in Figure 7.11, together with the frequencies associated with several components, such as the core, riser and the whole loop itself. The latter frequencies are calculated by taking the inverse transit time, i.e. integrated steady state velocity over component length. Following the analogy with BWR stability, low frequencies should relate to the riser length (type I instability) and high frequencies to the core length (type II instability). These relations are however not obvious for the current case, despite the fact that the NSB displays a similar ‘bump’ as observed for the BWR (Van Bragt and Van der Hagen, 1998). The low, mid and high frequency modes correspond roughly to the transit time of the downcomer, riser and core. A similar analysis

Figure 7.9: Stability map of the R23 loop for two placements of the reservoir: in the top of the downcomer (a) and at the bottom of the downcomer (b). Indicated are the effects of defining zero core- or heat exchanger friction and of applying core in- or outlet frictions (the latter effect is only shown in case the reservoir is located in the top of the downcomer).
7.2. LITERATURE BENCHMARKS

Figure 7.10: Full PSD data along the R23 loop NSB (left) and comparison of the PSD maxima with the frequency data reported by T’Joen et al. (2012) (right). The transitions between the distinct frequency groups are made at $N_{PCH} = 0.6$ and $0.8$, the same location as the kinks in the NSB.

is made for the CO$_2$ loop of which the results can be found in Appendix D.3.

Type II instabilities are driven by the frictional pressure drop in the core (Van Bragt and Van der Hagen, 1998). In order to further exclude the presence of type II instabilities, the core wall friction is set to zero in a small selection of working points. The heat exchanger has the inverse function of the core and is considered in the analysis as well. For both core and heat exchanger, no significant changes are observed in the resonance decay ratio and frequency if the friction is set to zero (see Figure 7.9), implying that the instabilities have a

Figure 7.11: Frequency identification in the R23 loop in case the reservoir is placed at the bottom of the downcomer (left) or at the top (right). Note that core and heat exchanger have the same length and (opposite) heat flux, the residence time of both components is therefore the same.
different origin. It must be noted that the loop of Van Bragt and Van der Hagen (1998) has a large diameter riser whereas the riser of the R23 loop has the same diameter as the core. The different friction distribution in- and around the core may disrupt the direct analogy to the BWR findings.

Changing the heat exchanger length, and thus transit time, by a factor of two has no significant effect on the stability line (see Appendix, Figure D.4), confirming again that the heat exchanger does not contribute to system instability. As last note, it is remarkable that the low frequency branch of the NSB line occurs at an approximately constant mass flow rate of 0.018kg/s (shown in Figure D.4 as well).

Indicated in Figure 7.9 is the effect of applying core in- and outlet frictions. Inlet friction stabilizes whereas outlet frictions destabilize, as is observed as well by for instance Ortega Gómez (2009). According to Boure et al. (1973), inlet friction tends to dampen oscillations in the high density inflow, thereby stabilizing the system. Imposing extra friction at the core outlet increases the core outlet pressure drop and the corresponding gain of the feedback, thereby amplifying type II instabilities (see discussion on Type II instabilities in Section 1.2).

The combined error in the decay ratio and frequency is given by the squared sum of absolute non-linear fit and temporal and spatial discretization errors. In all cases the fitting error is negligible with respect to the discretization errors. At higher frequencies the solution becomes more sensitive to the spatial step size. The discretization error made in this work is relatively large (6 and 10% for the R23 and CO$_2$ loops respectively), possibly explaining the deviations of the NSB with the references at large $N_{PCH}$.

### 7.3 DeLight benchmark

#### 7.3.1 Steady state

**Reactor start-up and steady state profiles**

The natural circulating flow is started by increasing the core power up to the steady state power. Several heating curves are considered; see Figure 7.12. The steady state is found to be independent of the start-up history, as expected. The S-shaped heating curve is selected for further simulations as it shows a minimal amount of oscillating behaviour (thereby minimizing the gradients in the system). Figure 7.12 illustrates that the core outlet enthalpy is directly related to the core power and that the mass flow rate follows the trajectory of a typical power flow map.

Steady state profiles of enthalpy, density, pressure and velocity for the DeLight geometry are presented in Figure 7.13 to illustrate the system during typical operation. The mass flow rate is constant over the length of the loop. Several sections in the loop can be identified in these profiles, as indicated. Here, it can for instance be seen that enthalpy increases linearly along the heated sections while density decreases in a non-linear manner (according to the non-linearity of the EOS, Figure 1.4). Note the HPLWR core power distribution (53/30/17% to evaporator, superheater 1 and 2) is visible in the enthalpy profile. The loop contains contractions at the core entrance and exit that cause a velocity increase and decrease respectively. The velocity increases along the core sections are due to the decrease in density upon heating. The same but opposite behaviour of the velocity is observed in the heat exchanger.

At zero power (and flow) the pressure profile is fully determined by static effects, as
indicated by the dashed line. Due to low steady state velocities in the downcomer, the pressure drop in the downcomer is mainly determined by static effects. In core- and riser sections however, the hydrostatic pressure reduces because of decreasing density. At the same time, the frictional pressure drop due to wall- and local friction increases, resulting in a rather different pressure profile. For instance, the local frictions in- and around the core become apparent as small steps in the pressure profile.
Figure 7.13: Steady state pressure, velocity, enthalpy and density profiles along the length of the DeLight loop. Locations of several loop elements (preheater, evaporator, super heater 1, super heater 2 and heat exchanger) are indicated. Working point: core power = 7 kW, $T_{inlet} = 0^\circ\text{C}$. 
7.3. DELIGHT BENCHMARK

Steady state benchmark

The power flow maps of the DeLight geometry are plotted in Figure 7.14. The relative error between measurement and simulation remains below 5%, except for the case with an inlet temperature of 0°C, where errors up to 8% are found. The latter case is built up out of two separate measurement series, performed with distinct heat exchanger outlet temperatures of -29 and -11°C respectively. Preheater powers are selected such that the core inlet temperature is equal to 0°C. The system is modelled accordingly, however, in contrast to the measurement, the numerical model predicts a discontinuity in the power flow map. The discontinuity is caused by the fact that the higher heat exchanger outlet temperature decreases the downcomer density by 8%, thereby reducing the driving force and corresponding mass flow rate. Note that the friction factor is modelled according to the combination of Blasius, McAdams and Haaland relations. The transitions between these models are not necessarily smooth and can possibly result in discontinuities in the power flow maps. The Reynolds number for cases with inlet temperatures of 0°C is however such that only the Haaland friction factor is applied in all control volumes of the loop. The transition between friction models is thereby excluded as cause for the kink in the power flow map. The fact that the discontinuity is not observed in the measurements indicates that there are remaining physical aspects of the facility that have not been identified yet.

In general, the power flow maps of the model display the same trends as the experiment.

![Figure 7.14:](image)

Figure 7.14: Power flow map benchmark for the DeLight geometry at several core inlet temperatures. The results for the cases with inlet temperatures of -27, -12 and 17°C are within 5% of relative error, the case of 0°C within 8%.
This implies that friction is correctly distributed over the downcomer and riser. One could argue that the flow rate is determined by the integral friction over the loop and not the local distribution. As the flow rate matches for the entire operating window, in which each working point has a different density distribution, we can however safely assume that friction is distributed correctly.

### 7.3.2 Stability

**Thermal hydraulic calculations**

First the thermal hydraulic stability (i.e. not including density reactivity feedback) of the DeLight facility is predicted by the numerical model. The resulting NSB line is presented in the bottom right plot of Figure 7.15. No thermal hydraulic instabilities were observed during measurements, however, an unstable system is predicted by the model. Interestingly, this observation has also been made for the loop at Argonne National Laboratory by Jain and Corradini (2006), who did not find the cause of the discrepancy.

![Stability map for the DeLight geometry](image)

**Figure 7.15:** Stability map for the DeLight geometry, top: comparison of the experimental and numerical results for several fuel time constants, bottom: the effect of the time constant on the experimental and numerical results separately. The thermal hydraulic case is indicated as 'zero reactivity', the other simulations are performed with a HPLWR reactivity constant of $3.5 \times 10^{-5}$ kg/m$^3$. The dashed line indicates where the core outlet enthalpy is at the pseudo critical value.
Several types of errors are made in the modelling of DeLight, these include: errors in identifying the physics of the system, errors in the modelling of the identified physics and discretization errors. The discretization error leads to numerical diffusion and would in fact stabilize the system, in contrast to what is observed (i.e. the model prediction is more unstable than the measurement).

With respect to the modelling errors, the thermal hydraulic model was benchmarked with the two literature cases, as described in the previous section. This benchmark validates the implementation of the conservation laws. However, several simplifications with respect to the modelling of some specific components of DeLight, such as the core, heat exchangers and tubing, are made.

One of the simplifications is the instantaneous supply of the core power to the coolant, by which it is essentially assumed that the tubing has zero heat capacity. In reality, the tubing causes thermal inertia and the heat transfer from wall to coolant depends on the difference between coolant and wall temperature. The resulting dynamic behaviour can dampen enthalpy oscillations, thereby stabilizing the system. The assumption of zero heat capacity of core tubes may explain the more unstable NSB predicted by the model, especially at high powers (and \( N_{PCH} \)) were the effect is more pronounced (Ambrosini, 2012).

In addition, the core power is adjusted for heat losses to the environment (that are obtained from core in- and outlet thermocouple measurements), thereby lumping all local losses together. The heat loss, however, depends on the wall temperature, which increases along the length of the core, and is therefore in fact non-uniformly distributed. Also, the Haaland friction model, for subcritical, isothermal flows is not valid in the heated sections, were the radial flow profile differs from developed flow. Due to these approximations, the actual enthalpy is distributed differently along the length of the core than predicted by the model, possibly affecting the stability.

Similar errors are made in the modelling of the heat exchangers. On top of that, the geometry of the heat exchangers is considerably more complex than the tubing in the core and is not specified exactly by the manufacturers. The large volume of the Vahterus heat exchanger is not included in the loop during the benchmarks. The inertia of the large coolant mass present in the Vahterus may have a dampening effect on inflow oscillations. Additional simulations, however, show that including the Vahterus volume, using various combinations of length and diameter, does not significantly affect system stability.

Core inlet frictions are known to have a stabilizing effect whereas core outlet frictions destabilize (Ortega Gómez, 2009). Hence, an incorrect friction model can affect the location of the NSB. The correct trend in power flow maps implies that the friction distribution is represented well and is unlikely to cause the discrepancy between model and measurement, unless system stability is more sensitive to small deviations in the friction distribution (e.g. due to uncertainties in the wall roughness). T’Joen et al. (2011) report that the selection of friction model can affect the stability line of heated vertical pipes up to 18% (comparing Haaland and Blasius). Small variations in tube diameter (1.6%) resulted in shifts of stability line by 6 to 12%, indicating that system stability may in fact be very sensitive to uncertainties in the friction distribution.

Last but not least, there may be several physical phenomena present in the DeLight facility that have strong impact on the NSB but are not yet identified.
Reactor physics calculations
The presence of density reactivity feedback decreases the system stability (see Figure 7.15), as is observed in experiments as well. However, the location of the NSB differs, especially at high $N_{PCH}$. The obtained NSB is similar to the result of Kam (2011), even though the original buffer model, affecting system stability in a non-physical way (see Appendix C), is now replaced by the $p' = 0$ definition (see Section 4.1.6).

Variation of the fuel time constant has only little impact on the location of the modelled NSB. This is not expected according to measurements. Van Bragt and Van der Hagen (1998) observe for BWR’s that low frequency, type I, oscillations are stabilized by intermediate fuel time constants. Small and large constants have a stabilizing effect. Although the NSB’s of $\tau = 2, 4, 6s$ in Figure 7.15 lay close to each other and are therefore hard to distinguish, an analogous trend is observed here.

The same reactor physics model, including all constants, is implemented in DeLight and the numerical model. Therefore similar results are expected and the deviation between model and experiment is more likely caused by the issues concerning the thermal hydraulics model, that were discussed in the above paragraphs.
Chapter 8

Conclusions

8.1 Conclusions

The aim of the current work was to develop a numerical model capable of predicting the Neutral Stability Boundary (NSB, i.e. decay ratio = 1) of natural circulation SCWRs, in particular of the DeLight experimental facility. First, computational demands of the existing model were reduced by 60% by replacing the slow NIST REFPROP fluid property database with pressure independent splines. The assumption of pressure independent fluid properties resulted in an overdetermined system of equations in the pressure correction model. This was resolved by defining zero pressure correction in one of the control volumes as is done by Patankar (1980). The pressure cannot change in this control volume and, effectively, acts as if it is connected to a mass buffer that maintains constant system pressure. The original buffer model implemented by Kam (2011), that was shown to affect system stability in an undesired manner, is thereby made obsolete.

8.1.1 Literature benchmarks

A time step independency test showed that the steady state solution can be evaluated with coarse time steps; this allowed the calculations to be performed within 15 minutes. The steady state solution was not affected by the shape of the start-up power curve. The model was benchmarked with the steady state solutions of the cases presented by Jain and Rizwan-Uddin (2008) and T’Joen et al. (2012). The results matched within 1% of relative error.

The stability analyses presented by Jain and Rizwan-Uddin (2008) and T’Joen et al. (2012) were used to benchmark the model under purely thermal hydraulic conditions. Grid and time step independency tests showed that the discretization error (with respect to the decay ratio) decreased linearly with step size whereas the computational time increased non-linearly. No fully grid independent decay ratio was obtained within reasonable computational times, therefore a trade-off between computational time and error was made while selecting the grids. Temporal- and spatial steps of 1ms and 0.25-5cm were selected, where the smaller grids were used for working points with high frequency resonances. The consequent error made in the decay ratio was of the order of 5-10% for high frequencies. Despite this error, the thermal hydraulic model was capable of accurately reconstructing the location and characteristics of the NSBs presented by Jain and Rizwan-Uddin (2008) and T’Joen et al. (2012). These benchmarks validated the thermal hydraulics model.
The benchmarks confirmed the presence of regions of dominant frequencies in the stability plane of the R23 and CO\textsubscript{2} loops, as observed in the results of the linear, frequency domain COMSOL model of T’Joen et al. (2012). In addition, it was found that the system destabilized if the reservoir (that implies constant enthalpy and pressure) was placed close to the core, possibly due to presence of density fluctuations in the downcomer that may induce gravitationally driven instabilities. The distinct frequencies did not occur if the reservoir was placed at the top of the downcomer, an observation for which no explanation was found within this work. Linking the frequencies to the inverse transit time of several loop components (core, riser, whole loop) did not result in a further physical understanding of their occurrence (e.g. by linking them to analogous BWR instabilities).

8.1.2 DeLight benchmark

The steady state mass flow rates of the experimental DeLight facility were predicted within 8\% of relative error over the whole operating range of core inlet temperatures and powers. The accurate prediction of the trend in flow rate as function of core power was achieved by implementing all local pressure drops due to bends, valves, expansions and the T-junctions at sensor entry points. The DeLight stability boundary was, however, not predicted accurately by the model. Experiments show that DeLight is thermal hydraulically stable whereas the model predicts an unstable operating window. Including neutronic-thermal hydraulic coupling into the model destabilized the system, as was observed by experiment. The location of the NSB differs however, especially at high core powers, where the model predicted a more unstable system. The same reactor physics model was applied in the DeLight facility and the numerical model. The deviation of the NSB calculated with density reactivity feedback is therefore most likely related to the offset already introduced by errors in the thermal hydraulic model. According to the parameter study for the fuel time constant, the heat transfer delay due to the fuel pellets and claddings has only little effect on the NSB, which is not expected according to experiment. Hence, it is concluded that the current model is not able to accurately predict the physics related flow instability of experimental systems.

8.2 Outlook

The discrepancy between the numerical and experimental NSBs of the DeLight facility may be caused by one of the simplifications made while modelling the physics of DeLight, e.g.: the implementation of a subcritical, isothermal friction model in a supercritical heated flow or the assumption of zero heat capacity of the heated sections. The last approximation may be improved by modelling the wall temperature of the core and heat exchangers, including appropriate transfer functions to the coolant and environment. By the initiative of Ambrosini et al., a joint investigation is started to further assess the impact of this kind of heat transfer models.

Another approach is to perform a sensitivity analysis to reveal which parameters in fact have an impact on system stability. This study can include uncertainties in, for instance, wall roughness, reactivity constant and heat losses to the environment. Other parameters known to affect stability, such as local friction distribution and the location of the reservoir, can be considered as well. As a result of this studies, the models that specifically involve the more
sensitive parameters can be identified and improved. This work will be part of future studies performed in the PNR group.

The current model is discretized using a first order upwind scheme, which is susceptible to numerical diffusion. Higher order schemes, such as second order upwind (optionally with flux limiters to be Total Variation Diminishing (TVD)), can be implemented to acquire more accurate solutions. In this case, the computational time can be reduced further while maintaining the same discretization error.

To obtain more physical insight into the origin of system instabilities, system identification methods (possibly in the frequency domain) may be considered. These methods can provide phase / gain information for the several loop components. Components may be identified as the origin of system instability if large phase shifts or gains are found at the observed oscillation frequency.
Bibliography


Appendix A

DeLight technical drawing

Figure A.1: DeLight technical drawing. Indicated are the measures of the components and the location of some sensors (legend: F - flow meter, T - thermocouple, P - absolute pressure sensor). See Figure 2.2 for a more complete indication of the sensors.
Appendix B

Modelling of the SWEP heat exchanger

The SWEP heat exchanger consists of 28 parallel plates, resulting in 14 primary- and secondary side parallel channels. The hydraulic diameter of a single channel is found from the dimensions provided on the SWEP website. Objective here is to find the single pipe model equivalent of the parallel channel heat exchanger, as indicated in Figure B.1.

The pressure drop over each parallel channel,

\[ \Delta p = \frac{1}{2} \rho \left( u_{HX,\text{channel}} \right)^2 f \left( Re_{HX} \right) \frac{L_{HX}}{D_{h,HX}} \]  

(B.1)

equals to the overall pressure drop over the heat exchanger. If scaling of transient and convective terms is neglected, the pressure drop over the heat exchanger has to equal the model pressure drop:

\[ \Delta p = \frac{1}{2} \rho \left( u_{\text{model}} \right)^2 f \left( Re_{\text{model}} \right) \frac{L_{\text{model}}}{D_{h,\text{model}}} \]  

(B.2)

The total mass flow rate \( M \) is the same for model and physical heat exchanger. Then:

\[ u_{\text{model}} = \frac{M}{\rho A_{\text{model}}} \]  

(B.3a)

\[ u_{HX,\text{channel}} = \frac{M}{N_{\text{channels}} \rho A_{HX,\text{channel}}} \]  

(B.3b)

It can be assumed that the density profile along the length of modelled and physical heat exchangers is the same. Equalling Equations B.1 and B.2 while neglecting differences in

\[ L, \Delta p_{\text{channel}}, u_{\text{channel}} \]  
\[ L_{\text{model}}, \Delta p_{\text{model}}, u_{\text{model}} \]

Figure B.1: The parallel channel SWEP heat exchanger depicted with hydraulic diameter equivalent channels (a) and the single pipe heat exchanger for modelling purposes (b).
friction factors and density profiles results in:

\[
\frac{L_{\text{model}}}{L_{\text{HX}}} = \left( \frac{D_{h,\text{model}}}{D_{h,\text{HX}}} \right)^5 \left( \frac{1}{N_{\text{channels}}} \right)^2
\]  
(B.4)

The occurrence of instabilities is related to the residence times in the system (see Chapter 1.2). Therefore, equal residence times \((\tau = \frac{L}{u})\) are posed for the heat exchanger and its model. This leads to the second scaling relation of the SWEP heat exchanger:

\[
\frac{L_{\text{model}}}{L_{\text{HX}}} = \frac{D_{h,\text{channel}}^2}{D_{h,\text{model}}^2} N_{\text{channels}}
\]  
(B.5)

Solving Equations B.4 and B.5 leads to:

\[
D_{h,\text{model}} = (N_{\text{channels}})^{3/7} D_{h,\text{channel}} \quad \text{(B.6a)}
\]

\[
L_{h,\text{model}} = (N_{\text{channels}})^{1/7} L_{h,\text{channel}} \quad \text{(B.6b)}
\]
Appendix C

Analysis of the original buffer model

Pressure was kept constant in the original model by including a mass outflow term;

\[ M_{\text{buffer},i} = F(p_i - p_{\text{set}}) \]  \hspace{1cm} (C.1)

This buffer model was originally defined over multiple (~100) control volumes but is reduced to a single control volume to keep the following analysis comprehensible. First, the magnitude of the model constant \( F \) greatly affects the resonance decay ratio of the loop, shown in Figure C.1. No buffering (\( F = 0 \)) is indicated here by the dashed line.

![Figure C.1: Decay ratio as function of buffer proportionality constant \( F \).](image)

In the limit of \( F \) to zero the two lines merge asymptotically. In this region (\( F < 10^{-8} \)) only little mass is removed, as is seen by the small amplitude difference in the time series of buffer control volume in- and outflows, displayed in Figure C.2(a,b). With increasing \( F \), the inflow oscillation is dampened as more mass is removed due to the larger gain of the system. A minimum in decay ratio is observed around \( F = 10^{-7} \) where the perturbation on the inflow is removed nearly instantaneously; amplitudes of inflow and flow to the buffer are equal (Figure C.2c). This is a turning point. For larger \( F \) the gain is such that the flow rate to the buffer is actually larger than the inflow. More mass is removed than present in the flow, leading to a 180° phase shift between in- and outflows, plus an amplification of the resonance. Interesting is the stabilization of this behaviour for \( F > 10^{-5} \) (Figure C.2(d,e)).
It is questionable which model constant $F$ to use. Only the limit of $F$ to zero appears to be appropriate as the decay ratio is not sensitive to changes in $F$ in this region and that no more mass is removed than flowing into the system. The DeLight facility works with a movable piston. The expected time constant of this system is too large to effectively dampen incoming oscillations of about 1Hz. Hence, for this case the best choice would be $F = 0$ as well. Defining the buffer over multiple control volumes can result in a series of phase shifts for large $F$ and is therefore not advised.

In the current, pressure independent, model, as described in Section 4.1.6, the issue of maintaining the loop pressure constant is solved by the $p' = 0$ definition in one of the control volumes. The advantage of this approach is that no $F$ has to be selected.
Appendix D

Additional results

D.1 Grid and time step in dependency tests

Steady state

Figure D.1: Steady state grid and time step independency test for the CO$_2$ loop (working point: $N_{PCCH},N_{SUB} = 0.438, 0.229$).
Figure D.2: Steady state grid and time step independency test for DeLight (working point: \(N_{PCH}, N_{SUB} = 0.260, 0.360\)).

**Stability**

Figure D.3: Stability analysis grid and time step independency test for DeLight (working point: \(N_{PCH}, N_{SUB} = 1.75, 0.09\)).
D.2 Variation of heat exchanger length in R23 loop

Figure D.4: Stability map of the R23 loop for two placements of the reservoir: in the top of the downcomer (a) and at the bottom of the downcomer (b). Indicated as well are the effects of defining zero core- or heat exchanger friction.
D.3 Resonance frequencies CO₂ loop

Figure D.5: Frequencies along the NSB of the CO₂ loop.

Figure D.6: Identification of frequencies in the CO₂ loop.
Appendix E

Derivation of a semi-implicit scheme

The implicit time stepping scheme is unconditionally stable but is prone to numerical diffusion. Explicit schemes on the other hand, are accurate but require small time steps to assure stability. The advantages of both schemes are combined in the semi-implicit scheme, in which a weighted average of both explicit and implicit terms contributes. Following up on the compressible flow model, this leads to the following model adaptations (Bijl, 1999).

Continuity

\[ A_j \frac{\rho_j^{n+1} - \rho_j^n}{\Delta t} + \theta \left( \frac{M_i^{n+1} - M_i^{n+1}}{\Delta x_j} \right) + (1 - \theta) \left( \frac{M_i^n - M_i^n}{\Delta x_j} \right) = 0 \]  (E.1)

Enthalpy

Introducing the semi-implicit scheme to the discretized enthalpy balance (Equation 4.6):

\[ A_j \frac{\rho_j^{n+1} h_j^{n+1} - \rho_j^n h_j^n}{\Delta t} + \frac{M_i^{n+1} h_j^{n+1} - h_j^{n+1} - M_i^{n+1} h_j^{n+1} - M_i^{n+1} h_j^{n+1} - M_i^{n+1} h_j^{n+1}}{\Delta x_j} + (1 - \theta) \left( \frac{M_i^n h_j^{n}}{\Delta x_j} \right) = \theta q_j^{n+1} + (1 - \theta) q_j^n - \theta A_j \rho_j^{n+1} \left( h_j^{n+1} - h_H X \right) C_t,i - (1 - \theta) A_j \rho_j^n \left( h_j^n - h_H X \right) C_t,i \]  (E.2)

Subtraction of the continuity equation (Equation E.1) multiplied with \( h_j^{n+1} \) results in:

\[ A_j \rho_j^n \frac{h_j^{n+1} - h_j^n}{\Delta t} + \rho_j^n \frac{h_j^{n+1}}{\Delta x_j} \left( M_i^{n+1} - M_i^{n+1} \right) + (1 - \theta) \left( \frac{M_i^n h_j^{n+1}}{\Delta x_j} \right) = \theta q_j^{n+1} + (1 - \theta) q_j^n - \theta A_j \rho_j^{n+1} \left( h_j^{n+1} - h_H X \right) C_t,i \]  (E.3)

\[- (1 - \theta) \left( \frac{M_i^n - M_i^n}{\Delta x_j} \right) h_j^{n+1} = \theta q_j^{n+1} + (1 - \theta) q_j^n - \theta A_j \rho_j^{n+1} \left( h_j^{n+1} - h_H X \right) C_t,i \]

Introducing iteration variables and estimating \( M_j^{k+1} \) and \( \rho_j^{k+1} \) with the value of iteration \( k \):

\[ A_j \rho_j^n \frac{h_j^{k+1} - h_j^n}{\Delta t} + \rho_j^n \frac{h_j^{k+1}}{\Delta x_j} \left( M_i^n - M_i^n \right) + (1 - \theta) \left( \frac{M_i^n h_j^{k+1}}{\Delta x_j} \right) = \theta q_j^{k+1} + (1 - \theta) q_j^n - \theta A_j \rho_j^k \left( h_j^{k+1} - h_H X \right) C_t,i \]  (E.4)
This system can be solved for $h^{k+1}$. Density, temperature and viscosity at iteration $k + 1$ are now obtained using the splines.

**Momentum**

The discretized equation with iteration variables (Equation 4.8b) in semi-implicit form:

$$
\frac{M_i^{k+1} - M_i^n}{\Delta t} + \theta \frac{M_i^{k+1} - M_i^{n+1}}{\Delta x_i} \frac{M_i^{k+1} - M_i^{k-1}}{A_j\rho_j} + (1 - \theta) \frac{M_i^n - M_i^{n-1}}{A_j\rho_j} = 
$$

$$
- \theta A_i \frac{p_j^{k+1} - p_j^k}{\Delta x_i} - (1 - \theta) A_i \frac{p_j^{n+1} - p_j^n}{\Delta x_i} - \theta K_i \frac{M_i^{k+1} + M_i^k}{2\Delta x_i A_i\rho_i^{k+1}} - (1 - \theta) K_i \frac{M_i^n + M_i^n}{2\Delta x_i A_i\rho_i^n} 
$$

$$
- \theta f_i^{k+1} P_{w,i} \frac{M_i^{k+1} |M_i^k|}{8A_i^2\rho_i^{k+1}} - (1 - \theta) f_i^n P_{w,i} \frac{M_i^n |M_i^n|}{8A_i^2\rho_i^n} + \theta g_i A_i\rho_i^{k+1} + (1 - \theta) g_i A_i\rho_i^n 
$$

(E.5)

**M\textsuperscript{s}** equation:

$$
\frac{M_i^* - M_i^n}{\Delta t} + \theta \frac{M_i^* - M_i^{n+1}}{\Delta x_i} \frac{M_i^* - M_i^{n-1}}{A_j\rho_j} + (1 - \theta) \frac{M_i^n - M_i^{n-1}}{A_j\rho_j} = 
$$

$$
- \theta A_i \frac{p_j^{k+1} - p_j^k}{\Delta x_i} - (1 - \theta) A_i \frac{p_j^{n+1} - p_j^n}{\Delta x_i} - \theta K_i \frac{M_i^* |M_i^k|}{2\Delta x_i A_i\rho_i^{k+1}} - (1 - \theta) K_i \frac{M_i^n |M_i^n|}{2\Delta x_i A_i\rho_i^n} 
$$

$$
- \theta f_i^{k+1} P_{w,i} \frac{M_i^* |M_i^k|}{8A_i^2\rho_i^{k+1}} - (1 - \theta) f_i^n P_{w,i} \frac{M_i^n |M_i^n|}{8A_i^2\rho_i^n} + \theta g_i A_i\rho_i^{k+1} + (1 - \theta) g_i A_i\rho_i^n 
$$

(E.6)

Subtracting both equations while neglecting differences in convective and friction terms leads to the velocity correction equation:

$$
M_i' = \theta \frac{\Delta t}{\Delta x_i} A_i (p_j - p_j^{k+1}) 
$$

(E.7)

The pressure correction equation is found again by taking the continuity equation,

$$
A_i \frac{\rho_j^{k+1} - \rho_j^n}{\Delta t} + \theta \left( \frac{M_i^{k+1} - M_i^{k-1}}{\Delta x_i} \right) + (1 - \theta) \left( \frac{M_i^n - M_i^{n-1}}{\Delta x_i} \right) = 0 
$$

(E.8)

and substituting:

$$
M_i^{k+1} = M_i^* + M_i' = M_i^* + \theta \frac{\Delta t}{\Delta x_i} A_i (p_j' - p_j^{k+1}) 
$$

(E.9)

to give:

$$
\frac{\Delta t}{\Delta x_i} \left( A_i \frac{p_j^{k+1} - p_j^k}{\Delta x_i} - A_i \frac{p_j^n - p_j^{n-1}}{\Delta x_i} \right) = A_i \frac{p_j^{k+1} - p_j^n}{\theta^2} \frac{\Delta t}{\Delta t} + \frac{1}{\theta^2} \frac{M_i^* - M_i^{n-1}}{\Delta x_j} 
$$

(E.10)
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<td>$b$</td>
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<td>Constant</td>
</tr>
<tr>
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<td>$#/m^3$</td>
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<td>Heaviside step function</td>
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**Greek symbols**

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<td>--------</td>
<td>-----------</td>
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</tr>
<tr>
<td>Λ</td>
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</tr>
<tr>
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<td>Pa s</td>
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<tr>
<td>φ</td>
<td>J/m$^3$ s</td>
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<td>τ</td>
<td>s</td>
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Subscripts
- 0: Steady state value
- coolant: Coolant property
- core: Core property
- eff: Effective instantaneous quantity after delay by fuel transfer function
- F: Fuel property
- HX: Heat exchanger property
- i: Precursor group
- (i): Spatial discretization index of staggered grid
- (i)]: Spatial discretization index in case of negative flows
- j: Spatial discretization index
- reactivity: Density reactivity
- w: Wall property

Superscripts
- ′: Pressure correction
- ˜: Perturbation
- k: Pressure correction iteration index
- n: Time stepping index

Dimensionless groups
- $N_{PCH}$: \( \frac{P}{\frac{M_{n}h_{pc}}{h_{pc}-h_{in}}} \)
- $N_{SUB}$: \( \frac{h_{pc}}{MD_{pc}} \)
- $Re$: \( \frac{MD}{A\mu} \)

Acronyms
- BWR: Boiling Water Reactor
- DeLight: Delft Light water reactor
- DWO: Density Wave Oscillation
- EOS: Equation Of State
- ESBWR: Economic Simplified Boiling Water Reactor
- HPLWR: High Performance Light Water Reactor
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