TURBULENT MIXING MODEL APPLICABLE TO SUPERCRITICAL CONDITION

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Abstract

In the design of a nuclear reactor, it is very important to predict the detailed flow and temperature distributions in the reactor core. The turbulent velocity fluctuation across the gap is an important parameter determining the inter-channel exchange, but the existing correlations show a rather large discrepancy with each other under supercritical conditions. Two types of subchannel lattices, triangular and square arrays are selected to be investigated using the CFD tools. The thermal-hydraulic behavior was investigated between the subchannels. A turbulent mixing correlation developed applicable under the supercritical condition was conducted under the adiabatic condition, a modifying factor was given for heating. Finally, the model was compiled into the subchannel code to analyze the CANFLEX bundle.

1. Introduction

Different concepts on Supercritical Water-cooled Reactor (SCWR) have been announced all over the world [1-3]. The CANDU [4] also offers a SCWR system concept which has advantages in the areas of sustainability, economics, safety and reliability and proliferation resistance. Firstly, since the moderator is located in the calandria vessel and is separated from the coolant, the coolant has relatively less effect on the neutronics. Secondly, since the channel flows can be bi-directionally interlaced (opposite flow direction in adjacent channels), the density gradients are balanced and a more axially uniform flux profile is achievable. The other advantage is the pressure boundary (pressure tube) can be easier to be fabricated which can accommodate much higher pressure.

In the design of a nuclear reactor, it is very important to predict the detailed flow and temperature distributions in the reactor core. This is because a safe and reliable operation of a reactor system relies on an accurate thermal-hydraulic design. To calculate these distributions, the subchannel approach is frequently used. In a subchannel approach, the temperature, pressure and velocity in a subchannel is averaged, and one representative thermal-hydraulic condition specifies the state of the subchannel. To obtain the flow and temperature distributions with a subchannel analysis code, the conservations of the mass, momentum, and energy in a subchannel are modelled and solved. Therefore, it is required to simulate the inter-subchannel mixing phenomenon due to the cross flow between the adjacent subchannels as accurately as possible to enhance the predictability of a subchannel analysis code.

The designs of SCWRs aim to realize a safe, reliable operation with a low power cost due to the higher outlet temperature. Although there is no phase change in water under the supercritical pressure condition and the thermophysical properties of supercritical water vary continuously when temperature increases, strong variations of properties exist in the vicinity of the pseudo-critical temperature. When a single-phase flow exists in the subchannels, a mixing of the mass, energy and momentum between the subchannels consists of two parts, a forced mixing and a natural one. The natural mixing again consists of a diversion flow and a turbulent mixing. The diversion flow mixing is mainly caused by the net convective transport (diversion crossflow) of energy from one subchannel to another. This type of mixing would result from flow redistribution due to the pressure gradient between the subchannels.

Mixing of this type can be computed with reasonable accuracy from the momentum and energy equations. The turbulent mixing is attributed to the eddy motion of the fluid across the gap between adjacent subchannels, enhances the exchange of the momentum and the energy through the gap with no net transport of the mass. It is assumed to be superimposed upon the diversion component of mixing. And the forced mixing caused by the spacers or wire-wrap is corresponding to the natural one. The effects of a turbulent mixing are taken into account in the axial momentum equation and the energy conservation equation in the subchannel analysis codes such as COBRA-IV [5] and ATHAS [6]. The turbulent mixing model in a subchannel code determines the turbulent mixing flow rate w'. The turbulent mixing flow rate from subchannel i to j per unit length is defined with the effective mean fluctuating velocity, v_{eff} as follows:

$$w'_{ij} = \rho_i v_{eff} s_{ij} \tag{1}$$

There are several methods to evaluate the turbulent mixing flow rate and lots of investigation has been done world-widely under subcritical conditions. Some researchers have calculated the turbulent mixing flow rate from the measured subchannel temperature and a computer simulation. The chemical tracer method, the hot-wire anemometry, and the laser Doppler anemometry are other possible experimental techniques. However, each method has one or more limitations in an application to a rod bundle geometry and considerable caution is required to obtain accurate data by using these methods. Therefore, the data for rod bundles is not enough to develop a reliable correlation to a rod bundle geometry under subcritical condition. Although some correlations have been developed for use in rod bundles, they show a rather large discrepancy with each other. Shan [6] examined some correlations using ATHAS under supercritical condition, the results were largely scattering. There is no turbulent mixing correlation obtained under supercritical condition due to lack and difficulty of experiments, but the model is very important to the design of SCWRs. The validity of the existing correlations should be verified and a new correlation more reliable application to the supercritical condition should be developed in the present study.

The sharp variation of thermophysical properties in the vicinity of the pseudo-critical temperature brings large non-uniformity of properties and non-uniformity of buoyancy forces over the cross-section of channels. It results in different turbulent flow and heat transfer characteristics of supercritical water from those of sub-critical water. Accordingly, the understanding of the unique and complicated flow and heat transfer phenomena in supercritical water is very important for the thermal hydraulic designs of SCWRs.

Due to the cost and measurement techniques of the experiment which is not applicable to a rod bundle condition, and the numerical studies which is a useful tool to give a basic understanding of thermal-hydraulic behaviour mechanism is selected.

The main difficulties in the numerical analysis are related to the turbulence model at supercritical pressures. In recent years, lots of numerical studies were carried out by commercial CFD codes which include a number of first order closure turbulence models and some advanced turbulence models [7-11]. All the previous studies found that the heat transfer capability is strong in the region near pseudo critical point, and is weak outside this region especially in the region when the bulk temperature is above the pseudo critical temperature in accordance with the experimental results. CFD analysis is turned up to be a suitable approach for the study of the thermal-hydraulic behaviour of supercritical fluids and some special phenomenon of turbulent mixing under supercritical condition was found.

Although lots of investigation was carried out, all previous studies give the recommend turbulence modelling and the qualitative analysis in the supercritical condition. However, no systemic study on the turbulent mixing has been carried out and no law has been summarized under supercritical condition. According to the survey done by Jeong et al. (2007) [12], the difference among the results of the existing correlations is large and sometimes even contrast, and majority are derived from subcritical condition. The validity will be doubtful when they are applied under supercritical condition. So understanding the thermal-hydraulic behaviour and giving a reasonable correlation on turbulent mixing is the urgent affairs to the design of SCWRs.

The objective of the present study is to obtain better understandings about the thermal-hydraulic behaviour under Supercritical Reactor conditions. The commercial CFD code Fluent 6.1, which coupled the second order closure turbulence model, RSM model[13], having the capacity to simulate the anisotropic behaviour, is utilized to investigate heat transfer characteristic in the subchannels under supercritical condition. Two types of subchannel lattices, triangular to triangular and square to square lattices are selected. The effect of various parameters, geometric configuration and thermal conditions on the thermal-hydraulic behaviour is investigated and a turbulent mixing correlation applicable under the supercritical condition is proposed.

2. Turbulent mixing

The mixing flow rate w'_{ij} is expressed in Eq. (1). The heat flux per unit length between two subchannels due to the mixing process is given by

$$q' = w'_{ij} c_p (T_i - T_j) = \rho c_p \varepsilon S \left(\frac{dT}{dz} \right)_{ij} \tag{2}$$

The temperature gradient can be approximated by

$$\left(\frac{dT}{dz} \right)_{ij} = \frac{T_i - T_j}{z_{ij}} \tag{3}$$

By combining Eqs. (2) and (3), the mixing flow rate can be written as

$$w'_{ij} = \rho \varepsilon S / z_{ij} \tag{4}$$

ε and z_{ij} are unknown.

The different hypothesis on ε and z_{ij} results in different definition on turbulent mixing rate, and the most popular ones are turbulent mixing coefficient and turbulent mixing factor.

2.1 The definition of turbulent mixing coefficient

The existing correlations on a turbulent mixing in rod bundles have been developed with different definitions of the mixing parameters. The most general form of a correlation is the turbulent mixing coefficient, defined by the ratio of the effective mean mixing velocity to the axial velocity as follows:

$$\beta = \frac{v_{\mathrm{eff}}}{\overline{u}} \tag{5}$$

This mixing coefficient is essentially the same as the gap Stanton number, St_g. This definition of a mixing coefficient was used in the correlations suggested by Row and Angle [14]. The turbulent mixing coefficient is normally determined from the thermal mixing test for single-phase conditions. With this definition of a turbulent mixing coefficient, the turbulent mixing flow rate from channels i to j is

$$w'_{ij} = \beta S_{ij} \overline{G}_{ij} \tag{6}$$

Some researchers such as Rogers and Tahir [15] have suggested correlations with the mixing flow rate divided by the dynamic viscosity, which are easily converted to a correlation with the mixing coefficient, β per the relation of Eq. (6). In the paper, the turbulent mixing correlation applicable under the supercritical condition is proposed based on this definition.

2.2 The definition of turbulent mixing factor

The other type of mixing factor Y was first suggested by Ingesson and Hedberg [16]. Other researchers such as Rehme [17] and Moeller [18] have also adopted the same definition of a mixing factor in their studies.

Ingesson and Hedberg [16] approximated the temperature gradient in Eq. (3) by

$$\left(\frac{dT}{dz}\right)_{ij} = \frac{T_i - T_j}{\delta_{ij}} \tag{7}$$

In addition, for the eddy viscosity they set a mean value $\overline{\varepsilon}$ as in pipe flow. To correct for the error due to the approximation of the effective mixing distance z_{ij} by the distance between centroids of adjacent subchannels and to the approximation of the eddy viscosity ε in rod bundles by the viscosity $\overline{\varepsilon}$ in pipe flow, they defined a mixing factor Y as

$$Y = \varepsilon \delta_{ij} / \overline{\varepsilon} z_{ij} \tag{8}$$

Thus, Eq. (2) can be rewritten as

$$q' = \rho c_p \overline{\varepsilon} S Y \left(\frac{T_i - T_j}{\delta_{ij}}\right) \tag{9}$$

In their work, Ingesson and Hedberg used for $\overline{\varepsilon}$ the expression

$$\overline{\varepsilon} = \nu \frac{Re}{20} \sqrt{\frac{\lambda}{8}} \tag{10}$$

Where $\lambda = 0.18 Re^{-0.20}$ is the friction factor for smooth circular tubes.

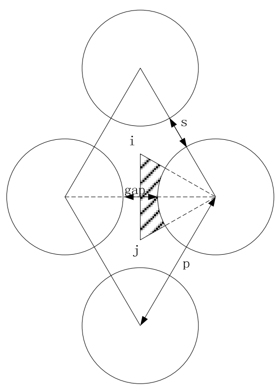
A comparison between Eqs. (1), (2) and (9) yields

$$Y = \frac{v_{eff}\,\delta_{ij}}{\overline{\varepsilon}} \tag{11}$$

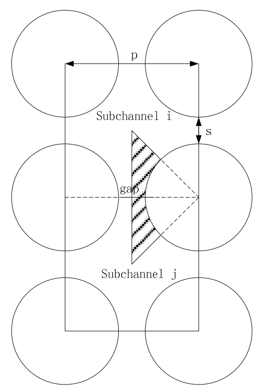
In the paper, the turbulent mixing factor is used to verify the new proposed correlation comparing with the existing ones.

3. Geometry and computational model

In the present study, two typical sub-channels of bare rod bundles are considered, including the triangular to triangular and square to square lattices arrangement, as indicated in Figure 1. Figure 1 depicts the schematics of rod bundles and the subchannels where the inter-subchannel mixing occurs. 1/6 of the triangular lattice and 1/8 of the square lattice which are covered by hatching in Figure 1 are taken as computational domain for the CFD analysis due to the symmetric feature. Subchannel parameters are selected based on the design parameters of CANDU type reactor bundle with variable gap width [4], so the dimensions of the rod diameter, the gap and the pitch are same for the two arrays. The subchannel parameters in the research are shown in Table 1.



(a)



(b)

Figure 1 Schematic diagram of rod bundle and flow channels. (a) triangular array; (b) square array. D=11.526mm

Table 1 The parameters of triangular array and square array

P/D	P /mm	s /mm
1.1	12.6786	1.1526
1.15	13.2549	1.7289
1.2	13.8312	2.3052
1.25	14.4075	2.8815
1.3	14.9838	3.4578
1.173521	13.526	2
1.347041	15.526	4

The RSM turbulent model with enhanced wall treatment [13]selected in this research is verified by comparing to the experiment data (Yamagata et al., 1972) [19] in the circular tube. Results are compared with the experimental data obtained by Yamagata et al. and the numerical results obtained by application of the RNG k-ε turbulent model with enhanced wall treatment which is the best one in the first closure order to predict the supercritical flow[7]. The comparison shows the RSM turbulent model which has the capacity to simulate the anisotropic behavior gives a more accurate prediction of the peak than the RNG k-ε turbulent model. And it can be concluded that the RSM model has the capacity to predict the heat transfer characteristic under the supercritical condition, which is in accordance with the result of Roelof [8]. Second moment closure turbulent model, e.g. RSM model, for solving seven equations consumed larger time than the first moment closure turbulent model, e.g. RNG k-ε model.

The RSM turbulent model is verified on the application to simulate rod-bundle-like flows to get an anisotropic result. For simplicity, we use the same idealized geometry as that in the GT experiments [20]. An essential objective of the present simulations is to accurately predict the flow field and to provide a proof of the capacity of RSM turbulent model on anisotropic flow. The results showed that the RSM turbulence model has the capacity to predict the anisotropic behaviour of the flow, and it can be proposed to be used to predict the supercritical flow in the subchannels.

4. The new turbulent mixing coefficient correlation

The v_{eff} was the key to obtain the turbulent mixing coefficient. From the definition of the Reynolds stress, which can be directly provided by the Fluent 6.1 code calculation using RSM turbulent model, one can obtain the relationship between the v_{eff} the Reynolds stress $\overline{vv}$. According to the analysis by Cheng (2007)[9], a Gaussian distribution of the probability distribution for the velocity fluctuation is assumed and the relationship between the Reynolds stress $\overline{vv}$ and the average amplitude of the velocity fluctuation across the gap $\overline{|v|}_{eff}$ is obtained as indicated in Equation (12).

$$\overline{|v|}_{eff} = \frac{\sqrt{\overline{vv}}}{\sqrt{\pi}} \tag{12}$$

Equation (12) is used in the present study to derive the average amplitude of the velocity fluctuation across the gap by knowing the Reynolds stress, which is obtained from the CFD analysis.

4.1 Turbulent mixing coefficient under adiabatic wall condition

To eliminate the effect of various thermal boundaries and obtain the characteristic of turbulent mixing, the calculations were carried out with the adiabatic boundary condition in different *P/D*. The geometries of the cases are shown in Table 1. The turbulent mixing coefficient can be obtained by the average amplitude of the velocity fluctuation across the gap normalized by the axial mean flow velocity across the gap, and the normalized velocity fluctuation is the local turbulent mixing coefficient actually.

In the previous research, the turbulent mixing coefficient was usually dependent on Reynolds number and the geometry parameters, such as *P/D*, and independent on the others. But the working fluids usually were the water or air, only the liquid or gas. Under supercritical condition, the density of the water will change about 8 times from 280 °C to 500 °C. The Reynolds number should be examined to be used as a determined parameter. Figure 2 shows the distribution of local turbulent mixing coefficient on the gap at various bulk temperatures at a pitch-to-diameter ratio of 1.173 in triangular lattice for a constant *Re* number. It can be found that the distribution of the local turbulent mixing coefficient is almost the same at different bulk temperature at a specified *Re*; the local turbulent mixing coefficient increases with the distance from the center to the wall with nearly linear law, and decreases sharply after reaching the peak.

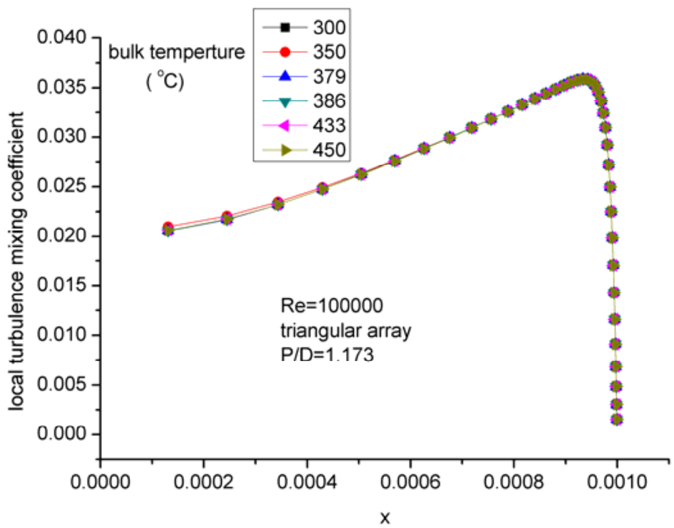


Figure 2 The local turbulence coefficient independent on the bulk temperature

After examined the *Re* number, a systemic calculation was carried out at different *Re* and *P/D*. The average turbulent mixing coefficients across the gap versus *Re* number at various pitch-to-diameter ratios are shown about triangular and square arrays in Figure 3 and Figure 4, respectively. It can be found that the average turbulent mixing coefficient decreases with the increased *Re* according to the exponential law, which is consistent to the previous study in subcritical condition. In the other hand, the average turbulent mixing coefficient is about 0.027, which is similar to the results obtained by Gu et al. [11] using CFX, and about two times larger than the value calculated using Roger's equation (0.008). The cause of the high turbulent mixing coefficient is the higher turbulence intensity under the supercritical condition.

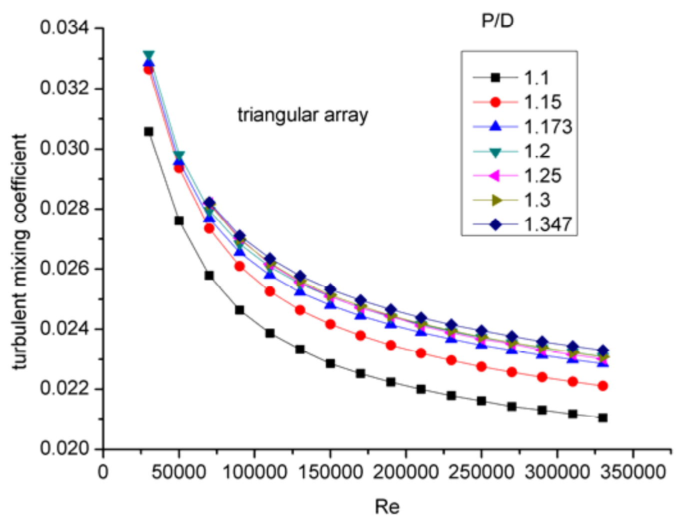


Figure 3 Turbulent mixing coefficient versus the Reynolds number in triangular arrays

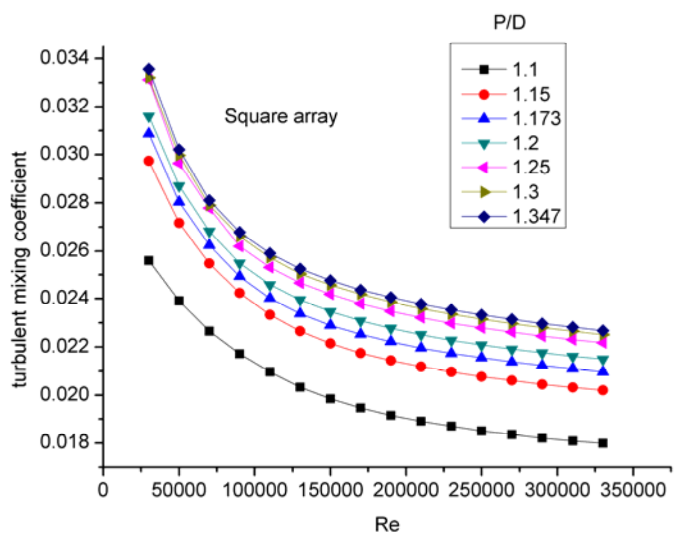


Figure 4 Turbulent mixing coefficient versus the Reynolds number in square arrays

The figures indicated that the turbulent mixing coefficient is almost a constant in a certain *Re* and independent on the geometry for the small *P/D* geometry for triangular array. Although the variation under the small *P/D* cases is obvious, the total error in the triangular array is about 0.002 which is less than 10 percent of the turbulent mixing coefficient, and the turbulent mixing coefficient is thought to be the function of only one variable, *Re*. In contast, the turbulent mixing rate is dependent on the *P/D* for the square array. And simple correlations with the similar form as that proposed by Rogers & Todreas (1969) [21] based on the figure are proposed, respectively in the two arrays. The mixing coefficient under adiabatic condition can be derived as

$$\beta_{\text{adi}} = \frac{|\overline{v}|}{W} = 0.11 \cdot \text{Re}^{-0.125} \tag{13}$$

$$\beta_{\text{adi}} = \frac{|\overline{v}|}{W} = 0.1391 \cdot \left(\frac{s}{D}\right)^{0.1679} \cdot \text{Re}^{-0.125} \tag{14}$$

The Equation (13) is used in triangular array and the Equation (14) is used in the square one. At the Reynolds number of 10^6 and a *P/D* of 1.2, Equation (13) and (14) give a mixing coefficient of about 0.026085 and 0.025175, respectively.

4.2 Turbulent mixing coefficient under heated wall condition

In the subchannel, the boundary condition has a great effect on the turbulent intensity distribution on the plane, and the correlation obtained under the adiabatic condition can't be used under the heated wall condition directly. To obtain the effect of thermal boundaries on the characteristic of turbulent mixing, the calculations were carried out in the subchannel varying the mass flux and the heat flux.

Figure 5 showed the turbulent mixing coefficient varied with the bulk temperature. It can be found that the turbulent mixing coefficient changed quickly in the pseudo critical region, which is different from the adiabatic condition. The corresponding figure of the turbulent mixing coefficient versus the *Re* number is shown in Figure 6. The figure indicated the turbulent mixing coefficient is smaller than the adiabatic condition, and it also is dependent on the *Re* number except the region near the pseudo critical point. To obtain a correlation to describe the phenomena, the modification on the equation (13) and (14) is taken.

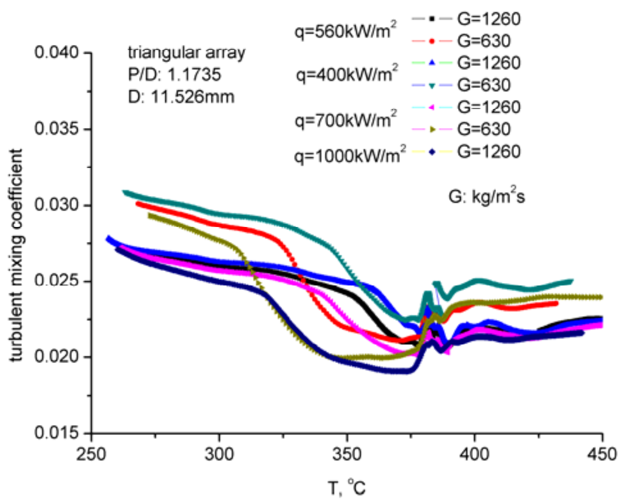


Figure 5 Turbulent mixing coefficient versus the bulk temperature under heated condition

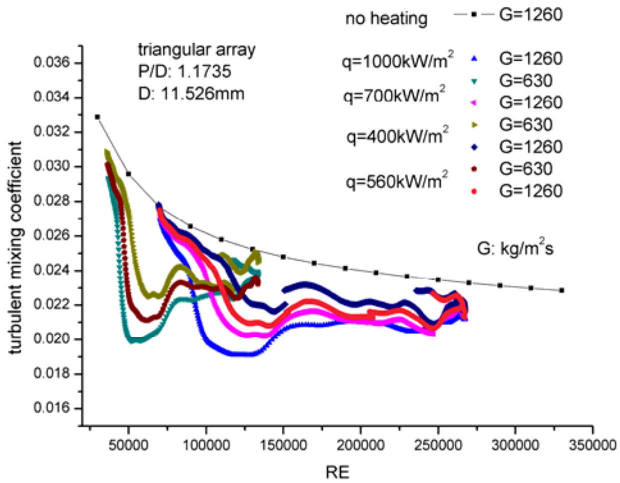


Figure 6 Turbulent mixing coefficient versus the *Re* number under heated condition

The difference between the adiabatic condition and the heated condition is caused by the temperature distribution on the wall, so the modification variable should consider the one which can describe the characteristic on the wall. The density ratio between the wall and bulk fluids which usually used in the thermal-hydraulics analysis is selected. The correlation obtained here is to be used in to the subchannel code which can only calculate the average temperature on the wall, not the detailed temperature distribution across the rod. And the average temperature on the wall is dealt with as the equation (15),

$$T_w = \frac{\int T ds}{\int ds} \cdot \frac{T\max + T\min}{2} \tag{15}$$

The turbulent mixing coefficient under the heated condition is obtained as equation (16):

$$\beta_{\text{heat}} = \beta_{\text{adi}} \left(\frac{\rho_{\text{W}}}{\rho_{\text{b}}} \right)^{0.2} \tag{16}$$

The ratio of the results by the correlation and the CFD analysis corresponding to Figure 5 is shown in Figure 7. The error of the two results is less than ten percent except extreme case like the deteriorated condition. The majority of the CFD results are higher and the calculation by the equation (16) is smaller.

Figure 8 give the results under a *P/D* of 1.347 in the triangular and square arrays. They give the similar results as under a *P/D* of 1.1735 in the triangular array and can testify the equation (16). It can be concluded that the equation (16) can give a reasonable prediction of the turbulent mixing coefficient under the heated condition.

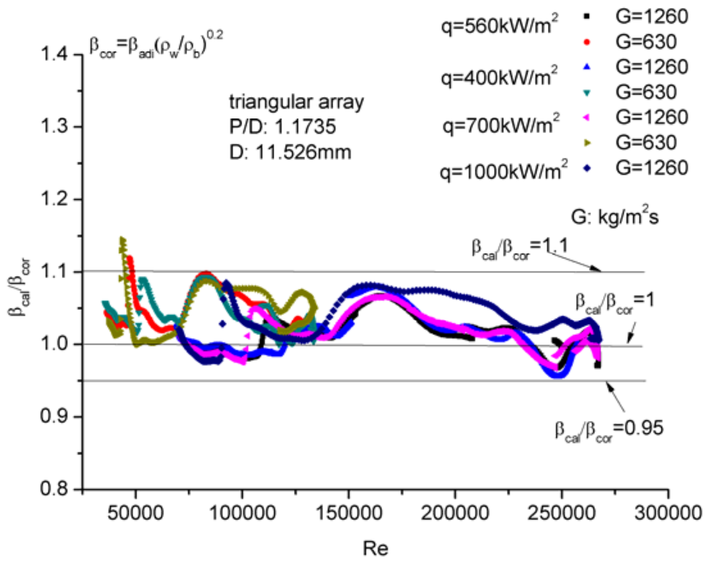
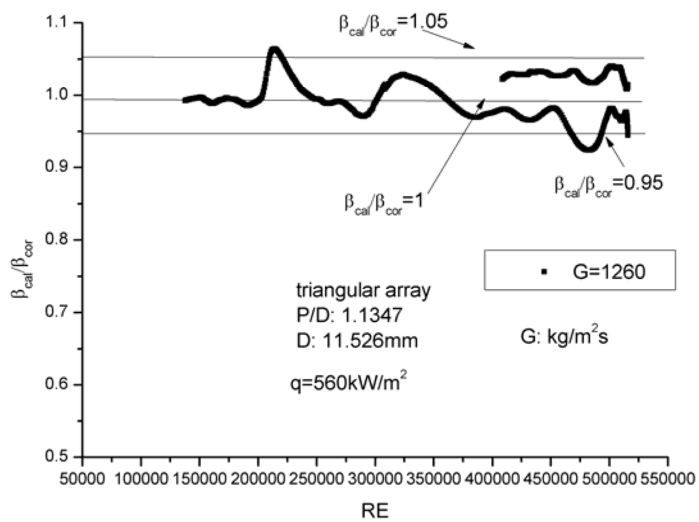
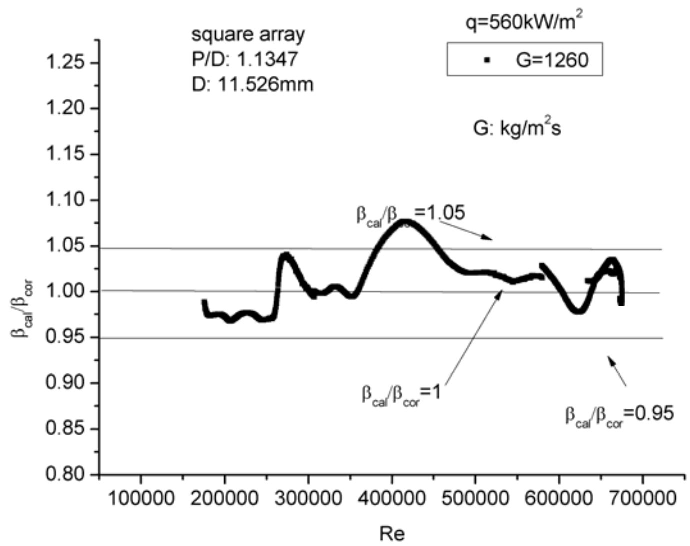


Figure 7 The ratio of the results by the correlation and the CFD analysis corresponding to Figure 5



(a) triangular array



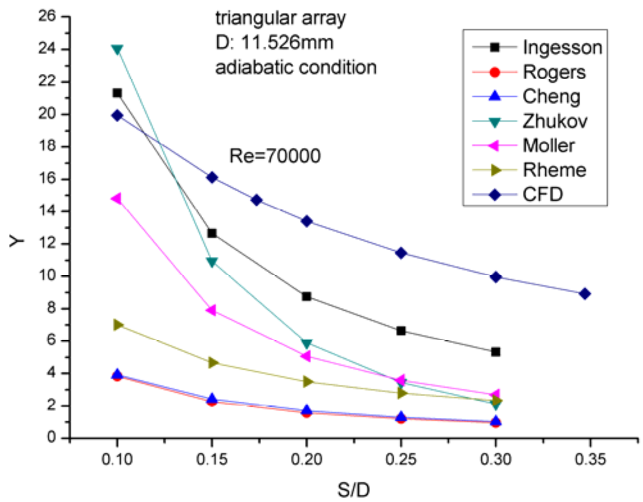
(b) square array

Figure 8 The ratio of the results by the correlation and the CFD analysis at a higher *P/D*

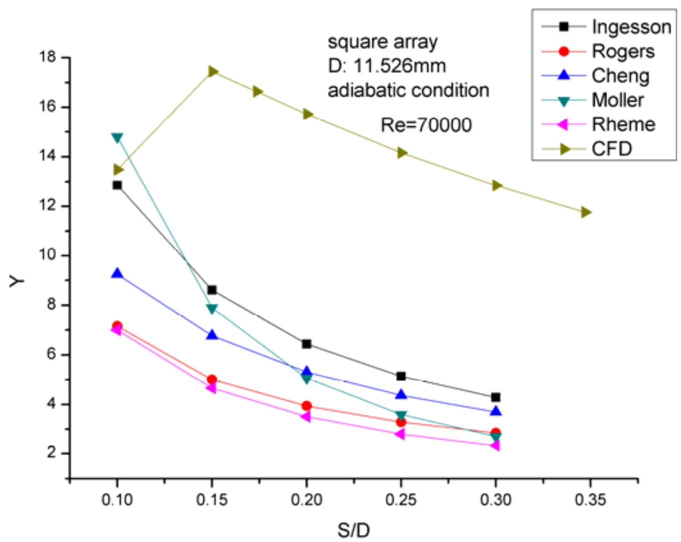
4.3 Turbulent mixing factor compared with the existing correlations

To compare the calculated turbulent mixing factor with some correlations reported in the literature [22], six correlations were chosen and recalculated as *Y*-factors to verify the new turbulent mixing coefficient model.

The comparison was performed for *Re*=70000. Figure 9 shows the comparison for triangular and square arrays. The calculated turbulent mixing factor is the biggest for the larger *P/D*, which is due the higher turbulent intensity under the supercritical condition. And there is a large difference among the different correlations, which all predict an increase of *Y* with decreasing *S/D*. If extrapolated towards the zero gap, this trend would imply that, as the gap vanishes, cross-gap mixing would increase without bounds, rather than also vanish, as common sense dictates. And the peak of square arrays gave a more reasonable trend[23], which the correlation can be proved.



(a) triangular array



(b) square array

Figure 9 The calculated turbulent mixing factor comparison with the existing correlations

4.4 The new model used in subchannel code

The turbulent mixing coefficient, Eq. (16), is compiled in the subchannel analysis code ATHAS [6]. It is compared with other correlations compiled in ATHAS by the analysis of the CANFLEX bundle, whose configuration is shown in Figure 10, under supercritical condition. The calculated MCST using the turbulent mixing coefficient recommended by Rowe et al. [24] was 780.1^{o}C, and located on the cladding of Rod 32 facing to Subchannel 34. The result using Eq. (16) was 800.2^{o}C, and located on the cladding of Rod 33 facing to Subchannel 60. It is higher but the location was changed, where the flow area and the mass flow rate was small. It is more reasonable due to the buoyancy in the cross-section of the bundle, and can prove the validity of Eq. (16).

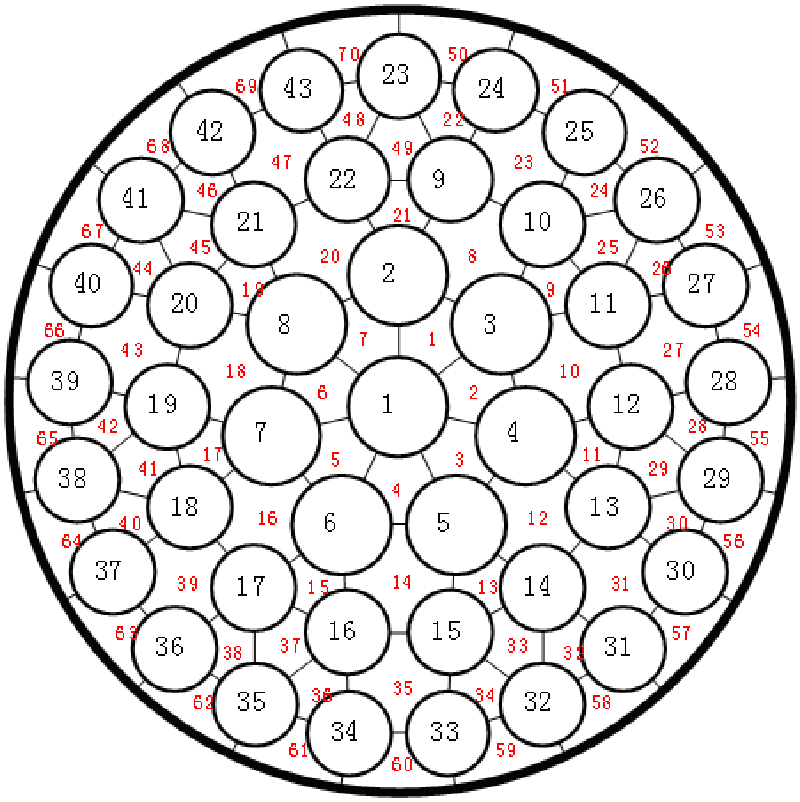


Figure 10 Subchannel identification in a CANDU CANFLEX fuel bundle

5. Conclusion

CFD analysis has been carried out to have more understandings about the thermal-hydraulic behavior in the typical flow channels under Supercritical Reactor conditions. Two types of subchannel lattices, triangular and square arrays are selected. The effect of various parameters, geometric configuration and thermal conditions on the thermal-hydraulic behavior is investigated and a turbulent mixing correlation developed applicable under the supercritical condition is conducted. Some main results achieved can be summarized as follows:

(1) The second order closure turbulence model, RSM model, which has the capacity to simulate the anisotropic behavior and gives a more accurate prediction on heat transfer characteristic than the first order closure turbulence models, is testified and recommended to predict the thermal hydraulic characteristic in the subchannel under the supercritical condition.

(2) Three-dimensional calculations for subchannel lattices, triangular and square arrays are carried out. Simple correlations of the mixing coefficient under adiabatic condition with the similar form as that proposed by Rogers & Todreas (1969) are proposed for the two arrays, respectively. And a modification variable is recommended under heated condition.

(3) According to the definition of the turbulent mixing factor *Y*, the results of the study were re-calculated. The turbulent mixing in the study is compared with the experimental data and the existing correlations which gives a proof for the correlations of the mixing coefficient. It can be seen that the turbulent mixing factor for the triangular decreases with the increased *S/D* monotonously, but there is a peak for the square array. This unique phenomena was also found by Wu [23] and Chang [25], which is

in according to the fact.

(4) The turbulent mixing coefficient is compiled into the subchannel analysis code ATHAS. It is compared with other correlations compiled in ATHAS by the analysis of the CANFLEX bundle under supercritical condition. The result using Eq. (16) was 800.2 ^{o}C, and located on the cladding of Rod 33 facing to Subchannel 60, which is more reasonable due to the buoyancy in the cross-section of the bundle. It can prove the validity of Eq. (16).

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NOMENCLATURE

C_p	Specific heat (kj/(kg K))
G	Mass flux (kg/m^{2}s)
P	Pressure (Pa)
q'	Heat flux per unit length (KW/m)
Re	Reynolds number
S	Gap width (m)
St_g	Gap Stanton number,
T	Temperature (^{o}c)
v_{eff}	Effective mean fluctuating velocity (m/s)
w'	Turbulent mixing flow rate (kg/ms)
Y	Turbulent ming factor
z_{ij}	Effective mixing distance (m)

Greek symbols

β	Turbulent mixing coefficient
λ	Friction factor
ν	Kinematic viscosity (m^2/s)
δ	Distance between centroids of subchanel

ε Eddy viscosity (m^2/s)

$\bar{\varepsilon}$ Eddy viscosity in pipe flow (m^2/s)

ρ Density (kg/m^3)

Subscripts

i Subchannal i

j Subchannal j

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