

Equation of state of chain molecules

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The formerly proposed equation of state of fused hard-sphere molecules is applied to evaluate the compressibility factor of systems of flexible chains. A fair agreement with the available Monte Carlo data is obtained. Next, the equation of state extended to mixtures is used to predict the P - V - T behavior of binary systems composed of simple hard-body chains differing in the number of atoms in molecules. Good accordance of the calculated and pseudoexperimental values—within the experimental errors of the data—is obtained. To get further experimental data for pure chain molecules and their mixtures Monte Carlo simulations were performed for the system of linear tetraatomic molecules with the site-site length $l^* = 1$ and their equimolar mixtures with hard dumbbells at several densities. Comparison of the results for the linear tetraatomics with data on the corresponding flexible chain molecule system reveals a good agreement of the data. The proposed equation of state describes adequately the behavior of both the pure fluid and mixtures.

I. INTRODUCTION

Equations of state of hard-body fluids have been studied intensively for several years. Recently, the effort has been focused on the prediction of the equilibrium behavior of systems of associating molecules including (longer) chain molecules. In a series of articles Wertheim¹⁻⁴ applied the graph theory to tackle the problem of the description of the behavior of systems of associating hard spheres forming the pearl-necklace chain (the bond length of which is just equal to the sum of radii of neighboring spheres) taking into account the condition of the bond saturation. Gubbins and co-workers⁵⁻⁶ applied the theory of associating fluids to characterize the equilibrium behavior of several model systems.

Another approach has been followed by Hall and co-workers⁷⁻⁹ who interpreted their simulation results for flexible chains of 4, 8, and 16 atoms in terms of generalized Flory and Flory-Huggins theory.¹⁰⁻¹¹ In these generalized versions of the mentioned theories they made use of the Carnahan-Starling and (in the latter case) Boublík equations of state of hard spheres and hard dumbbells, respectively. With the recent version Honnell and Hall⁹ obtained very good accord with the pseudoexperimental data for the chain and some other fused hard-sphere model systems. However, problems encounter when one tries to apply the theory to systems of chains with spheres of different radii or mixtures of different chains.

On the basis of the results of Wertheim and of Gubbins *et al.* one of the present authors¹² formulated an equation of state of fluids of linear fused hard-sphere bodies. It has been shown that the proposed equation of state yields very good agreement of the calculated and simulation values of the virial coefficients and of the compressibility factor of dumbbells, linear triatomic and tetraatomic molecules. The discussion of the results obtained within the theory of associating hard spheres, given by Wertheim, however, makes it clear that the expressions, employed by us as the basis for the derivation of the equation of state (EOS), are

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valid not only for the linear molecules but also for the chain molecules with bond angles differing substantially from the π value. Thus, also our recent EOS is not limited to the linear fused hard-body molecules and can be applied for flexible hard-sphere chains as well.

In this paper we examine the applicability of the formerly proposed EOS to predict the P - V - T behavior of higher members of the family of flexible chains. Then, the extension of the EOS to mixtures is given and employed to evaluate the compressibility factor of the simplest chain molecule mixtures for which pseudoexperimental data are available in the literature. In order to get experimental evidence for the idea that systems of linear molecules and those of flexible chains do not differ substantially in their P - V - T behavior and also to get data for a more severe test of the EOS of mixtures we performed the Monte Carlo simulations in the system of linear tetraatomic molecules and in the equimolar mixtures of tetraatomics and dumbbells, all with the same site diameter and the reduced site-site distance equal to one.

II. THEORY

The equation of state proposed recently for fused hard-sphere molecules is based on the expression developed by Wertheim¹⁻⁴ and by Gubbins and co-workers:⁵⁻⁷ the compressibility factor of the spherical associating molecule system is expressed in terms of the compressibility factor of hard spheres and chain contribution,

$$P/\rho_0 kT = Z_{hs} + Z_{chain} \quad (1)$$

with $\rho_0 = m\rho$ (where ρ is the number density of a chain and ρ_0 that of the associating molecules). Z_{chain} is

$$Z_{chain} = -\frac{m-1}{m} \left[1 + \rho \left(\frac{\partial \ln g}{\partial \rho} \right) \right]. \quad (2)$$

For the compressibility factor Z_{hs} and g , the contact value of the corresponding distribution function, one can employ the expressions due to Carnahan-Starling¹³ or those due to Kolafa (see Ref. 14). If y is the packing fraction we have in the latter case¹²

$$Z = \beta P / \rho = m \frac{1 + y + y^2 - 2y^3/3 - 2y^4/3}{(1 - y)^3} - (m - 1) \frac{1 + y - y^2/4 - 2y^3/3 + y^4/6}{(1 - y)(1 - y/2 + y^2/12 - y^3)}. \quad (3)$$

In the virial expansion of (3) all the virial coefficients are linear functions of the parameter m —the number of hard spheres in a chain. Thus, e.g., the second virial coefficient is

$$B = \frac{3}{2} m - \frac{5}{2}. \quad (4)$$

In order to get agreement with the well known expression for B in terms of the parameter of nonsphericity, α ($= RS/3V$), i.e.,

$$B = 3\alpha + 1, \quad (5)$$

it must hold

$$m = 2\alpha - 1 \quad \text{or} \quad \alpha = (m + 1)/2. \quad (6)$$

From (6) one obtains for the higher virial coefficients

$$C = 14.167\alpha - 4.167, \quad (7)$$

$$D = 31.667\alpha - 13.333, \quad (8)$$

etc.

Considering the general form of the EOS that follows from the scaled particle theory, extended to the nonspherical hard-body system, one obtains¹²

$$Z = \frac{1}{(1 - y)} + \frac{3\alpha y}{(1 - y)^2} + \frac{y^2[(49\alpha - 31) - y(11\alpha - 7) - y^2(25\alpha - 21)]}{6(1 - y)^3}, \quad (9)$$

where $y = \rho V_c$ is the packing fraction of hard chains.

The parameter of nonsphericity, α , should be within the theory of associating hard-sphere systems the same for all the different configurations of the considered flexible chains (as long as neighboring spheres to the given site do not overlap). Thus, the geometric quantities—volume, surface area, and the mean curvature integral divided by 4π , V_c , S_c , and R_c —can be evaluated for the linear form according to the standard procedure with R_c obtained for the enveloping hard spherocylinder. In the case of the chain molecule composed of hard spheres of the same diameter, all in contact, the parameter α is just

$$\alpha = (m + 1)/2. \quad (10)$$

Equation (9) is, however, valid also for chains of mutually overlapping spheres ($l < \sigma$). Defining the reduced site-site distance, $l^* = l/\sigma$ (where σ stands for the hard-sphere diameter, the same for all the sites) it holds true

$$R_c = [(m - 1)l^* + 2]\sigma/4, \quad (11)$$

$$S_c = [(m - 1)l^* + 1]\pi\sigma^2, \quad (12)$$

$$V_c = [\frac{1}{2}(m - 1)(3l^* - l^{*3}) + 1]\pi\sigma^3/6, \quad (13)$$

$$l^* > 0.5$$

so that

$$\alpha = [(m - 1)l^* + 2][(m - 1)l^* + 1]/[(m - 1) \times (3l^* - l^{*3}) + 2], \quad l^* > 0.5. \quad (14)$$

For the heteronuclear diatomic molecules with the respective diameters σ_a , σ_b and the site-site distance $l = a + b$, (where a is the distance from the center of site A to the intersecting plane)

$$a = l/2 + (\sigma_a^2 - \sigma_b^2)/8l, \quad (15)$$

we have

$$R_c = [\sigma_a + \sigma_b + l + (\sigma_a - \sigma_b)^2/4l]/4, \quad (16)$$

$$S_c = \pi[\sigma_a^2 + \sigma_b^2 + 2\sigma_a a + 2\sigma_b b]/2, \quad (17)$$

$$V_c = \pi[\sigma_a^3 + \sigma_b^3 + 3\sigma_a^2 a + 3\sigma_b^2 b - 4a^3 - 4b^3]/12. \quad (18)$$

The geometric quantities of more complex molecules follow from the extension of the above expressions for the considered chain.

The extension of the EOS to multicomponent systems is very simple. In the case of mixtures with the composition given by the mole fraction x_i , the packing fraction y_s is

$$y_s = \rho \sum x_i V_{ci}, \quad (19)$$

whereas for the nonsphericity parameter of the mixture, α_s , one has

$$\alpha_s = \sum x_i R_{ci} \sum x_i S_{ci} / 3 \sum x_i V_{ci}. \quad (20)$$

In the special case of the mixture of chain molecules with $l^* = 1$, with different number of spheres in their molecules, α is given by relationship

$$\alpha_s = \frac{1}{2} \sum x_i m_i + \frac{1}{2}. \quad (21)$$

In the third part of this paper some examples of the use of the proposed equation of state to predict the equilibrium behavior of pure fluids and mixtures are given together with the comparison with the results obtained from the "improved scaled particle theory" (ISPT) equation of state^{15,16}

$$Z = \frac{1 + (3\alpha - 2)y + (3\alpha^2 - 3\alpha + 1)y^2 - \alpha^2 y^3}{(1 - y)^3} \quad (22)$$

and predictions from the equation proposed for flexible hard chain molecule systems by Honnell and Hall.⁹ Their equation is given by a sum of the expressions for the compressibility factors of hard spheres and hard dumbbells (usually with $l^* = 1$) multiplied by $(1 + Y_n)$ and Y_n , where Y_n stands for the insertion factor, given by a ratio of the excluded volumes of one, two, and n molecules; i.e.,

$$Z = (1 + Y_n)Z_{db} - Y_n Z_{hs}. \quad (23)$$

For the compressibility factor of hard spheres Honnell and Hall employed the Carnahan-Starling equation, for Z_{db} the expression due to Tildesley and Street¹⁷ or Eq. (22) with $\alpha = 1.5$. This last choice appeared to yield the best results and will be used by us, too. To our best knowledge Eq. (23) has not been extended to mixtures and this extension is not straightforward.

III. MONTE CARLO SIMULATIONS

The standard Monte Carlo method with Metropolis' sampling and periodic conditions¹⁸ were used in our study both in the case of pure fluids and mixtures. In the former case we considered a system of linear molecules composed of

four equal hard spheres in contact (so that $l^* = 1$). We performed simulations with 128 particles in the cubic box; the initial configuration contained molecules equally distributed in the direction of the three edges of the cell. In the case of the two-component systems we considered equimolar mixtures of the above tetraatomics and hard dumbbells with $l^* = 1$; the cubic box contained 80 tetraatomics and 80 dumbbells. Also in this case the special initial configuration in which both the tetraatomics and dumbbells were equally distributed with respect to the main axis of the coordinate system was used in order to shorten the time necessary to reach the equilibrium in the studied system. Originally the molecules fill the available volume; by changing their size we obtained the wanted density. For the pure fluid we considered the packing fractions $y = 0.205, 0.289, \text{ and } 0.359$; these values were chosen among those for which Monte Carlo simulations had been performed by Dickman and Hall.⁷ For the equimolar mixtures we made simulations at the packing fraction $y, = 0.2, 0.3, \text{ and } 0.35$.

In the case of the pure fluid the initial part of the experiment included 8000 trial moves per particle whereas the equilibrium properties were evaluated from the run of 4000 moves per particle; in the case of mixtures 2000 trial moves in the initial and 2000 in the equilibrium part were employed except of the highest density where twice as many configurations were used. In every trial move the center of mass was displaced and the orientation of only one molecule changed. The acceptance ratio varied in the range 30%–50%. After each 5 trial moves we sampled the structural quantities considering shells of the width 0.02σ ; a linear interpolation was used to get the scalar products $\langle \mathbf{r}_{12} \mathbf{u}_{\alpha\beta} \rangle$ and majority of the site–site distribution functions (in some cases, however, quadratic dependence was used). Besides the site–site distribution functions also the center–center distribution function and first terms of the spherical harmonic expansion were evaluated. In order to know whether the system is isotropic or anisotropic we evaluated the tensor Q , the components of which were¹⁹

$$Q_{\alpha\beta} = \frac{1}{2N} \sum 3\mathbf{u}_{i\alpha} \mathbf{u}_{i\beta} - \delta_{\alpha\beta} \quad (24)$$

(where \mathbf{u} is a unit vector along the molecular axis) and took the medium eigenvalue λ_0 to get the order parameter S ,

$$S = -2\langle \lambda_0 \rangle. \quad (25)$$

The contact values of the site–site distribution functions $g_{\alpha\beta}$ and scalar products were used to evaluate the compressibility factor $\beta P / \rho$,

$$Z = \beta P / \rho = 1 + \frac{3}{2} \pi \rho \sum x_i x_j \sum n_{\alpha\beta} \sigma^2 g_{\alpha\beta} \langle \mathbf{r}_{12} \mathbf{u}_{\alpha\beta} \rangle, \quad (26)$$

where $n_{\alpha\beta}$ denotes the number of site–site interactions of the given type (outmost–outmost, outmost–inner, inner–inner sites). The values of the compressibility factors of pure tetraatomics and of the equimolar mixture of tetraatomics and dumbbells are given in Table I. For the sake of comparison also the Monte Carlo data of Dickman and Hall⁷ at the same packing fractions are listed in the first part of the table.

The comparison reveals the fact that for all the densities the compressibility factors for the linear and flexible chain molecules agree perfectly (within the respective error bars).

TABLE I. The compressibility factors of pure linear tetraatomics (of the same site diameter and with all the reduced lengths equal to 1) and of the equimolar mixtures of dumbbells and tetraatomics.

y	$\beta P / \rho_{MC}$		$\beta P / \rho_{calc}$	
	This work ^a	Ref. 7 ^b	Eq. (9)	Ref. 9
Pure fluid				
0.205	4.85 ± 0.10	4.73 ± 0.05	4.88	4.73
0.289	8.68 ± 0.17	8.70 ± 0.07	8.87	8.73
0.359	13.81 ± 0.30	13.50 ± 0.10	14.54	14.28
Mixture				
0.20	3.94 ± 0.10	...	3.94	...
0.30	7.70 ± 0.20	...	7.72	...
0.35	10.65 ± 0.30	...	10.83	...

^a Linear tetraatomics or its mixture with dumbbells.

^b Flexible chain $r = 4$.

In the case of the highest packing fraction, however, we observed that the order parameter S even after long run did not tend to zero. This fact could indicate formation of an ordered phase; this would be in agreement with the behavior of hard spherocylinders of the similar elongations and densities (see Ref. 20). In the case of mixtures there were no signs of a formation of an ordered phase—a fact easily understandable when one takes into account the relatively spherical shape of one of the components, i.e., hard dumbbells.

IV. APPLICATIONS

In the previous paper¹² dealing with the proposed equation of state the high quality of the prediction of the compressibility factor and virial coefficients of molecules formed by several hard spheres of the same diameter and reduced bond length equal to one have been demonstrated. Here we will first consider systems of longer flexible chains— r -mers. From the Monte Carlo simulations of Dickman and Hall⁷ the data for $r = 4, 8, \text{ and } 16$ are available. In order to get experimental evidence for the result of the theory of associating molecule systems, namely, that the rigid linear fused hard-sphere models and the corresponding flexible chain molecules (without overlapping of the next neighbors) do not differ in their P – V – T behavior, we performed simulations on the linear tetraatomics (with bond lengths equal to the diameter σ). The results are listed in the first part of Table I, where also the values of Dickman and Hall are given. Full agreement—within combined errors of the data—is found.

In Fig. 1, these data are used to examine quality of prediction of the P – V – T behavior from Eq. (9) in comparison with that from Eq. (23). One can see that the theoretical curves differ only very slightly in the whole density range; Eq. (23) is slightly better at the packing fraction $y = 0.3$ – 0.4 whereas Eq. (9) performs better at the highest densities. Similar conclusion can be drawn from Fig. 2, where the compressibility factor of the 8-mer system is plotted vs the packing fraction y ; in comparison with Fig. 1 both the curves and experimental points are shifted to lower values of y . Next we will consider the system of 16-mers (Fig. 3). The nonspheri-

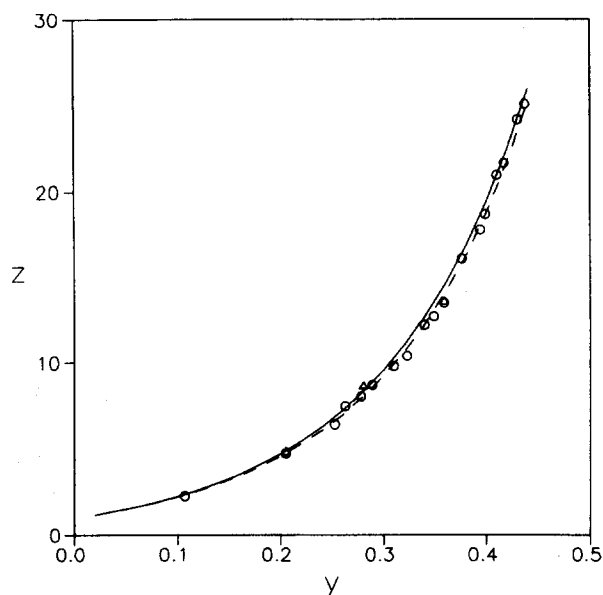


FIG. 1. Compressibility factor of the system of chains of $r = 4$ from the equation of state Eq. (9) (—), Eq. (23) (---), from the MC study of Dickman and Hall (\circ), and from our simulations on the linear hard tetraatomics (\triangle).

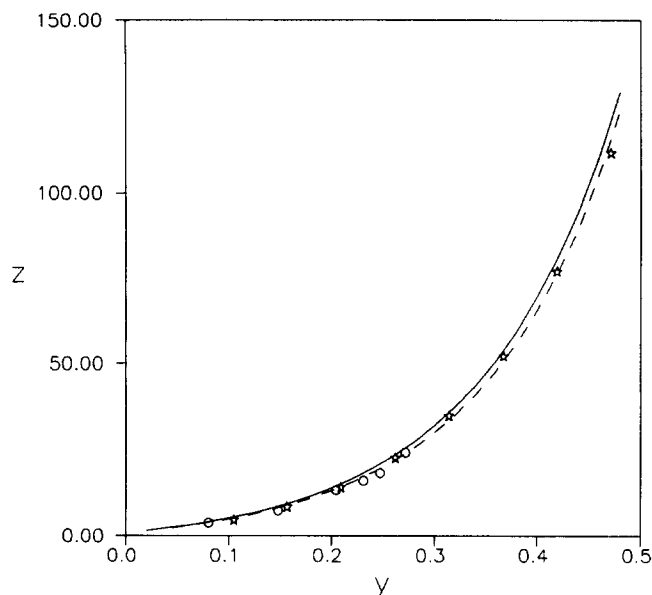


FIG. 3. Compressibility factor of the system of chains of $r = 16$ from Eq. (9) (—), Eq. (23) (---), the MC study of Dickman and Hall (\circ), and MD simulations of Gao and Weiner (*).

city of molecules of this system is quite high and with it increases also the difference in courses of the two theoretical curves. Besides the experimental data of Dickman and Hall (denoted by circles) also results of simulations of Gao and Weiner²¹ are available in the literature. The authors studied systems of flexible soft-sphere chains with number of bonds, N , equal to 15, 50, and 200. Experiments were performed at such conditions that the results correspond to flexible hard-sphere chains; it has been claimed that with the used MD method higher accuracy for systems of long chains was attained. The data for $N = 15$ are included in Fig. 3, too; they are denoted by asterisk. It is apparent that Eq. (9) repro-

duces the data for 16-mers very well up to the highest values of the packing fraction. In Figs. 4 and 5, similar comparisons are given for the systems of $N = 50$ and $N = 200$. It is evident that Eq. (9) yields very good prediction of the P - V - T behavior even for these systems. It slightly overestimates and Eq. (23) slightly underestimates the real P - V - T behavior. One can conclude saying that Eq. (9) predicts the compressibility factor for the different homonuclear fused hard-sphere models including hard-sphere flexible chains with high accuracy up to the highest densities. By passing we note that the ISPT EOS, Eq. (22) yields for the last system too great values of Z .

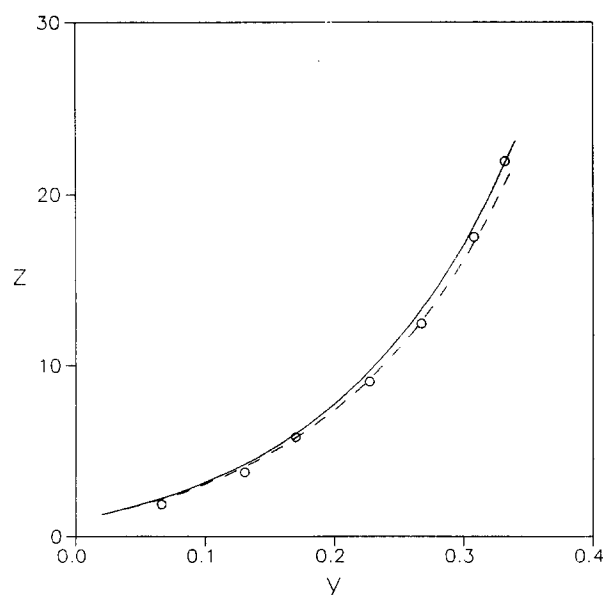


FIG. 2. Compressibility factor of the system of chains of $r = 8$ from Eq. (9) (—), Eq. (23) (---), and the MC study of Dickman and Hall (\circ).

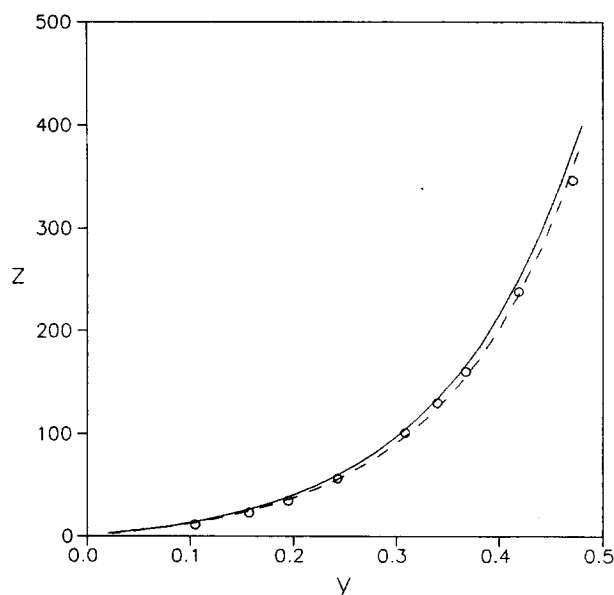


FIG. 4. Compressibility factor of the system of chains with $N = 50$ from Eq. (9) (—), Eq. (23) (---), and the MD simulation of Gao and Weiner (\circ).

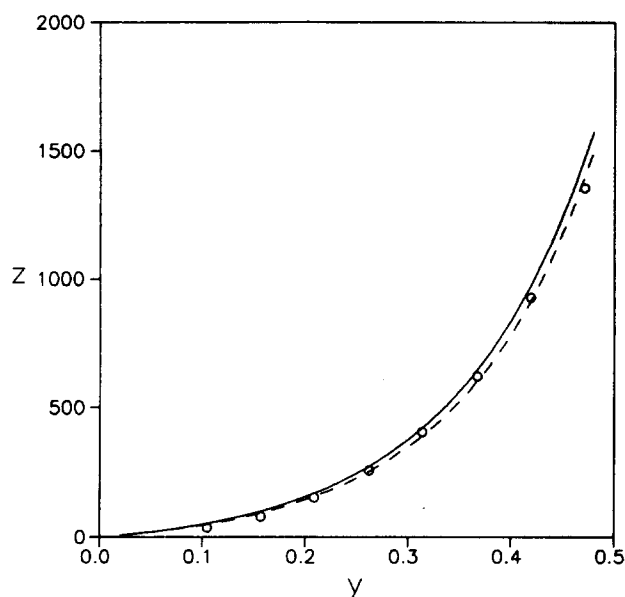


FIG. 5. Compressibility factor of the system of chains with $N = 200$ from Eq. (9) (—), Eq. (23) (---), and the MD simulations of Gao and Weiner (○).

Next, we will consider models where the reduced distance $l^* < 1$. The homonuclear dumbbells were studied in the previous paper; here we will focus on heteronuclear dumbbells and homonuclear triatomics. In Table II, the compressibility factor is given for three models of triatomics—two linear with $l^* = 0.4485$ and 0.5 and one with the right angle between bonds and with $l^* = 0.5$. From the table we see that Eq. (9) yields for the first system Z larger than the corresponding MC value (which, however, possesses quite high estimated error²²) but very good predictions for the remaining systems;²³ Eq. (23) considerably underestimates the P - V - T behavior of the second system. The ISPT EOS gives $\beta P/\rho$ close to those of Eq. (9). In the case of the heteronuclear dumbbells which are considered in Table III, Eq. (23) cannot be applied. The comparison of the calculated [from Eq. (9)] and experimental²⁴ compressibility factors reveals perfect accord, especially at high densities.

Finally, we will consider the case of mixtures of fused hard-sphere models. Unfortunately, to date only binaries composed of the simplest molecules are available in the literature. Mixtures of hard spheres and hard dumbbells have been investigated most thoroughly. In Table IV, the comparison of theoretical and experimental values of Z is given for hard spheres and homonuclear dumbbells (or dumbbells of different shapes) at three different mole fractions x_1 . The

TABLE III. The compressibility factor $\beta P/\rho$ of the heteronuclear hard dumbbells of $l/\sigma_a = 0.625$ and $\sigma_b/\sigma_a = 0.5$.

y	Eq. (9)	Eq. (22)	MC (Ref. 24)
0.2500	3.50	3.45	3.46 ± 0.12
0.3000	4.62	4.55	4.58 ± 0.15
0.3500	6.18	6.07	6.04 ± 0.25
0.4000	8.37	8.21	8.44 ± 0.32
0.4084	8.82	8.65	8.90 ± 0.62

error of the MC data of Wojcik and Gubbins²⁵ are estimated to be 3%. It is evident that the theoretical $\beta P/\rho$ is in perfect accord with the MC data. The same is true also for the mixture of hard spheres and heteronuclear dumbbells whose behavior is investigated in Table V. Also the comparison of values from Eq. (9) with experiments^{24,26} (accurate to 3.5%) shown in Table VI reveals the fact that the proposed EOS predicts the behavior of these simple mixtures very well.

In order to get data for a more severe test of Eq. (9) we performed the MC simulations in the equimolar mixture of hard dumbbells and hard tetraatomics of the same diameter and $l^* = 1$. The resulting data are listed in the second half of Table I, where also theoretical values from Eq. (9) are given. One can see that the theoretical prediction is in good accord with experiments at all the values of the packing fractions, i.e., within the estimated error of the data. Thus all the comparisons of the predicted and experimental compressibility factors of the studied mixtures reveal the fact that Eq. (9) describes the behavior of mixtures with high degree of precision.

V. CONCLUSION

The present paper brings further study of the applicability of the fused hard-sphere equation of state proposed recently on the base of the results obtained within the theory of associating molecule systems. It has been shown that the equation of state, while being only linear in the nonsphericity parameter and retaining the scaled particle theory form, yields very accurate prediction of the first few virial coefficients and of the compressibility factor of different molecular models including hard spheres and hard dumbbells as well as flexible chains with up to 200 bonds in the molecule. The way of determining the nonsphericity parameter of the chain molecules has been shown; the equation can be used without further problems to chains composed of spherical particles of different size. Also mixtures of different fused

TABLE II. The compressibility factor $\beta P/\rho$ of the hard triatomics (Monte Carlo data taken from Ref. 22 (*) and Ref. 23 (+)).

Model	l^*	y	Eq. (9)	Eq. (23)	Eq. (22)	MC
Linear*	0.4485	0.4697	13.81	12.76	13.54	12.84 ± 0.64
Linear +	0.5	0.4533	12.94	12.17	12.69	12.88 ± 0.32
Rt. angle +	0.5	0.3988	8.35	8.49	8.19	8.34 ± 0.21

TABLE IV. The compressibility factor $\beta P/\rho$ of the binary mixtures of homonuclear hard dumbbells.

y	$x_1 = 0.25$		$x_1 = 0.5$		$x_1 = 0.75$	
	Eq. (9)	MC (Ref. 25)	Eq. (9)	MC (Ref. 25)	Eq. (9)	MC (Ref. 25)
			$l_1^* = 0.6, l_2^* = 0.0, \sigma_1 = \sigma_2$			
0.30	4.25	4.20
0.45	9.80	9.78	10.28	10.15	10.82	10.76
			$l_1^* = 1.0, l_2^* = 0.0, \sigma_1 = \sigma_2$			
0.30	4.92	4.88
0.35	5.92	5.95	7.33	7.26
0.43	9.63	9.74	10.95	11.06	12.27	12.31
			$l_1^* = 0.6, l_2^* = 0.0, V_1 = V_2$			
0.30	4.26	4.25
0.45	9.89	9.76	10.39	10.27	10.88	10.82
			$l_1^* = 1.0, l_2^* = 0.0, V_1 = V_2$			
0.30	4.87	4.83
0.43	10.82	10.71
			$l_1^* = 0.6, l_2^* = 0.3, V_1 = V_2$			
0.30	4.36	4.30
0.45	10.64	10.52
			$l_1^* = 1.0, l_2^* = 0.6, V_1 = V_2$			
0.45	12.39	12.14	13.43	13.27	14.49	14.37

TABLE V. The compressibility factor $\beta P/\rho$ of mixtures of hard spheres and heteronuclear dumbbells ($l/\sigma_a = 0.625, \sigma_b/\sigma_a = 0.5, \sigma_{hs} = \sigma_a$).

y	$x_1 = 0.25$		$x_1 = 0.5$		$x_1 = 0.75$	
	Eq. (9)	MC (Ref. 26)	Eq. (9)	MC (Ref. 26)	Eq. (9)	(Ref. 26)
0.25	3.39	3.40	3.29	3.26	3.18	3.19
0.30	4.46	4.45	4.30	4.26	4.14	4.17
0.35	5.94	5.88	5.70	5.66	5.46	5.50
0.40	8.01	7.96	7.66	7.73	7.30	7.35

TABLE VI. The compressibility factor $\beta P/\rho$ of mixtures of hard spheres with linear symmetric triatomics ($l/\sigma_c = 0.8, \sigma_a/\sigma_c = 1, \sigma_{hs} = \sigma_c$).

y	$x_1 = 0.25$		$x_1 = 0.5$		$x_1 = 0.75$	
	Eq. (9)	MC (Ref. 24)	Eq. (9)	MC (Ref. 25)	Eq. (9)	MC (Ref. 24)
0.25	4.19	4.11	3.80	3.69	3.42	3.36
0.30	5.69	5.56	4.51	4.50
0.35	7.79	7.68	6.88	6.68	6.01	5.98
0.40	10.76	10.44	8.12	8.01

hard-sphere models (including mixtures of flexible chain molecules) can be treated quite easily. This allows a broad application of the new equation of state in different fields of theory.

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