

c_2	= second-stage impeller level from vessel bottom	[cm]	= surface tension	[g/cm ²]
Δc	= clearance between impellers	[cm]		
D	= vessel diameter	[cm]		
D_L	= liquid-phase diffusivity	[cm ² /s]		
d	= impeller diameter	[cm]		
g	= gravitational acceleration	[cm/s ²]		
H	= liquid height in vessel	[cm]		
$k_L a$	= capacity coefficient in gas absorption	[s ⁻¹]		
$(k_L a)_0$	= $k_L a$ obtained in vessel with single-stage impeller where $H/D=1$	[s ⁻¹]		
N_p	= power number	[—]		
n	= impeller speed	[s ⁻¹]		
n_B	= number of baffle plates	[—]		
n_p	= number of impeller blades	[—]		
P_{av}	= aeration power per unit mass of liquid	[cm ² /s ³]		
P_{gv}	= agitation power per unit mass of liquid	[cm ² /s ³]		
	= liquid viscosity	[g/cm · s]		
	= liquid density	[g/cm ³]		

Literature Cited

- 1) Fukuda, H., Y. Sumino and T. Kanzaki: *J. Ferment. Technol.*, **46**, 829 (1968).
- 2) Nishikawa, M., M. Nakamura, H. Yagi and K. Hashimoto: *J. Chem. Eng. Japan*, **14**, 219 (1981).
- 3) Nishikawa, M., M. Nakamura and K. Hashimoto: *J. Chem. Eng. Japan*, **14**, 227 (1981).
- 4) Nishikawa, M., S. Nishioka and F. Fujieda: *Kagaku Kogaku Ronbunshu*, **9**, 76 (1983).
- 5) Nishikawa, M., K. Ashiwake, N. Hashimoto and S. Nagata: *Kagaku Kogaku Ronbunshu*, **2**, 426 (1976).
- 6) Tuffile, C. M. and F. Pinho: *Biotech. and Bioeng.*, **12**, 849 (1970).
- 7) Yagi, H. and F. Yoshida: *Ind. Eng. Chem., Process Des. Dev.*, **14**, 488 (1975).

SECOND VIRIAL COEFFICIENT OF ETHANE AT 423.15 K AND PREDICTION OF SECOND VIRIAL COEFFICIENTS FOR NORMAL ALKANES

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Key Words: Physical Property, Second Virial Coefficient, Ethane, Normal Alkane, Molecular Potential Model

In a previous paper,⁷⁾ a simple potential model based on a group-contribution concept was proposed for predicting second virial coefficients of linear symmetric molecules. At that time, fundamental group parameters of the methyl group for the model were determined tentatively from literature values of second virial coefficients for ethane.

In the present study, the second virial coefficient of ethane at 423.15 K was measured by the Burnett method. Thereafter, by use of the value at 423.15 K and that at 298.15 K obtained previously,⁴⁾ the group parameters of the methyl group for the model have been redetermined.

1. Second Virial Coefficient of Ethane at 423.15 K

The experimental apparatus and procedures used in the present study were identical to those described in a previous paper.⁶⁾

Research-grade ethane supplied by Phillips

Petroleum Co. had a specified minimum purity of 99.99 mol% and was used without further purification in the experiments.

The method of data reduction based on the virial equation of Berlin-form is the same as that used in a previous paper.⁴⁾

The second virial coefficient of ethane obtained in the present study is compared with literature values in Table 1. The values of Dymond-Smith²⁾ and of Douslin-Harrison¹⁾ are larger than the value obtained in the present study by about 2–3 cm³ · mol⁻¹. The value of Eubank-Mansoorian³⁾ is in good agreement within experimental uncertainty. On the other hand, the prediction result of Tsonopoulos⁸⁾ is smaller by about 2 cm³ · mol⁻¹ in absolute terms.

2. Prediction of Second Virial Coefficients for Normal Alkanes

A simple potential model (abbreviated OK model hereafter), proposed for predicting second virial coefficients of linear symmetric molecules in the previous

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Table 1. Second virial coefficient of ethane at 423.15 K

	B [cm ³ ·mol ⁻¹]
Present work	-86.3 ± 0.5
Literature	$-84.4 \pm 1.0^{(2)}$ $-83.6^{(1)}$ $-85.7 \pm 1.3^{(3)}$

paper,⁷⁾ is based on a group-contribution concept. According to the model, an ethane molecule is regarded as consisting of two methyl groups combined with a C-C bond. Every functional group has two characteristic parameters of the Lennard-Jones potential. At that time, however, accurate data for ethane were not available in a wide temperature range, as described in the paper.⁷⁾ Therefore, the moderate parameters for the methyl group were estimated from the data of Dymond-Smith by way of trial.

From experimental data of the present work and those in our previous paper,⁴⁾ the potential parameters of the methyl group in the OK model were redetermined in the present study. The bond length of ethane used in the calculation is identical to the previous one ($l=0.169$ nm), which was obtained from X-ray analysis. The characteristic parameters revised are $\sigma=0.3908$ nm and $\varepsilon^\circ/k=143.8$ K.

The second virial coefficients for some hydrocarbons smaller than heptane were predicted by use of the revised parameter set. Since the calculation procedures are presented in the appendix of the previous paper,⁷⁾ readers are referred to the paper.

Although most literature values of second virial coefficients for normal alkanes longer than ethane are given without clearly defined uncertainty, for the cases of propane and butane only the values are recommended with their uncertainty by Dymond-Smith. Calculated results for propane and butane are listed in **Tables 2** and **3** together with the literature values. Although the uncertainty is considerably large in both systems, the agreement between predicted and literature values is within their uncertainty.

The results predicted by use of the revised parameter set are more satisfactory than those by the previous ones, especially for propane. For pentane or hexane, however, the difference between them is not significant.

Table 2. Comparison between predicted and experimental second virial coefficients for propane

T [K]	B [cm ³ ·mol ⁻¹]	
	Literature ²⁾	OK model
350	-276 ± 10	-273
400	-208 ± 10	-207
430	-177 ± 5	-177
470	-143 ± 5	-145
500	-124 ± 5	-125
550	-97 ± 5	-98

Table 3. Comparison between predicted and experimental second virial coefficients for butane

T [K]	B [cm ³ ·mol ⁻¹]	
	Literature ²⁾	OK model
400	-370 ± 20	-360
440	-298 ± 15	-296
500	-219 ± 10	-225
560	-164 ± 10	-172

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Nomenclature

B	= second virial coefficient	[cm ³ ·mol ⁻¹]
k	= Boltzmann's constant	[J·K ⁻¹]
l	= bond length	[nm]
ε°	= energy depth	[J]
σ	= hard sphere diameter	[nm]

Literature Cited

- 1) Douslin, D. R. and R. H. Harrison: *J. Chem. Thermodyn.*, **5**, 491 (1973).
- 2) Dymond, J. B. and E. B. Smith: "Virial Coefficients of Pure Gases and Mixtures," Oxford University Press, New York (1980).
- 3) Eubank, P. T., H. Mansoorian and K. R. Hall: *Proc. 7th Symp. Thermophys. Props.*, Am. Soc. Mech. Engrs., New York, 456 (1977).
- 4) Katayama, T., K. Ohgaki and H. Ohmori: *J. Chem. Eng. Japan*, **13**, 257 (1980).
- 5) Ohgaki, K., T. Mizuhaya and T. Katayama: *J. Chem. Eng. Japan*, **14**, 71 (1981).
- 6) Ohgaki, K., Y. Nakamura, H. Ariyasu and T. Katayama: *J. Chem. Eng. Japan*, **15**, 85 (1982).
- 7) Ohgaki, K. and T. Katayama: *J. Chem. Eng. Japan*, **17**, 65 (1984).
- 8) Tsonopoulos, C.: *AIChE J.*, **20**, 263 (1974).