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Abstract

The large change in density which occurs when supercritical water is heated above or near to the pseudocritical temperature in a vertical channel can result in the onset of flow instabilities (density wave oscillations). Near to the critical point, substance properties such as enthalpy, density, viscosity… all have larger relative uncertainties compared to subcritical conditions. The goal of this study is to quantify the effect of these property uncertainties and system uncertainties on numerically determined stability boundaries. These boundaries were determined through an eigenvalue analysis of the linearised set of equations. The sensitivity analysis is performed in a forward way. The results show that the impact of the density and viscosity tolerance individually as well as that of the uncertainty of the imposed pressure drop are negligible. The tolerance on the derivative of the density with regard to the enthalpy propagates only noticeably at low N_{SUB} numbers (T_{in} > 370°C). The friction factor and the heat flux distribution uncertainties have a comparable effect, being more pronounced near the bend in the stability curve. The most significant uncertainty was found to be that of the geometry, even a ± 25µm uncertainty on length scales results in a large uncertainty. The results also showed that the stability boundary is linked to the friction distribution rather than its average value, and that different correlations result in strong changes of the predicted boundary. This emphasizes the need for an accurate friction correlation for supercritical fluids. These findings are important to assess the design of experimental facilities which use scaling fluids.

Keywords: supercritical fluid, linear stability analysis, uncertainty boundaries

Introduction

Despite the harsh requirements a supercritical fluid imposes on applications (due to the high pressure and temperature and possible strong corrosion), a strong drive exists to use supercritical fluids in a range of different applications. One of the prime movers is the power cycle for electricity generation (e.g. the Rankine cycle with a turbine). By raising the working pressure and temperature of the fluid, the cycle efficiency can be increased (Carnot law). This has lead to the development of (ultra-) supercritical coal fired electricity plants with a steam pressure as high as 33 MPa which are currently in operation worldwide (e.g. in Japan, Denmark or the United States [1]). Using supercritical water has also been proposed for the power cycle of the Generation IV advanced nuclear reactor designs (the Supercritical Water Reactor – SCWR, [2]), as this not only results in increased thermal efficiency but also result in a reduced complexity of the auxiliary systems and components, cutting investment costs, as highlighted by Buongiorno and Macdonald [3]. On a smaller power scale there has been a lot of interest to use supercritical CO_2 as a natural refrigerant instead of Freon based hydrocarbons in compression cooling cycles as part of the ongoing struggle to reduce greenhouse gas emissions (see e.g. Kim et al. [4]). Supercritical organic fluids are also considered for ORC cycles aimed at low temperature energy recovery, Schuster et al. [5].

As such, supercritical fluids have attracted and continue to attract a lot of research interest. This has resulted in a very large number of papers published in technical literature dealing with different aspects of these fluids or the technical systems in which they are used. This paper focuses on the aspect of the *stability of the flow in a vertical heated channel*. It is well known from earlier research in boiling channels that the flow can become unstable. Bouré et al. [6] presented a classification of the different types of instabilities. A static instability (flow excursion, the so called Ledinegg instability) can be described using only the steady state equations. In this case, a small change in the flow conditions will result in a new steady state not equal to the original one. For dynamic instabilities, such as density wave oscillations or DWO, the steady equations are not sufficient to predict the system behavior, or the threshold of instability. March-Leuba and Rey [7] presented a detailed explanation of the DWO and the feedback mechanisms, which is driven by the interaction of inertia and friction for the thermo-hydraulic modes. In a nuclear reactor another feedback mechanism is present: the neutronic feedback which couples the instant fluid density to the power production through the moderation and a fuel time constant. This results in a much more complex behavior, as shown by Van Bragt et al. [8] for the ESBWR reactor and recently by Yi et al. [9] for the US design of a SCWR.

This study considers a heated channel with supercritical fluid flowing upwards. This case is identical to the one considered by Ambrosini and Sharabi [10] and will be described in detail in the next section. Neutronic feedback is not considered. As is well known, the uncertainty on fluid properties near the critical point can be quite large. There is also no consensus with regards to the friction correlations

which should be used for supercritical fluids. This study thus aims at quantifying the impact of the substance property and system uncertainties on the predicted linear stability boundaries. This study is also interesting from a scaling view point as well. In experimental facilities often other fluids are used to alleviate pressure and temperature constraints (e.g. supercritical R23 to mimic the behavior of supercritical water, Rohde et al. [11] or boiling R134a to mimic water in Marcel et al. [12]). It would be interesting to know the significance of the uncertainties in this scenario, and see how this affects the idea of scaling.

Model description

The proposed system is a single heated vertical tube with a length of 4.2672 m (14 feet) with upwards flow, shown in Fig. 1. It is identical to the one considered by Ambrosini and Sharabi [10], but for clarity the geometric parameters will be repeated here. Ambrosini and Sharabi [10] state that the geometric and operational properties were freely inspired by those proposed for a square lattice in a previous stability analysis (e.g. Yi et al. [13]). In such a lattice the fuel rods are enclosed between two parallel plates due to the presence of a moderator box. This type of fuel assembly is typical for thermal reactors with supercritical water. The tube connects two reservoirs with a fixed pressure, so the pressure drop over the channel is a constant imposed value (0.14 MPa). The proposed system thus mimics a single fuel channel present in a reactor core, whereby the pressure drop is imposed by the remainder of the core. The temperature and pressure are set at the inlet of the channel and local orifices can be placed at the inlet and outlet of the channel. The geometric data of the system can be found in the left column of Table 1.

To describe the thermo-hydraulic behavior of this system, a set of equations is needed. For this study a 1-D approach was chosen, whereby the properties are averaged out over the cross section of the tube. The code thus calculates so called ‘bulk averaged properties’. This is a standard approach in many system codes used today in the nuclear industry (TRACE, LAPUR, RELAP5 among others) as it allows to model large complex systems within a reasonable time frame. The equation set consists of the time dependent conservation of mass, momentum and energy, expressed as a function of the mass flux (G), pressure (p) and enthalpy (h). These are equations (1)-(3). To close this system of equations an equation of state is needed, linking the fluid density to the variables. Because the density varies much less with pressure than with enthalpy, and the pressure change of the system is small (0.14 MPa compared to the system pressure of 25 MPa), the density is described as a function of enthalpy only (Eq. (4)). In the equation for the momentum conservation, the Darcy-Weisbach friction factor is used in combination with local C_j friction values for the orifices (as indicated by the delta function). θ indicates the angle relative to the horizontal axis, which is set to 0° in this study.

$$\frac{\partial \rho}{\partial t} + \frac{\partial G}{\partial z} = 0 \qquad (1)$$

$$\frac{\partial G}{\partial t}+\frac{\partial}{\partial z}\left(\frac{G^2}{\rho}\right)=-\frac{\partial p}{\partial z}-g\rho\sin\theta-\frac{G^2}{2\rho}\left[\frac{f}{D_h}+C_j\delta\left(z-z_j\right)\right] \tag{2}$$

$$\frac{\partial \rho h}{\partial t}+\frac{\partial\left(Gh\right)}{\partial z}=\frac{q''P_h}{A} \tag{3}$$

$$\rho=f\left(h\right) \tag{4}$$

To describe the behavior of a supercritical system non-dimensional numbers have been derived. These have been mostly inspired by the earlier work done on boiling systems, seeking to extend the concept of the subcooling number and the phase change number into the supercritical range, as can be read in Ortega Gómez et al. [14] and Ambrosini and Sharabi [10]. Ambrosini [15] showed that the stability of a heated pipe with a supercritical fluid is similar to that of a boiling channel, experiencing both Ledinegg instabilities and DWO. Based on his analysis, he defined the 'sub pseudocritical number' N_{SUBPC} and the 'trans pseudocritical number' N_{TPC} to define the stability plane. Based on the considered set of equations ((1)-(4)) Marcel et al. [16] proposed a scaling procedure to preserve the stability behavior of a supercritical loop system. They suggested the pseudo phase change number N_{PCH} (Eq. (5)) and used the conditions at the inlet of the tube as reference values. This procedure was later slightly modified by Rohde et al. [11] to include friction scaling. They also used the pseudo phase change number and defined a subcooling number (Eq. (6)), but suggested to use the pseudocritical values as reference. As a result the non-dimensional numbers used by Rohde et al. [11] only differ from those suggested by Ambrosini [15] by replacing the constant ($\frac{\beta_{pc}}{C_{p,pc}}$) with ($\frac{1}{h_{pc}}$). The pseudocritical values which were used as reference value are presented in Table 2. In the remainder of this work N_{PCH} and N_{SUB} will be used.

$$N_{PCH}=\frac{q''\cdot P_h\cdot L}{G_{in}\cdot A\cdot h_{pc}} \tag{5}$$

$$N_{SUB}=\frac{\left(h_{pc}-h_{in}\right)}{h_{pc}} \tag{6}$$

Different methods exist to study the stability behavior of the proposed system. First, the steady state solution of the equations is determined given a set of boundary conditions. In this case, the boundary conditions are the imposed pressure drop, the inlet enthalpy and the heat flux on the wall. Based on this solution, different numerical methods can be used to determine the stability, these include transient simulations [15] and [19], Laplace transformation [8], eigenvalue analysis of the linearized set of perturbed equations [17] and derivation of a characteristic equation based on the linearized set of perturbed equations [18]. In this study, an eigenvalue analysis is used. Ambrosini [20] and Ambrosini and Sharabi [10] compared three different methods to determine the stability

boundary for a similar system as studied in this paper: a linearised code using eigenvalue analysis (non dimensional form), a transient dimensional code and a system code (RELAP5). The results showed very good agreement, and considering the diversity of these tools, they provide adequate confidence on their general reliability.

Numerical implementation

To simulate the system, a numerical model is required. This model was built in the Comsol© software package. This is a finite element analysis software environment for the modelling and simulation of so called 'multi-physics' problems where different phenomena interact. Standard modules exist to add e.g. 1-D flow and heat transfer problems, but in this study the basic 1-D PDE coefficient mode was used whereby the equations are added to the model, and Comsol acts as the solver. To fit in the predefined Comsol© PDE coefficient structure, the equations had to be rewritten in a slightly different form from Eqs. (1-3) to Eqs. (7-9). Important to note is that to this end the static pressure *p* was transformed into the dynamic pressure *P* in the momentum equation (Eq. (10)), to result in a form with only one spatial partial derivative. As such the solved variables are now enthalpy *h*, dynamic pressure *P* and mass flux *G*. The derivative of the specific volume with regards to the enthalpy can be rewritten through Eq. (11) as a function of the density derivative. Ortega Gómez et al. [14] previously used the same set of equations in Comsol©. By neglecting the coupling between the momentum and energy conservation equation (pressure work term), it is easier to solve the set of equations. By making an initial guess for the mass flux, the enthalpy profile can be determined. These enthalpy values can then be used to compute the substance properties and then solving the momentum equation. By then iterating until the pressure difference over the tube equals the prescribed value, the solution can be found.

$$\frac{\partial h}{\partial t} = \upsilon^2 \frac{\partial G}{\partial z}\left(\frac{\partial \upsilon}{\partial h}\right)_p^{-1} \tag{7}$$

$$\frac{\partial G}{\partial t} = -\frac{\partial P}{\partial z} - \frac{g}{\upsilon}\sin\theta - \frac{G^2\upsilon}{2}\left[\frac{f}{D_h} + C_j\delta\left(z - z_j\right)\right] \tag{8}$$

$$\frac{\partial h}{\partial t} + G\upsilon\frac{\partial h}{\partial z} = \frac{q''P_h\upsilon}{A} \tag{9}$$

$$p + G^2\upsilon = P \tag{10}$$

$$\left(\frac{\partial \upsilon}{\partial h}\right)_p = -\frac{1}{\rho^2}\frac{\partial \rho}{\partial h} \tag{11}$$

This set of equations was programmed in combination with the geometry and the boundary conditions. The numerical domain consists of three separate zones, one for the heated section and then upstream and downstream a small section for the orifice. Local frictions are thus implemented as short tube sections. The length of these sections was set to 0.05 m in order to be consistent with the results presented by Ambrosini and Sharabi [10]. Their steady state pressure graph shows a sharp drop in pressure at the inlet consistent with the local orifice over a distance of 0.05m. In these sections the effects of gravity and wall friction are neglected, to clearly separate these effects from the local friction. To start the calculations, all the variables are initialized in the domain. An initial mass flux value G is guessed and applied to all cells. Based on the imposed heat flux q'' and the inlet enthalpy h_{in} (fixed value) the enthalpy profile is computed and imposed. The pressure drop is imposed by setting the static pressure p at the inlet to 0 and to 0.14 MPa at the end. The dynamic pressure is initialized as a linear function between these two values.

Model verification

Comsol makes use of 'shape functions' to build the final solution. Different types of shape functions are available (Lagrange, Hermite) of which the order can be set as well, ranging from 1^{st} to 5^{th} order. In this study Lagrange elements were used of order 5, similar to what was used by Ortega Gomez et al. [14]. It was found that reducing the order of the elements down to two or changing the type to Hermite had no effect on the final solutions (both the predicted steady state and the predicted stability line were the same). It was verified that the variables were conserved. A grid independence study was performed. It was found that the predicted steady state mass flux and the stability line are very insensitive to the number of elements used in the simulations: the largest difference in N_{PCH} values between a simulation with 22 cells and the reference case (220 cells) was less than 0.5%. The convergence time for a simulation was slightly reduced by having more than one cell describing the local orifices. A grid distribution of 110 cells was selected with 5 cells in each orifice zone, and 100 in the heated section. This grid was used for the presented simulations.

To determine the steady state solution a numerical solver routine has to be selected. Different solvers were compared, and the UMFPACK routine was finally selected. The convergence criterion was set to 1e-8, and most cases converged within 20 iterations. Setting this value lower had no effect on the mass flux prediction. To determine the stability behavior of the system, the eigenvalue approach was selected. Comsol© offers the option to linearize the system around the computed steady state solution, and then to determine the eigenvalues of this new set of equations. The sign of the eigenvalue with the largest real part then indicates if the system is stable or not. The same solver routine was used (UMFPACK) and a set of 10 eigenvalues were determined and sorted.

To define the substance properties, the NIST REFPROP (v7) database was used. The density and viscosity at 25 MPa were determined as a function of the enthalpy over a wide range of temperatures (20°C to 1500 °C). Ortega Gómez et al. [14] previously studied the effect of various approximations to define supercritical fluid properties (e.g. a two or three region model, as introduced by Zhao et al. [21]), and they found that these approximations have a significant impact on the results. This was also reported by Jain and Corradini [22] who found that a very small change in the equation of state near the pseudocritical point had a very significant impact on the computed eigenvalues. Therefore great care was taken to ensure the fluid properties are well defined by using a series of splines. These are based on data points which are carefully spread over the selected temperature range, concentrating more points near the pseudocritical point to capture the steep change. A comparison between the density and viscosity data from the NIST REFPROP data between 20 °C and 1500 °C evaluated every 0.1 °C shows a maximum difference of 0.2% compared to the spline interpolations. In particular care had to be taken to define $\frac{\partial \rho}{\partial h}$. To determine this property, the central difference approximation was used on a fine mesh of tabulated density and enthalpy values. It is important that this mesh is sufficiently fine, as determining the derivative based on a coarse mesh will result in a very different curve shape of the derivative as a function of the enthalpy. This is shown in Fig. 2, where the $\frac{\partial \rho}{\partial h}$ is set out as a function of h for different meshes which vary in mesh size from 10°C to 0.1°C. As can be seen in Fig 2 the effect is obvious near the pseudocritical point, and very significant for the coarser meshes. The mesh of 10°C and 5°C clearly show a very different trend with an additional saddle point, a higher minimum value which occurs at lower temperatures. Only at smaller mesh sizes the curves converge to the same shape and the same minimum value. The impact of the mesh size is summarized further in Table 3. As can be seen, provided the mesh size is smaller than or equal to 0.5°C, the location of the minimum can be well predicted. However to make sure the difference between the predicted value at the minimum is small enough, a mesh size of 0.2°C or smaller is needed. In the remainder of this work, the derivative data is based on the mesh of 0.1°C.

Model validation

To ensure the proposed model results in an accurate simulation of the steady state and the stability behavior, a detailed comparison will be presented to the data of Ambrosini and Sharabi [10]. The considered operational parameters can be found in the right column of Table 1. As can be seen the friction factor in the heated section was set to a constant value of 0.0352, eliminating the dependence on the Reynolds number. Ambrosini and Sharabi [10] compared the results of two different codes and found good agreement with regards to the predicted stability boundary. However, for these two codes the inlet and exit orifice pressure drop coefficient values were different (20 and 1, versus 10.5 and 0).

They state this is due to "*the different formulation of the pressure drop and the particular treatment of the inlet and exit acceleration losses*". Considering our code has no additional treatment for these losses, the orifice pressure drop coefficient values had to be varied in order to match with their presented pressure drop profile. This resulted in the values of 27 and 0.75 for inlet and exit orifice coefficient respectively. The resulting agreement can be seen in Fig. 3. As can be seen the model with the fitted orifice coefficients provides a good agreement with the pressure distribution. It was verified that including the gravity and frictional terms in the momentum equation for the orifices has a negligible effect. The differences with the reported values in the paper by Ambrosini and Sharabi [10] can in part due to the data being read manually from a graph. Figure 4 shows a comparison of the predicted temperature and velocity distribution. This figure thus highlights that the code predicts the mass flow rate correctly as the temperature increase is the same; the agreement between the velocity distributions further shows that the density distribution is also captured well. As such the steady state characteristics of the proposed model are well validated.

As a second validation task, the ability to predict the stability boundary must be verified. To this end an iterative algorithm was written which scans the stability plane. This algorithm requires a scanning range of N_{SUB} numbers to be provided, the number of points to be considered in between and an initial power (heat flux). It then starts off at the highest N_{SUB} value, determines a steady state solution and the accompanying eigenvalue set and examines the sign of the eigenvalue with the largest real part. It then changes the power (decreasing if the system is unstable, increasing if it is stable) until the eigenvalue changes sign. It will then iterate in between these two eigenvalues with different signs using the 'pegasus' approach [23], to converge up to 1e-6. Once this eigenvalue is found, it moves to the next N_{SUB} value and the same process repeats itself. The resulting stability boundary can be seen in Fig 5, where it is compared to the results of Ambrosini and Sharabi [10] (black symbols). Note that they presented their data using N_{SUBPC} and N_{TPC}, and that these were converted using the values listed in Table 2. As can be seen the agreement is good, however there were some small differences as the model predicted the boundary at slightly lower N_{PCH} values for high N_{SUB} and at slightly smaller N_{PCH} values for low N_{SUB}. In a personal communication Ambrosini [24] provided an updated version of his stability boundary based on a finer grid of 96 cells..As can be seen there are small shifts in the boundary (white symbols) and these move towards the solution of our model. The same trend was shown for a comparable geometry in a recent paper (Ambrosini [20]). This validates our models ability to predict the stability boundary, and this model can now be applied to study the impact of any uncertainties on the result.

Unfortunately there are no experimental stability data available to validate these simulations further, so only numerical data can be used. This is of course due to the complexity of setting up such an experiment, in particular the difficulties related to the very high pressure and temperature when

operating with water, the high power requirements, and the difficulty in maintaining a constant pressure drop over the channel as a boundary condition. This could be realized by having a very large bypass operating in parallel with the studied tube, but this further makes the system even more expensive. From a code validation point, such experimental data could be of great use. Perhaps by using scaling analysis, a feasible experimental setup could be developed in the future to provide this kind of validation data.

Results

The proposed validated model will now be used to study the impact of different parameter uncertainties on the predicted stability boundary. Three different types of uncertainties are considered: the fluid properties, the geometry and the system parameters.

Impact of the substance properties

The IAPWS formulation for the substance properties of water provides an overview of the estimated uncertainty on the calculated density [25] and enthalpy [26]. These estimates were derived based on a comparison of various sets of experimental data, and are presented in the form of charts which indicate regions of relative tolerance $\frac{\Delta\rho}{\rho}$ and $\frac{\Delta h}{h}$. There is a strong increase in the relative tolerance values near to the critical point, with the maximum occurring in a triangle region bordered by the two isochores of 527 and 144 kg/m³ and 30 MPa. A conservative estimate was done for the tolerance for densities lower than 144 kg/m³: the graphs presented in [25]- [26] suggest that the density tolerance first decreases to 0.05% before increasing again to 0.25% starting from 500 °C, it was chosen to neglect this small zone (90°C width) with lower tolerance, and just have the higher tolerance start from 144 kg/m³. This had only a negligible effect on the final results. Table 4 lists the used values within this study and their ranges. In the computations these values were considered as the 1σ bounds, and as such twice these values were used as the upper and lower uncertainty bound.

Figure 6A illustrates the effect of the density. This was determined by calculating the upper and lower density bounds ρ^+ and ρ^- and the corresponding spline sets (e.g. $\rho^+ = \rho + 2\Delta\rho$). As can be seen, the effect of the density tolerance on the stability boundary is negligible. For most N_{SUB} values the curves almost collapse, only at very small values (< 0.1) and near the ‘bend’ of the stability line there are noticeable differences. Near the bend the difference between the curves is in the order of 0.4%; and for very low N_{SUB} values this difference increases to 1%. A comparison of the predicted steady state mass flux values as a function of power for three different N_{SUB} values (0.1, 0.5 and 0.9) indicated that the largest difference induced by the density tolerance was 0.4%.

The difference increases as N_{SUB} becomes lower and N_{PCH} increases (larger relative impact of the density tolerance), which explains the trend of the increasing difference between the stability curves for lower N_{SUB} values.

Figure 6B illustrates the combined effect of the enthalpy and density tolerance. As the code computes the enthalpy profile *h*, the spline formulation for the density and the density derivative was done as follows. Firstly, one assumes that the computed h profile actually represents either the upper (h^+) or lower bound (h^-) of the actual enthalpy profile h^*. This actual profile can be determined based on the known enthalpy tolerance Δh (see Table 4 for the tolerance values, $h^* = h \pm 2\Delta h$). A density profile ρ^* is linked to this enthalpy profile h^* through the original spline, and this density profile has a tolerance $\Delta\rho$, resulting in a ρ^+ and ρ^- profile. The derivative $\frac{\partial \rho}{\partial h}$ can then be computed using a sufficiently fine temperature mesh (0.1°C). Four combinations can be realised: $\frac{\partial \rho^+}{\partial h^+}$, $\frac{\partial \rho^-}{\partial h^+}$, $\frac{\partial \rho^+}{\partial h^-}$ and $\frac{\partial \rho^-}{\partial h^-}$. These were then added to the code as series of splines as a function of h^*. As such e.g. for $\frac{\partial \rho^+}{\partial h^+}$ and ρ^+ are a function of h^* and not of the computed enthalpy profile *h*. This results in a small shift of the derivative profile shown in Fig. 2 to either left or right depending on the selection of h^+ or h^-. Also, the N_{SUB} values must be computed based on h^* and not *h*, resulting in a small shift of the stability boundary to higher or lower N_{SUB} values. At high N_{SUB} values, the curves (Fig 6B) are very close to each other with a difference of less than 1% for $N_{SUB} > 0.2$. But for lower N_{SUB} values this difference quickly grows to 6% as the stability curve has a very steep gradient in this zone. In this section of the stability plane, the resulting variation in N_{SUB} number is about 0.015, which for an N_{SUB} value of 0.15 corresponds to an inlet temperature variation of 2.5°C. Near to $N_{SUB} = 0$ this difference of course quickly reduces as the temperature-enthalpy curve is very flat near T_{pc}.

Just as other substance properties, the dynamic viscosity μ has a tolerance, which varies over the considered temperature range, as described in [27]. The values used in this study are listed in Table 5. So similar as for the density, two new spline sets were generated μ^+ and μ^-, which were then used to compute the stability boundary. In order for the viscosity to affect the result, the friction factor must be a function of the Reynolds number instead of a constant value in the heated channel. The Haaland friction relationship ([28], Eq. (12)) was chosen to this end. It is an approximation of the more exact but implicit Colebrook equation for a fully turbulent flow in a tube. It is one of many different explicit formulations but it does provide a good accuracy over a wide range of conditions ($4000 < Re < 10^8$, $10^{-6} < \frac{\varepsilon}{D_h} < 5.\ 10^{-2}$), as shown by e.g. Sonnad and Goudar [29]. It was also used by Ortéga Gómez et al. [14] in their study. To compute the friction factor using Eq. (12) a surface roughness value is needed. This value was set to $4\ 10^{-6}$ m, which results in averaged values ranging from 0.025 to 0.023 for points on the stability boundary. This is significantly different from the model constant of 0.0352. The

selected roughness value was specified for the stainless steel tubes which are used in the experimental setup DeLight [11]. Ortéga Gómez et al. [14] and Ambrosini [20] previously considered a roughness value of 3 10^{-5} and 2.5 10^{-5} respectively, which provide a closer match to the model constant of 0.0352. The results are shown in Fig. 7. As can be seen, just as for the density, this tolerance has only a negligible effect. Only at the lowest N_{SUB} numbers the μ^+ and μ^- stability boundaries deviate slightly from the base case (~ 1.6%).

$$f = \left[-1.8 \log\left(\left(\frac{\varepsilon}{3.7 \cdot D_h} \right)^{1.11} + \frac{6.9}{\mathrm{Re}} \right) \right]^{-2} \tag{12}$$

Impact of the geometric parameters

When constructing a fuel assembly, a tolerance will be specified which the final result must comply with. As such, all dimensions are specified with an uncertainty value. In this study two uncertainty values were considered all for the geometric properties (fuel rod diameter, rod-to-wall distance and lattice pitch): 50 µm and 25 µm. Using standard error propagation rules (as described by e.g. Taylor [30]) the uncertainties ΔA and ΔD_h were determined. By adding/subtracting twice these values (for a 95% confidence interval) to A and D_h the upper and lower bounds of the geometric parameters were computed: A^+, A^-, D_h^+ and D_h^-. No tolerance was imposed on the length L, as it was preferred to always use exactly the same numerical domain. Also, because of the high manufacturing standard in the nuclear industry, any relative tolerance on the length can be estimated to be small to negligible. The results are shown in Fig. 8. As can be seen, the geometric parameters have a very significant impact on the stability boundary, much stronger than the density and enthalpy combined. As expected, the ±25 µm curve lies halfway between the ±50 µm curves. The ±50 µm tolerance corresponds to an uncertainty of ±1.6% on the hydraulic diameter and ±2.4% of the surface area. The resulting tolerance on the boundary varies between 6% and 12% (±50 µm), with the highest difference occurring at the lowest N_{SUB} values. A relative increase of the surface area and hydraulic diameter reduces friction, and thus stabilizes the system, whereas a decrease destabilizes it. This strong effect of the geometry is driven by two interactions. Firstly, in the momentum equation (Eq. (8)) a reduction of D_h corresponds to a relative increase of the friction factor. At the same time the reduction of the surface area A results in a increased heat flux through the energy equation (Eq. (9)). This further increases the density gradient, promoting instabilities. This is an important finding for setting up an experimental facility: small surface area and D_h uncertainties have a significant impact.

Impact of the friction factor relationship

Figure 9A shows the stability boundary for a constant (black) and a variable friction factor (Haaland relationship, red). The variable friction scenario is more stable (shifted to the right) due to the lower friction values. The curve shape is not exactly the same, it is slightly 'tilted' compared to the original curve. This is because the friction profile over the tube length changes significantly as N_{SUB} varies. This is highlighted in Fig. 9B. The two red curves show the tube friction profile at two extreme N_{SUB} values (0.9 and 0.1). At high N_{SUB} values (cold inlet), the friction is high at the inlet of the tube, while at low N_{SUB} values, the friction increases towards the exit of the tube. This is linked to the dynamic viscosity, which has a minimum at the pseudocritical temperature, and as such high N_{SUB} values result in a strong rise of the *Re* values through the pipe, whereas for low N_{SUB} values, a moderate drop off occurs. To better highlight the impact of the friction distribution, two artificial friction curves were programmed: 'linear upward' and 'linear downward'. These are shown in Fig. 9B (blue and green). They have the same mean value (0.0352), but the end points are shifted 10% higher or lower than the mean value. As can be seen from Fig 9A, having more friction in the first half of the tube stabilizes the system, with a slight shift to the right, and adding more friction in the second half of the tube destabilizes the system. As such it is clear that it is not the mean friction value which is of importance, but the overall friction distribution through the system. This finding is important when considering the scaling of these systems, as previously noted by Rohde et al. [11]. These results are consistent with the effects of adding a local friction: increasing C_{in} stabilizes the system, whereas increasing C_{out} destabilizes it. This was reported by e.g. Ambrosini and Sharabi [10] and Sharma et al. [18].

The Haaland relationship is valid for fully turbulent isothermal flow in a rough circular tube. In some previous studies smooth tube relationships have been used, neglecting the roughness effect. Jain and Uddin [19] used a combination of the Blasius (Eq.(13)) and McAdams relationship (Eq. (14), valid for *Re* between 30.000 and 10^6) in their stability study of a natural circulation CO_2 loop, resulting in a small discontinuity at *Re* = 30000. The Filonenko relationship (Eq. (15)) is often used in combination with the Gnielinski correlation [31] to determine heat transfer and pressure drop for fully developed turbulent pipe flow. These four relationships are compared in Fig 10B over the *Re* range or interest in this study. All friction factor relations have a certain tolerance as well, apart from those which are theoretically derived. If a tolerance of 10% is assumed on the Haaland correlation (*f*+ and *f*-, black dashed lines in Fig 10B), it is evident that the differences are only significant at the highest *Re* considered here. Figure 10A shows a comparison between the stability boundary determined with the Blasius, Haaland and Filonenko relationships. Due to the lower mean friction, the Blasius and Filonenko relationships result in a more stable system. However its clear the shape of the curve is also different, especially at low N_{SUB} values. Figure 10A also shows the impact of the friction factor tolerance for the Haaland relationship (dashed lines). As can be seen, the impact is small, but not negligible, especially near the bend where the difference is about 1.5%. The difference with the Blasius and Filonenko curves however is much larger, ±5.5-18% N_{PCH}. This again shows that it is the

friction distribution which determines the stability, rather than the mean value, as the f^- curve results in lower friction values than the Blasius curve up to *Re* 35000.

$$f = 0.316 \cdot \mathrm{Re}^{-0.25} \tag{13}$$

$$f = 0.184 \cdot \mathrm{Re}^{-0.2} \tag{14}$$

$$f = \left(-1.82 \cdot \log \mathrm{Re} - 1.64\right)^{-2} \tag{15}$$

However, Eqs. (13)-(15) are all isothermal friction factor relationships. Some correction methods exist to account for cross sectional property variation, e.g. Pethukov [32] suggested Eq. (16) which uses the ratio of the viscosity evaluated at the bulk and the wall temperature. This approximation is only valid up to *Re* of 23000, which is much lower than the considered values here, and these results were also never compared to supercritical fluid data, which shows much stronger property changes. Pioro et al. [33] provided an overview of friction correlations for supercritical fluids and found that there is no correlation suited for predicting the hydraulic resistance of supercritical fluids in reactor bundles. One of the listed correlations is that of Kirillov et al. [34] which is valid in a wide range of *Re* (up to 1.5 10^6) and which uses a density correction term, Eq. (17). The Filonenko relationship (Eq. (15)) is used to determine f_{cp}. To compute the wall temperature, the local heat transfer coefficient must be known. A large number of correlations have been suggested in the past. However, as shown in reviews (Pioro et al. [35], Cheng and Schulenberg [36]) these different relations can predict significantly different values near the pseudocritical point. This is due to the onset of heat transfer deterioration which is not captured in the correlation modeling. The Bishop correlation (Eq. (18)) was selected to compute the local wall temperature as it based on experiments conducted over a range of experimental conditions which cover the range considered here (22.6 MPa < p < 27.5MPa, 2.5 mm < D < 5.1 mm, 680 kg/m²s < G < 3600 kg/m²s, 0.31 MW/m² < q" < 3.5 MW/m²). The cross sectional averaged *Cp* value, $\bar{C}_p$, was approximated through Eq. (19).

$$\frac{f}{f_{cp}} = \frac{1}{6}\left(7 - \frac{\mu}{\mu_{wall}}\right) \tag{16}$$

$$\frac{f}{f_{cp}} = \left(\frac{\rho}{\rho_{wall}}\right)^{0.4} \tag{17}$$

$$Nu = 0.0069 \cdot \mathrm{Re}^{0.9} \cdot \mathrm{Pr}^{0.66} \cdot \left(\frac{\overline{C}_p}{C_p}\right)^{0.66} \left(\frac{\rho_{wall}}{\rho}\right)^{0.43} \left(1 + 2.4\frac{D_h}{L}\right) \tag{18}$$

$$\overline{C}_p = \left(\frac{H - H_{wall}}{T - T_{wall}}\right) \tag{19}$$

To determine the stability boundary in this case an additional iteration loop is required: after a first calculation of the bulk temperature, a guess is made for the wall temperatures by considering the Bishop relation and neglecting the wall temperature dependent parts. Using this wall temperature the heat transfer coefficients are updated allowing for new wall temperatures to be determined. This is repeated until the results no longer change (tolerance set to 0.1°C). This final wall temperature profile is then used to correct the friction factor, and these updated friction values are used to determine the new mass flux estimate. This was repeated until the mass flux no longer changed. The results are shown in Fig. 10A. As can be seen the results are quite different from all other friction relationships; the system is more unstable, in particular at higher N_{SUB} values. This is related to the strong change in friction profile compared to the isothermal correlations, as illustrated in Fig 9B for $N_{SUB} = 0.5$. In a recent benchmark exercise of the IAEA ([37]) on the stability of a supercritical fluid in a heated channel the results by VTT also showed a similar sensitivity to the chosen friction relationship (they compared the correlations of Filonenko, Colebrook and Kirillov, the latter combined with the Jackson-Fewster correlation to determine T_w). However, considering the large uncertainties on the heat transfer coefficients, in particular near to T_{pc}, and the uncertainties related to the friction factor modeling, it is difficult to assess the bounds of this prediction. This clearly shows that more experimental data and modeling effort is required to understand the hydraulic behavior of these flows in order to assess their stability using computational tools.

Impact of boundary condition uncertainties

When comparing experimental data to numerical simulation, it is important to assess the uncertainty on the imposed experimental boundary conditions as these can have a significant impact. For the considered case here the pressure drop over the channel has to be imposed in combination with a uniform heat flux on the wall. Considering the accuracy of pressure drop sensors, a tolerance of 1000-2500 Pa seems achievable. This would result in a channel pressure drop varying between 1.35 (Δp^-) and 0.145 MPa (Δp^+). The resulting stability boundaries for these two scenarios are compared to the original case with a constant friction factor in Fig. 11. As shown, the effect is negligible. Imposing a constant heat flux boundary seems trivial by using current heating of a tube as is commonly done in experiments, see e.g. Yamagata et al. [38]. However, due to the increase of the fluid temperature a comparable temperature gradient will also be present in the tube. For the points on the stability boundary the fluid temperature change from inlet to outlet varies between 400°C (near the bend) to 1000°C (at the lowest N_{SUB} values). As the temperature increases, so does the local resistivity of the metal tube material, resulting in a strong heat flux gradient when using current heating. However, the local heat losses also increase along the tube length as these are directly related to the surface temperature (radiation and convection). These two effects thus work in an opposite sense, and it can be expected that the non-uniformity of the heat flux is limited, partially also because of the good thermal

conductivity of the metal which will reduce the temperature gradient. To investigate the impact, a linearly varying heat flux profile was imposed in the simulation with the highest value near the exit of the tube (5% higher than the average). The results are shown in Fig. 11. The increasing heat flux profile makes the system slightly more stable with a difference of 1.7-3% for most of the considered N_{SUB} values. The curves almost coincide at the lowest N_{SUB} values, which is related to the small shifts in the density profile affecting the friction.

Comparison of scaled systems

As stated above, thermo-hydraulic or stability experiments are often conducted using a scaling fluid to reduce the high pressure and power constraints imposed by the studied system. Careful scaling laws are derived considering the relevant physics (see e.g. Marcel et al. [12], Rohde et al. [11], Cheng et al. [39]) and facilities are designed based on these laws. Based on the selection of R23 (CHF3) at 5.7 MPa as the scaling fluid, Rohde et al. [11]derived a set of scaling factors to model the stability of the HPLWR design (described by Fisher et al. [40]). As shown, the proposed scaling strategy preserves the stability behavior, but there are small deviations between the stability line for water and that of R23, in the order of a few percent. In light of the current study, these deviations are clearly negligible, considering the manufacturing and fluid property uncertainties, and it can be said that the results in fact agree to within their uncertainties.

Conclusions

This paper presents an overview of the impact of different substance property tolerances (enthalpy, density, viscosity and derivative of the density with respect to the enthalpy) and of system uncertainties on numerically predicted stability boundaries. The considered system here is a heated tube with supercritical water flowing upwards. A pressure drop is imposed over the channel, mimicking a reactor fuel assembly. It has been found that the individual tolerance of the density and viscosity and the uncertainty of the imposed pressure drop have a negligible impact. The tolerance on the enthalpy and derivative of the density with respect to the enthalpy only noticeably affect the result for very low N_{SUB} values (<0.1). The friction factor relation and the heat flux distribution (uniform or linear increasing) uncertainties have a comparable effect of about 1.7-3%, being more pronounced near the bend of the stability curve (N_{SUB} ~ 0.3). The most significantly propagating uncertainty was found to be that of the geometry, as even a ± 25µm uncertainty would result in a tolerance as high as 10%.

The results further showed that the stability boundary is linked to the friction distribution rather than its average value, and that different friction correlations result in strong changes of the predicted boundary. This emphasizes the need for a more accurate friction correlation for supercritical fluids in order to better assess stability boundaries. Also, from an experimental point of view, these results are

interesting for designing a new (scaled) setup, as they indicate that great care should be taken in selecting the scaled dimensions and their tolerances to preserve stability behaviour. Furthermore, no data was found in open literature to assess the actual heat flux profile which occurs when using current heating (a common experimental practice). As the heat flux distribution has a clear effect on the stability, a careful assessment is needed in order to allow for a better comparison between experiments and computations.

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Nomenclature

A	flow surface area [m²]
C_k	local friction value (orifice)
C_p	specific heat capacity [J/kgK]
D_h	hydraulic diameter [m]
f	Darcy Weisbach friction factor [-]
g	gravimetric acceleration [m/s²]
G	mass flux [kg/m²s]
h	enthalpy [J/kg]
L	length of the heater [m]
p	static pressure [Pa]
P	dynamic pressure [Pa]
P_h	heated perimeter [m]
Δp	pressure drop [Pa]
q'	linear power [W/m]
q''	heat flux [W/m²]
q'''	volumetric heat input [W/m³]
Re	Reynolds number, $\frac{G.D_h}{\mu_b}$ [-]
t	time [s]

w	velocity [m/s]
z	coordinate [m]

Greek symbols

β	isobaric thermal expansion coefficient [1/K]
δ	Dirac delta function
ε	surface roughness [m]
θ	angle relative to the horizontal axis, 0° in this study
μ	dynamic viscosity [Pa s]
ρ	density [kg/m³]
υ	specific volume [m³/kg]

Subscripts

cp	evaluated using constant properties
in	inlet
out	outlet
pc	value at the pseudocritical point
ref	value at the reference point
wall	value at the wall temperature

Superscripts

+	upper bound
-	lower bound

Figure Captions

Figure 1. Studied heated channel.

Figure 2. Impact of the temperature mesh choice on the derivative of the density with respect to the density, A: full view over the considered enthalpy range, B: zoom in near the pseudocritical point

Figure 3. Comparison of the predicted steady state pressure distribution by the proposed model and the data of Ambrosini and Sharabi [10]

Figure 4: Comparison of the predicted temperature (A) and velocity (B) distribution by the proposed model and the data of Ambrosini and Sharabi [10]

Figure 5. Comparison of the predicted stability boundary of the model to the data of Ambrosini and Sharabi [10] and of Ambrosini [20]

Figure 6. A: Impact of the density tolerance on the predicted stability boundary, B**:** impact of the combined density and enthalpy tolerance on the predicted stability boundary.

Figure 7. Impact of the viscosity tolerance on the predicted stability boundary using the Haaland friction relationship.

Figure 8. Impact of the geometric tolerance (D_h and A) on the predicted stability boundary for two values of the tolerance.

Figure 9. A: Impact of the variable friction profile on the stability boundary, B: comparison of the different considered variable friction profiles.

Figure 10. A: Impact of the viscosity tolerance, friction factor correlation (Blasius, Filonenko, Haaland and Kirilov (combined with the Bishop heat transfer correlation) correlation) and the tolerance of the Haaland relationship on the stability boundary, B: comparison of different friction correlations in the considered Re range.

Figure 11. Impact of the boundary conditions (imposed pressure drop and surface heat flux) on the stability boundary.