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A simple model for temperature-independent k_{ij} of the PR-vdW model for mixtures containing HCs, HFCs, PFCs, HFOs, CO_2, RE170 and R13I1

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ABSTRACT

The purpose of this paper is to establish a simple model for temperature-independent binary interaction parameter k_{ij} of the PR-vdW model (Peng-Robinson equation of state with van der Waals one-parameter mixing rules). The model was proposed as $k_{ij} = w_j k_i + w_i k_j$ $(i \neq j)$. In the present model, every pure component was considered to have a constant contribution k_i to k_{ij}, constant w_i is the contribution coefficient of component j mixing with component i. k_{ij} can be determined by summing the contribution coefficient of each pure component times its contribution. By regressing the vapor-liquid equilibrium (VLE) data of binary mixtures, 119 k_{ij} were obtained and used to optimize the constant contribution k_i and contribution coefficient w_i. k_{ij} of 351 binary systems were predicted and used to describe the VLE data of binary and ternary mixtures. Better performs could be found in the present model than the available models on VLE description of the mixtures.

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1. Introduction

Traditional chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs) have already been or will be replaced by refrigerants with zero ODP and low GWP values such as hydrocarbons (HCs), hydrofluoroolefins (HFOs), a part of hydrofluorocarbons (HFCs) and so on [1]. Owing to the better performance, mixed refrigerants especially the azeotropic mixtures are considered to be much promising alternative refrigerants [2–13]. Vapor-liquid equilibrium (VLE) data are essential to get the thermodynamic properties of refrigerant mixture, and can be used to evaluate the performance in a refrigeration cycle indirectly. Many experimental VLE studies are available in the open literature. Although experiments can provide accurate data, they are time consuming and expensive. Thus, reasonable predictions for the VLE properties of mixtures are of great importance.

The SRK [14] and PR [15] cubic equations of state (EOS) with the vdW [16], WS [17] and HV [18,19] mixing rules (MR) are usually employed to predict the VLE data of mixtures. Hu et al. [20] pointed out that the mixing rules for the parameters in cubic equations of state are difficult to be applied in a predictive model. But if the binary interaction parameters in cubic equations of state with mixing rules could be predicted, it would be much convenient for the calculation of VLE behaviors by using equation of state directly. A number of models for k_{ij} are available in the open literature. They can be classified into three groups: empirical or semi-empirical model (group 1), theoretical model (group 2), and group contribution model (group 3). In group 1, Chen et al. [21] developed a k_{ij} differential-model (ODM) in PR-vdW model for HFCs + HCs mixtures, in this model each pure component was assumed to have a mixing factor k_i, and the k_{ij} was simply assumed to be the difference between the two mixing factors of the pure components $k_{ij} = k_i - k_j$ $(i < j)$. Hu et al. [20] developed a modified differential-model (MDM) by introduced a weight coefficient. However, the above two models do not have a symmetrical structure in mathematics $k_{ji} = k_{ij}$, which is the request of the vdW one-parameter MR. Thus the calculation of k_{ij} must be in a certain sequence like $i < j$ to meet the symmetrical requirement, that is not convenient. Besides, the choice of the form of weight coefficient in MDM was not

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Nomenclature

Abbreviations

AAD	average absolute deviation
AARD	average absolute relative deviation
Ar	argon
CFCs	chlorofluorocarbons
CH_4	methane
C_6H_6	benzene
C_7H_8	toluene
C_8H_{10}	m-xylene
CO	carbon monoxide
CO_2	carbon dioxide
EOS	equations of state
E-PPR78	enhanced predictive Peng–Robinson EOS, 1978
GCM	group contribution method
GWP	global warming potential
H_2	hydrogen
H_2O	water
H_2S	hydrogen sulfide
HCs	hydrocarbons
HCFCs	hydrochlorofluorocarbons
He	helium-4
HFCs	hydrofluorocarbons
HFOs	hydrofluoroolefins
HV	Huron-Vidal
MAD	maximum absolute deviation
MDM	modified differential-model
MHV1	Michelsen-Huron-Vidal
MR	mixing rules
N_2	nitrogen
NO	nitric oxide
NRTL	non-random two-liquid
O_2	oxygen
ODM	original differential-model
ODP	ozone depletion potential
O.F	objective function
PFCs	perfluorocarbon
PR	Peng-Robinson
PPR78	predictive Peng-Robinson EOS, 1978
R13I1	trifluoroiodomethane
R14	tetrafluoromethane
R23	trifluoromethane
R32	difluoromethane
R50	methane
R116	hexafluoroethane
R125	pentafluoroethane
R134	1,1,2,2-tetrafluoroethane
R134a	1,1,1,2-tetrafluoroethane
R143a	1,1,1-trifluoroethane
R152a	1,1-difluoroethane
R227ea	1,1,1,2,3,3,3-heptafluoropropane
R236ea	1,1,1,2,3,3-hexafluoropropane
R236fa	1,1,1,3,3,3-hexafluoropropane
R245fa	1,1,1,3,3-pentafluoropropane
R290	propane
R600	*n*-butane
R600a	isobutane
R610	decafluorobutane
R1150	ethene
R1216	hexafluoropropene
R1234yf	2,3,3,3-tetrafluoroprop-1-ene
R1234ze(E)	trans-1,3,3,3-tetrafluoropropene
R1270	propene
RE170	dimethylether
SO_2	sulfur dioxide
SPM	“simple plus model”
SRK	Soave-Redlich-Kwong
T-p-x-y	temperature-pressure-liquid mole fraction-vapor mole fraction
vdW	van der Waals
VLE	vapor-liquid equilibrium
WS	Wong-Sandler

Symbols

a	energy parameter, $J \cdot cm^3 \cdot mol^{-2}$
b	covolume, $cm^3 \cdot mol^{-1}$
k_i	constant contribution of component i to k_{ij}
k_{ij}	binary interaction parameter
l	parameter
m	number of k_{ij} in the database
n	number of pure component in the database
n_{var}	number of variables, $n_{\mathrm{var}} = 2n$
N	number of experimental VLE data of each binary system
p	pressure, MPa
p_{c}	critical pressure, MPa
R	universal gas constant, 8.314472 $J \cdot mol^{-1} \cdot K^{-1}$
T	temperature, K
T_{c}	critical temperature, K
T_{nb}	normal point temperature, K
T_{r}	reduced temperature
w_i	contribution coefficient of component j mixing with component i
x	liquid mole fraction
y	vapor mole fraction

Greek letters

α	alpha function
ω	acentric factor

Subscripts

c	critical characteristic
cal	calculated data
cor	correlated value
exp	experimental data
i	component or experimental data index
j	component index
l	binary interaction parameter index
m	mixture
opt	optimal solution
pre	predicted value

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