NUMERICAL SIMULATION OF HEAT TRANSFER OF SUPERCRITICAL FLUIDS UNDER SCWR CONDITIONS (REVIEW)

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Abstract

SCWR was proposed as a type of generation IV reactors. The numerical simulation becomes a useful method for studying supercritical fluids in SCWR. The objective of this paper is to review the works that have been published in the numerical simulation of heat transfer of supercritical fluids under the SCWR conditions. Literatures show that there are still limits in the study of the fluid flow and the heat transfer of supercritical water in fuel channels. Due to this deficiency, the full-scale 3-D CFD simulations on the heat transfer of supercritical fluids are highly required for the design of SCWR.

1. Introduction

Supercritical fluids have been widely used in various industries, such as air-conditioning and heat pump systems in refrigeration engineering, cooling in rocket propulsion system in aerospace engineering, and cooling of superconducting electronics in cryogenics engineering [1, 2]. In nuclear industry, a supercritical water-cooled reactor (SCWR) was proposed as a type of generation IV reactors in order to improve the performance and efficiency of nuclear reactors [3].

The SCWR system has advantages in sustainability, economics, safety, and reliability. These systems may have a thermal or fast-neutron spectrum, depending on the core design. An SCWR system is shown in Figure 1 [3]. The main objectives of using supercritical fluids in nuclear reactors are: (a) to improve the performance and efficiency of nuclear power plants from 33%-35% to about 40%-45%; (b) to decrease the operational and capital costs (about \$1000 US/kW).

Many researchers have experimentally studied the heat transfer of supercritical fluids in circular tubes. Detailed reviews on heat transfer at supercritical pressures were provided by several authors [4-6]. However, representative experiments on large-scale models of the fuel elements can be performed only to a limited extent and at very great expense. The need for more accurate methods of predicting the behavior of coolant flow and heat transfer in SCWR has given rise to CFD methods.



Figure 1 Schematic of SCWR system [3].

Two approaches are currently used in the numerical study of SCWR: (a) numerical simulations in a single subchannel of SCWR with the assumption of periodical boundary conditions and (b) the subchannel approach where the flow in each subchannel is assumed uniform and the turbulent mixing coefficient is used to account for the turbulent effect [7, 8]. The objective of this paper is to understand thermal-hydraulic behavior of supercritical fluids and to review the works that have been published in the numerical simulation of heat transfer of supercritical fluids under the SCWR conditions.

2. Thermal-physical properties of supercritical fluids

A supercritical fluid is a fluid of which the pressure and the temperature are higher than the values at the critical point. The position of the supercritical fluid can be shown in projection of phase diagram of water in Figure 2. The critical pressure of water is 22.1 MPa and the critical temperature is 374.12°C. However, in the present monograph, the term supercritical fluid includes: (a) the fluid of which both pressure and temperature are higher than the critical values; (b) the compressed fluid of which the pressure is higher than the critical value [9, 10]. The point at which the specific heat of the fluid has a peak value is known as the pseudo-critical point, which is above the critical point.



Figure 2 Phase diagram of water in the P-T plane.

The most important characteristic of supercritical fluids is that their thermal-physical properties exhibit rapid variations with the change of temperature and pressure. The physical properties of water at a pressure of 25 MPa is shown in Figure 1.3 [11]. In general, all thermal-physical properties undergo significant changes near the pseudo-critical point. The density, the thermal conductivity, and the dynamic viscosity undergo a significant drop within a very narrow temperature range.

This strong variation in thermal-physical properties has a great impact on the characteristics of fluid flow and heat transfer. Near the pseudo-critical line the water density decreases dramatically with the increase in temperature, which will result in a strong buoyancy force. For the turbulent water flow, there is a rapid change in the heat transfer coefficient when the temperature approaches to the pseudo-critical value. The closer the temperature is to the critical point, the higher is the heat transfer coefficient.





Figure 3 Physical properties of water at a pressure of 25 MPa [11].

In the 1930s, researchers started to study the problem of heat transfer at supercritical pressures. The heat transfer coefficient of supercritical fluids is compared with the Dittus-Boelter equation which calculates the heat transfer coefficient for ordinary fluids. The Dittus-Boelter equation is known as [12]

$$Nu = 0.023 \,\mathrm{Re}^{0.8} \,\mathrm{Pr}^n \tag{1}$$

where *n*=0.4 for heating and 0.3 for cooling.

At low heat fluxes, the heat transfer coefficient for supercritical fluids is higher than the value predicted by the Dittus-Boelter equation, which is called heat transfer enhancement. At high heat fluxes, the heat transfer coefficient for supercritical fluids is lower than that computed by the Dittus-Boelter equation. Under some specific conditions, a sharp decrease in the heat transfer coefficient may occur in supercritical fluids. This phenomenon is called heat transfer deterioration.

Correlations of the heat transfer coefficient for supercritical fluids can be obtained empirically based on experimental data. Most empirical correlations for the heat transfer of supercritical fluids have the general form of a modified Dittus-Boelter equation [13]

$$Nu_X = C \cdot \operatorname{Re}_X^n \cdot \operatorname{Pr}_X^m \cdot F \tag{2}$$

The subscript X indicates the reference temperature which is used for calculating the properties. The coefficient C, and the exponents n and m are determined using experimental data. The correction factor F takes into account the effect of property variation and the entrance effect.

3. Numerical simulation of heat transfer of supercritical fluids

3.1 CFD analysis in circular tubes

Numerical simulations of heat transfer of supercritical fluids in circular tubes were carried out by many researchers using CFD methods. The most important and difficult things are related to turbulence modeling.

In the earlier works, turbulence modeling was carried out by the simple eddy diffusivity approach [14, 15]. These studies only provided qualitative information of heat transfer mechanisms and did not give quantitative agreement with experimental data over a wide range of flow conditions.

With the development of the computer technology in recent years, k- ε turbulence models have been widely applied in numerical studies. Renz and Bellinghausen [16] solved the near-wall region by using the k- ε model of Jones and Launder. They introduced an additional term to the turbulence model to account for the gravity influence. The results showed that heat transfer enhancement occurs at low heat fluxes and at the bulk temperature close to the pseudo-critical line.

Koshizuka et al. [17] performed a 2-D numerical analysis for heat transfer of supercritical water in a 10 mm circular tube. An excellent agreement between their results and the test data was obtained. Based on numerical results, an empirical correlation of heat transfer coefficient was derived.

Kim et al. [18] studied turbulence models for upward flows in circular tubes at supercritical pressures with 2-D calculations by FLUENT. They concluded that among the selected turbulence models, the RNG *k*- ε model with enhanced wall treatment gives the best prediction results. It was also concluded that the wall function approach shows an acceptable prediction capability.

He et al. [19] conducted simulations of heat transfer of CO_2 at supercritical pressure using various low-Reynolds numbers turbulence models.

Kitou et al. [20] used STAR-CD to simulate the heat transmission behavior in circular tubes and in single-rod channels for HCFC-22 with three-dimensional calculations. The two-layer k- ε turbulence model was used.

Seo et al. [21] used the standard k- ε model with wall functions to predict heat transfer. However, the model was not able to predict heat transfer deterioration under conditions of high heat flux or low mass flux. He et al. [22] numerically studied on the convection heat transfer to carbon dioxide. The low Reynolds number turbulence models are used and the results were comparied with the experimental data. The results showed that the effect of buoyancy on turbulence production and heat transfer in fluids at supercritical pressures can be very significant.

Gallaway et al. [23] did 3-D simulations of fluid flow and heat transfer in SCWR channel (circular tube) using the NPHASE computer code. It showed that the local flow and heat transfer are very important in the evaluation of the heated wall temperature. The use of a proper approach to the modeling of local changes in the fluid properties across the turbulent boundary layer is the key factor affecting the accuracy of predictions of the peak heat transfer coefficient.

3.2 CFD analysis in subchannels

Some researchers have studied the heat transfer of subchannels for ordinary fluids. Baglietto and Ninokata [24, 25] numerically studied the heat transfer of liquid sodium flowing in a rectangular channel in which four heated rods were arranged. Cheng [26] performed a CFD analysis for thermal-hydraulic behavior of heavy liquid metal flows in subchannels of both triangular and square lattices. Chang and Tavoularis [27] studied turbulent flow and analyzed the effect of diminishing gap size on local flow and heat transfer of ordinary fluid in subchannels by using Reynolds stress model. They also numerically studied the flow in a 60° sector of a 37-rod bundle of a nuclear reactor [28].

The numerical analysis on heat transfer of supercritical fluids in subchannels is very limited. During the last few years, several researches [13, 29-31] have made efforts to assess the applicability of existing CFD methods to the simulation of heat transfer at the supercritical pressure conditions in subchannels.

Cheng et al. [13, 29] investigated heat transfer of supercritical water in various flow channels using the software CFX. 3-D calculations for subchannels of triangular and square bundles were carried out. Strong circumferential non-uniformity of heat transfer and cladding surface temperature distributions in subchannels was found. The non-uniformity is more significant in a tighter lattice than in a wider lattice. However, the reason for this non-uniformity was not clarified.

Yang et al. [30] numerically investigated the heat transfer in upward flows of supercritical water in circular tubes and tight fuel rod bundles using the commercial software STAR-CD. 3-D simulations were carried out in subchannels of tight square lattice and triangular lattice fuel bundles at supercritical pressures. Results showed that there is a strong non-uniformity of the circumferential distribution of the cladding

surface temperature in the square lattice bundle with a small pitch-to-diameter ratio (P/D); however, it does not occur in the triangular lattice bundle.

Gu et al. [31] studied the thermal-hydraulic behavior of supercritical water flows in subchannels of a typical SCWR fuel assembly using the commercial software CFX. Three types of subchannels including regular subchannel, wall subchannel and corner subchannel were analyzed. Effects of various parameters, such as boundary conditions and pitch-to-diameter ratios, on the mixing phenomenon in subchannels and heat transfer were investigated. The amplitude of turbulent mixing in wall subchannel is slightly higher than that in regular sub-channel and is close to that in corner subchannel. The mass mixing due to cross flow in wall subchannel is much stronger than that in regular subchannel at the same P/D.

3.3 Subchannel thermal-hydraulic analysis for SCWR

Mukohara et al. [32] applied the subchannel approach in a high temperature fast reactor cooled by supercritical water (SCWR-H) to estimate the effect of local power peaking and cross flow. The results were compared with experimental data of High Conversion Pressurized Water Reactor (HCPWR). It was found that sensitivities of the outlet coolant and the cladding temperature to the subchannel flow area and the local power peaking are high.

Chatoorgoon [33] examined supercritical flow stability in a single-channel, natural-convection loop using a non-linear numerical code. A theoretical stability criterion was also developed to verify the numerical prediction. Good agreement between the numerical and analytical results was obtained.

Dimmick et al. [34] investigated the feasibility of natural-convection cooling for the SCWR designs by using the subchannel approach.

Cheng et al. [35] summarized the main results related to a thermal-hydraulic design analysis of applicable fuel assemblies. The sub-channel analysis code Sub-channel Thermal-hydraulic Analysis in Fuel Assemblies under Supercritical conditions (STAFAS) was developed, which has a higher numerical efficiency compared to the conventional sub-channel analysis codes. The effect of several design parameters on the thermal-hydraulic behavior in sub-channels was investigated. Based on the results achieved so far, two fuel assembly configurations were recommended for further design analysis.

Yu et al. [36] developed a sub-channel thermal-hydraulic analysis code named SUBCHAN to analyse CANDU-SCWR. Thermal-hydraulic model of SUBCHAN is based on four partial differential equations that describe the conservation of mass, energy and momentum vector in axial and lateral directions for the water liquid/vapor

mixture. By calculating the case and comparing with the results of ASSERT-PV code, they concluded that the SUBCHAN code with supercritical water property package can provide reasonable simulation results.

Yoo et al. [37] carried out the subchannel analysis for Supercritical water Cooled Fast Reactor (SWFR) fuel assembly by using the subchannel approach. Since there was no available experiment data at supercritical pressures in bundle scale, the code has been verified with the results of ASFRE-III.

Li [38] developed a sub-channel code (ATHAS) for fuel bundle analysis of supercritical water. The code was applicable for transient and steady state calculations. A total of 13 heat transfer correlations, 6 frictional resistance correlations, and 13 turbulence mixing models were implemented into the code. In addition, an azimuthal conduction model was implemented to establish the fuel temperature. Preliminary analysis of the cladding surface temperature of 43-rod bundles and 37-rod bundles in a fuel channel was performed using this sub-channel code.

4. Conclusion

SCWR was proposed as a type of generation IV reactors in the 1990s. This SCWR concept requires researchers to demonstrate that the reactor and the fuel design limits can be met under the supercritical conditions. This has led researchers to investigate the fluid flow and heat transfer of supercritical fluids in fuel channels. The experimental study of supercritical fluids in the SCWR fuel channels is very costly and time-consuming. Therefore, the CFD method, which is less expensive and which can reduce the need for prototype testing, becomes a useful and attractive method for studying supercritical fluids in SCWR. This literature review is on numerical simulation of supercritical fluids in both subchannels and channels under the SCWR conditions. In general, although investigations on the thermal-hydraulic behavior in SCWR have obtained the attention of many researchers, there are still limits in the study of the fluid flow and the heat transfer of supercritical water in fuel channels.

The literature review showed that although a large number of numerical studies on the heat transfer of supercritical fluids have been carried out, these studies are mainly on the heat transfer of supercritical fluids in circular tubes. Very few researchers devoted to heat transfer in square/triangular tubes. In the flow channels other than a circular tube, such as subchannels of a fuel rod bundle in nuclear reactor, anisotropic behavior of turbulence and secondary flow are observed. Therefore, different turbulence models need to be assessed for subchannel studies. In addition, most of the previous studies have been performed on supercritical fluid in vertical tubes; thus, more studies need to be carried out for the reactors whose bundles are horizontally arranged. Further studies on the modeling of the heat transfer of supercritical fluids in tubes and subchannels need to be down for the design of SCWR.

The subchannel approach, which is widely used in the thermal-hydraulic design and analysis of nuclear fuel bundles, takes into account turbulent interactions between subchannels by using the turbulent mixing coefficient. In order to enhance the reliability, accuracy, and predictability of the subchannel approach, a reliable correlation of the turbulent mixing coefficient under supercritical conditions is needed. However, the current simulations are based on the turbulent mixing coefficient for ordinary fluids, because the correlation of the turbulent mixing coefficient for supercritical fluids has not yet been developed. Therefore, numerical investigations using CFD methods are needed to provide a basic understanding of inter-subchannel turbulent mixing phenomena and to obtain the correlations of the turbulence mixing coefficient for supercritical fluids. The mixing coefficient correlations for supercritical fluids need to be further studied using the CFD method and embedded into subchannel analysis codes.

In addition, the maximum local cladding surface temperature is an important value to ensure that nuclear reactors operate safely; yet, the subchannel approach for SCWR is not able to provide 3-D cladding surface temperature distributions. However, based on the literatures in subchannel studies, it can be seen that there is a strong non-uniformity of the circumferential distribution of the cladding surface temperature. Moreover, the geometry and the arrangement of the bundles have great influence on the cladding surface temperature in each subchannel is assumed to be uniform in the circumferential direction. This assumption results in inaccurate prediction of the subchannel approach, the full-scale 3-D CFD simulations on the heat transfer of supercritical fluids in fuel channels are highly required for the thermal-hydraulic design of SCWR.

5. References

- P.X. Jiang, Y. Zhang, Y.J. Xu, R.F. Shi., "Experimental and numerical investigation of convection heat transfer of CO₂ at supercritical pressures in a vertical tube at low Reynolds numbers", *International Journal of Thermal Sciences*, vol. 51, Iss. 11-12, 2008, pp. 3052-3056.
- [2] Y. Zhang, "Convection heat transfer of CO₂ at supercritical pressures in mini/micro scale tubes", M.Sc Thesis, Tsinghua University, China, 2006.
- [3] "A technology roadmap for generation IV nuclear energy systems", Issued by the U.S. DOE nuclear energy research advisory committee and the generation IV international forum, December, 2002.
- [4] X. Cheng and T. Schulenberg, "Heat transfer at supercritical pressures literature review and application to a HPLWR", Scientific report FZKA6609. Forschungszentrum Karlsruhe, 2001.

- [5] I.L. Pioro, H.F. Khartabil, R.B. Duffey, "Heat transfer to supercritical fluids flowing in channels-empirical correlations (survey)", *Nuclear Engineering and Design*, vol. 230, 2004, pp. 69-91.
- [6] I.L. Pioro, H.F. Khartabil, R.B. Duffey, "Heat transfer at supercritical pressure (survey)", <u>11th International Conference on Nuclear Engineering</u> (ICONE11), Paper-36454, Tokyo, Japan, 2003 April 20-23.
- [7] K. Rehme, "The structure of turbulence in rod bundles and the implications on natural mixing between the subchannels", *International Journal of Heat and Mass Transfer*, vol. 35, Iss. 2, 1992, pp. 567-581.
- [8] L.N. Carlucci, N. Hammouda, D.S. Rowe, "Two-phase turbulent mixing and buoyancy drift in rod bundles", *Nuclear Engineering and Design*, vol. 227, 2004, pp. 65-84.
- [9] I.L. Pioro and R.B. Duffey, "Heat transfer and hydraulics resistance at supercritical pressure in power-engineering applications", ASME, New York, 2007.
- [10] Y. Arai, T. Sako, Y. Takebayashi, "Supercritical fluids molecular interactions, physical properties, and new applications", Spring-Verlag Berline Heidelberg, New York, 2002.
- [11] W. Wagner and A. Kruse, "Properties of water and steam: the industrial standard IAPWS-IF 97 for the thermodynamic properties and supplementary equations for other properties", Springer, New York, USA, 1998.
- [12] F.P. Incropera, D.P. Dewitt, T.L. Bergman, A.S. Lavine, "Fundamentals of heat and mass transfer (sixth edition)", John Wiley & Sons, Inc., USA, 2006.
- X. Cheng, B. Kuang, Y.H. Yang, "Numerical analysis of heat transfer in supercritical water cooled flow channels", *Nuclear Engineering and Design*, vol. 237, 2007, pp. 240-252.
- [14] R.G. Deissler and O. Cleveland, "Heat transfer and fluid friction for fully developed turbulent flow of air and supercritical water with variable fluid properties", Transactions of ASME, vol. 76, 1954, pp. 73-85.
- [15] N.M. Schnurr, V.S. Sastry, A.B. Shapiro, "A numerical analysis of heat transfer to fluids near the thermodynamic critical point including the thermal entrance region", *Journal of Heat Transfer* (November), 1976, pp. 609-615.
- [16] U. Renz and R. Bellinghausen, "Heat transfer in a vertical pipe at supercritical pressure", <u>8th International Heat Transfer Conference</u>, 3, 1986, pp. 957-962.
- [17] S. Koshizuka, N. Takano, Y. Oka, "Numerically analysis of deterioration phenomena in heat transfer to supercritical water", *International Journal of Heat and Mass Transfer*, vol. 38, Iss. 16, 1995, pp. 3077-3084.

- [18] S. H. Kim, Y.I. Kim, Y.Y. Bae, B.H. Cho, "Numerical simulation of the vertical upward flow of water in a heated tube at supercritical pressure", <u>Proceedings of</u> <u>International Congress on Advances in Nuclear Power Plants</u>, Paper-4047, Pittsburgh, PA, USA, 2004 June 13-17.
- [19] S. He, W.S. Kim, Jiang W.S., J.D. Jackson, "Simulation of mixed convective heat transfer to carbon dioxide at supercritical pressure", *Journal of Mechanical Engineering and Science*, vol. 218, 2004, pp. 1281-1296.
- [20] K. Kitou, M. Chaki, Y. Ishii, M. Matsuura, A. Shioiri, H. Mori, S. Yoshida, "Three dimensional heat transmission simulation of supercritical pressure fluid", <u>Proceedings of International Congress on Advances in Nuclear Power Plants</u> (ICAPP05), Paper-5428, Seoul, Korea, 2005 May 15-19.
- [21] K.W. Seo, M.H. Anderson, M.L. Corradini, B.D. Oh, M.H. Kim, "Studies of supercritical heat transfer and flow phenomena", <u>11th International Topical</u> <u>Meeting on Nuclear Reactor Thermal Hydraulics (NURETH 11)</u>, Avignon, France, 2005 October 2-6.
- [22] S. He, W.S. Kim, J.D. Jackson, "A computational study of convective heat transfer to carbon dioxide at a pressure just above the critical value", *Applied Thermal Engineering*, vol. 28, 2008, pp. 1662-1675.
- [23] T. Gallaway, S.P. Antal, M.Z. Podowski, "Multi-dimensional model of fluid flow and heat transfer in Generation-IV Supercritical Water Reactors", *Nuclear Engineering and Design*, vol. 238, 2008, pp. 1909-1916.
- [24] E. Baglietto and H. Ninokata, "Turbulence models for heat transfer simulation in tight lattice fuel bundles", <u>10th International Topical Meeting on Nuclear</u> <u>Reactor Thermal Hydraulics</u> (NURETH-10), Seoul, Korea, 2003 October 5-9.
- [25] E. Baglietto and H., Ninokata, "A turbulence model study for simulating flow inside tight lattice rod bundles", *Nuclear Engineering and Design*, vol. 235, Iss. 7, 2006, pp. 773-784.
- [26] X. Cheng and N.I. Tak, "CFD analysis of thermal-hydraulic behaviour of heavy liquid metals in sub-channels", *Nuclear Engineering and Design*, vol. 236, 2006, pp. 1874-1885.
- [27] D. Chang and S. Tavoularis, "Simulations of turbulence, heat transfer and mixing across narrow gaps between rod-bundle subchannels", *Nuclear Engineering and Design*, vol. 238, 2008, pp. 109-123.
- [28] D. Chang and S. Tavoularis, "Numerical simulation of turbulent flow in a 37-rod bundle", *Nuclear Engineering and Design*, vol. 237, 2008, pp. 575-590.
- [29] X. Cheng, E. Laurien, Y.H. Yang, "CFD analysis of heat transfer in supercritical water in different flow channels", <u>Proceedings of International Conference</u>

Nuclear Energy Systems for Future Generation and Global Sustainability (GLOBAL 2005), Paper-369, Tsukuba, Japan, 2005 Oct 9-13.

- [30] J. Yang, Y. Oka, Y. Ishiwatari, J. Liu, J. Yoo, "Numerical investigation of heat transfer in upward flows of supercritical water in circular tubes and tight fuel rod bundles", *Nuclear Engineering Design*, vol. 237, 2007, pp. 420-430.
- [31] H.Y. Gu, X. Cheng, Y.H. Yang, "CFD analysis of thermal-hydraulic behavior of supercritical water in sub-channels", *Nuclear Engineering and Design*, vol. 238, 2008, pp. 3348–3359.
- [31] T. Mukohara, S. Koshizuka, Y. Oka, Subchannel analysis of a fast reactor cooled by supercritical light water", *Progress in Nuclear Energy*, vol. 37, No. 1-4, 2000, 197–204.
- [32] V. Chatoorgoon, "Stability of supercritical fluid flow in a single-channel natural-convection loop", *International Journal of Heat and Mass Transfer*, vol. 44, 2001, pp. 1963-1972.
- [33] G.R. Dimmick, V. Chatoorgoon, H.F. Khartabil, R. B. Duffey,
 "Natural-convection studies for advanced CANDU reactor concepts", *Nuclear Engineering and Design*, vol. 215, 2002, pp. 27-38.
- [34] X. Cheng, T. Schulenberg, D. Bittermann, P. Rau, "Design analysis of core assemblies for supercritical pressure conditions", *Nuclear Engineering and Design*, vol. 223, 2003, pp. 279-294.
- [35] J. Yu, S. Wang, B. Jia, "Development of sub-channel analysis code for CANDU-SCWR", *Progress in Nuclear Energy*, vol. 49, 2007, pp. 334-350.
- [36] J. Yoo, Y. Oka, Y. Ishiwatari, J. Yang, J. Liu, "Subchannel analysis of supercritical light water-cooled fast reactor assembly", *Nuclear Engineering and Design*, vol. 237, 2007, pp. 1096–1105.
- [37] C. Li, "Subchannel analysis of supercritical water reactor", Master thesis, Xi'an Jiaotong University, China, 2008.