

Extrapolating Phenomena Observed with Carbon Dioxide to Supercritical Water Reactor Conditions

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ABSTRACT

In the present paper, Supercritical Water Reactor (SCWR) fuel rod cooling conditions are addressed by a Computational Fluid Dynamic (CFD) model, in the light of the phenomena observed in experiments performed with carbon dioxide as a surrogate fluid. The discussion aims at highlighting how the interesting phenomena observed in these experiments may compare to those expected in actual reactor conditions. Making use of a fluid-to-fluid similarity theory recently developed by the authors for heat transfer applications and of the mentioned CFD model, possible counterpart experiments to be performed with carbon dioxide are envisaged, comparing them with the predictions obtained for water and drawing conclusions on their meaningfulness in view of SCWR behaviour prediction.

1 INTRODUCTION

Supercritical Water Reactors constitute the only Generation IV concept based on the long-term operating experience achieved with light water reactors (see, e.g., classical textbooks [1-3] and a recent review [4]). As such, the technological leap for achieving an advanced reactor concept may appear more feasible than for other technologies, in front of advantages as the higher energy conversion efficiency and a more compact design with respect to pressurized water reactors.

Studies are being performed since decades in this field, in the aim to achieve a better knowledge of the very peculiar heat transfer and dynamic phenomena occurring when fluids at pressures beyond the critical threshold approach the pseudo-critical conditions, being the locus of rather sharp local maxima of the specific heat, also marking a dramatic change in other thermodynamic properties. The transition from liquid-like to gas-like conditions, i.e., from a higher to a lower density fluid remaining substantially a single-phase one, adds considerable complexity to a behaviour that was initially believed simpler than at subcritical pressure, owing to the lack of phase change with the related phenomena of departure from nucleate boiling. Actually, in place or as a sort of reminder of the boiling crisis occurring at subcritical pressures, fluids beyond the critical pressure exhibit a departure from the normal heat transfer expected for a single-phase fluid that, especially in mixed convection conditions occurring in heated ducts in upward flow, appears in the form of "heat transfer deterioration". Phenomenological analogies between flow boiling and forced convection conditions at supercritical pressures

have been established for both heat transfer and flow dynamics, benefitting of modelling techniques applicable to both cases.

Two past Coordinated Research Projects of the International Atomic Energy Agency (IAEA) and an ongoing one contributed and are contributing to summarise the knowledge available worldwide in support to the design of SCWRs [5-7]. In past research activities, the authors of this paper have investigated both the flow dynamic and the heat transfer aspects of fluids at supercritical pressures, developing fluid-to-fluid similarity theories applicable to flow stability and to the various heat transfer regimes that are encountered in experimental tests [8-13]. The development of a CFD model based on an algebraic expression of the turbulent heat flux available in literature (namely the Algebraic Heat Flux Model, AHFM) has been an important step in providing a means for predicting observed heat transfer phenomena with unprecedented accuracy with respect to some experimental data [14]. The model was successfully applied to supercritical carbon dioxide data collected at the University of Ottawa [15-16], which revealed particularly useful for describing a full range of heat transfer phenomena occurring when a fluid at supercritical pressure undergoes heating starting with the liquid-like region and reaching the gas-like one, as it is expected for water in SCWR fuel channels. In particular, the data by Kline at the University of Ottawa involve normal heat transfer, the start of heat transfer deterioration, a full deterioration to a higher wall temperature manifold, very similar to a sort of boiling crisis, and a final recovery of turbulence occurring when the density in bulk becomes so similar to the one at the wall that buoyancy effects causing flow laminarisation are no more effective. Such a range of behaviours is not easily found in water experiments, owing to temperature and safety limitations, often suggesting to avoid overcoming the threshold of pseudocritical temperature in the bulk fluid during experimental activities, and stimulated interesting reflections about their origin [17-18].

Thanks to the predictive accuracy achieved in the developed CFD model and to the knowledge about heat transfer phenomena acquired by its application to actual experimental data with different fluids, it is now possible to envisage the behaviour expected to occur in a realistic SCWR subchannel configuration, exhibiting features in close similarity to those observed in CO₂ experiments, duly transposed to the operating domain of a supercritical water nuclear reactor. In this aim, a specific rod-and-coolant configuration already considered in previous analyses [19, 8] has been here addressed from the heat transfer point of view, making use of the mentioned AHFM model implemented under the STAR-CCM+ code [20].

The understanding gained by the experiments and transposed to water by the predictive capabilities of the CFD model provides a synergic and revealing description of expected phenomena, in a convincing picture that is proposed in the paper for reflection about the heat transfer behaviour that is envisaged in nuclear reactors. This behaviour should be confirmed by experiments that hardly exist at the moment, being anyway necessary for a safe design of SCWRs. In addition to the description of these expected phenomena, hints for conducting such experiments with water and CO_2 as a surrogate fluid are proposed, discussing predictions of results expected from experiments to be performed in future research activities.

2 ADDRESSED ROD AND COOLANT SYSTEM AND MODELLING CHOICES

The reference reactor channel condition is related to a fuel bundle already addressed in previous work on flow stability [see e.g., 19, 21], representing one of the possible reactor subchannel conditions. A sketchy representation of the rod with the related coolant is reported in Figure 1. These conditions have been used in a number of previous studies by the authors for sensitivity analyses on flow stability, made also with CFD codes [8, 22]; in those analyses heat transfer was obviously simulated, but it was not the first concern, considering that the focus of the studies was flow stability at imposed power conditions. In the present work, instead, profit is taken from the experience gained in the use of CFD models in simulating experimental data of wall temperature at supercritical pressure in different configurations, in

order to predict the possible trends of temperature along the fuel rod. A limitation of this first work on this subject is that the power of the rod is assumed to be uniform along the axis, something that is certainly not the case in actual operating conditions. Future work will take into account possible nearly sinusoidal distributions along the core height.



- fuel rod diameter: 10.2 mm;
- lattice pitch: 11.2 mm;
- rod-to-wall distance: 1 mm;
- coolant flow area: $5.49 \times 10^{-5} \text{ m}^2$;
- hydraulic diameter : 3.4 mm;
- channel length: 4.2672 m (14 ft);
- system pressure: 25 MPa;
- inlet temperature: 280 °C;
- individual rod coolant flow: 0.055 kg/s;
- linear power: 25 kW/m;

Figure 1. Addressed subchannel conditions and assumed working parameters.

A further simplification introduced in this work is the use of a 2D configuration for the fluid gap between the rod and the external box wall appearing in Figure 1, allowing to use the Algebraic Heat Flux Model (AHFM) introduced in STAR-CCM+ [14], which has received validation only in axial-symmetrical conditions. Given the fact that the diameter of the rod is 10.2 mm, in order to approximately preserve the flow area and the range of the hydraulic diameter, in the chosen 2D conditions the outer channel diameter was selected equal to 13.2 mm, providing a hydraulic diameter of 3 mm (vs. the actual 3.4 mm) and a cross section of 5.5×10^{-5} m² very close to the actual one.

The channel length is 4.2672 m (14 ft) and has been axially discretised with nodes of 1 cm. In the radial direction a well assessed technique is used, adopting prism layers close to the walls, aiming to refine the mesh to obtain a wall y+ lower than 1 at the heated wall and equally spaced elsewhere, except close to the non-heated wall, anyway, tolerating a higher wall y+ close to the latter (anyway less than 7). A total of 80+10+10 radial meshes, respectively in the prism layer close to the heated wall, in the bulk and in the prism layer close to the non-heated surface, have been used. The solid rod has not been simulated, imposing only the surface heat flux. An all-y+ approach (allowing for a low-Reynolds approach close to the heat wall and a blend of low- and high-Reynolds approaches at the non-heated one) has been adopted. This meshing technique was adopted for the water cases, adapting the values of its parameters in the case of the carbon dioxide analyses to be described below in consequence of the different values of the fluid properties and of the similarity principles.

3 PHENOMENA OBSERVED IN CO₂ EXPERIMENTS

Kline's experiments [15] have been collected in vertical bare tubes of different diameters making use of a variety of boundary conditions, using carbon dioxide at the supercritical pressure of 8.35 MPa. The great value of these data lies in the wide range of boundary conditions adopted, which allows to observe interesting phenomena, quite relevant for our present discussion. In particular, Figure 2 presents experimental and calculated trends of wall temperature as a function of bulk specific enthalpy, showing the following phenomena: 1) normal heat transfer (e.g., at low bulk enthalpy in Figure 2b); 2) inlet peaks of deterioration with temperature oscillations, which may be also a local phenomenon not leading to subsequent deterioration; 3) an envelopment of deteriorated heat transfer conditions (see the black dots in Figure 2b), showing a deteriorated manifold attracting temperature profiles at different inlet temperatures after the initial oscillations; 4) a heat transfer recovery after deterioration, occurring when buoyancy forces are no more strong enough to lead to laminarization, owing to the transition between liquid-like and gas-like conditions in the bulk fluid.





Figure 2. Kline's experimental data and CFD predictions showing the involved phenomena.

The richness of these phenomena is relevant to our reactor case, in which it is assumed that light water enters the core at about 280 °C (in liquid like-conditions at 25 MPa), exiting at a temperature of 500 °C or more, well beyond the pseudo-critical transition marking the boundary between the regions of liquid-like and gas-like conditions. Experiments with water in similar conditions, whether in bare tubes or rod bundle conditions, are scarce or even not existing, owing to the high temperatures involved in running the apparatuses, thus justifying the present attempt to extrapolate the behaviour observed with CO_2 to reactor postulated conditions. In this aim, use is made of the fluid-to-fluid similarity theory recently assessed by several CFD analyses [10-13], trying to estimate possible carbon dioxide experimental conditions that could be considered for experiments similar to the target water conditions.

4 RESULTS OBTAINED FOR WATER COOLING

The use of the AHFM implemented in STAR-CCM+ allowed to obtain results concerning the heated wall and the bulk fluid temperatures in the annulus representing the fuel rod with the related coolant in the nominal conditions for power and flow rate. As it can be noted in Figure 3a, the heated wall temperature shows a first deterioration while crossing the pseudocritical temperature (T_{pc}); then, the temperature keeps increasing also when the bulk temperature crosses T_{pc} . So, in this condition the final restoration at the transition to the gaslike phase is not observed. However, in sensitivity analyses performed by progressively decreasing flow rate at the same heat flux, shown in Figure 3b, it is noted that this phenomenon, clearly observed in Kline's data, starts appearing together with the previously mentioned wall temperature oscillations.



Figure 3. Results of the CFD model for the reactor channel water conditions.

410.5

Indeed, it must be recognised that the high values of the heated wall temperature obtained in the cases with low flow represent conditions in which the reactor should not be operated at full power, as it is in any case of loss of flow accidents. It can be also noted that assuming a uniform power profile along the channel axis contributes to the high values of temperature and represents a simplification that is here retained only for postulating possible experiments, which only in a few known cases have been run with the sinusoidal power profile which is more suitable to represent actual SCWR conditions. While this effect will be taken into account in a subsequent phase of the research, it is here useful to retain this assumption for comparison with the experiments by Kline, which were run with axially uniform power profile.

5 PREDICTING RESULTS OF CO_2 EXPERIMENTS TO BE PERFORMED IN SIMILARITY

Owing to space restrictions, it is not possible to recall here in sufficient detail the features of the similarity theory adopted in this work, referring the reader to the several papers published which describe its principles and methodology [10-13]. For the sake of clarity, here we simply recall that the theory is based on the link observed between a dimensionless form of the fluid density and the one of specific enthalpy, which is found nearly the same for some relevant fluids (water, carbon dioxide, ammonia, R23) in a large range of supercritical pressures. Since heat transfer phenomena at supercritical pressures are strongly affected by fluid density difference (e.g., by buoyancy and acceleration effects), two different fluid conditions are considered similar if the dimensionless enthalpy (hence the dimensionless density) has a similar distribution along and across the heated duct. This compels to use the same values of the dimensionless subcooling with respect to pseudo-critical conditions, represented by the number N_{SPC} , and the same dimensionless enthalpy jump, represented by the number N_{TPC} . Further considerations suggest imposing the same Froude and Reynolds numbers at the channel inlet, to make sure that the ratio between buoyancy and inertia will be preserved all along the duct and to maintain at least approximately the same level of turbulence. Corresponding pressures must be also selected according to a rationale summarised in the mentioned papers; in the present case, previous analyses showed that 25 MPa for water and 8.35 MPa for carbon dioxide correspond sufficiently well in terms of thermodynamic properties to allow for establishing a sufficient degree of similarity between corresponding two fluid conditions.



Figure 4. Comparison in dimensionless form of wall temperatures for water and CO₂.

Figure 4 shows the comparison in terms of dimensionless wall specific enthalpy of the results obtained for wall temperature in similar cases identified for CO_2 in comparison with the nominal case above presented for water. Note that a dimensionless enthalpy equal to zero means that the fluid is at the pseudocritical threshold. The different wall heat fluxes appearing in the plot represent corresponding attempts to obtain the closest behaviour from a quantitative point of



Figure 5. Wall temperature and Reynolds number for CO₂ cases at different heat fluxes

Figure 5 shows the values of wall temperature for the CO₂ cases corresponding in the similarity theory to the nominal water case, obtained at slightly different heat fluxes, and the corresponding trends of the Reynolds number for water and carbon dioxide. A striking aspect of these results is indeed the fact that for assuring the same dimensionless subcooling with respect to pseudo-critical conditions as in water at 280 °C the theory suggests that carbon dioxide should be chilled well below the water freezing temperature at the inlet of the test section, something that complicates the experimental procedure. This explains an observed difficulty to compare presently available results obtained with CO₂ (rarely below 0° C) with those obtained with water, pointing out an intrinsic problem in reverting to the most used and perhaps advisable surrogate fluid in supercritical pressure experiments applicable to water reactor conditions. In particular, 280 °C in water at 25 MPa corresponds to a value of N_{SPC} equal to about 1.55, resulting in a corresponding carbon dioxide temperature of -21.2 °C (251.95 K). So, since the degree of subcooling at the inlet determines the trend of fluid density along the heated duct in the transformation of the liquid-like fluid to a gas-like one owing to the consequent enthalpy change, it is necessary (though not sufficient) to keep the same value of subcooling at the inlet to assure a similar phenomenological behaviour.

On the other hand, the plot of the Reynolds number in Figure 5 shows that, even assuming the same value of the Reynolds number at channel inlet for the two fluids, it is unavoidable to witness strong discrepancies when the fluid is subsequently heated up, reaches the pseudocritical conditions and expands well beyond them. This is an unavoidable problem due to the different trends of the dynamic viscosity as a function of dimensionless enthalpy for different fluids: even assuming different diameters of the test sections to impose the equality of the Froude number and of the Reynolds number at the inlet, while the Froude number will keep similarity in the two cases (as it can be easily demonstrated), the Reynolds number, it is thus necessary to admit that only a partial similarity can be achieved along the pipe, to be possibly mitigated by a future recipe, e.g., suggesting imposing the same Reynolds number somewhere at middle length, in order to minimise differences in defect or in excess.

In order to carry on further the comparison of phenomena predicted by the CFD code for the two fluids with the phenomenological trends shown by Kline's data, Figure 6 reports in dimensional (wall temperature vs. bulk enthalpy) and dimensionless (wall dimensionless enthalpy vs. bulk dimensionless enthalpy) forms trends of wall temperature at a flow rate decreased to 70% of the nominal value, for different heat fluxes. As it can be noted, the initial peak of deterioration, the migration to a stable deteriorated regime at higher wall temperature and a final recovery before the transition to gas-like conditions in bulk are phenomena that can

be easily identified in the plots, closely reminding the trends observed in Figure 2 and in Figure 3b, respectively related to Kline's data and to predictions for water conditions. This information clarifies what can be reasonably expected from experiments with either fluid that would represent the addressed low flow reactor conditions.



*Figure 6. Wall temperature and wall dimensionless enthalpy for CO*₂ *at 70% flowrate, also in comparison with dimensionless trends for water*

6 CONCLUSIONS

The research whose first results are presented in this paper is aimed at exploring the consequences that experimental observations with surrogate fluids have on the postulated supercritical water reactor heat transfer behaviour. The scarcity or absence of data in which supercritical pressure water is let to be transformed from a liquid-like fluid to a gas-like one, as it is in postulated SCWR designs, is motivating to adopt fluid-to-fluid similarity theories to translate the broader information obtained by surrogate fluids to the conditions envisaged for nuclear reactors. In particular, it was shown here that the experimental data obtained by Kline at the University of Ottawa [15] can provide such relevant information, possibly only limited in significance by the fact that it was obtained for bare tubes instead of rod bundles. The large number of different boundary conditions adopted in those experiments makes them indeed valuable for a rather complete inquiry about phenomena to be expected in different regions of the operating regimes of interest.

The translation of Kline's experimental data to equivalent SCWR information has been made in previous work [13]. The specific task here has been to check if the phenomena pointed out by these experiments could be witnessed in postulated experiments related to the behaviour of a fuel rod in a reactor assembly. The results discussed in the previous sections above show that it is the case: temperature oscillations, deterioration with stable migration to a higher temperature manifold, heat transfer restoration at the transition to gas-like fluid in bulk are phenomena that can be observed in the results obtained for water and CO₂ in similar conditions. The limitation pointed out herein about the need of a substantial carbon dioxide subcooling for having meaningful experiment is an aspect to be carefully borne in mind.

The research is continuing by refining the modelling tools and by addressing non-uniform heat flux conditions, to make the obtained predictions more relevant for SCWR design.

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