A Generalized Correlation for Pool Boiling Heat Transfer Coefficient Based on Corresponding State Rule for Pure Compounds and Binary Mixtures

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Abstract: - A generalized correlation for prediction of pool boiling heat transfer coefficient of pure compounds and their binary mixtures is presented. The proposed correlation is based on the corresponding state rule and is applicable to ideal and non-ideal solutions. The effect of phase behavior has been considered and an activity coefficient model has been used to describe the non-ideality of mixture.

The global parameters and system specific parameters for 19 binary systems have been determined and reported. The overall absolute percentage deviation from experimental heat transfer coefficients are 15.31 and 14.50 for pure compounds and their binary mixtures, respectively. The accuracy of the proposed correlation is also compared with other correlations.

Keywords: - Pool boiling, heat transfer coefficient, corresponding state rule, non-ideal solution

1 Introduction

The pool boiling of pure compounds and their binary mixtures is of practical significance for design of heat transfer equipment. Pool boiling has many chemical engineering and heat pump applications. Therefore, there have been many researches for measurement of heat transfer coefficients for pure compounds and binary mixtures as a function of heat flux, temperature, pressure, and compositions [1-4]. There have been also several attempts to develop theoretical or semiempirical models to predict the heat transfer coefficients [1-6].

Modeling and correlation of heat transfer coefficient as function of design variables such as pressure, temperature, composition and heat flux depends strongly on the thermodynamic nature of the system. In other words the vapor-liquid equilibrium plays an important role. The ideal behavior binary mixture such as benzene + toluene is much easier to model than a non-ideal system such as n-propanol + water mixture which may go through azeotrope point. Therefore; the effect of phase behavior should be taken into account.

Due to the importance of pool heat transfer coefficient in the design and simulation of heat transfer equipment, an attempt has been made to develop a generalized heat transfer coefficients based the corresponding state rule. The aim was to develop a correlation to predict the pool heat transfer coefficient for pure compounds, their binary mixtures which may form ideal or non-ideal solution, thermodynamically. In the following sections, the VLE phase behavior calculation is presented, previous work has been reviewed and then the development of the model is discussed and finally the accuracy of the proposed model is studied. The accuracy of the model is compared against other available models.

2 Vapor-Liquid – Equilibrium (VLE)

The VLE phase behavior has a great impact on the mechanism of pool boiling. The driving force for mass transfer from liquid phase to vapor phase is the difference between the equilibrium vapor phase mole fraction, y, and the liquid phase mole fraction, x. Normally, pressure, heat flux, and liquid phase composition are measured. By performing a standard bubble point calculation one can determine, the bubble point temperature and equilibrium vapor phase composition. Figure 1 presents the calculated equilibrium vapor phase mole fraction of its liquid phase mole fraction at several isobars for mixtures of benzene and toluene. For the same system, the calculated bubble temperatures have been plotted as a function of both y and x of benzene and shown in Figure 2.

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Benzen Mole Fraction, x and y Figure 2. T-x-y diagram at constant pressure for benzen-toluene system

Similar plots for binary mixtures of acetone and nbutanol are presented in Figures 3 and 4. At low pressure, this system behaves ideally; however, as the pressure increases, the system deviates from ideal phase behavior and eventually it forms an azeoptropic solution and become non-ideal solution. At azeotropic point, y and x become equal and practically the net mass transfer will become zero. Therefore; care should be taken to consider the effect of VLE phase behavior. The Soave-Redlich-Kwong [7, 8] equation of state and the NRTL [9, 10] activity coefficient model were used to perform these VLE calculations by ASPEN PLUS [11] software.

3 Experimental Data Bank

Through literature survey, 19 sets of experimental heat transfer data on pure and binary mixtures consisting of 586 data points were collected. From these data points, 120 of them are for pure compounds. Table 1 presents the information about these 19 systems used in this study. Some of the literature data were read from graphs since they were not available in tabular form.



Table 1. The summary of data bank used in this work

Mix	Com 1 - Comp 2	Ref	Ν	P, bar	Q, kW/m ²
1	Benzene-Toluene	13	56	0.98 to 9.81	50 to 250
2	i-Propanol – W ater	13	33	1	70 to 200 100 to
3	n-Propanol – Water	4	25	1.01	400
4	Ethanol – Water Methylethylketone-	22	8	1	200
5	Toluene	15	24	1 to 10	100
6	CCl3F - C2Cl3F3	15	66	1.75	16 to 86
7	Methanol - Water	15	76	1	50 to 232
8	i-Propanol - Water	15	30	0.98	50 to 200
9	Acetone - Water	15	26 10	1	50 to 200
10	Acetone - n-Butanol	15	2	0.98 to 9.81	50 to 232
11	Benzene – Toluene	15	18	0.5 to 2	100
12	Acetone - Methanol	15	24	1	50 to 100
13	Methanol - Benzene	15	30	0.98	50 to 200
14	Ethanol – Water	16	11	1.01	232
15	Ethanol – Benzene	16	15	1.01	232
16	Ethanol - Acetone	16	11	1.01	232
17	Water - Ethanol	17	9	1.01	116
18	Methanol - Water	17	11	1.01	116
19	n-Butanol – Ethanol	17	11	1.01	116

4 Previous Work

Mostinski [5] has applied the rule of corresponding states for the calculation of heat transfer to boiling liquids. His correlation was for pure compounds only and presented as:

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$$h = 0.10P_c^{0.69}q^{0.7} \left| 1.8 \left(\frac{P}{P_c}\right) + 4\left(\frac{P}{P_c}\right) + 10\left(\frac{P}{P_c}\right) \right| \left(1\right) \qquad f(y-x) = \frac{\left[1-4\left(y-x\right)\right]\left[1+5\left(y-x\right)\right]}{1+12\left(y-x\right)^2} \qquad (9)$$

He reported the accuracy of this expression within ± 30 % and is valid for heat flux, $q_{,} \leq$ critical heat flux, q_{c} . This equation was applied to the pure compounds consisting of 120 data points and the average absolute percent deviation (AAPD) was 16.26 %. Attempt to extend this correlation to binary mixtures, was not successful.

Based on Stephan and Körner [12] suggestion, an empirical correlation of the following form was developed.

$$\Delta T = \left[x \Delta T_1 + (1 - x) \Delta T_2 \right] \left[1 + A(y - x) \right]$$
⁽²⁾

in which A is an empirical constant different for every binary mixture and (y-x) is the mass transfer driving force. Then the heat transfer coefficient is calculated by $h = q / \Delta T$ (3)

Other form of Eq 2 has been reported [6].

$$\Delta T = \left[x \Delta T_1 + (1 - x) \Delta T_2 \right] \left[1 + A \left| y - x \right| \left(0.88 + 0.12x 10^{-5} P \right) \right]$$
(5)

Calus and Leonidopolous [4] modified Eq 5 for npropanol-water mixture and presented the following equation.

$$\Delta T = \left[x \Delta T_1 + (1 - x) \Delta T_2 \right] \left[1 + (x - y) \left(\frac{\alpha}{D} \right)^{0.5} \left(\frac{C_L}{h_{fg}} \right) \left(\frac{dT}{dx} \right) \right]$$
(6)

This correlation has no empirical constants but the knowledge of boiling curves for the two pure liquids, obtained on the same heat transfer surface, are necessary. The largest deviation of the predicted coefficients from the experimental values was 16.6% [4].

Since the subject being dealt with is too complex to tackle analytically, Ünal [6] used dimensional analysis to incorporate the effect of pressure and mass deriving force and suggest the following correlation.

$$\Delta T = \left[x \Delta T_1 + (1 - x) \Delta T_2 \right] \left[1 + (b_1 + b_2)(1 + b_3) \right] \left[1 + b_4 \right]$$
(7)

Using experimental data, Ünal presented expressions for b₁ through b₄ as a function of pressure, vapor and liquid phase mole fractions. All together a minimum of 8 constants in addition to ΔT_1 and ΔT_2 are required. The RMS error of 13 binary mixtures consisting of 388 points was 14.8% [6]. Equation 7 predicts the heat transfer coefficients from the data accurate to 30% for 97% of the time. The rest of the time, this equation is accurate to 38.8%.

5 Development of Model

Due to the complexity of the binary mixtures pool boiling and in line with Mostinski [5] correlation based the corresponding state rule and using dimensional analysis, we propose the following correlation for pool boiling heat transfer coefficients.

$$h = \frac{f(y-x)f(Pr)f(q)}{f(Tr)}$$
(8)

where f(y-x) represents the mass transfer driving force and is defined by:

$$f(Pr) = C_1 P r^{C_2} + C_3 P r^{C_4}$$
(10)

$$f(q) = q^{\lfloor C_s + C_6(y-x)^2 \rfloor}$$
(11)

which will reduce to q^{C_5} for pure compounds. The last term is the temperature effect which is defined by:

$$f(Tr) = C_7 T r^{C_8} + C_9 T r^{C_{10}}$$
(12)

In the above equations, Pr and Tr are the reduced temperature and pressure, respectively. They are calculated using conventional linear mixing rule (Kay's rule) as follows:

$$Pr = \frac{P}{xPc_1 + (1-x)Pc_2}$$
(13)

and

$$Tr = \frac{T}{xTc_1 + (1 - x)Tc_2}$$
(14)

where T is the bubble point temperature of the mixture at system pressure and calculated with the aid of an equation of state and activity coefficient model.

In order to determine the correlation parameters C_1 through C_{10} an objective function was defined.

$$Objective \ Function = \sum_{i=1}^{N} \left[\frac{Experimental \ h - Calculated \ h}{Experimental \ h} \right]_{i}^{2} \quad (15)$$

A nonlinear regression software was used to determine the correlation parameters by minimizing this objective function. Overall, 586 data points for pure compounds and their mixtures shown in Table 1 were used in this study. The global parameters obtained are presented in Table 2. The correlation parameters were also determined for each binary system independently and are reported in Table 2. For each case, the average absolute percent deviation was calculated and reported in the last row of Table 2.

6 Results and Discussion

Using the proposed correlation and the global parameters reported in Table 2, the pool boiling heat transfer coefficients for 586 data points consisted of pure compounds and their mixtures were predicted and compared with the corresponding experimental values. This comparison is shown graphically in Figure 5 and the majority of predictions fall within $\pm 30\%$ of experimental values. The overall average absolute percentage error for all points was 14.5%. Figure 6 presents the error percent of each predicted heat transfer coefficients for all 19 binary systems. As can be seen from this figure, the majority of error falls within the $\pm 30\%$ boundaries and only a few points are outside of these ranges. Some of the large deviation may be attributed to inherent experimental error.

С	Global	Benzene Toluene	i-Propanol Water	n-Propanol Water	Ethanol Water	Methylethylketon e Toluene	CCI3F C2CI3F3
1	1.70E-09	8.8990E-13	1.1875E-06	2.9141E-10	6.9051E-08	1.6442E-11	3.3328E-10
2	0.0380	0.8965	2.2729	-1.2641	1.4151	-1.0987	-6.2823
3	1.20E-14	2.7404E-15	7.2837E-13	-6.5222E-13	2.9786E-13	4.0373E-12	-2.7394E-13
4	-2.2600	-0.4516	-1.4334	10.1951	-1.5546	50.0000	50.0000
5	0.7260	0.7086	0.7900	0.7445	0.8747	0.3265	0.6871
6	0.3650	0.0752	0.3128	0.6848	0.4133	0.6267	0.9053
7	5.70E-10	2.2131E-13	6.9673E-11	2.0732E-09	8.7788E-11	2.6432E-14	2.1552E-09
8	-2.1200	3.8033	-5.2876	-8.3025	-6.8096	-13.5866	-43.9571
9	132.0000	-200.0000	132.0000	132.0000	132.0000	-200.0000	132.0000
10	189.4000	200.0000	189.4000	189.4000	189.4000	200.0000	189.4000
AAPD	14.50	13.79	19.50	14.51	15.41	11.29	4.08
APD	-3.15	11.28	-19.39	-5.31	-15.41	-7.23	-1.44
APD ^a		-0.38	-0.68	-0.96	0.23	-0.75	-0.20
AAPD ^a		4.48	6.43	8.16	3.95	6.92	3.55

Table 2. The global and system specific correlation parameters

Table 2. (Continued)

С	Methanol Water	i-Propanol Water	Acetone Water	Acetone n-Butanol	Benzene Toluene	Acetone Methanol	Methanol Benzene
1	1.4417E-06	2.9472E-09	2.1395E-07	1.6022E-09	1.0000E+02	-3.5849E-11	2.1778E-07
2	5.4997	0.7523	0.9042	0.0870	12.2985	50.0000	2.1850
3	4.4459E-14	0.0000E+00	0.0000E+00	0.0000E+00	9.4571E-14	1.8133E-13	0.0000E+00
4	1.9382	0.0000	0.0000	0.0000	0.3979	-1.9045	0.0000
5	0.8048	0.7437	0.6443	0.7454	1.1295	0.7522	0.5131
6	-0.1036	0.3606	0.2020	0.3568	0.4957	0.5321	0.2120
7	2.8013E-11	1.3494E-09	1.3761E-08	6.1348E-10	5.2411E-12	8.5178E-11	1.8376E-09
8	30.0752	5.8010	6.0899	-1.6385	2.4715	-4.8350	13.0415
9	132.0000	132.0000	132.0000	0.0351	132.0000	132.0000	132.0000
10	189.4000	189.4000	189.4000	129.4980	189.4000	189.4000	189.4000
AAPD	18.14	15.95	21.01	8.83	19.49	19.55	14.63
APD	-5.04	15.95	-17.6	-3.91	-19.43	-19.55	1.20
APD ^a	-3.69	-0.34	-0.39	-0.93	-0.41	-0.04	-0.52
AAPD ^a	14.71	4.63	5.00	7.52	3.91	1.45	5.83
$44PD = \frac{10}{2}$	$0 \sum_{k=1}^{N} \left(Experimental h - Calculated h \right) and APD = \frac{100}{N} \sum_{k=1}^{N} \left(Experimental h - Calculated h \right)$)	
$I = \frac{1}{N}$	$V = \frac{1}{i=1}$	Experimenal h	\int_{i}	$D = N \sum_{i=1}^{n} ($	Experime	malh),

a Using system specific parameters





The accuracy of system specific parameters and global parameters is compared in Figure 7 for CCl₃F – C₂Cl₃F₃ mixture which exhibits an ideal solution behavior. Both sets of parameters display very good accuracy for this particular system. Similar trends were observed for other ideal solution system. Figure 8 presents the accuracy of the proposed correlation for prediction of n-propanol-water system against Calus and Leonidopolous model [4] with an AAPD of 10.38% and Stephan and Korner [12] correlation with AAPD=30.64%. As can be seen from this figure, for the proposed model with mixture data only (the same condition as the other two model), the AAPD is 7.56% but with all points including the pure compound data, the AAPD is 8.43%. Using all of the points for this binary system and global parameters, the AAPD is 14.51%. It should be noted that the n-propanol- water exhibits non-ideal solution behavior.

The same set of global parameters was used to predict the heat transfer coefficients of 120 points of pure compounds only and the overall absolute percent deviation was 15.31. Using Mostinski [5] correlation for the same 120 points, the overall absolute percent deviation was 16.26. Even though the proposed correlation was developed for binary mixtures, it is more accurate than the generalized Mostinski correlation of the same type.



20 10 0 % -10 Error -20 -30 -40 -50 -60 0 0.2 0.4 0.6 0.8 Mole fraction of n-propanol Figure 8. Comparison of the proposed heat transfer coefficients correlation accuracy with others for n-propanol+water system, experimental data [4]

7 Conclusions

The proposed generalized correlation for pool boiling heat transfer coefficient handles both ideal solutions and non-ideal solutions with good accuracy. Its global parameters and system specific parameters have been determined and reported for 19 binary mixtures. The correlation is robust and can handle pure compounds and their binary mixtures with the same set of global parameters. The accuracy of the proposed correlation for pure compounds is better than Mostinski correlation. The proposed model is relatively simple and does not require transport properties such as thermal diffusivity, mass diffusivity, heat of vaporization and etc. The only required parameters are the liquid phase composition, heat flux and pressure. The bubble point temperature and the equilibrium vapor phase composition are calculated by standard VLE calculations using an equation of state and an activity coefficient model.

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- A System specific parameters in Eq. 2
- bi Correlation parameters in Eq. 7, i=1 to 4
- C_i Coefficients in the proposed model, i=1 to 10
- C_L Liquid phase specific heat, J/kg-K
- D Mass diffusivity
- h Heat transfer coefficient, W/m²-h-K
- hfg Heat of vaporization, J/kg
- N Number of data points
- P Pressure, bar
- Pc Critical pressure, bar
- Pr Reduced pressure
- Q Heat flux, W/m^2 -K
- T Bubble point temperature, K
- Tc Critical temperature, K
- Tr Reduced temperature
- x Liquid phase mole fraction of component 1
- y Vapor phase mole fraction of component 1 in equilibrium with x.
- ΔT Apparent temperature difference
- ΔT_1 Apparent temperature difference for component 1
- ΔT_2 Apparent temperature difference for component 2

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