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MOLECULAR BEAM SOURCES FABRICATED FROM MULTICHANNEL ARRAYS. PART IV. SPEED DISTRIBUTION IN THE CENTER-LINE BEAM

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ERRATA

TO: All recipients of UCRL-19084

FROM: Technical Information Division

RE: MOLECULAR BEAM SOURCES FABRICATED FROM MULTICHANNEL ARRAYS - Part IV: Speed Distribution in the Center-line Beam, by D. R. Olander, R. H. Jones and W. Siekhaus, Inorganic Materials Research Division, LRL, Department of Nuclear Engineering, College of Engineering, University of California, Berkeley, Calif. dated November 1969.

Please correct title of subject report to read as above. Note that this is Part IV and not Part III as was previously indicated.

Part III is UCRL-19603.

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MOLECULAR BEAM SOURCES FABRICATED FROM MULTICHANNEL ARRAYS

Part III Speed Distribution in the Centerline Beam

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ABSTRACT

The collision model utilized by Giordmaine and Wang to describe the centerline beam intensity from long tubes has been extended to account for molecular speed effects. The modification was accomplished by utilizing the velocity dependent mean free path instead of the Maxwellian averaged value. The analysis shows that the centerline beam intensity (or peaking factor) is practically unaffected by explicitly accounting for the distribution of molecular speeds. The speed distribution on the axis of the beam, however, is depleted of slow speed molecules. The perturbation of the Maxwellian spectrum begins at a Knudsen number based on tube length of ~10. For Knudsen numbers less than ~0.1, the spectrum is no longer dependent of the Knudsen number. The average translational energy of the centerline beam in the low Knudsen number limit is 5-1/2% greater than that of a Maxwellian beam.

Non-Maxwellian distributions of molecular speeds in a molecular beam from thin-walled orifices have frequently been observed. The perturbed spectrum, which is deficient in low speed molecules, has been explained in terms of beam-background scattering by Manista[1] and ascribed to beam-beam scattering by Estermann et al.[2]

The angular distribution of the efflux from a long tube has been shown by Giordmaine and Wang[3] to be governed by intermolecular collisions within the channel proper. In the following analysis, the model proposed by Giordmaine and Wang is extended and shown to produce a non-Maxwellian speed distribution of the molecular beam as well.

The total flow rate through a channel can be represented by the Knudsen formula provided that the Knudsen number based on tube diameter is of order unity or greater. The angular and velocity distributions, on the other hand, are much more sensitive to intermolecular collisions within the channel than is the total flow. In order to achieve the angular distribution calculated by Clausing[4] and a Maxwellian speed spectrum, the Knudsen number based upon tube length must be greater than unity.

In the speed-independent model of Giordmaine and Wang[3] the center-line intensity of the molecular beam consists of two parts: 1) a component due to intermolecular collisions within the channel which result in scattered molecules directed along the tube axis, 2) a component due to molecules from the source reservoir which succeed in travelling down the tube axis without colliding with other molecules.

In order to formulate the quantitative contributions of these two components, the number density within the tube is a priori assumed to vary linearly from a specified value n_s in the source reservoir to zero at the tube exit. At any point in the channel, the gas in which

intermolecular collisions occur is assumed to possess an isotropic angular distribution and a Maxwellian speed distribution. Intermolecular scattering is of the classical hard sphere type, with a cross section of $\pi\sigma^2$.

This model is depicted in Fig. 1 for a single circular tube of length L and radius a. Collision-free flow is considered to prevail downstream of the exit. (In a multichannel source, each channel is assumed to behave independently of its neighbors.) The two contributions to the centerline beam intensity, $j_1(v)$ and $j_2(v)$, are drawn off-axis in Fig. 1 for clarity of illustration only.

In the one speed model considered by Giordmaine and Wang, the probability that a molecule produced at location y in the tube escaped without further collisions was taken as $\exp[-\int_0^y dy/\lambda(y')]$, where $\lambda(y)$ is the local mean free path corresponding to the gas density at position y. Since the gas density is assumed to vary as:

$$n(y) = n_s\, y/L \tag{1}$$

and

$$\lambda(y) = [\sqrt{2}\pi\sigma^2\, n(y)]^{-1} \tag{2}$$

the escape probability can be written as $\exp[-(y/L)^2/2Kn]$, where Kn is the Knudsen number based on channel length:

$$Kn = \lambda_s/L \tag{3}$$

λ_s is the mean free path in the source reservoir.

This model may be modified to allow for velocity dependence by utilizing the classical expression for the mean free path of a molecule of specified speed in a Maxwellian gas:[5]

$$\lambda(z,y) = \lambda(y)/\psi(z) \tag{4}$$

$\lambda(y)$ is given by Eq. (2) and z is the reduced speed v/α, where $\alpha = (2kT/m)^{1/2}$ is the most probable speed of a Maxwellian gas at the source temperature. The function $\psi(z)$ is:[5]

$$\psi(z) = \frac{ze^{-z^2} + \frac{\sqrt{\pi}}{2}(1+2z^2)\,\mathrm{erf}(z)}{\sqrt{2\pi}\ z^2} \qquad (5)$$

If the velocity dependent mean free path of Eq. (4) is utilized in place of the average mean free path of Eq. (2) the escape probability for molecules of reduced speed z is $\exp[-\psi(z)(y/L)^2/2Kn]$. The function $\psi(z)$ approaches infinity as $z \to 0$ and has a limiting value of $1/\sqrt{2}$ as $z \to \infty$. Because of this dependence on speed, slow molecules have a lower escape probability than high speed ones. Manista[1] has applied the concept of the velocity dependent mean free path to successfully predict the spectrum hardening of a beam from an orifice after passage through a constant density background gas. In the present analysis, however, collisions occur within the beam-forming channel itself, and do not involve background species.

Consider the contribution of intermolecular collisions within the tube to the centerline beam intensity (j_1). The probability per second of a collision between a molecule of reduced speed z with a Maxwellian gas at a total density of n(y) is the distance travelled in one second divided by the mean free path of the molecule, or $\sqrt{2\pi}\ \sigma^2\ n(y)\alpha z\ \psi(z)$.[5] The number of molecules per second per unit volume in the reduced speed range between z and z + dz entering collisions is this collision probability multiplied by the number of molecules with speeds in this range, which is $n(y)f_M(z)\,dz$. Here $f_M(z)$ denotes the Maxwellian speed distribution:

$$f_M(z) = \frac{4}{\sqrt{\pi}}\ z^2\ e^{-z^2} \qquad (6)$$

According to the principle of detailed balance, the number of molecules in a particular speed range entering collisions is equal to the number of molecules in the same speed range produced by collisions. Of the $\sqrt{2}\pi\sigma^2[n(y)]^2\ \alpha z\psi\ (z)\ f_M(z)\ dz(\pi a^2\ dy)$ molecules with speeds between z and z + dz which are produced per second in a slice dy of the channel, a fraction $1/4\pi$ is emitted into a unit solid angle along the tube axis. Finally, of the molecules produced by collisions in dy which have the proper direction and speed, only a fraction $\exp[-\psi(z)(y/L)^2/2Kn]$ succeeds in passing through the remaining gas in the tube and contributing to the molecular beam. The j_1 contribution to the beam (in units of molecules/sec-sr-unit reduced speed) can be written as:

$$j_1(z) = \int_0^L (\pi a)^2 \sqrt{2}\pi\sigma^2\ n_s^{\ 2}\ \alpha_z\ \psi(z)\ f_M(z)(y/L)^2 \times (1/4\pi)\ \exp[-\psi(z)(y/L)^2/2Kn] \qquad (7)$$

Performing the integration over y yields:

$$j_1(z) = j_M(z)\left\{-e^{-\psi(z)/2Kn} + \frac{\sqrt{\pi}}{2}\ \frac{\operatorname{erf}\sqrt{\psi(z)/2Kn}}{\sqrt{\psi(z)/2Kn}}\right\} \qquad (8)$$

where $j_M(z)$ is the Maxwellian speed spectrum of the centerline flux from an ideal orifice of radius a:

$$j_M(z) = (1/4)\ n_s\ a^2\ \alpha z\ f_M(z) \qquad (9)$$

The component of the flux due to molecules which originate in the source reservoir and pass through the channel without collision is:

$$j_2(z) = j_M(z)\ e^{-\psi(z)/2Kn} \qquad (10)$$

Adding Eqs. (8) and (10), the centerline beam intensity can be written as the product of the ideal orifice Maxwellian distribution and a perturbation function:

$$j(z) = j_M(z)\ P[Kn,\ \psi(z)] \tag{11}$$

where

$$P[Kn,\ \psi(z)] = \frac{\sqrt{\pi}}{2}\ \frac{\operatorname{erf}\sqrt{\psi(z)/2Kn}}{\sqrt{\psi(z)/2Kn}} \tag{12}$$

If $\psi(z)$ is set equal to unity in Eq. (12), integration of Eq. (11) over all reduced speeds yields the total centerline intensity deduced by Giordmaine and Wang[3] for the one-speed model (given as Eq. (8) in Ref. 6).

The normalized number density speed distribution of the centerline beam can be written from Eqs. (9) and (11) as:

$$f(z) = \frac{f_M(z)\ P[Kn,\psi(z)]}{\int_0^\infty f_M(z)\ P[Kn,\psi(z)]\,dz} \tag{13}$$

As $Kn \to \infty$, the perturbation function approaches unity and the speed distribution in the beam becomes Maxwellian:

$$\lim_{Kn \to \infty} f(z) = f_M(z) \tag{14}$$

As the Knudsen number becomes small, however, the perturbation function behaves as $[\pi\ Kn/2\psi(z)]^{1/2}$ and the speed spectrum approaches a limiting shape which is independent of the Knudsen number:

$$\lim_{Kn \to 0} f(z) = \frac{f_M(z)/[\psi(z)]^{1/2}}{\int_0^\infty f_M(z)/[\psi(z)]^{1/2}\,dz} \tag{15}$$

The Maxwellian and the fully saturated spectrum are shown in Fig. 2. By comparison to a Maxwellian distribution, the saturated spectrum is

deficient in low speed molecules. This shape is quite similar to that calculated and observed by Manista[1] for an originally Maxwellian beam traversing an isotropic background gas. However, the phenomenon of a limiting distribution is unique. Saturation occurs when the Knudsen number is small enough so that all direct flight molecules from the source reservoir are removed from the beam (i.e., $j_2 \approx 0$). The entire centerline beam is then due to molecules which have undergone collisions with other molecules in a region upstream of the exit (i.e. only the j_1 contribution remains). Further increase in either the length of the tube or in the source reservoir pressure (provided that hydrodynamic flow does not become significant) no longer affects the velocity distribution of the molecular beam. The change from Maxwellian to saturation distributions occurs over the range $0.1 < Kn < 10$.

The Peaking Factor

The degradation of the peaking factor according to the one-speed model of Giordmaine and Wang was discussed in Part I (Ref. 6). The effect of employing a velocity dependent mean free path in place of the Maxwellian averaged value can be calculated by integrating Eq. (11) over all reduced speeds and using the resulting expression for the total centerline intensity instead of Eq. (8) of Part I. This procedure yields:

$$\chi/\chi_{max} = \frac{\sqrt{\pi}}{2} \int_0^\infty z\, f_M(z)\, P[Kn, \psi(z)]\, dz \qquad (16)$$

The original formula due to Giordmaine and Wang is recovered by inserting the perturbation function of Eq. (12) with $\psi(z)$ set equal to unity into Eq. (16):

$$(\chi/\chi_{max})_{G\text{-}W} = P[Kn,1] = \frac{\sqrt{\pi}}{2}\, \frac{\operatorname{erf}\sqrt{1/2Kn}}{\sqrt{1/2Kn}} \qquad (17)$$

The peaking factors of Eqs. (16) and (17) are plotted as functions of the reciprocal Knudsen number in Fig. 3. The difference between the two curves is never greater than a few percent, which is insignificant from a practical point of view. The single speed model of Eq. (17) is therefore perfectly adequate for predicting beam intensities from near-effusive channel sources.

Average Translational Beam Energy

The average translational energy of a molecule in the beam is an important factor in determining the probability of interaction between a beam particle and a target. This same parameter also provides a convenient means for quantifying the "hardness" of the centerline speed distribution. The average translational energy of a molecule in the beam is:

$$\bar{\epsilon} = 1/2(m\,\alpha^2)\,\frac{\int_0^\infty z^3\, f(z)\, dz}{\int_0^\infty z f(z)\, dz} \tag{18}$$

If the speed distribution is Maxwellian, the average beam energy is $m\alpha^2$. If the average energy of Eq. (18) is referenced to the Maxwellian value, $\bar{\epsilon}_M$, one obtains:

$$\bar{\epsilon}/\bar{\epsilon}_M = \frac{\int_0^\infty z^3\, f_M(z)\, P[Kn,\psi(z)]dz}{2\int_0^\infty z\, f_M(z)\, P[Kn,\psi(z)]\, dz} \tag{19}$$

Equation (19) is plotted on Fig. 4. The average beam energy increases by only 5.5% between the very low pressure Maxwellian limit and the high pressure saturation region. The one-speed model of course gives an average energy characteristic of a Maxwellian beam.

The average beam energy and the peaking factor both begin to be affected

by intermolecular collisions in the channel at Kn < 10. (If the length-to-diameter ratio of the tube is 10, non-Maxwellian behavior can be expected for diameter based Knudsen numbers of 100 or less.)

For Knudsen numbers (based on length) of less than 0.1, the spectrum has achieved its limiting shape, the average translational energy is constant at a value 5.5% greater than a Maxwellian beam at the same source temperature, and the peaking factor varies as the square root of the source reservoir pressure. At very small Knudsen numbers the system approaches the behavior of a hydrodynamic jet. For a completely expanded nozzle beam (i.e., complete conversion of thermal energy to directed kinetic energy) the beam energy ratio is $\gamma/2(\gamma-1)$ where γ is the specific heat ratio of the gas. The beam energy ratio in this limit is 1.25 for a monatomic gas and 1.75 for a diatomic gas.

Limitations of the Model

The analysis presented here contains all of the basic limitations of the Giordmaine and Wang model. These are:

1) The total number density varies linearly with distance in the tube.

2) The gas within the tube is isotropic.

3) The number density at the inlet and exit are specified as the source reservoir density and zero, respectively.

4) Collisions are of the hard sphere type.

Specifications 1-3 amount to judicious a priori estimates of several features of the exact solution to the kinetic theory problem, which, of course, has not been solved. Assumptions 2 and 3 are increasingly valid as the length-to-diameter ratio becomes large. Because of the net flow through the tube, the gas within the tube cannot be isotropic, nor can the

density at the exit (which is the flow rate divided by the average velocity component along the axis) be zero. Relaxation of assumption 3, within the context of the one-speed model, has been accomplished.[7,8]

The model (with or without the velocity dependence of the mean free path) is tenable mainly because of the simplicity of the calculations compared to an exact solution and because of the reasonable agreement with peaking factor measurements reported in Ref. 6 and with the spectrum hardening measurements reported in the following paper.

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LIST OF FIGURES

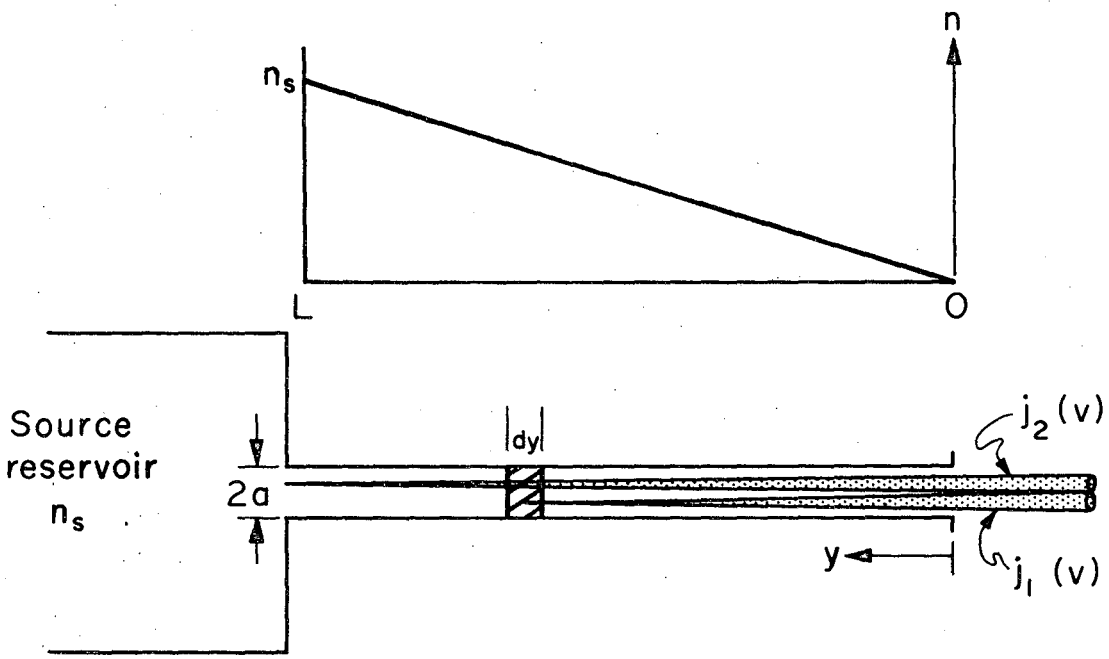

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Fig. 1

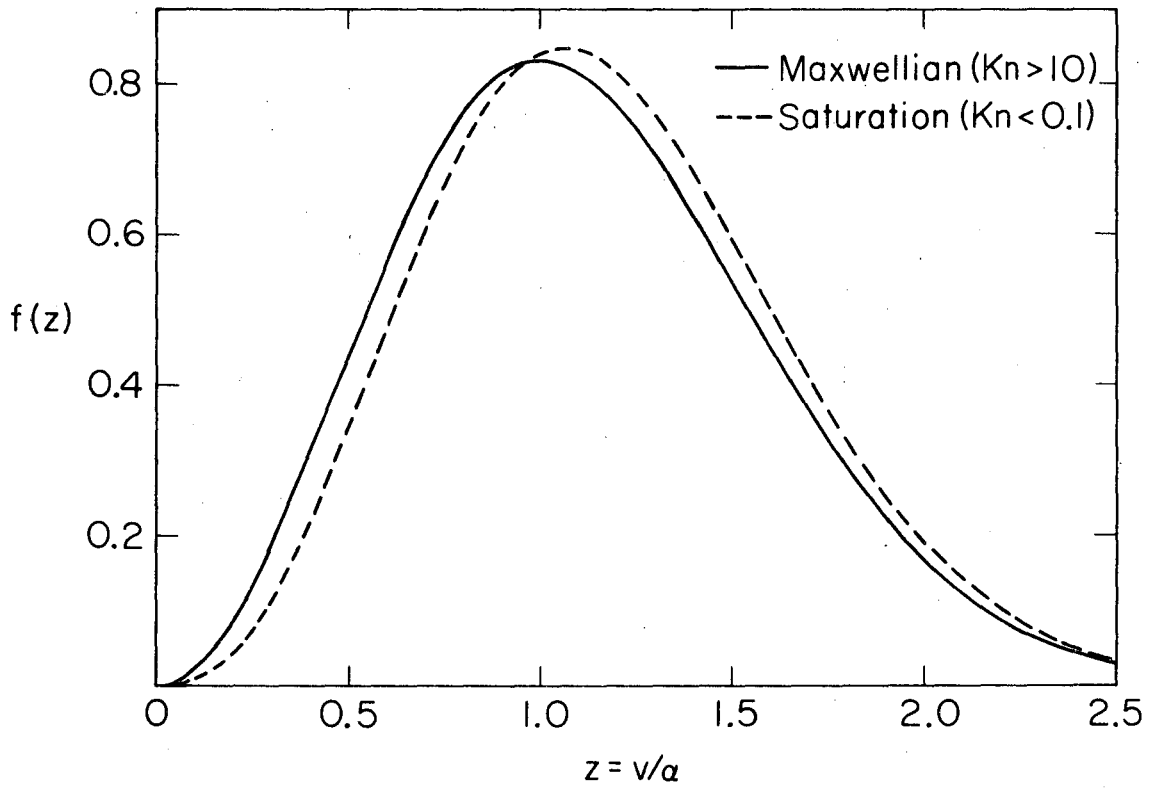

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Fig. 2

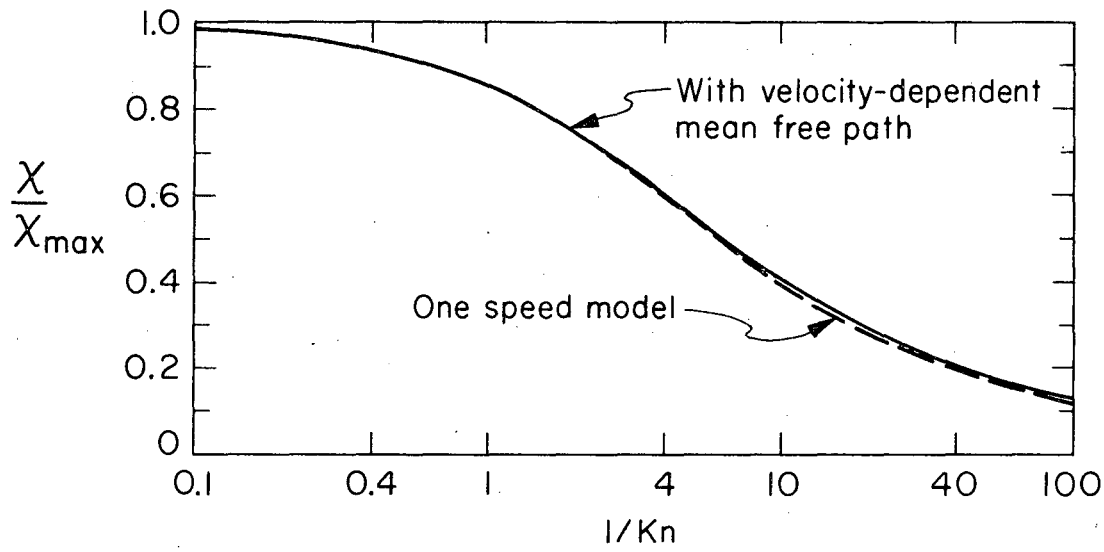

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Fig. 3

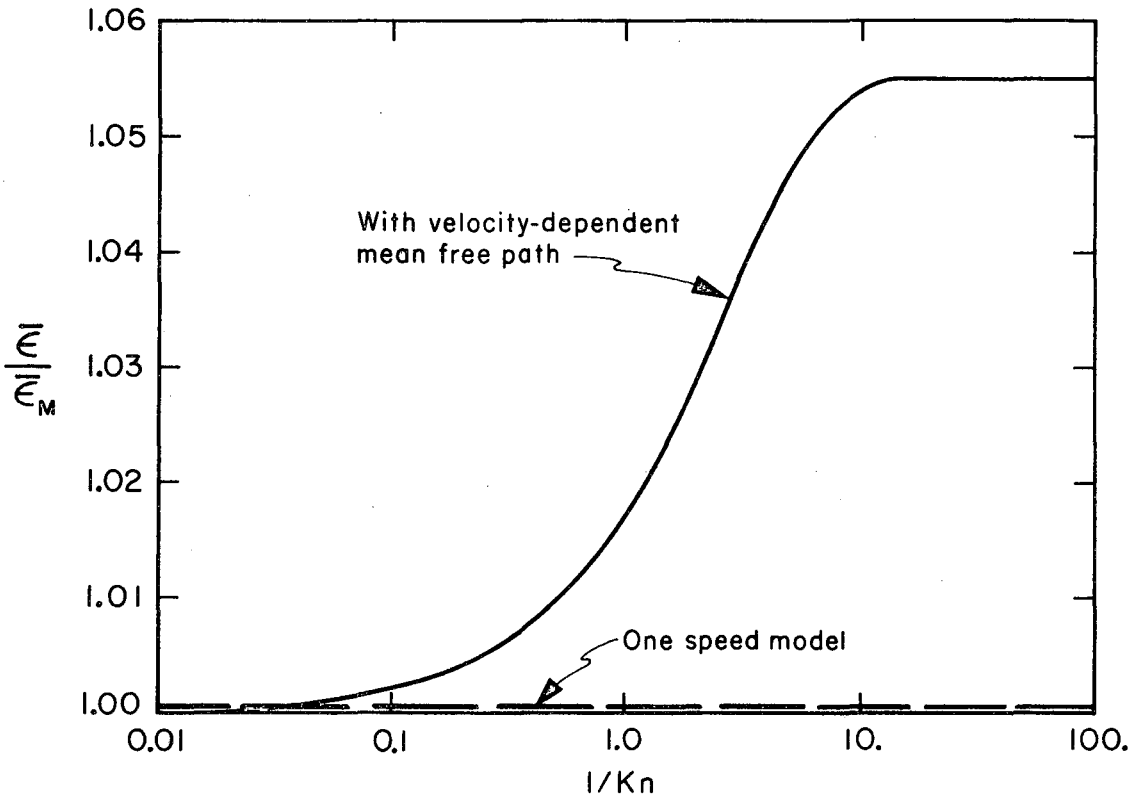

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Fig. 4

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