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Virial coefficients and vapor-liquid equilibria of the EXP6 and 2-Yukawa fluids

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Virial coefficients B_2 through B_4 and the vapor-liquid equilibria for the EXP6 and 2-Yukawa (2Y) fluids have been determined using numerical integrations and Gibbs ensemble simulations, respectively. The chosen 2Y models have been recently determined as an appropriate reference fluid for the considered EXP6 models.

Key words: *EXP6 fluid, 2-Yukawa fluid, virial coefficients, vapor-liquid equilibrium, critical point*

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1. Introduction

Simple fluids, i.e., the fluids whose molecules interact via a spherically symmetric potential, $u = u(r)$, are most commonly modeled as Lennard-Jones (LJ) fluids. When applied to simple real fluids, the LJ performs reasonably well at subcritical and slightly supercritical conditions. However, for quite obvious reasons it fails at high temperatures/pressures: Repulsive interactions at these conditions are very soft and it has been well established that the EXP6 potential provides much more faithful description of the intermolecular interactions [1]. Furthermore, the exponential repulsion agrees with molecular beam scattering data as is also known from theoretical studies. It is therefore highly desirable, particularly from the point of geochemical and industrial (conditions of detonations and propagation of shock waves) applications, to reach a similar level of understanding and theoretical description of the EXP6 fluids similar to that of the LJ fluid.

A number of simulation data for the EXP6 fluid are available in literature along with early theoretical attempts (see [2] and references therein). The problem of theory is that all common methods are based on the assumption of the presence of very steep repulsions at short separations and thus make use of, either directly or indirectly, the known properties of the fluid of hard spheres. Consequently, they are not applicable to models with soft repulsion. To overcome this problem we have recently developed an alternative to HS-based theories, a theory based on the Yukawa (Y) model as a reference [3]. The Y potential seems to be a 'universal' simple fluid model because it is possible, by changing its parameter [see equation (2) below], to change both its range and repulsive softness. This is the reason why the Y potential is used in applications to describe of a variety of physical phenomena (see [4] and references therein).

The Y potential is a model belonging to the family of van der Waals models, i.e., the model with a hard core and approximating interactions outside the core. A large body of results, both theoretical and simulation, is available in literature (see, e.g., references [5–7] and references therein) for the Y fluid. However, to apply the Y potential to more realistic models with a soft repulsive part (i.e., without a hard core), it is necessary to use a combination of two (or even more) Y functions which results in a model without any hard core.

In a recent paper [2] we investigated, by means of molecular simulations, the structure of the EXP6 fluids and formulated the criteria for determining a Y model [more accurately, two Yukawa model (2Y)] which could be used as a reference system for developing an analytic theory of the EXP6 fluids. Unlike the one Y model (1Y), multiple Y models have not been investigated in detail yet and only a handful of results are available [8, 9]. To accomplish the goal, i.e., to develop an analytic theory for the EXP6 fluid, we should first know the properties of the 2Y fluids accurately and in detail and this has been the motivation for the present study.

Since the virial coefficients provide the basic information on the properties of the fluid and can be used in various theoretical methods, we computed the first four virial coefficients of both the parent EXP6 fluid and descending 2Y fluids. Furthermore, we have also determined the vapor-liquid equilibrium (VLE) of the 2Y fluid and located the critical point which is an important information for setting the criteria of determining the 2Y fluid associated with the EXP6 fluid.

2. Basic definitions and computational details

The EXP6 fluid is a collection of additive species (atoms, molecules, etc.) interacting via the EXP6 potential (also referred to as a modified Buckingham potential),

$$u_{\mathrm{EXP6}}(r) = \begin{cases} \infty, & \text{for } \ r < r_{\max}\,, \\ \epsilon\left(\dfrac{6}{\alpha-6}\exp\left[\alpha(1-r/r_{\mathrm{m}})\right] - \dfrac{\alpha}{\alpha-6}(r_{\mathrm{m}}/r)^6\right), & \text{for } \ r > r_{\max}\,, \end{cases} \tag{1}$$

where $r_{\max}$ and r_{m} is the location of the potential maximum and minimum, respectively, and ϵ is the depth of the minimum. Parameters r_{m} and ϵ are used henceforth as the length and energy units; dimensionless number density, ρ^*, temperature, T^*, pressure, P^*, and internal energy, U^*, are thus defined as $\rho^* = \rho r_{\mathrm{m}}^3$, $T^* = Tk_{\mathrm{B}}/\epsilon$, $P^* = Pr_{\mathrm{m}}^3/\epsilon$, and $U^* = U/\epsilon$, respectively, where k_{B} is the Boltzmann constant.

The hard core 1Y potential is defined as

$$u_{\mathrm{Y}}(r) = \begin{cases} +\infty, & \text{for } r < \sigma, \\ (\sigma/r)\exp(-zr), & \text{for } r \geqslant \sigma, \end{cases} \tag{2}$$

where z is the parameter governing the range of the interaction.

The 2Y potential is a model made up of two Yukawa tails without, in general, any hard core,

$$u_{2Y}(r) = \epsilon_1\frac{\sigma}{r}\exp[-\kappa_1 r] - \epsilon_2\frac{\sigma}{r}\exp[-\kappa_2 r]\,, \tag{3}$$

where $\epsilon_1 > 0$ and $\epsilon_2 > 0$ are the strengths of the repulsive and attractive contributions, respectively, while κ_1^{-1} and κ_2^{-1} are the measures of the range of the corresponding tails.

The virial coefficients, B_i , of the virial expansion,

$$\frac{P}{\rho k_{\mathrm{B}}T} = 1 + \sum_{i>1} B_i\rho^{i-1}\ , \tag{4}$$

were evaluated numerically up to B_4 over a wide range of temperatures using the Mayer sampling [10]. We have recently examined another version of the virial expansion, the perturbed expansion around a suitable reference system similarly to the theories of liquids,

$$\frac{P}{\rho k_{\mathrm{B}}T} = \left(\frac{P}{\rho k_{\mathrm{B}}T}\right)_{\mathrm{ref}} + \sum_{i>1}\left[B_i(T) - B_{i,\mathrm{ref}}(T)\right]\rho^{i-1}\ , \tag{5}$$

where subscript "ref" refers to a reference system. To determine the VLE envelope we used the common Gibbs ensemble with the total number of particles $N = 512$ and applied the long-range correction in order to truncate the potential at $r_{\mathrm{c}} = 0.45\sqrt[3]{N/\rho^*}$.

3. Results and discussion

When the EXP6 model is applied to real fluids by adjusting its parameter α, its resulting values typically vary between 11 and 15. To keep contact with our previous papers [2, 11] we have chosen the bracketing values, $\alpha = 11.5$ and 14.5. Parameters of the 2Y model descending from these EXP6 models were determined in our previous paper [2] and are given in table 1.

Table 1. The parameters of the 2Y potential function defined by equation (3) which are used to represent the EXP6 fluid.

	α	ϵ_1/ϵ	$\kappa_1 r_m$	ϵ_2/ϵ	$\kappa_2 r_m$	$\sigma/r_{\rm m}$
SET I	11.5	15026.86	9.4548	227.61	4.650	0.872
SET II	14.5	389565.31	13.344	148.24	4.514	0.892

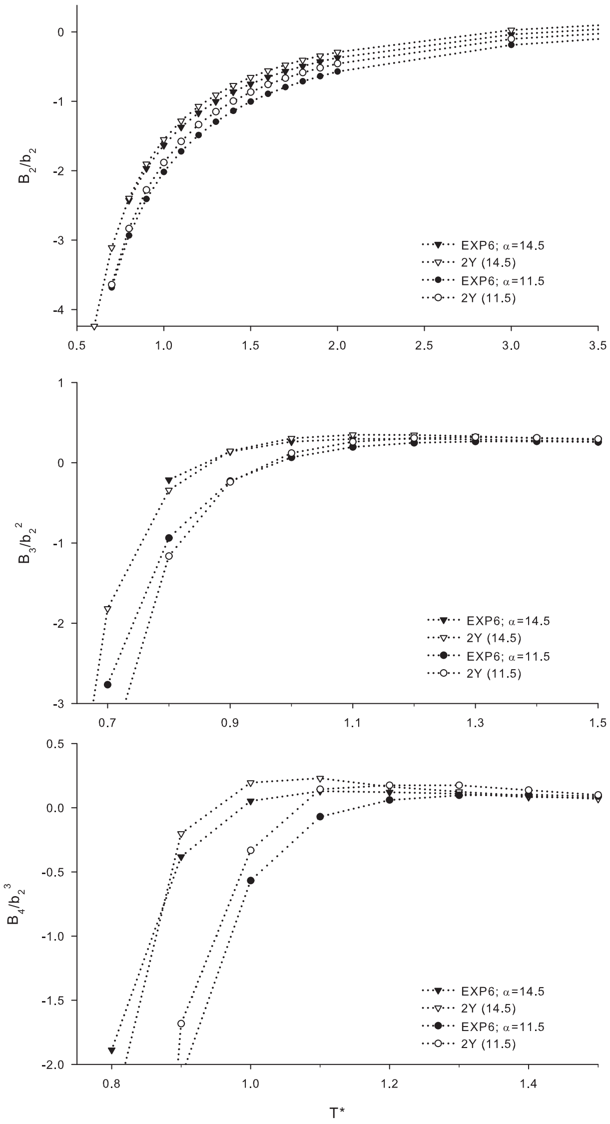

Figure 1. Comparison of the virial coefficients B_2–B_4 of the considered models. The dotted line has been drawn as a guide for eye.

Table 2. Virial coefficients of the EXP6 potential with α=11.5; $b_2 = (2/3)\pi r_{\mathrm{m}}^3$.

T^*	B_2/b_2	B_3/b_2^2	B_4/b_2^3
50.00	0.254 ± 0.001	0.049 ± 0.001	0.045 ± 0.026
40.00	0.263 ± 0.001	0.057 ± 0.001	0.000 ± 0.009
30.00	0.272 ± 0.001	0.066 ± 0.001	0.011 ± 0.003
20.00	0.275 ± 0.001	0.080 ± 0.001	0.016 ± 0.001
15.00	0.268 ± 0.001	0.090 ± 0.001	0.022 ± 0.002
14.00	0.263 ± 0.001	0.092 ± 0.001	0.028 ± 0.007
13.00	0.260 ± 0.001	0.094 ± 0.001	0.022 ± 0.001
12.00	0.253 ± 0.001	0.097 ± 0.001	0.021 ± 0.003
11.00	0.245 ± 0.001	0.100 ± 0.001	0.023 ± 0.001
10.00	0.234 ± 0.001	0.103 ± 0.001	0.022 ± 0.003
9.00	0.219 ± 0.001	0.106 ± 0.001	0.027 ± 0.001
8.00	0.200 ± 0.001	0.111 ± 0.001	0.029 ± 0.001
7.00	0.173 ± 0.001	0.115 ± 0.001	0.030 ± 0.001
6.00	0.135 ± 0.001	0.120 ± 0.001	0.031 ± 0.001
5.00	0.076 ± 0.001	0.127 ± 0.001	0.031 ± 0.001
4.00	−0.018 ± 0.001	0.138 ± 0.001	0.031 ± 0.001
3.00	−0.190 ± 0.001	0.158 ± 0.001	0.030 ± 0.001
2.00	−0.573 ± 0.001	0.210 ± 0.001	0.046 ± 0.002
1.90	−0.640 ± 0.001	0.219 ± 0.001	0.048 ± 0.002
1.80	−0.714 ± 0.001	0.228 ± 0.001	0.057 ± 0.002
1.70	−0.798 ± 0.001	0.239 ± 0.001	0.066 ± 0.002
1.60	−0.895 ± 0.001	0.249 ± 0.001	0.076 ± 0.002
1.50	−1.006 ± 0.001	0.258 ± 0.001	0.089 ± 0.003
1.40	−1.139 ± 0.001	0.266 ± 0.001	0.101 ± 0.004
1.30	−1.296 ± 0.001	0.264 ± 0.001	0.096 ± 0.005
1.20	−1.489 ± 0.001	0.247 ± 0.001	0.059 ± 0.006
1.10	−1.723 ± 0.002	0.196 ± 0.001	−0.071 ± 0.009
1.00	−2.020 ± 0.002	0.066 ± 0.002	−0.569 ± 0.014
0.90	−2.408 ± 0.003	−0.229 ± 0.003	−2.104 ± 0.041
0.80	−2.934 ± 0.003	−0.939 ± 0.004	−7.230 ± 0.230
0.70	−3.682 ± 0.004	−2.767 ± 0.009	−24.997 ± 0.649

Table 3. Virial coefficients of the EXP6 potential with $\alpha = 14.5$; $b_2 = (2/3)\pi r_{\mathrm{m}}^3$.

T^*	B_2/b_2	B_3/b_2^2	B_4/b_2^3
50.00	0.340 ± 0.001	0.083 ± 0.001	0.016 ± 0.002
40.00	0.351 ± 0.001	0.091 ± 0.001	0.023 ± 0.004
30.00	0.360 ± 0.001	0.103 ± 0.001	0.023 ± 0.003
20.00	0.364 ± 0.001	0.116 ± 0.001	0.030 ± 0.002
15.00	0.358 ± 0.001	0.126 ± 0.001	0.039 ± 0.007
14.00	0.355 ± 0.001	0.129 ± 0.001	0.036 ± 0.002
13.00	0.351 ± 0.001	0.131 ± 0.001	0.034 ± 0.002
12.00	0.347 ± 0.001	0.135 ± 0.001	0.035 ± 0.001
11.00	0.340 ± 0.001	0.135 ± 0.001	0.033 ± 0.007
10.00	0.330 ± 0.001	0.138 ± 0.001	0.042 ± 0.001
9.00	0.318 ± 0.001	0.142 ± 0.001	0.044 ± 0.002
8.00	0.301 ± 0.001	0.144 ± 0.001	0.041 ± 0.002
7.00	0.278 ± 0.001	0.147 ± 0.001	0.045 ± 0.001
6.00	0.245 ± 0.001	0.150 ± 0.001	0.049 ± 0.001
5.00	0.195 ± 0.001	0.154 ± 0.001	0.048 ± 0.001
4.00	0.112 ± 0.001	0.160 ± 0.001	0.047 ± 0.001
3.00	−0.039 ± 0.001	0.171 ± 0.001	0.043 ± 0.001
2.00	−0.373 ± 0.001	0.209 ± 0.001	0.039 ± 0.001
1.90	−0.429 ± 0.001	0.216 ± 0.001	0.041 ± 0.001
1.80	−0.495 ± 0.001	0.225 ± 0.001	0.045 ± 0.001
1.70	−0.568 ± 0.001	0.236 ± 0.001	0.051 ± 0.002
1.60	−0.652 ± 0.001	0.249 ± 0.001	0.056 ± 0.002
1.50	−0.751 ± 0.001	0.263 ± 0.001	0.078 ± 0.006
1.40	−0.863 ± 0.001	0.276 ± 0.001	0.082 ± 0.003
1.30	−1.003 ± 0.001	0.289 ± 0.001	0.108 ± 0.004
1.20	−1.169 ± 0.001	0.297 ± 0.001	0.120 ± 0.005
1.10	−1.373 ± 0.002	0.296 ± 0.001	0.128 ± 0.007
1.00	−1.635 ± 0.002	0.262 ± 0.002	0.052 ± 0.010
0.90	−1.969 ± 0.002	0.137 ± 0.002	−0.382 ± 0.019
0.80	−2.427 ± 0.002	−0.213 ± 0.002	−1.888 ± 0.160

Table 4. Virial coefficients of the 2-Yukawa potential mimicking the EXP6 potential with $\alpha = 11.5$; $b_2 = (2/3)\pi\sigma^3$.

T^*	B_2/b_2	B_3/b_2^2	B_4/b_2^3
50.00	0.268 ± 0.001	0.052 ± 0.001	0.007 ± 0.001
40.00	0.278 ± 0.001	0.059 ± 0.001	0.010 ± 0.001
30.00	0.290 ± 0.001	0.069 ± 0.001	0.013 ± 0.001
20.00	0.297 ± 0.001	0.081 ± 0.001	0.017 ± 0.001
15.00	0.293 ± 0.001	0.092 ± 0.001	0.019 ± 0.003
14.00	0.291 ± 0.001	0.094 ± 0.001	0.022 ± 0.001
13.00	0.287 ± 0.001	0.097 ± 0.001	0.023 ± 0.001
12.00	0.282 ± 0.001	0.100 ± 0.001	0.015 ± 0.013
11.00	0.276 ± 0.001	0.103 ± 0.001	0.024 ± 0.001
10.00	0.268 ± 0.001	0.106 ± 0.001	0.025 ± 0.001
9.00	0.257 ± 0.001	0.108 ± 0.001	0.028 ± 0.001
8.00	0.241 ± 0.001	0.112 ± 0.001	0.030 ± 0.001
7.00	0.218 ± 0.001	0.116 ± 0.001	0.031 ± 0.001
6.00	0.186 ± 0.001	0.120 ± 0.001	0.032 ± 0.001
5.00	0.134 ± 0.001	0.127 ± 0.001	0.032 ± 0.001
4.00	0.051 ± 0.001	0.137 ± 0.001	0.032 ± 0.001
3.00	−0.104 ± 0.001	0.159 ± 0.001	0.028 ± 0.001
2.00	−0.458 ± 0.001	0.223 ± 0.001	0.038 ± 0.001
1.90	−0.520 ± 0.001	0.234 ± 0.001	0.042 ± 0.001
1.80	−0.588 ± 0.001	0.249 ± 0.001	0.051 ± 0.002
1.70	−0.669 ± 0.001	0.262 ± 0.001	0.068 ± 0.005
1.60	−0.760 ± 0.001	0.278 ± 0.001	0.087 ± 0.003
1.50	−0.870 ± 0.001	0.295 ± 0.001	0.099 ± 0.003
1.40	−0.998 ± 0.001	0.310 ± 0.001	0.136 ± 0.004
1.30	−1.151 ± 0.001	0.319 ± 0.001	0.174 ± 0.006
1.20	−1.338 ± 0.002	0.307 ± 0.001	0.174 ± 0.008
1.10	−1.580 ± 0.002	0.260 ± 0.002	0.143 ± 0.012
1.00	−1.883 ± 0.002	0.119 ± 0.002	−0.333 ± 0.021
0.90	−2.278 ± 0.002	−0.240 ± 0.003	−1.683 ± 0.308
0.80	−2.834 ± 0.003	−1.165 ± 0.004	−8.430 ± 0.150

Table 5. Virial coefficients of the 2-Yukawa potential mimicking the EXP6 potential with $\alpha = 14.5$; $b_2 = (2/3)\pi\sigma^3$.

T^*	B_2/b_2	B_3/b_2^2	B_4/b_2^3
50.00	0.355 ± 0.001	0.087 ± 0.001	0.015 ± 0.002
40.00	0.363 ± 0.001	0.095 ± 0.001	0.027 ± 0.006
30.00	0.376 ± 0.001	0.106 ± 0.001	0.021 ± 0.002
20.00	0.383 ± 0.001	0.120 ± 0.001	0.031 ± 0.001
15.00	0.380 ± 0.001	0.130 ± 0.001	0.028 ± 0.006
14.00	0.378 ± 0.001	0.131 ± 0.001	0.036 ± 0.002
13.00	0.374 ± 0.001	0.134 ± 0.001	0.035 ± 0.004
12.00	0.371 ± 0.001	0.135 ± 0.001	0.039 ± 0.001
11.00	0.365 ± 0.001	0.137 ± 0.001	0.046 ± 0.005
10.00	0.359 ± 0.001	0.140 ± 0.001	0.042 ± 0.001
9.00	0.348 ± 0.001	0.143 ± 0.001	0.042 ± 0.001
8.00	0.334 ± 0.001	0.145 ± 0.001	0.045 ± 0.001
7.00	0.314 ± 0.001	0.147 ± 0.001	0.046 ± 0.001
6.00	0.284 ± 0.001	0.150 ± 0.001	0.049 ± 0.001
5.00	0.239 ± 0.001	0.153 ± 0.001	0.049 ± 0.001
4.00	0.163 ± 0.001	0.158 ± 0.001	0.047 ± 0.001
3.00	0.026 ± 0.001	0.168 ± 0.001	0.041 ± 0.001
2.00	−0.292 ± 0.001	0.214 ± 0.001	0.033 ± 0.001
1.90	−0.345 ± 0.001	0.225 ± 0.001	0.031 ± 0.001
1.80	−0.407 ± 0.001	0.236 ± 0.001	0.038 ± 0.002
1.70	−0.478 ± 0.001	0.250 ± 0.001	0.043 ± 0.002
1.60	−0.560 ± 0.001	0.268 ± 0.001	0.050 ± 0.002
1.50	−0.655 ± 0.001	0.286 ± 0.001	0.068 ± 0.002
1.40	−0.771 ± 0.001	0.306 ± 0.001	0.091 ± 0.004
1.30	−0.909 ± 0.001	0.329 ± 0.001	0.124 ± 0.005
1.20	−1.074 ± 0.001	0.345 ± 0.001	0.162 ± 0.006
1.10	−1.283 ± 0.001	0.348 ± 0.001	0.229 ± 0.010
1.00	−1.553 ± 0.001	0.304 ± 0.002	0.195 ± 0.015
0.90	−1.904 ± 0.002	0.146 ± 0.002	−0.202 ± 0.023
0.80	−2.397 ± 0.002	−0.342 ± 0.003	−2.433 ± 0.056
0.70	−3.108 ± 0.003	−1.818 ± 0.007	−14.300 ± 0.330
0.60	−4.239 ± 0.004	−6.815 ± 0.025	−86.259 ± 2.362

Numerical values of the virial coefficients of all four fluids considered are given in tables 2 through 5 and are also compared in figure 1. Examination of the tables/figure shows that the coefficients of the EXP6 and 2Y fluids are very similar. This is a consequence of the fact that the repulsive parts of the EXP6 and 2Y models have been used to fit the corresponding 2nd virial coefficients [2]. In other words, the similarity of all the virial coefficients means that the long-range part of the models does not affect them to any important extent.

Table 6. Vapor-liquid equilibrium data of the 2Y fluid mimicking the EXP6 potential with $\alpha = 11.5$.

T^*	ρ_v^*	ρ_l^*
0.700	0.0073 ± 0.0031	1.1798 ± 0.0130
0.800	0.0194 ± 0.0060	1.1097 ± 0.0162
0.900	0.0438 ± 0.0086	1.0331 ± 0.0177
1.000	0.0886 ± 0.0159	0.9327 ± 0.0294
1.030	0.1107 ± 0.0183	0.9012 ± 0.0352
1.050	0.1333 ± 0.0253	0.8748 ± 0.0387
1.070	0.1567 ± 0.0288	0.8540 ± 0.0353
1.100	0.1930 ± 0.0439	0.7805 ± 0.0610
1.120	0.2324 ± 0.0282	0.7203 ± 0.0577
1.140	0.2732 ± 0.0502	0.6241 ± 0.0717

Table 7. Vapor-liquid equilibrium data of the 2Y fluid mimicking the EXP6 potential with $\alpha = 14.5$.

T^*	ρ_v^*	ρ_l^*
0.600	0.0054 ± 0.0028	1.1571 ± 0.0113
0.700	0.0172 ± 0.0049	1.0863 ± 0.0152
0.800	0.0454 ± 0.0105	0.9983 ± 0.0193
0.850	0.0688 ± 0.0132	0.9437 ± 0.0219
0.900	0.1055 ± 0.0167	0.8799 ± 0.0283
0.930	0.1394 ± 0.0251	0.8287 ± 0.0459
0.950	0.1533 ± 0.0256	0.7852 ± 0.0603
0.970	0.1948 ± 0.0257	0.7512 ± 0.0462
0.975	0.2072 ± 0.0319	0.7287 ± 0.0576
0.980	0.2157 ± 0.0341	0.7078 ± 0.0584
0.985	0.2211 ± 0.0348	0.6920 ± 0.0604
0.990	0.2320 ± 0.0238	0.6677 ± 0.0527
0.995	0.2474 ± 0.0548	0.6012 ± 0.0720

Table 8. Critical properties of the 2Y fluids determined from the vapor-liquid coexistence data. Numbers in parentheses give results of the perturbed virial expansion (first row) and the virial expansion (second row) of the second order.

Model	ρ^*	T^*
2Y–11.5	0.452	1.171
		(1.18)
		(1.43)
2Y–14.5	0.295	1.00
		(1.05)
		(1.24)

The VLE results for the equilibrium densities of the 2Y fluids are given in tables 6 and 7. With these data, the critical point was determined using the rectilinear rule and the common analytic parametrization expression

$$\rho_{\mathrm{l}} - \rho_{\mathrm{v}} = B_0 \, |t|^{\beta} + B_1 \, |t|^{\beta+\Delta_1} , \tag{6}$$

and

$$\frac{\rho_{\mathrm{l}} + \rho_{\mathrm{v}}}{2} = \rho_{\mathrm{c}} + C_1 \, |t|^{\psi} + C_2 \, |t| + C_3 \, |t|^{\psi+\Delta_1} , \tag{7}$$

where $t = 1 - T/T_{\mathrm{C}}$ and B_i, C_i, β and ψ are parameters to be fitted to the simulation data; $\Delta_1 = 0.5$ for the vapor-liquid equilibria [12]. The results are given in table 8. In this table we also give an estimate of the critical temperature obtained using the common virial expansion and the perturbed virial expansion of the 2nd order [13, 14]; in the perturbed expansion we used the fluid of hard spheres of diameter σ as the reference. As we see, the perturbed method provides a very good estimate which further confirms its superiority over the common virial expansion.

4. Conclusions

In this paper we have presented results for the first four virial coefficients of the EXP6 fluid and the associated 2-Yukawa fluids, and vapor-liquid equilibria in the latter models. These data are necessary for a subsequent development of a theory for the 2-Yukawa fluids which further provides an alternative to hard core (van der Waals type) equations of state. In addition to the determination of the critical point from the vapor-liquid coexistence data, we have used the computed virial coefficients to determine the critical temperature from the virial expansions. The obtained results further confirm the recently reported applicability and accuracy of the perturbed expansion.

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Віріальні коефіцієнти і фазова рівновага пара-рідина у EXP6 та 2-Юкава плинах

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Віріальні коефіцієнти від B_2 до B_4 і фазова рівновага пара-рідина у EXP6 та 2-Юкава (2Y) плинах розраховані, відповідно, з допомогою чисельного інтегрування та на основі комп'ютерного експерименту з використанням ансамблю Гібса. Вибрані 2Y модельні системи нещодавно були запропоновані як базисні для EXP6 плинів, що розглядаються.

Ключові слова: *EXP6 плин, 2-Юкава плин, віріальні коефіцієнти, фазова рівновага пара-рідина, критична точка*