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Heat transfer to water near the critical point: evaluation of the ATHLET thermal-hydraulic system code

The heat transfer coefficient is an essential measure in the pre-design of supercritical water-cooled reactors (SCWRs). At supercritical pressures, three distinct heat transfer modes exist: normal, improved, and deteriorated. The heat transfer behavior of supercritical water in the pseudo-critical range is different from that of single-phase fluids in the subcritical range. These heat transfer modes differ from those of single-phase flow at subcritical pressures, resulting in an unusual behavior of the heat transfer coefficients. Moreover, during accidental scenarios, when the operating pressure is reduced from supercritical to subcritical conditions, a boiling crisis may occur. During pressure reduction, temporary phenomena such as superheating of the cladding temperature can endanger the safe operation of SCWRs. In order to analyze operational and accidental scenarios of SCWRs, thermal-hydraulic system codes such as ATHLET are applied. However, the prediction capabilities of thermal-hydraulic system codes rely on a comprehensive validation work based on experimental data. This study presents an extensive analysis of the applicability of ATHLET at the near-critical pressure range. ATHLET is assessed against the LESHP-database and two trans-critical transient experiments. At supercritical pressures, the heat transfer coefficient correlations are evaluated with regard to their prediction accuracy and numerical problems including the "multiple solutions problems". The trans-critical transient experiments are used to test the prediction capability of ATHLET with respect to transient heat transfer phenomena including critical heat flux, film boiling and return to nucleate boiling.

Wärmeübergang an Wasser in der Nähe des kritischen Punkts: Evaluierung des Thermohydraulik-Rechenprogramms ATHLET. *Der Wärmeübergangskoeffizient ist essentiell bei der Auslegung von überkritischen wassergekühlten Reaktoren (SCWR) im Hinblick auf den Wärmeübergang im Reaktorkern. Das Wärmeübergangsverhalten von überkritischem Wasser weicht insbesondere im pseudo-kritischen Bereich vom typischen Wärmeübergangsverhalten einphasiger Fluide im unterkritischen Bereich ab. Im überkritischen Druckbereich untergliedert man das Wärmeübergangsverhalten deshalb in drei verschiedene Wärmeübertragungsbereiche: normal, verbessert und verschlechtert. Zudem kann bei Störfällen in SCWRs eine Druckabsenkung vom überkritischen in den unterkritischen Druckbereich erfolgen, die zu einer Siedekrise führt. Dabei können zeitlich begrenzte Phänomene wie eine Überhitzung der Rohrwand mit anschließender Wiederbenetzung auftreten. Um Betriebs- und Unfallszenarien von SCWRs zu analysieren, werden im Allgemeinen Thermohydraulik-Systemrechenprogramme wie ATHLET eingesetzt. Zur genauen Vorhersage sowie Validierung der Simulationsergebnisse stützen sich Thermohydraulik-Systemrechenprogramme auf die Ergebnisse experimenteller Untersuchungen. Entsprechend ist es Ziel dieser Studie, ATHLET im Hinblick auf den nah-kritischen Druckbereich zu testen. Dazu werden die Simulationsergebnisse mit der LESHP-Datenbank und zwei transienten Experimenten im transkritischen Druckbereich verglichen. Die überkritischen Wärmeübergangskorrelationen werden hinsichtlich ihrer Vorhersagegenauigkeit und der auftretenden numerischen Probleme einschließlich des Problems von Mehrfachlösungen untersucht. Die transkritischen transienten Experimente dienen dazu, die Anwendbarkeit der in ATHLET implementierten Modelle im Hinblick auf den kritischen Wärmestrom, Filmsieden und Rückkehr zum Blasensieden zu testen.*

1 Introduction

As part of the Generation IV reactors, various Supercritical Water-Cooled Reactor (SCWR) concepts have been pursued worldwide in recent years, offering many advantages compared to state-of-the-art nuclear power plants. Among others, these advantages include improved economics with respect to capital costs and levelized cost of electricity, a simplified design, and higher thermal efficiencies (> 43 %) [1, 2]. The latter advantage is due to the high temperatures and pressures within the reactor core of SCWRs. SCWRs are designed to operate at pressures above 24 MPa and outlet temperatures of up to 625 °C using light or heavy water as the coolant [3]. In general, the reactor core of SCWRs is designed as a once-through direct-cycle without coolant recirculation in the vessel [4]. Although the once-through concept as well as the operating temperatures and pressures of SCWRs are well known from commercial supercritical fossil-fired boilers, several technological challenges remain. According to [5], one key challenge is related to the basic thermal-hydraulic phenomena at near-critical pressures within the reactor core. These include the important phenomena of heat transfer deterioration (DHT) at supercritical pressures and boiling crisis at sub-critical conditions. Both phenomena can lead to local temperature peaks, and hence overheating and damage to the cladding material. Particularly accidental conditions – resulting in depressurization from super- to subcritical pressures – might cause a temporary phenomenon resulting in significantly higher temperatures than expected at steady-state conditions [6]. In consequence, enormous efforts have been made in recent years to understand these critical phenomena. Experimental investigations at supercritical pressures were performed in round tubes [7–10], annular channels [11–14] and rod bundles [15–17], whereas only a few trans-critical transient experiments are reported in the literature [18–21]. Analytical studies have mainly focused on the heat transfer to supercritical water using experimental data at steady-state conditions. Over 30 correlations describing the heat transfer coefficient (HTC) and more than 10 criteria predicting the onset of DHT are found in the literature. A thorough review of the different correlations is, for example, presented by [22–25]. In order to find the most appropriate correlations, various studies have assessed the different correlations and the criteria. In view of the limited correlations, varying experimental datasets, different assessment methods and ambiguous results due to the nonlinear behavior of most of the HTC correlations, the assessment studies have presented inconsistent results [26]. Moreover, different databases for thermophysical fluid properties used in developing and evaluating correlations reduce the degree of prediction accuracy, especially in the pseudo-critical region. All of these issues significantly complicate predesign studies of SCWRs, including those for start-up and shut down procedures, safe plant operations or even accidental scenarios.

In general, when it comes to plant analyses of nuclear power plants (NPP), thermal-hydraulic system codes such as ATHLET are used. ATHLET is an advanced best-estimate code developed for the simulation of current light water reactors and advanced Generation III+ and IV reactors [27]. Since ATHLET aims to accurately and as realistically as possible predict the behavior of NPPs, it relies on validation using experimental measurements. While a rigorous validation basis exists for common light-water reactors, up to now ATHLET has not yet been systematically validated for GEN IV reactors [28]. In the field of SCWRs only a few studies have been published addressing the applicability of ATHLET at supercritical pressures [29–32]. *Fu et al.* [29] modified ATHLET by applying the pseudo two-phase method using a fictitious latent heat region in order to simulate trans-critical transient processes. Based on the pseudo two-phase method of *Fu et al.* [29], *Zhou et al.* [30] evaluated the capability of ATHLET in simulating fast depressurization from super- to subcritical pressures (*Edwards and O'Brien* blow-down test). In addition, *Zhou et al.* [30] extended the heat transfer module of ATHLET by five HTC correlations and assessed them against an experimental database. However, since the latest version of ATHLET Mod 3.1 Cycle A treats the supercritical fluid as a single-phase fluid (liquid phase) [27], studies on the pseudo two-phase method are limited in validating and providing a guidance for the current version of ATHLET.

Hegyi et al. [32] assessed nine correlations against a set of experimental data by modifying ATHLET Mod 2.1 Cycle A. They found a large scattering of the different HTC correlations when compared to experimental data. Overall, the *Watts and Chou* correlation [33] provided the best results. *Samuel et al.* [31] evaluated the correlations provided in the latest ATHLET version (Mod 3.1 Cycle A). *Samuel et al.* created a numerical model in ATHLET representing the test section of the Supercritical-Pressure Test Facility SKD-1 loop and compared the numerical results to 12 experimental runs. The experimental data covered mass fluxes ranging from 220 to 1,500 kg/m^2/s, heat fluxes from 70 to 1,240 kW/m^2 and bulk temperatures from 320 to 450 °C at a pressure of 24 MPa. The results showed that, depending on the parameter range, certain correlations perform better, whereas overall none of the HTC correlations were able to predict the heat transfer with acceptable accuracy. Although the latest two studies addressed the heat transfer at supercritical pressures, they are limited in that

1. the parameter range of the experimental dataset was limited and
2. only the prediction accuracy was investigated.

However, the influence of nonlinear behavior of the thermophysical fluid properties of supercritical water on the HTC correlations and hence on the simulation results and numerical stability of ATHLET was not investigated. In fact, *Gschnaidtner et al.* [26] showed that, depending on the HTC correlation, numerical stability problems can exist resulting in unrealistic, multiple solutions or no solutions with regard to predicting the wall temperature.

Moreover, to the best of the authors' knowledge so far only the heat transfer capability of ATHLET was investigated at sub- and supercritical pressures as well as the trans-critical transient thermal-hydraulics of water. In contrast, this article tests the trans-critical transient heat transfer capability of ATHLET in predicting the wall temperature. No validated models are provided in ATHLET predicting the temporary behavior of the wall temperature during depressurizations for pressures especially in the pressure range near the critical point from 20 to 22.1 MPa.

In view of the difficulties of predicting the heat transfer at pressures near the critical point and the associated numerical problems, this work evaluates the ATHLET thermal-hydraulic system code with respect to the above mentioned issues. Simple numerical models are therefore developed in ATHLET and assessed against the LESHP-database and two trans-critical transient experiments.

2 The ATHLET Mod 3.1 Cycle A thermal-hydraulic system code

ATHLET (Analysis of THermal-hydraulics of LEaks and Transients) is an advanced best-estimate code developed by GRS (Gesellschaft für Anlagen- und Reaktorsicherheit)[Global research for safety] for the simulation of current light water reactors and advanced Generation III+ and IV reactors including SCWRs [28]. Advanced thermal-hydraulic modeling, heat generation, heat conduction and heat transfer to single- or two-phase fluid are among the main features of ATHLET. Since ATHLET Mod 3.0 Cycle A, the applicability of ATHLET has been extended to supercritical water considering the transition from super- to subcritical pressures. At supercritical pressures, ATHLET treats the supercritical fluid as a single-phase fluid and solves the mass, momentum and energy balance only for the liquid phase. At subcritical pressures, ATHLET provides the 6-equation model and solves the mass, momentum and energy balance for the liquid and vapor phases separately. A staggered grid is applied, where the pressure, temperature and steam mass quality are calculated at the center of a control volume (CV) and the flow related variables at the junction between the CVs. Generally, ATHLET uses the Jacobian matrix for the underlying equation system and applies the fully implicit scheme (general ODE-solver Forward-Euler, Backward-Euler) for the time integration. The complete system is initialized with a steady-state simulation.

In the heat conduction and heat transfer module, ATHLET provides a one-dimensional heat conductor model in radial direction with the option of including axial heat conduction. In order to calculate wall to fluid heat transfer, empirical correlations for different heat transfer regimes are implemented. Since most of the empirical heat transfer models implemented in ATHLET are of an implicit nature, i.e. dependent on the wall temperature, the actual heat transfer mode and HTC rely on the wall temperature of the previous time step throughout the transient calculation.

At supercritical pressures, ATHLET provides a total of seven HTC correlations, of which six correlations were developed for supercritical water.

While no distinction is made between the different heat transfer phenomena at supercritical pressures, – improved heat transfer (IHT), normal heat transfer (NHT) and deteriorated heat transfer (DHT) –, ATHLET distinguishes between three main heat transfer levels for the heat flow from wall to fluid at subcritical pressures:

1. Natural and forced convection, subcooled and saturated nucleate boiling
2. Transition boiling
3. Stable film boiling

The selection logic of the heat transfer mode and hence the choice of the corresponding HTC correlation are based on the fluid and wall temperature, the critical heat flux and return to nucleate boiling temperature, enthalpy quality, and the void fraction. Therefore, ATHLET offers a wide range of models in order to select the heat transfer mode and predict the HTC including models for calculating the HTC, the critical heat flux, the minimum film boiling temperature and the rewetting temperature. For more information about ATHLET Mod 3.1 Cycle A please refer to [27].

3 Methodology

In order to investigate the numerical issues related to the nonlinear thermophysical fluid properties of water as well as the applicability to predict the heat transfer to water near the critical point, ATHLET was assessed against the LESHP-database and two trans-critical transient experiments. The experimental data and numerical models used throughout this study are described in the following subchapters.

Table 1. LESHP-database for supercritical water flowing upwards in vertical bare tubes

	LESHP-database
Number of data sources	44
Number of data points	15,840
Heat flux range	37 to 4,521 kW/m^2
Mass flux range	55 to 3,700 kg/m^2/s
Pressure range	22.5 to 34.5 MPa
Inside diameters	1.5 to 38 mm

3.1 Experimental data

3.1.1 Supercritical experimental data

Since the 1950 s, numerous experimental studies from different research institutes all over the world have been published for supercritical water in round tubes, annular channels and rod bundles. However, due to a limited number of experimental data points in annular channels and rod bundles and since all supercritical HTC correlations currently implemented in ATHLET are based on round tubes, we decided to assess ATHLET only against experimental data for supercritical water flowing upward in vertical bare tubes. The experimental data were chosen following the selection process proposed by [26]. The LESHP-database contains a total of 15,840 data points collected from 44 different sources in the literature. The database comprises experimental data points of supercritical water for a pressure range from 22.5 to 33.5 MPa, heat flux range from 37 to 4,521 kW/m^2, mass flux range from 55 to 3,700 kg/m^2/s, specific enthalpies from 105 to 3,275 kJ/kg and hydraulic diameters from 1.57 mm to 38.13 mm.

3.1.2 Transient trans-critical experimental data

Only a few transient trans-critical experiments are available in the literature: In bare round tubes the well-known experiment by *Hein et al.* [20, 21] and the experiment by *Kohlhepp et al.* [19] and in a 2 × 2 rod bundle with wire wraps around the rods, the experimental runs conducted by *Li et al.* [18]. To investigate the influence of accident conditions, such as those occurring in a loss of coolant accident (LOCA), or the flexible operation of boilers using supercritical water, *Hein et al.*, *Kohlhepp et al.* and *Li et al.* carried out depressurization experiments from supercritical to subcritical pressures. The experiments showed that overheating of the wall temperature – including fast heat-up and conduction controlled rewetting – may occur when the pressure falls below the critical pressure. However, only the experiments for round tubes [19–21] were considered in this study. The important data of these two experiments are summarized in Table 2. A detailed description of the experimental apparatus can be found in [19–21, 34].

Table 2. Transient trans-critical experiments considered in this study

Experiment	*Hein et al.* [1, 2]	*Kohlhepp et al.* [3]
Tube dimensions (L/d_i/d_o)	6,000 mm/14 mm/18 mm	7,000 mm/15.81 mm/26.63 mm
Material	1.4981	1.4903
Heat flux	619 kW/m^2	302 kW/m^2
Mass flux	2,000 kg/m^2/s	751 kg/m^2/s
Pressure reduction	From 24.7 to 19.1 MPa	From 24.7 to 19.1 MPa
Inlet enthalpy	1,630 kJ/kg	1,700 kJ/kg

3.2 Numerical models

3.2.1 Numerical model and procedure for the steady-state supercritical experiments

Numerical model:
In order to simulate the LESHP-database, a simple model was developed in ATHLET. The model implementation (see Fig. 1) consists of two thermo-fluid-dynamic objects (TFOs): PIPE and BRANCHOUT. The pipe object (PIPE) represents the pipe and describes the one-dimensional fluid transport within the pipe. For assessing ATHLET against each data point from the database, the pipe object consists of one CV with a length of 10 mm. A heat conduction object (HCO) coupled to the pipe serves as pipe wall as well as the heat source. Although the thickness and material of the pipe wall are irrelevant for this study, here the wall consists of austenitic steel and was modeled with a thickness of 2 mm consisting of five layers of equal thickness. The outer surface was chosen adiabatic. The rod model of ATHLET was used to simulate the electrical heat source in the HCO. The fill simulation model was applied to the left-most junction of the pipe object (i.e. the bottom edge) in order to determine the mass flow rate and inlet temperature. At the right end of the pipe object (i.e. the top edge), the BRANCHOUT, a p-h boundary model, allows control of the pressure and enthalpy at the outlet of the pipe. In order to control the p-h boundary, the general control simulation module (GCSM) is used.

Procedure:
In general, ATHLET starts each simulation with a steady-state calculation. Therefore, ATHLET initializes the system based on specific data including the geometry of the pipe, the underlying models, mass and heat flow, as well as pressure and temperature at the starting point of the TFD system, i.e. at the inlet of the pipe. Then ATHLET starts the transient simulation based on the initialization results. During the transient simulation, ATHLET relies on the enthalpy provided by the p-h boundary at the outlet of the pipe in order to simulate the behavior within the pipe. Since both the temperature and enthalpy are specified using the experimental data from the database, a very slight deviation may be expected between the steady-state calculation and the steady-state result of the transient calculation, especially for low mass flow rates and in the vicinity of the pseudo-critical points. Therefore, two simulation times were chosen for the transient calculation: 50 s and 500 s. In case the simulation did not converge for 50 s, a simulation time of 500 s should guarantee steady-state conditions for unambiguous results. The convergence criterion, i.e. steady-state condition, was set to 10^{-3} for five consecutive time steps considering the quantities of interest: HTC, bulk and wall temperature, mass flow rate, and bulk enthalpy. In addition to the prediction accuracy, this criterion also allows the investigation of ATHLET with respect to numerical instabilities such as oscillations and bifurcations. Code was written in Python in order to realize an automatic simulation of all data points. A flow chart of the code structure is shown in Fig. 2.

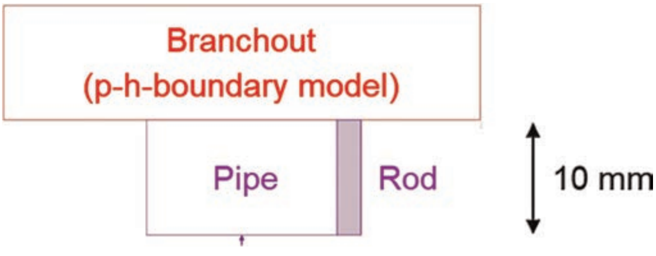


Fig. 1. Scheme of the numerical model in order to assess ATHLET against the LESHP-database

Just like in *Gschnaidtner et al.* [26], the statistical measures' relative error (RE), mean absolute relative error (MARE), root-mean-square relative error (RMSRE) and the standard deviation (SD) in this study are applied to analyse the converged results.

3.2.2 Numerical model and procedure for the transient trans-critical experiments

Numerical model:
The numerical model for the transient trans-critical experiments is similar to the model developed to assess ATHLET against the database. It only differs in that the pipe object is represented by more CVs. The number of CVs was chosen for the simulation of both experiments of *Hein et al.* and *Kohlhepp et al.* in such a way that numerical instabilities are assured to not occur.

(A grid independency study was carried out for the *Hein et al.* experiment as the originally-planed simulation with 300 CVs each of a length of 20 mm resulted in numerical issues leading to no solution: The simulation results using 60, 120 and 240 CVs showed no significant differences during depressurization and the final solution representing the steady-state boiling crisis. Hence, 60 CVs were chosen for the *Hein et al.* experiment reducing the simulation time drastically. However, the *Kohlhepp et al.* experiment could be performed with a total of 350 CVs (20 mm length of one CV) without producing any numerical problems.) Moreover, since axial conduction plays an important role in conduction-controlled rewetting processes, the axial heat conduction module was also activated for the transient calculation. An exemplary scheme of the transient trans-critical numerical model is shown in Fig. 3.

Procedure:
The transients start with a settling time of 20 s to assure a steady-state operating point at the beginning of the depressurization process. During the transient simulation, the pressure of the p-h boundary is however changed according to the pressure history of the experimental data via GCSM. For the transient simulations, a convergence criterion was not found to be necessary, as the comparison of the temporal experimental and simulation data is of utter interest. In this study in total 360 different combinations were tested by varying the models for the critical heat flux, return to nucleate boiling and film boiling. Therefore, a Python code was developed whose structure is illustrated in Fig. 4. At supercritical pressures, the explicit correlation of *Cheng et al.* that was explicitly developed for the upward flow in vertical pipes was chosen in order to avoid any ambiguous results (see discussion and analysis of the results – "multiple solutions problems").

4 Results

In total, 15,840 data points at supercritical conditions and two transient trans-critical experiments were simulated using ATHLET. The results are presented in the following.

4.1 Results at supercritical conditions

All correlations available at ATHLET Mod 3.1 Cycle A and explicitly developed for supercritical water were assessed against the database. Since the database also contains experimental data not closely related to the proposed parameter range in the core of SCWRs, the following two categories were considered for analysis of the results:

1. The whole database
2. Experimental data in the pressure range from 22.1 MPa to 26.5 MPa, temperature range from 200 to 625 °C and diameters from 6 to 16 mm

The latter set represents the data for the typical pressure range of SCWRs including start-up and shut down procedures and accidental scenarios.

The results of the whole database are outlined in Table 3, and a reduced dataset related to SCWRs in Table 4. In order to assess the prediction accuracy of each correlation, only the results of the converged data points were chosen. The statistical measures are based on the deviation of the HTC from the simulation and the HTC from the experimental data. Irrespective of the assessed dataset, all correlations have data points with no convergence, inclusive of the explicit correlations of *Cheng et al.* [35] and *Zhao et al.* [36]. While the convergence is only a minor issue for most correlations (less than 0.3 % of all data points), the *Gupta et al.* [37] correlation fails to assure convergence for more than 1.5 % of all data points. With regard to MRE, all correlations, except for the *Mokry et al.* [38] correlation, tend to over-predict the HTC. Although the *Watts and Chou* [33] correlation demonstrates a superior performance over all other correlations in terms of MARE, RMSE, and SD, it is not able to achieve deviations of less than 30 %. The comparison of all correlations to the reduced dataset considering only data points for which all correlations yielded converging results is shown in Fig. 5.

4.2 Results for the transient trans-critical experiments

In total, 360 different combinations of available models in ATHLET were simulated concerning the critical heat flux, return to nucleate boiling and film boiling. At supercritical pressures, the HTC was calculated based on the correlation by *Cheng et al.* [35]. Here, the accuracy of the correlations at

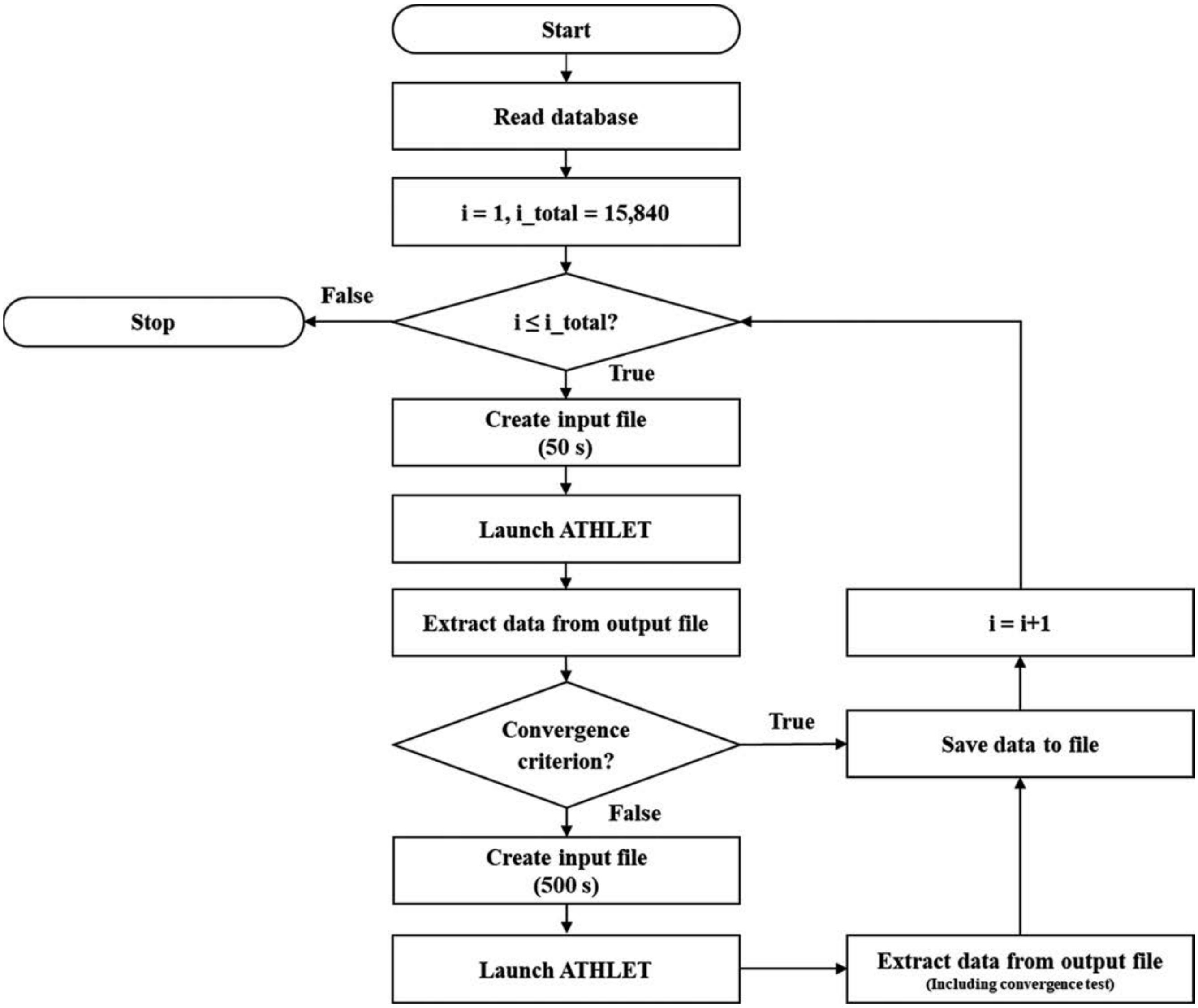


Fig. 2. Flow chart of the Python code structure for the database

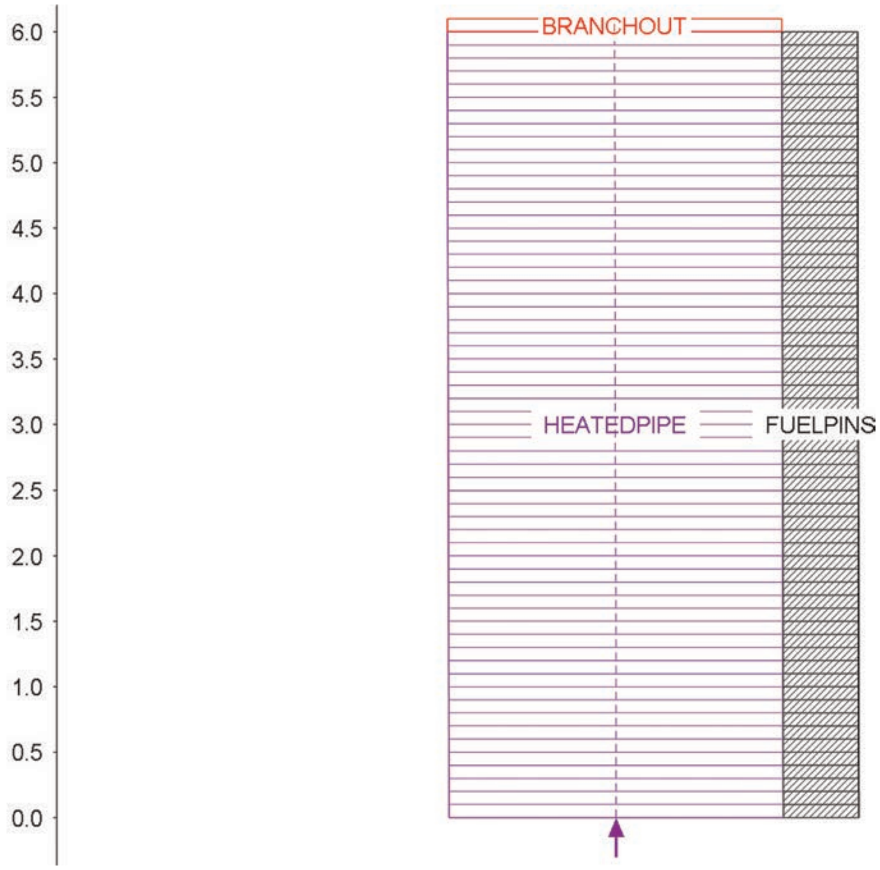


Fig. 3. Exemplary scheme of the numerical model for the transient trans-critical experiments of Hein et al. with 60 CVs

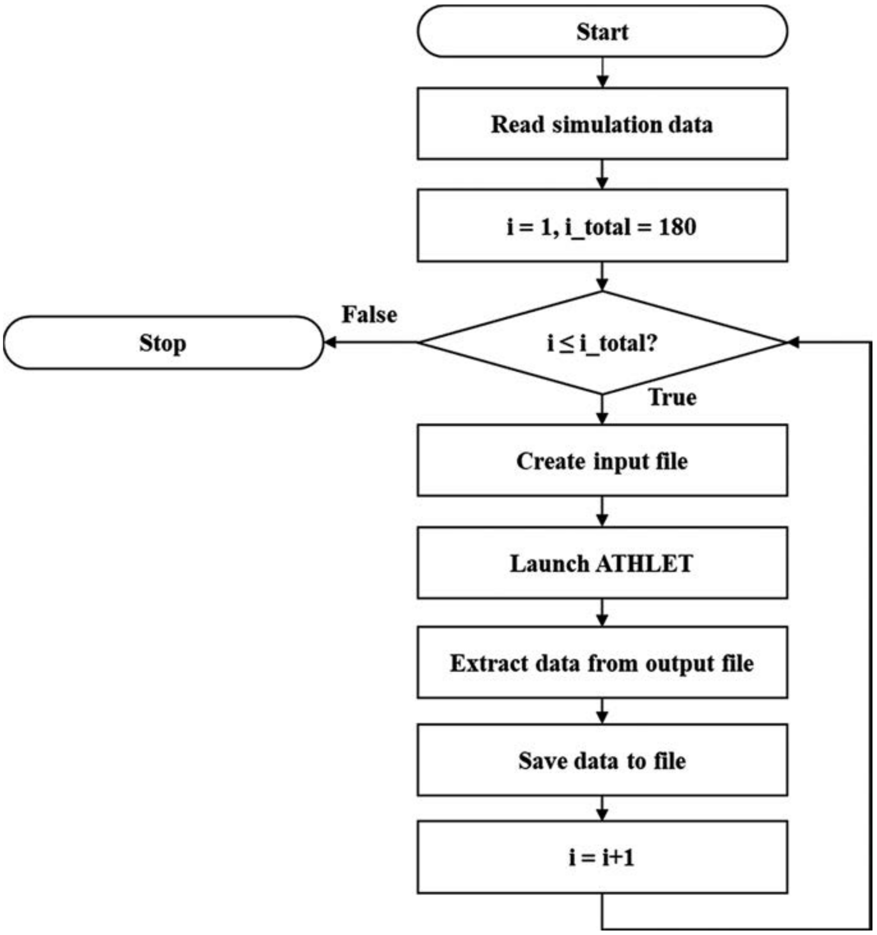


Fig. 4. Flow chart of the Python code structure for the transient trans-critical simulation

supercritical pressure is not of utmost importance. In fact, the main objective of these simulations was to test the capability of ATHLET to simulate a boiling crisis and conduction-controlled rewetting process during pressure reduction from super- to subcritical pressures. The results of both experiments are described in the following subsections. Emphasis is put on the models that best describe the transient heat transfer behavior.

4.2.1 Results of the Hein et al. experiment

For simulation of the *Hein et al.* experiment, the critical heat flux model was the parameter that influenced the results of the simulations the most. All simulation results reflected a boiling crisis, but differed in the position of the onset of the boiling crisis. Depending on the applied model, the onset of the boiling crisis occurred between enthalpies of 1,911 kJ/kg (Westinghouse W-3) and 2,024 kJ/kg (Groeneveld look-up table). Although the final location of the boiling crisis was well predicted by the Groeneveld look-up table, none of the results predicted the transient behavior accurately, inclusive of position of the quench front and the conduction-controlled rewetting as it occurs in the experiment. In fact, only a small shift of the location of the boiling crisis moving against the flow direction was calculated by ATHLET. Moreover, all results over predict the maximum wall temperature registered during the experiment by more than 200 °C. In all simulations, almost steady-state was reached after about 300 s with wall temperatures of more than 750 °C for the correlation of *Bromley* [39] and more than 1 000 °C for the correlation of *Berenson* [40] for the region with inverted annular film boiling. Neither the return to nucleate boiling models nor the rewetting temperature models affected the results of the simulation significantly. Figure 6 shows the exemplary simulation results based on the *Biasi et al.* correlation [41] for the critical heat flux (CHF) and the *Bromley* correlation [39] for the inverted annular film boiling together with the experimental data. The simulation results, represented by the full and dashed lines, represent the experimental data (crosses) quite well at supercritical pressures (see Fig. 6a)), whereas at subcritical pressures the above-mentioned discrepancies occur (see Fig. 6b)).

4.2.2 Results of the Kohlhepp et al. experiment

In the *Kohlhepp et al.* experiment, a boiling crisis occurred at subcritical pressures resulting in a higher maximum wall temperature than at supercritical pressures. For the *Kohlhepp et al.* experiment, only ATHLET simulations considering the CHF look-up table by *Groeneveld et al.* [42] predicted a boiling crisis similar to that in the experiment. Following the trend of the experimental results, in the simulation the boiling crisis shifts slightly against the flow direction. Here, the different models implemented in ATHLET for the rewetting tem-

Table 3. Results of the assessment of ATHLET against the whole database containing 15,840 data points

		Based on $RE = \frac{\alpha_{cor.} - \alpha_{exp.}}{\alpha_{exp.}}$			
Correlation	Converged data points	MRE	MARE	RMSE	SD
Cheng et al. [4]	15,838	56.5 %	76.5 %	161.4 %	151.2 %
Gupta et al. [5]	15,602	1.7 %	48.5 %	300.8 %	300.8 %
Jackson and Hall [6]	15,832	38.8 %	51.0 %	108.1 %	100.9 %
Mokry et al. [7]	15,810	–1.1 %	37.0 %	110.3 %	110.3 %
Watts and Chou [8]	15,803	8.9 %	34.2 %	71.4 %	70.9 %
Zhao et al. [9]	15,838	48.0 %	73.0 %	156.0 %	148.4 %

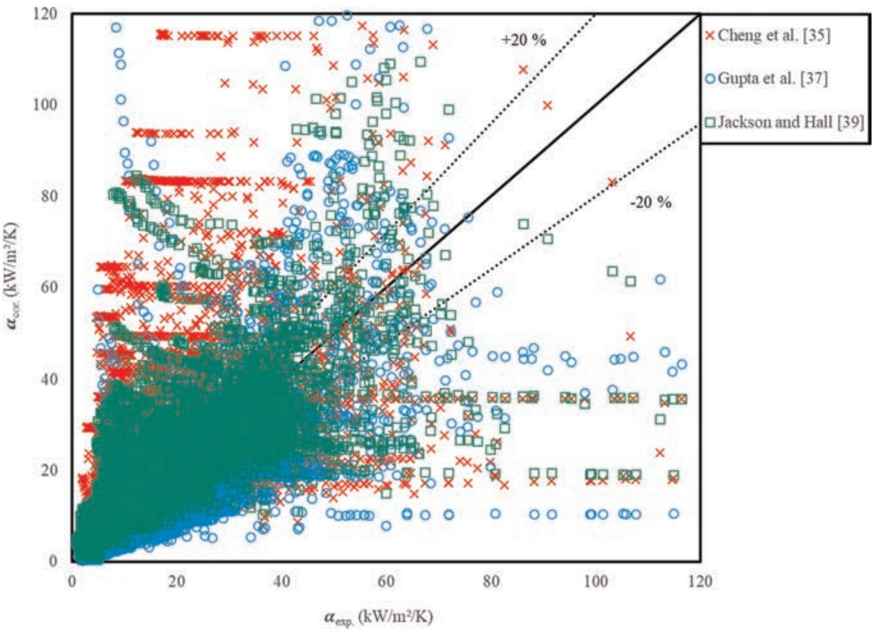
Table 4. Results of the assessment of ATHLET against the database containing 10,029 data points in a pressure range from 22.1 to 26.5 MPa, a temperature range from 200 to 625 °C, and diameters from 6 to 16 mm.

		Based on $RE = \frac{\alpha_{cor.} - \alpha_{exp.}}{\alpha_{exp.}}$			
Correlation	Converged data points	MRE	MARE	RMSE	SD
Cheng et al. [4]	10,027	61.6 %	79.5 %	146.4 %	132.8 %
Gupta et al. [5]	9,849	2.0 %	49.1 %	335.3 %	335.4 %
Jackson and Hall [6]	10,022	42.2 %	52.0 %	90.4 %	79.9 %
Mokry et al. [7]	10,011	–4.2 %	36.1 %	103.3 %	103.2 %
Watts and Chou [8]	10,000	11.7 %	31.4 %	57.9 %	56.8 %
Zhao et al. [9]	10,027	53.2 %	76.1 %	140.2 %	129.8 %

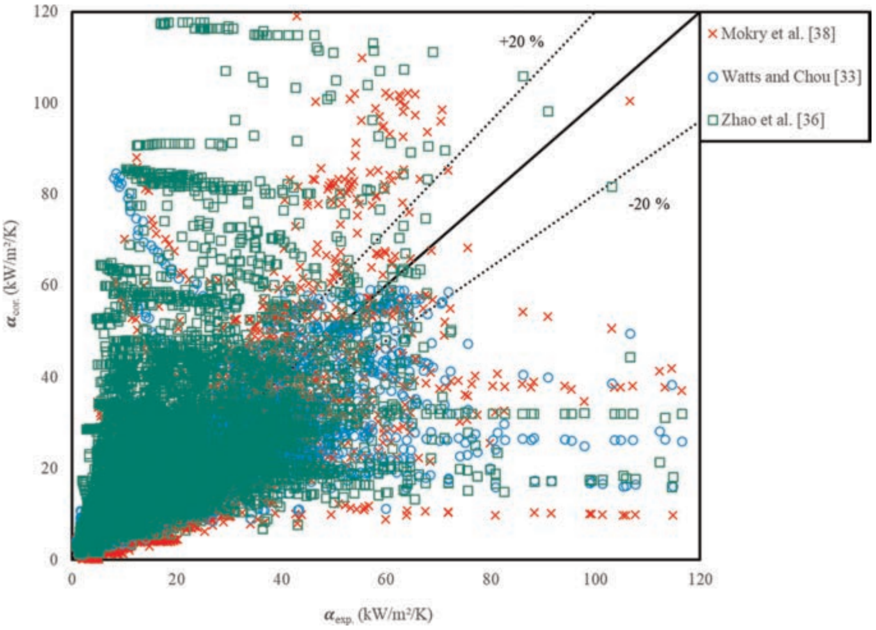
perature, minimum film boiling temperature and return to nucleate boiling temperature had no significant effects on the results. The final solution of ATHLET (t = 500 s) overestimates the maximum wall temperature by more than 100 °C compared to the experimental data when using the *Bromley* correlation [39] and by more than 150 °C for the correlation of *Berenson* [40] for the region with inverted annular film boiling. However, the transient behavior with respect to the onset of the boiling crisis is quite well predicted. The exemplary simulation results of ATHLET based on the CHF look-up table by *Groeneveld et al.* and the *Bromley* correlation [39] for the inverted annular film boiling are shown in Fig. 7.

5 Discussion and analysis of results

This chapter provides a detailed analysis of the simulation results of the supercritical database with respect to the convergence issues and takes the not yet discussed multiple solution possibilities into account. Although the majority of the simulations did converge for all investigated supercritical HTC correlations (see Table 3 and 4), convergence issues occurred for a small number of data points. Since convergence issues can lead to termination of the simulation or may produce misleading results, the non-convergence cases are analyzed in more detail. Moreover, according to *Gschnaidtner et al.* [26], in addition to convergence issues, implicit correlations may result in multiple solutions for the identical parameter set. Both, the non-convergence cases as well as the multiple solu-



(a) Cheng et al. [35], Gupta et al. [37] and Jackson and Hall [39]



(b) Mokry et al. [38], Watts and Chou [33] and Zhao et al. [36]

Fig. 5. Comparison of the correlations with experimental data for the typical pressure range of SCWRs considering only data points for which all correlations yielded converging results

tions problems are discussed in the following. A detailed assessment of the HTC correlations against NHT and DHT cases is not presented here, but can be found in [31].

Furthermore, the simulation results of the transient experiments are also discussed and analyzed in this chapter.

5.1 Analysis of non-convergence/unrealistic cases

The analysis of the non-convergence cases showed the following common problems for the wall temperatures:

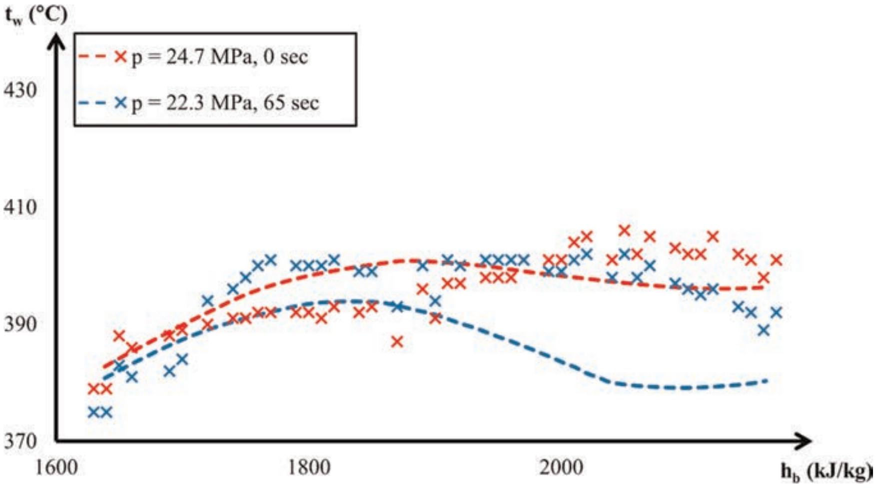
a. Oscillations for case dependent correlations.
b. Bifurcations for implicit correlations in case the resulting wall temperature is in the vicinity of the pseudo-critical point. However, the maximum amplitude of the bifurcations observed throughout the simulations was within a few tenth of °C.
c. Unrealistic high solutions of more than 1000 °C with asymptotical behavior, but no convergence in case of implicit correlations. Bulk temperatures are in general below the pseudo-critical temperature.
d. No solution in case of implicit correlations without ATHLET producing an error message.

Table 5 outlines what problems have been observed for each correlation. Examples for cases a) to c) are shown in Fig. 8.

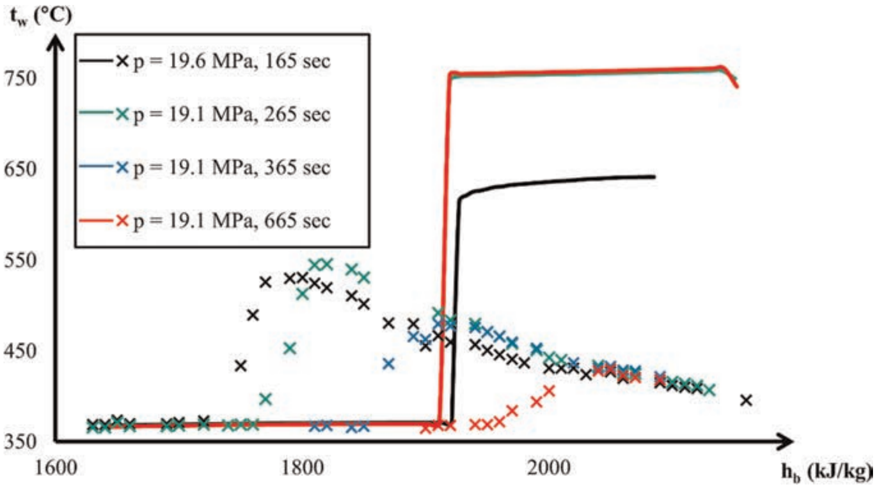
The convergence issue cases a) and b) may be regarded as issues related to the case dependency or the implicit nature of the corresponding correlation and the non-linearity of the thermophysical properties near the pseudo-critical line. These two cases make up most of the convergence issues cases. Particularly the correlation by *Gupta et al.*, which strongly depends on the thermophysical properties evaluated at the wall temperature, shows most of the convergence issues related to case b).

Case c) can be attributed to the procedure of the solver: While the initialization, i. e. steady-state solution, relies on the bulk temperature and pressure, the transient simulation is based on the enthalpy of the p-h- boundary. Since both parameters are specified by the database and since ATHLET especially uses a slightly modified version of the IAPWS-IF97 formulation (see [27]) in the pseudo-critical region and for high heat flux to mass flux ratios, a deviation may be expected for the steady-state and transient calculation. Depending on the correlation, this can result in a drastic change of up to 300 °C in the simulated wall temperature, as is the case in Fig. 8c).

Irrespective of the convergence issues, the Gupta et al. (up to 1,680 °C) and Mokry et al. (up to 6,250 °C) correlations may predict unrealistically high wall temperatures. In fact, too high wall temperatures exceeding the limits of ATHLET



(a) At supercritical pressures



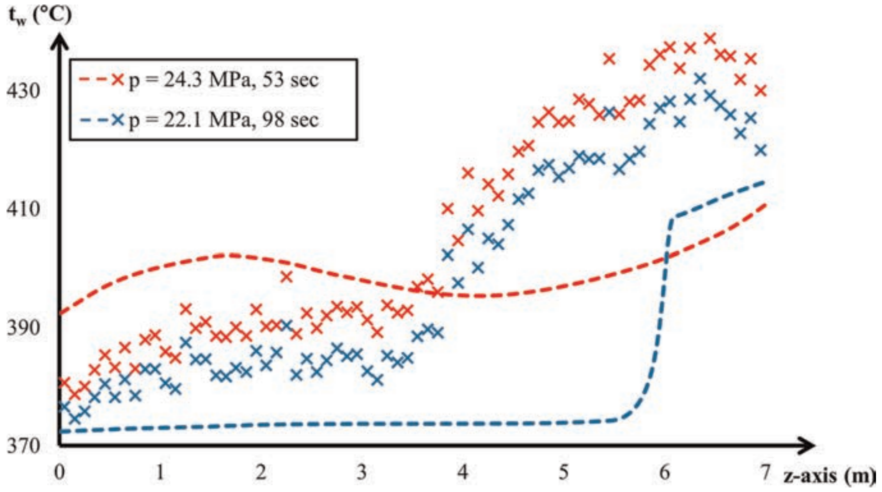
(b) At subcritical pressures

Fig. 6. Simulation results of the Hein et al. experiment using the Biasi correlation for predicting the CHF and the Bromley correlation for the inverted annular film boiling (crosses represent experimental data and dashed/full lines represent simulation data)

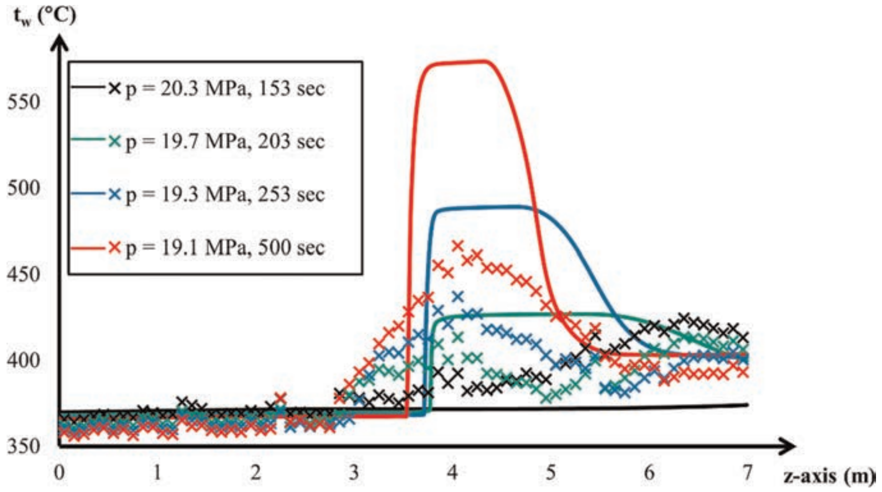
are assumed to terminate the simulations – representing case d).

5.2 *Analysis of multiple solutions problems*

Besides the convergence issues outlined in the previous section, implicit HTC correlations tend to gain multiple solutions for the same set of fluid parameters at supercritical pressures, i. e. heat flux, mass flux, bulk temperature and pressure [26]. In general, properties determining the heat transfer undergo a sharp increase or decrease at supercritical pressures and can have a peak near the pseudo-critical line. This behavior can lead to ambiguous results for the wall temperature in case of implicit correlations. Since the wall temperature must exceed the bulk temperature of the fluid for heating surfaces, the phenomenon of multiple solutions may primarily be ex-



(a) At supercritical pressures



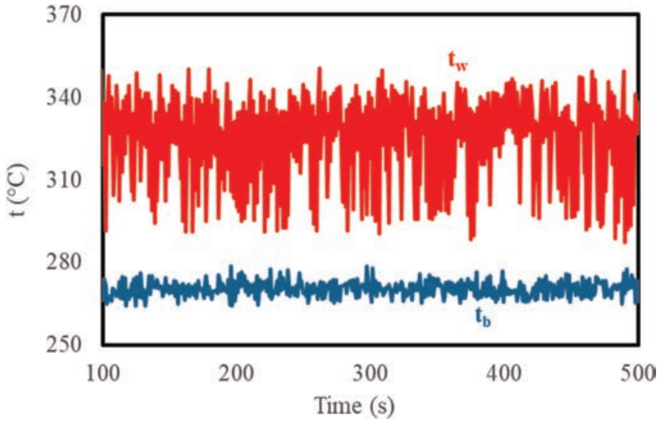
(b) At subcritical pressures

Fig. 7. Simulation results of the Kohlhepp et al. experiment using the Groeneveld look-up table for predicting the CHF and the Bromley correlation for the inverted annular film boiling (crosses represent experimental data and dashed/full lines represent simulation data)

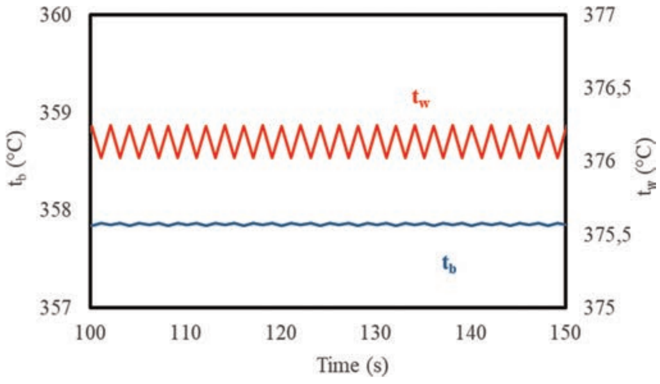
Table 5. Non-convergence issues associated to the corresponding correlation

Correlation	Oscillations	Bifurcations	Tw > 1 000 °C	No solution
Cheng et al. [4]	x			
Gupta et al. [5]		x	x	
Jackson and Hall [6]	x		x	x
Mokry et al. [7]		x	x	x
Watts and Chou [8]	x	x		
Zhao et al. [9]	x			

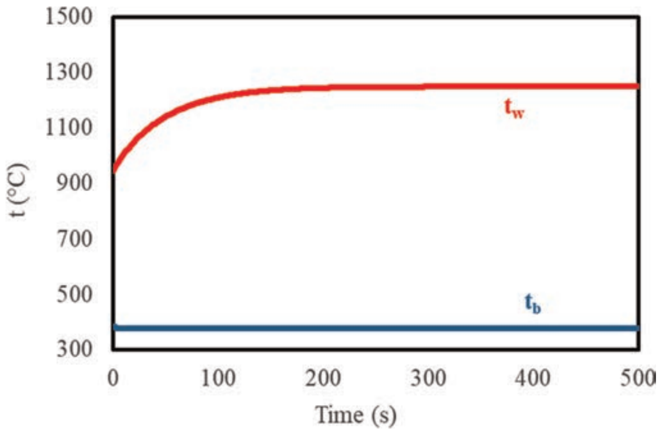
pected for bulk temperatures below or slightly above the pseudo-critical temperature. This was also observed by *Gschnaidtner et al.* [26]. Although the multiple solutions problem might produce misleading results, to the best of the authors' knowledge no study has identified or discussed the multiple solutions problem with respect to thermal-hydraulic system codes to date. However, in order to identify the cases with possible multiple solutions, a detailed screening of the HTC correlations is necessary [26]. Therefore, the data base was assessed applying the method proposed by *Gschnaidtner et al.* [26]. The results for the whole database according to this method are outlined in Table 6.



(a) Oscillations: Cheng et al. correlation, 267 kW/m^2, 55 kg/m^2/s, 24.5 MPa, 16 mm



(b) Bifurcations: Mokry et al. correlation, 800 kW/m^2, 2,250 kg/m^2/s, 22.5 MPa, 10 mm



(c) Unrealistic high solutions with no convergence: Mokry et al. correlation, 372 kW/m^2, 188 kg/m^2/s, 24.5 MPa, 16 mm

Fig. 8. Problems associated with non-convergence cases: (correlation, heat flux, mass flux, pressure, inner diameter)

Similar to the non-convergence data, most ambiguous results can be assigned to the correlation by *Gupta et al.*. This might be due to the strong dependence of the *Gupta et al.* correlation on the wall temperature: Most of the properties are calculated based on the wall temperature. A typical example for a multiple solutions problem is shown in Fig. 9a). Up to three possible solutions may be obtained for this set of parameters (see intersection points of blue and red dotted line) using the correlation by *Mokry et al.* (represented by the blue line). Here, the experimental solution is highlighted as a green star.

In order to analyze ATHLET with respect to the multiple solutions problem, the specific set of parameters was approached from two sides:

1. The first starting point was set to a lower bulk temperature than the corresponding bulk temperature of the parameter set. During the transient simulation, the enthalpy was gradually increased to the desired bulk temperature. The final result was taken at steady-state conditions, i. e. a simulation time of at least 500 s with no change in the final temperatures.
2. The second starting point was set to a higher bulk temperature than the corresponding bulk temperature of the parameter set. Furthermore, the bulk temperature was chosen in such a way that the wall temperature exceeded the wall temperature of the second or third solution possibility. During the transient simulation, the enthalpy was gradually decreased to the desired bulk temperature. The final result was taken at steady-state conditions, i. e. a simulation time of at least 500 s with no change in the final temperatures.

Various data points from the multiple solutions cases were selected and analyzed based on the above procedure. The results indicate that different results might be obtained depending on the starting bulk/wall temperature. Figure 9b) shows the exemplary simulation results for the *Mokry et al.* correlation. In this simulation, the results aim for the first and third solution identified by the method proposed by *Gschnaidtner et al.* [26]. This proves that implicit HTC correlations can in fact result in ambiguous results. However, in this study multiple solutions were only found in the relevant parameter range for SCWRs for the *Gupta et al.*, *Jackson and Hall* and *Mokry et al.* correlations.

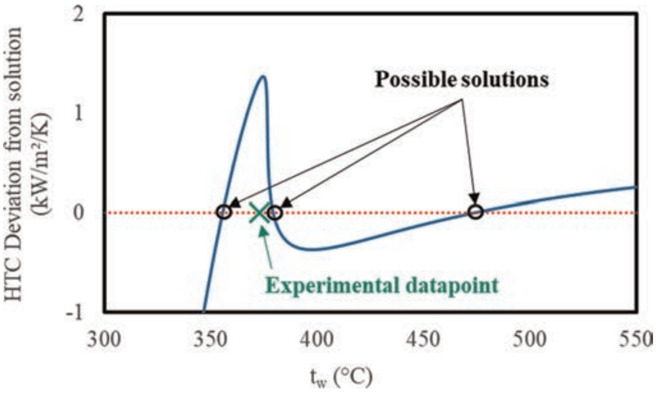
5.3 Analysis of the transient simulation results

5.3.1 Analysis of the Hein et al. experiment

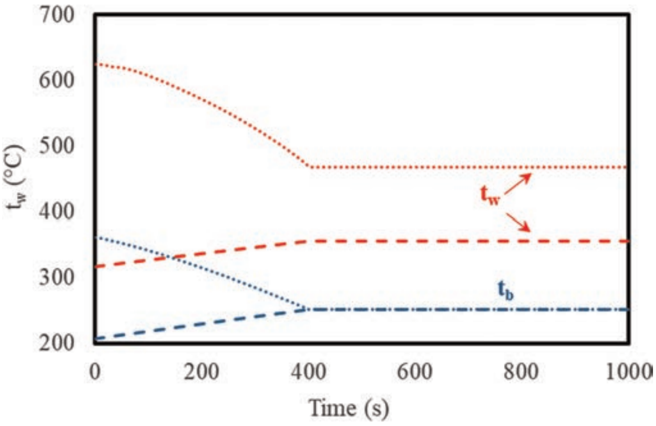
During the *Hein et al.* experiment temporary superheating and conduction controlled rewetting occurred. The superheating phenomena could not accurately be predicted by ATHLET: The onset of the boiling crisis was predicted at an almost constant value of the enthalpy, while the enthalpy increases constantly in the experiment. The final location of the onset was quite well predicted by the *Groeneveld* look-up table. The reason why the *Groeneveld* look-up table well predicts the final location of the boiling crisis is that it is the only correlation considering CHF data up to 21 MPa, while the validity range of all other correlations is limited to 17 MPa. However, the transient behaviour of the quench front could not be reproduced at all. At the time steps at 165 s and 265 s in the experiment, the location of the boiling

Table 6. Multiple solutions of the whole database according to the method proposed by Gschnaidtner et al. [10] and the maximum bulk temperature up to which multiple solutions may be expected in this study

Correlation	2 Solutions	3 Solutions	Max. bulk temperature
Cheng et al. [4]	0	0	–
Gupta et al. [5]	0	194	344 °C
Jackson and Hall [6]	0	9	270 °C
Mokry et al. [7]	35	72	322 °C
Watts and Chou [8]	0	7	190 °C
Zhao et al. [9]	0	0	–



(a) Multiple solutions possibilites of the wall temperature according to the method proposed by Gschnaidtner et al. [26]



(b) Multiple solutions of the wall temperature using the thermal-hydraulic system code ATHLET

Fig. 9. Multiple solutions problem using the correlation by Mokry et al.: 252 °C, 1,203 kW/m^2, 1,221 kg/m^2/s, 22.7 MPa, 9.4 mm

crisis is below the saturation temperature and shifts in flow direction towards the steady state solution. Although the conservation equations for the fluid and the tube wall are solved dynamically, it seems that the transient heat up process with respect to the heat transfer and in particular, the onset of the CHF is represented by a series of quasi-steady states. All CHF correlations were developed based on steady-state experiments and cannot reproduce the actual position of the quenching front. Although the *Cheng et al.* correlation quite well reproduces the experimental data of the wall temperature at supercritical pressures, the maximum wall temperature of the experimental data at subcritical pressures was over predicted by more than 200 °C. According to [27] for a dry wall and void fraction values of less than or just above 0.75 – as is the case in this experiment – the wall temperature is predicted using the HTC correlations by either *Berenson* [40] or *Bromley* [39]. Both correlations are based on experiments for a horizontal plate/tube and fluids other than water (i. e. benzene, carbon tetrachloride, n-pentane). Moreover, the experimental data were taken at atmospheric pressure [40]. Therefore, the applicability of both correlations is questionable at near-critical pressures.

5.3.2 Analysis of the Kohlhepp et al. experiment

Whereas throughout the *Hein et al.* experiment fast heat up and conduction controlled rewetting occurred, the experimental results by *Kohlhepp et al.* yielded only a slow heat up of the wall temperatures. However, the wall temperatures increased comparatively slowly to the *Hein et al.* experiment. Only the *Groeneveld* look-up table [42] predicted the onset of the boiling crisis quite accurately between 3 to 6 meters downstream of the inlet. This range corresponds to an enthalpy range from 2,052 to 2,295 kJ/kg. As mentioned before, the *Groeneveld* look-up table is the only correlation considering CHF data up to 21 MPa. Although the quench front is much steeper in the simulations, for slow transients, i. e. no fast heat up, the *Groeneveld* look-up table yields satisfactory results. However, all other CHF correlations predicted no boiling crisis at all or wall temperatures below the wall temperatures at supercritical pressures. Similar to the *Hein et al.* experiment the applied HTC correlations by *Berenson* [40] or *Bromley* [39] over predicted the final wall temperature of the experiment within the enthalpy range from 2,048 to 2,190 kJ/kg. At high void fraction values of more than 0.85 all correlations implemented in ATHLET are in good agreement with the experimental data. The reason is, that, for example, the correlation by *Groeneveld and Moeck* [43] was developed for water in vertical tubes for a pressure range up to 21.5 MPa.

6 Conclusions and final remarks

This study presents an extensive assessment of the ATHLET thermal-hydraulic system code and its implemented models. The capability of ATHLET was analyzed in predicting the heat transfer at steady-state and transient conditions in the near-critical pressure range. The HTC correlations for supercritical water were assessed against a database containing more than 15,000 data points from over 40 sources from the literature. In addition to the prediction accuracy, the numerical stability of the supercritical HTC correlations was analyzed. The applicability of ATHLET in describing the transient heat transfer behavior during a depressurization from supercritical to subcritical pressures was investigated based on two experiments.

The results of the assessment can be summarized as follows:

1. Assessing the HTC correlations for supercritical water implemented in ATHLET against the LESHP-database shows that overall none of the HTC correlations predict the heat transfer with satisfactory accuracy. Overall, the HTC correlation by *Watts and Chou* [33] gave the best results in terms of MARE, RMSE and SD followed by the correlations of *Jackson and Hall* [44] and *Mokry et al.* [38].
2. A detailed analysis of the numerical stability of the supercritical HTC correlations revealed that the following problem cases exist: oscillations, bifurcations, unrealistic high solutions and no solution. Most of these cases did not satisfy the convergence criterion of this study. In terms of unrealistic high solutions – wall temperatures exceeding 1,000 °C – temperatures of up to 6,250 °C were calculated by ATHLET.
3. In addition to non-convergence issues, all implicit correlations may yield ambiguous results for the same set of parameters. Depending on the starting point, i. e. below or above the desired bulk temperature, ATHLET calculated two different solutions for specific cases. This is related to the multiple solutions problem of implicit correlations resulting from the non-linear behavior of the thermophysical properties of supercritical water.
4. In general, numerical problems occur more likely for HTC correlations that strongly depend on the wall temperature: Since most of the properties are evaluated at the wall, the non-linear behavior of the thermophysical properties has a greater impact on the solution and hence on numerical stability.
5. The results of the transient trans-critical experiments showed that ATHLET is accurately capable of predicting the location of the onset of the boiling crisis based on the Groeneveld look-up table [42]. However, this is only the case for transient experiments without temporary superheating and conduction controlled rewetting phenomena. In case of transients including temporary superheating and conduction controlled rewetting process, ATHLET is not able to reproduce the position of the quench front and hence neither the temporary superheating nor the conduction controlled rewetting process.
6. In general, ATHLET over predicted the maximum occurring wall temperatures by more than 100 °C for both transient experiments. Moreover, the final temperature profile at steady-state conditions of the simulation did not match the experimental data of both experiments.

Although ATHLET is able to perform steady-state and transient simulations in the near-critical pressure range, the experimental heat transfer data cannot be reproduced or can only be reproduced to a certain degree. At supercritical pressures, more accurate models are required considering the numerical issues outlined in this study. At the current state, ATHLET cannot calculate temporary phenomena including the superheating and conduction controlled rewetting process. A new method is therefore required to predict the quench front. In addition, the steady-state results at subcritical pressures indicate the need for more accurate heat transfer models under inverted annular flow boiling conditions in the near-critical pressure range from 18 to 22 MPa.

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Nomenclature

d	diameter (m)
h	enthalpy (J/kg)
i	index variable (-)
L	length (m)
p	pressure (Pa)
t	temperature (°C)

Greek symbols

α	heat transfer coefficient (W/m^2/K)

Subscripts

b	at bulk conditions
cor	correlation
exp	experimental
i	internal
o	external
w	at internal tube wall conditions

Abbreviations

ATHLET	Analysis of THermal-hydraulics of LEaks and Transients
CHF	critical heat flux

CV	control volume
DHT	deteriorated heat transfer
GCSM	general control simulation module
GRS	Gesellschaft für Anlagen- und Reaktorsicherheit [Global research for safety]
HCO	heat conduction object
HTC	heat transfer coefficient
IHT	improved heat transfer
LESHP	Lehrstuhl für Energiesysteme High Pressure database
MARE	mean absolute relative error
MRE	mean relative error
NHT	normal heat transfer
NPP	nuclear power plants
RE	relative error
RMSE	root-mean-square relative error
SCWR	supercritical water-cooled reactor
SD	standard deviation
TFO	thermo-fluid-dynamic objects

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