COMMUNICATIONS TO THE EDITOR

An Example of the Use of Combined Models: Mixing in a Tubular Reactor with Return Bends

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Recently, some data on axial mixing in a tubular high-pressure reactor with a large proportion of return bends were presented by Carter and Bir (*4*). They found, as would be qualitatively expected, that the axial mixing was somewhat greater than that observed for straight pipe flow. Thus, they concluded that more experimenetal work is needed for systems of this type.

It would seem that a reactor of this type could be broken up naturally into two sections. First, the straight, tubular part, and second, the return bends. The axial mixing in the straight portion could be found then from correlations such as Levenspiel's (*6*), and the bends might be approximately treated as perfect mixers. This latter approximation is probably a rather poor one, since the bends would not act as perfect mixers under all flow conditions. A better representation could be found by experimentally measuring mixing in bends, but this information is not available at the present time. Thus the results of the analysis to be presented will be limited to relatively crude estimates of the total axial dispersion and will serve more as an indication of what could be done if more data were available.

Models of this type, which were given the name of *mixed models* or *combined models* (*9*), and organized and generalized by Levenspiel (*7*) have been found to be useful in other types of complex flow situations. Thus, one of the earlier applications was to the flow in fluidized beds as discussed, for example, by May (*10*). Another application to flow in real stirred tanks was by Cholette and Cloutier (*5*). The advantages of such a procedure are mainly that the mixing characteristics of each individual section may be obtained from standard correlations such as those for empty pipes, perfectly mixed regions, etc., and then combined for the total system. Thus, the very extensive experimental testing of every possible type of system made up of combinations of the single elements, which would be almost impossible, is avoided. The correlation of mixing data then becomes less voluminous.

DEVELOPMENT OF MODELS

The model that lumps the straight-pipe and return-bend mixing into one effective axial dispersion coefficient, as used by Carter and Bir, is represented

(Continued on page 593)

Kihara and Lennard-Jones Parameters for the Isomeric Hexanes

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Precise methods of estimating physical data are quite useful and are often the sole source of such information for the process engineer. One such method is the estimation of transport properties (*1* to *4*) using the parameters of the Lennard-Jones intermolecular potential (*5*):

$$U(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{1}$$

Another technique is the estimation of vapor-liquid equilibrium constants (*6*) using parameters of the Kihara intermolecular potential (*7*):

$$U_p = U_o\left[\left(\frac{\rho_o}{\rho}\right)^{12} - 2\left(\frac{\rho_o}{\rho}\right)^{6}\right] \tag{2}$$

The Lennard-Jones potential assumes a spherical molecule with *r*-to-*r* spacing between molecules. Although specifically designed to describe spherical molecules, it is applicable to nonspherical molecules, especially over short temperature ranges.

(Continued on page 591)

TABLE 1. KIHARA AND LENNARD-JONES PARAMETERS FOR THE ISOMERIC HEXANES

Compound	l_1	l_2	l_3	V_o	S_o	M_o	ρ_o	U_o/k	σ(Å)	ϵ/k (°K.)
2,2-dimethylbutane	0.862	0.543	2.51	3.35	39.6	17.65	2.50	1060	7.614	266
2,3-dimethylbutane	0.783	0.788	1.57	4.02	30.8	19.65	2.50	1070	6.751	412
2-methylpentane	0.783	0.684	2.51	3.35	36.7	18.4	2.50	1130	8.065	267
3-methylpentane	0.862	0.543	2.51	3.35	35.3	17.6	2.50	1178	8.587	265

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The Relationship between the Froude and Reynolds Numbers in Falling Vertical Films

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Numerous workers in the field of falling liquid films have accepted the Froude number as a very appropriate dimensionless group for correlating their experimental results (*1, 2, 14*). Jackson (*14*) used the Froude number in the form

$$N_{Fr}' = \frac{V}{(gm)^{1/2}} \tag{1}$$

as a criterion for wave inception on films. His definition of the Froude number in this way must have been influenced by the fact that long gravity waves in a shallow, horizontal, open

(Continued on page 586)

(Continued from page 584)

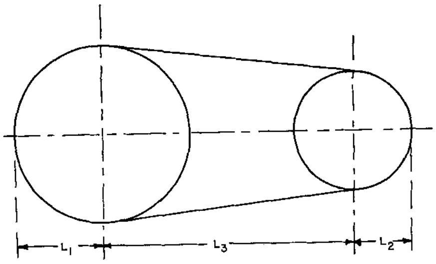

Fig. 1. Kihara core model.

The Kihara potential applies equally well to spherical or nonspherical molecules. This potential assumes impenetrable cores (whose shapes are related to intramolecular distances) separated by a distance ρ. A specific model must be derived for a molecule in order to obtain its Kihara parameter.

Both potentials may be determined from second virial coefficients-temperature data. The techniques for doing this have been described by Hirschfelder, Curtiss, and Bird (*8*) and Kihara (*7*).

The present investigation determined the Kihara and Lennard-Jones parameters for the isomeric hexanes (2-methylpentane, 3-methylpentane, 2, 2-dimethylbutane, 2,3-dimethylbutane) from second virial coefficient data (*9*).

Table 1 lists the Lennard-Jones and Kihara parameters. A spherocylindrical model (Figure 1) was used to determine the Kihara parameters. Average deviations between experimental and calculated virial coefficients were 3.19% (Kihara) and 2.28% (Lennard-Jones).

The Lennard-Jones parameters could be checked by comparing transport properties calculated from them with experimentally determined values. Unfortunately, very little experimental data was available for the isomeric hexanes. The only information found were some viscosities for 2,3-dimethylbutane (*10*). Values of viscosity calculated from the equation

$$\mu = 2.6693 \times 10^{-5} \frac{\sqrt{MT}}{\sigma^2 \, \Omega \, \mu} \quad (3)$$

compared favorably to the experimental values (see Figure 2).

A further check could also be made on the Kihara parameters if vapor-liq-

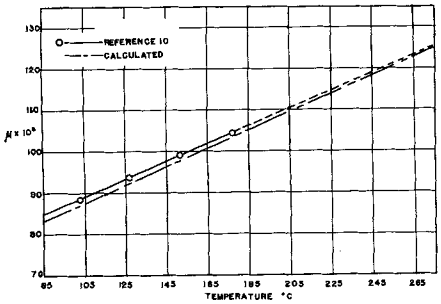

Fig. 2. Comparison estimated and experimental viscosities for 2,3-dimethylbutane.

INFORMATION RETRIEVAL

(*Continued from page 590*)

The prediction of the viscosity of nonpolar binary gaseous mixtures at atmospheric pressure, Strunk, Mailand R., Wayne G. Custead, and Gerald L. Stevenson, **A.I.Ch.E. Journal, 10,** No. 4, p. 483 (July, 1964).

Key Words: Predicting-8, Estimating-8, Nonpolar Gases-8, Viscosity-8, Lennard-Jones-, Binary-, Viscosity-9, Pure Component-, Force Constants-9, Atmospheric Pressure-9, Mixture-, Force Constants-10.

Abstract: A method for predicting the viscosity of binary nonpolar gaseous mixtures from the pure component Lennard-Jones force parameters and composition is presented. Force parameters, representative of the particular binary mixture, can be obtained and used to compute the viscosity in a manner similar to that for a pure component gas. Based on two hundred and one viscosity mixtures examined over a temperature range from 80° to 550°K. the limits of the predicted viscosity can be expected to fall between +5.5 and —6.7% of the observed viscosity 95% of the time.

Compressibility of ammonia and its mixtures with nitrogen and hydrogen, Lichtblau, I. M., R. H. Bretton, and B. F. Dodge, **A.I.Ch.E. Journal, 10,** No. 4, p. 486 (July, 1964).

Key Words: Ammonia-5, Binary System-8, Compressibility-7, Gases-5, Nitrogen-5, Pressure-6, Temperature-6, Volume-7.

Abstract: An apparatus has been developed to take compressibility data on gases from 500 to 2,500 atm. at temperatures ranging from 300° to 500°C. Compressibility data were obtained with this equipment for pure ammonia and a mixture of 19 mole % nitrogen and 81% ammonia at three temperatures, 350°, 400°, and 450°C. The pressures ranged from 500 to 2,500 atm. at each temperature. The data are internally consistent to 0.1%, and the maximum absolute error is estimated to be 0.32%. A comparison is made with literature data for pure ammonia at 300°C. for pressures ranging from 500 to 1,600 atm. No data were available for a comparison with the mixture data of the present paper. The results are presented as compressibility factors Z in two tables, one giving smoothed observations and the other data interpolated to even values of pressure.

Resistance to mass transfer inside droplets, Skelland, A. H. P., and R. M. Wellek, **A.I.Ch.E. Journal, 10,** No. 4, p. 491 (July, 1964).

Key Words: Mass Transfer Rates-8, Liquid Extraction-7, 8, Drops-10, Dispersed-Phase Mass Transfer Coefficient-7, 8, Physical Properties-6, Circulation-8, Oscillation-8, Correlations-9, Glyceryl Triacetate-5, Glycol Diacetate-5, Ethyl Acetoacetate-5, Ethyl Acetate-5.

Abstract: Effects of physical properties on the dispersed-phase mass transfer coefficient were determined for nonoscillating and for oscillating liquid droplets falling through stationary liquids. Equations were developed, involving the dimensionless time group, which correlated the mass transfer rates better than existing mathematical models. The binary systems studied were water with ethyl acetate, glyceryl triacetate, glycol diacetate, and ethyl acetoacetate.

Selectivity in hydrocarbon oxidation, Spielman, Maurice, **A.I.Ch.E. Journal, 10,** No. 4, p. 496 (July, 1964).

Key Words: Oxidation-8, Hydrocarbons-1, Liquid Phase-5, Correlations-8, Kinetics-8, Reactor-10, Design-6, Plug Flow-6, Continuous-6, Batch-6, Selectivity-7, 8, Yield-7, 8, Air-1, Conversion-7, 8, Intermediate Products-2, Cyclohexane-1, Cyclohexanone-2, Cyclohexanol-2, Boric Acid-4, Cyclohexyl Esters-2, Organic Acids-3.

Abstract: Two reaction sequences postulated for liquid phase hydrocarbon oxidation are studied from a kinetic and flow standpoint. Considering that the desired products are degradable intermediates, the interrelationships between conversion of feed, selectivity to intermediate, yield, and reactor type are discussed. Comparison with experimental data on cyclohexane oxidation is given.

(*Continued on page 594*)

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uid equilibrium constants were available for the isomeric hexanes with other compounds. However, no such data were found.

CONCLUSIONS

1. Kihara and Lennard-Jones parameters were determined for the isomeric hexanes.
2. Values of 2,3-dimethylbutane viscosity estimated from Equation (3) were close to experimental data.

NOTATION

$A_o{}^o$ = Angstrom unit
B = second virial coefficient, cc./g. mole
M = molecular weight
M_o = surface integral of mean curvature of the Kihara model over the model surface $(A_o{}^o)^2$
S_o = surface area of Kihara model
T = temperature, °K.
$U(r)$ = Lennard-Jones potential energy
$U(\rho)$ = Kihara potential energy
U_o = maximum potential energy
V_o = volume of Kihara model, $(A_o{}^o)^3$
k = Boltzmann constant
l_1, l_2, l_3 = characteristic dimensions of Kihara model, $A_o{}^o$

Greek Letters

ϵ = parameter of Lennard-Jones potential
σ = parameter of Lennard-Jones potential
ρ = minimum distance separating Kihara cores
ρ_o = shortest distance between Kihara cores and energy minimum
μ = viscosity g./cm. sec.
$\Omega\mu$ = function of kT/ϵ

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