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Development of a new criterion for predicting critical heat flux in rod bundles with supercritical water flowing upward

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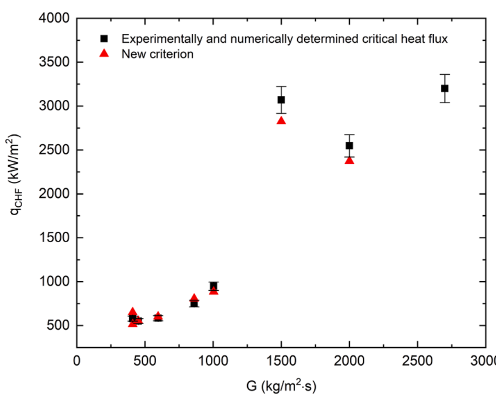
HIGHLIGHTS

- Sudden wall temperature gradient increase indicates heat transfer deterioration.
- Existing criteria for predicting critical heat flux underestimate that in rod bundles.
- Criteria considering only mass flux does not perform well.
- Proposed new criterion performs better than existing criteria with errors within ± 20 %.

GRAPHICAL ABSTRACT



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ABSTRACT

Investigations of heat transfer characteristics in channels with supercritical fluids are crucial for power cycle applications, such as supercritical water-cooled reactors. To ensure the safety of the system, heat transfer deterioration (HTD) should be avoided. The criteria to identify the onset of HTD in heated rod bundles are still not determined. This study summarizes indicators for the onset of HTD in a rod bundle with supercritical water flowing upward based on observations from experimental data. Existing criteria for the tube flow are assessed by comparing predicted critical heat flux (CHF) values with experimentally identified values. Considering effects of different operating parameters, a new criterion for predicting HTD behavior in rod bundles is developed. The results indicate that the new criterion has a better performance than all existing criteria, with a mean average relative deviation of 0.26 %. Predicted CHF values are within ± 20 % of the respective experimentally identified CHF values.

Abbreviation: CHF, Critical Heat Flux; HTD, Heat Transfer Deterioration; HTE, Heat transfer Enhancement; NHT, Normal Heat Transfer; RE, Relative Error; SC, Supercritical; SCW, Supercritical Water; SCWR, Supercritical Water-Cooled Reactor.

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Nomenclature

Symbols

c_p	specific heat, J/kg K
C	constant coefficients
D,d	diameter, m
$f(x)$	function of x
g	gravitational acceleration, m/s^2
G	mass flux, kg/m^2 s
h	enthalpy, J/kg
i_{pc}	enthalpy at the pseudo-critical point, $i_{pc} = c_{p,pc}/\beta_{pc}$, J/kg
N	number of total cases
Nu	Nusselt number, $Nu = q_w D/(k_b(T_w - T_b))$
P	operating pressure, Pa
Pr	Prandtl number, $Pr = c_p\mu/\lambda$
q	heat flux, W/m^2
Re	Reynolds number, $Re = \rho uD/\mu$
T	temperature, K
u	velocity, m/s
x	position vector
z	axial location, m
Δ	change/difference
&	and

Greek letters

β	thermal expansion coefficient, 1/K
μ	dynamic viscosity, Pa s
λ	thermal conductivity, W/m K
ρ	density, kg/m^3

Subscripts

CHF-criteria	critical heat flux predicted by criteria
CHF-exp	experimentally identified critical heat flux
MRD	mean relative error
MARD	mean absolute relative error
SD	standard deviation of relative error
b	bulk fluid
c	critical
db	Dittus-Boelter
exp	experimental
h	hydraulic
i, j	data/vector index
in	inlet
pc	pseudo-critical
t	turbulent
w	wall

1. Introduction

Supercritical fluids are extensively used in thermodynamic processes, such as heat pump systems, refrigerating systems, and power plants [1]. The term, supercritical fluid, usually refers to the fluid at a pressure higher than the critical pressure while the temperature could be lower than the critical temperature. The critical pressure and temperature for water are 22.1 MPa and 374 °C, respectively. Thermophysical properties of the supercritical water exhibit sharp variations in a narrow temperature range around the pseudocritical point, as shown in Fig. S1 in Supplementary Materials. The specific heat reaches the maximum value at the pseudocritical temperature, which implies that the heat absorption at this point is stronger than at other temperatures. This could enhance the heat transfer performance. In the power plant, the thermal efficiency can be up to 55 % with the supercritical steam at a pressure ranging from 23.5 MPa to 38 MPa and the turbine inlet temperature from 540 °C to 625 °C [2]. In addition, there is no phase change for the supercritical water. Therefore, steam generators and separators are not needed, which could reduce capital cost. Such benefits have motivated the design and development of supercritical water-cooled reactors (SCWRs) in last two decades. Accordingly, the interest in the study of heat transfer behavior of supercritical water in channels is increased. However, both the thermal conductivity and density fall significantly at the same time when the fluid temperature is within ± 25 °C around the pseudo-critical temperature. The consequent buoyancy effect and flow acceleration would suppress turbulent diffusion, resulting in the possibility of heat transfer deterioration. Such non-monotonic effects caused by variations of different thermophysical properties could induce different heat transfer mechanism at various operating conditions. This adds to the complexity of heat transfer behavior of the supercritical water in upward channels. Therefore, in order to achieve a safe and efficient application of supercritical water, it is necessary to explore the heat transfer mechanism in upward supercritical water channels.

Different heat transfer scenarios could occur for supercritical water in heated tubes [1], [3,4]: normal heat transfer (NHT), heat transfer enhancement (HTE), and heat transfer deterioration (HTD). The NHT region is characterized by generally no great change in the difference between the wall temperature and the bulk fluid temperature in the whole tube. The HTE region refers to the flow domain where the increase in the wall temperature is moderate and the difference between the wall temperature and the bulk fluid temperature gets smaller. In the HTD region, the increase in the wall temperature is significant and the difference between the wall temperature and the bulk fluid temperature arises. Some studies have devoted to investigations of onset of HTD for supercritical fluids in channels. The earliest HTD phenomenon was discovered by Shitsman in experiments for supercritical water heated in upward tubes [5]. The operating conditions covered pressures: 23.3 MPa, 24.3 MPa, and 25.3 MPa, mass fluxes: 300 kg/m^2·s, 430 kg/m^2·s, 700 kg/m^2·s, and 1500 kg/m^2·s, and heat fluxes up to 1162.2 kW/m^2. The heat transfer is impaired with the increase of heat flux until the onset of HTD. The location where HTD occurs moves from regions near the exit towards the inlet with the increase in the heat flux. Such findings were also reported in later studies [6–10]. From these studies, it was found that several parameters govern the heat transfer behavior of supercritical water in upward heated tubes, including heat flux, mass flux, operating pressure, flow direction, and flow geometry. HTD is found mostly exists under high heat fluxes or low mass fluxes conditions in these investigations. It also showed that there exists a critical heat flux (q_{CHF}). When the heat flux is above q_{CHF}, HTD will appear, leading to an unusually sharp increase in the wall temperature, which consequently could damage the tube.

The flow in a rod bundle is different from that in a simple tube. Therefore, heat transfer characteristics for the supercritical water in heated tubes can not directly represent those in heated rod bundles. Razumovskiy et al. [11,12] found that the heat flux for the onset of HTD in rod bundles is 1.6–1.8 times higher than that in bare tubes under the same operating conditions. Several experimental investigations were conducted in upward annular channels [13–15]. The results indicated that HTD is more intense when the gap area is smaller or the pressure is lower. Researchers also investigated heat transfer phenomenon in different rod assemblies numerically [16–18] under various operating parameters. HTD zones mainly exist in the region around the pseudocritical temperature. With the increase in the heat flux and the mass flux, HTD could be avoided. The dynamic viscosity and thermal conductivity are generally higher at a higher supercritical pressure. Experiment results for annular channels by Gang et al. [15] indicated that the heat transfer is enhanced with the increase in the pressure when the mass flux

$G = 350\ kg/m^2 \cdot s$, which is a high heat to mass flux ratio case, while impaired with the increase in the pressure when $G = 1000\ kg/m^2\ s$, which is a low heat to mass flux ratio case.

In the literature, the definition of HTD for supercritical flows in heated tubes could be divided into two types: qualitative and quantitative definitions. The qualitative definition of HTD is based on the direct observation of the occurrence of peak wall temperatures within some part of or the entire heated length [19–21]. On the other hand, HTD phenomenon could be characterized by comparisons of heat transfer quantitatively. The commonly used criterion is Nu_{db}, which is the Nusselt number calculated by the Dittus-Boelter equation [22]. The Nusselt number for supercritical flows in heated tubes is represented as Nu. Some researchers [23–25] indicated that HTD appears in the tube when $Nu/Nu_{db} < 0.3$, where Nu_{db} is obtained by:

$$Nu_{db} = 0.023Re^{0.8}Pr^{0.4}. \tag{1}$$

In contrast, in the investigation on the heat transfer behavior in the rod bundles with supercritical water flowing upward, few studies gave a clear definition of HTD. In addition, existing studies proposed criteria to determine CHF for the occurrence of HTD in upward supercritical tube flow only. The CHF is usually considered directly relevant to the mass flux. There is still a lack of criteria for predicting the onset of HTD in rod bundles with the supercritical water flowing upward now. Although the existence of rods in channels provides the possibility of heat transfer enhancement [11,12], the fluid flow and heat transfer characteristics in the cross-section of channels also lead to non-uniform distributions of wall temperatures circumferentially. When HTD appears in the SCWR, certain parts of claddings on fuel rods could be overheated, which will consequently cause safety issues. During the operation of SCWRs, it is important to reduce or avoid the possibility of the occurrence of HTD so that a safe and efficient application can be achieved.

In this paper, the definition of the onset of HTD for supercritical water flow in upward rod bundles is proposed based on available experimental data in the open literature. The existing criteria for predicting HTD in supercritical tube flows are evaluated against experimentally identified HTD conditions for supercritical water flows in upward rod bundles. Based on the evaluation of existing criteria, a new criterion is proposed for predicting the onset of HTD for upward supercritical water flow in rod bundles.

2. Evaluation of existing criteria

2.1. Experimental HTD data collection of upward supercritical water flows in rod bundles

In order to assess the existing criteria for predicting the onset of HTD, it is essential to compare prediction results by using criteria with experimentally identified data. The selected cases where the onset of HTD were observed in experiments for supercritical water flow in upward rod bundles in the open literature are listed in Table 1. Corresponding operation parameters cover pressures from 22.6 MPa to 27.5 MPa, mass fluxes from 410 $kg/m^2 \cdot s$ to 2700 $kg/m^2 \cdot s$, heat fluxes from 551 kW/m^2 to 3200 kW/m^2, and hydraulic diameters from 2.4 mm to 7.6 mm.

2.2. HTD indicators for onset of HTD in a rod bundle with supercritical water flowing upward

Based on the cases used in the experimental work where HTD occurs [11,12], [26,27], the HTD indicators for predicting the onset of HTD in rod bundles with supercritical water flowing upward are proposed in this study and summarized below:

(a) The increase of the circumferential wall temperature gradient along the axial direction $\Delta T_w/\Delta z$ is more than 100 °C/m.

Table 1
Heat transfer deterioration experimental data for upward supercritical water flow in rod bundles.

Reference	Rod bundle geometry	p (MPa)	G (kg/m² s)	D_h (mm)	q (kW/m²)
Razumovskiy et al. [12]	Annular, with helical ribs along each rod	22.6	2000	2.67	2547
Li et al. [26]	Annular, bare rod bundle	23	596.5	7.3	584
		23	596.5	7.3	669.8
		23	596.5	7.3	768.3
		23	1004.3	7.3	948.4
		23	1004.3	7.3	1035.6
		23	1004.3	7.3	1065.1
Razumovskiy et al. [12]	3-rod, with helical ribs along each rod	24.5	2700	2.4	3200
		27.5	1500	2.4	3070
Gu et al. [27]	4-rod, with wire wraps along each rod	25	410	4.77	580
Li et al. [26]	4-rod, with grid spacers along each rod	25	451.2	7.6	551.6
	4-rod, with wire wraps along each rod	25	410.5	7.6	578.3
Razumovskiy et al. [11]	7-rod, with helical ribs along each rod	22.6	2000	2.67	2547

(b) (b)The normalized wall temperature gradient along the axial direction, which is defined as $\Delta T_w/\Delta T_b$ is above 2.

If at least one of the two conditions mentioned above is satisfied, HTD is considered to have happened under the corresponding operating parameters. A graph showing how to identify heat transfer deterioration zones is presented in Fig. S2 in Supplementary Materials.

2.3. Existing HTD criteria

In this work, the criteria for the prediction of critical heat flux (q_{CHF}) causing the occurrence of HTD in tubes with supercritical fluids flowing upward by several researchers in the literature are considered. They are classified and summarized in Table 2.

2.4. Evaluation of existing HTD criteria against experimental data

The existing criteria for the prediction of the CHF leading to the onset of HTD are assessed first. Comparisons between of q_{CHF} predicted by these criteria ($q_{CHF\text{-}criteria}$) and identified experimentally ($q_{CHF\text{-}exp}$) are presented in Fig. 1. Table S1 in Supplementary Materials illustrates parameters used in the criteria for predicting the CHF. The relative deviation of $q_{CHF\text{-}criteria}$ from $q_{CHF\text{-}exp}$ in each case is calculated by the following equation:

$$REi = \frac{q_{CHF\_criteria,i} - q_{CHF\_exp,i}}{q_{CHF\_exp,i}}. \tag{2}$$

$RE_i > 0$ indicates the criterion overpredicts the CHF while $RE_i < 0$ the criterion underpredicts the CHF.

In addition, the prediction uncertainty using the criteria is evaluated through several parameters in this study, which are defined below:

$RE_i > 0$ indicates the criterion overpredicts the CHF while $RE_i < 0$ the criterion underpredicts the CHF.

$$REMRD = \frac{1}{N}\sum_{i}^{N} RE_i, \tag{3}$$

$$REMARD = \frac{1}{N}\sum_{i}^{N} |RE_i|, \tag{4}$$

Table 2
Existing criteria for predicting critical heat fluxes for supercritical fluid flows in upward heated tubes.

Reference	Criterion (G: kg/m^2·s, D or d: mm, i_{pc}: kJ/kg, h_{pc}: kJ/kg, P: MPa, T_{in}: °C)	Correlation types	Fluids	Application range
Yamagata et al. [9]	$q_{CHF} = 0.2\ G^{1.2}$	q - G	SCW	D = 10 mm, P = 22.6–29.4 MPa
Mokry et al. [28]	$q_{CHF} = -58.97 + 0.745\ G$		SCW	D = 10 mm, P = 24 MPa G = 200, 500, 1000, 1500 kg/m^2·s q = 70–1250 kW/m^2 T_{in} = 320–350 °C
Yin et al. [29]	$q_{CHF} = 1/2.16\ G$		SCW	D = 26 mm with inclined angle of 20° from the horizon P = 23–30 MPa G = 600–1200 kg/m^2·s q = 200–600 kW/m^2
Kline et al. [30]	$q_{CHF} = 0.0002\ G^2\ [0.7 + 0.3/(1 + e^{4/(D/8-2.35)})]$	q - G & D	SC CO_2	D = 4.6–22 mm G = 300–1500 kg/m^2·s P/P_c = 1.13
Deev et al. [31]	$q_{CHF} = 5.32\ G^{1.265}(0.001D)^{0.865}$		SCW	widely
Cheng et al. [23]	$q_{CHF} = 0.001354\ G\ i_{pc}$	q - G & i_{pc}	SCW	D = 10 mm, 20 mm P = 22.5, 23.5, 24, 25 MPa G = 700, 1000 1500, 2250, 3500 kg/m^2·s q = 300–2000 kW/m^2 T_b = 300–450 °C
Luo et al. [19]	$q_{CHF} = 1.578 \times 10^{-6} i_{pc} G^2$		SCW, SC CO_2	SCW: D = 6–26 mm P = 22–30 MPa G = 201–2500 kg/m^2·s q = 129–2328.6 kW/m^2 SC CO2: D = 2–22 mm P = 7.5–10.5 MPa G = 100–2000 kg/m^2·s q = 2.9–436 kW/m^2
Urbano and Nasuti [32]	$q_{CHF} = 0.001(1.8 \times 10^{-6} i_{pc} - 91.9)G$		SC CH_4	Not stated
Zhu et al. [33]	$q_{CHF} = 5.126 \times 10^{-4} G h_{pc}$	q - G & h_{pc}	SC CO_2	D = 10 mm P = 7.5–21.1 MPa G = 488–1600 kg/m^2·s q = 74–413 kW/m^2
Schatte et al. [24]	$q_{CHF} = 1.942 \times 10^{-6}\ G^{0.795} \times (30 - D)^{0.339} i_{pc}^{2.065}$	q - G & D & i_{pc}	SCW	D = 7.6–26 mm P = 22.5–30 MPa G = 203–1500 kg/m^2·s q = 166–1200 kW/m^2
Kong et al. [20]	$q_{CHF} = 0.457\ G^{1.09}[1-0.035(\frac{D}{20})^{1.96}(\frac{p}{22.1})^{7.16}]$	q - G & D & P	SCW	D = 3–38 mm P = 22.5–31 MPa G = 200–2150 kg/m^2·s q = 148–1810 kW/m^2
Ma et al. [25]	$q_{CHF}=8255.2117\times G^{0.8325} d^{-0.4958} p^{-0.7486} T_{in}^{-0.8125}$	q - G & D & P & T_{in}	SCW	D = 0.7–38.1 mm P = 22.5–31 MPa G = 203–3000 kg/m^2·s q = 166–2960 kW/m^2 T_{in} = 103.49–372.28 °C h_b = 451.30–3162.85 kJ/kg

$$RESD = \sqrt{\frac{1}{N-1} \cdot \sum_{i=1}^{N} (RE_i - RE_{MRD})^2}, \tag{5}$$

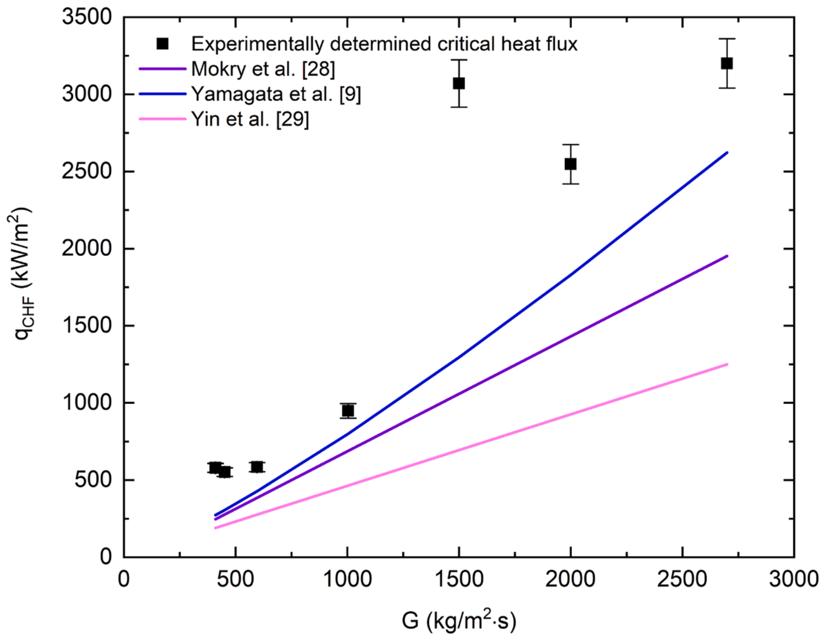
$$RE20 = N_{|RE_i|<0.2} / N. \tag{6}$$

In Eqs. (3) – (6), RE_{MRD}, RE_{MARD}, and RE_{SD} are the mean relative error, mean absolute relative error, and standard deviation of the relative error, respectively. N is the number of total cases considered. $N_{|RE_i|<0.2}$ are numbers of cases where RE_i of $q_{CHF\text{-}criteria}$ is within ± 20 % range around $q_{CHF\text{-}exp}$. Therefore, RE_{20} represents the ratio of predicted HTD cases whose relative error is within ± 20 % around the $q_{CHF\text{-}exp}$ value.

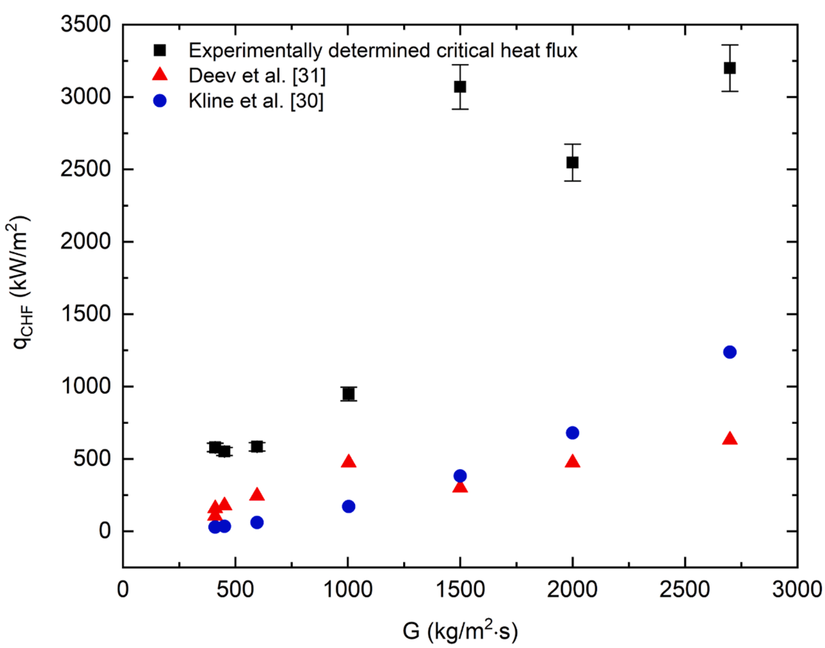
Table 3 summarizes the prediction uncertainty using all criteria considered in this study. In terms of RE_{MRD} and RE_{MARD}, the four criteria with the least relative errors are those proposed by Ma et al. [25], Zhu et al. [33], Urbano and Nasuti [32], and Kong et al. [20]. The results given in Table 3 basically show that predictions by all criteria for critical heat fluxes are conservative since all of RE_{MRD} are less than zero. The RE_{20} ranges from 23.1 % to 76.9 %. Taking RE_{SD} of these four criteria into consideration, the three better criteria are those proposed by Zhu et al. [33], Urbano and Nasuti [32], and Kong et al. [20]. However, the criteria proposed by Urbano and Nasuti [32], and Zhu et al. [33] were based on the data for supercritical CH_4 and CO_2, respectively, whose critical pressures and temperatures of CH_4 and CO_2 are much lower than those of supercritical water. Therefore, from the comparison between $q_{CHF\text{-}criteria}$ and $q_{CHF\text{-}exp}$ by existing criteria and if only the criteria for supercritical water is considered, the criterion by Kong *et al.* [20] is the best one for predicting q_{CHF} for the supercritical water flows in upward rod bundles.

2.5. Evaluation of existing criteria against numerical data

Given the limited HTD experimental cases available in the open literature, numerical cases are used as supplements to evaluate the performance of the existing criteria. In this study, numerical investigations of HTD for supercritical water flow upward in a 64-element rod bundle with D_h = 9.3 mm are carried out under operating conditions of q from 600 kW/m^2 to 879.9 kW/m^2, G from 861 kg/m^2·s to 4385 kg/m^2·s, and P from 23 MPa to 29 MPa.



(a) q - G type criteria (Mokry *et al.* [28]: —, Yamagata *et al.* [9]: —, Yin *et al.* [29]: —).



(b) q - G & D type criteria (Deev *et al.* [31]: ▲, Kline *et al.* [30]: ●).

Fig. 1. Comparison of experimentally determined critical heat fluxes with those predicted by existing criteria.

2.5.1. Numerical methods

In this work, the fluid flow and heat transfer of supercritical water flow upward in the rod bundle are considered under steady state conditions, which are governed by conservations of mass, momentum, and energy, given by the following equations [34]:

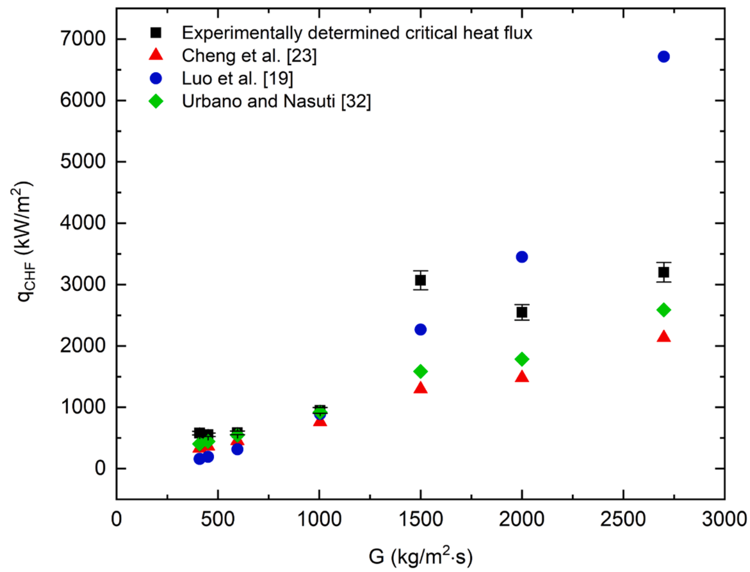
The finite volume method based on integration variables over control volumes is used to solve governing equations. The Fluent software from ANSYS is used for conducting numerical simulations. Details of simulations could be found in the previous work [18].

2.5.2. Prediction of HTD by selected criterion

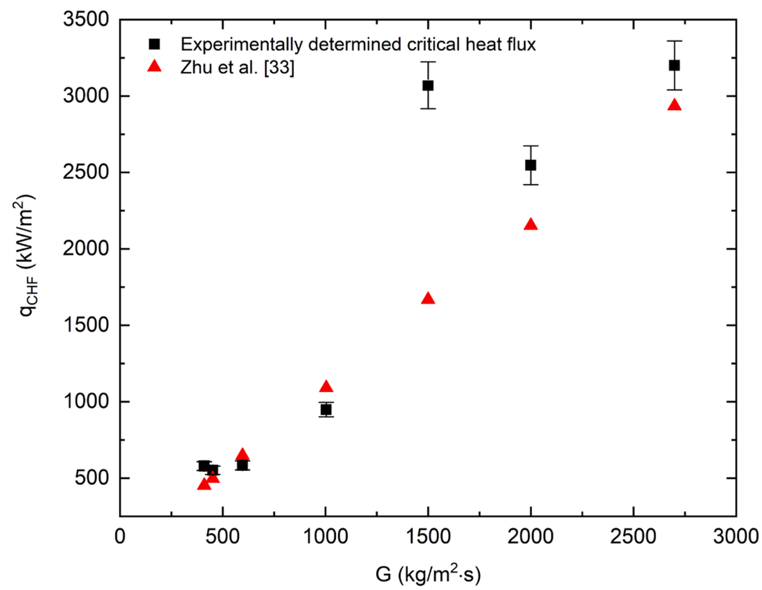
Based on the evaluation of existing criteria against experimentally identified q_{CHF} data, the criterion proposed by Kong *et al.* [20] is adopted to predict q_{CHF} for numerical cases under different operating conditions. Predicted operating conditions when HTD occurs in different numerical cases are summarized in Table S2 in Supplementary Materials.

2.5.3. Verification of numerical HTD cases

The onset of HTD predicted using the criterion from Kong *et al.* [20] for numerical cases need to be further verified whether the HTD



(c) q - G & i_{pc} type criteria (Cheng *et al.* [23]: ▲, Luo *et al.* [19]: ●, Urbano and Nasuti [32]: ♦).



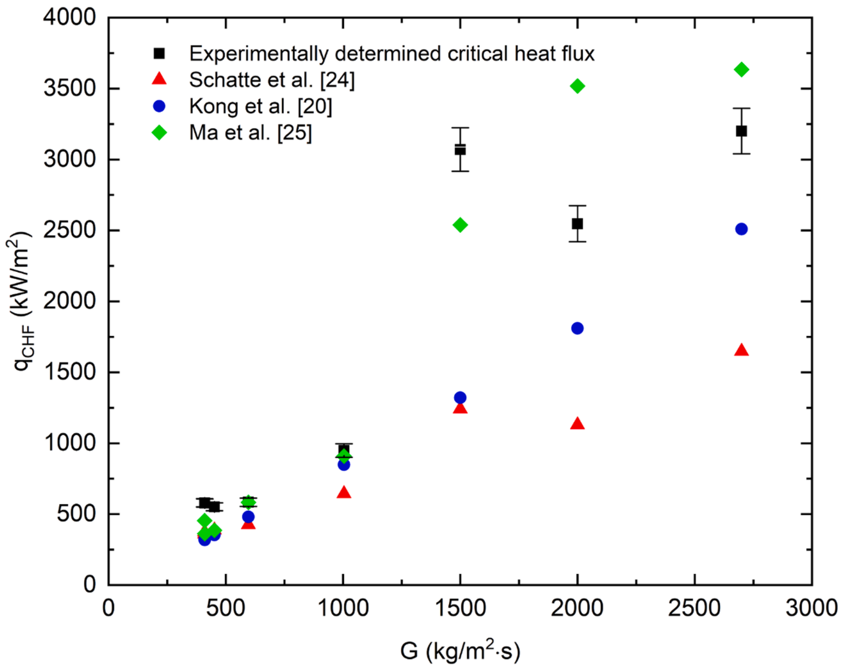
(d) Zhu et al.'s criterion (Zhu *et al.* [33]: ▲).

Fig. 1. (*continued*).

indicators presented in Section 2.2 can be satisfied. Cases having HTD predicted by Kong' s criterion and satisfying HTD indicators at the same time are listed in Table 4, which could be used as supplements to HTD database for future study. It can be seen that the criterion proposed by Kong *et al.* [20] can predict the occurrence of HTD in these numerical cases. In summary, the criterion proposed by Kong *et al.* [20] gives a better performance in predicting HTD scenarios for both experimental and numerical cases than other criteria.

2.6. Analysis of difference between predicted and experimentally identified q_{CHF}

From the evaluation results, existing criteria generally give conservative q_{CHF} predictions for supercritical water flow in the rod bundle. This supports the statement in the literature [35] that critical heat flux in a rod bundle is higher than that in a bare tube under the same operating conditions. Mass flux, operating pressure, and hydraulic diameter all have impacts on heat transfer of upward supercritical water flow in rod bundles [15,18,36], which will also influence q_{CHF} that causes the onset of HTD. Therefore, reasons for deviations between predicted and experimentally identified q_{CHF} can be: (1) Most existing criteria only considered the relationship between q_{CHF} and mass flux, and few criteria took operating pressure and hydraulic diameter into consideration, (2) Existing criteria were developed for predicting the onset of HTD in tubes, not rod bundles, and (3) The definitions of HTD scenarios for supercritical water flow in a tube and a rod bundle are different.



(e) Criteria from Schatte et al. [24] (▲), Kong et al. [20] (●), and Ma et al. [25] (♦).

Fig. 1. (*continued*).

Table 3
Deviations between predicted critical heat fluxes by existing criteria and experimentally identified critical heat fluxes.

Criteria	RE_{MRD} [a]	RE_{MARD} [b]	RE_{SD} [c]	RE_{20} (%) [d]
Yamagata et al. [9]	-0.348	0.348	0.142	15.4
Mokry et al. [28]	-0.445	0.445	0.111	0
Yin et al. [29]	-0.615	0.615	0.0705	0
Kline et al. [30]	-0.847	0.847	0.102	0
Deev et al. [31]	-0.696	0.696	0.128	0
Cheng et al. [23]	-0.358	0.358	0.103	7.69
Luo et al. [19]	-0.193	0.471	0.534	23.1
Urbano and Nasuti [32]	-0.223	0.223	0.123	53.8
Zhu et al. [33]	-0.095	0.147	0.162	76.9
Schatte et al. [24]	-0.415	0.415	0.105	0
Kong et al. [20]	-0.303	0.303	0.133	23.1
Ma et al. [25]	-0.063	0.205	0.241	53.8

[a] RE_{MRD} - mean relative error.
[b] RE_{MARD} - mean absolute relative error.
[c] RE_{SD} - standard deviation of the relative error.
[d] RE_{20} - ratio of predicted HTD cases whose relative error is within ± 20 % around the $q_{CHF\text{-}exp}$ value.

$$\frac{\partial \rho \overline{u_i}}{\partial x_i} = 0, \tag{7}$$

$$\frac{\partial(\rho \overline{u_i} \overline{u_j})}{\partial x_j} = -\frac{\partial \overline{P}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial \overline{u_i}}{\partial x_j} - \rho \overline{u_i' u_j'}\right) + \rho g_i, \tag{8}$$

$$\frac{\partial}{\partial x_i}\left(\overline{u_i} \rho c_p T\right) = \frac{\partial}{\partial x_i}\left[\left(\lambda + \frac{c_p \mu_t}{\mathrm{Pr}_t}\right)\frac{\partial T}{\partial x_i}\right]. \tag{9}$$

3. A new criterion for predicting onset of HTD in rod bundles with supercritical water flowing upward

3.1. Requirements for new criterion

In the process of developing a criterion for predicting q_{CHF} for upward supercritical water flow in a rod bundle, several requirements need

Table 4
Operating conditions of numerical cases satisfying heat transfer deterioration indicators.

P (MPa)	G (kg/m^2·s)	q (kW/m^2)	Axial location z (m)	Maximum $\Delta T_w/\Delta z$ (C/m)	$\Delta T_w/\Delta T_b$
25	861.2	750	4.6–4.7	161.1	1.4
25	861.2	800	4.6–4.7	182	1.5
25	861.2	850	0.8–0.9	474.7	19.1
25	861.2	879.9	0.8–0.9	578	22.4

to be fulfilled: (1) The construction of the new criterion should include as many operating parameters as possible since they affect q_{CHF}, (2) Accuracy of the new criterion should be higher than existing ones, (3) Applicability of the criterion should be determined.

3.2. Development of new criterion

Database used for developing the new criterion is summarized in Table S3 in Supplementary Materials. To satisfy all requirements stated above, the new criterion will include mass flux, hydraulic diameter, and operating pressure into account. A multiplicative function form of the criterion is used as:

$$q_{CHF} = C_1 \cdot f_1(G) \cdot f_2(D_h) \cdot f_3(P), \tag{10}$$

According to effects of operating parameters on heat transfer and formulas of existing criteria, the new criterion is further constructed as:

$$q_{CHF} = C_1 \cdot G^{C2} \cdot (D_h/10)^{C3} \cdot (P/22.1)^{C4}, \tag{11}$$

where q_{CHF} is in kW/m^2, G is in kg/m^2·s, D_h is in mm, and P is in MPa. The reference hydraulic diameter is selected as 10 mm to cover the maximum hydraulic diameter in the database. The reference pressure is the critical pressure of supercritical water (22.1 MPa). The constants C_1, C_2, C_3, and C_4 in Eq. (11) need to be determined. If taking natural logarithms on both sides of Eq. (11), it will be converted into:

$$\ln(q_{CHF}) = \ln(C_1) + C_2 \cdot \ln(G) + C_3 \cdot \ln(D_h/10) + C_4 \cdot \ln(P/22.1). \quad (12)$$

The problem is simplified into a multiple linear regression problem as:

$$Y = XB + U, \quad (13)$$

where U is the error which needs to be minimized. Y, X and B are illustrated as:

$$Y = \begin{bmatrix} \ln(q_{CHF\_exp,1}) \\ \ln(q_{CHF\_exp,2}) \\ \vdots \\ \ln(q_{CHF\_exp,N}) \end{bmatrix}, \quad (14)$$

$$X = \begin{bmatrix} 1 & \ln(G(1)) & \ln(\frac{D_h}{10}(1)) & \ln(\frac{P}{22.1}(1)) \\ 1 & \ln(G(2)) & \ln(\frac{D_h}{10}(2)) & \ln(\frac{P}{22.1}(2)) \\ \vdots & \vdots & \vdots & \vdots \\ 1 & \ln(G(N)) & \ln(\frac{D_h}{10}(N)) & \ln(\frac{P}{22.1}(N)) \end{bmatrix}, \quad (15)$$

$$B = \begin{bmatrix} \ln(C_1) \\ C_2 \\ C_3 \\ C_4 \end{bmatrix}. \quad (16)$$

To minimize U and solve the regression problem, B can be solved as [37]:

$$B = (X'X)^{-1}X'Y, \quad (17)$$

where X' is the transpose of X, and $(X'X)^{-1}$ is the inverse of X'X. Based on the calculation, the resulting B is presented as:

$$B = \begin{bmatrix} 1.4448 \\ 0.7401 \\ -0.5029 \\ 1.6988 \end{bmatrix}. \quad (18)$$

Therefore, the new criterion is constructed and shown as:

$$q_{CHF} = 4.241 \cdot G^{0.7401} \cdot (D_h/10)^{-0.5029} \cdot (P/22.1)^{1.6988}. \quad (19)$$

The range of applicability for using this criterion to predict q_{CHF} is determined based on the database used. It is valid for heated supercritical water flowing upward in rod bundles with mass flux from 550 kg/m^2·s to 3200 kg/m^2·s, hydraulic diameter from 2.4 mm to 9.3 mm, and operating pressure from 22.6 MPa to 27.5 MPa.

3.3. Performance evaluation of new criterion

The comparison between experimentally identified CHFs and those predicted by the new criterion given in Eq. (19) is shown in Fig. 2, indicating predicted CHFs by the new criterion are close to experimentally identified values. To evaluate the prediction uncertainty using the new criterion, errors using the best four existing criteria and the new criterion given in Eq. (19) are summarized in Table 5. It can be seen that relative errors using the new criterion are much lower than using the existing criteria although the new criterion overestimates CHFs a little bit. This can be due to the fact that some experimentally determined critical heat fluxes adopted to derive the new criterion are for rod bundles with either helical ribs, grid spacers, or wire wraps along each rod. Critical heat fluxes in such rod bundles are higher than those in bare rod bundles under the same operating conditions. In addition, all CHFs predicted by the new criterion given in Eq. (19) are within ± 20 % of the respective experimentally identified CHFs in all cases considered. Therefore, the new criterion developed in this study satisfies the requirements mentioned above. It can be used to predict CHFs for supercritical water heated in rod bundles and help to determine the safety boundary of operating conditions in industry applications, such as in the development of SCWRs.

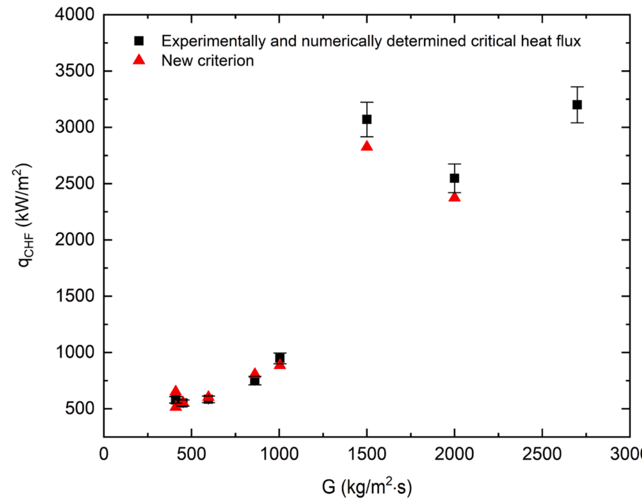


Fig. 2. Comparison of experimentally identified critical heat fluxes given in Table S3 in Supplementary Materials (■) with those predicted by new criterion given in Eq. (19) (▲).

Table 5
Prediction difference between existing criteria and new criterion.

Criteria	RE_{MRD} [a]	RE_{MARD} [b]	RE_{SD} [c]	RE_{20} (%) [d]
Urbano and Nasuti [32]	-0.223	0.223	0.123	53.8
Zhu et al. [33]	-0.095	0.147	0.162	76.9
Kong et al. [20]	-0.303	0.303	0.133	23.1
Ma et al. [25]	-0.063	0.205	0.241	53.8
New Criterion given in Eq. (19)	0.0026	0.075	0.089	100

[a] RE_{MRD} - mean relative error.
[b] RE_{MARD} - mean absolute relative error.
[c] RE_{SD} - standard deviation of the relative error.
[d] RE_{20} - ratio of predicted HTD cases whose relative error is within ± 20 % around the $q_{CHF\text{-}exp}$ value.

4. Conclusions

In this study, the concept of HTD for supercritical water flow in rod bundles is introduced according to observations from experimental data. Existing criteria for predicting critical heat flux causing the onset of heat transfer deterioration for supercritical fluid flow in tubes are first assessed against extensive experimental data for supercritical fluid flows in rod bundles. Extensive numerical simulations are conducted to not only further verify the onset of heat transfer deterioration, but also to provide a supplement database used for constructing the new criterion to predict the onset of HTD. Based on errors between predicted and experimentally identified CHFs, it is found that Kong's criterion gives the best accuracy. Operating parameters include mass flux, hydraulic diameter, and operating pressure, which have impacts on CHF for supercritical fluid flow in rod bundles, are considered in developing the new criterion. Through the comparison with experimentally identified CHFs, the new criterion shows a better performance than all existing criteria. Predicted CHFs by the new criterion are within ±20 % around the respective experimentally identified CHFs in all cases considered. With more experimental and numerical data on CHFs for supercritical water flow in rod bundles in the future, the criterion could be further improved.

CRediT authorship contribution statement

Jing Jiang: Supervision. **Huirui Han:** Writing – original draft, Validation, Methodology, Conceptualization. **Chao Zhang:** Writing – review & editing, Supervision, Project administration.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.supflu.2024.106263.

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