NUCLEAR ENERGY RESEARCH INITIATIVE

Development of Modeling Capabilities for the Analysis of Supercritical Water-Cooled Reactor Thermal-Hydraulics and Dynamics

PI: *Dr. Michael Z. Podowski, Rensselaer Polytechnic Institute*

Collaborators: *None*

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Research Objectives

- Develop an experimental and theoretical data base for heat transfer in tubes and channels cooled by water and CO_2 at supercritical pressures.
- Develop mechanistic computational models of local turbulence-driven heat transfer in forced-convection flows of supercritical fluids experiencing strong variations of physical properties.
- Implement the new models in the NPHASE-CFD computer code, and perform model testing and validation against available experimental data for both water and CO_2.
- Test the proposed models using water and carbon dioxide (CO_2) as working fluids. Perform parametric analyses on the effect of different models of turbulence, including both kinematic and, in particular, thermal aspects of turbulence.
- Perform numerical simulations to validate the new models against experimental data, to show their applicability in the analysis of SCWR thermal-hydraulics.
- Perform numerical simulations of supercritical water system dynamics based on the NPHASE code. In particular, investigate transient response of a heated channel to power and flow variations. Analyze the effect of both heat transfer enhancement and heat transfer degradation.
- Investigate the effect of fluid property variations at supercritical pressures on thermal-hydraulics of SCWRs.

A summary of the major research accomplishments is give below. Details concerning specific issues can be found in the publications listed at the end of this report.

Major Research Accomplishments

(1) Development of Data Base for Model Validation of Heat Transfer in Supercritical Fluids

In collaboration with Royal Institute of Technology (KTH) in Stockholm, Sweden, and with Korea Atomic Energy Research Institute (KAERI), an extensive study has been performed on the development of a data base for heat transfer in tubes and channels cooled by water and CO_2 at supercritical pressures.

A schematic of a new Supercritical Water Loop (SCWL) test facility at KTH is shown in Figure 1. A schematic of supercritical CO_2 test facility, SPHINX, test at Korean Atomic Energy Research Institute (KAERI) is shown in Figure 2.

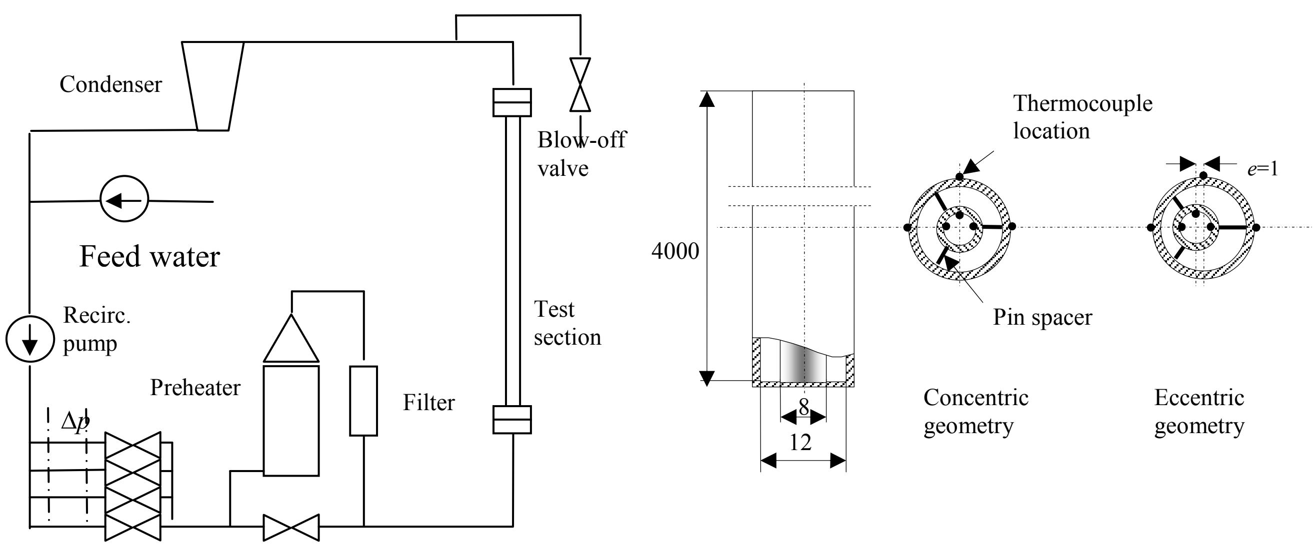


Figure 1. Supercritical water loop (SCWL) at KTH:

(a) a schematic of the test facility,

(b) details of proposed test sections.

In particular, the results of experiments at the SPHINX test facility have been examined and selected results have been identified as suitable for multidimensional simulations and model validation. As shown in Figure 2, two geometries of a heated section have been included in both the experiments and the simulations: a cylindrically heated tube insulated from outside and an annulus with a heated rod inside.

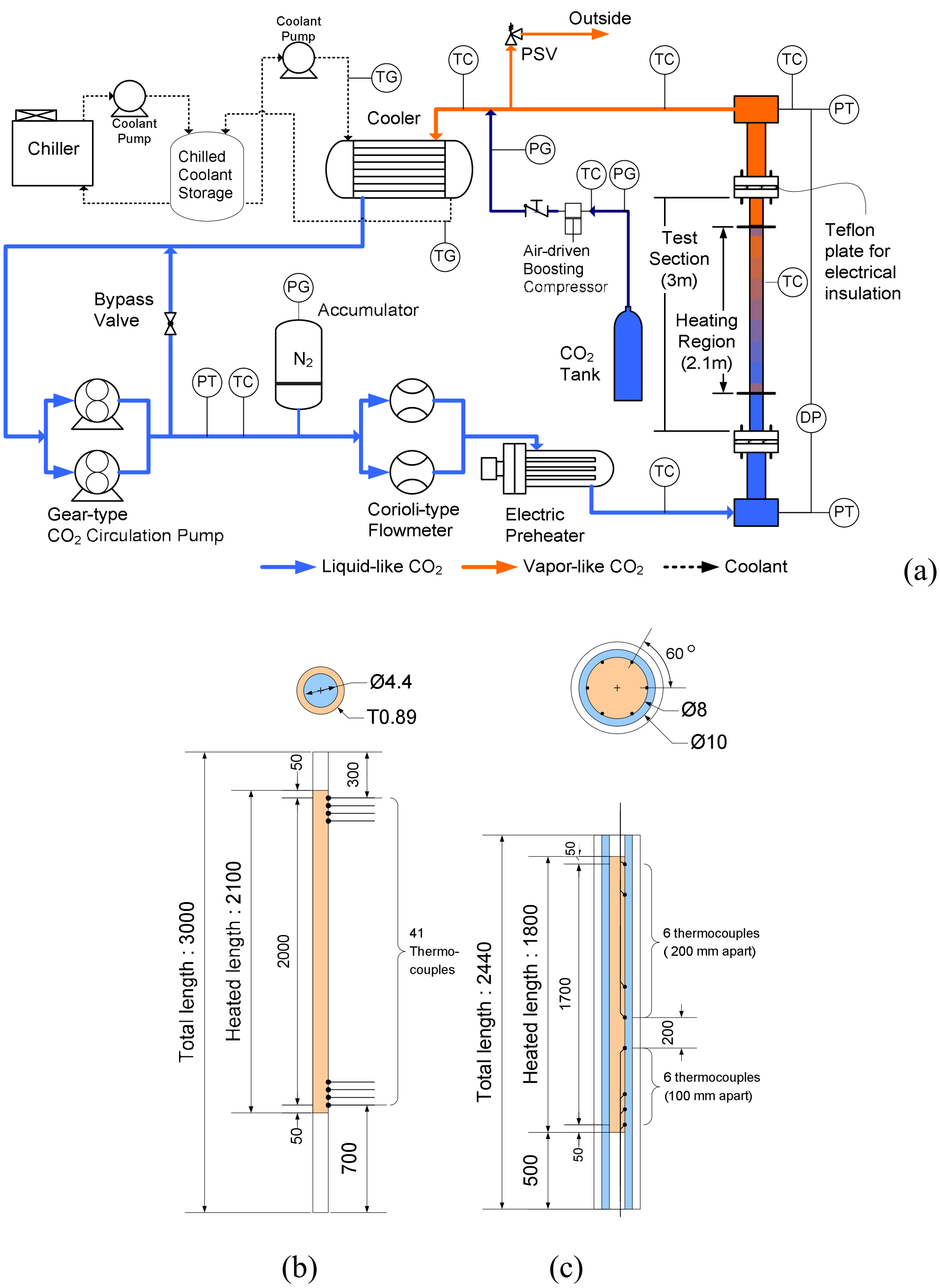


Figure 2. SPHINX test facility:
(a) schematic diagram,
(b) cylindrical-heated-tube test section,
(c) annular test section.

(2) Development of Computational Models of Supercritical Fluid Properties

New analytical models have been developed for all major properties of water (i.e., density, viscosity, specific heat, thermal conductivity, and Prandtl number) as functions of temperature and pressure, for pressures varying between 23.5 MPa and 25 MPa. The new models have been converted into a non-dimensional form based on the ratios of actual-to-critical pressure and actual-to-critical temperature (using the absolute temperature scale). Furthermore, similar models have also been developed for supercritical carbon dioxide (CO_2).

For computational purposes, all major thermo-fluid properties of both CO_2 and water at supercritical pressures have been converted into analytical expressions based on a spline-type formulation given by

$$\Psi(T,p) = a_{\zeta,i}(P) + b_{\zeta,i}(P)T + c_{\zeta,i}(P)T^2 + d_{\zeta,i}(P)T^3 \quad \text{for} \quad T_i \le T \le T_{i+1}, \quad (i = 1,2,...N)$$

where Ψ represents one of the following properties: density, ρ, specific heat, c_p, dynamic viscosity, μ, thermal conductivity, k, and Prandtl Number, Pr, and N is the total intervals needed to sufficiently resolve the property dependence on temperature.

The new models were first validated for fixed pressures; then the effect of pressure has been be accounted for as an independent variable in a manner similar to that used for temperature variations. Typical results showing a comparison between the new models and experimental data are shown in Figure 3.

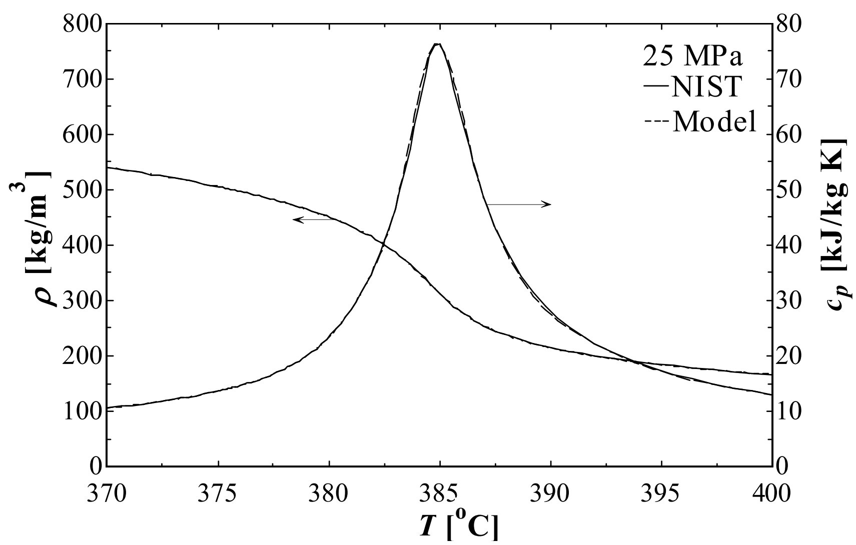


Figure 3. Temperature-dependent density and specific heat of water at a supercritical pressure of 25 MPa; a comparison between the current model and the official NIST data.

(3) Improvements in the NPHASE-CMFD Computational Solver

As a result of the present work, several contributions have been made to upgrade some of the existing models in the NPHASE-CMFD code, and to develop and implement new models pertinent to the objectives of the current project.

The new models include:

- Thermodynamic property routines for water and carbon dioxide at supercritical pressures; see Item (2) above.

- A model of transient heat conduction/convection between the hated wall and the fluid flowing along the wall has been developed and encoded in NPHASE-CMFD. A schematic of the new model is shown in Figure 4. The main rationale behind the model is to properly capture the effect of heater inertia during transients on the interfacial conditions at the heated wall surface in contact with a variable-property fluid at a supercritical pressure. Both annular and solid-cylinder type heater geometries have been accounted for.

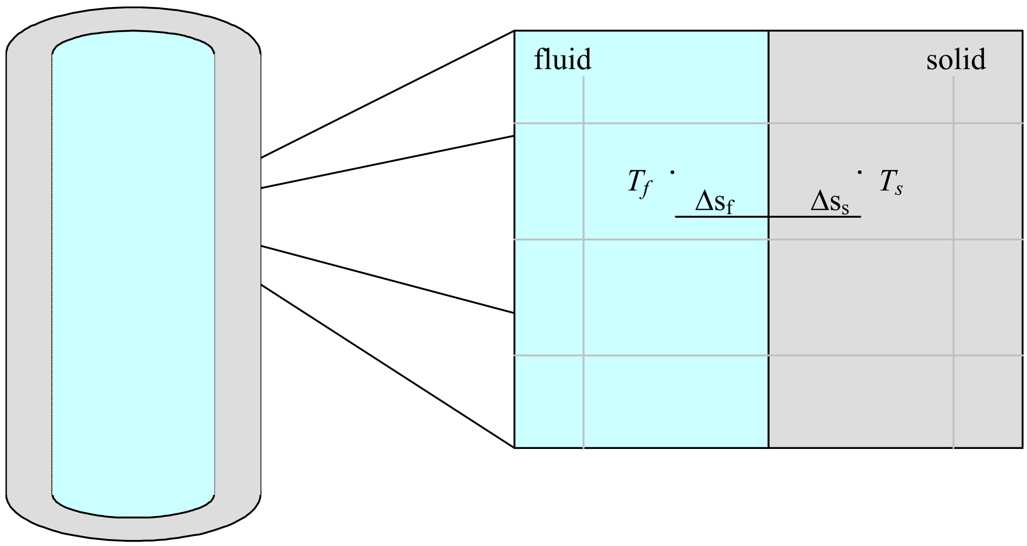


Figure 4. A schematic of the computational model of solid/liquid interface at transient conditions.

The models which have been the subject of major upgrades and modifications included the following:

- near-wall heat convection based on a High-Reynolds Number (HRN) k-ε model of turbulence,
- variable property models of turbulence based on both HRN and Low Reynolds Number (LRN) k-ε models.

Selected results obtained using the modified models are shown in Items (4) and (5) below.

(4) Effect of Fluid Properties Variations on Local Velocity and Temperature Fields in Heated Channels

Extensive testing and validation have been carried out of the proposed multi-dimensional model of flow of heat transfer for both supercritical water and CO_2 as coolants. Typical results are shown in Figures 5 and 6. The results at a reference pressure of 25 MPa are shown in Figure 6. In order to demonstrate the ability of NPHASE to quantify the effect of system pressure on flow and heat transfer conditions, calculations were also performed for a pressure of 24 MPa.

As it can be readily noticed, the overall results are numerically consistent and they show correct physical trends.

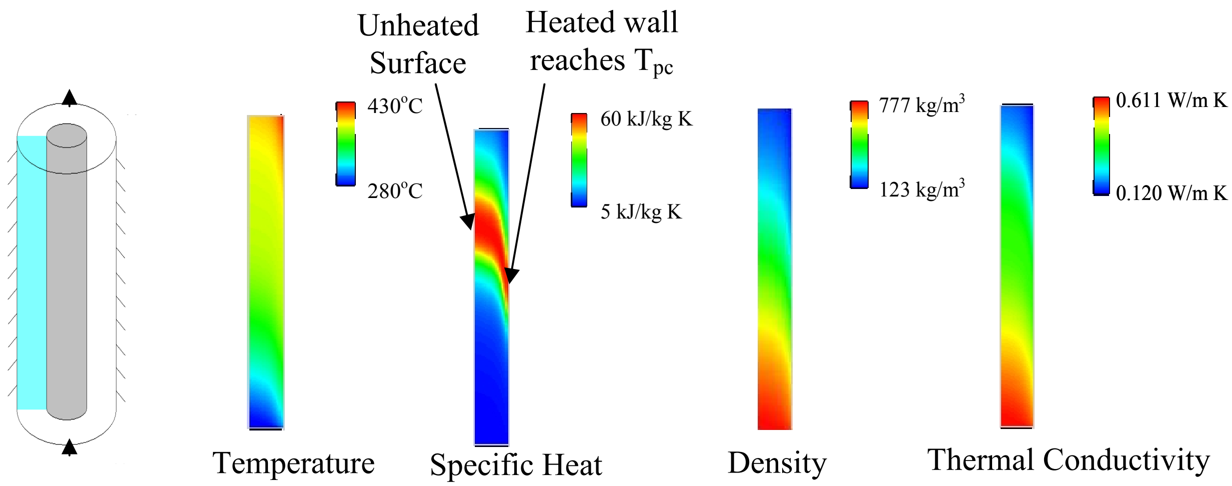


Figure 5. Heated channel geometry and contour plots of various parameters for water at 25 MPa.

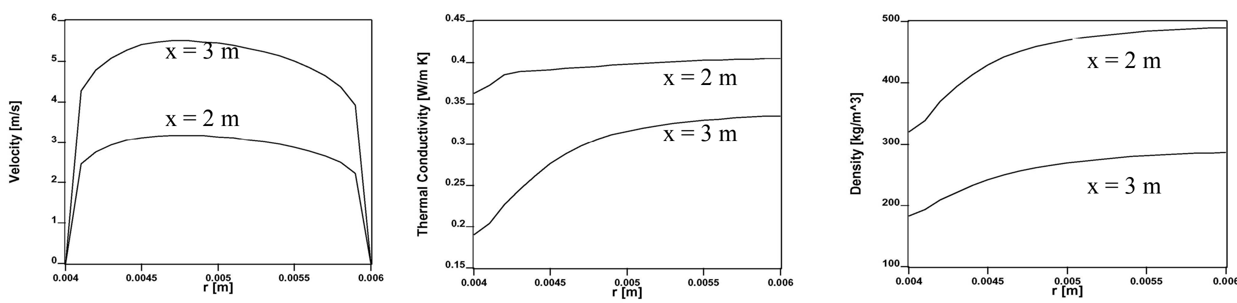


Figure 6. Radial plots at two axial locations along a 4 m long heated channel at 25 MPa.

(5) Effect of Turbulence Model on Wall Temperature and Local Heat Transfer Coefficient in Heated Channels Cooled by Fluids at Supercritical Pressures

The effect of variable properties of supercritical water has been analyzed on the heat transfer in heated channels cooled by both water and CO_2.

The radial velocity and temperature profiles at two axial locations, shown in Figure 7, indicate that the Low-Reynolds Number (RRN) model predictions match and extend upon radial trends predicted by the High-Reynolds Number (HRN) model. It is also seen from these plots that the dominant temperature and velocity changes in each cross-section occur within the boundary layer, and are predicted by the LRN model.

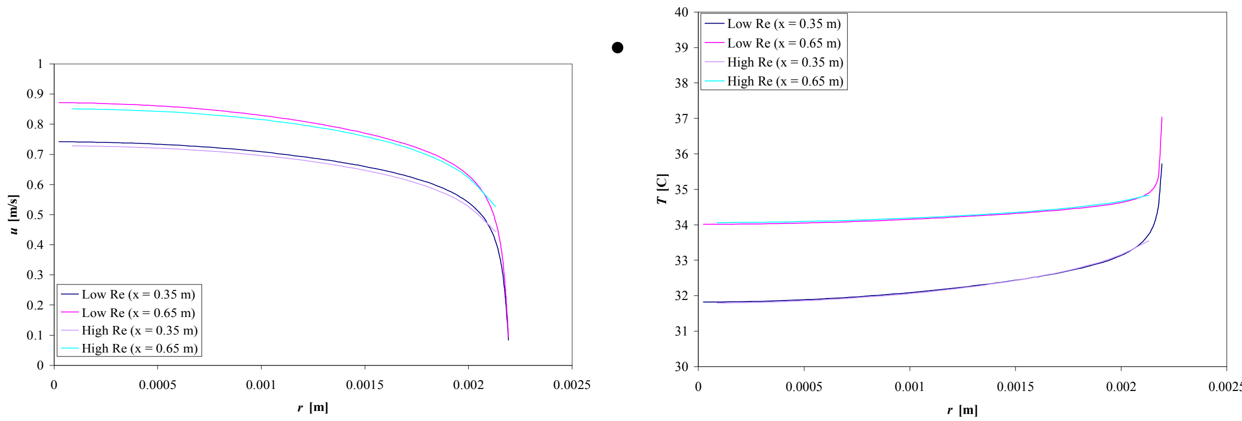
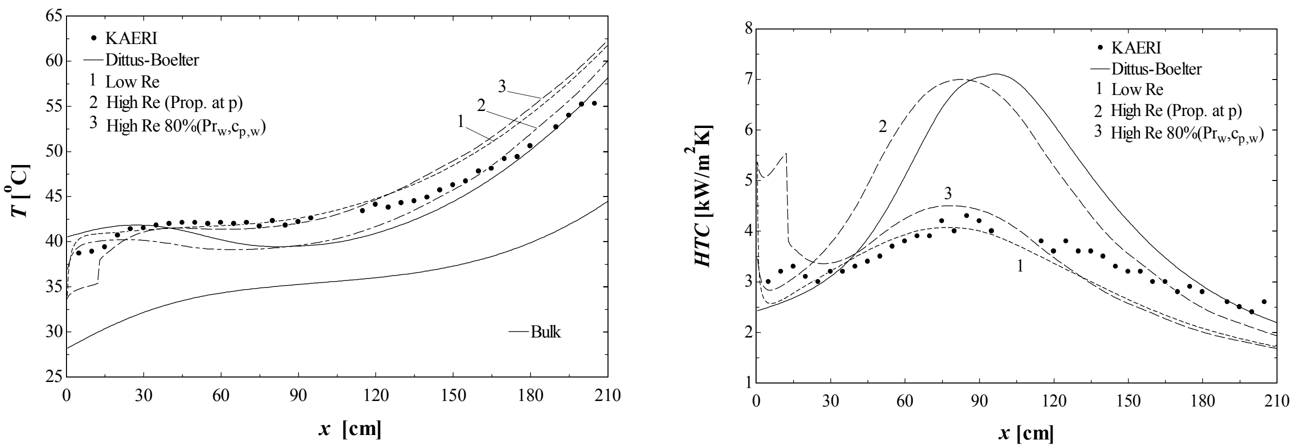


Figure 7. Radial velocity and temperature profiles for flow in heated channel with variable properties.

Figure 8 shows the axial profiles of temperature and the heat transfer coefficient along the heated channel, as predicted by the Low- and High-Reynolds Number (LRN and HRN) turbulence models, as compared against the corresponding experimental results. The Low-Reynolds Number model predicts the wall temperature crossing the pseudo-critical temperature near the entrance to the channel. Also, the bulk fluid temperature crosses the pseudo-critical temperature at a distance of approximately one meter from the entrance of the channel. Figure 8(a) shows that the Low-Reynolds Number model correctly predicts the wall temperature before the bulk temperature reaches the pseudo-critical region, then begins to overpredict the experimental data as the bulk fluid crosses the pseudo-critical region. Figure 8(b) shows that the Low-Reynolds model did not capture the subtle peak in heat transfer coefficient at the entrance of the channel, but predicts the experimental data well after this peak up to the position at which the bulk temperature reaches the pseudo-critical value. The heat transfer coefficient is under-predicted after this point, and just as in Figure 8(a), the wall temperature was slightly over-predicted. However the Low- Reynolds Number model prediction for the heat transfer coefficient is of a similar magnitude as the experimental heat transfer coefficient, showing that the finer resolution in the near wall region accounts for a lower overall heat transfer coefficient than that predicted by the Dittus-Boelter correlation. The temperature in the last half of the channel, after the bulk fluid temperature has passed the pseudo-critical point, is generally overpredicted by the multi-dimensional models. This difference may be caused by the fact that the derivation of the transport equations for momentum, mass, and turbulent quantities. Clearly, additional work is still needed to fully resolve the current small differences between the predictions and data.



(a) Temperature (b) Heat Transfer coefficient

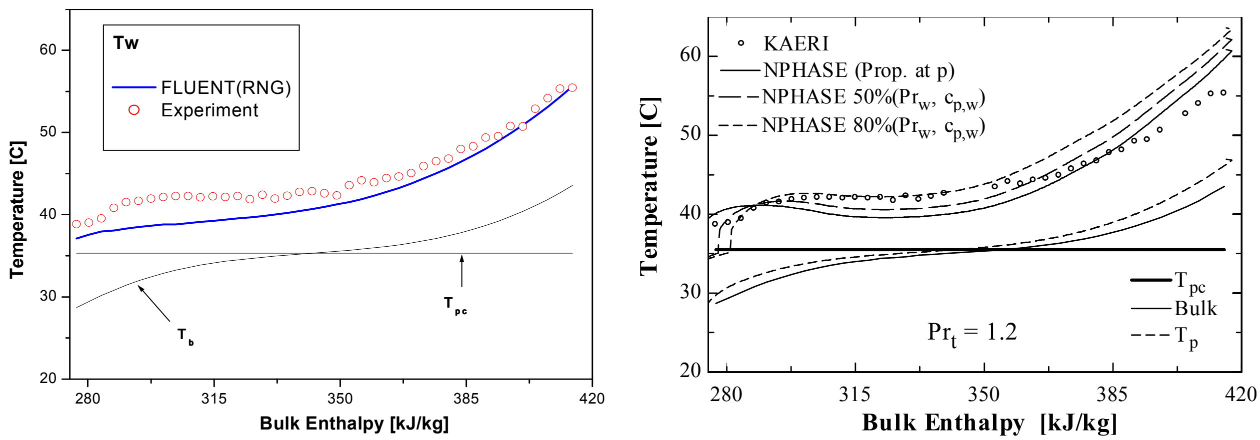
Figure 8. Axial profiles of watt temperature and heat transfer coefficient for flow in a heated channel with variable properties.

(6) Analysis of Uncertainties Associated with using Different Computational Tools

A comparative analysis has been performed between two CFD computer codes: FLUENT and NPHASE-CMFD. Two heater geometries have been investigated: flow in a tube heated from outside and an annulus with a central heated rod. The results of simulations have been compared against experimental data and empirical correlations. Typical results are shown in Figures 9 and 10.

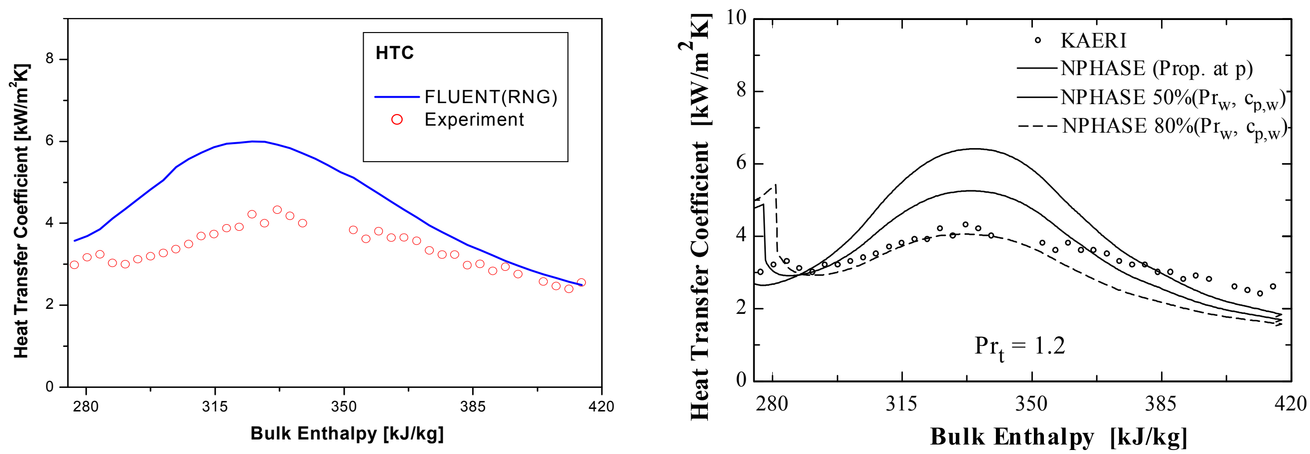
Figure 9 display shows that the Fluent RNG model overpredicts the heat transfer coefficient at the point where the bulk temperature crosses the pseudo-critical temperature, much like in the NPHASE predictions if the properties are evaluated at the near-wall nodal point, *P*. At the same time, the FLUENT RNG model predicts the heat transfer coefficient in the high temperature region (i.e., after the bulk and wall temperatures have surpassed the pseudo-critical temperature) slightly better than the NPHASE simulations. These results suggest that both properly accounting for the cross-sectional property variation and the modeling of turbulence may be the keys for improving the accuracy of heat transfer predictions in supercritical fluids.

Figure 10 displays a comparison between FLUENT and NPHASE predictions with the experimental results for the channel with a heated inner rod. The Fluent RNG model is used, as before, to model the effect of turbulence. As can be seen in Figure 10(a), the heat transfer coefficient predicted by FLUENT is much higher than the experimental values. A similar trend, but of a much (3 times) smaller magnitude, is observed in the NPHASE predictions for the case of fluid properties taken at the near-wall nodal point, *P,* inside the logarithmic wall-of-the wall region (it is important to mention here that the result is practically independent of the specific distance between point-*P* and the wall as long as $10 < y_P^+ < 300$). At the same time, if the fluid properties used in the calculation of wall temperature are used, the error in the NPHASE-predicted peak heat transfer coefficient is less than 10%. Thus, one concludes that the cross-sectional property variation plays the dominant role in the prediction of the peak heat transfer coefficient in the region where the local fluid temperature passes through the pseudo-critical temperature range.



(a) FLUENT (b) NPHASE

Figure 9. Temperature distribution predictions compared with experimental data for Case A1.



(a) FLUENT (b) NPHASE

Figure 10. Heat transfer coefficient predictions compared with experimental data for Case E1.

(7) Flow Dynamics

A model has been developed and implemented in the NPHASE-CMFD code for the analysis of local phenomena at non-steady and transient flow conditions in heated channels cooled with fluids at supercritical pressures. The major features of the new model are: it includes complete models of variable properties of both supercritical water and CO_2, and it accounts for thermal inertial of the heater. The model is applicable to both tubes with a central heated rod and to pipes with directly heated walls (annular heater geometry). Initial testing of the new model has been performed. In particular, simulations have been carried out for the transient response of a heated annular channel subject to changes in the wall heat flux and inlet mass flux. Figure 11 shows a comparison between the NPHASE-CMFD predictions and the results obtained using a simplified one-dimensional (1-D) model. As can be seen, the agreement between the two models is quite good, although slight differences have been observed, which can be explained by the fact that the NPHASE-CMFD model accounts for local (across the channel) effects in both flow and heat transfer.

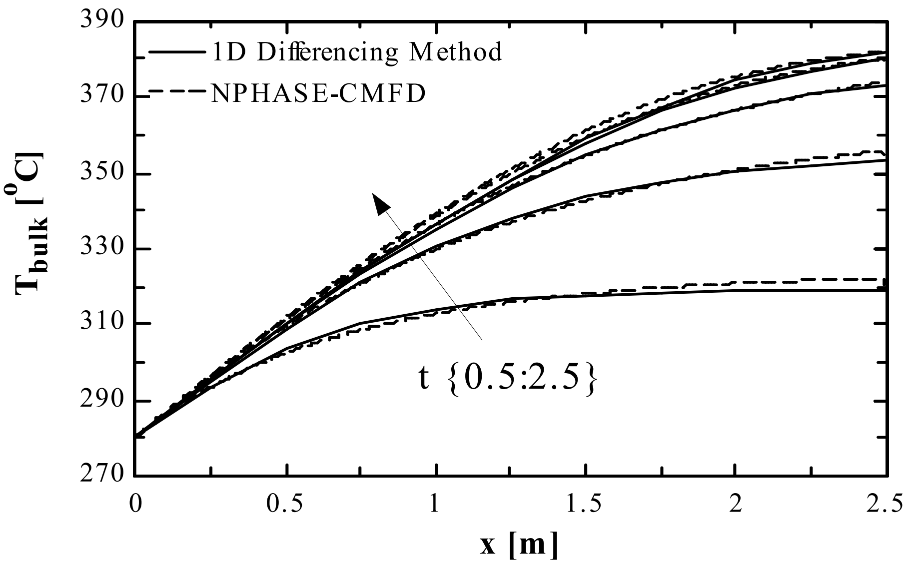


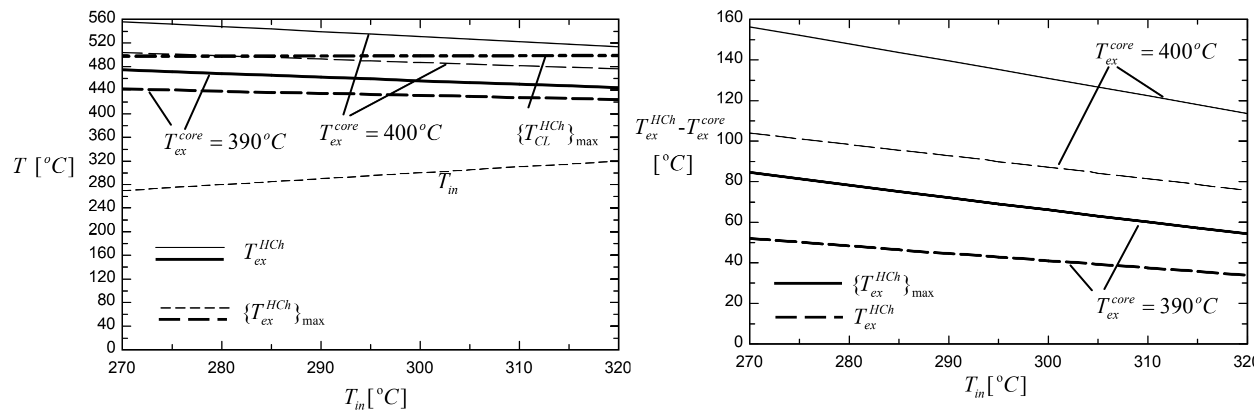
Fig. 11. Time and axial-position-dependent bulk temperature in a heated channel subject to a sudden increase in wall heat flux.

(8) Effect of Properties of Supercritical Water on Thermal-Hydraulic Aspects of SCWR Design

An important feature of most Supercritical Water-Cooled Reactor (SWCR) designs that have been proposed to date is a highly nonuniform temperature distribution inside the reactor core. This is mainly due to the combined effects of core peaking factors and limits imposed on coolant flow rate. Furthermore, statistical uncertainties in the evaluation of hot spot factors normally contribute to an increase in the range of temperature distribution that must be considered in reactor design. Thus, it is important that the effect of variable properties of supercritical water be properly be understood to identify possible methods of reducing the maximum coolant temperature and improving the thermal-hydraulic characteristics of the proposed reactor system.

Typical results of a parametric study are shown in Figures 12 and 13, aimed at analyzing the effect of core inlet temperature on the core exit temperature, the corresponding hot channel exit temperature, and the maximum cladding temperature. As both Figures indicate, whereas a significant degree of nonuniformity is anticipated to occur between the coolant temperature at hot channel exit and the exit temperature averaged over the entire core flow area, the magnitude of the actual temperature difference strongly depends on the average core exit temperature.

Other results of the present study show that by modifying the reactor operating conditions and/or core design characteristics, significant improvements can be achieved aimed at mitigating the effect of variable properties of supercritical water on the local nonuniform temperature distributions across the reactor core in general, and the exit coolant temperature in particular. Thus, various possible modifications in the current reactor design should be investigated in future works. In particular, the effect of small design changes of core layout should be considered, aimed increasing the coolant flow rate. For example, an increase in the inlet velocity by as much as 50% should be quite feasible. Also, the effect of coupling between the thermal/hydraulic and neutronic characteristics of the SCWR core should be thoroughly investigated using state-of-the art models and computational tools, such as those developed in this project.



(a) (b)

Figure 13. The effect of uncertainties in the evaluation of various SCWR parameters on the: (a) maximum hot channel exit temperature and maximum cladding temperature, (b) maximum coolant temperature increase along the reactor core.

(9) Conclusions and Plans for Work Continuation.

Several thermal-hydraulic issues arising from using fluids at supercritical pressures as coolants in heated channels in general, and future Gen. IV Supercritical Water Reactors (SCWRs) in particular, have been investigated in the present project. It has been shown that a multidimensional approach based on CFD concepts is capable of properly capturing local effects that may lead to either heat transfer deterioration or enhancement. Still additional work is still needed in order to develop fully-mechanistic models applicable to different fluids and a broad range of operating conditions.

It is important to mention that the research at RPI will continue on selected issues addressed in the project, at no cost to the sponsor. This is possible thanks to the fact that this project has been a part of PhD research requirements by a doctoral student who will still work on several unresolved issues needed for the PhD program completion. Specifically, those issues will include a new approach to the modeling of turbulence in supercritical fluids, further model testing for both heat enhancement and heat deterioration conditions, and the analysis of local multidimensional aspects of unsteady states in heated channels and SCWRs.

Finally, a complete list of publications documenting the results of the research on this project is shown below. It should be noticed that this list includes papers which have been submitted (and already accepted) to several conferences planned after the termination of the project. This is why we have recently submitted a final request for a no-cost extension, to cover the travel expenses associated with attending those conferences and presenting our most recent results there.

Publications Documenting the Results of Current Research

1. Podowski, M.Z., Antal, S.P. and Anglart, H., "Development of Mechanistic Modeling Capabilities for Generation-IV Supercritical Water-Cooled Reactor (SCWR)", with S.P. Antal and H. Anglart, Proc. ICAPP'06 Conf., Reno, NV, 2006.
2. Gallaway, T., Antal, S.P. and Podowski, M.Z., "Local Multidimensional Model of Fluid Flow and Heat Transfer in Generation-IV Supercritical Water Reactors", Proc. ICONE-14 Conf., Miami, FL, 2006.
3. Podowski, M.Z., "Thermal-Hydraulic Aspects of SCWR Design", Proc. 15th International Conference on Nuclear Engineering, ICONE15-10285, Nagoya, Japan, 2007.
4. Gallaway, T., Antal, S.P. and Podowski, M.Z., "Effect of Physical Properties of Fluids at Supercritical Conditions on Local Flow and Heat Transfer in Heated Channels", Proc. Int. Congress on Advances in Nuclear Power Plants, Nice, France, 2007.
5. Anglart, H., Gallaway, T., Antal, S.P. and Podowski, M.Z., "Prediction and Analysis of Onset of Turbulent Convective Heat Transfer Deterioration in Supercritical Water Flows", Proc. Int. Congress on Advances in Nuclear Power Plants, Nice, France, 2007.
6. Gallaway, T., Antal, S.P., Podowski, M.Z., Bae, Y.Y. and Cho, B.H., "The Development of a Modeling Framework for Multidimensional Analysis of Flow and Heat Transfer in Supercritical Fluids", Proc. Twelfth International Topical Meeting on Nuclear Reactor Thermal-Hydraulics (NURETH-12), Pittsburgh, PA, 2007.
7. Gallaway, T., Antal, S.P. and Podowski, M.Z., "On the Modeling of Thermal Aspects of Turbulence in Heated Channels Cooled using Supercritical Fluids", Proc.16th International Conference on Nuclear Engineering (ICONE-16), Florida, FL, Orlando, 2008.
8. Gallaway, T., Antal, S.P., and Podowski, M.Z., "Multidimensional Model of Fluid Flow and Heat Transfer in Generation-IV Supercritical Water Reactors", *Nuclear Science and Engineering*, 238, 2008, pp.1909–1916.
9. Podowski, M.Z., "Thermal-Hydraulic Aspects of SCWR Design", *Journal of Power and Energy Systems*, **2**, 1, 2008, pp. 352-360
10. Gallaway, T., Antal, S.P. and Podowski, M.Z., "Mechanistic Multidimensional Analysis of Heat Transfer in Fluids at Supercritical Pressures ", Proceedings of ICAPP '09, Tokyo, Japan, May 10-14, 2009 (to be published).

11. Gallaway, T., Antal, S.P. and Podowski, M.Z., “Multidimensional Modeling of Flow and Heat Transfer to CO2 at Supercritical Pressures”, Proceedings of International Supercritical CO_2 Power Cycle Symposium, Troy, NY, April 29-30, 2009.
12. Gallaway, T., Antal, S.P. and Podowski, M.Z., ”Mechanistic Multidimensional Analysis of Heat Transfer in Fluids at Supercritical Pressures“, Proceedings of ICAPP ’09, Tokyo, Japan, May 10-14, 2009 (to be published).
13. Gallaway, T., Antal, S.P. and Podowski, M.Z., “Multidimensional Analysis of Turbulence in Forced Convection Heat Transfer for Fluids at Supercritical Pressures”, 13th International Topical Meeting on Nuclear Reactor Thermal-Hydraulics (NURETH-13), Kanazawa City, Japan, September 27 – October 2, 2009 (in preparation).