Purdue University
Purdue e-Pubs

International Refrigeration and Air Conditioning
Conference

School of Mechanical Engineering

2014

Vapor-liquid equilibrium properties of binary mixture refrigerants (R1234ZE+R290, R290+R227ea)

Yingxia Qi
University of Shanghai for Science and Technology, China, People's Republic of, qipeggy@126.com

Hua Zhang
University of Shanghai for Science and Technology, China, People's Republic of, zhanghua3000@163.com

Wei Zhao
University of Shanghai for Science and Technology, China, People's Republic of, zw_cherry@163.com

Yefeng Liu
University of Shanghai for Science and Technology, China, People's Republic of, yfliu209@163.com

Xunhai Liu
University of Shanghai for Science and Technology, China, People's Republic of, brownliu2004@163.com

Follow this and additional works at: http://docs.lib.purdue.edu/iracc

Prediction of Gas-liquid Equilibrium Properties of two Binary Refrigerants (R1234ze(E)+R290, R290+R227ea) with COSMO-RS Model

Yingxia QI*, Hua ZHANG, Wei ZHAO, Yefeng LIU, Xunhai LIU

College of Energy and Power Engineering, University of Shanghai for Science and Technology
Shanghai, 200093, China

E-mail: qipeggy@126.com
* Corresponding Author

ABSTRACT

The gas-liquid equilibrium data is an important part of thermophysical properties of a new refrigerant. Theoretical predictions and experimental measurements of gas-liquid equilibrium data of a new mixed working fluid become to be an urgent need for the researches on alternative refrigerants. The gas-liquid equilibrium curves of binary mixtures (R1234ze(E)+R290, R290+R227ea) were simulated by COSMO-RS model which are based on quantum chemistry. The simulation results could accord with the experimental data well. It was concluded that COSMO-RS simulation method is feasible to predict the gas-liquid equilibrium properties of mixed refrigerants.

Keywords: gas-liquid equilibrium; quantum chemistry; COSMO-RS; R1234ze+R290; R290+R227ea

1. INTRODUCTION

The use of the chlorofluorocarbon (CFC) and hydrochlorofluorocarbon (HCFC) refrigerants has been prohibited with the implementation of the Montreal protocol because of their high ozone depletion potential (ODP) values and its amendments because of global environmental concerns (Creazzo, 1993, Zipfel, 1999). Searching for the high efficient and environment friendly alternative refrigerants becomes one of the most important tasks for the refrigeration industry. Several hydrofluorocarbons (HFCs), hydrofluoroethers (HFEs) and hydrocarbons (HCs) have been considered as promising alternatives due to their zero ozone depletion potentials and low global warming potentials. Unfortunately, only a few existing pure fluids can ensure performances equal or at least comparable to those of the banned substances. Thus, the main search for substitute refrigerants nowadays is devoted to mixtures. Vapor–liquid equilibrium (VLE) data for such mixtures are required as fundamental data for evaluating the performance of refrigeration cycles and determining optimal compositions (Valtz, 2004, Hou, 2005). However, the number of potentially useful mixtures is huge, and it would be extremely uneconomic, if not even inconceivable, to evaluate experimentally the thermodynamic properties of all possible alternatives. Theoretical and computational models can be valuable tools for the estimation of the thermodynamic properties of such mixtures, thus reducing time, resources and overall cost in the selection of the correct fluids.

Since its first publication in 1995, the quantum chemically based Conductor-like Screening Model for Realistic Solvation (COSMO-RS) (Klamt, 1995, 1998, 2000, 2004, 2007, Eckert, 2002, 2003, Milocco, 2002, Hsieh, 2010) has developed to a widely accepted and independent novel approach to the simulation of fluid phase equilibria. It

starts directly from quantum chemical calculations for the individual molecules and expresses the intermolecular interactions based on this quantum chemical information. The combination of this relatively fundamental description of intermolecular interactions with a fast and accurate statistical thermodynamics of interacting surfaces led to an efficient and broadly applicable new approach to the prediction of the thermodynamic properties of liquid mixtures. R1234ze(E) and R290 are good components with zero ODP and very low global warming potential (GWP) values. Their mixtures are friendly to the environment (Valtz, 2002, Dong, 2011). This article is trying to simulate the gas-liquid equilibrium properties of new mixed refrigerants (R1234ze(E)+R290) and (R290+R227ea) with COSMO-RS model.

2. COSMO-RS PRINCIPLE

2.1 COSMO-RS concept

COSMO (conductor-like screening model) is a continuum solvation model(Klamt, 1993), in the which the dielectric constant is set to infinite (ideal), and the screening charges are limited on the interface, thus there is no electric field among molecules and solvent, and no charges in the conductors. On the basis of COSMO, combining the method of statistical thermodynamics, Klamt developed COSMO-RS (real solvents) (Klamt, 1995) for quantitative calculation solvation phenomenon which predicts the properties of phase equilibrium of multi-component system. Since the full description of the COSMO-RS theory is beyond the scope this article and has been given in several recent articles (Klamt, 1998, 2000), we restrict ourselves to a short introduction of the basic features required for the understanding this article.

2.2 COSMO-RS simulation steps

COSMO-RS is a two step procedure. In a first step, quantum chemical calculations were performed for all components of interest. In these calculations, the continuum solvation model COSMO was applied in order to simulate a virtual conductor environment for the molecule. In this environment, the solute molecule induces a polarization charge density on the interface of the molecule to the conductor, i.e. on the molecular surface, and these charges act back to the solute, generating a more polarized electron density than in vacuum. During the quantum chemical self-consistency algorithm, the solute molecule is thus converged to its energetically optimal state in a conductor with respect to electron density and geometry. The standard quantum chemical method for COSMO-RS is density functional theory (DFT) and the DFT functional B88-PW86 with a triple zeta valence polarized basis set (TZVP) was used throughout this study. All DFT/COSMO calculations have been performed using the quantum chemical program ADF program package (ADF, 2012). The molecules considered in this contest were relatively small. Hence none of the calculations for the four molecules took longer than 5 min on a single 800MHz CPU.

The polarization charge density σ is a good local descriptor of the molecular surface polarity. In the second step of COSMO-RS, the statistical thermodynamics of the molecular interactions, this polarization charge density is used for the quantification of the interaction energy of pair-wise interacting surface segments with regard to the most important molecular interaction modes, i.e. electrostatics and hydrogen bonding. The less specific van der Waals (vdW) interactions or dispersive interactions are taken into account in a more approximate way by element specific dispersion coefficients.

All COSMO-RS calculations of this paper are performed using the ADF program package [ADF, 2012], which

provides an efficient and flexible implementation of the COSMO-RS method. The total CPU time spent for each calculation took only about 2 min on a 900MHz laptop computer. The ADF default parameterization of (Pye, 2009) was used. Detailed values of the parameterization used are given there.

2.3 The gas-liquid equilibrium of the binary system

The total pressure P^{total} was calculated by the following equation (1):

$$P^{total} = x_1\gamma_1 P_1^{sat} + x_2\gamma_2 P_2^{sat} \tag{1}$$

Here, P^{total} means the total pressure of the system, P_1^{sat}, P_2^{sat} means the saturated vapor pressure, x_1, x_2 the mole fraction, γ_1, γ_2 the activity coefficient of pure component 1 and component 2, respectively, which is calculated with COSMO-RS model.

The vapor mole fraction y_1 was calculated by the following equation (2).

$$y_1 = \frac{x_1\gamma_1 P_1^{sat}}{x_1\gamma_1 P_1^{sat} + x_2\gamma_2 P_2^{sat}} \tag{2}$$

3. SIMULATION RESULTS

3.1 Gas-liquid equilibrium R1234ze(E)+R290

R1234ze, also named as HFO-1234ze or 1,1,1,3-terafluoropropene(R1234), has a molecular formula of CF3CH=CHF. Its molecular weight is 114 and boiling point is 9℃ with ODP=0 and GWP=6. It is non-toxic and non-flammable. Its atmospheric residence time is short and chemical property is stable. It's an important hydrofluoroolefins (abbreviation HFOs). R290, also named propane or C3H8, has a molecular weight of 44.9. Its boiling point is -42.2℃ with ODP=0 and GWP=0.01. It is used to be substitution for R22 and R502.

An attempt was done to obtain complementary advantages by mixing of the two refrigerants. The gas-liquid equilibria of (R1234ze+R290) mixtures at fixed temperatures (258.15K, 263.15K, 273.15K, 283.15K) were simulated using COSMO-RS model. The simulation results were shown in table 1. For comparisons, the experimental results from (Dong, 2011) were also shown in table 1. From table 1, it was known that the maximum relative errors of the liquid phase compositions x_1 and the gas phase pressures P between the calculations and experiments were 3.94% and 9.60%, respectively. To see visually, the gas-liquid equilibrium curves made according to table 1 were shown in figure 1. From figure 1, it could be seen that there was a good consistency between the calculated and experimental results (Dong, 2011). The relative errors of the gas pressures collected in table 1 were graphically presented in figure 2, too. From figure 2, it was known readily that the deviations of the gas pressures were distributed uniformly except the points around $x_1 = 0.9$. From figure 1, the azeotropic points were determined. They were shown in the table 2 and figure 3. The relative errors of the mole fractions x_1 between the calculations and the experiments were – 5.07% to -7.19%, while the relative errors of the gas pressures were 0.39% to 0.53%. So it was reasonable to predict the gas-liquid equilibrium data of refrigerant mixtures using COSMO-RS method.

Table 1. Gas-liquid equilibrium data of the (R1234ze+R290) mixtures
at temperatures (258.15K, 263.15K, 273.15K, 283.15K).

x_1	P^e(Mpa)	P^s(Mpa)	$\delta(P)$	y_1^e	y_1^s	$\delta(y_1)$
			258.15K			
0	0.2916	0.29162	0.01%	0	0	
0.122	0.3021	0.303032	0.31%	0.131	0.1295	-1.15%
0.203	0.3016	0.302138	0.18%	0.181	0.17281	-4.52%
0.387	0.2918	0.292808	0.35%	0.251	0.23029	-8.25%
0.465	0.2846	0.28607	0.52%	0.279	0.25383	-9.02%
0.622	0.2632	0.263491	0.11%	0.346	0.31799	-8.10%
0.683	0.2525	0.24982	-1.06%	0.378	0.35534	-5.99%
0.786	0.2249	0.221887	-1.34%	0.46	0.43813	-4.75%
0.901	0.181	0.173866	-3.94%	0.619	0.62669	1.24%
1	0.1194	0.12	0.50%	1	1	0.00%
			263.15K			
0	0.3453	0.34528	-0.01%	0	0	
0.12	0.3576	0.35903	0.40%	0.131	0.13086	-0.11%
0.203	0.3574	0.3582	0.22%	0.183	0.17578	-3.95%
0.388	0.3458	0.347291	0.43%	0.257	0.23644	-8.00%
0.463	0.3374	0.339101	0.50%	0.287	0.26192	-8.74%
0.627	0.3111	0.311287	0.06%	0.357	0.33188	-7.04%
0.685	0.2983	0.296927	-0.46%	0.394	0.36661	-6.95%
0.785	0.267	0.264579	-0.91%	0.476	0.4503	-5.40%
0.902	0.2153	0.209232	-2.82%	0.639	0.63939	0.06%
1	0.1464	0.14736	0.66%	1	1	0
			273.15K			
0	0.4745	0.47446	-0.01%	0	0	
0.12	0.4915	0.493875	0.48%	0.131	0.13321	1.69%
0.203	0.4918	0.493324	0.31%	0.187	0.18117	-3.12%
0.39	0.4762	0.477785	0.33%	0.27	0.25089	-7.08%
0.463	0.4648	0.467891	0.67%	0.292	0.27551	-5.65%
0.626	0.4267	0.430579	0.91%	0.388	0.35074	-9.60%
0.685	0.4099	0.411234	0.33%	0.424	0.38785	-8.53%
0.784	0.3697	0.368697	-0.27%	0.505	0.47487	-5.97%
0.904	0.3	0.295863	-1.38%	0.678	0.66481	-1.95%
1	0.2154	0.2164	0.46%	1	1	0.00%
			283.15K			
0	0.6367	0.6366	-0.02%	0	0	
0.121	0.6598	0.663113	0.50%	0.132	0.13514	2.38%
0.205	0.6601	0.663118	0.46%	0.191	0.18487	-3.21%
0.388	0.6404	0.64421	0.59%	0.281	0.25706	-8.52%

0.629	0.5735	0.580651	1.25%	0.412	0.36948	-10.32%
0.782	0.4995	0.502633	0.63%	0.534	0.49478	-7.34%
0.909	0.4097	0.403716	-1.46%	0.705	0.6976	-1.05%
1	0.307	0.30833	0.43%	1	1	0.00%

Superscript e: experimental; s: simulation. δ: relative error; $\delta(y_1) = (y_1^s - y_1^e)/y_1^e(\%)$; $\delta(P) = (P^s - P^e)/P^e(\%)$. x_1: liquid phase composition; y_1: gas phase composition.
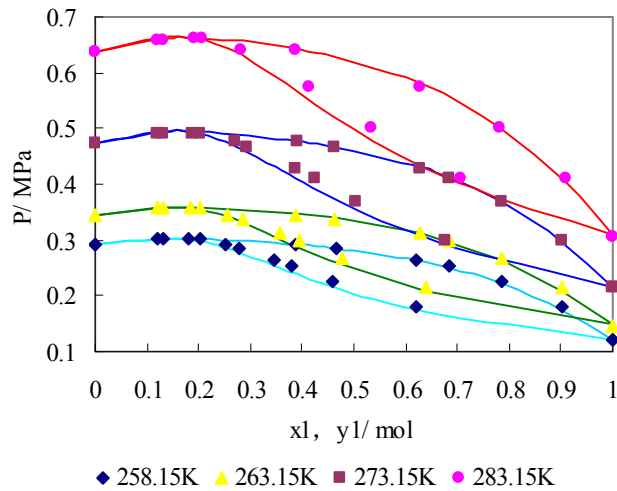

Figure 1. Gas-liquid equilibrium curves of the (R1234ze+R290) mixtures. The solid lines: calculations; the dots: experiments (Dong , 2011).
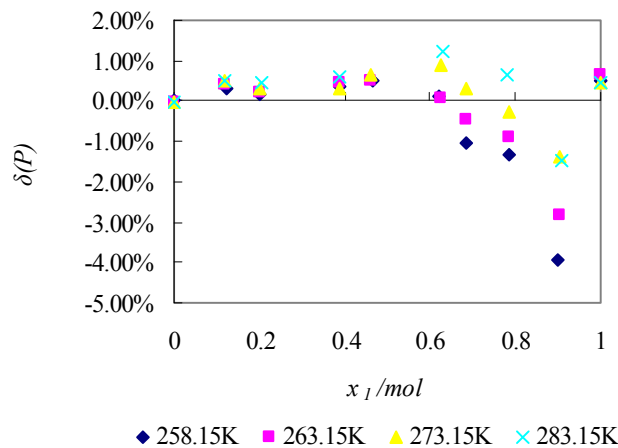

Figure 2. The relative errors of the gas pressures between the calculated and the experimental results for the (R1234ze+R290) mixtures.

Table 2. The azeotropic compositions (x_1) and gas pressures (P) at temperatures (258.15K, 263.15K, 273.15K, 283.15K) for the (R1234ze+R290) mixtures.

T(K)	x_1^e(mol)	x_1^s(mol)	$\delta(x_1)$	P^e(MPa)	P^s(MPa)	$\delta(P)$
258.15	0.153	0.142	-7.19%	0.302	0.30317	0.39%

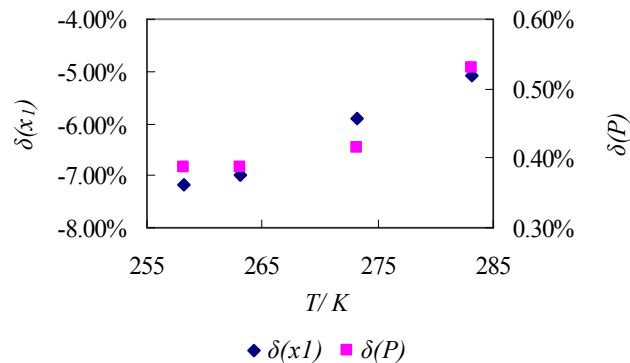| 263.15 | 0.157 | 0.146 | -7.01% | 0.3579 | 0.35928 | 0.39% |
| 273.15 | 0.164 | 0.15429 | -5.92% | 0.4924 | 0.494437 | 0.41% |
| 283.15 | 0.17 | 0.16138 | -5.07% | 0.6607 | 0.664207 | 0.53% |

Figure 3. The relative errors of the azeotropic composition (x_1)and gas pressure (P) between the calculated and experimental results for the (R1234ze+R290) mixtures.

3.2 Gas-liquid equilibrium of R290+R227ea

HFO-227ea, 1, 1, 1, 2, 3, 3, - heptafluoropropane is a kind of new substitute proposed recently internationally which doesn't destroy the ozone layer. It has been treated as a fire extinguishing instead of halon and it is regarded as a promising alternative refrigerants, especially used as an alternative component of mixtures in R502 and R22. R290, propane C_3H_8 is a kind of environment-friendly refrigerant and can be used to replace R22, R114.

An attempt was done on the mixing of the two refrigerants to have complementary advantages. The gas-liquid equilibrium of the mixture (R290+R227ea) at fixed temperatures (293.16 K, 303.15 K, 313.14 K, 333.15 K, 343.16 K, 353.188 K) was simulated using COSMO-RS model. The simulation results were shown in table 3 and in figure 4. At the same time, the experimental results from (Valtz, 2002) were also shown in table 3 and figure 4. The relative errors of the total pressure between the experimental and calculated were shown in figure 5, too. From table 3, it was known that the maximum relative error of the total pressure was 4.33%. From figure 4, it could be seen that there was a good consistency between the calculated and experimental results (Valtz, 2002), and the consistency was better in the lower temperature region. In figure 5, the distribution of the relative errors of the pressure was shown. It can be seen that the maximum errors occurred around x_1=0.2 mole fraction.

From figure 4, the azeotropic points were determined. They were shown in the table 4, and the relative errors of the mole fractions and the pressures calculated compared to the experimental results were shown in figure 6. The relative errors of the mole fractions were 2.10% to 3.22%, while the relative errors of the pressures were -0.05% to -0.46%. So it could be said that the predicting of the gas-liquid equilibrium data of refrigerant mixtures using COSMO-RS method was reasonable.

Table 3. Gas-liquid equilibrium data of the (R290+R227ea) mixtures
at temperatures (293.16 K, 303.15 K, 313.14 K, 333.15 K, 343.16 K, 353.188 K)

293.16K						
x_1	P^e(MPa)	P^s(MPa)	$\delta(P)$	y_1^e	y_1^s	$\delta(y_1)$
0.0000	0.38921	0.38921	0.00%	0.0000	0.0000	

0.0388	0.4515	0.4505	-0.22%	0.1612	0.1928	19.60%
0.1442	0.5948	0.5919	-0.49%	0.4111	0.4645	12.99%
0.2515	0.7019	0.6974	-0.64%	0.5457	0.5906	8.23%
0.4213	0.8082	0.8048	-0.42%	0.6693	0.6897	3.05%
0.6985	0.8734	0.8789	0.63%	0.7988	0.7774	-2.68%
0.7526	0.8756	0.8847	1.04%	0.8235	0.7956	-3.39%
0.8469	0.8719	0.8878	1.82%	0.8728	0.8369	-4.11%
0.9467	0.8541	0.8694	1.79%	0.9446	0.917	-2.92%
1.0000	0.8365	0.8365	0.00%	1.0000	1.0000	0.00%
			303.15K			
0.0000	0.5284	0.5284	0.00%	0.0000	0.0000	
0.04	0.6061	0.607	0.15%	0.147	0.1632	11.02%
0.1578	0.7923	0.7953	0.38%	0.3965	0.4318	8.90%
0.3346	0.9797	0.9832	0.36%	0.5813	0.6131	5.47%
0.5234	1.0877	1.089	0.12%	0.6961	0.709	1.85%
0.6513	1.1227	1.1273	0.41%	0.7589	0.7545	-0.58%
0.743	1.1329	1.1423	0.83%	0.8043	0.7869	-2.16%
0.8197	1.1318	1.147	1.34%	0.8466	0.8199	-3.15%
0.9529	1.1018	1.1178	1.45%	0.9471	0.9244	-2.40%
1.0000	1.079	1.079	0.00%	1.0000	1.0000	0.00%
			313.14K			
0.0000	0.7023	0.7023	0.00%	0.0000	0.0000	
0.055	0.8226	0.8313	1.06%	0.1673	0.2008	20.02%
0.1529	1.0031	1.0177	1.46%	0.3558	0.4075	14.53%
0.245	1.1374	1.154	1.46%	0.4691	0.523	11.49%
0.3725	1.2747	1.2881	1.05%	0.5775	0.6226	7.81%
0.4673	1.3464	1.3568	0.77%	0.6393	0.6739	5.41%
0.5482	1.3905	1.3981	0.55%	0.6856	0.7087	3.37%
0.6204	1.4181	1.4243	0.44%	0.7245	0.7357	1.55%
0.7118	1.4384	1.447	0.60%	0.7737	0.7694	-0.56%
0.8197	1.4409	1.4568	1.10%	0.8375	0.8166	-2.50%
0.9503	1.4014	1.419	1.26%	0.9421	0.9213	-2.21%
1.0000	1.3694	1.3694	0.00%	1.0000	1.0000	0.00%
			333.15K			
0.0000	1.1759	1.1759	0.00%	0.0000	0.0000	
0.1713	1.6134	1.6615	2.98%	0.3200	0.4039	26.22%
0.3368	1.9149	1.9602	2.37%	0.4883	0.5721	17.16%
0.4229	2.0308	2.0640	1.63%	0.5547	0.6280	13.21%
0.5194	2.1312	2.1490	0.84%	0.6214	0.6776	9.04%
0.6331	2.2110	2.2141	0.14%	0.6956	0.7268	4.49%
0.7304	2.2450	2.2450	0.00%	0.7596	0.7679	1.09%

0.8283	2.2430	2.2520	0.40%	0.8296	0.8178	-1.42%
0.9316	2.1892	2.2100	0.95%	0.9197	0.8987	-2.28%
1.0000	2.1168	2.1168	0.00%	1.0000	1.0000	0.00%
			343.16K			
0.0000	1.4874	1.4874	0.00%	0.0000	0.0000	
0.1637	1.9623	2.0331	3.61%	0.2801	0.3792	35.38%
0.3110	2.2891	2.3610	3.14%	0.4327	0.5396	24.71%
0.5108	2.5976	2.6220	0.94%	0.5890	0.6649	12.89%
0.6246	2.7060	2.7038	-0.08%	0.6713	0.7170	6.81%
0.7369	2.7579	2.7468	-0.40%	0.7540	0.7671	1.74%
0.8341	2.7505	2.7512	0.03%	0.8303	0.8196	-1.29%
0.9401	2.6709	2.6897	0.70%	0.9285	0.9099	-2.00%
1.0000	2.5868	2.5868	0.00%	1.0000	1.0000	0.00%
			353.18K			
0.0000	1.8583	1.8583	0.00%	0.0000	0.0000	
0.1541	2.3607	2.4593	4.18%	0.2374	0.3529	48.66%
0.2343	2.5808	2.6925	4.33%	0.3236	0.4552	40.67%
0.3865	2.9276	3.0134	2.93%	0.4565	0.5846	28.06%
0.4511	3.0486	3.1089	1.98%	0.5078	0.6244	22.96%
0.5681	3.2264	3.2340	0.24%	0.6011	0.6851	13.97%
0.6538	3.3157	3.2934	-0.67%	0.6729	0.7249	7.73%
0.7653	3.3629	3.3317	-0.93%	0.7690	0.7785	1.24%
0.8119	3.3391	3.3390	0.00%	0.8096	0.8048	-0.59%
0.9450	3.2341	3.2430	0.28%	0.9354	0.9167	-2.00%
1.0000	3.1319	3.1319	0.00%	1.0000	1.0000	0.00%

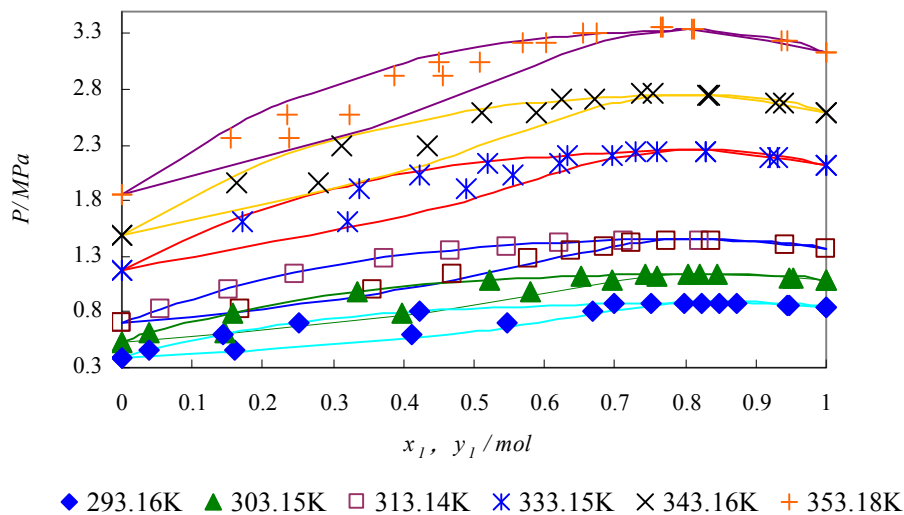◆ 293.16K ▲ 303.15K ☐ 313.14K ✳ 333.15K ✕ 343.16K ＋ 353.18K

Figure 4. Gas-liquid equilibrium curves of the (R290+R227ea) mixtures. The solid lines: calculated; the dots: experimental (Valtz, 2002).
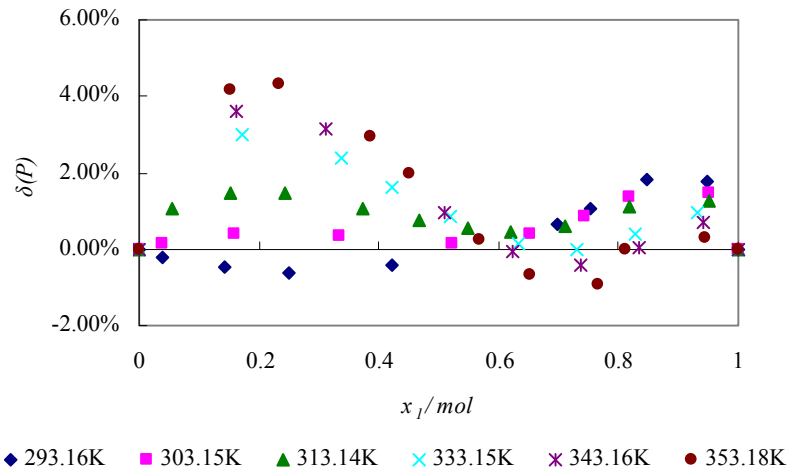
Figure 5. The relative errors of the gas pressures between the calculated and experimental results for the (R290+R227ea) mixtures.

Table 4. The azeotropic compositions (x_1) and gas pressures (P) for the (R290+R227ea) mixtures at temperatures (293.16 K, 303.15 K, 313.14 K, 333.15 K, 343.16 K, 353.188 K).

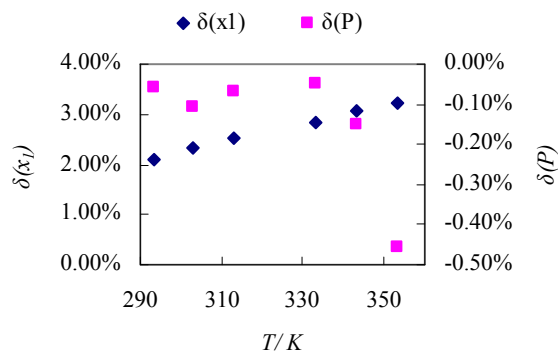| T(K)	x_1^e(mol)	x_1^s(mol)	$\delta(x_1)$	P^e(MPa)	P^s(MPa)	$\delta(P)$
293.16	0.8090	0.8260	2.10%	0.8886	0.8881	-0.06%
303.14	0.8012	0.8200	2.35%	1.1482	1.1470	-0.10%
313.15	0.7940	0.8139	2.51%	1.4578	1.4568	-0.07%
333.15	0.7813	0.8035	2.84%	2.2548	2.2537	-0.05%
343.15	0.7754	0.7991	3.06%	2.7582	2.7541	-0.15%
353.15	0.7700	0.7948	3.22%	3.3523	3.3370	-0.46%

Figure 6. The relative errors of the azeotropic compositions (x_1) and the gas pressures (*P*) between the calculated and the experimental results for the (R290+R227ea) mixtures.

4. CONCLUSION

The gas-liquid equilibrium properties of new mixture refrigerants (R1234ze+R290) and (R290+R227ea) were studied by simulations using COSMO-RS model. The relative errors of the gas pressures and mole fractions in liquid phase between the calculated and the experimental results were in the ranges acceptable to the engineering

applications, i.e., within 1% and 7%, respectively. It was concluded that the prediction of the gas-liquid equilibrium data of refrigerant mixtures using COSMO-RS model was reasonable. Further efforts would be put on improving the accuracy of the data in high temperature region.

REFERENCES

ADF COSMO-RS Manual., ADF program System Release 2012., *Scientific Computing & Modelling NV, Vrije Universiteit, Theoretical Chemistry, De Boelelaan* 1083; 1081 *HV Amsterdam*; The Netherlands.

The Montreal Protocol on Substances that Deplete the Ozone Layer, 2000, Ozone Secretariat, *United Nations Environment Program*.

Creazzo, J.A., Hammel, H.S., Cicalo, K.J., Schindler, P., 1993, Zero-ODP blowing agents for polyurethane foams, in: *Presented at the Polyurethane World Congress*.

Dong, X., Gong, M., Shen, J., Wu, J., 2011, Experimental measurement of vapor-liquid equilibrium for (trans-1,3,3,3-tetrafluoropropene (R1234ze(E))+propane (R290)). *International Journal of Refrigeration* 34 (2011) 1238–1243.

Eckert, F., Klamt, A., 2002, *AICHE J.* 48 (2002) 369–385.

Eckert, F., Klamt, A., 2003, Prediction of halocarbon thermodynamics with COSMO-RS. *Fluid Phase Equilibria* 210 (2003) 117–141.

Hsieh, C., Sandler, S.I., Lin, S., 2010, Improvements of COSMO-SAC for vapor–liquid and liquid–liquid equilibrium predictions. *Fluid Phase Equilibria* 297 (2010) 90–97.

Hou, S.X., Duan, Y.Y., Wang, X.D., 2007, *Ind. Eng. Chem. Res.* 46 (2007) 9274–9284.

Klamt, A., Schuurmann, G., 1993, COSMO: a new approach to dielectric screening in solvents with explicit expressions for the screening 8energy and its gradient. *Journal of Chemical Society*, *Perkin Transactions,* 5:799-805.

Klamt, A., 1995, Conductor-like screening model for real solvents: A new approach to the quantitative calculation of solvation phenomena. *J. Chem. Phys*. 99:2224-2235.

Klanlt, A., Jonas, V., Burger, T., and et al., 1998, Refinement and Parameterization of COSMO-RS. *The Journal of Physical Chemistry*, 102(26):5074-5085.

Klamt, A., Eckert, F., 2000, COSMO-RS: a novel and efficient method for the a priori prediction of thermophysical data of liquids. *Fluid Phase Equilibria*, 172(1):43-72.

Klamt, A., Eckert,F., 2004, Prediction of vapor liquid equilibria using COSMOtherm. *Fluid Phase Equilibria*, 217:53–57.

Klamt, A., Eckert, F., 2007, Prediction, fine tuning, and temperature extrapolation of a vapor liquid equilibrium using COSMOtherm. *Fluid Phase Equilibria* 260:83–189.

Milocco,O., Fermeglia, M., Pricl, S., 2002, Prediction of thermophysical properties of alternative refrigerants by computational chemistry. *Fluid Phase Equilibria*, 199:15–21.

Pye, C.C., Ziegler, T., Lenthe, E., Louwen, J.N., 2009, An implementation of the conductor-like screening model of solvation within the Amsterdam density functional package. Part II. COSMO for real solvents. *Can. J. Chem.* 87:790.

Valtz, C., Coquelet, D., Richon, D., 2004, *Fluid Phase Equilib*. 220:77–83.

Valtz, A., Coquelet, C., Baba-Ahmed, A., Richon, D., 2002, Vapor–liquid equilibrium data for the propane+ 1,1,1,2,3,3,3-heptafluoropropane (R227ea) system at temperatures from 293.16 to 353.18 K and pressures up to 3.4 MPa. *Fluid Phase Equilibria* 202:29–47.

Xu, T., Cui, X., Li, Z., et al. Experimental study on thermal performance of oscillating heat pipe with mixture of ethanol and bits of acetone. J. University of Shanghai for Science and Technology. 35(6): 581-585.

Zipfel, L., Barthelemy, P., Dournel, P., 1999, *Cell Plast,* 35:345–364.