

Comments on “Intermolecular Forces: Thermal Diffusion and Diffusion in He-Kr and H₂ - Kr”

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Citation: [Physics of Fluids](#) **12**, 1531 (1969); doi: 10.1063/1.1692706

View online: <http://dx.doi.org/10.1063/1.1692706>

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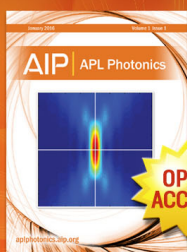
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$$\begin{aligned}
 E'_x &= i \left(\Psi \frac{\partial E}{\partial x} - \frac{\bar{\omega} B}{kc} \frac{\partial \Psi}{\partial x} \right), \\
 E'_y &= \bar{\omega} \frac{B}{c} \Psi, \\
 V'_x &= \bar{\omega} \Psi, \\
 V'_y &= \frac{i}{k} \left[\frac{kcE}{B} \Psi \left(\eta - \frac{1}{E} \frac{\partial E}{\partial x} \right) + \bar{\omega} \frac{\partial \Psi}{\partial x} \right], \\
 j'_z &= \frac{1}{4\pi} \left[\Psi \left(\omega \frac{\partial E}{\partial x} - kc\eta B \right) - \frac{\bar{\omega} B}{kc} \frac{\partial \Psi}{\partial x} \right], \\
 j'_x &= -\frac{i}{4\pi} \left[\Psi \left(\omega \bar{\omega} \frac{B}{c} + c \frac{\partial^2 B}{\partial x^2} \right) + c\eta B \frac{\partial \Psi}{\partial x} \right], \\
 B' &= i\eta B \Psi, \\
 \rho' &= i\Psi \frac{\partial \rho}{\partial x}, \\
 p' &= i\Psi \frac{\partial p}{\partial x}, \\
 R' &= i\Psi \frac{\partial R}{\partial x},
 \end{aligned}
 \tag{10}$$

and

$$\begin{aligned}
 \sigma' &= \frac{i}{4\pi} \left[\Psi \left(\frac{\partial^2 E}{\partial x^2} + \frac{kB}{c} \bar{\omega} \right) \right. \\
 &\quad \left. + \frac{\partial \Psi}{\partial x} \left(2 \frac{\partial E}{\partial x} - \frac{\omega \eta B}{kc} \right) - \frac{\bar{\omega} B}{kc} \frac{\partial^2 \Psi}{\partial x^2} \right].
 \end{aligned}$$

In writing these expressions Maxwell's equations and relation (9) have been used wherever necessary.

Finally taking the Z component of the curl of the linearized form of Eq. (6) and using relations (10) we obtain (after some algebraic reductions)

$$\frac{\partial}{\partial x} \left(\rho T \frac{\partial \Psi}{\partial x} \right) - k^2 \rho T \Psi + k^2 \sum g \frac{\partial \rho}{\partial x} \Psi = 0 \tag{11}$$

with

$$T = (1 + b^2) \bar{\omega}^2 + \frac{k \bar{\omega}}{\rho \Omega} \left(\frac{\partial p}{\partial x} + \eta p \right) + \frac{k^2 \eta}{\rho \Omega^2} \frac{\partial R}{\partial x}$$

and

$$b^2 = B^2 / 4\pi \rho c^2.$$

Equation (11) agrees with Eq. (45) of Ref. 6. For a low β plasma ($\eta = 0$) this equation immediately reduces to Eq. (3.12) of Ref. 1.

¹ M. N. Rosenbluth and A. Simon, *Phys. Fluids* **8**, 1300 (1965).

² N. K. Bajaj and J. N. Tandon, *Nucl. Fusion* **8**, 297 (1968).

³ R. Hardan and B. S. Liley, *Rev. Mod. Phys.* **32**, 731 (1960).

⁴ N. K. Bajaj, *Phys. Fluids* **11**, 2059 (1968).

⁵ A. A. Ware, *Phys. Fluids* **9**, 816 (1966).

⁶ L. D. Pearlstein and N. A. Krall, *Phys. Fluids* **9**, 2231 (1966).

Comments on "Intermolecular Forces: Thermal Diffusion and Diffusion in He-Kr and H₂-Kr"

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(Received 30 December 1968)

In the paper by Annis, Humphreys, and Mason,¹ deviations from the geometric mean combining rule for the characteristic energy parameter were suggested as the major cause of disagreement between theoretical and experimental diffusion properties. These deviations from the geometric mean rule are also found by evaluating phase equilibrium and volumetric data.

A comprehensive study of phase equilibrium properties of binary systems containing helium, neon, and hydrogen with light hydrocarbons led us to relate the deviations from the geometric mean combining rule to the ionization potentials I of the component species. This relation, presented earlier² in a preliminary way, is expressed as

$$k_{12} = 0.17(I_1 - I_2)^{1/2} \ln(I_1/I_2), \tag{1}$$

where k_{12} is defined by

$$\epsilon_{12} = (1 - k_{12})(\epsilon_{11}\epsilon_{22})^{1/2}. \tag{2}$$

The magnitude of k_{12} must be a fundamental property of the binary interaction. It was found³ that Eq. (1) predicts k_{12} values of the correct magnitude for a variety of binary systems, though experimental values of k_{12} were obtained with different models.

In Table I, column 2 shows k_{12} values computed from the beam-scattering data of Helbing *et al.*⁴ (cited in the subject paper) for the systems listed in column 1. Corresponding values computed from Eq. (1) are given in column 3. Ionization potentials used in Eq. (1) were taken from the Handbook of

TABLE I. Deviations from geometric mean combining rule.

System	k_{12}		
	Beam scattering ^a ($L - J$ 12:6)	Eq. (1)	Equilibrium data ^b
He-Ne	0.119	0.038	0.07
He-Ar	0.253	0.237	0.22
He-Kr	0.359	0.312	...
He-Xe	0.406	0.422	0.40
Ne-Kr	...	0.203	0.20
H ₂ -Ne	0.152	0.132	...
H ₂ -Ar	-0.099	0.001	0.00
H ₂ -Kr	0.007	0.026	...
H ₂ -Xe	0.047	0.082	...

^a Reference 4.

^b Reference 3.

Chemistry and Physics, with the exception of that for Ar, 15.4 eV, taken from the International Critical Tables. Column 4 gives values of k_{12} computed for Eq. (2) from experimental equilibrium data. Except for k_{12} values for the He-Ne and H₂-Ar systems from the beam-scattering data, there is good agreement in all cases.

Annis *et al.* found that ϵ_{12}/k values for the exp-6 potential, obtained from the geometric mean combining rule, required adjustment by amounts equivalent to k_{12} values of 0.35 and 0.00 to best represent

experimental diffusion properties of the He-Kr and and H₂-Kr systems, respectively. Values of k_{12} computed from Eq. (1) support their findings.

¹ B. K. Annis, A. E. Humphreys, and E. A. Mason, *Phys. Fluids* **11**, 2122 (1968).

² M. J. Hiza and A. G. Duncan, in *Advances in Cryogenic Engineering*, K. D. Timmerhaus, Ed. (Plenum Press, Inc., New York, 1969), Vol. 14.

³ M. J. Hiza and A. G. Duncan, *A. I. Ch. E. J.* (to be published).

⁴ R. Helbing, W. Gaide, and H. Pauly, *Z. Physik* **208**, 215 (1968).