

COMPARATIVE STUDY OF DIFFERENT FLOW MODELS USED TO PREDICT CRITICAL FLOW CONDITIONS OF SUPERCRITICAL FLUIDS

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Abstract

Present models used to predict supercritical choking flows have been developed for fluids under subcritical conditions. Most of these models can be classified in the following three principal categories: Homogeneous equilibrium, slip flow and disequilibrium. In some models a thermal disequilibrium is more or less empirically introduced. None of these models are developed to handle the expansion of supercritical fluids. In addition, from the experimental viewpoint, information about critical discharge flows of supercritical fluids is nowadays very scarce and in most cases the data are collected under conditions that are not representative of future Supercritical-Cooled Water Reactors (SCWR's), e.g., using fluids different from water. In the present work, few existing data are used to compare the ability of some of the aforementioned modeling approaches to handle choking flow of water under supercritical conditions. In general, it is observed that critical discharge mass fluxes depend on the degree of thermodynamic disequilibrium as well as on stagnation conditions. It is also observed that for temperatures above and below 50°C from the critical one, the discharge of supercritical water can be predicted using a simple ideal gas modeling approach.

1. Introduction

The International Atomic Energy Agency (IAEA) has stipulated that by the year 2030 world primary energy requirements will increase by up to 45%. It is obvious that to assure a vigorous world economy as well as adequate social standards, new energy conversion technologies are mandatory. Further, it is apparent that present observed trends in energy supply and consumption do not satisfy environmental sustainability. To fulfill this requirement, the participation of 10 countries has made it possible to establish a Generation IV International Forum (GIF). Within this framework, GIF members' have proposed the development of new generation of nuclear power reactors to replace actual technologies. The principal goals of these nuclear-power reactors, among others are: economic competitiveness, sustainability, safety, reliability and resistance to proliferation. Besides the high efficiency that should characterize such systems, future nuclear reactors must also permit other energy applications, i.e., hydrogen production, sea water desalinization or petroleum extraction, to be achieved. To this aim, the Canadian nuclear industry is involved in developing a SCWR technology similar to actual CANDU systems that will run at a coolant outlet temperature of about 625°C and at pressure of 25 MPa [1-4].

Even though the power industry has more than 60 years of experience in using fossil-fuelled supercritical boilers, the available scientific information is very scarce [5]. Consequently, the appropriate design and safety analyses of future SCWRs will require fundamental research to be

accomplished. The European Nuclear Commission and the University of Tokyo have jointly studied the feasibility of a High Performance Light Water Reactor under supercritical pressure and temperature conditions [6]. This study was based on several years of well-established European experience in operating fossil fuelled supercritical once-through boilers. As part of this ambitious work, some recommendations that involve fundamental research and the production of data required for carrying out both the design and the safety analyses of such a reactor were clearly identified. Some of these aspects, among others are: *i)* Due to the large density variations of a supercritical coolant, there is an imperative necessity for developing new coupled neutronic-thermohydraulic calculation techniques; *ii)* In the case of a depressurization during a normal reactor shutdown or an emergency, a transition of the supercritical fluid towards two-phase flow conditions may occur. This will require advanced thermal-hydraulic models that will be able to handle such a flow transition condition; *iii)* In order to carry out appropriate core design, out-of-pile heat transfer and pressure drop experiments with supercritical water are also mandatory and *iv)* There is an urgent need for experimental data on the discharge flow rate of supercritical water expanding across orifices and breaks. It was also argued that the amount of data on this particular field is very scarce which may seriously compromise the design and safety analyses of future SCWRs. Furthermore, few models are able to predict choking flow of water under supercritical conditions.

Present models used to predict supercritical choking flows have been developed by assuming two-phase flow mixtures, i.e., discharge of fluids under subcritical conditions. Most of these models can be classified in the following three principal categories: Homogeneous Equilibrium Model (HEM), slip flow and disequilibrium. In the first case, it is assumed that during the expansion the supercritical fluid enters into the liquid-vapor mixture zone where two-phases coexist forming a homogeneous pseudo fluid [7]. This approach allows pseudo-physical properties of the mixture to be used in the model. Furthermore, it is assumed that along the expansion a strong coupling between the phases exists; thus, mechanical and thermal dissipation between the phases are neglected. Thus, the phases are considered to be at the same temperature and pressure (i.e., thermodynamic equilibrium). In addition, the expansion is assumed as isentropic (which sounds as a contradiction from thermodynamics point of view) starting from the initial supercritical thermodynamic state up to the end of the process, i.e., low pressure reservoir.

In some models a thermal disequilibrium is more or less empirically introduced. If a total thermal disequilibrium is taken into account, then the Homogeneous Frozen Model is obtained [8]. Instead, if only a fraction of thermal disequilibrium is introduced a well known Henry-Fauske model is obtained [9]. In general, non-homogeneous models, where thermal disequilibrium is considered, have been developed based on the homogeneous one [8, 10-13]. A non-homogeneous disequilibrium formulation was proposed and applied by Trapp & Ransom [14] to simulate the discharge of two-phase flows.

In the present work, limited experimental data on supercritical choking flows is used to compare the ability of some of the aforementioned modeling approaches to handle choking flow. For completeness of the work, both Henry-Fauske and HEM are also compared with subcritical steam-water data.

2. Existing modeling approaches

In this section four choking flow modeling approaches are briefly presented and then compared in Section 3 with data given in Chen et al. [15, 16] and Lee & Swinnerton [17]. The first model is the well known Henry-Fauske equation largely used to predict critical discharges in boiling water nuclear power reactors. The second one is the HEM that is developed by assuming an expansion of homogeneous two-phase flow mixtures. It must be pointed out that this model has been also applied to simulate the critical discharge of supercritical fluids [15-17]. The third approach that has been used for treating supercritical fluids is Bernoulli's equation [16]. In addition, a simple analytical polytropic equation is also presented in this paper before comparing it with the same data set.

2.1 Henry-Fauske Model

The thermal non-equilibrium model developed by Henry and Fauske [9] assumes that entropy is constant and the steam phase behaves as an ideal gas during the expansion process. These hypotheses are then used to write a model for predicting critical mass fluxes, i.e., choking flow. Using these assumptions, under isentropic flow conditions (i.e., adiabatic, frictionless flows), the critical mass flux is written at the throat as:

$$G_{cr}^2 = \left[\frac{x_o v_g}{n P} + (v_g - v_{lo}) \left\{ \frac{(1-x_o)N}{s_{gE} - s_{lE}} \cdot \frac{ds_{lE}}{dP} - \frac{x_o C_{pg} (1/n - 1/\gamma)}{P(s_{go} - s_{lo})} \right\} \right]_{throat}^{-1} \quad (1a)$$

With the pressure ratio calculated by:

$$\eta = \frac{P_t}{P_0} = \left[\frac{\frac{1-\alpha_0(1-\eta) + \frac{\gamma}{\gamma-1}}{\alpha_0}}{\frac{1}{2\beta\alpha_t^2} + \frac{\gamma}{\gamma-1}} \right]^{\frac{\gamma}{\gamma-1}} \quad (1b)$$

and

$$\beta = \left[\frac{1}{n} + \left(1 - \frac{v_{lo}}{v_g} \right) \left[\frac{(1-x_o)NP}{x_o(s_{gE} - s_{lE})} \cdot \frac{ds_{lE}}{dP} \right] - \frac{C_{pg} (1/n - 1/\gamma)}{(s_{go} - s_{lo})} \right]_{throat} \quad (1c)$$

where, C_{pg} is the specific heat of the gas phase at constant pressure, P is the pressure, s is the specific entropy, v is the specific volume, x is the thermodynamic quality, α_o and α_t are the stagnation and throat averaged void fractions respectively, and γ is the isentropic expansion coefficient of steam. Subscripts E , g , l , and o represent equilibrium, vapor, liquid and stagnation flow conditions, respectively. The quantity N is used to account for partial phase change occurring in the throat. Henry and Fauske have correlated the value of N as a function of throat

equilibrium quality. This model is largely used in the nuclear industry to perform nuclear power reactor safety analyses.

2.2 Homogeneous Equilibrium Model (HEM)

The HEM is also a frequently used model to calculate critical flow rates, especially for saturated liquid-vapour mixtures [15-17]. In this model, it is assumed that the two-phases are strongly coupled thermal and mechanically; thus, velocities, temperatures and pressures acting on the phases are equal. Thus, it must be pointed out that this model is developed to treat the critical discharge of two-phase flow mixtures by assuming that there is no slip between the phases and that both heat and mass transfer between them are negligible. The critical mass flux given by this model is expressed as:

$$G_{cr} = \frac{[2(h_o - (1 - x_E)h_{lE} - x_E h_{gE})]^{1/2}}{(1 - x_E)v_{lE} + x_E v_{gE}} \quad (2)$$

where h_o is the stagnation specific enthalpy and x_E is the thermodynamics equilibrium quality. According to the open literature, it seems that this model provides better results for high stagnation pressures and qualities, i.e., when the two-phases approach saturation vapour conditions. Moreover, it is observed that increasing the residence time of the fluid in the channel (i.e., higher length to diameter ratios) increases the accuracy of the HEM, which is coherent with the assumption of thermal equilibrium.

2.3 Bernoulli's Model

The critical flow rate of frictionless, incompressible and potential single-phase flows can be estimated by using Bernoulli's equation which is written as [16]:

$$G_{cr} = 0.61 \sqrt{2\rho(P_o - P_d)} \quad (3)$$

where P_d is the discharge pressure and ρ is the fluid density determined at stagnation conditions (P_o, T_o). Even though this formulation is straightforward (i.e., conversion of potential into kinetic energy), it is included in the paper to compare with supercritical water choking flow data.

2.4 Proposed Polytropic Expansion Approach

Based on mass and momentum conservation equations and using similar hypotheses applied by Henry & Fauske [9], a basic polytropic equation is written as:

$$G_{cr}^2 = \frac{n p}{v} \quad (4)$$

where p is the critical discharge pressure, n is a polytropic expansion coefficient and v is the specific volume determined at pressure p and at the critical temperature. Herewith, we assume that the flow can expand within a full range of thermodynamic conditions, i.e., complete thermal equilibrium ($n = 1$) or fully out of equilibrium ($n = k$). Notice that these two extreme cases can easily be controlled by a single correlation parameter (n). When the flow expands isentropically, i.e., out of equilibrium, the isentropic expansion coefficient, k , is considered constant during the whole process. It is calculated from small changes of the pressure and the temperature around the critical point, by keeping the entropy constant.

3. Comparison of model predictions with experimental data

Existing experimental data on choking water flows under supercritical conditions are very scarce. Therefore, to determine the ability of the aforementioned models to predict critical flows under different inlet water conditions, the data of Lee & Swinnerton [17] and Chen et al. [15, 16] are used in this work. Calculations performed with the models described in the former section are carried out using the Matlab software (version R2008a, 2008) and the X-Steam library [19]. Before conducting simulations, the thermo physical properties predicted by this library are compared with data given in the steam-water table of Schmidt [20] for a wide range of temperature and pressure conditions.

Figure 1 shows that for flow conditions far away from the critical one, in general the X-Steam library is able to predict enthalpies, entropies and mass volume densities quite well. Close to the critical point, however, errors of up to 1.1% are obtained for the enthalpy and the entropy. Instead, within the same region, the errors for calculated densities are much higher (up to 3%).

Figure 2 shows the variation of water density with temperature for a constant pressure of 240 bars. This figure includes values calculated using the X-Steam library [19] as well as those given in Schmidt [20]. It can be observed that for temperatures higher than the critical one (i.e., $T_{cr} - T_o < 0$), the change of density with temperature occurs at a much slow pace. Close to the critical value, however, a very fast change in density occurs. Further, only small differences can be observed between densities calculated with X-Steam and those given in Schmidt's table.

The polytropic model presented in Section 2.4 is developed based on similar hypothesis used by Henry & Fauske [9]. Therefore, this model is first compared with steam-water data under subcritical conditions (i.e., two-phase flow mixtures). Figure 3 shows a comparison of the predictions obtained with Henry-Fauske model and the experimental data collected for reservoir pressures ranged from 200 psi(a) to 500 psi(a). Notice that herewith the imperial system of units is used to facilitate the reader to perform a direct comparison of present results with those given in Henry & Fauske [9]. In general it is observed that under relative low pressure conditions the Henry-Fauske model is able to catch the experimental trends. For high and medium pressures, however, it has been determined that this model underestimates the experiments by up to 40% [21, 22].

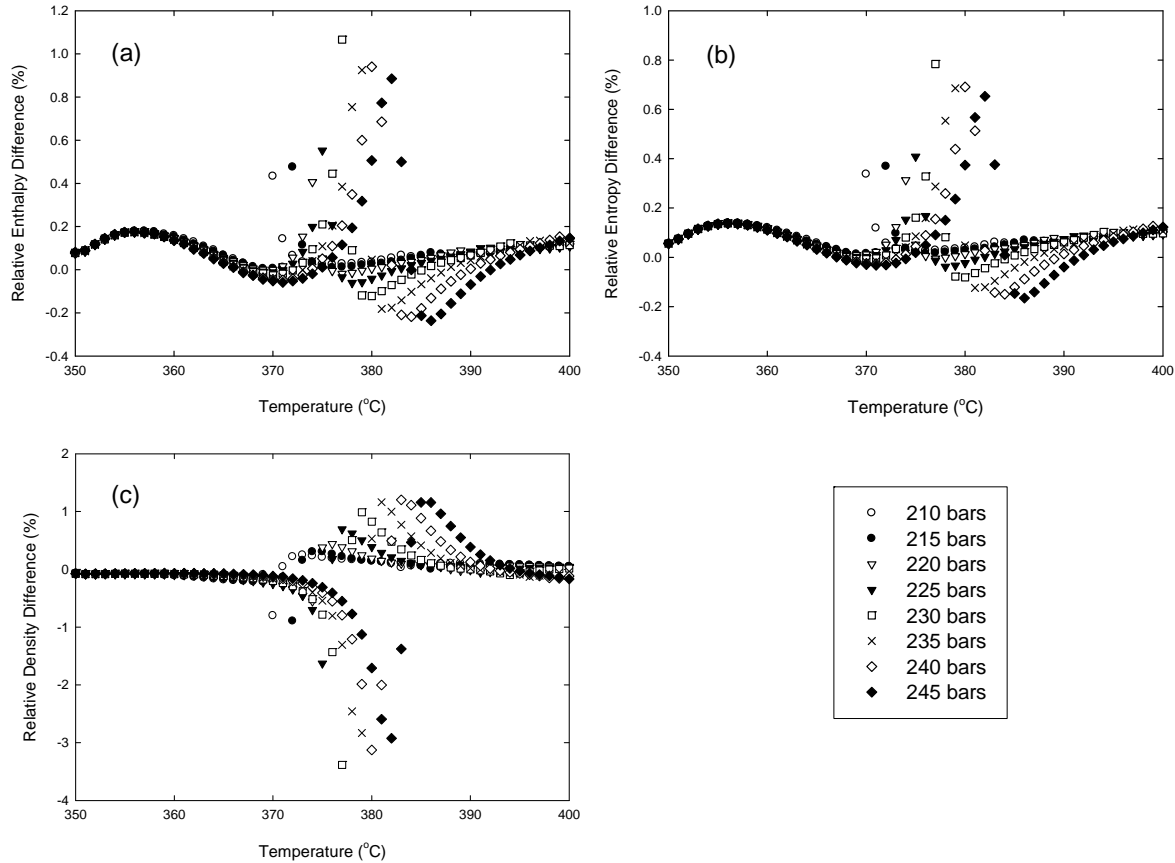


Figure 1 Comparison of thermodynamic properties calculated using the X-Steam library [19] and the steam-water table of Schmidt [20].

Predictions of critical mass fluxes obtained with HEM for a single pressure of 500 *psi*(a) (Equation 2) are also presented in Figure 3. It must be pointed out that this approach is sensitive to both reservoir pressure and quality (see Equation 2). It is apparent that this approach is able to handle stagnation quality conditions higher than 10%, however, it is unable to perform well for low values of qualities.

Even though for relatively high stagnation quality conditions both Henry-Fauske and HEM models follow almost the same trends, the latter predicts lower critical mass fluxes. For stagnation qualities lower than 10%, the HEM behavior could be explained by the fact that the number of liquid droplet entrained within the flow increases with decreasing quality. In fact, the higher is the droplet density the lower is the probability of the flow to reach mechanical and thermal equilibrium; two hypotheses used to develop the HEM given in Equation (2).

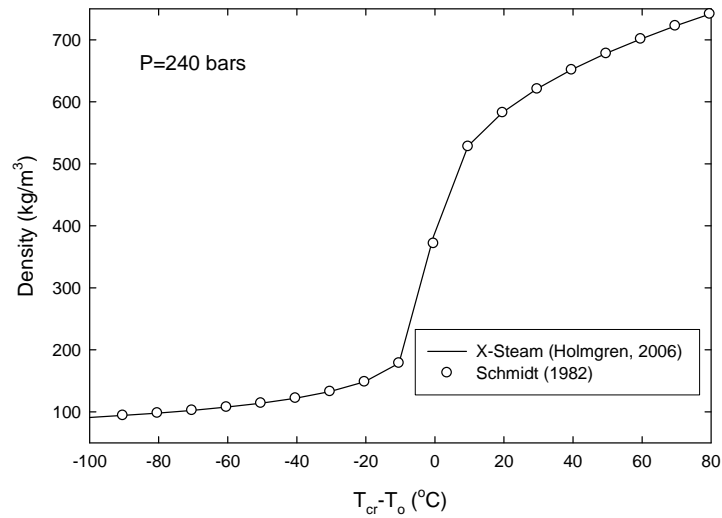


Figure 2 Variation of the density with temperature.

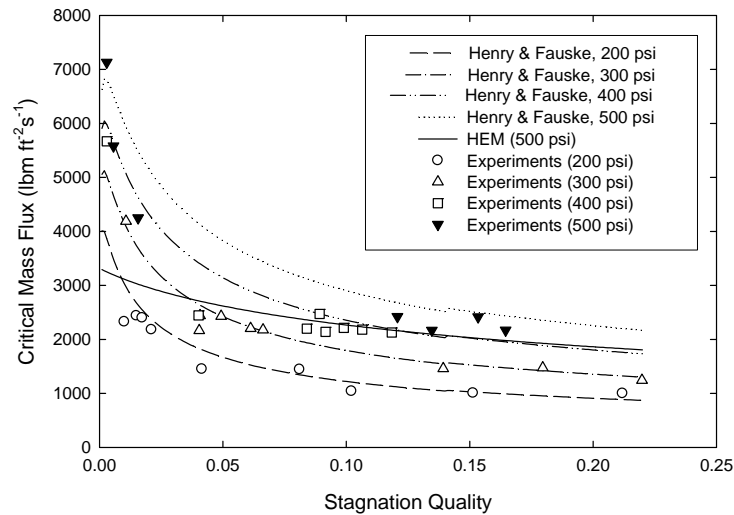


Figure 3 Comparison of the predictions of the Henry-Fauske and HEM models with data.

From Equation (1a), it is apparent that the Henry-Fauske model cannot properly work under supercritical water conditions because this model requires a steam quality determined at reservoir pressure conditions. Nevertheless, as mentioned in Section 2.4, similar hypotheses are used to write a polytropic expansion model. Moreover, to fulfill the gap that exists in modeling supercritical water choking flows, Bernoulli (Equation 3) and HEM (Equation 2) are also used. Figure 4 shows a comparison of the prediction of these models with data collected under supercritical water conditions [15-17]. Notice that only experimental data of Lee & Swinnerton that correspond to pressure conditions close to those used by Chen et al. are shown in the figure.

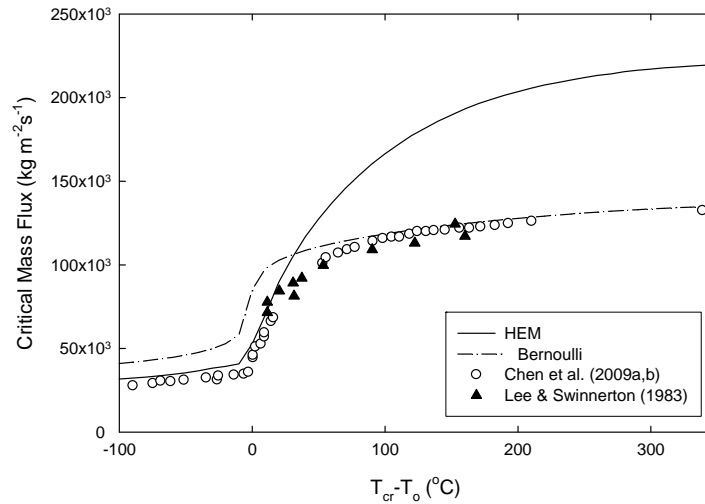


Figure 4 Comparison of predictions obtained with HEM and Bernoulli's model with supercritical water experimental data. ($P_o = 22.1\text{--}26.8\text{ MPa}$ for Chen et al. and EPRI; $P_o = 24.5\text{ MPa}$ for HEM and Bernoulli)

It is surprisingly observed that Bernoulli's model is able to produce excellent results for flow temperatures much lower than the critical one (i.e., $T_{cr} - T_o > 50^\circ\text{C}$). In turn, for temperatures close to and higher than the critical one, the model overpredicts the data. Figure 4 also presents a comparison of HEM predictions with the same data set. It is apparent that for flow temperatures ($T_{cr} - T_o$) lower than 25°C this modeling approach does not work. In fact, to perform calculations using this model the flow conditions are estimated by assuming an isentropic flow expansion (Equation 2); thus, the exit quality decreases with decreasing the inlet flow temperature. It is obvious that such situations can bring about low discharge qualities where the homogeneous two-phase mixture is not completely transformed into steam. Therefore, the flow becomes two-phase with a relatively high content of water in the form of very small droplet. It is quite possible that under such conditions the use of a homogeneous two-phase flow approach is not necessarily appropriate [21, 22]. Furthermore, there is an apparent contradiction when the HEM formulation is applied to isentropic conditions. In fact, mechanical and thermal equilibrium between the two-phases cannot be achieved isentropically. It is then quite possible that the flow undergoes an expansion process that does not satisfy the hypotheses required to write Equation (2).

This behavior seems to be confirmed by the results of the HEM obtained for temperatures higher than the critical and a pressure of 24 MPa , as shown in Figure 5. Herewith, the same model is compared with similar calculations carried out by Chen et al. [15]. For low stagnation temperatures, up to the critical one, the results are very similar. The critical discharge pressure presents a maximum and then start decreasing with increasing temperature and reaches a plateau at about 380°C . Nevertheless, starting at about 430°C , the HEM predicts a constant critical discharge pressure that is almost independent of the temperature while Chen et al. have predicted different trend (i.e., the critical pressure decreases with increasing temperature). Based on

thermodynamics of perfect gases, HEM results seem physically correct because the gas velocity is given by:

$$v_{cr} = c = \sqrt{\frac{k P_{cr}}{\rho}} \quad \text{or} \quad P_{cr} = \frac{c^2 \rho}{k} \quad (5)$$

where c represents the speed of sound. Therefore, the HEM seems to indicate that for temperatures much higher than the critical one, supercritical water behaves almost as an ideal gas which is not shown by Chen et al. [15]. Furthermore, Equation (5) shows a linear relationship between the critical discharge pressure and the fluid density. The Figure 2 shows that higher is the temperature with respect to the critical one, the lower is the dependency of the density with temperature. Thus, results obtained with the HEM approach for temperature higher than the supercritical value encouraged us to write the model described in Section 2.4.

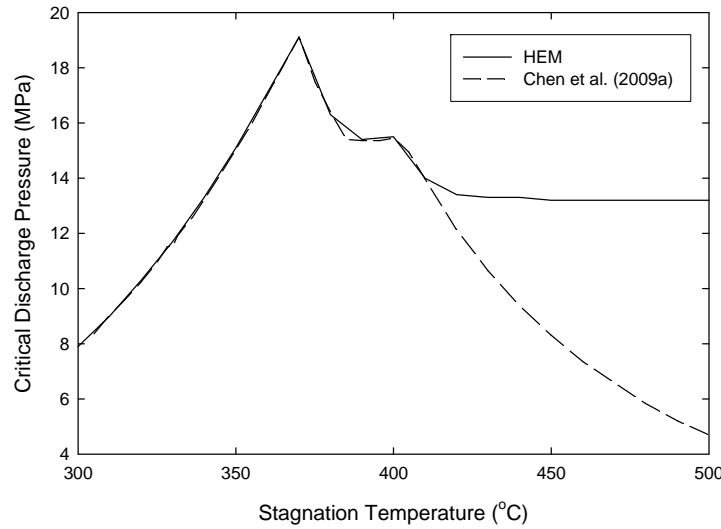


Figure 5 Comparison of calculations performed using the HEM ($P_o=24$ MPa) with those given in Chen et al. [15].

We have performed calculations using Equation (4) with isentropic and polytropic expansion coefficients equal to $k=1.302$ and $n=1.0$, respectively. As mentioned before, the coefficient k is previously determined numerically using the X-Steam library [19] and very small incremental changes of both the pressure and the temperature by maintaining the entropy constant. Predictions obtained from this model are compared with the same experimental data set in Figure 6.

For flow temperatures above and below 50°C of the critical value, it is obvious that the polytropic expansion equation is able to predict the experimental data. It is interesting to note that for temperatures higher than the critical one ($T_{cr} - T_o < 0$), this approach suggests that an isothermal expansion behaves much better, i.e., $n=1$ provides better results than $n=k$. However, for temperatures close to the critical one, this simple analytical approach is unable to

predict the experimental trends. An error propagation analysis is performed by using the uncertainties shown in Figure 1. To this aim a differential form of Equation (4) is given as:

$$dG_{cr} = \frac{\partial G_{cr}}{\partial P} dP + \frac{\partial G_{cr}}{\partial \rho} d\rho \quad (6)$$

For a constant pressure this equation is rewritten as a function of relative variable changes by:

$$\frac{dG_{cr}}{G_{cr}} = \frac{d\rho}{\rho} \rightarrow \varepsilon_{G_{cr}} = \varepsilon_{\rho} \quad (7)$$

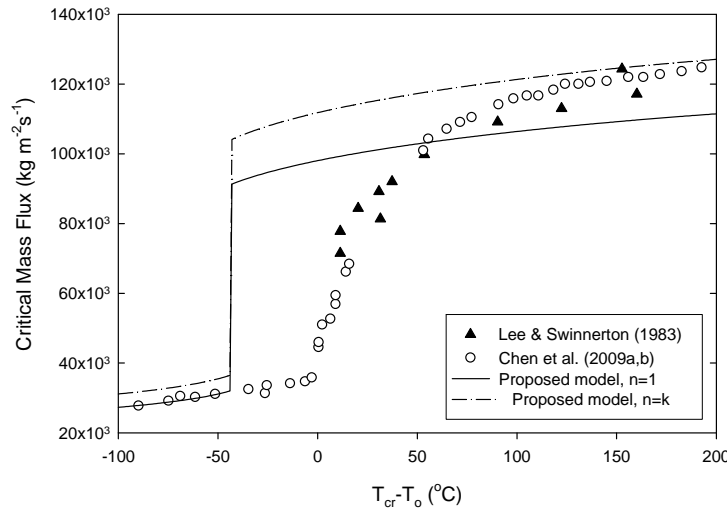


Figure 6 Comparison of polytropic expansion model with experimental data.

Equation (7) predicts a maximum error of around 3%, which does not explain the differences observed in Figure 6. Several physical reasons may explain the departure of the predictions from the data around the critical region. For instance, it is quite possible that when the fluid approaches the pseudo-critical temperature, a rapid modification of the flow structure occurs. To this aim, Sakurai et al., [23] and Okamoto et al., [24] have observed that supercritical fluids show two-phase like configurations. If the difference between the relaxation of these structures and the fluid residence time in the throat becomes important, then the flow structures will not have enough time to reach isothermal conditions as indicated in Figure 6 (i.e., for flow temperature lower than the critical one). In fact, for flow conditions close to the critical point, the expansion could bring about both flow structure and phase flow transformations that cannot be correctly represented by such a simplified analytical approach. Additional work is still required to better understand the physical phenomena of choking flows for fluids close to subcritical-to-critical transition conditions.

4. Conclusion

Predictions obtained using several well known choking flow models are compared with experimental data. In general, for steam-water flows under subcritical conditions it is observed

that the models are modestly able to predict experimental trends. For subcritical conditions Bernoulli's equation gives good results. Instead, for supercritical water flows, it seems that HEM is the most appropriate for predicting choking flow conditions. In turn, the behavior of the HEM within this region provides some indications that supercritical choking flows behave like an ideal gas. Based on this observation and using similar hypotheses introduced by Henry & Fauske [9], a simple polytropic critical mass flux equation is presented. The predictions obtained by using this approach show that for temperatures not too close to the critical one this method gives relatively good results. However, close to the critical value, it is not able to predict the experimental data. In this region, it is apparent that additional physical insights of the flow discharge process as well as more appropriate adjustment of the model are required. Since in this region the flow may undergo internal structure as well as phase changes, further work is still necessary to provide more physical foundation that could help us in obtaining a better correlation of this approach with the data.

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5. References

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