NUMERICAL SIMULATION OF FLOW AND HEAT TRANSFER OF FLUIDS AT SUPERCRITICAL PRESSURE

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Abstract

Simple geometries such as circular pipes or annular channels have been used to investigate the heat transfer experimentally in the vicinity of the pseudo-critical temperature using water or CO_2. A large database exists worldwide. In these experiments large deviations from the 'normal' heat transfer behaviour were documented, in particular a strong dependency of the heat transfer coefficient on high wall heat fluxes and a sharp, sometimes unexpected drastic rise of the wall temperature, known as the 'heat transfer deterioration'. This body of data is also useful for model testing. Our own efforts were directed towards an analytic modelling of the near-wall turbulent layer and the laminar sub-layer in order to derive RANS turbulence model parameters and CFD wall functions, which are reliable for a large range of the flow and wall heat flux parameters. A close investigation on the flow mechanisms under deterioration conditions reveals that the thickness of the laminar, heat-conducting sub-layer must be modelled accurately as a function of the local Prandtl number. Furthermore it is necessary to take account of the drastic property changes, in particular of the heat capacity, with temperature or enthalpy in the turbulent near-wall layer. An attempt to model this effect has been made by using a probability-density function approach (pdf model). Buoyancy effects must also be modelled.

Various three-dimensional numerical examples of the flow and heat transfer within the reactor core cooling channels of the European High-Performance Light-Water Reactor (HPLWR) are presented. An important geometrical element of its core, are the wires wrapped around each rod as spacers. The wires enhance mixing and mass exchange between the sub-channels of an assembly, but they also may cause a non-uniform wall temperature distribution with local high-temperature regions. In order to validate our models, an experiment of a single rod with wrapped wire has been performed in the supercritical water flow loop of Xi'an Jiaotong University, China. The comparison of these and other experiments with CFD models shows, that great achievements have been made but the reliability of our models for supercritical flow conditions must be further improved.

1. Introduction

The Supercritical Water Reactor (SCWR) is presently studied as one of the six Generation IV nuclear reactor concepts due to its high thermodynamic efficiency and its economic advantages [1]. At supercritical pressure the cooling water is heated similar to a single-phase flow at high, supercritical pressure: thus no departure from nucleate boiling or dry-out can occur. However, in the vicinity of the pseudocritical temperature (382°C at 25 MPa) the fluid properties undergo drastic changes leading to nonlinear behaviour of the heat transfer, the mixing properties, and the moderation of neutrons. This has led to a complex geometrical design of an SCWR core, with separate moderator channels, wrapped-wire spacers, and support structures with thin walls. Therefore, design studies and safety analyses of such a core are often performed or supported by a detailed three-dimensional numerical flow simulation (CFD). In the present paper the ability of CFD methods to predict this complex heat transfer behaviour of turbulent flows at supercritical conditions is discussed. In particular such effects as heat transfer enhancement, deterioration and the formation of local high-temperature wall regions are of interest.

These systems make use of the high heat capacity of water at pressures not far above the critical pressure, by operation at typical system pressures in the range 22,5-27,0 MPa (the critical pressure for water is at 22,1 MPa). In Europe this reactor concept is denoted as the High-Performance Light-Water Reactor (HPLWR); a first design concept has been presented in [2-5]. A supercritical steam cycle with pre-heater (economizer), inlet and outlet of the Reactor Pressure Vessel (RPV), high pressure (HP) turbine, intermediate (IP) and low pressure (LP) turbines is used. Here, the ´phase change´ from compressed water to compressed steam occurs continuously in absence of phenomena such as film boiling or surface dry-out, which are associated with an abrupt temperature rise. Also, a Pressurized Water-cooled Reactor with supercritical pressure in the primary circuit hat been considered [6].

In order to prevent material overheating of the core cooling channels it is particularly important to predict the heat transfer accurately for very high heat fluxes and all mass fluxes in the bulk temperature range between 280 to 500 °C. Interesting for an HPLWR are pipe diameters between 5 and 20 mm, pressures between 22,5 and 29,0 MPa enthalpies between 1000 and 3000 MJ/(kg K), mass flow rates between 300 and 2000 kg/m^2 and wall heat fluxes up to 1500 kW/m^2.

The flow and heat transfer to fluids above the thermodynamic critical pressure, e.g. strongly heated pipe or channel flows, are influenced by the nonlinear variations of the fluid properties (density, viscosity, heat conductivity, enthalpy and heat capacity) with temperature near the critical point. The enthalpy and the heat capacity exhibit the most pronounced changes: in the above given pressure and temperature range the heat capacity has a local maximum at the pseudo-critical temperature (e.g. 656 K at 245 bar), with values as much as 25 fold compared to neighbouring temperatures.

This lecture gives an overview on the most important flow and heat transfer effects and mechanisms in supercritical flows with heat transfer. The present status of relevant CFD models is presented. Another overview has been given in [7-9].

2. Heat Transfer Phenomena at Supercritical Pressure

a. Experimental Observations

Simple geometries such as circular pipes or annular channels have been used to investigate the heat transfer experimentally in the vicinity of the pseudo-critical temperature using water or CO_2. Some heat transfer mechanisms are discussed in [10] and [11]. A large database exists worldwide, see [12,13]. In these experiments large deviations from the ‘normal’ heat transfer behaviour were documented, in particular a strong dependency of the heat transfer coefficient on high wall heat fluxes and a sharp, sometimes unexpected drastic rise of the wall temperature, known as the ‘heat transfer deterioration’. This body of data is also useful for model testing.

Various experimental investigations have been performed at supercritical conditions with water flowing upward or downward in circular pipes under intense electrical heating [14-19]. In these and other studies the various nonlinear effects of heat transfer enhancement and deterioration were identified, correlated, and classified. The data were summarized in a look-up table [20]

In media other than water similar phenomena occur: In gas flows within strongly heated channels an increase of the wall temperature may be observed, which is sometimes attributed to re-laminarization due to flow acceleration [21]. To take advantage of its relatively low critical pressure and temperature CO_2 can be used as a medium, e.g. [22-24], to understand the effects of property variations or to calibrate models.

At positions where the pseudo-critical temperature (defined as the temperature where the specific heat at constant pressure has a local maximum), lies between the bulk and the wall temperatures, the heat transfer may exhibit unusual behaviour such as enhancement or ´deterioration´. Often the heat transfer coefficient increases near the pseudo-critical temperature for low heat flux (denoted as ´enhancement´), but often decreases relative to this measure when the wall heat flux is increased.

These are local phenomena, which can be correlated purely on the basis of local parameters, i.e. without any upstream effects taken into consideration. The dramatic rise in the wall temperature for some cases at high heat flux and low mass flux is denoted as ′deterioration′.

b. Insights from Direct Numerical Simulation

The governing principles of continuum motion and heat transport are the conservation of mass, momentum end energy within a spatially fixed infinitesimal control volume, i.e. the ‘Euler’ frame of reference. For a Newtonian fluid such as water or water vapour these equations are known as the Navier-Stokes Equations of fluid mechanics. We consider these equations to be ‘exact’ in the sense that they describe all flows, even the very complex and unsteady turbulent flows, without further modelling. The simulations based on these equations are denoted as ‘direct’. Direct numerical simulations (DNS) of isothermal single phase turbulent flows have extensively been performed; a relevant review article is given in [25]. The method has extensively been applied to isothermal transitional [26, 27] and turbulent flows [28].

For non-isothermal flows, when heat transfer between the wall and the fluid is relevant, we have in addition the energy equation, in which the temperature, the heat capacity and the heat conductivity appear. Dissipation of kinetic energy into heat has been neglected. Simulations of channel flows heve been performed [29]. For natural convection bouyancy can be introduced into the system, making e.g. the DNS of supercritical pipe flows with heat transfer possible. In a gas flow the effect of re-laminarization could be reproduced [30]. In a supercritical flow of CO_2 the effect of density variations in the fluctuations could be identified [31,32].

c. Results from Analytical Modelling

Fundamental theories on the modelling of wall-bounded turbulence, see e.g. [33-35] may serve as the basis for the analytical modelling of variable-property flows. Various efforts were directed towards an analytic modelling of the near-wall turbulent layer and the laminar sub-layer in order to derive RANS turbulence model parameters and CFD wall functions, which are reliable for a large range of the flow and wall heat flux parameters [36-39]. A close investigation on the flow mechanisms under deterioration conditions reveals that the thickness of the laminar, heat-conducting sub-layer must be modelled accurately as a function of the local Prandtl number. Furthermore it is necessary to take account of the drastic property changes, in particular of the heat capacity, with temperature or enthalpy in the turbulent near-wall layer. Buoyancy effects must also be modelled.

In [40] an attempt is made to extend existing models for heat transfer in channel or pipe flows to variable-property fluids, i.e. supercritical water in a pipe. Emphasis is laid on the effect of the local maximum of the Prandtl number and the heat capacity near the pseudo-critical temperature on the laminar or turbulent heat transport. The one-dimensional near-wall momentum equation (to determine the mean velocity) and the energy equation (to determine the temperature, including the wall temperature) in the wall normal direction are used as a strarting point of the analysis. We use Prandtl’s algebraic mixing-lengh turbulence model. For the temperature, which is of primary interest here, the wall layer is subdivided into a heat conducting, laminar sub-layer and a logarithmic layer. In the sub-layer the heat transfer is determined by the Prandtl number of the fluid, which may vary depending on the temperature distribution across the layer. In the logarithmic region the heat transfer depends only on the turbulence Prandtl number. The thickness of the laminar sub-layer is very important for the heat transfer deterioration and must be modelled in a physical correct manner.

The result is expressed in ‘wall units’ y+. The temperature rise in the logarithmic layer depends only on the turbulence Prandtl number and the van Karman constant, both being parameters of the turbulence model. The temperature rise across the heat conducting (laminar) sub-layer depends on the Prandtl number of the fluid and on the thickness of the heat conducting sub-layer, which in general differs from the thickness of the viscous (laminar) sub-layer of the velocity. Both mechanisms as an effect of the property change on laminar and turbulent flow regions or layers are modelled. Thus heat transfer deterioration is captured qualitatively and, with some restrictions, quantitatively. A close investigation on the flow mechanisms under deterioration conditions reveals that the thickness of the laminar, heat-conducting sub-layer must be modelled accurately as a function of the local Prandtl number. Furthermore it is necessary to take account of the drastic property changes, in particular of the heat capacity, with temperature or enthalpy in the turbulent near-wall layer.

The theory [40] contributes to a better understanding of heat transfer of supercritical flows. It can also be used for the development of numerical wall functions, which are needed for an efficient numerical simulation using Computational Fluid Mechanics. By comparison with experiments it is demonstrated, that it is able to capture the effects of heat transfer deterioration quantitatively well. Improvements of the accuracy, however, may be achieved by a further investigation of two important model parameters: the thickness of the heat-conducting sub-layer and the turbulence level, here represented by the width of the fluctuation spectrum.

3. Accuracy of Present CFD and Turbulence Models

The first to simulate such conditions numerically using a two-dimensional CFD model were Koshizuka et al. [41] using a low-Re k-ε turbulence model with fine resolution of the near-wall region. Acceptable qualitative agreement with the experimental data [19] was achieved. In the meantime, however, a large database of other experimatal investigations on supercritical heat transfer has been established, see chapter 2.1. A large variety of flow and turbulence mechanisms exist in these flows, such as heat transfer deterioration, enhancement, buoyancy effects, re-laminarisation and more. The heat transfer to supercritical water in the cooling channels of a Supercritical Light Water Reactor (SCLWR) has been investigated by using CFD in numerous studies. Such investigations rely on the ability of a turbulence model to predict the wall temperatures accurately under the respective flow conditions

A brief overview on some of these studies is given in the following:

- The accuracy of the RNG-k-ε model was investigated in [42] and some guidelines for the near-wall numerical resolution were derived. It was found that some kind of heat transfer deterioration could be predicted.
- Another study has been performed in [44]. The k-ω model is recommended to simulate heat transfer deterioration.
- The authors of [45] were able to predict the onset of overheating using the k-ω-model with very fine wall resolution.
- The analysis [46] focuses on results obtained by a low-Reynolds number k-ε model. The obtained results allow comparing the trends observed for heat transfer deterioration at supercritical pressure with those typical of the thermal crisis in boiling systems.
- In a preliminary study [47] five turbulence model were used. All models were able to reproduce the general trend.
- [48] concluded from their study of 14 different turbulence models that the RNG-k-ε model with enhanced wall treatment gave the most outstanding results.
- Based on sensitivity tests of [49] with several FLUENT's models, the standard k-ε model was found be sufficient as a base model for further development to handle supercritical flow.

It becomes obvious, that the respective recommendations about the best turbulence model depends on the flow parameters of the respective test case as well as on some details on the near-wall numerical grid. To date, a reliable turbulence model for CFD, which covers all phenomena of supercritical water flow and is able to predict the wall temperature accurately in all cases, does not exist. This lack maybe due to the fact that none on the models, which have been implemented in commercial CFD codes, has been developed for supercritical flows. In particular the large changes of the heat capacity and the Prandtl number with temperature near the pseudo-critical point were not considered during the development of those models. It is therefore not yet permissible to conclude about the flow physics or special turbulence mechanisms, e.g. re-laminarization, from the results of RANS simulations of supercritical flows.

4. Three-Dimensional Effects at Supercritical Pressure

Three-dimensional effects occur in the core cooling channels or in the mixing chambers below and above a core section [50]. We will focus on the core cooling channels, in which the noncircular shape is the main deviation from the pipe flows as discussed above. Although analytical criteria exist [51], many three-dimensional numerical examples of the flow and heat transfer within the reactor core cooling channels of an SCWR exist.

In [52] investigated the heat transfer of supercritical water in various flow channels using the computational fluid dynamics (CFD) code CFX-5.6. In their paper and in [53,54] CFD analyses are carried out to study the flow and heat transfer behaviour of supercritical water in sub-channels of both square and triangular rod bundles. In [55] heat transfer in upward flows of supercritical water in circular tubes and in tight fuel rod bundles is numerically investigated by using the commercial CFD code STAR-CD 3.24. Other on smooth channels can be found in [56-58].

An important geometrical element of the core of the HPLWR are the wires wrapped around each rod as spacers. The wires enhance mixing and mass exchange between the sub-channels of an assembly, but they also may cause a non-uniform wall temperature distribution with local high-temperature regions. An attempt to determine the mixing coefficients for this geometry by unstedy RANS has been performed in [59].

Attempts were made to compute the flow in parts of the fuel bundle [60] using symmetries or the whole bundle [61]. A section with one revolution located in the evaporator region of the HPLWR core is investigated using hydraulic (to ensure fully developed flow inlet boundary conditions and reference for heated cases) and thermal-hydraulic boundary conditions. The geometry of wrapped wires gives rise to additional mixing and a circulating or ‘sweeping’ flow near the outer and inner regions of the fuel element next to the wall of the so called fuel assembly and moderator box. Some interesting flow features associated with the complex three-dimensional flow with significant transverse velocity components are visualized as the first evaluated result of this diversified investigation. The aim of this investigation is to gain experience about CFD modelling of the whole perimeter HPLWR fuel assembly and to provide firstly qualitative and then quantitative insight about the inter-channel cross flow and mixing. Considering the high number of computational cases relatively coarse numerical meshes have been used to discretize the geometry. Fine boundary mesh is not applied to model suitably the near wall region. That is why the wall temperature and the near wall fields are not accurate enough to be investigated in detail but the physically valid demonstration of qualitative features of the flow in such geometry is expected. The scalable wall function has been used to model the near wall region. The geometry and mesh (with the automatic tetra meshing method) was created in the ANSYS ICEM CFD 11 SP1. The unstructured tetrahedral meshes of the cases differ only in the total number of nodes due to different global mesh size.

These computations were performed on a NEC Xeon EM 64T type cluster named “cacau1” at HLRS (Peak Performance: 2.5 TFlops). Cacau1 has 200 dual nodes with 400 Intel Xeon EM64T CPU's (3.2GHz) for high performance computation. ANSYS CFX 11 SP1 has been used in parallel mode on cacau1 for the computations. Table 2 summarizes the used number of processors, wall clock times, maximal residual and imbalance values for each computational group. Four so called “User Point” were monitored during the calculations: the area average of the pressure and velocity on the inflow and outflow regions. The User Points and the imbalances indicated that all of the cases are well converged which means each value converged to a certain value (almost zero for imbalances) and does not changing with the iterations any more. The convergence values are acceptable considering the proposal of the guidelines. Not swirling flows are well converged with a reduction of only 3-4 orders of the final/peak RMS residual ratios. In case of swirling flow (which is valid for all cases presented here) 5-6 orders of the final/peak RMS residual ratios is necessary and acceptable for converged CFD calculation.

The expected flow properties such as additional mixing and the sweeping flow are qualitatively reproduced as expected. A quantitative comparison to the results of a sub-channel code has now become possible in order to better understand and possibly improve the sub-channel models for wrapped-wire geometries. The expected counter-clockwise (outer swiping cycle) and clockwise (inner swiping cycle) swiping flow is demonstrated next to the fuel assembly and moderator box walls respectively which helps to eliminate the hot spots confirmed by previous studies. Unidirectional inter-channel cross flows have been proven between sub-channels in the inner and outer sweeping cycle and bidirectional inter-channel cross flows have been found through such gaps which are between two fuel rods (gaps far from fuel assembly and moderator box walls). Such work demonstrates, that with reasonable numerical effort a sufficient accuracy of the CFD calculations can be achieved using unstructured tetrahedral grids, the Reynolds-stress turbulence model and a combination of cases with hydraulic and thermo hydraulic boundary conditions.

In order to validate our models for a complex geometry, an experiment of a single rod with wrapped wire has been performed [62,63]. The comparison of these and other experiments with CFD models shows, that some achievements have been made but the reliability of our models for supercritical flow conditions must be further improved.

The work [64-65] presents a three-dimensional simulation of the conjugated heat transfer to supercritical water flowing upward in a square annular channel around a single wire-wrapped rod. Some efforts have been made previously without taking the heat transfer of cladding material into consideration, in which a very high temperature region is observed in the upwind side of the wire on the rod surface. In these investigations a Local Deteriorated Heat Transfer (LDHT) occurs at a high heat flux over mass flux ratio, i.e. the wall temperature rises significantly within a hotspot. However, when the heat conduction in the cladding material is taken into account (conjugate heat transfer), the maximum wall temperature is reduced and the prediction reaches a better agreement of the mean surface temperature compared with experiments. The cladding temperature within the hotspots is remarkably reduced with elimination of the local heat transfer deterioration due to the heat conduction of the cladding material. However, the conjugate heat transfer does not remove the hotspot completely. In the paper investigations of a smooth rod (no wire) in a square and in an annular channel are also presented for comparison.

5. Improvements of CFD Models

a. Wall Functions

In turbulence modelling there are two alternative approches for the treatment of the near-wall turbulent layer including the laminar, heat conducting sublayer a) full resolution schemes using a 'low-Reynolds number' turbulence model, or b) wall functions. An important parameter of these models is the non-dimensional wall distance of the first data point adjacent to the wall y_1^+. Here the index + refers to the non-dimensional 'wall units' and the index 1 to the first, wall-adjacent discretization point or cell. A small required value of y_1^+ means, that the first grid point or cell must be close to the wall and therefore a fine near-wall grid is required.

In order to achieve acceptable accuracy of method a) as well as to capture the complex heat transfer behaviour of supercritical turbulent flows, the near-wall region of the turbulent boundary layer has to be resolved with large numerical effort ($y_1^+ << 1$) and numerically inefficient low-Reyonolds number turbulence models have to be applied. Method b) can only be applied when the state-of the art (standard) wall-functions are extended to variable-property fluids. Wall functions allow a much coarser grid resolution ($y_1^+ > 30$) giving approximately the same results as low-Reynolds number turbulence models.

Recently, the near-wall turbulence processes, which are responsible for heat transfer enhancement and deterioration, have been much better understood and documented than in the past and thus analytic modelling of this near wall behaviour can be used to develop wall functions for supercritical flows [65]. Standard wall functions can be extended to supercritical flows with variable properties. In the heat-conducting sub-layer the temperature-dependency of the molecular Prandtl number can be taken into account by a subdivision into intervals and numerical integration. In the turbulent wall layer the enhanced transport by the high heat-capacity turbulent flow is taken into account by a modified turbulence Prandtl number. The nonlinear dependency of all properties on the temperature is modelled. As a result we get analytic expressions for the heat transfer coefficient, which must be solved by an iteration.

In [65] we have used the wall functions with a set of constant model parameters for all cases. By comparison with experiments it is demonstrated, that our wall functions are able to capture the effects of heat transfer deterioration quantitatively well. Improvements of the accuracy, however, may be achieved by a further investigation of two important model parameters: the thickness of the heat-conducting sub-layer and the turbulence level. Improvements may also be achieved by modelling further details of the flow such as the buffer layer.

b. Modification of the Turbulence Model

In [67] we proposed a pdf model to take account of the important temperature fluctuations in the definition of an average (or turbulent) heat capacity, which exhibits the largest variation near the pseudo-critical temperature. This approach introduces an assumption about the amplitude and frequency spectrum of the turbulent temperature fluctuations, which is parameterized by using a Gaussian probability density (filter-)function. The model takes these average mean properties on physical grounds in contrast to other models, in which the fluid properties are simply determined at the local, average temperature or enthalpy. In the approach the local turbulence level is taken into account as a model parameter.

We found in [67], that the agreement of CFD results with experiments [19] can be improved, when a turbulent heat capacity is modelled. Due to the nonlinear dependency of all fluid properties on the temperature the process of averaging must be modified. In general, any property taken at the local mean temperature may be different from a property arising from temporal averaging at fluctuating temperature. In particular the avaraging of the heat capacity is important. A parameter is introduced as a measure for the fluctuation intensity of turbulence, because the range of instantaneous temperature values increases with it. Our new pdf-model is tested for a case of super-critical heat transfer of pipe flows to water, using a semi-analytical method, in which the one-dimensional momentum and energy equations for turbulent flows are integrated numerically [68]. Quasi-fully developed flow is assumed, buoyancy is not considered. Good agreement with various experiments is achieved. The present results are independent of a particular CFD-code or numerical grid. Our pdf-model can be implemented as a modification of existing turbulence models into any CFD code.

6. Conclusion

The goals of a CFD analysis in reactor safety is to provide a reliable tool for the physical understanding of a flow and for the scaling between the spatial dimensions of laboratory experiments and a power plant. In order to meet these goals, turbulence models must to be physically correct (up to a high degree) and scalable. The consequences of these requirements on the choice of CFD turbulence models is discussed along with examples of present model developments. Some aspects towards a turbulence modelling strategy for the application of CFD methods in nuclear reactor safety have been discussed.

7. References

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