The Dilute-Gas Properties of Some Systems Containing CO_2

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The SSR-MPA potential model is used to correlate and extrapolate the dilute-gas properties of some systems containing CO_2. With parameters determined from a consistent set of second virial and Joule–Thomson data, the third virial coefficient of CO_2 as well as the second virial coefficients of various mixtures containing CO_2 can be predicted very well. The Mason–Monchik approximation fails for a complicated molecule such as CO_2, although at least a viscosity prediction of technical accuracy is obtained. If parameters fitted to the CO_2 viscosity are used, excellent predictions can be made for the viscosity of gaseous mixtures containing CO_2.

1. INTRODUCTION

In a recent article we developed a new potential model for linear molecules, to which we refer as the SSR-MPA model [1]. This potential, which uses "site–site" repulsive interactions plus the well-known long-range interactions from quantum mechanical perturbation theory in the multipole expansion form, was applied to N_2, O_2, and C_2H_6 [1], to mixtures of these molecules with themselves and the noble gases [2], and to their third virial coefficients [3] with remarkable success. Starting from three parameters fitted to a consistent set of second virial coefficient and Joule–Thomson coefficient data, all other dilute-gas properties including viscosity could be predicted essentially within experimental error. In view of the success for these simple molecules, it was decided to test the new model on a

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considerably more complicated molecule, for which we chose CO_2. The more complicated force field of this molecule arises from a significant anisotropy of its shape as well as from a significant quadrupole moment. Further, contrary to C_2H_6, it cannot reasonably by modeled as a symmetric diatomic, such that the site–site repulsive parameters are not determined by the closure condition discussed in Ref. 1. Finally, there are quite reliable data for a wide range of different gas mixtures containing CO_2, recommending this substance as a further test for the SSR-MPA potential model.

2. POTENTIAL MODELS

2.1. Long-Range Forces (MPA)

The long-range contributions to the potential are taken as the standard expressions from quantum mechanical perturbation theory in connection with the multipole expansion. For the pair potential we have [4]

$$
\begin{aligned}
\phi^{\mathrm{MPA}} = {} & -4\varepsilon_{\alpha\beta} \left(\frac{\sigma_{\alpha\beta}}{r_{\alpha\beta}}\right)^6 \Bigg\{ 1 + \frac{\kappa}{2}\,(3\cos^2\vartheta_\alpha + 3\cos^2\vartheta_\beta - 2) \\
& + \frac{3}{2}\,\kappa^2 \big[(\sin\vartheta_\alpha \sin\vartheta_\beta \cos\varphi - 2\cos\vartheta_\alpha \cos\vartheta_\beta)^2 \\
& \quad - \cos^2\vartheta_\alpha - \cos^2\vartheta_\beta\big] \Bigg\} \\
& + \frac{3\theta^2}{4r_{\alpha\beta}^5}\,\big[1 - 5\cos^2\vartheta_\alpha - 5\cos^2\vartheta_\beta - 15\cos^2\vartheta_\alpha \cos^2\vartheta_\beta \\
& \quad + 2(4\cos\vartheta_\alpha \cos\vartheta_\beta - \sin\vartheta_\alpha \sin\vartheta_\beta \cos\varphi)^2\big] \\
& - \frac{9\alpha\theta^2}{8r_{\alpha\beta}^8}\,\big[\sin^4\vartheta_\alpha + \sin^4\vartheta_\beta + 4\cos^4\vartheta_\alpha + 4\cos^4\vartheta_\beta\big] \\
& - \frac{9\kappa\alpha\theta^2}{8r_{\alpha\beta}^8}\,\big[6\sin^2\vartheta_\alpha \sin^2\vartheta_\beta \cos 2\varphi(\cos^2\vartheta_\alpha + \cos^2\vartheta_\beta) \\
& \quad + (3\cos^2\vartheta_\beta - 1)(11\cos^4\vartheta_\alpha - 8\cos^2\vartheta_\alpha + 1) \\
& \quad + (3\cos^2\vartheta_\alpha - 1)(11\cos^4\vartheta_\beta - 8\cos^2\vartheta_\beta + 1) \\
& \quad - 12\sin\vartheta_\alpha \cos\vartheta_\alpha \sin\vartheta_\beta \cos\vartheta_\beta \cos\varphi(3\cos^2\vartheta_\alpha + 3\cos^2\vartheta_\beta - 2)\big]
\end{aligned}
\tag{1}
$$

Here $r_{\alpha\beta}$ is the distance between molecular centers, (ϑ, φ) are the Euler angles of the molecule defined in a space-fixed coordinate system with its z

axis along the connecting line of the molecular centers, κ is the anisotropy of the polarizability, α is the isotropic polarizability, and θ is the quadrupole moment.

The nonadditive three-body induction forces have the form [4, 5]

$$
\phi_{\alpha\beta\gamma}^{\text{ind}} = \frac{45}{320} \frac{\alpha_\alpha \theta_\beta \theta_\gamma}{r_{\alpha\beta}^4 r_{\alpha\gamma}^4} \cdot \{\sin^2 \vartheta_\beta'(3\cos^2 \vartheta_\gamma' - 1)
$$

$$
\times [10\cos(2\varphi_\beta' - 3\theta_\alpha) + 2\cos(2\varphi_\beta' - \theta_\alpha)]
$$

$$
+ \sin^2 \vartheta_\gamma'(3\cos^2 \vartheta_\beta' - 1)
$$

$$
\times [10\cos(2\varphi_\gamma' + \theta_\alpha) + 2\cos(2\varphi_\gamma' - \theta_\alpha)]
$$

$$
- \sin^2 \vartheta_\beta' \sin^2 \vartheta_\gamma'[5\cos(2\varphi_\beta' + 2\varphi_\gamma' - 3\theta_\alpha)
$$

$$
+ 25\cos(2\varphi_\beta' - 2\varphi_\gamma' - 3\theta_\alpha)
$$

$$
+ \cos(2\varphi_\beta' - 2\varphi_\gamma' - \theta_\alpha) + 5\cos(2\varphi_\beta' + 2\varphi_\gamma' - \theta_\alpha)]
$$

$$
- 32\sin \vartheta_\beta' \cos \vartheta_\beta' \sin \vartheta_\gamma' \cos \vartheta_\gamma'[\cos(\varphi_\beta' + \varphi_\gamma' - \theta_\alpha)
$$

$$
+ \cos(\varphi_\beta' - \varphi_\gamma' - \theta_\alpha)] - 4(3\cos^2 \vartheta_\beta' - 1)(3\cos^2 \vartheta_\gamma' - 1)\cos \theta_\alpha\}
$$

$$
+ \frac{45}{320} \frac{\alpha_\beta \theta_\alpha \theta_\beta}{r_{\alpha\beta}^4 r_{\beta\gamma}^4} \cdot \{\sin^2 \vartheta_\alpha'(3\cos^2 \vartheta_\gamma' - 1)
$$

$$
\times [10\cos(2\varphi_\alpha' - 2\theta_\alpha + \theta_\beta) - 2\cos(2\varphi_\alpha' - \theta_\alpha + \theta_\gamma)]
$$

$$
+ \sin^2 \vartheta_\gamma'(3\cos^2 \vartheta_\alpha' - 1)
$$

$$
\times [10\cos(2\varphi_\gamma' - \theta_\beta + 2\theta_\gamma) - 2\cos(2\varphi_\gamma' - \theta_\alpha + \theta_\gamma)]
$$

$$
- \sin^2 \vartheta_\alpha' \sin^2 \vartheta_\gamma'[-5\cos(2\varphi_\alpha' + 2\varphi_\gamma' - 3\theta_\alpha + \theta_\gamma)
$$

$$
+ 25\cos(2\varphi_\alpha' - 2\varphi_\gamma' + 3\theta_\beta)
$$

$$
+ \cos(2\varphi_\alpha' - 2\varphi_\gamma' + \theta_\beta) - 5\cos(2\varphi_\alpha' + 2\varphi_\gamma' - \theta_\alpha + 3\theta_\gamma)] \tag{2}
$$

$$
+ 32\sin \vartheta_\alpha' \cos \vartheta_\alpha' \sin \vartheta_\gamma' \cos \vartheta_\gamma'[\cos(\varphi_\alpha' + \varphi_\gamma' - \theta_\alpha + \theta_\gamma)
$$

$$
- \cos(\varphi_\alpha' - \varphi_\gamma' + \theta_\beta)] - 4(3\cos^2 \vartheta_\alpha' - 1)(3\cos^2 \vartheta_\gamma' - 1)\cos \theta_\beta\}
$$

$$
+ \frac{45}{320} \frac{\alpha_\gamma \theta_\alpha \theta_\beta}{r_{\alpha\gamma}^4 r_{\beta\gamma}^4} \cdot \{-\sin^2 \vartheta_\alpha'(3\cos^2 \vartheta_\beta' - 1)
$$

$$
\times [10\cos(2\varphi_\alpha' - \theta_\gamma) + 2\cos(2\varphi_\alpha' + \theta_\gamma)] - \sin^2 \vartheta_\beta'(3\cos^2 \vartheta_\alpha' - 1)
$$

$$
\times [10\cos(2\varphi_\beta' + 3\theta_\gamma) + 2\cos(2\varphi_\beta' + \theta_\gamma)]
$$

$$
+ \sin^2 \vartheta_\alpha' \sin^2 \vartheta_\beta'[5\cos(2\varphi_\alpha' + 2\varphi_\beta' + \theta_\gamma)
$$

$$
+ 25\cos(2\varphi_\alpha' - 2\varphi_\beta' - 3\theta_\gamma) + \cos(2\varphi_\alpha' - 2\varphi_\beta' - \theta_\gamma)
$$

$$+ 5 \cos(2\varphi'_\alpha + 2\varphi'_\beta + 3\theta_\gamma)]$$

$$+ 32 \sin \vartheta'_\alpha \cos \vartheta'_\alpha \sin \vartheta'_\beta \cos \vartheta'_\beta [\cos(\varphi'_\alpha + \varphi'_\beta + \theta_\gamma)$$

$$+ \cos(\varphi'_\alpha - \varphi'_\beta - \theta_\gamma)] + 4(3 \cos^2 \vartheta'_\alpha - 1)(3 \cos^2 \vartheta'_\beta - 1) \cos \theta_\gamma \}$$

where $(\vartheta'_i, \varphi'_i, 0)$ are the Euler orientational angles of the molecule i in a different space-fixed coordinate system defined in Fig. 1 ıand θ_α is the angle between $r_{\alpha\beta}$, $r_{\alpha\gamma}$ of the triangle with analogous definitions for θ_β and θ_γ. For the nonadditive three-body dispersion forces we used the expression as documented in Ref. 3. Transformation formulas between the two different space-fixed coordinate systems are provided in Ref. 3.

2.2. Anisotropic Repulsion (SSR)

For the anisotropic repulsion forces we use the "site–site" repulsion model. The site–site repulsive potential with an r^{-12} distance law is defined as

$$\phi_{\alpha\beta}^{\text{rep}} = \sum_a \sum_b 4\varepsilon_{a_\alpha b_\beta} \left(\frac{\sigma_{a_\alpha b_\beta}}{r_{a_\alpha b_\beta}} \right)^{12} \tag{3}$$

where $\varepsilon_{a_\alpha b_\beta}$, $\sigma_{a_\alpha b_\beta}$ are the potential parameters of the site–site repulsive energy and $r_{a_\alpha b_\beta}$ is the distance between site a of molecule α and site b of
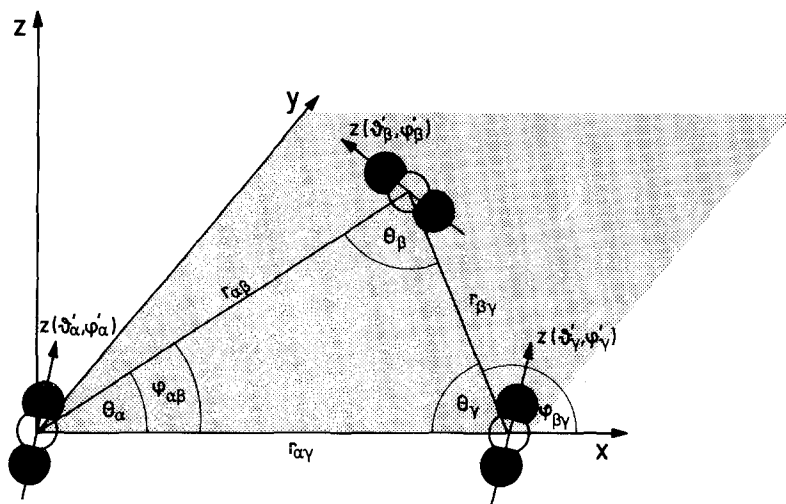

Fig. 1. The coordinates of the three molecules in the space-fixed coordinate system.

molecule β. Equation (3) can be transformed into a function explicit in the center-to-center distance between the molecules, the Euler orientational angles, and the elongation of the molecules [4]. The site–site parameters are subjected to the condition

$$\sum_a \sum_b 4\varepsilon_{a_\alpha b_\beta} \sigma^{12}_{a_\alpha b_\beta} = \varepsilon_{\alpha\beta} \sigma^{12}_{\alpha\beta} \tag{4}$$

where $\varepsilon_{\alpha\beta}$ and $\sigma_{\alpha\beta}$ are the center-to-center potential parameters. Equation (4) ensures the proper limiting case when the elongation of the molecule reduces to zero. Contrary to the molecules discussed in Ref. 1, this condition is not sufficient to determine the site–site parameters of CO_2. It is complemented by the following ad hoc rule [4]:

$$\varepsilon_{a_\alpha a_\alpha} \sigma^{12}_{a_\alpha a_\alpha} = \left(\frac{m_a}{m_b}\right)^2 \varepsilon_{b_\alpha b_\alpha} \sigma^{12}_{b_\alpha b_\alpha} \tag{5}$$

where m_a and m_b are the atomic masses of atoms a and b, respectively. The results are not very sensitive to this rule. An additional combination rule [4] is needed for the unlike "site" interaction:

$$\varepsilon_{a_\alpha b_\alpha} \sigma^{12}_{a_\alpha b_\alpha} = \left[\frac{\left(\varepsilon_{a_\alpha a_\alpha} \sigma^{12}_{a_\alpha a_\alpha}\right)^{1/13} + \left(\varepsilon_{b_\alpha b_\alpha} \sigma^{12}_{b_\alpha b_\alpha}\right)^{1/13}}{2} \right]^{13} \tag{6}$$

Equation (5) introduces the essential feature that the strength of the repulsive forces between two large and heavy atoms is greater than between two small and light ones. While not too significant for CO_2, the recognition of this effect becomes absolutely crucial in a case such as HCl. Equation(6) can be derived from a mechanical spring model [4].

3. RESUTS FOR PURE CO₂

The potential parameters for pure CO_2 were obtained from a simultaneous fit to a consistent set of data for the second virial coefficient

Table I. Values of the Parameters of the SSR-MPA Potential Function for N_2, O_2, C_2H_6, and CO_2 and the Molecular Constants [6]

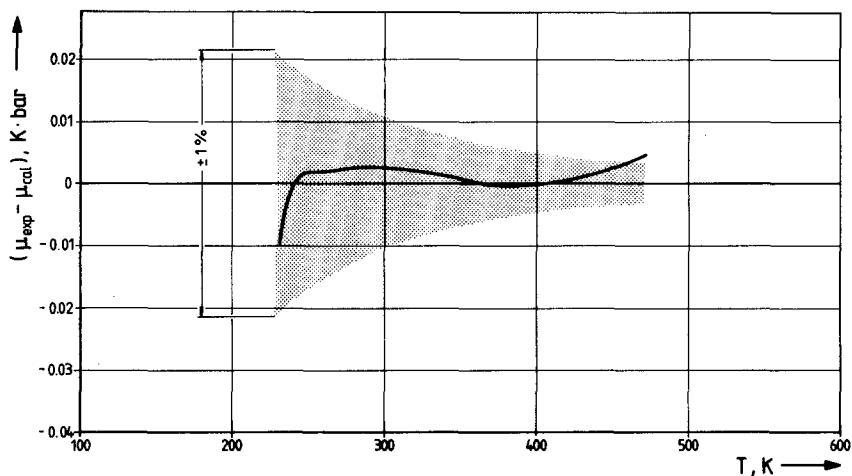| Gas	ε/k (K)	σ (Å)	r_d/σ	θ (10^{-26} esu · cm²)	α (Å³)	κ
N_2	257.89	2.9728	0.23455	−1.4	1.74	0.133
O_2	329.94	2.7678	0.22564	−0.4	1.58	0.232
C_2H_6	553.85	3.6438	0.22254	−1.2	4.44	0.0578
CO_2	830.20	2.8794	0.36896	−4.3	2.65	0.264

Fig. 2. Deviation plot of experimental Joule–Thomson coefficients of CO_2 for the SSR-MPA potential. Data from Ref. 9.

and the Joule–Thomson coefficient. They are summarized in Table I, along with the corresponding parameters for N_2, O_2, and C_2H_6 from Ref. 1 and the molecular constants from Ref. 6. Figures 2 and 3 demonstrate the perfect representation of the second virial coefficient and the Joule–Thomson coefficient that is obtained for the SSR-MPA model.
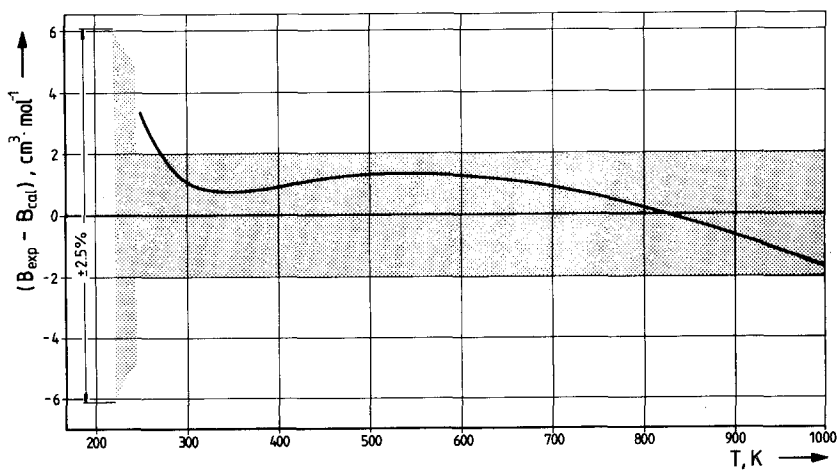

Fig. 3. Deviation plot of experimental second virial coefficients of CO_2 for the SSR-MPA potential. Data from Ref. 10.
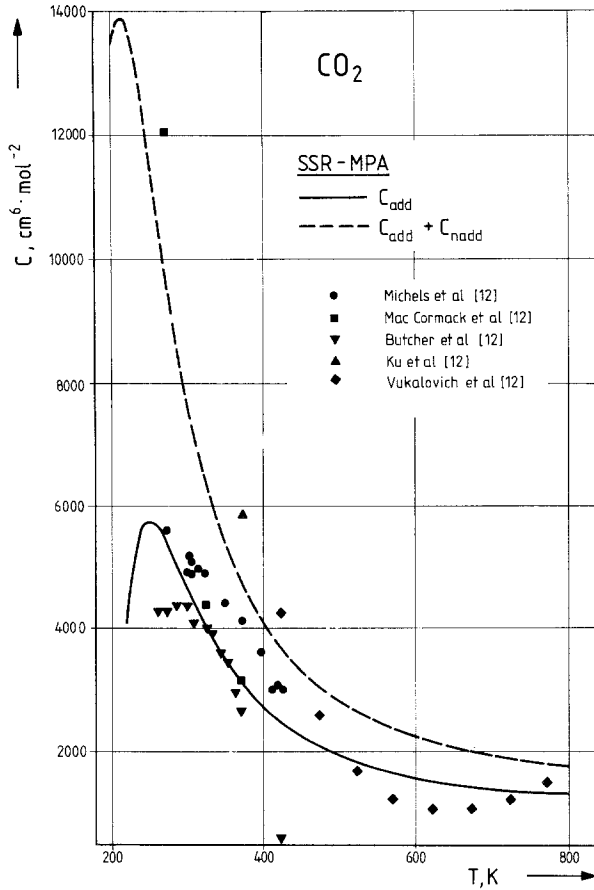
Fig. 4. The third virial coefficient for CO$_2$.

Table II. Contributions to the Third Virial Coefficient of CO$_2$

T (K)	C_{add} (cm$^6 \cdot$ mol^{-2})	C_{000}^{dis} (cm$^6 \cdot$ mol^{-2})	$C_{\neq 000}^{dis}$ (cm$^6 \cdot$ mol^{-2})	C^{ind} (cm$^6 \cdot$ mol^{-2})
200	−2,519	13,998	2,065	−1,162
220	4,043	8,414	1,435	−598
240	5,615	5,606	1,053	−342
260	5,627	4,026	807	−212
280	5,174	3,057	640	−140
300	4,628	2,420	524	−98
340	3,660	1,664	374	−54
400	2,700	1,101	253	−26
500	1,924	689	158	−11

With this same set of potential parameters, the third virial coefficient of CO_2 is predicted in Fig. 4. The factor k_c is defined as

$$k_c = \frac{C_{nadd}^{eff}}{C_{nadd}} \tag{7}$$

and takes recognition of the fact that a Lennard–Jones model tends to overestimated the third virial coefficient; the overestimation increases with increasing reduced polarizability [3]. The value of k_c is taken from the generalized correlation given in Ref. 3 and is zero in the case of CO_2. Thus, the nonadditive three-body forces for CO_2 are effectively taken care of by the pair potential plus the nonadditive induction forces used in this work. It should be noted that this is due to the large reduced polarizability of CO_2 and does not hold generally [3]. It can be seen from Fig. 4 that the SSR-MPA model predicts the third virial coefficient of CO_2 in excellent agreement with the data. Table II shows the different contributions to the third virial coefficient of CO_2.

It is further interesting to check the predicted gas viscosity of CO_2. It must be realized that there is as yet no rigorous kinetic theory of dilute polyatomic gases which lends itself to practical evaluation. The Mason–Monchik approximation [7] is quite successful for the particular simple molecules discussed in Ref. 1 but is known to fail in the general case. Figure 5 shows that the predicted viscosity for the SSR-MPA model is
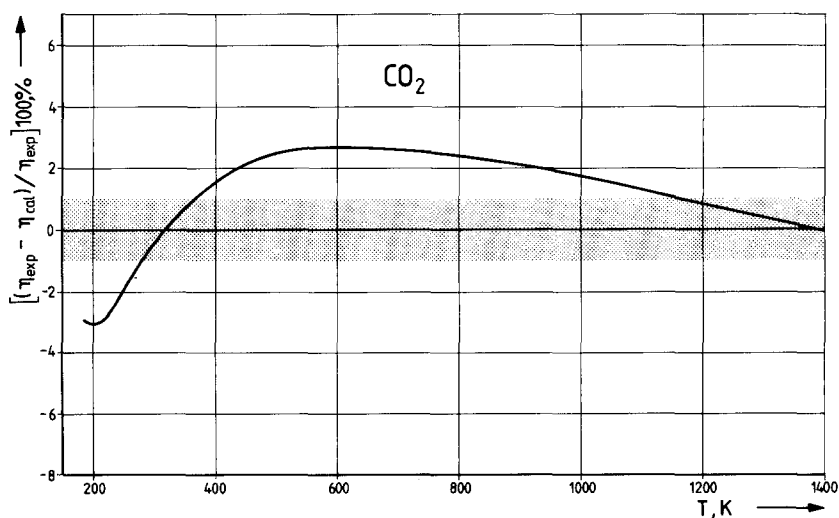

Fig. 5. Percentage deviation plot of xperimental dilute-gas viscosity for CO_2. Data from Ref. 11.

Table III. The Energy Parameter for Effective Viscosity and
Second Virial Coefficient Lennard–Jones Interaction

Gas	ε/k (K)	
	Viscosity	Second virial coeff.
He	8.162	8.592
Ne	56.850	35.519
Ar	140.671	119.105
Kr	199.843	173.242
H$_2$	43.157	31.785

essentially within $\pm 3\%$ of the data, which is outside their stated accuracy as indicated by the shadow. We attribute this to a failure of the Mason–Monchik approximation and not necessarily to a weakness of the SSR-MPA model.

4. RESULTS FOR SOME MIXTURES CONTAINING CO$_2$

For mixture calculations, we need combination rules for the potential parameters. For the SSR-MPA model, two sets of combination rules are required, one for the parameter $\varepsilon_{a_\alpha b_\beta} \sigma^{12}_{a_\alpha b_\beta}$ and the other for the parameter $\varepsilon_{\alpha\beta} \sigma^6_{\alpha\beta}$. Consistent with Eq. (6), we use

$$\varepsilon_{a_\alpha b_\beta} \sigma^{12}_{a_\alpha b_\beta} = \left[\frac{\left(\varepsilon_{a_\alpha a_\alpha} \sigma^{12}_{a_\alpha a_\alpha}\right)^{1/13} + \left(\varepsilon_{b_\beta b_\beta} \sigma^{12}_{b_\beta b_\beta}\right)^{1/13}}{2} \right]^{13} \tag{8}$$

Table IV. The Distance Parameter for Effective Viscosity and
Second Virial Coefficient Lenard–Jones Interaction

Gas	σ (Å)	
	Viscosity	Second virial coeff.
He	1.9553	2.5389
Ne	2.6740	2.8016
Ar	3.3217	3.4292
Kr	3.5545	3.6115
H$_2$	2.8772	2.9550

while for the attraction term we use Kohler's rule [8], i.e.,

$$\varepsilon_{\alpha\beta}\sigma_{\alpha\beta}^6 = \frac{\varepsilon_{\alpha\alpha}\sigma_{\alpha\alpha}^6\varepsilon_{\beta\beta}\sigma_{\beta\beta}^6}{\varepsilon_{\alpha\alpha}\sigma_{\alpha\alpha}^6\alpha_\beta^2 + \varepsilon_{\beta\beta}\sigma_{\beta\beta}^6\alpha_\alpha^2}\alpha_\alpha\alpha_\beta \tag{9}$$

We look at mixtures of CO_2 with Kr, Ar, Ne, He, H_2, O_2, N_2, and C_2H_6. As noted in Ref. 2, for the noble gases effective Lennard–Jones (12-6) parameters, different for the second virial coefficient and viscosity, have to be used to evaluate these combination rules. For H_2 a Lennard–Jones + quadrupole model was found to describe its thermophysical data most adequately. Although for most of the components, the potential parameters have been determined before, we put them together for convenient reference in Tables III and IV for the noble gases and H_2.

In Figs. 6 and 7 we summarize the results for the second virial coefficients of the unlike interactions. The data of Brewer [13] were corrected slightly for more reliable second virial coefficients of pure CO_2 at 248.15
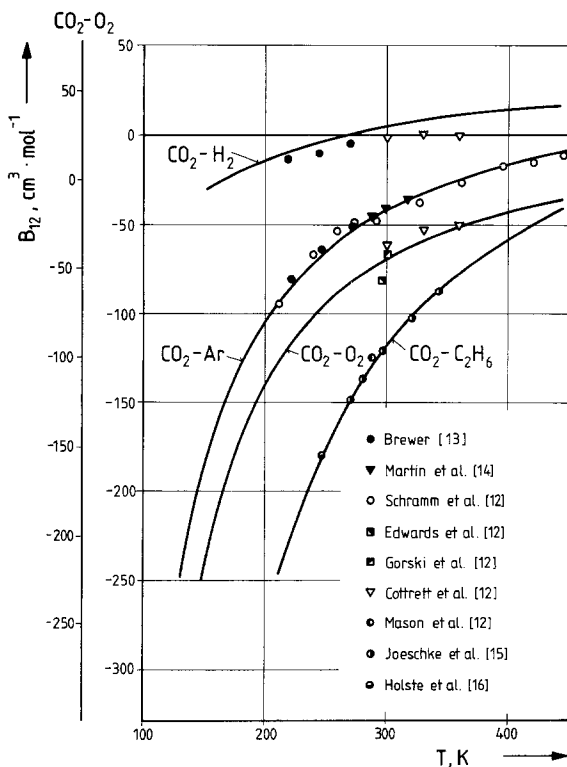
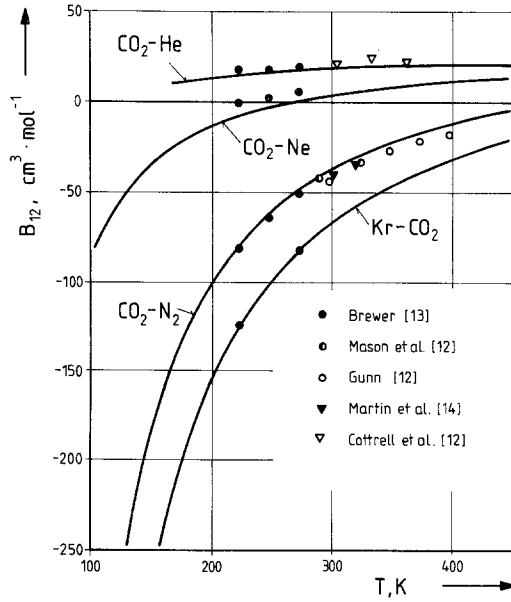Fig. 6. Predicted second interaction virial coefficients for $CO_2 - H_2$, CO_2–Ar, CO_2–O_2, and CO_2–C_2H_6.

Fig. 7. Predicted second interaction virial coefficients for CO$_2$–He, CO$_2$–Ne, CO$_2$–N$_2$, and Kr–CO$_2$.
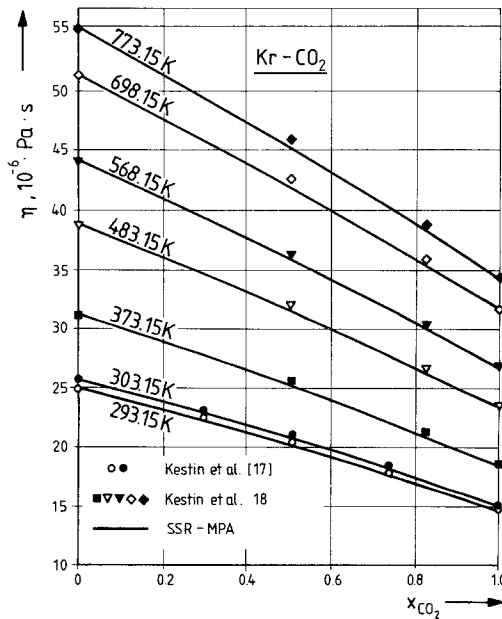

Fig. 8. Predicted viscosities of the system Kr–CO$_2$.
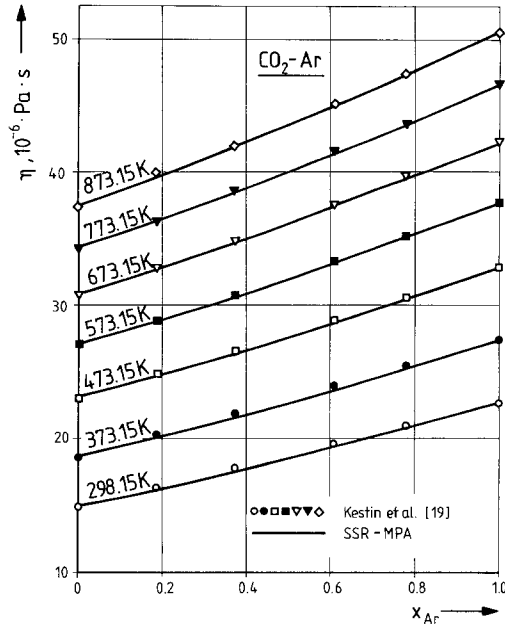
Fig. 9. Predicted viscosities of the system CO_2–Ar.
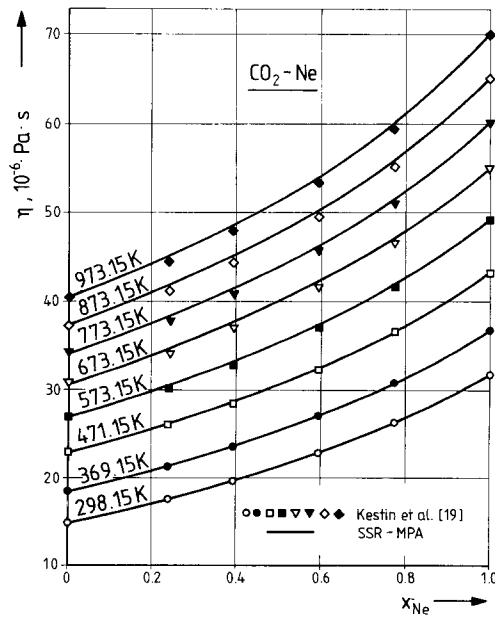

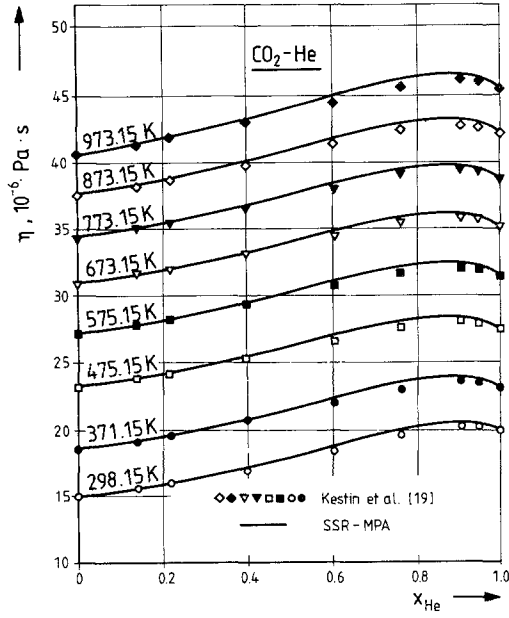**Fig. 10.** Predicted viscosities of the system CO_2–Ne.
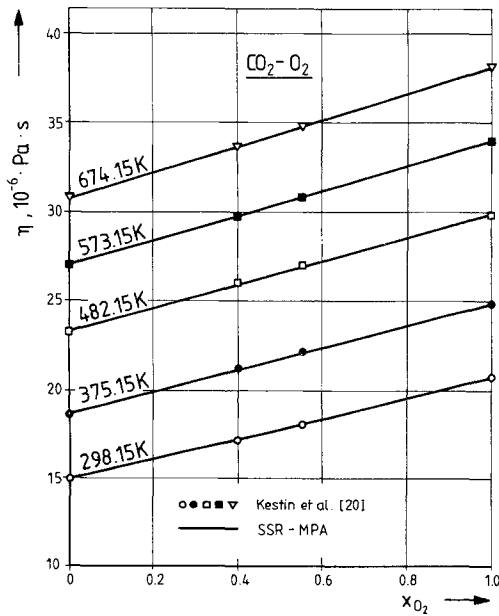
Fig. 11. Predicted viscosities of the system CO$_2$–He.
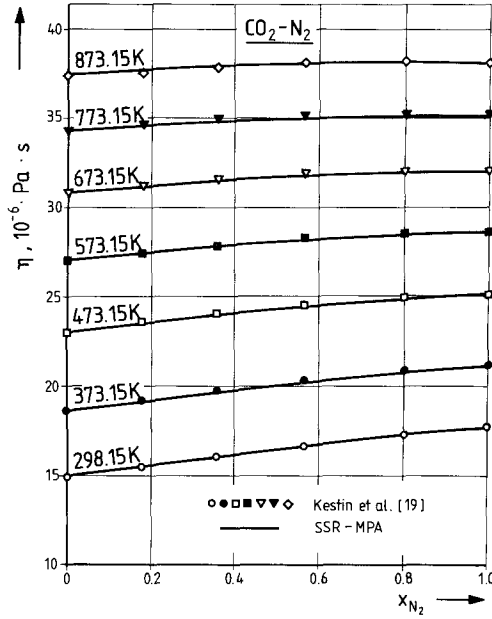

Fig. 12. Predicted viscosities of the system CO$_2$–O$_2$.

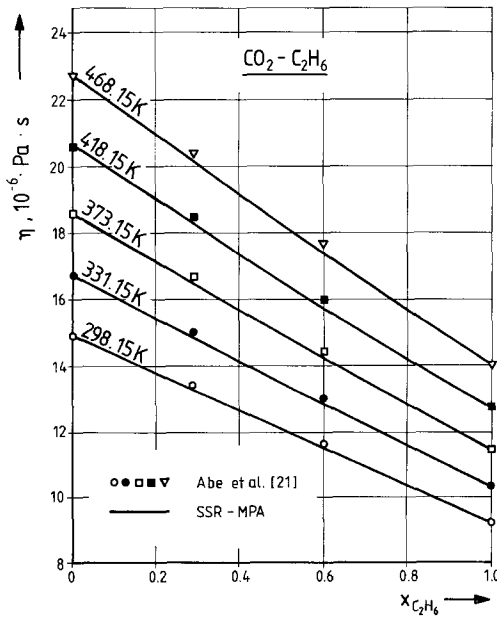**Fig. 13.** Predicted viscosities of the system CO_2-N_2.

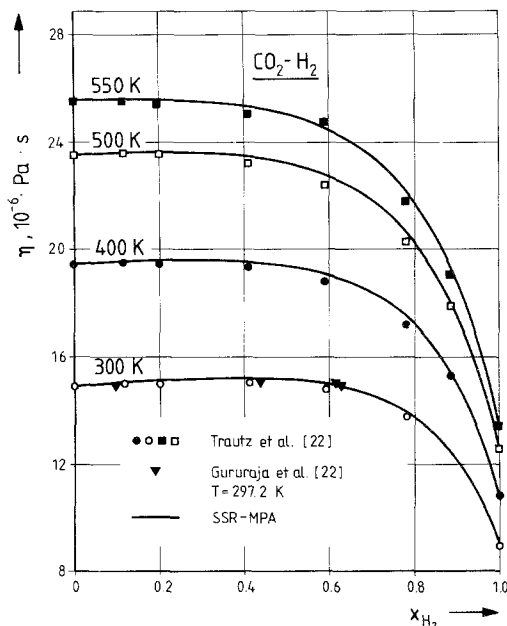**Fig. 14.** Predicted viscosities of the system CO_2-C_2H_6.

Fig. 15. Predicted viscosities of the system CO_2-H_2.

and 231.5 K, since they are inconsistent with the Joule–Thomson data [9] at these temperatures. It can be seen that the agreement of predicted and experimental B_{12} values is generally within a few $cm^3 \cdot mol^{-1}$, which is considered to be the experimental uncertainty, except, perhaps, for CO_2-H_2. It should be noted that this holds for interactions as complicated as CO_2-Ne and, in particular, CO_2-C_2H_6, where the unlike interaction coefficient falls slightly outside the range of the like interactions. Figures 8 to 15 show predictions of the dilute-gas viscosities of these mixtures. Since the viscosity of CO_2 cannot be predicted from the Mason–Monchik approximation with sufficient accuracy, we refitted the SSR-MPA model to the viscosity data of CO_2, resulting in the following set of parameters: $\varepsilon/k = 469.51$ K, $\sigma = 3.24810$, and $r_a/\sigma = 0.19430$. Using these parameters as well as the combination rules, the viscosity of all mixtures is predicted within 0 to 2%, which is essentially the accuracy of the data.

5. CONCLUSIONS

It has been shown that for dilute-gas systems containing the challenging molecule CO_2, the recently proposed SSR-MPA model with suitable combination rules is entirely satisfactory as a correlation and

extrapolation tool. This lends considerable support to this potential model for more complicated, nonlinear molecules, to which we shall address ourselves in a subsequent publication.

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