Comparisons of wall heat transfer models implemented in US TRACE and Korean MARS-KS system TH codes

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1. Introduction

System thermal hydraulic system analysis codes are commonly used for nuclear power plant simulation to evaluate the safety. Nearly all current thermal-hydraulic analysis codes adopted two-fluid model instead of homogeneous equilibrium model. Although the twofluid model has the advantage of being more accurate than homogeneous model, conservation equations for two phase contain some variables, such as wall-liquid heat transfer, friction, etc., so constitutive relations have to be included in the code. In addition, the accuracy of the system analysis codes depends on the development of physical models to close the governing equations. Despite this importance of constitutive relation models, accurate and in depth evaluation for constitutive relation models is still limited.

In this study, wall heat transfer models of TRACE version 5.0 patch 4 and MARS-KS version 1.5 are evaluated. TRACE and MARS-KS are very different in the implemented wall heat transfer models and correlations even though the governing equations are almost identical. Thus, it is expected that differences in the code calculations can be observed due to this difference. To compare different physical models and correlations packages of each code, each correlation package is extracted in a separate computational environment. Separate computational environment and methodology for evaluation is referred in the previous paper [1].

2. Wall heat transfer models of two codes

In order to solve energy conservation equations, information on amount of energy transfer from a heat structure to a fluid volume is required. Generally, wall heat transfer module is configured as follows: Firstly, the wall heat transfer (HT) regime is determined based on the thermo-hydraulic conditions. The amount of heat transfers from wall to fluid is evaluated by a correlation which matches the corresponding wall HT regime. Sometimes, if CHF value is required to select the wall HT regime, CHF is also calculated with the correlation. In other words, wall heat transfer modules of TRACE and MARS-KS are consisted of 3 components as shown in Fig 1: (1) wall HT regime selection logic, (2) CHF calculation model, and (3) various heat transfer models & correlations.



Fig1. Composition of wall HT modules.

2.1. Wall HT selection logic

Both codes determine the wall HT regime with the wall HT regime selection logic based on the thermalhydraulic conditions. Each code's selection logics of wall HT regime can be checked in each code's theory manual. In TRACE selection logic, wall temperature is compared with the temperatures at ONB, CHF, MFB and saturation temperature. TRACE has correlations to model temperature of ONB and MFB. TRACE applies Groeneveld's correlation for modeling temperature of MFB with upper and lower limits due to quenching. The implemented correlation is shown in equation (1).

In the similar way, MARS-KS determines wall HT regime with the selection logic. However, in MARS-KS, instead of temperature at ONB, the temperature T_{sat} + 0.001 is applied, because MARS-KS does not have correlations to model temperature for ONB. When distinguishing MFB point, criteria is comparing the heat flux obtained from correlations for transition and film boiling HT regimes as in equation (2). To check if the HT regime is in pre-CHF or post-CHF regime, heat flux criteria as in equation (5) is utilized instead of temperature criteria as in equations (3-4) of TRACE.

$$T_{MFB} = \max\left(\min\left(800, T_{MFB,sat} - \frac{x \cdot 10^4}{(2.82 + 1.22P)}\right), 725\right) (1)$$

$$q_{transition}^* \left((@, T_{MFB}) = q_{film}^* \left((@, T_{MFB})\right) \right) (2)$$

$$T_{w}(@,CHF) = T_{CHF}$$
(3)

$$q''_{CUE} = q''_{medente} \left(T_{CUE} \right) \tag{4}$$

$$q''_{CHE} = q''_{uvaluata} (T_{uv})$$
⁽⁵⁾

To select the wall HT regime, if TRACE or MARS-KS requires CHF information, CHF prediction model is used. To evaluate CHF, TRACE and MARS-KS use Groeneveld CHF look-up table as the default. However, two codes use different version of the table. TRACE uses 1995 version and MARS-KS uses 1986 version.

2.2. Wall heat transfer models of TRACE

In the single phase HT regime, TRACE selects the largest Nusselt number among laminar, turbulent, and natural convection Nusselt numbers. TRACE utilizes Sellars [2] correlation (6) for laminar flow, and Gnielinski [3] correlation (7) for turbulent flow. Generally, Dittus-Boelter correlation is used for turbulent flow, but the reason of using Gnielinski in TRACE is that Dittus-Boelter [4] correlation overpredicts HTC in transition regime between laminar and turbulent flows [5].

N

$$u_{lam} = 4.36$$
 (6)

$$Nu_{turb} = \frac{(f/2)(Re-1000)Pr}{1+12.7(f/2)^{0.5}(Pr^{2/3}-1)} \times \left(\frac{Pr_{l}}{Pr_{w}}\right)^{0.11}$$
(7)

In TRACE, a self-developed model is used for the nucleate boiling HT regime on the basis of additive contributions (8) in Chen [6] correlation. Additive contributions are firstly suggested by Rohsenow [7] in 1952, and then Gambill [8] applied the additive concept with burnout data in 1963. After that, Chen [6] added flow factor and suppression factor, because convective and boiling contributions could be superimposed in the saturated boiling regime without modifications. By using the flow factor, two-phase enhancement is accounted for and suppression of bubble due to convection is reflected in the suppression factor.

TRACE utilizes a newly suggested flow factor and a suppression factor, and applies different models for the forced convection and pool boiling heat transfer terms. Originally, in Chen correlation, the flow factor is a function of Martinelli parameter with flow quality, but the flow factor has oscillation when flow quality is illdefined. For this reason, TRACE uses Rezkallah & Sims [9] liquid-acceleration model (9) for the flow factor, where n is the exponent on the Reynolds number for single-phase heat transfer model. That is, two-phase enhancement effect can be considered by substituting newly defined Reynolds number (10) to a single-phase heat transfer model. For the same reason, the suppression factor is not used in TRACE.

Gorenflo [10] model is adopted for the pool boiling heat transfer term in equation (9). The reason for changing pool boiling model is the tendency to underestimate the heat flux in Chen correlation. More modern nucleate boiling correlation shows the dependency of the boiling heat flux on the wall superheat, where the exponent n is generally agreed to have a value between 3 and 4 [11]. From this reason, TRACE selects Gorenflo correlation (11).

$$h_{\rm NB} = F \cdot h_{\rm FC} + S \cdot h_{\rm PB} \tag{8}$$

$$h_{2\phi}/h_{l} = (1-\alpha)^{-n}$$
 (9)

$$\operatorname{Re}_{2\phi} = \frac{G_{l} \cdot D_{h}}{\mu_{l}} = \frac{(1-\alpha)\rho_{l}v_{l}D_{h}}{\mu_{l}}$$
(10)

$$h_{\rm PB} = \left(\frac{5600F_p}{20000^n}\right)^{1/(1-n)} \left(\left(T_w - T_{sat}\right)^{n/(1-n)} \right)$$
(11)

In transition boiling HT regime, TRACE uses interpolation approach suggested by Bjornard-Griffith [12] as shown in equation (12), where weighting function wf_{TB} is only a function of the wall temperature.

$$q''_{l} = wf_{TB}q''_{CHF} + (1 - wf_{TB})q''_{MFB,l}$$
(12)

$$wf_{TB} = \left(\frac{T_w - T_{MFB}}{T_{CHF} - T_{MFB}}\right)^2 \tag{13}$$

TRACE divides film boiling HT regime into 3 regimes: inverted annular film boiling (IAFB), inverted slug film boiling (ISFB) and dispersed flow film boiling (DFFB) HT regimes. In each regime, wall heat transfer phenomena are simulated differently and heat flux or HTC is evaluated with different models. Fig 2 shows heat transfer paths from wall to liquid or vapor in IAFB and DFFB HT regimes. In the IAFB HT regime, vapor film is near the wall and liquid core is inside the tube. It is assumed that wall heat is transferred to vapor by conduction and to liquid core by radiation. An additional term is included, which considers heat transfer from wall to vapor, from vapor to saturated interface, and finally from interface to liquid phase. To consider conductive and radiation heat transfer, laminar theory and Hannouda's model is applied respectively. In DFFB regime, there is a finely dispersed droplet mixture with the continuous phase being superheated. Major phenomena of wall heat transfer are forced convective heat transfer from wall to superheated vapor and thermal radiation. The forced convective heat transfer is estimated by a similar method as in the single phase HT regime and model for radiation is Sun [13] model. In ISFB regime, HTC or heat flux is determined by interpolating values in IAFB regime and in DFFB regime with respect to void faction.



Fig2. Schematic of heat transfer paths in the film boiling heat transfer regime.

2.3. Wall heat transfer models of MARS-KS

In MARS-KS, the largest Nusselt number is selected for the single phase HT regime as in TRACE, and Sellars [2] correlation (6) is implemented for laminar heat transfer model. Meanwhile, Dittus-Boelter [4] correlation (14) is used to model turbulent heat transfer. Churchill-Chu [14] correlation and McAdams [11] correlation are used for vertical and horizontal natural convective flows, respectively.

$$Nu_{uvb} = 0.023 \,\mathrm{Re}^{0.8} \,\mathrm{Pr}^{0.4} \tag{14}$$

MARS-KS applies Chen [6] model (8), which was developed for the saturated liquid condition. MARS-KS assumes that the wall is fully wet with water and uses Chen model in the subcooled HT regime with a slight modification. Chen selected Dittus-Boelter correlation for the forced convection term in equation (14) and Forster-Zuber [15] model (15) for the pool boiling model with flow factor and suppression factor. In the subcooled nucleate regime, MARS-KS modifies Chen model with suggestion by Bjornard and Griffith: the flow factor is set to unity and the total mass flux is used in Reynolds number, if the regime is in the subcooled nucleate boiling.

$$h_{\rm PB} = 0.00122 \left(\frac{k_l^{0.79} c_{pl}^{0.45} \rho_l^{0.49}}{\sigma^{0.5} \mu_l^{0.29} h_{fg}^{0.24} \rho_v^{0.24}} \right) \Delta T_w^{0.24} \Delta P^{0.75}$$
(15)

In transition boiling HT regime, MARS-KS uses Chen's transition correlation [16], where the factor A_f is depended on void fraction and mass flux in addition to the wall temperature.

$$q"_l = A_f q"_{CHF} \tag{16}$$

$$A_f = \exp\left(-\lambda \left(T_w - T_{sat}\right)^{0.5}\right) \tag{17}$$

$$\lambda = \max\left(C_1 - \frac{C_2 G}{10^5}, \frac{C_3 G}{10^5}\right)$$
(18)

$$C_1 = 2.4C_2$$
 (19)

$$C_2 = \frac{0.05}{1 - \alpha^{40}} + 0.075\alpha \tag{20}$$

$$C_3 = 0.2C_2$$
 (21)

All film boiling HT regimes include the following heat transfer models: conductive heat transfers from wall to vapor film, convective heat transfer from wall to vapor and droplet, and radiative heat transfer from heated wall to liquid core, liquid droplet and vapor. HT correlations of Bromley [17], Dittus-Boelter, and Sun are applied to evaluate conduction, convection, and radiation heat transfer, respectively.

3. Comparison results

Fig 3 shows a boiling curve calculated from separate platforms by setting no mass flux of liquid and vapor, which means pool boiling conditions. (a) and (b) in the figure represent the cases of 10MPa and ambient pressure for system pressure, respectively. More details will be explained later. There are two major causes that both codes calculate heat flux differently: (1) from different selection logic: Both codes select other heat transfer regime in the same thermal hydraulic conditions. (2) from different HT correlations: Both codes select the same HT regime, but use different correlations.



Fig 4 is the comparison of calculated heat flux values when both codes chose identical HT regime. In other words, the figures show deviation of wall heat transfer caused by having different heat transfer correlations in both codes. In Fig 4, HT regime, where the largest deviation between two codes exists, is the transition boiling HT regime which has -0.3637, -0.3667, -0.4237, 0.3416 R-square values. Equation (12) and Equation (16) show the heat transfer correlation in the transition HT regime of TRACE and MARS-KS, respectively. Interpolation approach of TRACE has a function of only the wall temperature, but Chen model of MARS-KS depends on void fraction and mass flux in addition to the wall temperature. The weight functions wf_{TB}, A_f of two codes are plotted with respect to the wall temperature as shown in Fig 5.



Fig4. Calculated wall heat flux in the case of selected same wall HT regimes

The weighting function of TRACE is linearly changing with the wall temperature between CHF and MFB but the weighting function of MARS is discontinuous. This causes major differences in the calculated heat flux in the transition boiling HT regime. An effect of the weighting function is also confirmed in the boiling curve as mentioned before in Fig 3. In the pool boiling curve, the heat flux of TRACE is linearly varying as transition boiling occurs just after CHF but MARS has a point where wall heat flux is abruptly reduced. The reason is that TRACE has linear weighting function with respect to the wall temperature but this is not the case in MARS.



Fig5. Interpolation weighting function with wall temperature in transition boiling HT regime.

Next, heat flux values are compared when MARS-KS and TRACE chose different HT regimes. It can be seen that the selected wall HT regimes are significantly different in both codes. In horizontal flow, 39.06% of total 920 data set is differently selected and in vertical flow, 22.21% is chosen differently for MARS-KS and TRACE. When both codes chose different wall HT regime, how both codes differently predict heat transfer regime can be observed in Fig 6.



The fraction of the case that TRACE predicts transition boiling HT regime while MARS-KS choose film boiling HT regime is highest than other cases. As presented in Fig 6, about 20% of all dataset is included in this case. This comes from that both codes have different logic to distinguish film boiling and transition boiling HT regime. In TRACE, MFB criteria is determined by equation (1), but two heat flux values from film and transition boiling HT correlations are the criteria in MARS-KS. When the TRACE and MARS-SK satisfy the conditions for the MFB point, i.e., equations (1) and (2), the wall temperature is shown in Fig 7. In the case of MARS-KS, the Newton-Raphson method is used to obtain the wall temperature at which two heat fluxes coincide. While the MFB temperature of the TRACE appears in the minimum and maximum limits, MARS-KS has a wide range of temperature for MFB. From this comparison, it is confirmed that the conditions to distinguish transition and film boiling HT regimes are quite different between TRACE and MARS-KS.



Fig7. Evaluated temperature of MFB in TRACE and MARS-KS.

In Fig 6, the second most frequent case is that TRACE selects single phase convection HT regime and MARS-KS chooses nucleate boiling HT regime, respectively. About 7% of the whole data sets are in this case. This is because both codes use different ONB criteria. TRACE uses ONB Basu's model but MARS-KS uses a value of Tsat - 0.001 instead of ONB temperature. Fig 8 shows ONB temperatures of both codes in 15.5MPa and 0.1MPa, respectively. Influence of ONB on the HT regime can be confirmed again in the previously mentioned pool boiling curve, which is plotted in Fig 3. At 10 MPa, the slopes for two codes are almost unchanged with respect to the heat flux until approaching to CHF because in high pressure both codes predict similar ONB temperature. In contrast, at ambient pressure, the slope before CHF does not change in MARS but TRACE has a point where the slope changes. While MARS-KS still predicts the nucleate boiling regime after $T_{wall} = T_{sat} - 0.001$ in ambient pressure, TRACE judges single phase HT regime until the inflection point and considers nucleate boiling regime after the point.



Fig8. Calculated temperature of ONB at 0.1MPa and 15.5MPa in TRACE and MARS-KS.

The third most frequent case is when TRACE and MARS-KS alternate between nucleate and transition boiling HT regimes. The case that TRACE selects film boiling HT regime while MARS-KS predicts nucleate boiling HT regime is 5% of the whole cases, and the opposite case that TRACE selects nucleate boiling HT regime while MARS chooses film boiling HT is 3% in fraction. To analyze the cause, the wall HT regime selection logic for CHF is checked. TRACE and MARS-KS use equation (3) and equation (5) as criteria for CHF, respectively. Since TRACE uses the wall temperature and MARS-KS uses the heat flux to determine CHF point, the two criteria seem to be different. However, T_{CHF} is obtained from condition (4) by using Newton-Rapson method, thus the logic for CHF is the same between TRACE and MARS-KS. It is questionable why TRACE and MARS-KS predict different CHF point even though the calculation logic is same. There are two reasons: (1) both codes refer CHF lookup table of different version (MARS-KS: 1986, TRACE: 1995) or different k-effects are used. (2) Different HT correlations in the nucleate boiling HT regime are implemented in the two codes. To find out which one is more significant cause, CHF values of both codes are calculated. Fig 9 represents CHF values calculated by both codes. When void fraction becomes large, TRACE slightly overestimates CHF values than MARS-KS but CHF values calculated by both codes are almost identical. To compare temperature of T_{CHF}, platform of MARS-KS is added with a function to solve for the CHF temperature by using Newton-Rapson method with condition (4) in the same way as implemented in TRACE. The calculated temperature of CHF is plotted in Fig 10. Unlike CHF values, the temperatures of CHF of both codes do not match with each other when void fraction becomes small. CHF values are similar for both codes, but CHF temperatures of both codes are substantially different. It is because the calculated heat flux values in logic equation (4) are not the same. In short, CHF point becomes different in both codes even though the logic is the same due to the differences in the implemented correlation for the nucleate boiling HT regime. Fig 11 shows the calculated HTC of the nucleate boiling HT regime with respect to various wall temperatures and fluid liquid temperatures. The trends in the figure look similar but the magnitudes of HTC are substantially different. For modeling nucleate heat transfer, correlations of TRACE and MARS-KS include forced convection and boiling heat transfer effects as shown in equation (8). The boiling HTC is more significant term than the forced convection term as different heat flux values are calculated in both codes. As shown in Fig 12, the pool boiling HTC of both codes are largely different similar magnitudes with in total HTC as shown in Fig 11. TRACE uses Gorenflo correlation as shown in equation (11) and MARS-KS uses Forster-Zuber correlation as shown in equation (15) for the pool boiling model. According to Forster-Zuber correlation, the exponent of dT_{wall} is a constant as described in $dT_w^{0.24} dP^{0.75}$, but the exponent of dT_{wall} in Gorenflo correlation is a function of pressure as expressed in $dT_w^{n/(n-1)}$. Fig 13 indicates exponents of dT_{wall} applied in pool boiling correlation by using Claperyon relations. As a result, exponents of TRACE are fairly larger than MARS-KS and moreover the lower pressure leads to more deviation.



Fig9. Calculated CHF in TRACE and MARS-KS.



Fig10. Calculated temperature of CHF in TRACE and MARS-KS.





Fig13. Calculated exponent of T_{wall} in pool boiling model in nucleate HT regime

As a summary, TRACE usually predicts higher ONB and MFB points and lower CHF point than MARS-KS does, which means TRACE judges single phase convection and transition boiling HT regimes to be broader than MARS-KS does.

4. Summary

System thermal hydraulic analysis codes such as TRACE and MARS-KS are developed with different constitutive relation models even though two codes have similar field equations. Thus, it is expected that differences in the code calculations can be observed due to this difference, but implemented constitutive relation models are hard to evaluate separately within the code. The authors suggest a new methodology based on comparison method to evaluate constitutive relations alone and the methodology is applied to evaluate wall heat transfer models of two codes. The suggested method involves setting up a separate computational platform which is constructed by extracting each wall heat transfer model calculation module to a separate computational environment. After successfully setting up the platform, the comparison was performed for the wall heat transfer models. Different heat transfer regimes are occasionally chosen in each code and shows substantial deviation and despite the two codes have different wall heat transfer models, the calculated wall friction values show quite a good agreement except for transition boiling HT regime. In the future work, the same methodology will be applied to other constitutive relations such as interfacial quantities to further identify the effect of constitutive relation on the code calculation results.

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