

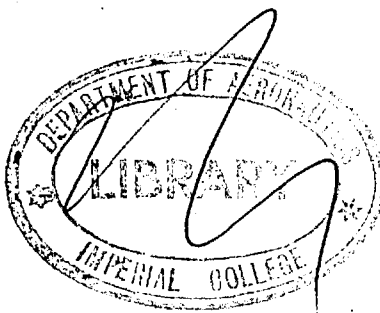
NUMERICAL SOLUTIONS TO TWO
PROBLEMS IN FLUID MECHANICS

PART I LEADING EDGE SEPARATION FROM
A YAWED SLENDER DELTA WING

PART II RAREFIED LEADING EDGE FLOW
OF A DIATOMIC GAS

BY

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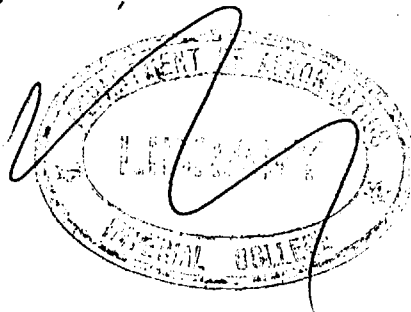
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PART I: LEADING EDGE SEPARATION FROM
A YAWED SLENDER DELTA WING

Abstract

The author's treatment of the Mangler and Smith vortex-sheet model of leading-edge separation is extended to the calculation of steady conical flow past a yawed slender delta wing. Introducing yaw destroys the symmetry property inherent in the unyawed problem necessitating that the two leading-edge vortex sheets be treated as independent but mutually interacting singularity distributions in the cross-flow plane of the slender-body theory. From the calculations, predictions are obtained of the variation of the principal quantitative flow characteristics - including the two primary vortex core positions and the wing rolling-moment coefficient - with the incidence and yaw parameters. Comparison of these predictions with experimental data is reasonable qualitatively but only fair quantitatively, the discrepancies being attributed to the neglect, in the flow model, of the effects of the secondary separation system on the windward side of the wing. The range of the present calculations is to some extent limited by an unexplained failure of the solution technique at lower values of the incidence parameter.



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NOTATIONSymbols

a	$= \alpha/K$, incidence parameter
A_j	coefficient in expression for vortex-sheet shape near a leading edge, see equation (26)
$A_{\ell m}$	coefficient in trapezoidal rule quadrature as defined for equations (24)
A_{-1}	coefficient of Z^{-1} in expansion of W for large Z
b	$= \beta/K$, yaw parameter
B_j	coefficient in expression for vortex-sheet shape near a leading edge, see equation (26)
C_j	denotes cross-section of j^{th} vortex-sheet in the Z -plane
C_j^*	transformed shape of C_j in the Z^* -plane
C_j^{i*}	image of C_j^* in the circle $ Z^* = s$
C_p	pressure coefficient
C_N	normal-force coefficient (z direction)
C_Y	side-force coefficient (y direction)
C_L	rolling-moment coefficient
$\left[\frac{C_N}{K^2} \right]_{\text{ATT}}$	$\frac{C_N}{K^2}$ in attached flow
$\left[\frac{C_L}{K^2} \right]_{\text{ATT}}$	$\frac{C_L}{K^2}$ in attached flow
C_{-1}	coefficient of ω^{-1} in expansion of W/KU_s for large ω

Symbols (cont.)

D_j	x-wise moment acting on j^{th} cut, see equation (33)
E_j	= 0, symbolic representation of j^{th} zero-force condition [equations (30)]
f_k	= 0, symbolic representation of k^{th} equation, in equations (36)
F	function used in constructing the complex velocity potential in the Z^* -plane
$F_{k\ell}$	matrix coefficient defined in equation (37)
g	function which appears in the slender-body theory, see equation (3)
G_j	= Γ_j/KU_s , nondimensional circulation about the j^{th} vortex-sheet
h_n	quantity defined in equation (21C)
H_{jn}	= 0, symbolic representation of finite difference form of equations (17) at j - n^{th} point
Im	imaginary part
K	= $\tan \delta$
ℓ	x-distance from apex, see equation (A2.1)
L_j	denotes j^{th} leading-edge in the Z -plane
L_j^*	point to which L_j is transformed, in the Z^* -plane
L	rolling moment
L_{ATT}	rolling moment in attached flow
M	= 0, symbolic representation of zero-moment condition [equation (35)]

Symbols (cont.)

M_0	free stream Mach number
N	normal force
p	static pressure
P_j	point on C_j in Z -plane
P_j^*	point on C_j^* in Z^* -plane
Q_j	$= 0$, symbolic representation of Kutta conditions [equations (28)]
r_j	scalar distance of P_j from the origin of the Z -plane
Re	real part
s	local wing semi-span
t_j^*	sliding point on the j^{th} vortex-sheet in the Z -plane [see equation (14)]
U	free stream speed
V	see equation (40)
W	complex velocity potential
x, y, z	rectangular cartesian co-ordinates, fixed on the wing
Y	total side (y-wise) force acting on wing plus vortex-sheets
Z	complex variable in the cross-flow plane
Z_j	a value of Z on the j^{th} vortex-sheet
Z^*	complex variable in the transformed plane
Z_j^*	a value of Z^* on the j^{th} vortex-sheet

Symbols (cont.)

α	incidence angle of the wing
β	yaw angle of the wing
γ	exponent defined for equation (27)
Γ_j	circulation about j^{th} vortex-sheet
δ	semi-apex angle of the wing
Δ	difference operator across vortex-sheet, see equations (4) and (5)
$\Delta\phi_j$	potential difference across j^{th} vortex-sheet
Δp_j	pressure difference across j^{th} cut in cross-flow plane
ΔC_{p_j}	pressure coefficient difference across j^{th} cut
η, η_j, η_{jn}	$= \text{Im}(\omega), \text{Im}(\omega_j), \text{Im}(\omega_{jn})$ respectively
$\eta^*, \eta_j^*, \eta_{jn}^*$	$= \text{Im}(\omega^*), \text{Im}(\omega_j^*), \text{Im}(\omega_{jn}^*)$ respectively
θ_j	angle in cross-flow plane, see Fig.2
λ_j	$= 1 - \Delta\phi_j/\Gamma_j$, nondimensional potential difference across j^{th} vortex-sheet
λ_{jn}	value of λ_j at ω_{jn} or ω_{jn}^*
$\lambda_{jn,n-1}$	value of λ_j defined in equations (23)
μ	exponent defined for equation (26)
ξ, ξ_j, ξ_{jn}	$= \text{Re}(\omega), \text{Re}(\omega_j), \text{Re}(\omega_{jn})$ respectively
$\xi^*, \xi_j^*, \xi_{jn}^*$	$= \text{Re}(\omega^*), \text{Re}(\omega_j^*), \text{Re}(\omega_{jn}^*)$ respectively

Symbols (cont.)

ρ	free stream density
σ_j	arc length along C_j [see equations (4) and (5)]
τ_j^*	$= \frac{t_j^*}{s}$
ϕ	quasi two-dimensional velocity potential
ϕ_0	slender-body theory perturbation potential
χ_j	angle in cross-flow plane, see Fig.2
Φ	complete velocity potential
ψ_j	angle in the cross-flow-plane, see Fig.2
ω	$= Z/s$, non-dimensional complex variable in the cross-flow plane
ω_j	a value of ω on the j^{th} vortex-sheet
ω_{jn}	complex co-ordinate of the n^{th} point on the j^{th} vortex-sheet, in the ω -plane
$\omega_{jn,n-1}$	point to which $\omega_{jn,n-1}^*$ is transformed, in the ω -plane
ω^*	$= \frac{Z^*}{s}$, non-dimensional complex variable in the transformed plane
ω_j^*	a value of ω^* on the j^{th} vortex sheet
ω_{jn}^*	complex co-ordinate of the n^{th} point on the j^{th} vortex sheet in the ω^* -plane
$\omega_{jn,n-1}^*$	midpoint of ω_{jn}^* and ω_{jn-1}^* , defined by equations (23)
Ω	vectorial representation of the unknowns of equations (36)

Symbols (cont.)

Ω_l l^{th} component of Ω

Ω^p p^{th} approximation to a solution of equations (36)

Ω_l^p l^{th} component of Ω^p

$\delta\Omega_l^{p,p+1} = \Omega_l^{p+1} - \Omega_l^p$

Subscripts

j refers to a quantity on a vortex-sheet, $j=1$, leeward sheet;
 $j=2$, windward sheet

k k^{th} equation in equations (36)

l, m dummy subscripts in summation terms; m also denotes the mean value across a vortex sheet

n refers to n^{th} point on a vortex-sheet

N number of points on the outer part of a vortex-sheet

1. INTRODUCTION

In recent years, many theoretical studies of the phenomenon of separated flow about unyawed slender delta wings have appeared in the literature^{(1),(2),(3)}. This work culminated in that of Smith⁽⁴⁾, who presented the first really adequate approach to the calculation of flows involving leading-edge separation. Following the earlier work of Mangler and Smith⁽³⁾, Smith considered a flow model, based on the slender-body theory, in which each of the two spiral vortex sheets representing leading-edge separation are broken up into an outer part, retaining a sheet-like character, and an inner part, the circulation of which is concentrated on to an isolated vortex. He developed an ad-hoc iterative technique for the numerical treatment of this model and used this scheme to calculate the flow, with leading edge separation, past an unyawed semi-infinite flat-plate delta wing. Levinsky and Wei⁽⁵⁾ have subsequently employed the same method to treat slender bodies formed of combinations of circular/elliptical cones and flat-plate delta wings. Smith⁽⁶⁾ has since extended his treatment to deal with leading-edge separation from slender rhombic cones thus calculating for the first time the formation of a free vortex sheet at a leading edge of non zero cross-section angle, while Barsby⁽⁷⁾ has used a variation of the Smith approach to investigate the effect of blowing from the leading-edge of a slender delta wing.

Earlier, an alternative model for the treatment of separated flows had been developed by Sacks et al.⁽⁸⁾. In this approach, the separated shear layers are represented by discrete vortices - shed from the wing leading-edges - which are allowed to convect in an inviscid unsteady flow. This model is suitable for the calculation of nonconical flows but, like all approaches based on the slender-body theory, trailing edge effects cannot be directly taken into account. Simplified flow models for low aspect-ratio wings in which trailing effects are included, have been presented by Garner and Lehrian⁽⁹⁾, by Polhamus⁽¹⁰⁾, and by Nangia and Hancock⁽¹¹⁾.

More recently, the author⁽¹²⁾ has developed an alternative technique to Smith, for the treatment of the slender-body theory vortex-sheet model of conical separated flow. This approach, following Legendre⁽¹⁾, formulates the general problem for an arbitrary number of vortex sheets, as a system of singular nonlinear integro-differential equations. A finite

difference representation of these equations, based on the Mangler and Smith vortex-sheet-cut-isolated-vortex model, is constructed, and a Newton-Raphson solution procedure is presented. Some calculated examples with simple leading-edge separation are given.

In all of the above-mentioned work, the slender bodies being treated have incidence to the oncoming stream, but not yaw, thus introducing a plane of symmetry into the problem. A slender conical body with both incidence and yaw may be expected to exhibit a region of approximately conical flow near the apex, and it therefore seems natural to extend the vortex-sheet model to the calculation of such flows. Ribner⁽¹³⁾ has treated attached flow past a yawed slender delta wing with and without dihedral, obtaining predictions of the lift and rolling moment, but to the author's knowledge no treatment of the yawed wing problem in which leading-edge separation is included, has yet appeared.

On the experimental side, Fink⁽¹⁴⁾ carried out some preliminary measurements of the pressure distribution on a thin yawed slender delta wing in a region of approximately conical flow. This experimental programme was completed by Harvey⁽¹⁵⁾, who, in addition to pressure measurements, took detailed flow field total head surveys from which the positions of the vortex cores of the windward (attacking edge) and leeward leading-edge vortex systems were obtained. By integration of the wing pressure distribution, he also obtained the local lift and rolling-moment coefficients.

From these experiments it was apparent that yawing the wing strengthened the windward vortex system which moved inboard and closer to the wing surface. Exactly the converse happened to the leeward system.

In the present work, the problem of flow with leading-edge separation past a semi-infinite flat plate delta wing - with both incidence and yaw - is treated using the inviscid slender-body theory. This allows the construction of a quasi two-dimensional complex velocity potential in the cross-flow plane. The flow is assumed to be conical and flow separation is taken to occur only at the wing "leading-edges". Firstly, the set of integro-differential equations for the strength and position of the two vortex sheets which represent the respective separated shear-layer core systems is derived, and a finite difference representation of these equations is formulated, based on the Mangler and Smith vortex-sheet-cut-

isolated-vortex model. A Newton-Raphson iterative procedure is then used to solve the resulting set of nonlinear algebraic equations for a range of values of the incidence and yaw parameters.

From the solutions, predictions are obtained of the positions of the vortex core centres of the leeward and windward separation systems, and also of the wing surface pressure distribution and hence of the wing normal-force and rolling-moment coefficients. Comparison of the variation of these quantities with incidence and yaw, with the experimental data of Harvey⁽¹⁵⁾ is fair, differences being largely attributed to the neglect of the influence of secondary separation on the windward side of the wing.

For an envelope of values of the incidence and yaw parameters, the Newton-Raphson procedure failed to yield solutions of the defining equations. This failure was associated with values of the incidence parameter in the low part of the range considered, and occurred, in particular, for flow situations for which experimental evidence might lead one to suspect that solutions should exist. The author can offer no satisfactory explanation for this failure.

It is perhaps of interest to note here, that solutions obtained for values of the yaw angle greater than half of the wing apex angle represent the calculation of a vortex-sheet from a trailing edge. The general approach to the present problem, including the formulation and solution of the relevant equations, is similar to that adopted in the author's treatment⁽¹²⁾ of the unyawed problem

2. THEORY

We consider conical inviscid separated flow about a semi-infinite flat-plate delta wing with both incidence and yaw, in which separation from the leading-edge is represented by free conical surfaces of discontinuity in the velocity potential known as 'vortex-sheets'. The effects of secondary and other separation, which might possibly be incorporated into such a flow model are ignored. The problem is formulated within the slender-body theory of Munk, Jones and Ward, of which the basic assumption is that stream wise gradients of the flow properties are much smaller than the corresponding gradients normal to the free stream. We are thus restricted to the treatment of delta wings of very small aspect ratio.

2.1 Statement of the Problem

Consider a slender semi-infinite delta wing in uniform stream and choose axes $O-x-y-z$ fixed in the wing as shown in Fig.1. The wing lies in the $x-y$ plane such that the x axis bisects its apex angle at O , and is semi-infinite in the positive x direction. Let δ , which is small, be the half apex angle of the wing and let U be the free stream velocity inclined at small angles α to the $x-y$ plane and β to the $x-z$ plane. The sense of these angles is taken such that for small α and β , to first order, the components of the free stream velocity relative to the wing are

$$U, -\beta U, \alpha U,$$

in the x, y and z directions respectively.

Then, since the flow is inviscid and irrotational, a velocity potential exists, which, within slender body theory will be of the form

$$\phi(x,y,z) = Ux + \phi_0(x,y,z), \quad (1)$$

for small α, β , and where ϕ_0 must satisfy

$$\frac{\partial^2 \phi_0}{\partial y^2} + \frac{\partial^2 \phi_0}{\partial z^2} = 0. \quad (2)$$

The most general solution of (2) is

$$\phi_0(x,y,z) = \phi(y,z;x) + g(x, M_0), \quad (3)$$

where M_0 is the free stream Mach number. The first term of (3) is a two-dimensional velocity potential in the y - z 'cross-flow' plane in which x appears as a parameter. The second term, $g(x, M_0)$, is a function which appears in the general slender-body theory, but which vanishes for the present case of a flat delta wing.

Figure 2 shows the cross-flow plane at some value of x for which the wing semi-span is $s = Kx$. The cross-section of the wing is represented by $L_1 A L_2 B$, a cut in the y - z plane, and the cross-sections of the leeward and windward vortex sheets by further cuts C_1 and C_2 respectively. The points L_1 and L_2 represent the leading-edges of the slender delta wing being considered. Free stream velocity components in the cross-flow plane are shown as $-\beta U$ in the y direction and αU in the z direction. Since the flow is assumed to be conical, the geometry of Fig.2 will be that for any cross-section $x = \text{const} > 0$, the scale being altered accordingly.

Mangler and Smith⁽³⁾ have shown that, for conical flow, within the context of slender-body theory, the appropriate conditions which must be satisfied at each point $P_j^\dagger$ on C_j , may be written as

$$\frac{\partial \phi}{\partial n_j} = -KU \left(\frac{r_j}{s} \right) \sin \chi_j, \quad (4)$$

for the condition that a vortex sheet is a stream surface of the three-dimensional flow, and

$$\Delta \phi_j = \Delta \left(\frac{\partial \phi}{\partial \sigma_j} \right) \left\{ r_j \cos \chi_j - s \left(\frac{\partial \phi}{\partial \sigma_j} \right)_m / KU \right\}, \quad (5)$$

for the condition that the pressure is continuous across the sheet, where

- σ_j is the arc length along C_j measured as positive from the appropriate leading edge L_j ,
- n_j is the normal to C_j as shown in Fig. 2,

[†]We introduce the convention that if a subscript j appears whose range is unspecified, it is to be taken to be $j = 1, 2$, referring to quantities on the leeward and windward sheets respectively as shown in Fig.2. In particular P_j represents a point on a vortex sheet.

Δ is the difference operator across either C_1 or C_2 , taken as left-right, where left and right are defined relative to increasing σ_j along the appropriate C_j , $\Delta\phi_j$ for instance, being the jump in the discontinuous velocity potential at P_j ,

$\frac{\partial\phi}{\partial n_j}$ is the velocity normal to and continuous across C_j , at P_j ,

and $\left(\frac{\partial\phi}{\partial\sigma_j}\right)_m$ is the mean of the discontinuous tangential velocity at P_j .

The other symbols are as defined in the notation.

Since by (2), ϕ is harmonic, it is convenient to introduce a complex velocity potential $W(Z)$, $Z = y + iz$, in the cross-flow plane, such that $\phi = \text{Re}(W)$. At infinity in the cross flow plane, the velocity must approach the appropriate components of the free stream velocity. Hence we may write, for the form of the velocity potential $W(Z)$ for large Z

$$W(Z) \sim -U(\beta + i\alpha)Z + O\left(\frac{1}{Z}\right), \quad (6)$$

since there must be no sources or overall circulation in the Z plane.

The problem is thus to find the velocity potential $\phi = \text{Re}(W)$, a solution of (2) which satisfies

- (a) Condition (6) in the Z plane
- (b) Conditions (4) and (5) on C_j , $j = 1, 2$,
- (c) Condition (4) on $L_1 A L_2 B$ (Fig.2), since the flat-plate delta wing must also be a stream surface of the flow.

2.2 The Integro-Differential Equations for The Yawed Wing Problem

In Ref.12, the system of integro-differential equations for a number of mutually interacting twin-vortex-sheet systems in an unyawed flow were derived. The symmetry of the problem about the $x-z$ plane was embodied in the form of the equations, and, in particular, in the transformation of the cross-flow plane introduced to facilitate construction of the complex velocity potential. In the present problem, we consider only one pair of vortex-sheets, but the introduction of yaw destroys the

symmetry inherent in the unyawed problem, and we must here regard the two leading-edge vortex-sheets as independent surfaces of discontinuity in the flow, whose shape and strength will be determined by the mutual and self interaction of the singularity distributions used to represent them, together with the action of the free stream and the effect of the wing. We now derive the pair of integro-differential equations expressing this interaction by considering the form of the velocity potential which satisfies conditions (a)-(c) outlined at the end of section 2.1.

Along any curve in the Z-plane, and in particular, at a point $P_j(Z_j)$ (Fig.2) we may write

$$\left(\frac{\partial \phi}{\partial \sigma_j}\right)_m - i \left(\frac{\partial \phi}{\partial n_j}\right) = \left(\frac{dW}{d\sigma_j}\right) = \left(\frac{dW}{dZ}\right)_{Z_j} \left(\frac{dZ_j}{d\sigma_j}\right) \quad (7)$$

But from conditions (4) and (5) on C_j

$$\left(\frac{\partial \phi}{\partial \sigma_j}\right)_m - i \left(\frac{\partial \phi}{\partial n_j}\right) = \left\{ r_j (\cos \chi_j + i \sin \chi_j) - \frac{\Delta \phi_j}{\Delta \left(\frac{\partial \phi}{\partial \sigma_j}\right)} \right\} \frac{KU}{s} \quad (8)$$

and combining expressions (7) and (8) gives:

$$KU \left\{ \left(\frac{r_j}{s}\right) e^{i\chi_j} - \frac{1}{s} \frac{\Delta \phi_j}{\Delta \left(\frac{\partial \phi}{\partial \sigma_j}\right)} \right\} \bigg/ \frac{dZ_j}{d\sigma_j} = \left(\frac{dW}{dZ}\right)_{Z_j} \quad (9)$$

Now for any curve in the Z-plane, $Z_j = Z_j(\sigma_j)$, we have

$$\left. \begin{aligned} \frac{dZ_j}{d\sigma_j} &= e^{i\psi_j} \\ \text{or alternatively} \quad \frac{d\bar{Z}_j}{d\sigma_j} &= e^{-i\psi_j} = 1 / \left(\frac{dZ_j}{d\sigma_j}\right) \end{aligned} \right\} \quad (10)$$

where ψ_j is the angle between the positive y-direction and the position vector to C_j , ^{at P_j} as shown for the windward vortex sheet in Fig.2. *tangent*

Substituting (10) into (9) and noting that *incorrect*

$$\Delta \left(\frac{\partial \phi}{\partial \sigma_j} \right) = \frac{\partial (\Delta \phi_j)}{\partial \sigma_j} ,$$

one obtains

$$KU \left\{ \left(\frac{r_j}{s} \right) e^{i(\chi_j - \psi_j)} - \frac{1}{s} \frac{\Delta \phi_j}{\frac{\partial (\Delta \phi_j)}{\partial \sigma_j} \frac{d\sigma_j}{d\bar{z}_j}} \right\} = \left(\frac{dW}{dZ} \right)_{Z_j} . \quad (11)$$

From simple geometrical considerations (Fig.2), we have

$$\theta_j = \psi_j - \chi_j$$

and thus expression (11) may be written as, at P_j

$$KU \left\{ \left(\frac{\bar{z}_j}{s} \right) - \Delta \phi_j \frac{d \left(\frac{\bar{z}_j}{s} \right)}{d(\Delta \phi_j)} \right\} = \left(\frac{dW}{dZ} \right)_{Z_j} , \quad (12)$$

where

$$\left(\frac{\bar{z}_j}{s} \right) = \left(\frac{r_j}{s} \right) e^{-i\theta_j} .$$

From equation (7), it can be seen that expression (12) represents the mean of the discontinuous complex velocity at P_j .

We now introduce the transformation

$$Z = \frac{1}{2} \left(Z^* + \frac{1}{Z^*} \right) , \quad (13)$$

which transforms a circle of radius s , $L_1^* A^* L_2^* B^*$ in the Z^* -plane (Fig.3A), to a slit of width $2s$, $L_1 A L_2 B$ in the Z -plane, and the curves C_j^* in the Z^* -plane to C_j in the Z -plane.

Working in the Z^* -plane, we can now construct a velocity potential which will satisfy condition (4) on $L_1 A L_2 B$, by applying the Milne-Thompson circle theorem to the function

$$F(Z^*) = -\frac{U}{2} (\beta + i\alpha) Z^* - \frac{1}{2\pi i} \int_{\Gamma_1}^0 \log\{Z^* - t_1^*(\Delta\phi_1)\} d(\Delta\phi_1) - \\ - \frac{1}{2\pi i} \int_{\Gamma_2}^0 \log\{Z^* - t_2^*(\Delta\phi_2)\} d(\Delta\phi_2) ,$$

and by disregarding a term in the resulting expression which represents an isolated vortex of strength $\Gamma_1 + \Gamma_2$ at $Z^* = 0$, in order to satisfy the required form of $W(Z)$ for large Z in the original cross-flow plane, as expressed by (6). Carrying this operation out, we obtain for the complex velocity potential

$$W(Z^*) = -\frac{U}{2} \left\{ (\beta + i\alpha) Z^* - (-\beta + i\alpha) \frac{s^2}{Z^*} \right\} - \\ - \frac{1}{2\pi i} \int_{\Gamma_1}^0 \log \left\{ \frac{Z^* - t_1^*(\Delta\phi_1)}{Z^* - s^2/\overline{t_1^*(\Delta\phi_1)}} \right\} d(\Delta\phi_1) - \\ - \frac{1}{2\pi i} \int_{\Gamma_2}^0 \log \left\{ \frac{Z^* - t_2^*(\Delta\phi_2)}{Z^* - s^2/\overline{t_2^*(\Delta\phi_2)}} \right\} d(\Delta\phi_2) , \quad (14)$$

where the first term represents the attached flow, which leads to velocity singularities at L_j in the Z -plane. The factor $\frac{1}{2}$ appears because of the form of the transformation, equation (13). The two integral terms represent the velocity potential at a point Z^* due to the two sheets C_j^* , together with their images $C_j'^*$ in the circle $|Z^*| = s$.

In expression (14) it should be noted that:

(1) The integrals are to be evaluated along C_j^* , $j = 1, 2$ respectively, $t_j^*(\Delta\phi_j)$ representing parametrically, in the integrals, the as-yet unknown shape of C_j^* .

(2) The potential difference $\Delta\phi_j$ across C_j^* , at some point P_j^* , is used in the same sense as in equation (5). It is to be considered as an independent variable along C_j^* . A given value of $\Delta\phi_j$, $|\Gamma_j| \geq |\Delta\phi_j| \geq 0$ will uniquely define a point P_j^* and will take the same value at corresponding points [through equation (13)] P_j in the Z -plane.

(3) $\Delta\phi_j$ is taken to be Γ_j at L_j^* and zero at the end points of C_j^* . Thus Γ_j is the total circulation around both C_j and C_j^* , at the particular value of x for which $s = Kx$. It represents the total circulation in the j^{th} separation shear layer at this x -station, and because of the assumed conicality of the flow, Γ_j is linear in x .

Differentiating expression (14) with respect to Z , and evaluating the resulting complex velocity at some point $Z_j^*(\Delta\phi_j)$ on C_j^* , we obtain[†]

$$\begin{aligned} \left(\frac{dW}{dZ}\right)_{Z_j} &= \left(\frac{dZ^*}{dZ}\right)_{Z_j^*} \left[-\frac{U}{2} \left\{ (\beta + i\alpha) + (-\beta + i\alpha) \frac{s^2}{Z_j^{*2}} \right\} \right. \\ &\quad - \frac{1}{2\pi i} \int_{\Gamma_1}^0 \left\{ \frac{1}{Z_j^* - t_1^*(\Delta\phi_1')} - \frac{1}{Z_j^* - s^2/t_1^*(\Delta\phi_1')} \right\} d(\Delta\phi_1') \\ &\quad \left. - \frac{1}{2\pi i} \int_{\Gamma_2}^0 \left\{ \frac{1}{Z_j^* - t_2^*(\Delta\phi_2')} - \frac{1}{Z_j^* - s^2/t_2^*(\Delta\phi_2')} \right\} d(\Delta\phi_2') \right]. \end{aligned} \quad (15)$$

Note that the whole expression is a function of $\Delta\phi_j$ defining Z_j^* or Z_j . For $j = 1$, the first integral in expression (15) is singular, and for $j = 2$, the second is singular. The integral in each case is interpreted as a Cauchy principle value integral, taking the mean of the two values obtained by approaching Z_j^* from either side of C_j^* .

Combining equations (15) and (12), and introducing the following non-dimensionalizing transformations

$$\left. \begin{aligned} \lambda_j &= 1 - \frac{\Delta\phi_j}{\Gamma_j} \\ \omega_j &= \frac{Z_j}{s} = \xi_j + i\eta_j \\ \omega_j^* &= \frac{Z_j^*}{s} = \xi_j^* + i\eta_j^* \\ \tau_j^* &= \frac{t_j^*}{s} \end{aligned} \right\} \quad j = 1, 2, \quad (16)$$

[†]In carrying out this operation we replace the integration variables $\Delta\phi_j$ in (14), by $\Delta\phi_j'$.

we obtain[†]:

$$\begin{aligned}
 & \left(\frac{d\omega}{d\omega^*} \right) \omega_j^* \left\{ \bar{\omega}_j + (1 - \lambda_j) \frac{d\bar{\omega}_j}{d\lambda_j} \right\} \\
 & = -\frac{1}{2} \left\{ (b + ia) + (b - ia)/\omega_j^{*2} \right\} \\
 & \quad + \frac{G_1}{2\pi i} \int_0^1 \left\{ \frac{1}{\omega_j^* - \tau_1^*(\lambda_1')} - \frac{1}{\omega_j^* - 1/\tau_1^*(\lambda_1')} \right\} d\lambda_1' \\
 & \quad + \frac{G_2}{2\pi i} \int_0^1 \left\{ \frac{1}{\omega_j^* - \tau_2^*(\lambda_2')} - \frac{1}{\omega_j^* - 1/\tau_2^*(\lambda_2')} \right\} d\lambda_2' \\
 & \qquad \qquad \qquad j = 1, 2, \qquad (17)
 \end{aligned}$$

where

$$\omega_j = \frac{1}{2} \left(\omega_j^* + \frac{1}{\omega_j^*} \right), \qquad (18)$$

$$G_j = \Gamma_j / K U_s,$$

$$a = \alpha / K, \quad b = \beta / K,$$

and $K = \tan \delta \approx \delta$, for small δ .

Equations (17) together with (18) are a pair of complex simultaneous integro-differential equations for the real and imaginary parts of

$$\omega_j^*(\lambda_j) = \xi_j^*(\lambda_j) + i\eta_j^*(\lambda_j), \quad 1 \geq \lambda_j \geq 0,$$

for $j = 1, 2$, where λ_j is the normalized non-dimensional potential difference across either C_j or C_j^* . The parameters a and b , which are to be specified when solving equations (17) and (18), represent incidence and yaw respectively. The parameters G_j are unknowns of the

[†] Terms involving a subscript j appearing twice, such as $\frac{d\bar{\omega}_j}{d\lambda_j}$, for example, are to be understood as not to be summed.

problem and represent the total circulation about C_j or C_j^* . They are made determinate within the mathematical model by applying closure conditions, namely the Kutta conditions, which require that the velocity be finite at the leading edges L_1 and L_2 in the cross flow plane.

These conditions may be expressed as

$$\left(\frac{dW/KUs}{d\omega^*} \right)_{\omega^* = \omega_{j0}^*} = 0 \quad j = 1, 2, \quad (19)$$

which by differentiation of equation (14), and application of relations (16), can be written in terms of the flow parameters as

$$\begin{aligned} a + \frac{G_1}{2\pi} \int_0^1 \left\{ \frac{1}{\omega_{j0}^* - \tau_1^*(\lambda_1')} - \frac{1}{\omega_{j0}^* - 1/\tau_1^*(\lambda_1')} \right\} d\lambda_1' + \\ + \frac{G_2}{2\pi} \int_0^1 \left\{ \frac{1}{\omega_{j0}^* - \tau_2^*(\lambda_2')} - \frac{1}{\omega_{j0}^* - 1/\tau_2^*(\lambda_2')} \right\} d\lambda_2' = 0 \end{aligned}$$

$j = 1, 2, \quad (20)$

where $j = 1$, $\omega_{10}^* = (-1, 0)$ is the first Kutta condition applied at L_1^* , and $j = 2$, $\omega_{20}^* = (1, 0)$ is the second Kutta condition applied at L_2^* , and (20) are two real equations since the expressions in brackets are real.

It should be noted that, in equations (17) and (20), the incidence and yaw angles appear only in ratio to $K = \tan \delta$. We may regard a and b as similarity parameters of the problem. Solutions of (17) and (20) and quantitative properties of these solutions, will therefore be functions of a and b only.

3. NUMERICAL TREATMENT

3.1 Finite Difference Form of the Equations and the Zero Force Conditions

We now formulate a closed set of non-linear finite difference equations to replace equations (17) and (20), based on the Mangler and Smith vortex-sheet-cut-isolated-vortex model, discussed in detail in Ref.4. Each sheet C_j^* in the ω^* -plane is broken up into an outer part defined over $\lambda_{jN} \geq \lambda \geq 0$, and an inner part, $1 \geq \lambda > \lambda_{jN}$. The outer part of C_j^* is represented by N discrete points in the ω^* -plane

$$\begin{aligned} \omega_{jn}^* &= \xi_{jn}^* + i\eta_{jn}^* & j &= 1, 2, \\ & & n &= 1, \dots, N, \end{aligned} \quad (21A)$$

and the outer part of C_j by N corresponding points in the ω -plane

$$\begin{aligned} \omega_{jn} &= \xi_{jn} + i\eta_{jn} & j &= 1, 2, \\ & & n &= 1, \dots, N. \end{aligned} \quad (21B)$$

The discrete values of λ corresponding to expressions (21A) and (21B), we write as

$$\begin{aligned} \lambda_{jn} &= h_n \lambda_{jN}, & j &= 1, 2, \\ & & n &= 1, \dots, N, \end{aligned} \quad (21C)$$

where

$$h_N = 1 > h_{N-1} > \dots > h_2 > h_1 > 0,$$

and the h_n are to be specified. Note that λ_{1N} and λ_{2N} are not necessarily equal.

The inner part of C_j^* is represented by an isolated vortex at a point ω_{jN+1}^* and is joined to ω_{jN}^* , the end of the outer part of C_j^* , by a cut in the ω^* -plane, introduced so as to define the potential ϕ unambiguously. This ensures that the velocities induced by the inner part of the sheet on the rest of the flow field are adequately modelled. Corresponding isolated vortices and cuts exist in the ω plane. The complex velocity $d(W/KUs)/d\omega^*$ is continuous across the cuts but the potential ϕ is not, suffering a discontinuity equal in magnitude to the circulation concentrated at the isolated vortex. Thus, while the outer part of the representation retains its sheet-like character within the

model, the inner part does not, any possibility of satisfying equations (17) in some form for $1 > \lambda > \lambda_{jN}$ being disregarded. The equivalent points representing $C_j^{!*}$, the image of C_j^* in the circle $|\omega^*| = 1$, are given by

$$\frac{1}{\omega_{jn}^*} = \frac{1}{\xi_{jn}^* - i\eta_{jn}^*} \quad \begin{matrix} j = 1, 2, \\ n = 1, \dots, N+1 \end{matrix} \quad (22)$$

Figure (3B) shows the break-up of C_j^* and $C_j^{!*}$ for the finite difference representation. Of the total non-dimensional circulation about C_j^* , a fraction λ_{jN} is distributed along the N elements of the outer part, and a fraction $1 - \lambda_{jN}$ will be concentrated at the isolated vortex ω_{jN+1}^* , or equivalently, at ω_{jN+1} in the ω -plane.

We then have $4N + 6$ unknowns given by:

- (1) The $N + 1$ real parts ξ_{jn}^* , and the $N + 1$ imaginary parts η_{jn}^* , of ω_{jn}^* , $j = 1, 2$, $n = 1, \dots, N+1$, that is $4N + 4$ unknowns, and
- (2) The circulations G_j , $j = 1, 2$.

We further choose to introduce an extra degree of freedom by allowing λ_{1N} to be a free parameter (arbitrarily chosen instead of λ_{2N}) while specifying λ_{2N} , giving now $4N + 7$ unknowns, which we represent vectorially by Ω , with components

$$\Omega_l \quad l = 1, \dots, 4N+7,$$

arranged in some arbitrary order, the details of which will not concern us here.

To find a suitable Ω representing a solution of the problem for given values of $a, b, h_n, n = 1, \dots, N$ and λ_{2N} , $4N + 7$ relations involving Ω are required. $4N$ of these are supplied by satisfying equations (17) in finite difference form along the outer part of the sheet, and 2 more are given by the finite difference form of equations (20). Four more relations are supplied by satisfying conditions of zero total force on each cut-isolated vortex system in the ω plane. This is introduced so as to make the inner part of the model force free in lieu of one in which the inner part retains its sheet-like character, each element being force and moment free. One final condition introduced is that the sum of the two moments due to the pressure difference on the cuts $\omega_{jN+1} - \omega_{jN}$, is zero.

It should be emphasized that this 'zero-moment condition' has no significance in the sense that the zero force condition has on each sheet. It is associated with the parameter λ_{1N} , and unlike the zero force conditions, it is not necessary to incorporate it into the model to obtain realistic solutions. We could for example specify λ_{1N} and drop the moment condition since it is unlikely that the main physical parameters of the problem - the sheet shape near the leading edge, the positions of the isolated vortices and the circulations - will be very dependent upon it. Nevertheless since it does ensure that overall, the fluid in the vicinity of the wing is moment free, and since it is easy to incorporate into the present method, we choose to include it.

We satisfy a finite difference form of equations (17) at points in the ω^* plane defined by

$$\left. \begin{aligned} \omega_{jn,n-1}^* &= \frac{1}{2} (\omega_{jn}^* + \omega_{jn-1}^*) \\ \lambda_{jn,n-1} &= \frac{\lambda_{jN}}{2} (h_n + h_{n-1}) \end{aligned} \right\} \quad \begin{aligned} j &= 1, 2, \\ n &= 1, \dots, N \end{aligned} \quad (23)$$

Corresponding points $\omega_{jn,n-1}$ in the ω plane are given through equation (18). The left-hand side of (17) is replaced by a two point differentiation rule along C_j and the integrals on the right-hand side in $\lambda_{jN} \geq \lambda \geq 0$, are evaluated at points given by (23) using the trapezoidal rule (ignoring the singularity), that part for $\lambda > \lambda_{jN}$ being given by the velocity field due to an isolated vortex. Thus a finite difference representation of equations (17) can be written as

$$\begin{aligned} H_{jn}(\Omega) &= - \left(\frac{d\omega}{d\omega^*} \right)_{\omega_{jn,n-1}^*} \left\{ \frac{1}{\omega_{jn-1}^*} \left(\frac{h_n - 1/\lambda_{jN}}{h_n - h_{n-1}} \right) - \frac{1}{\omega_{jn}^*} \left(\frac{h_{n-1} - 1/\lambda_{jN}}{h_n - h_{n-1}} \right) \right\} - \\ &\quad - \frac{1}{2} \left\{ (b + ia) + (-b + ia) / \omega_{jn,n-1}^{*2} \right\} + \\ &\quad + \frac{G_1}{2\pi i} \sum_{m=0}^{N+1} A_{1m} \left\{ \frac{1}{\omega_{jn,n-1}^* - \omega_{1m}^*} - \frac{1}{\omega_{jn,n-1}^* - 1/\omega_{1m}^*} \right\} + \\ &\quad + \frac{G_2}{2\pi i} \sum_{m=0}^{N+1} A_{2m} \left\{ \frac{1}{\omega_{jn,n-1}^* - \omega_{2m}^*} - \frac{1}{\omega_{jn,n-1}^* - 1/\omega_{2m}^*} \right\} = 0, \\ &\quad j = 1, 2, \quad n = 1, \dots, N, \end{aligned} \quad (24)$$

where

$$\begin{aligned} A_{\ell 0} &= h_1 \lambda_{\ell N} \\ A_{\ell m} &= (h_{m+1} - h_{m-1}) \frac{\lambda_{\ell N}}{2} \quad m = 1, \dots, N-1, \\ A_{\ell N} &= (1 - h_{N-1}) \frac{\lambda_{\ell N}}{2} \\ A_{\ell N+1} &= 1 - \lambda_{\ell N} \quad \ell = 1, 2. \end{aligned}$$

Expression (24) is complex and represents $4N$ equations, $2N$ real and $2N$ imaginary. The terms $(d\omega/d\omega^*) \omega_{jn, n-1}^*$, $\overline{\omega_{jn}}$ and $\overline{\omega_{jn-1}}$ in (24) can be evaluated in terms of $\overline{\omega_{jn}^*}$ and $\overline{\omega_{jn-1}^*}$ through equation (18).

In equations (20) for the Kutta conditions, the integrals over the outer part of the sheets may be written as

$$\frac{G_\ell}{2\pi} \sum_{m=1}^N \int_{\lambda_{\ell m-1}}^{\lambda_{\ell m}} \left\{ \frac{1}{\omega_{j0}^* - \tau_\ell^*} - \frac{1}{\omega_{j0}^* - 1/\overline{\tau_\ell^*}} \right\} d\lambda, \quad (25)$$

for both $\ell = 1, 2$ in each of (20), $j = 1, 2$.

The integral for $j = \ell$, $m = 1$ in the above has a singularity (not of the Cauchy principle value type) at the leading-edge L_j , where $\lambda_j = 0$ and $\tau_j^* = 1/\overline{\tau_j^*} = \omega_{j0}^*$. From solutions of equation (17) valid near L_j , that is, for small λ_j , it can be shown that the sheet shape is given by

$$\tau_j^* = \omega_{j0}^* + A_j \lambda_j^{\frac{1}{2}} + iB_j \lambda_j + O(\lambda_j^{1+\mu}), \quad (26)$$

where $\mu > 0$ and where A_j and B_j are real constants that depend on the overall flow. Substitution of this expression into the first integral for $j = \ell$ in expression (25) yields

$$\begin{aligned} & \frac{G_j}{2\pi} \int_0^{\lambda_{j1}} \left\{ \frac{1}{\omega_{j0}^* - \tau_j^*} - \frac{1}{\omega_{j0}^* - 1/\overline{\tau_j^*}} \right\} d\lambda \\ &= \frac{G_j h_1 \lambda_{jN}}{\pi} \left\{ \frac{4}{2\omega_{j0}^* - (\omega_{j1}^* + \overline{\omega_{j1}^*})} - \frac{1}{2\omega_{j0}^*} \right\} + O(\lambda_{j1}^{1+\gamma}) \end{aligned} \quad \text{where } \gamma > 0. \quad (27)$$

The other integrals in (25) are evaluated using the trapezoidal rule and thus the first Kutta condition $j = 1$, $\omega_{10}^* = (-1,0)$ in equations (20) can be replaced by, dropping the term of $O(\lambda_{j1}^{1+\gamma})$ in (27)

$$\begin{aligned}
 Q_1(\Omega) = & a + \frac{G_1 h_1 \lambda_{1N}}{\pi} \left\{ \frac{4}{2\omega_{10}^* - (\omega_{11}^* + \overline{\omega_{11}^*})} - \frac{1}{2\omega_{10}^*} \right\} + \\
 & + \frac{G_1}{2\pi} \sum_{m=1}^{N+1} A'_{1m} \left\{ \frac{1}{\omega_{10}^* - \omega_{1m}^*} - \frac{1}{\omega_{10}^* - 1/\overline{\omega_{1m}^*}} \right\} + \\
 & + \frac{G_2}{2\pi} \sum_{m=0}^{N+1} A_{2m} \left\{ \frac{1}{\omega_{10}^* - \omega_{2m}^*} - \frac{1}{\omega_{10}^* - 1/\overline{\omega_{2m}^*}} \right\} = 0 \quad (28A)
 \end{aligned}$$

$$\begin{aligned}
 \text{where } A'_{11} &= (h_2 - h_1) \frac{\lambda_{1N}}{2} \\
 A'_{1m} &= A_{2m}, \quad m \geq 2.
 \end{aligned}$$

The second Kutta condition, $j = 2$, $\omega_{20}^* = (1,0)$ can be written in a similar manner to equation (28A), with the subscripts 1 and 2 reversed. We represent this condition, symbollically as

$$Q_2(\Omega) = 0. \quad (28B)$$

From considerations of the three-dimensional flow, Smith⁽⁴⁾ shows that the conditions of zero force on each cut and isolated vortex may be written as

$$\begin{aligned}
 \lim_{\omega \rightarrow \omega_{jN+1}} \left\{ \frac{d(W/KU_s)}{d\omega} - \frac{G_j(1 - \lambda_{jN})}{2\pi i} \frac{1}{\omega - \omega_{jN+1}} \right\} - \\
 - 2\overline{\omega_{jN+1}} + \overline{\omega_{jN}} = 0 \quad (29) \\
 j = 1, 2,
 \end{aligned}$$

where the limit represents the velocity at ω_{jN+1} in the cross-flow plane, if the isolated vortex were not present. When this limit has been taken and the resulting integrals replaced by trapezoidal rule quadratures,

(29) can be written in finite difference form as

$$\begin{aligned}
 E_1(\Omega) = & \left[-\frac{1}{2} \left\{ (b + ia) + (-b + ia)/\omega_{1N+1}^{*2} \right\} + \right. \\
 & + \frac{G_1}{2\pi i} \left\{ \sum_{m=0}^N \frac{A_{1m}}{\omega_{1N+1}^* - \omega_{1m}^*} - \sum_{m=0}^{N+1} \frac{A_{1m}}{\omega_{1N+1}^* - 1/\omega_{1m}^*} \right\} + \\
 & + \frac{G_2}{2\pi i} \sum_{m=0}^{N+1} A_{2m} \left\{ \frac{1}{\omega_{1N+1}^* - \omega_{2m}^*} - \frac{1}{\omega_{1N+1}^* - 1/\omega_{2m}^*} \right\} \left/ \left(\frac{d\omega}{d\omega^*} \right)_{\omega_{1N+1}^*} \right. + \\
 & + \frac{G_1(1 - \lambda_{1N})}{4\pi i} \left\{ \frac{d}{d\omega^*} \left(\frac{d\omega^*}{d\omega} \right) \right\}_{\omega_{1N+1}^*} - \overline{2\omega_{1N+1}} + \overline{\omega_{1N}} = 0, \quad (30A)
 \end{aligned}$$

for the first zero-force condition, together with a similar equation with the subscripts 1 and 2 reversed for the second zero-force condition

$$E_2(\Omega) = 0, \quad (30B)$$

where the A_{jm} , $j = 1, 2$, $m = 1, \dots, N+1$, are as in equations (24), and equations (30) are 4 equations since (30A) and (30B) both have real and imaginary parts.

We now derive the condition of zero total moment on the two cuts $\omega_{jN+1} - \omega_{jN}$ in the ω plane. Within the context of slender body theory, the pressure coefficient at some point in the three-dimensional flow about the flat plate delta wing is given by (Ref.4)

$$C_P = 2 \left\{ y \frac{\partial \phi}{\partial y} + z \frac{\partial \phi}{\partial z} - \phi \right\} / Ux - \left\{ \left(\frac{\partial \phi}{\partial y} \right)^2 + \left(\frac{\partial \phi}{\partial z} \right)^2 \right\} / U^2 + \alpha^2 + \beta^2. \quad (31)$$

Now since both $\frac{\partial \phi}{\partial y}$ and $\frac{\partial \phi}{\partial z}$ are continuous across the cuts $\omega_{jN+1} - \omega_{jN}$, there will exist a constant pressure difference across each cut given by, from equation (31)

$$\begin{aligned}\Delta p_j &= \frac{1}{2} \rho U^2 \Delta C_{p_j} = - \frac{\rho U \Delta \phi_j}{x} \\ &= - \frac{\rho U \Gamma_j (1 - \lambda_{jN})}{x} .\end{aligned}\quad (32)$$

The x-wise moment per unit length in the x-direction, of this pressure difference about Z_{jN+1} in the Z plane can thus be written as

$$\begin{aligned}D_j &= \frac{1}{2} \Delta p_j (Z_{jN+1} - Z_{jN}) (\overline{Z}_{jN+1} - \overline{Z}_{jN}) \\ &= - \frac{\rho U}{2x} \Gamma_j (1 - \lambda_{jN}) (Z_{jN+1} - Z_{jN}) (\overline{Z}_{jN+1} - \overline{Z}_{jN}) \\ j &= 1, 2 .\end{aligned}\quad (33)$$

Then since the total force per unit length in the x direction on each cut-isolated-vortex system is zero, taking moments about the origin of the Z-plane yields the condition that the sum of the x-wise moments in the fluid, near the wing, due to the existence of the two cut-isolated-vortex systems is zero, viz :

$$\sum_{j=1}^2 D_j = 0 , \quad (34)$$

which can be transformed to non-dimensional variables using relations (16), to give

$$M(\Omega) = \sum_{j=1}^2 G_j (1 - \lambda_{jN}) (\omega_{jN+1} - \omega_{jN}) (\overline{\omega}_{jN+1} - \overline{\omega}_{jN}) = 0 , \quad (35)$$

where (35) is one real equation.

For the unyawed case ($b = 0$), equation (35) is satisfied by $G_1 = -G_2$, $\lambda_{1N} = \lambda_{2N}$ and $\omega_{1n} = -\overline{\omega}_{2n}$, $n = N, N+1$. This is automatically satisfied by symmetry in the formulations of the unyawed problem in References 4 and 12.

Equations (24), (28), (30) and (35) are the $4N+7$ equations involving the $4N+7$ unknowns of the problem. We represent these equations symbolically, their various real and imaginary parts assumed separated (which is actually not explicitly necessary for the solution procedure used

herein), as

$$f_k(\underline{\Omega}) = 0, \quad k = 1, \dots, 4N+7, \quad (36)$$

the order of k in respect to equations (24), (28), (30) and (35) being chosen in some arbitrary but convenient way.

3.2 Solution Procedure

For the present work, equations (36) were solved for fixed values of $h_1 \dots h_N$ and λ_{1N} , for a range of values of a and b , by a Newton Raphson technique previously developed by the author⁽¹²⁾. This method is a single iteration procedure and amounts to a full linearization of equations (36) about some known approximation to a desired solution. A full outline of this method is given in Ref. 12. Only sufficient details are given here to indicate its present application.

Each iteration of the above-mentioned scheme involves first the calculation of a $(4N + 7) \times (4N + 7)$ matrix, the components of which are

$$F_{k\ell} = \frac{\partial f_k}{\partial \Omega_\ell} \quad \begin{matrix} k = 1, \dots, 4N+7, \\ \ell = 1, \dots, 4N+7, \end{matrix} \quad (37)$$

and the subsequent solution of a set of $4N + 7$ linear equations of the form

$$\sum_{\ell=1}^{4N+7} F_{k\ell}(\underline{\Omega}^p) \delta \Omega_\ell^{p,p+1} = -f_k(\underline{\Omega}^p) \quad k = 1, \dots, 4N+7. \quad (38)$$

In equations (38), the f_k and the $F_{k\ell}$ are evaluated at a p^{th} approximation, say $\underline{\Omega}^p$, to a solution of equations (36). The $\delta \Omega_\ell^{p,p+1}$ are the unknowns of the linear system, from which a $(p+1)^{\text{th}}$ approximation given by

$$\Omega_\ell^{p+1} = \Omega_\ell^p + \delta \Omega_\ell^{p,p+1} \quad \ell = 1, \dots, 4N+7,$$

can be constructed. Repeated calculation of (37) and solution of equations (38) (by a standard method), for $p = 1, 2, \dots$, yields a sequence of approximations which should converge to a satisfactory solution of equations (36).

The derivatives $\partial f_k / \partial \Omega_\ell$ are determined by direct differentiation of equations (24), (28), (30) and (35) with respect to the various components of $\underline{\Omega}$. With regard to the real variables G_1 , G_2 and λ_{1N} , the differentiation is straightforward. With regard to the components of $\underline{\Omega}$ which represent the real and imaginary parts of

$\omega_{jn}^* = \xi_{jn}^* + i\eta_{jn}^*$, $n = 1, \dots, N+1$, $j = 1, 2$, the required derivatives are found by differentiation with respect to ω_{jn}^* and $\overline{\omega_{jn}^*}$, and use of the relations

$$\left. \begin{aligned} \frac{\partial f_k}{\partial \xi_{jn}^*} &= \left\{ \begin{array}{c} \text{Re} \\ \text{Im} \end{array} \right\} \left[\frac{\partial V}{\partial \omega_{jn}^*} + \frac{\partial V}{\partial \overline{\omega_{jn}^*}} \right] \\ \frac{\partial f_k}{\partial \eta_{jn}^*} &= \left\{ \begin{array}{c} \text{Re} \\ \text{Im} \end{array} \right\} \left[i \left(\frac{\partial V}{\partial \omega_{jn}^*} - \frac{\partial V}{\partial \overline{\omega_{jn}^*}} \right) \right] \end{aligned} \right\} \quad (39)$$

where f_k for some value of k , is either the real or imaginary part of the complex equation

$$V(\underline{\Omega}) = 0, \quad (40)$$

V being any of H_{jn} , $n = 1, \dots, N$, Q_j , E_j , $j = 1, 2$ or M in equations (24), (28), (30) and (35).

3.3 Choice of Numerical Parameters

Solutions of equations (36) will be of the form

$$\Omega_\ell = \Omega_\ell(a, b; h_1, h_2, \dots, h_N, \lambda_{2N}), \quad \ell = 1, \dots, 4N+7, \quad (41)$$

The work of Smith^{(4) (6)} on the unyawed problem, and the author's own experience indicates that solutions will not depend strongly on λ_{2N} , provided that sufficient of the outer part of the sheet is represented in a sheet-like manner. Sufficient in this context may be taken to mean:

(a) That at least that part of the sheet which extends from the leading edge of the wing to a point where it may be considered that the spiral "rolling up" process has properly begun, is included in the representation of the outer part.

(b) That enough of the sheet near the wing leading-edge is treated in a sheet-like manner to ensure that the velocity field in this region is adequately modelled.

Smith uses a geometrical variable - namely the polar angle θ (in Ref.4) taken around the isolated vortex in the transformed plane - to specify the extent of the outer part of the sheet and concludes, from numerical experiment, that the choice $\theta_{\max} = 157^\circ$ (maximum polar angle) gives an adequate representation. In the author's treatment of the unyawed problem⁽¹²⁾ for the flat plate, calculations were made for both $\lambda_{1N} = \lambda_{2N} = .45$, $N = 20$ and $\lambda_{1N} = \lambda_{2N} = .195$, $N = 10$ (roughly equivalent to $\theta_{\max} = 157^\circ$) which confirmed Smith's conclusion.

Hence, for the present work, $N = 10$ points were chosen on the outer part of the sheet and λ_{2N} was chosen as $\lambda_{2N} = .2$, that is, 20% of the total circulation on the windward system is distributed along the sheet and 80% is concentrated at the isolated vortex. The fraction of the total circulation distributed on the sheet in the leeward system is, of course, an unknown of the problem.

The values of h_n chosen were as follows:

TABLE 1

n	1	2	3	4	5	6	7	8	9	10
h_n	.01	.04	.10	.25	.375	.50	.625	.75	.875	1.0

3.4 Computational Details; Range of Solutions

A fortran IV computer programme (not included in the present report) was written embodying the solution procedure outlined above, in which the various numerical parameters of the problem - including an initial approximation - could be input as data. Using this programme, approximate numerical solutions to equations (36) were found, with the above values of $h_1, \dots, h_N$ and λ_{2N} , over a range of values of a and b . For given values of a and b , the solution procedure was terminated and a solution considered to be found, when an iterate, say Ω^P , was obtained which satisfied the condition

$$\frac{1}{4N+7} \sum_{k=1}^{4N+7} \left| f_k(\Omega^P) \right| \leq 10^{-8} . \quad (42)$$

It is believed (though it is not proved herein), that when (42) is satisfied, a solution to (36) has been found accurate to four significant figures in each of the components of Ω . This is considered to be more than sufficiently accurate given the limitations of the mathematical flow model, and the accuracy of the available experimental data. The conclusion that this degree of accuracy has been obtained was reached by observing that there was, in general, no change in the fifth significant figure of components of successive iterates, say Ω^P and Ω^{P+1} , when (42) had been satisfied by Ω^P . Usually 4-5 iterations were required to reduce the L.H.S. of (42) from $O(1)$ to $O(10^{-8})$, requiring about 10 seconds of CDC-6600 computing time. Often convergence was so fast in the later iterations that the L.H.S. of (42) was reduced to values several orders of magnitude lower than 10^{-8} .

Calculations were made for values of a up to 3.0, and values of b up to 2.0 along lines of constant a or b in the a - b plane. Starting approximations were obtained from solutions for $b = 0$, that is, from solutions to the unyawed problem. Solutions with yaw were then found by increasing b by intervals of 0.1 or smaller (where necessary), at fixed values of $a = 0.5, 1.0, 1.5, 2.0, 2.5$ and 3.0 . From solutions obtained along the $a = 3.0$ line in the a - b plane, further solutions were found by decreasing a by intervals of 0.1 at constant values of b given by $b = 0.5, 1.0, 1.5$ and 2.0 . In this way, a grid of solutions was obtained in the region $0 \leq b \leq 2.0$, $0 \leq a \leq 3.0$, of the a - b plane.

However, as mentioned in the introduction, it was found that at lower values of a , over the whole range of b , the Newton-Raphson scheme diverged, failing to yield solutions of the finite-difference equations. The lowest value of a for a given value of b , for which solutions could be obtained, was found to be given approximately by

$$a = 0.15 + 0.4b \quad (43)$$

Thus, in a significant part of that region of the a - b plane, in which solutions were sought, none could be found. This phenomenon is discussed in more detail in section 4.2.1.

4. RESULTS AND COMPARISON WITH EXPERIMENT

Table 2 gives a summary of the significant numerical parameters obtained from solutions of the defining equations. It lists the positions ξ_{jN+1} , η_{jN+1} , $j = 1, 2$, of the two isolated vortices in the ω plane, the total circulations G_j , $j = 1, 2$, of the two sheet-isolated vortex systems, and the fraction λ_{1N} of the total circulation distributed along the sheet in the leeward system, for values of a and b separated by 0.5. Also shown are the normal-force coefficient C_N/K^2 , calculated by the method of residues [equation (A2.4), Appendix A], and the rolling moment coefficient C_L/K^2 calculated by numerical integration of the first moment of the pressure coefficient across the wing surface, equation (A3.3).

4.1 Vortex Sheet Shapes

Vortex sheet shapes and isolated vortex positions are shown, for the values of a and b indicated, in Figs 4A, 5A and 6A for the leeward system and in Figs 4B, 5B and 6B for the windward system. They may be regarded as typical graphical representations of solutions obtained to the finite difference equations and serve to illustrate the principal features of, and in particular the extent of typical vortex sheet shapes in relation to the positions of the associated isolated vortices.

The sheet shapes presented were constructed by drawing smooth lines through the plotted solution points ξ_{jn} , η_{jn} , $n = 1 \dots, N$, $j = 1, 2$. A typical distribution of these points along the outer part of the sheet is shown in Figs 6A and 6B, where they are plotted for $a = 1.5$, $b = 2.0$. In Figs 4A and 4B, the sheet shapes for $a = 0.5$ and $b = 0.95$ represent the solution for the largest value of b (for $a = 0.5$) which could be obtained before the aforementioned failure of the iteration scheme occurred. For $a = 1.0$ (Figs 5A and 5B), failure occurred for values of b only slightly larger than 2.0, but for $a = 1.5$ (Figs 6A and 6B), the solution range could be extended considerably beyond $b = 2.0$. A general comment regarding Figs 4-6 worth mentioning here, is that for $b = 0$, the twin vortex sheet system exhibits, quite naturally, the symmetry property about the η axis expected for zero yaw.

It would seem, from Figs 4B, 5B and 6B, that the geometrical extent of the outer part of the windward vortex sheet is adequate even though only 20% of the total windward circulation is distributed along it, 80% being concentrated at the isolated vortex. In each of these figures, the extent of the outer part of the sheet increases with b indicating a movement of circulation towards the asymptotic centre of the system. As b increases at constant a , there appears to be a tendency for the whole windward sheet-vortex system to move closer to the wing surface, while the overall windward circulation G_2 (the variation of which with a and b , is shown in Fig. 10B), increases quite strongly. At higher values of a than those depicted in Figs 4B, 5B and 6B, the tendency is not so much a movement toward the wing, as a movement inboard toward the wing centre line. This is illustrated by the variation of the position of the isolated vortex, as shown by the heavy lines in Fig.9.

For all values of a calculated, at higher values of b , regions of negative curvature and associated points of inflection appeared in the windward vortex sheet shape near the leading edge. This phenomenon was noted by Smith in his treatment of the unyawed problem for the flat plate (Ref.4), and for a family of rhombic cones (Ref.6), but whereas in his calculations, inflection points appeared only at small values of the incidence parameter a , in the present work, they were found to arise at different values of b , over the whole range of a treated. Smith⁽⁶⁾ suggests that the phenomenon might arise from the necessity that a vortex sheet separating from a sharp leading edge must do so in a direction tangential to the lower surface. In the present calculations this condition has been applied implicitly by way of an assumption made in the derivation of equation (26) for the sheet shape near a leading edge, which is used in the finite difference formulation of the Kutta conditions.

The outer part of the leeward vortex sheet is not so well represented geometrically as that of the windward sheet. From Figs 4A, 5A and 6A, it can be seen that, as b increases, the distance between the free end of the sheet and the isolated vortex increases, and for higher values of b , it might well be argued that insufficient[†] of the

[†]see footnote next page

outer part of the sheet is represented, to satisfy condition (a) in section 3.3. The effect of this on the calculated position of the leeward vortex is that it is possibly too far to leeward, the velocity inducing effect of the "missing part" of the sheet, in the vicinity of the vortex being a component to windward. This is illustrated in Fig. 5A, where, for $a = 1.0$, $b = 1.0$, a leeward sheet and vortex position, calculated with λ_{1N} held fixed at $\lambda_{1N} = 0.20$, is shown. The solution for the same a and b , in which the zero moment condition is applied yields $\lambda_{1N} = 0.159$ (Table 2). For $a = 1.0$ and $a = 1.5$ (Figs 5A and 6A), as b increases, the isolated vortex approaches more nearly the tangent to the sheet at its free end. Although part of this effect can probably be attributed to the above-mentioned error in the calculation of the vortex position, it is nevertheless believed to be a genuine indication that the sheet (if it were continued) is becoming more tightly wound, geometrically, about its asymptotic centre.

The main effect, of increasing b , on the position of the leeward sheet and vortex can be seen to be a marked movement to leeward. For $b > 1$, the wing leeward edge must be considered to be a trailing edge, since for these cases $\beta > \delta$. Thus in solutions calculated for $b > 1$ the leeward vortex sheet can be interpreted as one emanating from a trailing edge, and the overall flow, as that in the tip region of a very highly forward swept wing with a pointed tip of small apex angle.

4.2 Isolated Vortex Positions; Circulation

4.2.1 Calculated vortex positions

The heavy lines in Figs 7 and 9 show the variation of the calculated position of the leeward and windward isolated vortices respectively, and also depict a comparison of the calculated values with Harvey's⁽¹⁵⁾

[†]Note, however, that at values of b near $b = 2.0$, the calculated value of λ_{1N} increases sharply (Table 2), which means that quite a substantial fraction of the total leeward circulation is distributed along the outer part of the sheet.

experimentally determined core positions. Figure 8 shows a similar comparison of the calculated vortex positions on the leeward side with the results of an experiment carried out by the author.

For $b > 0$, there is no longer symmetry of the two vortex-sheet-isolated-vortex systems about $\xi = 0$. As b increases at a fixed value of a , Figs 7 or 8 show that the leeward isolated vortex moves upwards away from the wing surface and towards, and eventually outboard of the leeward leading edge. This movement represents a general trend for all values of a . It is associated with a weakening of the leeward system which may be seen in Fig.10A as a decrease in the magnitude of the total circulation G_1 with b at constant a . However, while the rate of movement of the vortex position with b appears to increase with increasing b , the rate of change of $|G_1|$ seems to decrease to near zero. Thus at large yaw the leeward vortex moves rapidly outboard with increasing b while the overall leeward circulation remains nearly constant. The main effect on the position of the leeward vortex, of increasing a at constant b , is a marked vertical movement and a corresponding increase in $|G_1|$.

The effect of relaxing the zero moment condition, on the position of the leeward isolated vortex, is illustrated in Fig.8 where the dash-dotted line shows its variation with b for $a = 1.0$, obtained from solutions calculated with λ_{1N} held constant at $\lambda_{1N} = 0.20$. Differences between vortex positions given by this curve and those given by the heavy line (for $a = 1.0$), begin to become significant at values of b somewhat less than $b = 1.0$, where the calculated value of λ_{1N} associated with the zero moment condition begins to differ appreciably from $\lambda_{1N} = 0.2$ (see Table 2). Where this value exceeds 0.2, the vortex positions given by the heavy line are to be preferred, and where it is less than 0.2, those given by the dot-dashed line will be more accurate. The effect of holding λ_{1N} fixed, on the windward vortex position, is too small to be illustrated graphically. The effect on the normal-force and rolling-moment coefficients was found to amount to, except at very large yaw, a fractional change of less than 1%.

On the windward side of the wing, at high values of a , there can be discerned (Fig.9) a strong inboard movement of the vortex, without much variation in the height, as b increases at constant a . For intermediate incidence ($a = 1.5, 1.0$) the inboard movement is less marked

and there is a definite downward movement towards the wing surface. The variation of the vortex position with b is not very systematic for these values of a and is completely haphazard for $a = 0.5$, over the small range of b for which solutions could be obtained with $N = 10$, $\lambda_{2N} = 0.20$.

As a decreases at constant b , the vortex path can be seen to move outboard and downwards towards the windward leading edge, the loci for all values of b converging as a decreases, until failure of the iteration scheme is encountered. The extremities of the heavy lines in Figs 7, 8 and 9 at the lower values of a represent the first onset of failure for the values of b indicated. The appropriate values of a are given by equation (43). To verify that this failure was not a numerical effect associated with, say, the particular numerical parameters chosen, some solutions for $N = 8$, $\lambda_{2N} = 0.15$ were obtained for values of a below 1.0. In general, for a fixed b , the iteration scheme first diverged at about the same value of a for the $N = 10$, $\lambda_{2N} = 0.2$ cases. However, whereas for $a = 0.5$, no $N = 10$ solutions could be found for $0.08 < b < 0.5$ (although solutions could be obtained for $0.5 \leq b \leq 0.95$), $N = 8$ solutions could be found for all $0.0 \leq b \leq 0.95$. The vortex loci for these $N = 8$ solutions are shown in Figs 7, 8 and 9 as dotted lines. On the leeward side, the $N = 8$ isolated vortex positions are reasonably close to the $N = 10$ ones, except near the point of solution failure, but on the windward side, there is significant difference, the loci for both values of N being quite unrealistic.

There are two possible reasons for the failure to obtain solutions at low values of a . The first is that the integro-differential equations (17), and the Kutta conditions (20) [and hence the finite difference equations (24), (28), (30) and (35)] are inappropriate to the physical flow in this particular region of the a - b plane. This however seems unlikely as Harvey's experimental evidence indicates that well formed shear-layer core systems exist in the flow for values of α and β for which no solutions could be found. The second possible reason is that the divergence of the solution scheme is a result of the inability of the second order Newton-Raphson iteration technique to obtain solutions to what are in fact, well posed equations. Divergence always occurred quite suddenly (as a was decreased or b increased) and was not associated with any appreciable increase in the number of iterations

required for convergence to solutions, just prior to failure. It was, however, accompanied by a change in sign of the determinant $\|[\partial f_k / \partial \Omega_\ell]\|$, which implies complex behaviour of the strongly nonlinear finite difference equations.

4.2.2 Present experiment

In Ref.15 Harvey presents maps of the total head surveys (Figs 7-15) he obtained for various values of the incidence and yaw angles α and β and also a summary graph showing the variation of the leeward and windward vortex cores, taken as the positions of the respective total head absolute minima. Unfortunately there seems to be a discrepancy between the core positions that can be inferred from the total head maps and those presented in the summary graph. Discussion with Dr. Harvey led to the conclusion that the summary graph - Fig.16 in Ref.15 - in fact gives the correct experimental determination of the vortex cores, the total head maps being incorrect due to scale errors in the plotting process. Regrettably the original total head data has been lost.

To verify that Harvey's summary graph indeed gives the correct core positions, and to determine core positions for some values of a and b which were not covered in Harvey's work, a further experiment was carried out by the author, in the 5 ft. $\times$ 4 ft. low speed wind tunnel at Imperial College. This was performed with the same delta wing ($\delta = 10^\circ$) used by Harvey. Experimental conditions, and in particular the Reynolds number ($Re \approx 6.1 \times 10^5$, based on distance from the wing apex) were generally similar to those of Ref.15.

The leeward primary core positions were determined by searching for the absolute total head minima in the flow field, using a Kiel tube mounted on a Deiser traverse gear, for yaw angles of $\beta = 0^\circ, 5^\circ, 10^\circ, 15^\circ$ and 20° at each of 3 values of the incidence, $\alpha = 5^\circ, 10^\circ$ and 15° . Measurements were made only on the leeward side of the wing as it is believed that the effect of secondary separation on the windward side is so strong at higher values of b , as to make the extra data that might

be obtained not worthwhile in relation to the present work.

4.2.3 Comparison with experiment

Comparison of the calculated leeward vortex positions with the experimental[†] results of Harvey (Fig.7) and of the author^{††} (Fig.8) is fair and is similar to that obtained by Smith⁽⁴⁾⁽⁶⁾ for unyawed flow. As b increases and the primary vortex core moves past the leeward leading-edge, the leeward secondary separation system diminishes in size and influence, eventually vanishing completely. One might therefore expect that comparison with experiment would improve, the higher the value of b . From Figs 7 and 8 it can be seen that this is not the case; the measured core-positions being, in general, rather inboard of the calculated positions of the isolated vortex.

As was noted in section 4.1, as b increases, the geometrical extent of the outer part of the leeward vortex-sheet becomes less adequate, the probable effect on the calculated vortex position being an error to leeward. Since this is just the direction of the general theoretical-experimental discrepancy, we might perhaps interpret it as being the result of the improvement in the aptness of the flow model with increasing b (diminishing secondary separation), being to some extent offset by a slight worsening in the sufficiency of the present numerical representation.

It can be seen from Fig.9 that comparison with experiment on the windward side of the wing is not good and in fact worsens with increasing yaw. In general the height of the vortex core is well predicted but the lateral position is not, the calculated values being much too far inboard of the measured ones. These discrepancies are more than likely attributable to the neglect of the windward secondary separation shear-layer core system, the size of which, as noted by Harvey⁽¹⁵⁾, increases with

[†]In Figs 7, 8 and 9 similarly flagged symbols of different type (different incidence) represent experimental results at the same yaw angle.

^{††}Note that the present experimental leeward primary core positions, as they are based on one measurement only, must be considered to be less reliable than those of Harvey, which were inferred from detailed total head surveys.

increasing yaw. The fact that the windward core position is not well predicted will, of course, through the mutual coupling of the velocity inducing effects of the leeward and windward circulatory systems, introduce errors into the calculated position of the leeward isolated vortex. However, since the two systems are fairly remote from each other, this effect is thought to be small.

4.2.4 Circulation

Figures 10A and 10B show the variation of the total circulation of the leeward and the windward systems, G_1 and G_2 respectively, with b at constant a . That $|G_1|$ decreases with increasing b has been previously noted. The circulation of the windward system, on the other hand, can be seen to increase quite strongly with increasing b , the rate of increase rising with both a and b . Thus for intermediate and large yaw, the windward circulatory system is much the stronger of the two. These trends are confirmed qualitatively by Harvey's⁽¹⁵⁾ observations concerning the variation in strength of the absolute minima of his total head surveys, with α and β .

4.3 Wing Surface Pressure Distributions

The pressure coefficient - expressed as C_p/K^2 so as to be a function of a , b and $\xi = y/s$ only[†] - was calculated, for various a and b , at discrete points along the upper and lower wing surfaces using equations (A1.1)-(A1.5), Appendix A. Figures 11-16 show graphically the calculated pressure distributions, for the values of a and b indicated and compare them with measured distributions obtained by Fink⁽¹⁴⁾ and Harvey⁽¹⁵⁾ in regions of approximately conical flow.

It can be seen in Figs 11-16 that there appears to be a relative shift in the vertical scales of the calculated and measured distributions

[†]Integrals of the zeroth and first moments of $\Delta C_p/K^2$ about $\xi = 0$, being the normal-force and rolling-moment coefficients respectively, will thus only be functions of a and b .

amounting to about 1.5 units of C_p/K^2 . The present theoretical distributions for $b = 0$ are in good agreement with those of Ref.4, calculated for unyawed flow. Furthermore the centreline pressure coefficients on the underside of the wing are for all cases, slightly larger than the corresponding attached flow values

$$\left[\frac{C_p}{K^2} \right]_{ATT, \omega = (0, 0^-)} = a(a+2)$$

which is consistent with the additional velocity inducing effect of vortex sheets present in the separated flow. It is therefore believed that the experimental distributions presented in Refs (14) and (15) are slightly in error, a circumstance which is thought to have arisen due to a static pressure gradient which probably existed in the flow between the tunnel axis and the static pressureappings on the tunnel wall. This, of course, would not affect estimates of local lift and rolling moments obtained from them, which was the primary objective of the experiment.

Figure 11, for $a = 0.5$, figures 12 and 13, for $a = 1.0$ and figures 14-16 for $a = 1.5$ clearly indicate the effect of yaw on the calculated wing surface pressure distributions. As b increases from zero, the distributions lose their symmetry about $\xi = 0$. The windward upper surface suction peak follows the windward isolated vortex inboard and increases in strength, corresponding to the rise in the total circulation of the windward system and the slight downward movement of the isolated vortex. On the leeward side, the general effect is quite the opposite, the suction peak collapsing rapidly (as b increases), and moving outboard toward the leading edge in sympathy with the calculated movement of the isolated vortex, and the decrease in magnitude of the circulation of the leeward system. No pressure distribution is presented for which the leeward vortex is actually outboard of the leading edge, but for such cases the leeward suction peak vanishes completely.

Comparison of calculated and experimental distributions is generally quite good along the lower surface of the wing and fair on the leeward upper surface. The large discrepancies which exist between theory and experiment on the windward upper surface, and which increase with increasing yaw, are believed to be due to the effects of secondary separation. The presence of this phenomenon influences the pressure

distribution on the windward side of the wing directly in that it causes a reduction in the size of the suction peak and inhibits pressure recovery between the primary vortex core and the wing leading edge. An indirect effect is that it displaces the primary core inboard. Overall the effect might be described as a "flattening and broadening" of the windward suction peak. That the calculated suction peak is much too strong and is too far outboard is consistent with the discrepancies, previously noted, between the calculated and measured primary vortex positions. That the predicted shape is manifestly incorrect may be explained by the absence of the modifying effects of secondary separation as described above.

As the influence of secondary separation on the leeward side of the wing diminishes (with increasing b), comparison with experiment improves significantly and in fact the shape of the small leeward suction peak is quite well predicted for the higher values of b in figures 11C, 12B and 16.

It is interesting to note that at higher values of a and b , the calculated pressure distributions resemble more nearly those appropriate to a two-dimensional wing at incidence in a uniform stream. This is not surprising since with the present formulation, the limiting case

$$a \rightarrow \infty$$

$$b \rightarrow \infty$$

$$a/b \rightarrow \text{CONST} = \tan(\gamma), \text{ say,}$$

corresponds to a two-dimensional flow (at incidence γ) with both leading and trailing edge separation. Of course, for stability reasons it is unlikely that such a flow could exist.

4.4 Normal-Force Coefficient

Equation (A2.4) gives the complex lateral force coefficient $(C_Y + iC_N)/K^2$ for the entire wing vortex-sheet-isolated-vortex separated flow system. Since the wing has no thickness, and since there are no leading edge suction forces acting, the y -wise force on the wing must necessarily be zero. Because, however, of small residual forces acting in the fluid (due largely to the finite difference modelling of the integro-differential equations), the overall y -wise force will not vanish.

For the same reason, the overall normal-force coefficient obtained from the imaginary part of A2.4, will differ from that obtained by numerical evaluation of (A2.5), the integral of the pressure difference across the wing surface. In the present calculations, the magnitude of the real part of equation (A2.4) was always less than 0.5% of the imaginary part, and the fractional difference between the imaginary part, and numerical evaluation of (A2.5) (using a 5 point rule), was always less than 1.5%, and generally less than 1%.

The lift in attached flow is given by the first term of equation (A2.4)

$$\left[\frac{C_N}{K^2} \right]_{ATT} = 2\pi a ,$$

and is independent of yaw.

Figure 17 shows the variation of the imaginary part of $(C_Y + iC_N)/K^2$ with b for various values of a . Also shown are experimental values obtained in Ref.15 from integration of measured pressure distributions. These values actually represent local normal-force coefficients, but have been corrected to give overall coefficients by assuming that the flow is conical. They therefore exclude trailing edge effects.

It can be seen from Fig.17 that the calculated effect of yaw is to increase the separated flow lift, the rate of increase increasing with both a and b . Harvey's experimental data shows an initial decrease in the overall lift, with increasing yaw, which is not predicted by the present calculations, and a subsequent increase. It is difficult to say whether or not this experimental trend is genuine, although there is no reason to doubt it. Quite possibly it is a result, direct or otherwise, of the change in state of the secondary separation systems with yaw, or it could perhaps be a thickness effect. We may conclude that although the details of the pressure distribution are not well predicted on the windward upper surface, the normal force coefficient is reasonably well predicted, the regions of under and over prediction of the pressure coefficient, balancing in contribution thereto.

4.5 Rolling-Moment Coefficient

For separated flow, the rolling-moment coefficient C_L/K^2 cannot be evaluated by the method of residues (see Appendix A) and in the present work was calculated by numerical evaluation of a span-wise integral of the first moment of the pressure difference across the wing surface, equation (A3.3). Figure 18 shows the variation of C_L/K^2 with b for various values of a . The dotted lines give the attached flow rolling moment

$$[C_L/K^2]_{ATT} = \frac{\pi}{3} ab ,$$

obtained by Ribner⁽¹³⁾. As was mentioned in section 4.1, for $b > 1$, the leeward wing edge becomes, in fact, a trailing edge, at which it is necessary that the flow satisfy a Kutta condition. Since this is impossible without free circulation, the attached flow has no meaning for $b > 1$, and the dotted lines (in Fig.18) are therefore terminated at $b = 1$.

Figure 18 indicates that in general both the attached and separated flow rolling-moment coefficients[†] increase either with b at constant a or vice-versa. However, for $a = 3.0$, after an initial increase with b , the rolling-moment decreases for values of b greater than about 1.5. In general, the difference between the predicted attached and separated flow rolling-moments (for $b < 1$) can be seen to be significant, but not large. Thus although the separated flow considerably alters the wing pressure distribution from that obtained in attached flow, it produces rather smaller fractional changes in the rolling moment than it does in the lift. This may be interpreted as meaning that as b increases at constant a , both the attached and separated flow pressure distributions change - from the corresponding distribution at zero yaw - in roughly the same manner, even though they differ quantitatively and qualitatively from each other.

In Fig.19, the rolling-moment coefficient plotted as $C_L/(K^2b)$ is compared with Harvey's experimental values obtained as the first moment of the measured pressure distribution about $\xi = 0$. For $a = 0.5$, the

[†]The sense of positive rolling-moment is indicated in Fig.1.

comparison is quite good over the range for which solutions could be obtained. At higher α the experimental values generally lie between those predicted for the attached and separated flow. For the separated flow, the largest contribution to the rolling-moment will come from the windward suction peak region of the wing, and since it is here that the upper surface pressure coefficient is most poorly predicted, it is not surprising that there is large discrepancy between theory and experiment. Since the windward suction peak is calculated to be rather too far outboard, we might expect that the magnitude of the rolling moment might be over-predicted, as is the case for $\alpha = 1.0$ and $\alpha = 1.5$. The reasonable comparison with experiment obtained for $\alpha = 0.5$ must be regarded as fortuitous.

5. CONCLUSION

Numerical calculations have been made of the conical inviscid flow, with leading edge separation, past a yawed slender delta wing. The Newton-Raphson iterative technique employed yielded satisfactory solutions to the finite difference equations over ranges of the incidence and yaw parameters, but diverged, failing to do so in a region of the parameter space associated with lower values of the incidence.

For non-zero yaw, comparison of the calculated flow properties with experiment was generally no worse than for zero yaw, there being two notable exceptions, namely the position of the windward primary vortex core and the shape and strength of the associated pressure suction peak on the windward upper surface of the wing. The large theoretical-experimental discrepancies which were found to exist for these quantities were attributed to the increasing influence (with increasing yaw) of the secondary separation system, the effects of which were not included in the flow model.

There was good qualitative agreement between theory and experiment, both of which indicate that increasing the yaw angle:

- (a) strengthens the windward primary vortex core which moves inboard and slightly downwards,
 - (b) weakens the leeward core which moves markedly outboard of the wing centre line and upwards,
 - (c) causes an increase in strength of the pressure suction peak on the windward upper surface of the wing, and a decrease in that on the leeward upper surface,
 - (d) produces appreciable increase in the normal-force coefficient only at large yaw,
- and (e) induces a rolling-moment on the wing, not very much larger than that predicted by attached flow theory.

The failure of the solution method in the lower incidence range remains unexplained and clearly requires further investigation.

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Appendix A

Calculation of the Pressure Coefficient, Normal Force and Rolling Moment

In this appendix, the expressions used to calculate the wing pressure coefficient and the lift and rolling moment coefficients, are derived.

A1 Pressure Coefficient

For conical inviscid irrotational flow about a flat plate delta wing, the slender-body theory prediction of the pressure coefficient is given by (Ref.4)

$$\begin{aligned} \frac{C_P}{K^2} = & 2 \left(y \frac{\partial \phi}{\partial y} + z \frac{\partial \phi}{\partial z} - \phi \right) / K^2 U_x - \\ & - \left\{ \left(\frac{\partial \phi}{\partial y} \right)^2 + \left(\frac{\partial \phi}{\partial z} \right)^2 \right\} / K^2 U^2 + a^2 + b^2 \end{aligned} \quad (A1.1)$$

Note that the pressure coefficient is a quadratic function of the velocity components. Hence while solutions of equation (2) and the derived velocity fields may be superposed [since (2) is linear], pressure coefficients and lift and rolling moment coefficients, in general, may not be obtained by superposition.

It is easily verified that the various terms of (A1.1) may be expressed in terms of the complex velocity potential W , and the mapping $\omega(\omega^*)$, as follows.

$$\left\{ \left(\frac{\partial \phi}{\partial y} \right)^2 + \left(\frac{\partial \phi}{\partial z} \right)^2 \right\} / K^2 U^2 = \left| \frac{d(W/KUs)}{d\omega^*} \frac{d\omega^*}{d\omega} \right|^2, \quad (A1.2)$$

and

$$\left(y \frac{\partial \phi}{\partial y} - z \frac{\partial \phi}{\partial z} - \phi \right) / K^2 U_x = -2\text{Re} \left[\frac{W}{KUs} - \omega \frac{d(W/KUs)}{d\omega^*} \frac{d\omega^*}{d\omega} \right]. \quad (A1.3)$$

The last three terms of equations (24) (section 3.1) give the present representation of the complex velocity $d(W/KUs)/d\omega^*$, evaluated at a point $\omega_{jn,n-1}^*$ on a vortex sheet in the ω^* plane. By replacing

$\omega_{jn,n-1}^*$ in these terms by ω^* , we obtain an expression for the complex velocity at a general point in the ω^* plane:

$$\begin{aligned} \frac{d(W/KUs)}{d\omega^*} = & -\frac{1}{2} \left\{ (b+ia) + (-b+ia)/\omega^{*2} \right\} + \\ & + \frac{G_1}{2\pi i} \sum_{m=0}^{N+1} A_{1m} \left\{ \frac{1}{\omega^* - \omega_{1m}^*} - \frac{1}{\omega^* - 1/\overline{\omega_{1m}^*}} \right\} + \\ & + \frac{G_2}{2\pi i} \sum_{m=0}^{N+1} A_{2m} \left\{ \frac{1}{\omega^* - \omega_{2m}^*} - \frac{1}{\omega^* - 1/\overline{\omega_{2m}^*}} \right\}, \end{aligned} \quad (A1.4)$$

where the $A_{\ell m}$, $\ell = 1, 2$ are as in equations (24).

The associated expression for the complex potential W/KUs is obtained by integration of (A1.4) with respect to ω^* , which yields

$$\begin{aligned} W/KUs = & -\frac{1}{2} \left\{ (b+ia)\omega^* - (-b+ia)/\omega^* \right\} + \\ & + \frac{G_1}{2\pi i} \sum_{m=0}^{N+1} A_{1m} \log \left\{ \frac{\omega^* - \omega_{1m}^*}{\omega^* - 1/\overline{\omega_{1m}^*}} \right\} + \\ & + \frac{G_2}{2\pi i} \sum_{m=0}^{N+1} A_{2m} \log \left\{ \frac{\omega^* - \omega_{2m}^*}{\omega^* - 1/\overline{\omega_{2m}^*}} \right\}. \end{aligned} \quad (A1.5)$$

Using equations (A1.1)-(A1.5), the pressure coefficient can be evaluated at a point in the fluid, and in particular, at a point on the wing surface, provided that suitable branches of the logarithms appearing in (A1.5) are chosen.

A2 Normal Force

Sacks⁽¹⁶⁾, using the slender body theory, derives expressions for the overall forces and moments acting on a slender body in a generalized state of motion by considering various integrals of the pressure around contours adjacent to the body cross section in the cross-flow plane. In these expressions, where possible, contour integrals involving analytic

functions of the complex variable in the cross-flow plane are obtained. These integrals are treated by expanding the contour to infinity and applying the method of residues. Although only attached flows (i.e. those without vortex sheets) are considered in Ref.16 the arguments used and equations derived therein should be applicable to separated flow problems, provided that the contours considered surround the vortex sheets as well as the body, in the cross flow plane.

From equation (45) of Ref.16, the complex lateral force, acting up to a station $x = \ell$ on a flat plate delta wing with incidence and yaw, in a steady uniform stream may be written as

$$Y + iN = 2\pi\rho U \left\{ A_{-1} \right\}_{x=\ell}, \quad (A2.1)$$

where A_{-1} is the coefficient of Z^{-1} in the expansion for the appropriate complex potential[†] W , at large Z . The complex lateral force coefficient, when divided by K^2 , can be expressed as

$$\frac{C_Y}{K^2} + i \frac{C_N}{K^2} = \frac{Y + iN}{\frac{1}{2}\rho U^2 K^2 s \ell} \quad (A2.2)$$

where $s = K\ell$. Hence from equations (A2.1) and (A2.2) we may write

$$\frac{C_Y}{K^2} + i \frac{C_N}{K^2} = 4\pi C_{-1} \quad (A2.3)$$

where $C_{-1} = A_{-1}/(KU s^2)$ is the coefficient of ω^{-1} in the expansion of W/KUs for large ω . Note that (A2.3) is valid for either attached or separated flow.

For the present problem, C_{-1} can be evaluated using equations (A1.5) and (18) (from section 2.2), yielding for the overall complex lateral

[†]Note that in Ref.16, wing fixed axes are chosen on the moving body such that, at infinity, the lateral velocity components are zero. The different choice of axes for the present work will have no effect on the coefficient A_{-1} - merely adding a term linear in Z to the general form of the velocity potential used by Sacks - and thus the expressions derived in Ref.16 will be directly applicable to the present case.

force coefficient

$$\begin{aligned} \frac{C_Y}{K^2} + i \frac{C_N}{K^2} = 2\pi \left[ia + \frac{G_1}{2\pi i} \sum_{m=0}^{N+1} A_{1m} \left\{ \frac{1}{\omega_{1m}^*} - \omega_{1m}^* \right\} + \right. \\ \left. + \frac{G_2}{2\pi i} \sum_{m=0}^{N+1} A_{2m} \left\{ \frac{1}{\omega_{2m}^*} - \omega_{2m}^* \right\} \right] . \end{aligned} \quad (A2.4)$$

The first term on the R.H.S. of equation (A2.4) may be interpreted as the linear lateral force due to the attached flow, which, in fact, turns out to be independent of the yaw angle. The summation terms represent the lift due to the separated flow, which depends implicitly, through the solution points ω_{jn}^* , $j = 1, 2$, $n = 1, \dots, N+1$, on the incidence and yaw parameters.

Alternatively, the normal-force coefficient may be obtained by integration of the pressure coefficient over the wing upper and lower surface. Because of the conicality of the flow, this integral may be reduced to one along the wing cross section in the cross flow plane, viz:

$$\frac{C_N}{K^2} = \frac{1}{2} \int_{-1}^1 \frac{\Delta C_P}{K^2} d\xi , \quad (A2.5)$$

where ΔC_P is the pressure coefficient difference, lower surface minus upper surface, across the wing.

A3 Rolling Moment

Sacks also derives expressions for the rolling-moment acting on a slender body with a generalized motion, namely equation (52) of Ref.16. However, for the present case, the integrals appearing in this equation can only be evaluated by the method of residues if the initial contour taken about the wing (and vortex sheets, if any) has minor symmetry about the y and z axes. For separated flow, the presence of vortex sheets will mean that there can be no such symmetry, necessitating the use of other methods in the evaluation of the separated flow rolling-moment.

For attached flow, however, the required symmetry exists (for the present problem), and in this case, equation (52) of Ref.16 reduces to

$$L_{ATT} = - \frac{2\pi\rho K^4 U^2 \ell^3}{3} \operatorname{Im}[(b + ia)C_{-1}] , \quad (A3.1)$$

where $[L]_{ATT}$ is the attached flow rolling-moment and where C_{-1} is as defined for equation (A2.3). Using the expression

$$\left[\frac{C_L}{K^2} \right]_{ATT} = \frac{L_{ATT}}{\rho K^2 U^2 s^2 \ell} ,$$

and noting that for attached flow we have

$$C_{-1} = \frac{ia}{2} ,$$

we obtain for the attached flow rolling moment coefficient

$$\left[\frac{C_L}{K^2} \right]_{ATT} = - \frac{\pi ab}{3} . \quad (A3.2)$$

This result agrees with that obtained by Ribner⁽¹³⁾.

The rolling-moment coefficient for separated flow can be evaluated by a wing surface integration of the first moment of the pressure about the x axis. Reduction of this integral to one across the wing-span in the cross flow plane leads to

$$\frac{C_L}{K^2} = -\frac{1}{6} \int_{-1}^1 \frac{\Delta C_P}{K^2} \xi \, d\xi , \quad (A3.3)$$

where $\xi = (y/s)$. In equation (A3.3), ΔC_P is as for (A2.5). A positive C_L/K^2 acts in the sense indicated in Fig.1. As with (A2.5), (A3.3) can be evaluated numerically by a standard method.

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TABLE 2

PRINCIPAL SOLUTION PARAMETERS

$N = 10, \lambda_{2N} = 0.20$

a	b	ξ_{1N+1}	η_{1N+1}	G_1	λ_{1N}	ξ_{2N+1}	η_{2N+1}	G_2	$\frac{C_N}{K^2}$	$\frac{C_L}{K^2}$
0.5	0.0	-0.808	0.118	- 2.081	0.200	0.808	0.118	2.081	4.586	0.000
0.5	0.5	-0.849	0.162	- 1.649	0.131	0.815	0.097	2.469	4.622	-0.349
0.5	0.95	-0.949	0.232	- 1.237	0.152	0.815	0.088	2.841	4.807	-0.660
1.0	0.0	-0.704	0.246	- 4.610	0.200	0.704	0.249	4.610	10.94	0.000
1.0	0.5	-0.770	0.314	- 3.854	0.210	0.673	0.210	5.383	11.11	-0.668
1.0	1.0	-0.950	0.415	- 3.177	0.159	0.675	0.182	6.109	11.77	-1.317
1.0	1.5	-1.226	0.510	- 2.862	0.190	0.672	0.169	6.884	13.09	-1.882
1.0	2.0	-1.583	0.613	- 2.885	0.321	0.662	0.162	7.768	14.92	-2.245
1.5	0.0	-0.660	0.352	- 7.563	0.200	0.660	0.352	7.563	18.65	0.000
1.5	0.5	-0.746	0.431	- 6.560	0.199	0.608	0.308	8.595	18.96	-0.957
1.5	1.0	-0.922	0.551	- 5.704	0.186	0.563	0.285	9.681	20.07	-1.780
1.5	1.5	-1.190	0.688	- 5.220	0.223	0.528	0.271	10.85	22.16	-2.502
1.5	2.0	-1.530	0.822	- 5.138	0.310	0.517	0.255	12.00	24.94	-3.223
2.0	0.0	-0.643	0.428	-10.87	0.200	0.643	0.428	10.87	27.50	0.000
2.0	0.5	-0.742	0.515	- 9.68	0.181	0.579	0.384	12.12	27.94	-1.278
2.0	1.0	-0.915	0.640	- 8.66	0.169	0.513	0.368	13.48	29.55	-2.300
2.0	1.5	-1.168	0.796	- 8.10	0.208	0.442	0.366	14.98	32.48	-2.972
2.0	2.0	-1.481	0.969	- 7.98	0.298	0.377	0.365	16.56	36.17	-3.455
2.5	0.0	-0.637	0.486	-14.47	0.200	0.637	0.486	14.47	37.34	0.000
2.5	0.5	-0.746	0.579	-13.10	0.163	0.568	0.443	15.93	37.92	-1.635
2.5	1.0	-0.916	0.705	-11.98	0.151	0.490	0.433	17.55	40.08	-2.884
2.5	1.5	-1.159	0.870	-11.38	0.186	0.397	0.444	19.34	43.96	-3.501
2.5	2.0	-1.453	1.062	-11.29	0.269	0.304	0.457	21.20	48.63	-3.706
3.0	0.0	-0.638	0.533	-18.30	0.200	0.638	0.533	18.30	48.07	0.000
3.0	0.5	-0.755	0.632	-16.76	0.145	0.567	0.492	19.98	48.80	-2.068
3.0	1.0	-0.921	0.757	-15.57	0.135	0.482	0.487	21.86	51.58	-3.543
3.0	1.5	-1.157	0.925	-14.98	0.166	0.374	0.508	23.96	56.53	-4.106
3.0	2.0	-1.437	1.127	-14.98	0.243	0.259	0.536	26.11	62.25	-3.965

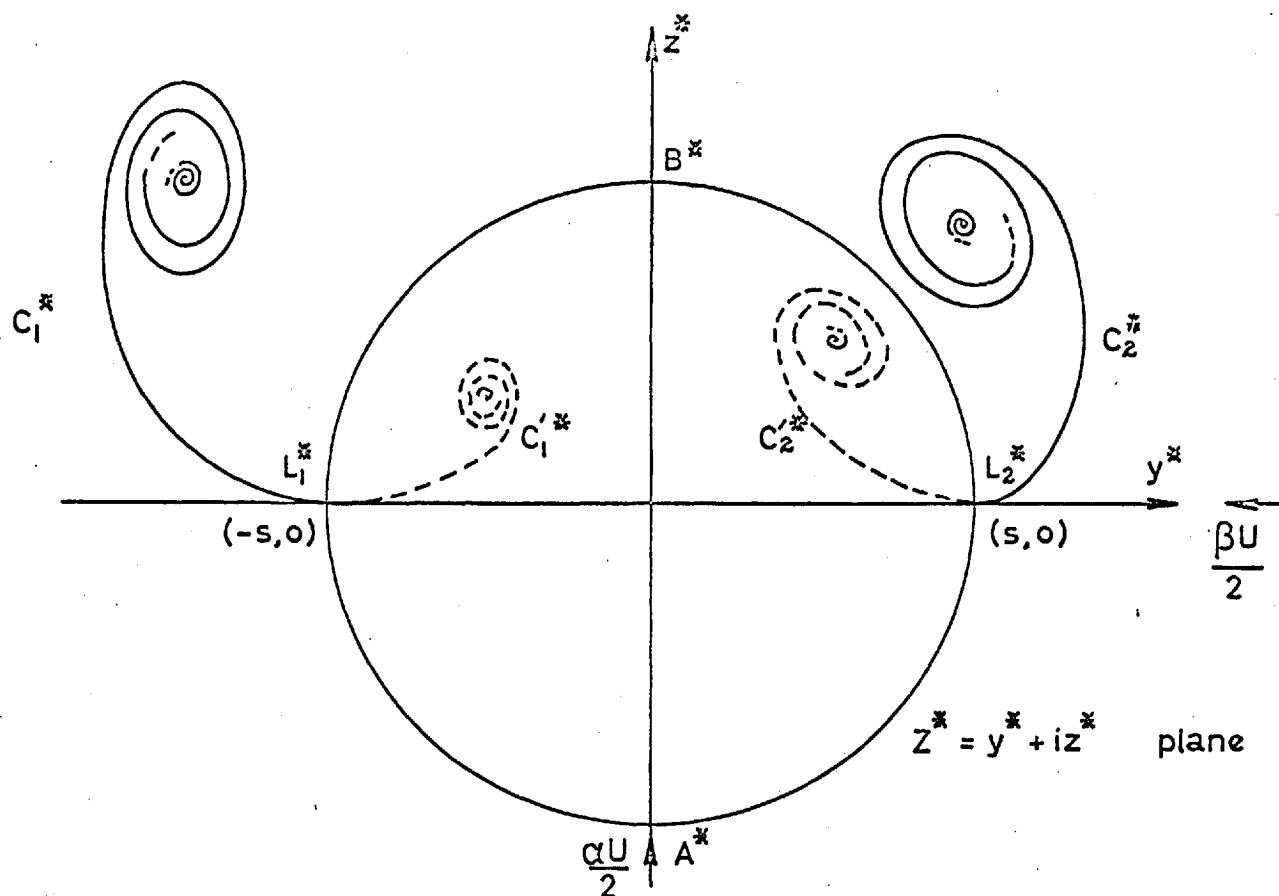


FIG. 3A VORTEX SHEETS IN THE TRANSFORMED PLANE.

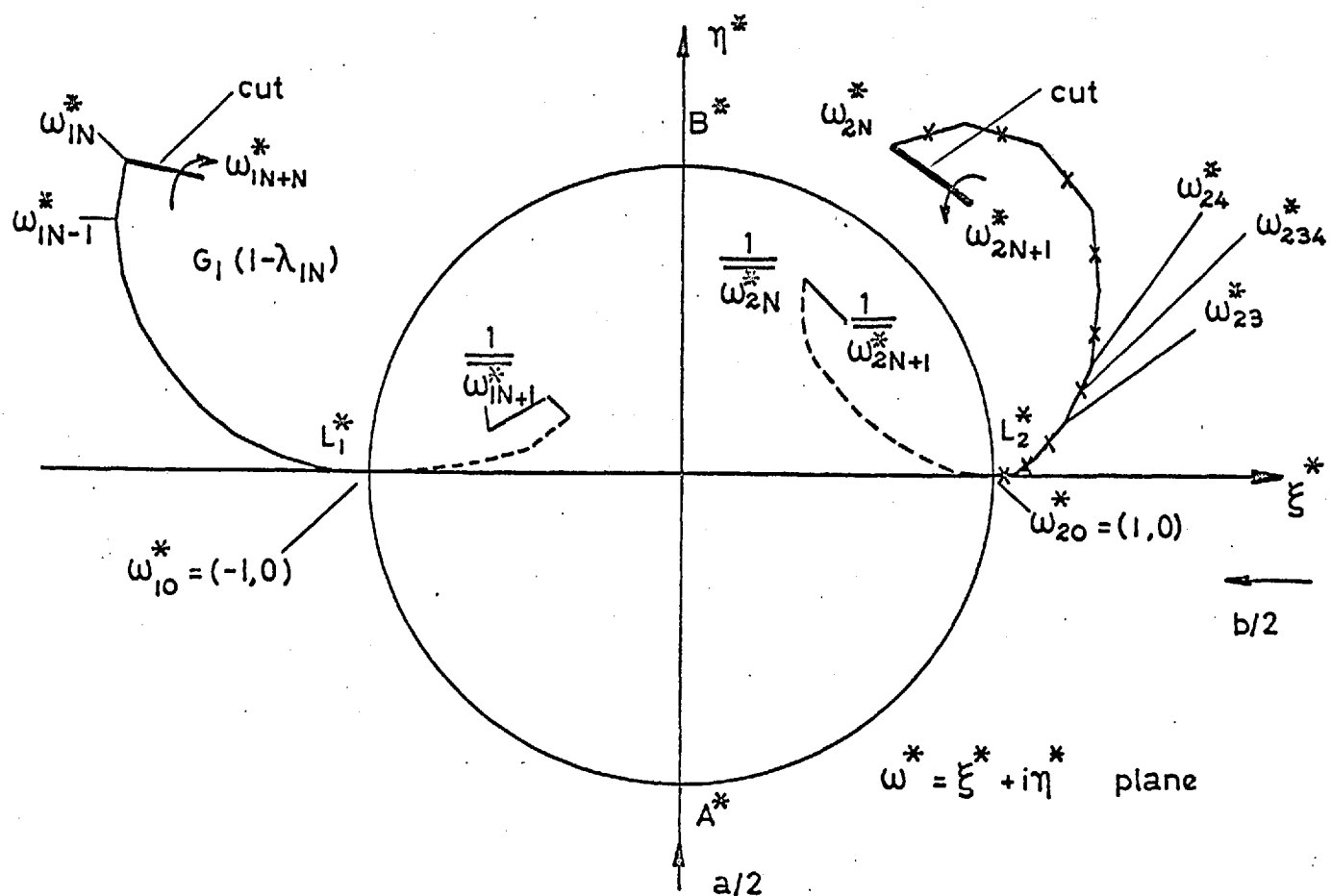


FIG. 3B BREAKUP OF VORTEX SHEETS FOR FINITE DIFFERENCE REPRESENTATION.

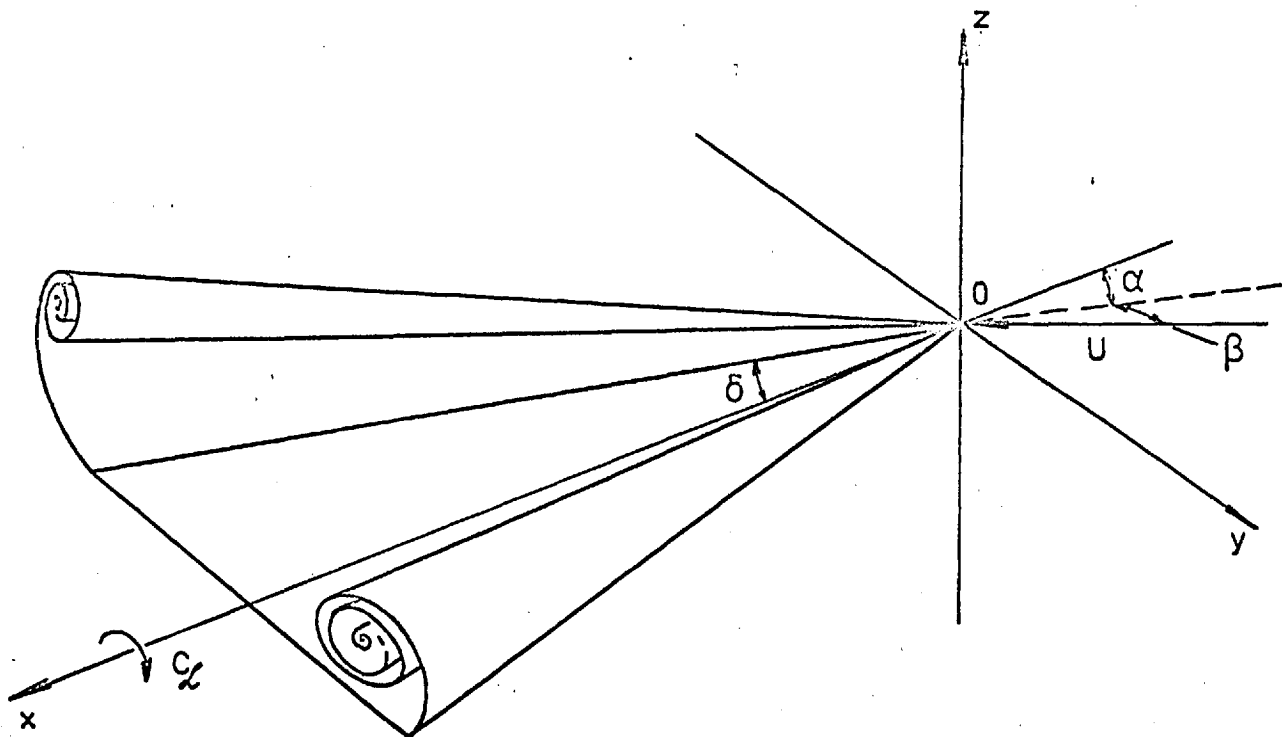


FIG. 1 THREE DIMENSIONAL VIEW OF CONICAL YAWED FLOW PAST A SLENDER DELTA WING WITH LEADING EDGE SEPARATION REPRESENTED BY VORTEX SHEETS.

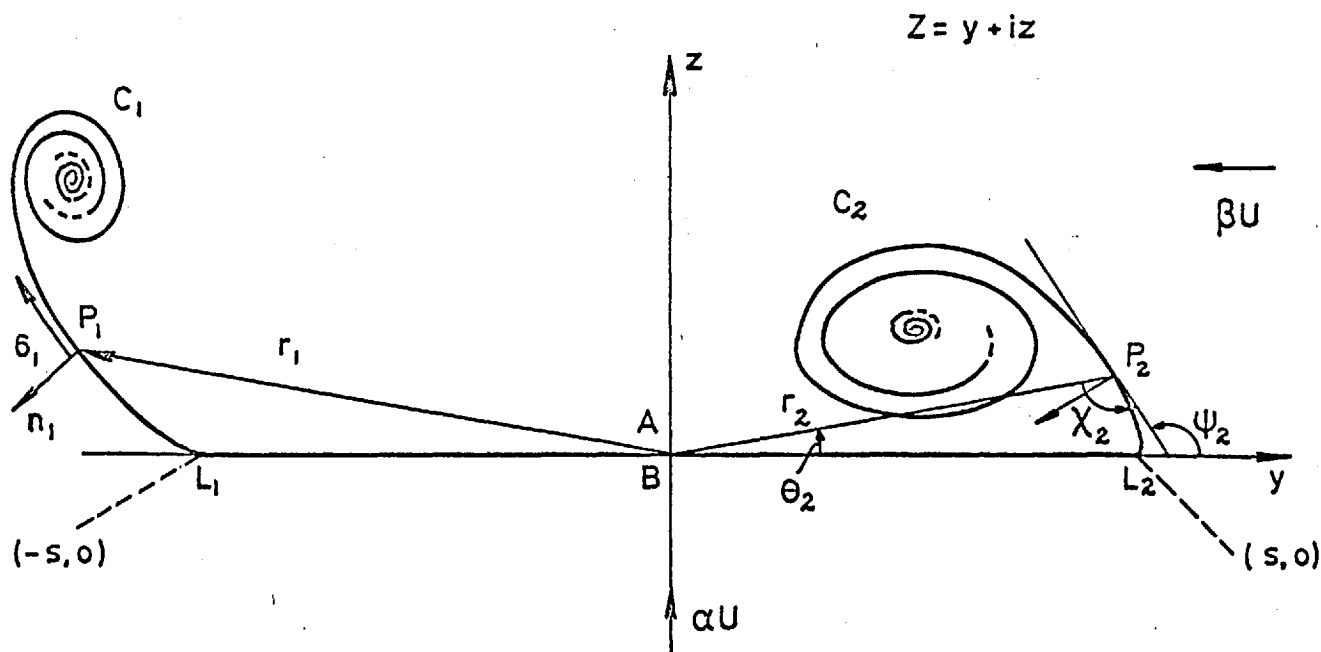


FIG. 2 CROSSFLOW PLANE SHOWING WING $(L, A, L_2 B)$, LEEWARD (C_1) AND WINDWARD VORTEX (C_2) SHEETS.

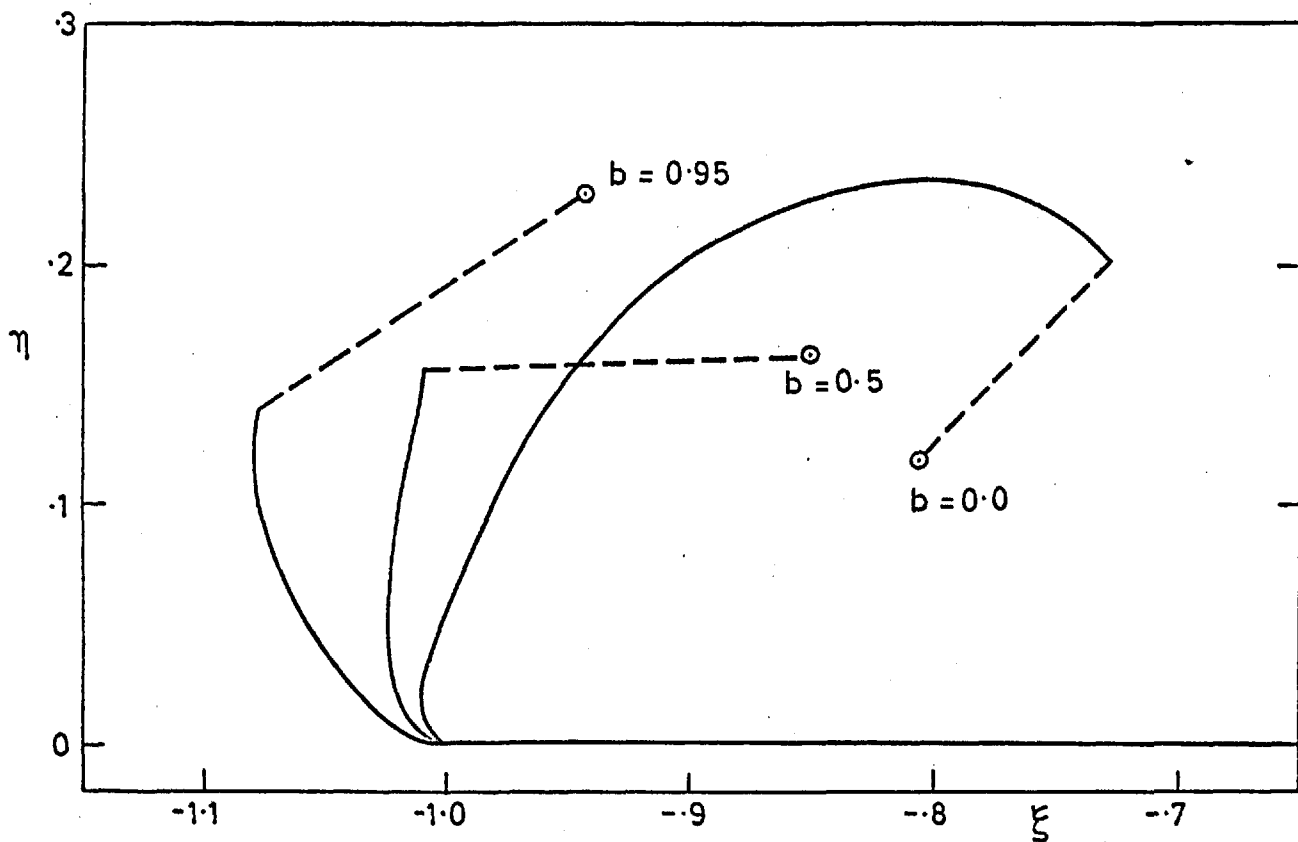


FIG. 4A LEEWARD SYSTEM; VORTEX SHEET SHAPE AND POSITION OF ISOLATED VORTEX FOR $a = .5$, VARIOUS b .

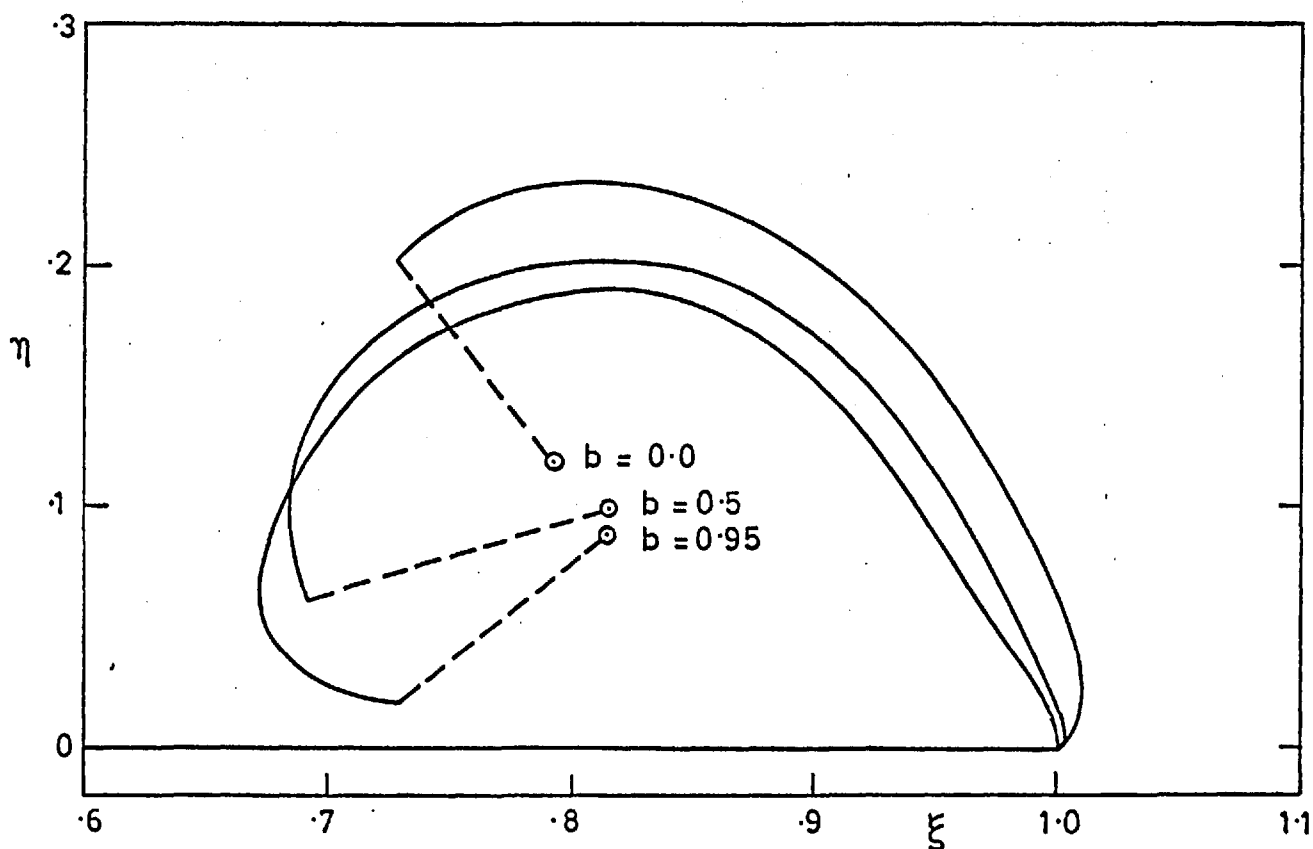


FIG. 4B WINDWARD SYSTEM; VORTEX SHEET SHAPE AND POSITION OF ISOLATED VORTEX FOR $a = .5$, VARIOUS b .

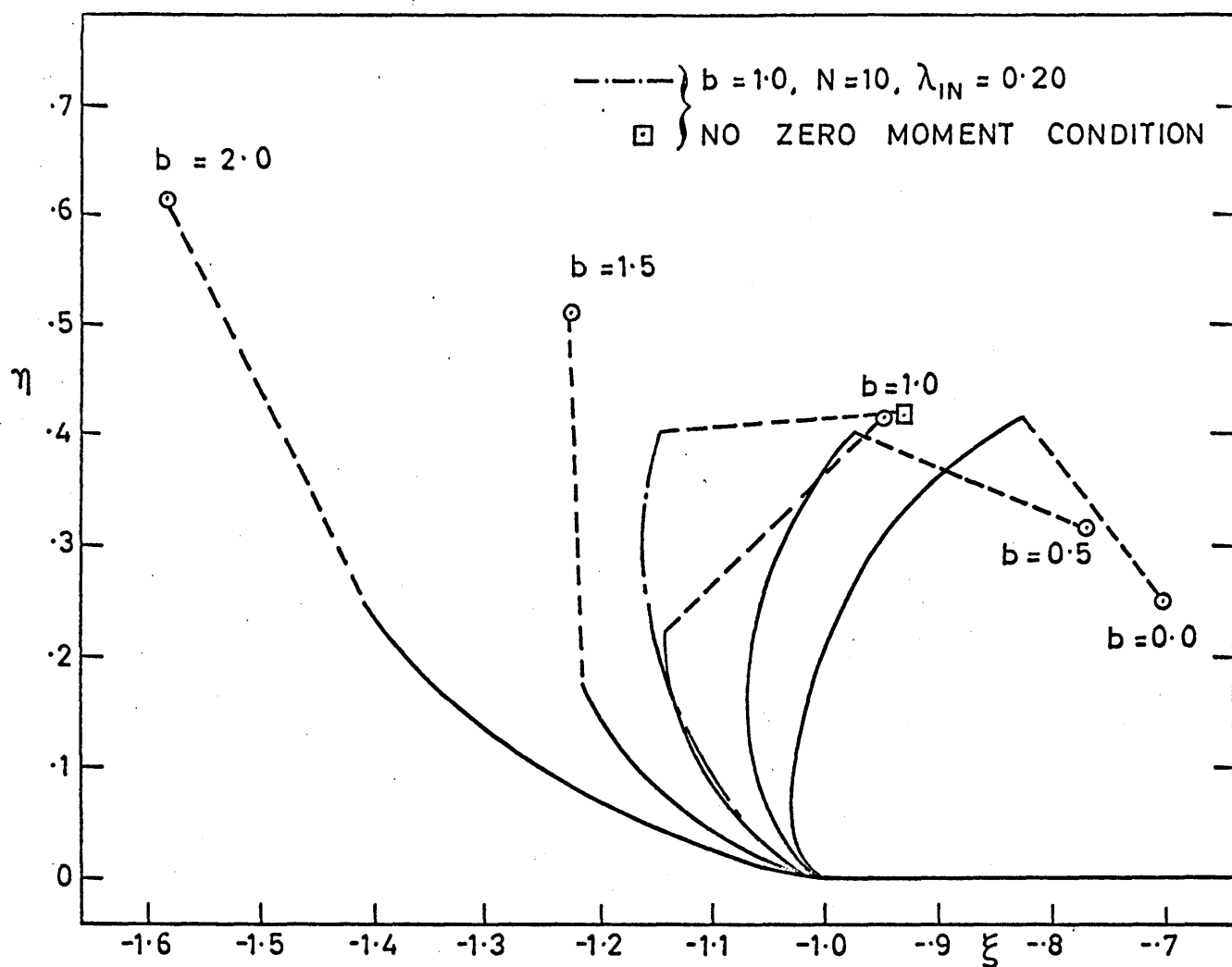


FIG. 5A LEEWARD SYSTEM; VORTEX SHEET SHAPE AND POSITION OF ISOLATED VORTEX FOR $a=1.0$, VARIOUS b .

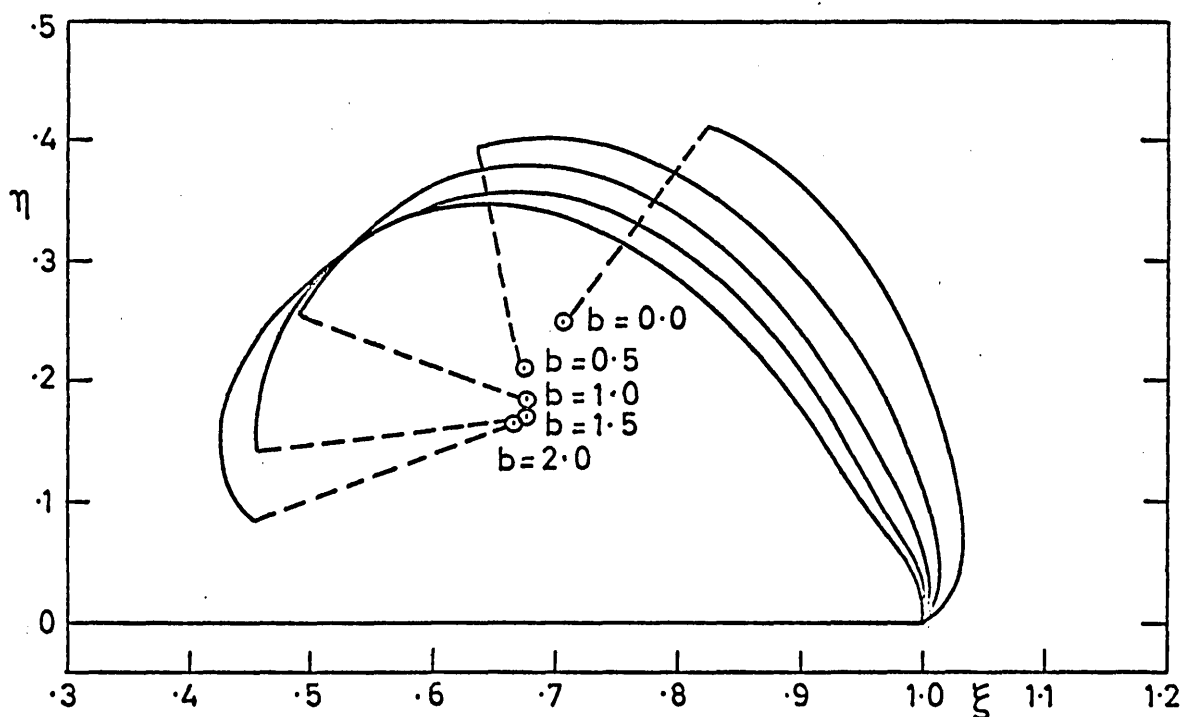
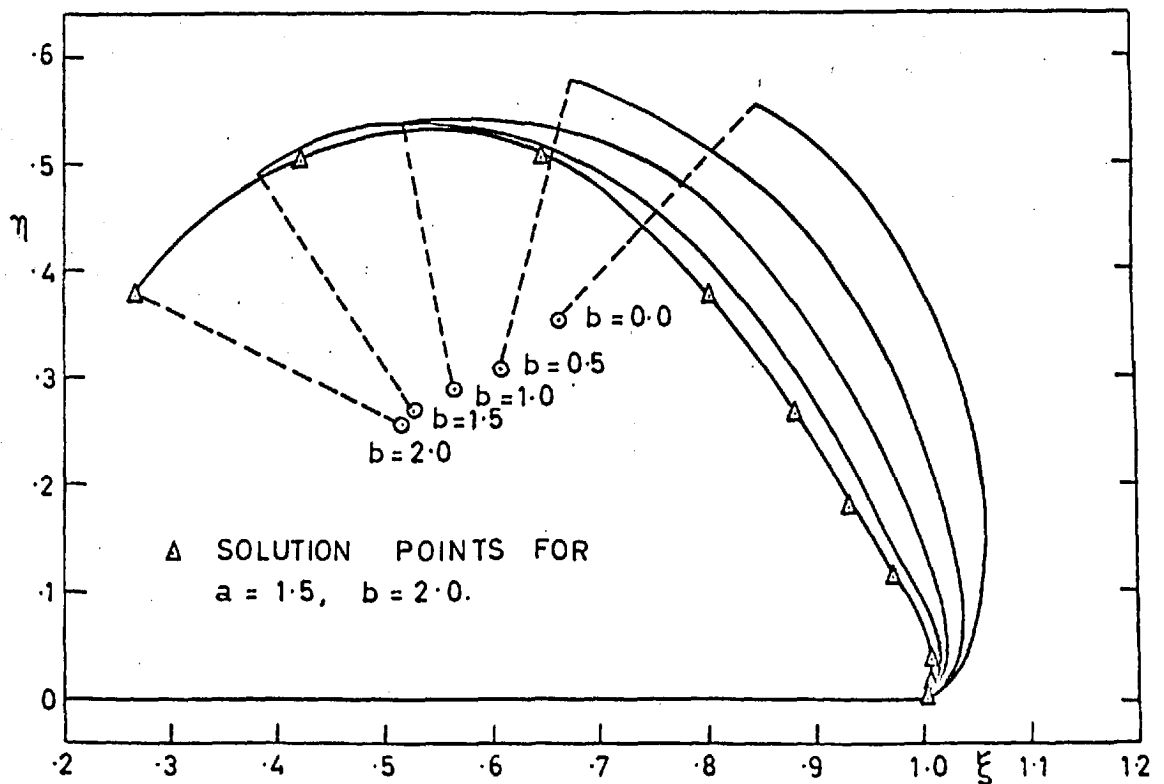
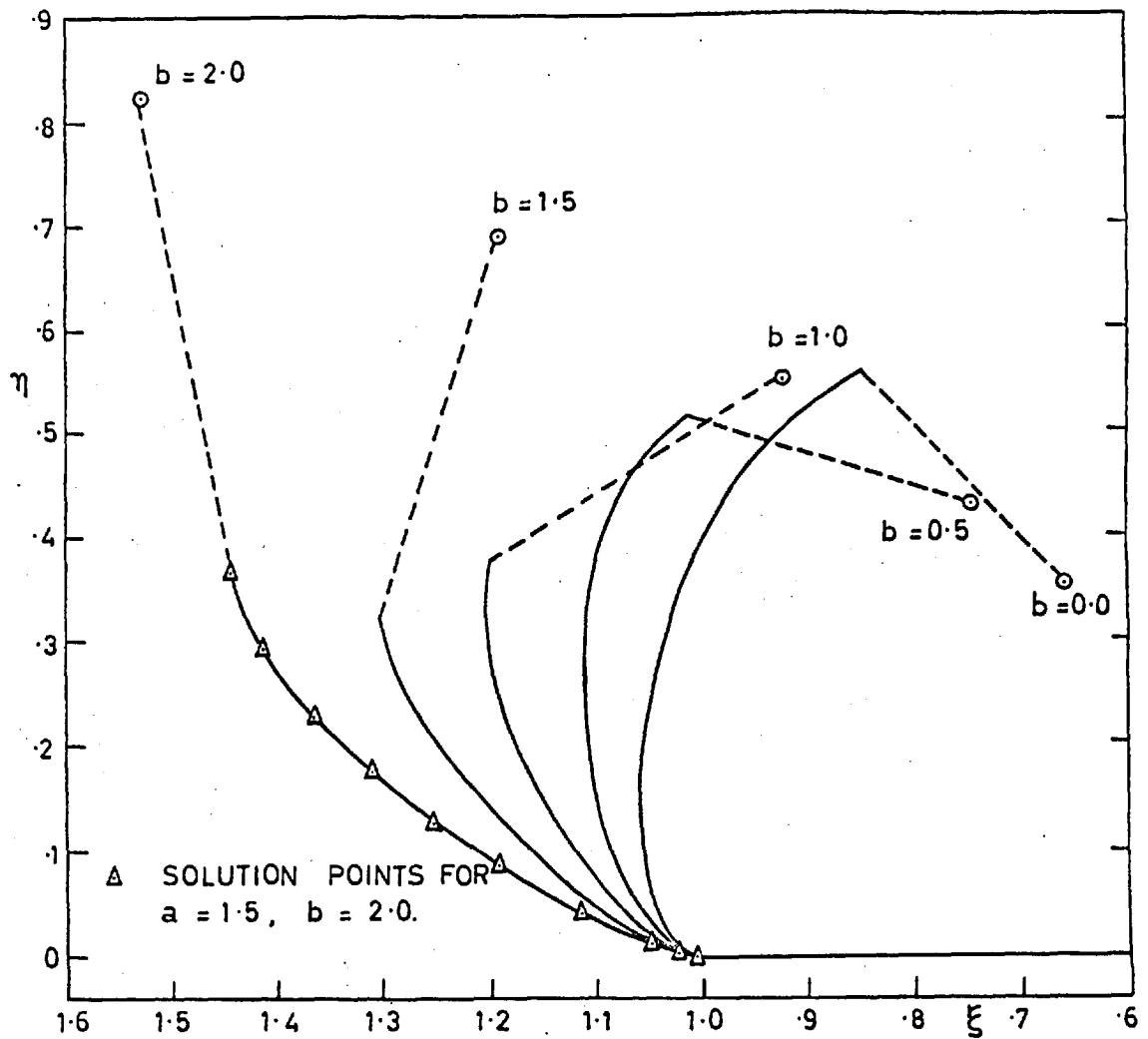


FIG. 5B WINDWARD SYSTEM; VORTEX SHEET SHAPE AND POSITION OF ISOLATED VORTEX FOR $a=1.0$, VARIOUS b .



FIGS. 6A TOP (LEEWARD SYSTEM) AND 6B BOTTOM (WINDWARD SYSTEM) VORTEX SHEET SHAPE AND POSITION OF ISOLATED VORTEX FOR $a = 1.5$, VARIOUS b .

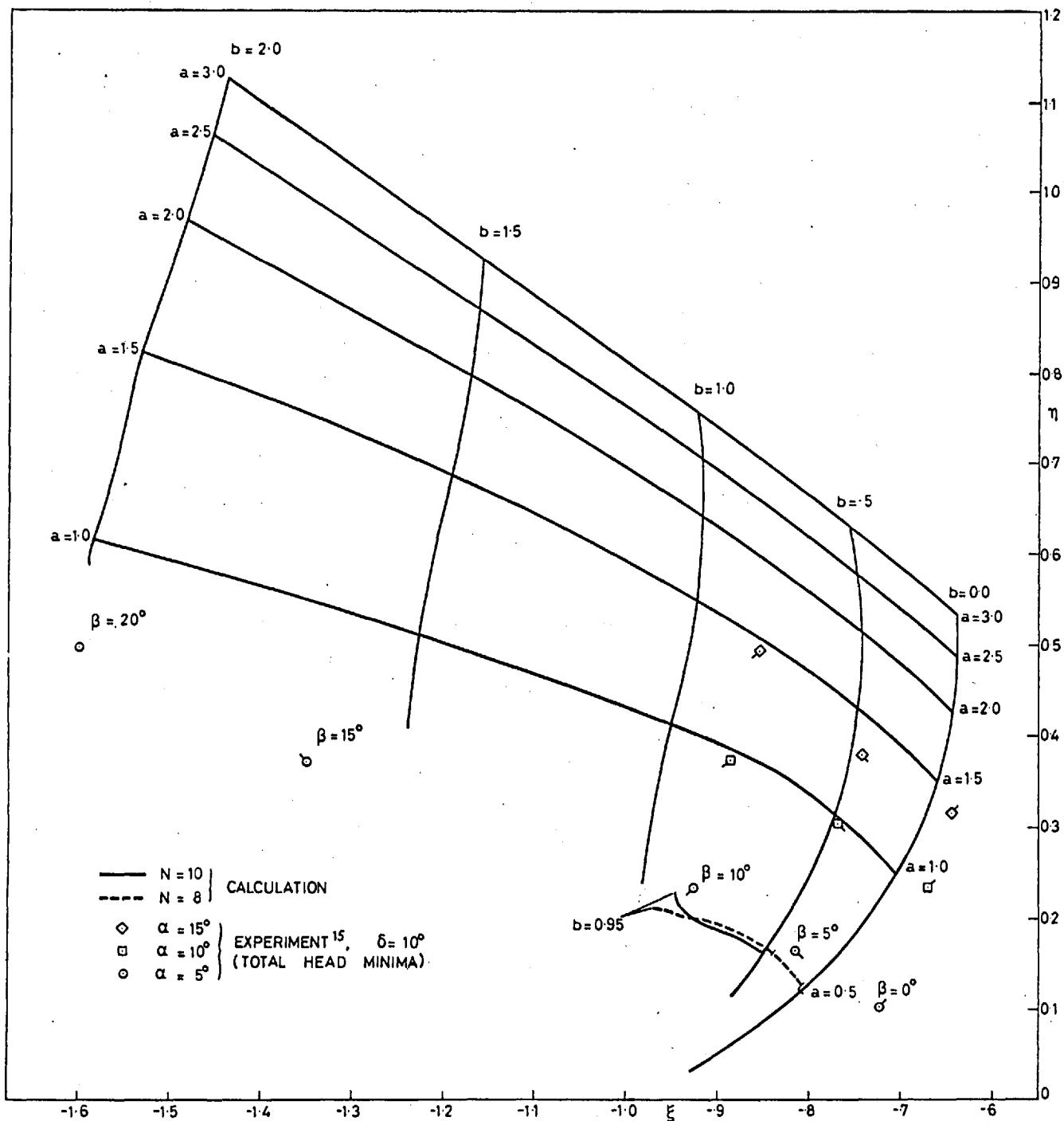


FIG. 7 VARIATION OF CALCULATED AND MEASURED POSITION OF LEEWARD VORTEX WITH INCIDENCE AND YAW.

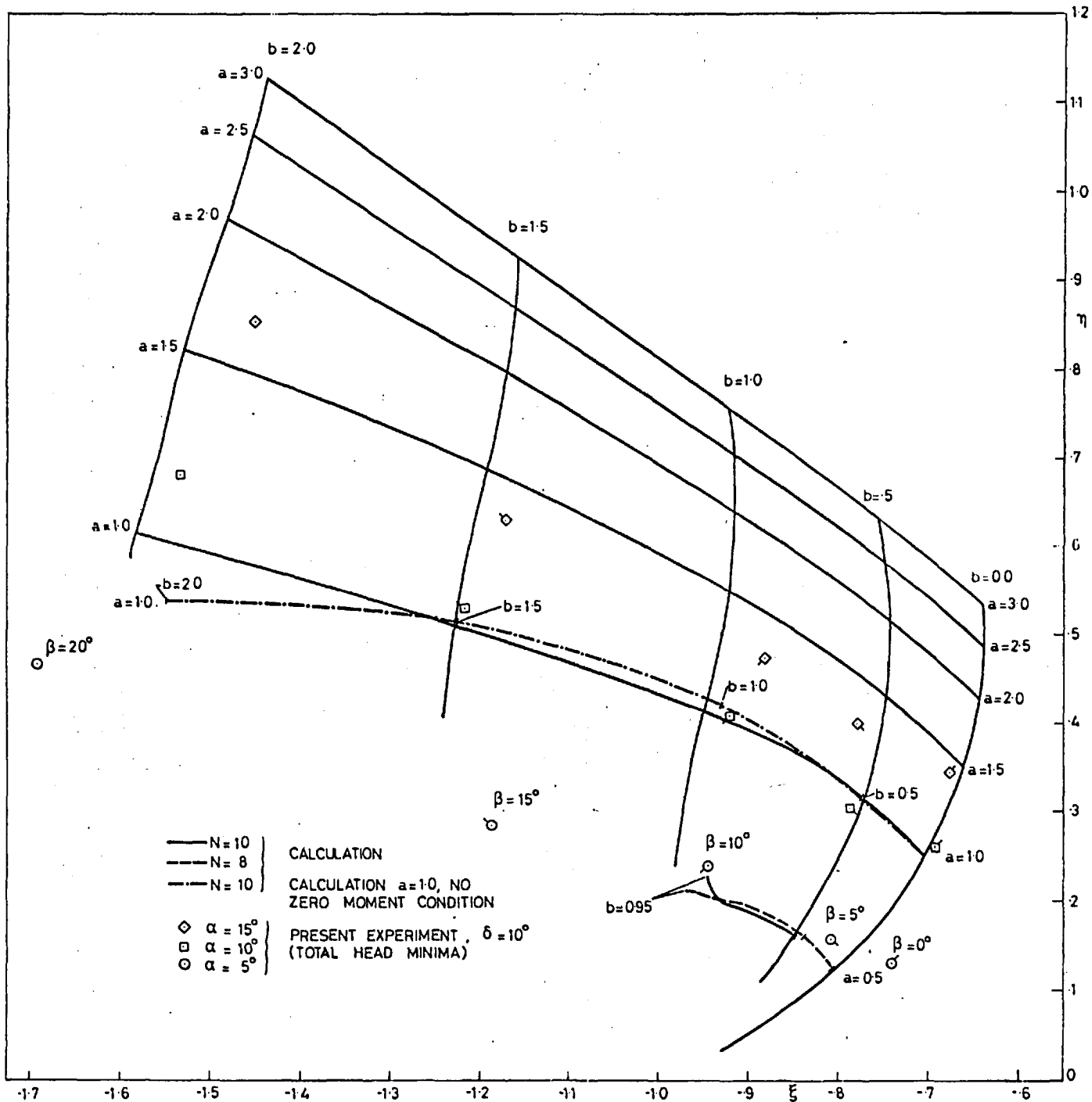


FIG. 8 VARIATION OF CALCULATED AND MEASURED POSITION OF LEEWARD VORTEX WITH INCIDENCE AND YAW.

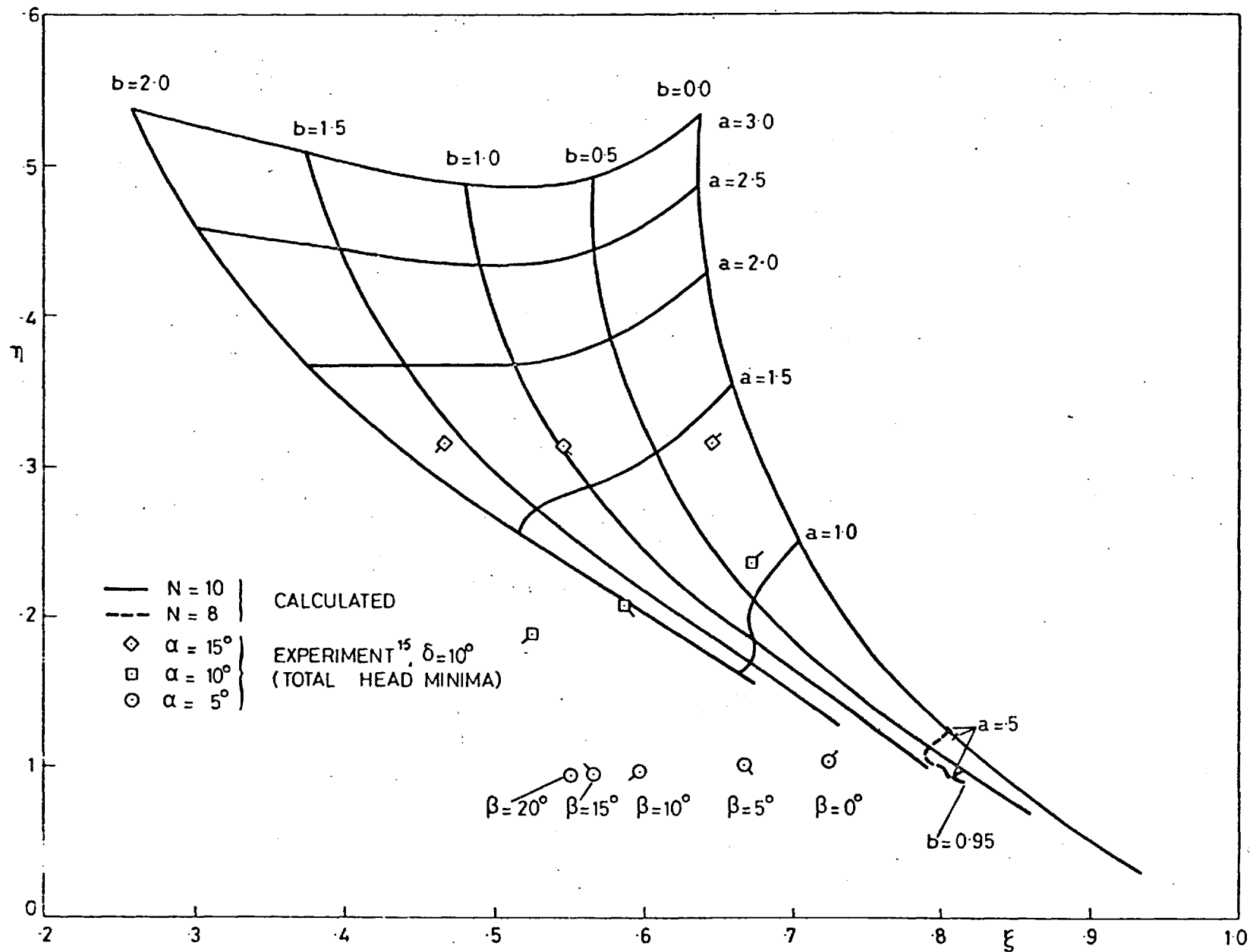


FIG 9 VARIATION OF CALCULATED AND MEASURED POSITION OF WINDWARD VORTEX WITH INCIDENCE AND YAW.

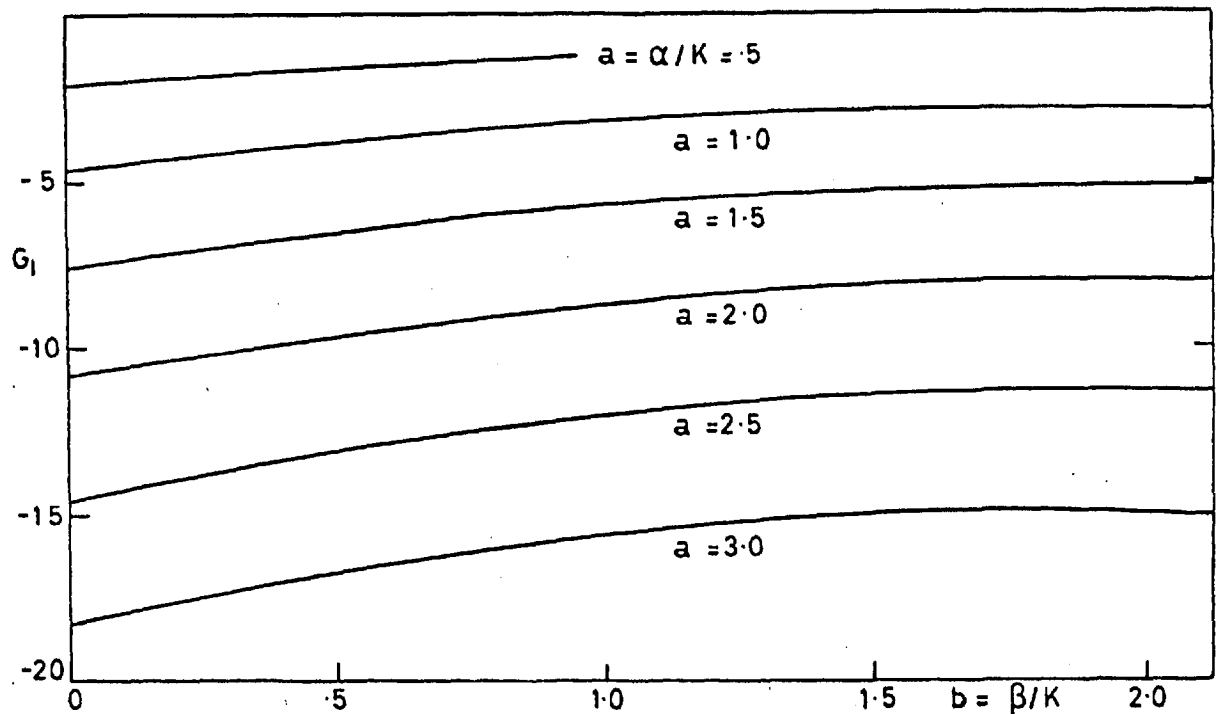


FIG. 10A VARIATION OF TOTAL CIRCULATION, $G_1 = \Gamma_2 / K U_s$ OF LEEWARD SHEET + VORTEX, WITH b FOR VARIOUS a .

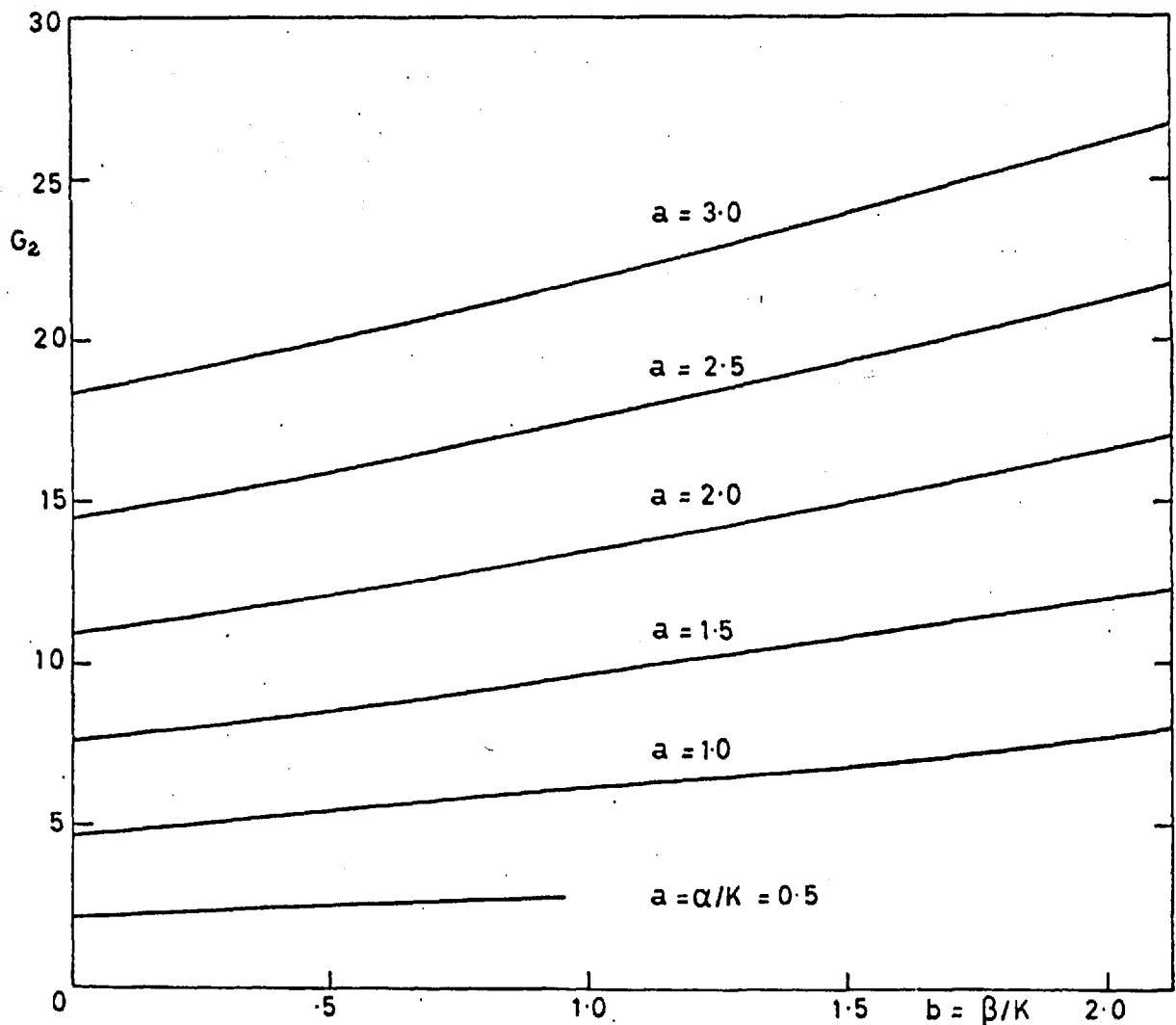


FIG. 10B VARIATION OF TOTAL CIRCULATION, $G_2 = \Gamma_2 / K U_s$ OF WINDWARD SHEET + VORTEX WITH b FOR VARIOUS a .

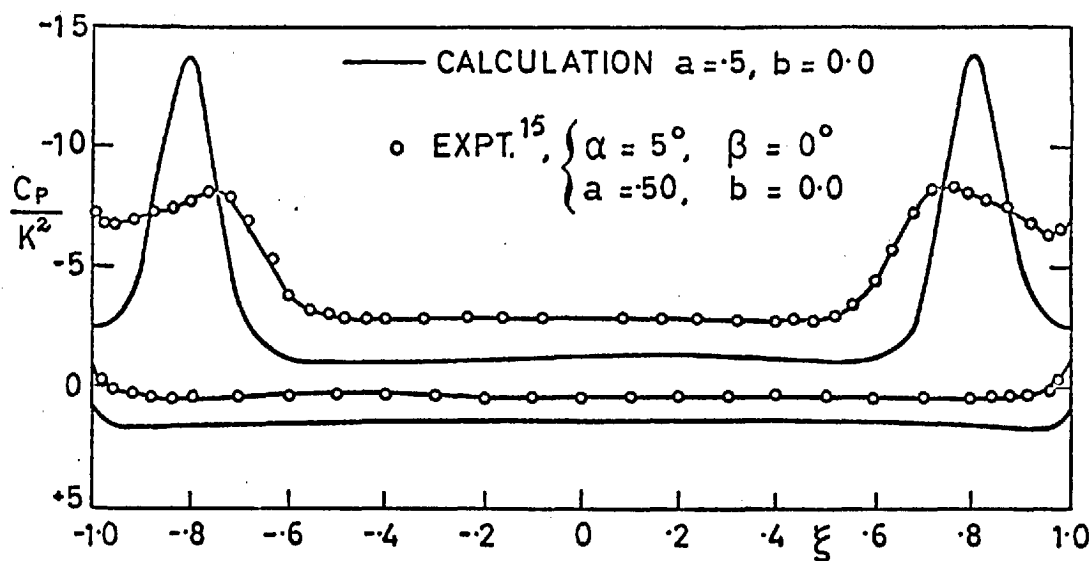


FIG. 11A

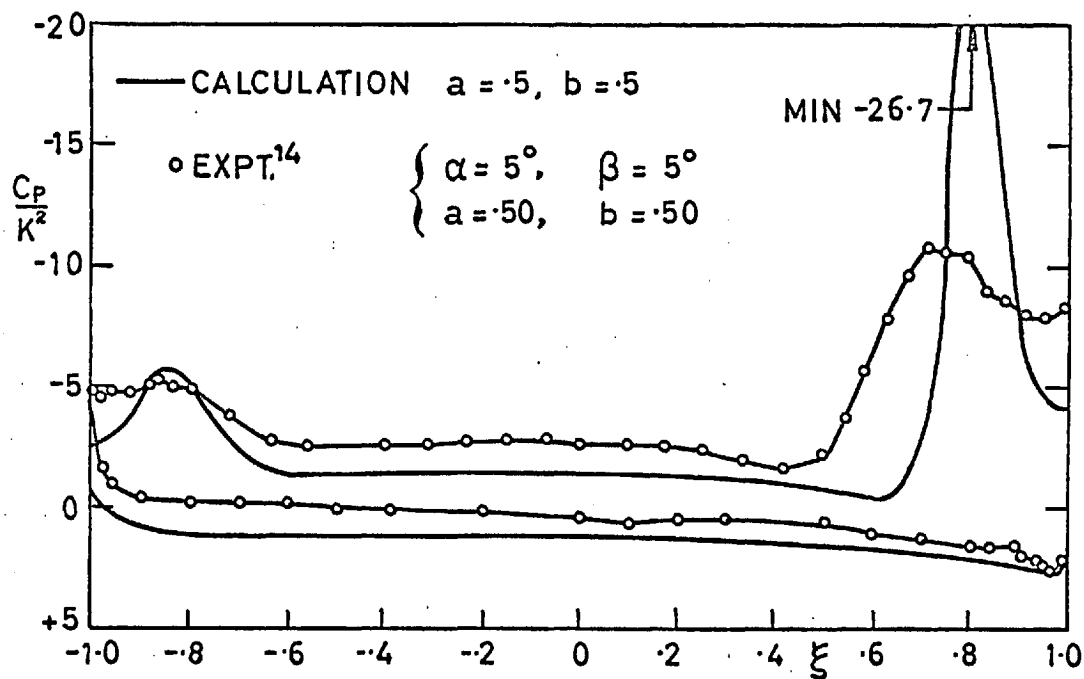
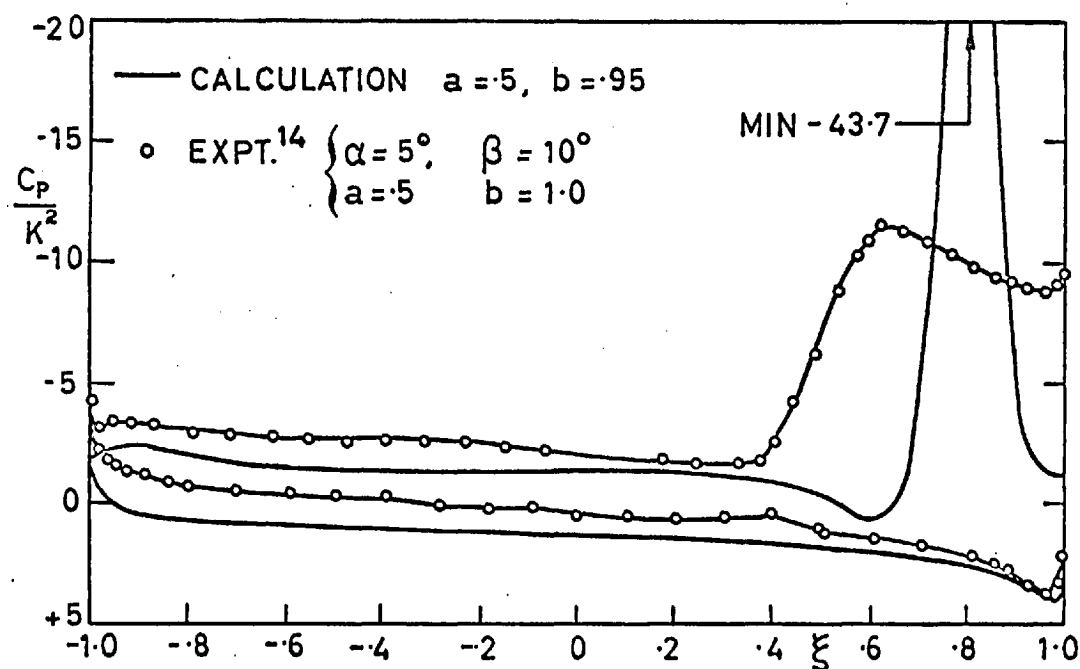
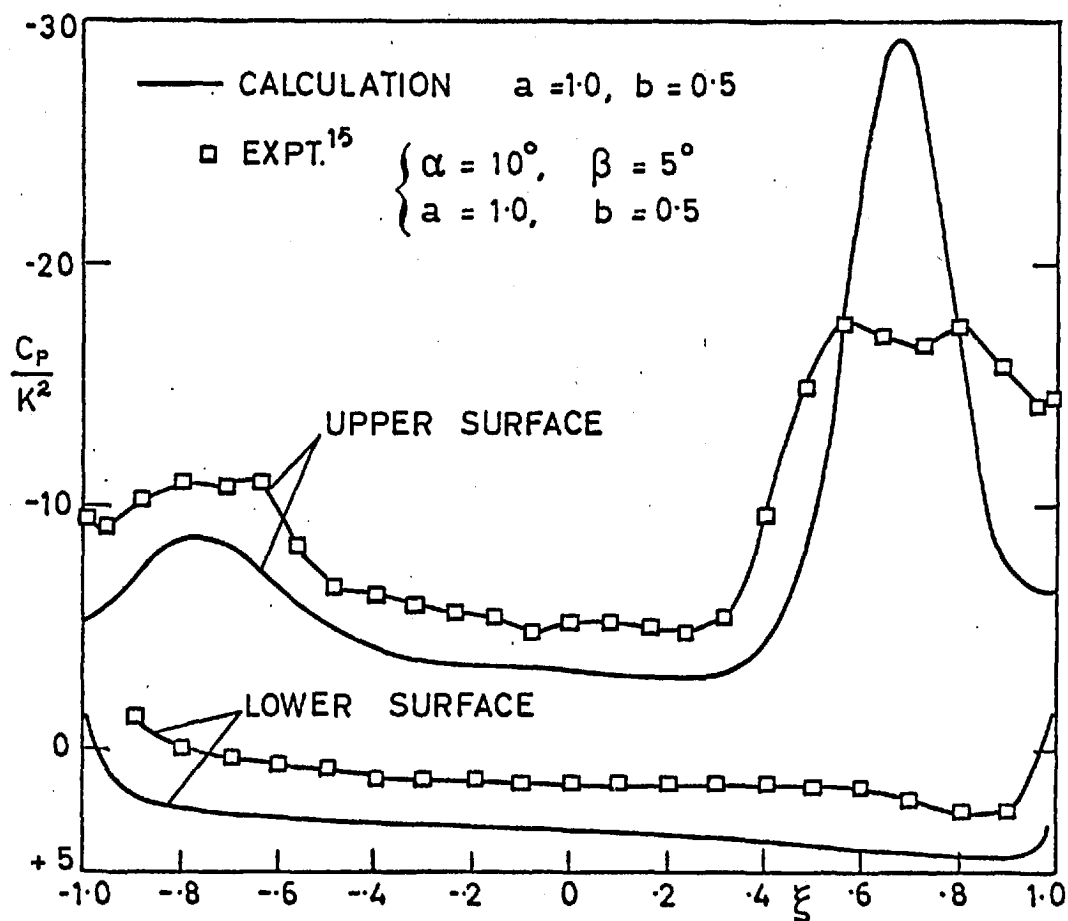
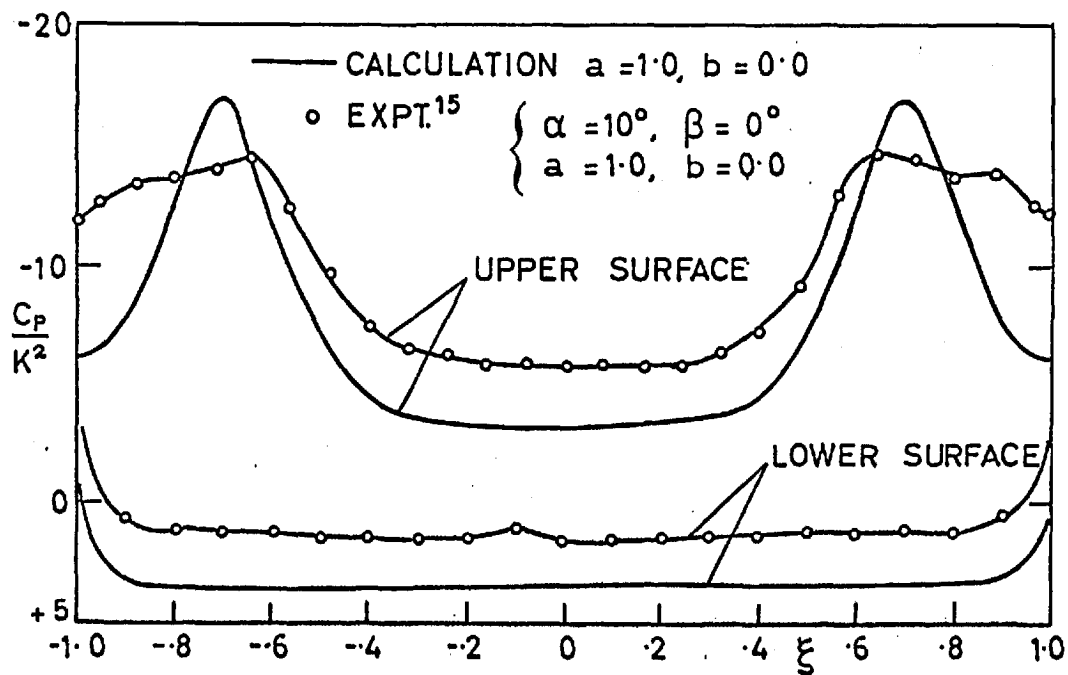


FIG. 11B



FIGS. 11A, 11B, & 11C PRESSURE ON WING UPPER AND LOWER SURFACE $a = .5$



FIGS. 12A & 12B PRESSURE ON WING UPPER AND LOWER SURFACE $a = 1.0$.

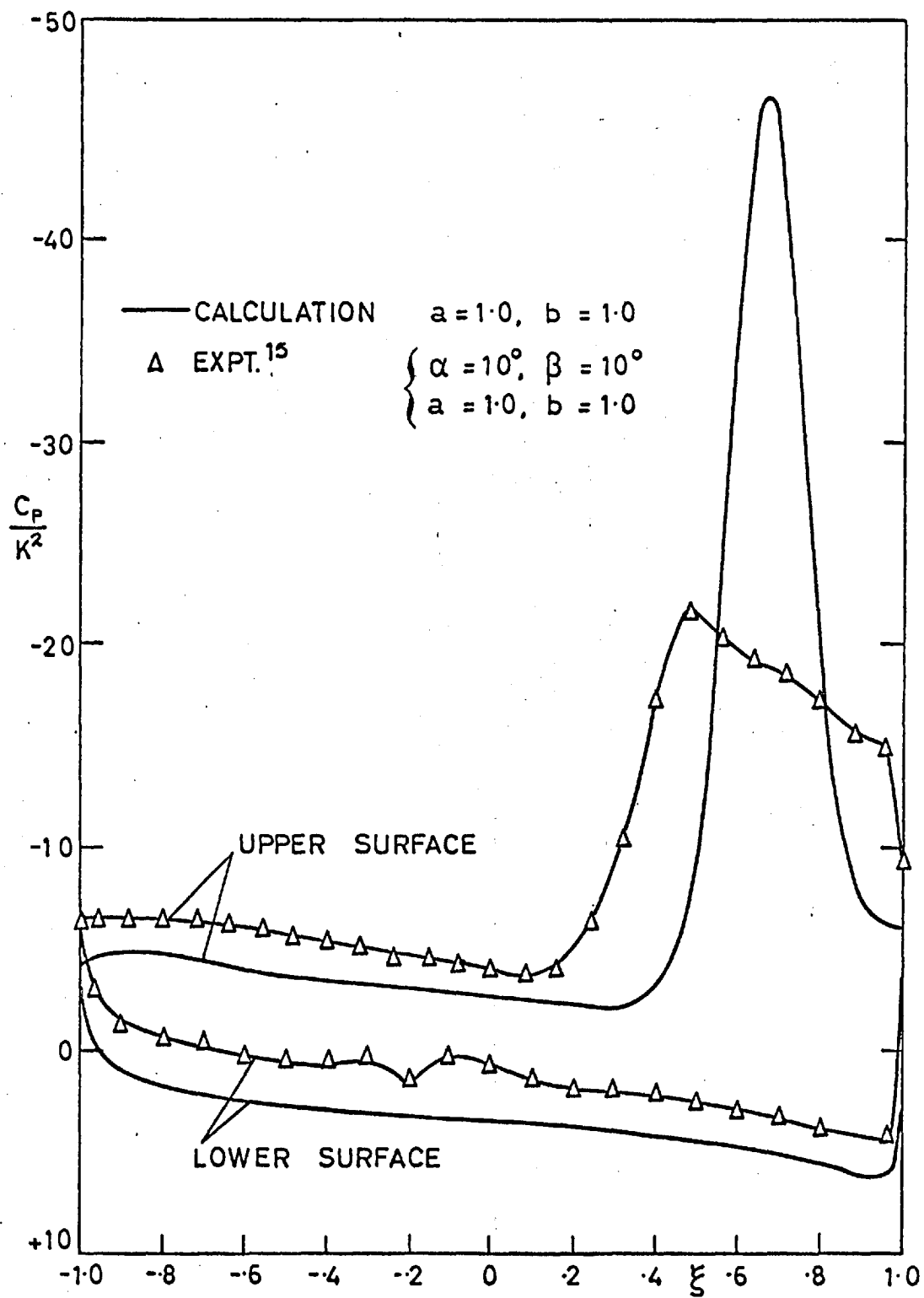


FIG. 13 PRESSURE ON WING UPPER AND LOWER SURFACE.

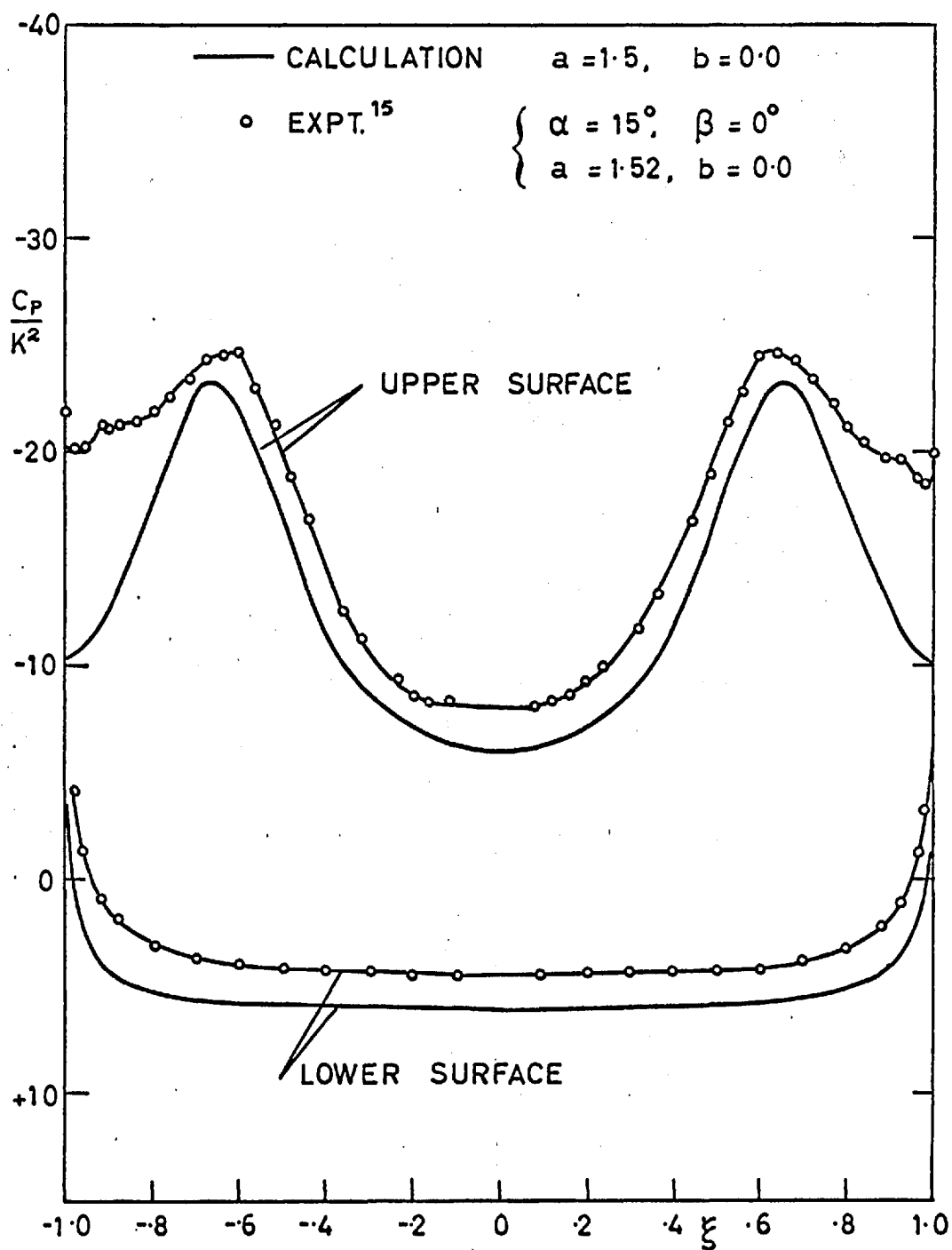


FIG. 14 PRESSURE ON WING UPPER AND LOWER SURFACE.

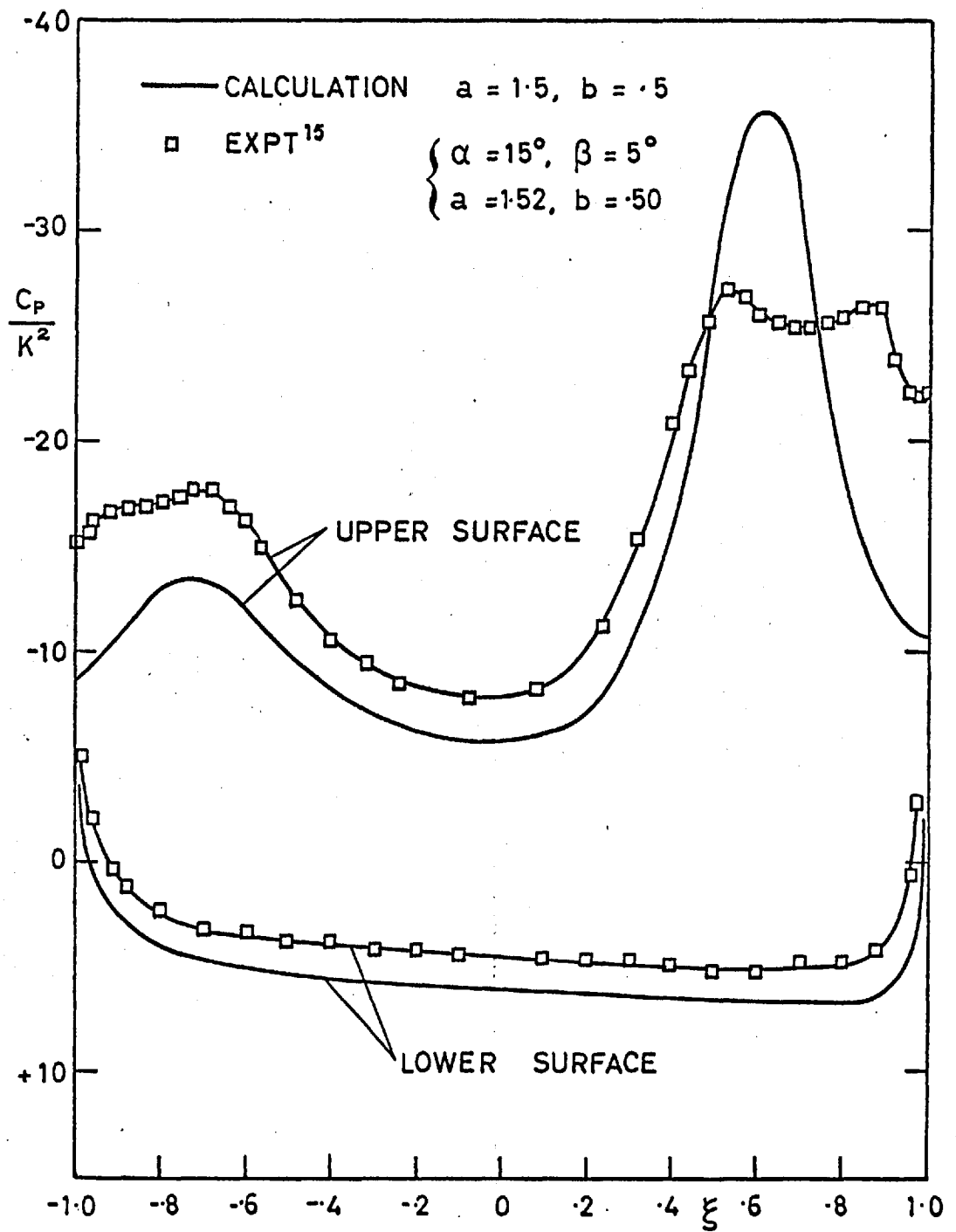


FIG. 15 PRESSURE ON WING UPPER AND LOWER SURFACE.

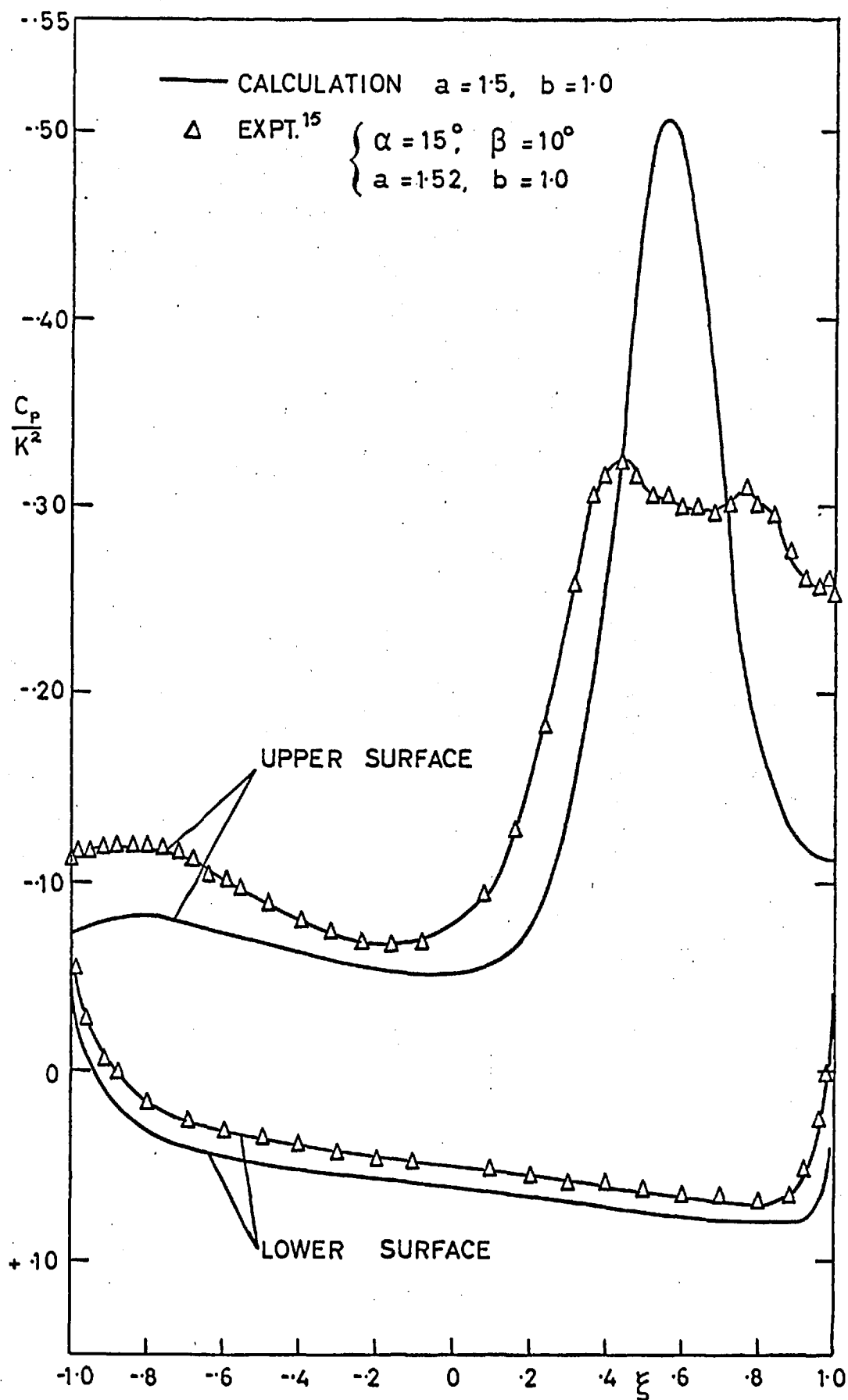


FIG. 16 PRESSURE ON WING UPPER AND LOWER SURFACE.

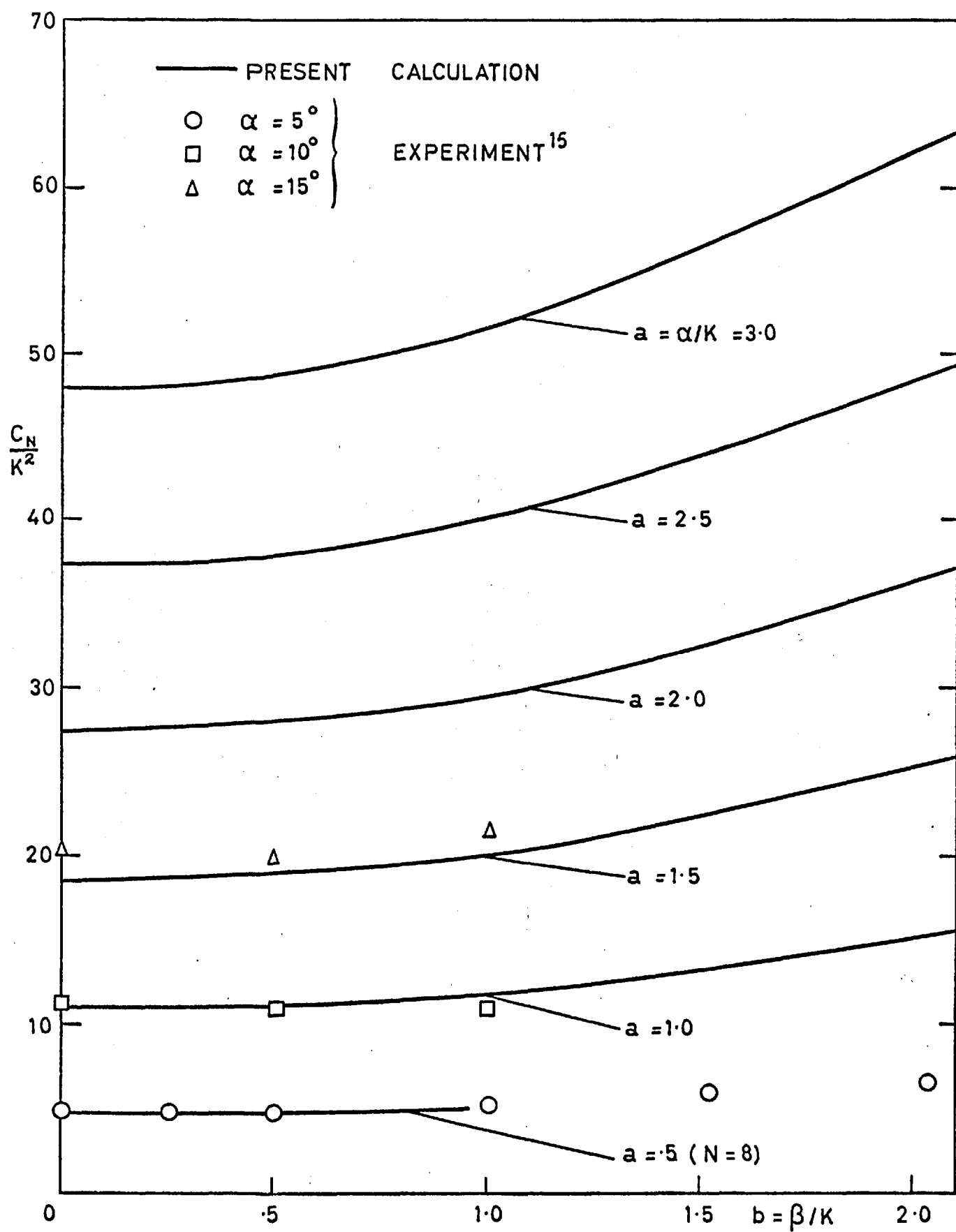


FIG. 17 VARIATION OF LIFT COEFFICIENT WITH b FOR VARIOUS a .

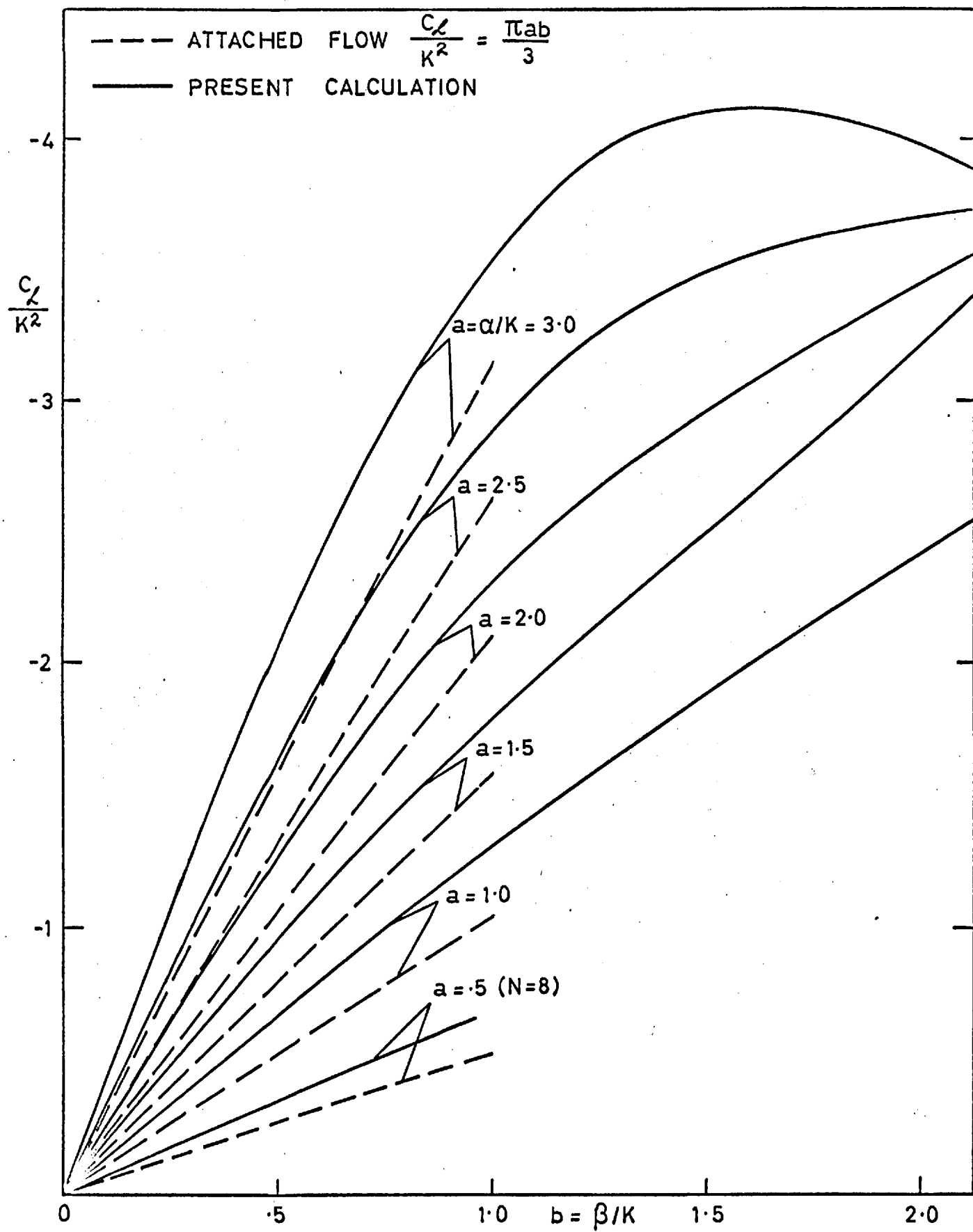


FIG. 18 VARIATION OF ROLLING MOMENT COEFFICIENT WITH b FOR VARIOUS a .

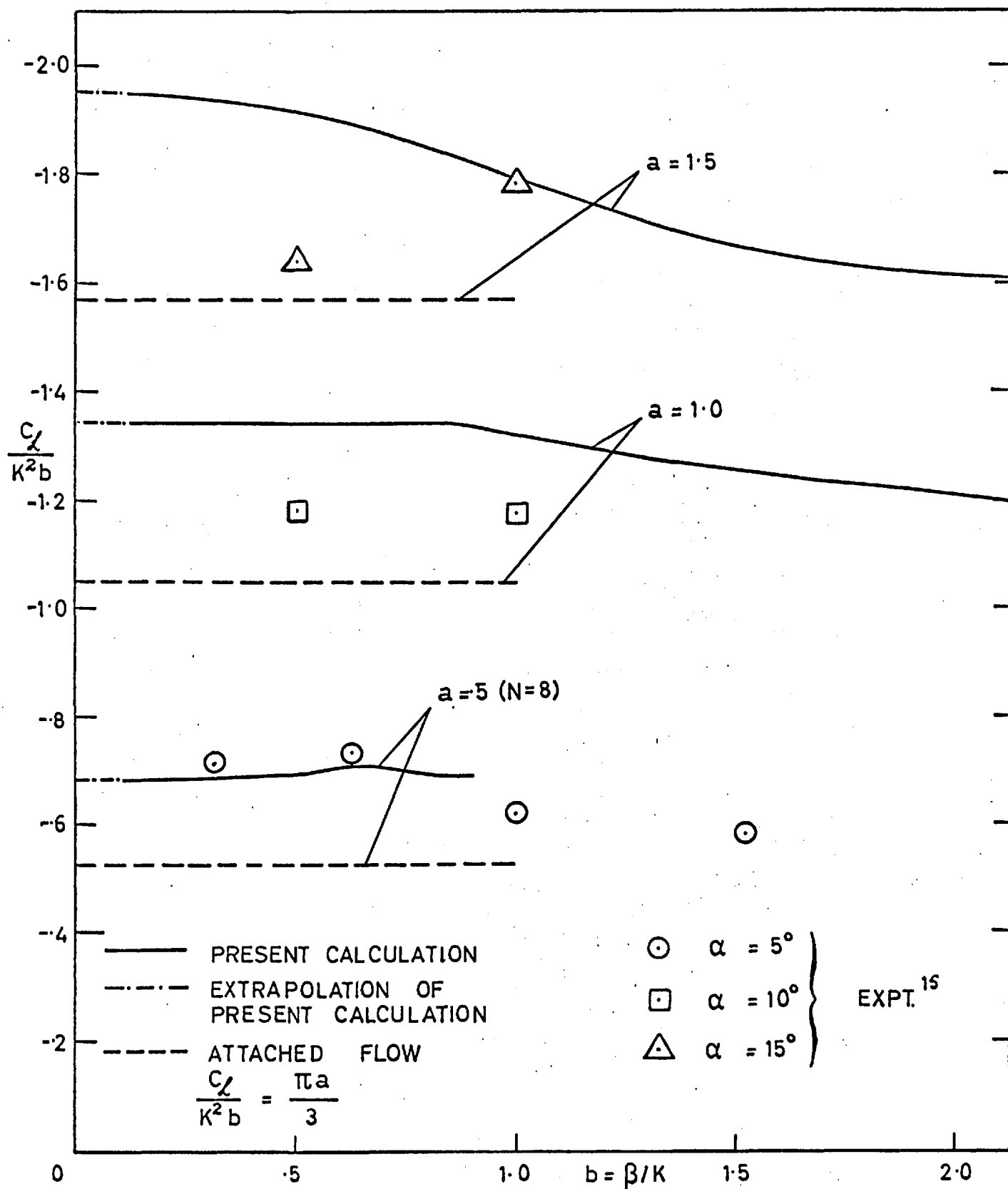


FIG. 19 VARIATION OF ROLLING MOMENT COEFFICIENT PLOTTED AS $C_L / (K^2 b)$, WITH b FOR VARIOUS a .

PART II: RAREFIED LEADING EDGE FLOW OF A DIATOMIC GAS

Abstract

The hypersonic flow of a rarefied diatomic gas past the sharp leading edge of a two-dimensional flat plate has been calculated using the Monte-Carlo Direct Simulation method. This technique simulates the full Boltzmann equation in a statistical manner by computing the simultaneous random motion, including binary collisions, of several thousand sample particles. To account for rotational-translational energy exchange in inelastic collisions, an approximate form of a classical, non-spherical soft potential collision model used recently in polyatomic transport theory calculations has been adapted for use in the Direct Simulation method. Although this model has certain limitations which are discussed in the text, it nevertheless appears to be adequate for the present calculations.

The majority of the flow calculations were performed for M_∞ in the range $M_\infty = 23-25$. For the fully diffuse completely accommodating gas-surface law assumed, these indicate that a highly nonequilibrium kinetic flow in which first collisions between incident free stream and body reflected particles play an important role extends to about $1.5\lambda_{fb}$ downstream of the leading edge. This is followed by transition to a merged layer flow. The influence of the body reflected particles extends forward of the leading edge with the result that some of the surface properties exceed their free molecule values near $x = 0$. For diatomic molecules the presence of rotational degrees of freedom which absorb energy in initial collisions has a substantial effect on the flow properties.

Macroscopic gas and surface properties obtained from the calculations have been compared with experimental data on the basis of the kinetic scales x/λ_{fb} and y/λ_{bf} .

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NOTATIONSymbols

a, A	see Eq.(35)
a'	$= \alpha\sigma$
b	binary collision impact parameter (miss distance)
b^*	$= b/\sigma$
b_0, b_0^*	elastic cutoff (maximum) values of b, b^*
c_i, c_i'	velocity of i^{th} particle before and after collision in lab. framework
$\bar{c}$	$= (8\pi kT/\pi m)^{1/2}$; mean thermal speed in Maxwellian gas
C^*	$= n(T'')T_\infty / n(T_\infty)T''$; modified Chapman-Rubeson constant
C_F	$= \tau_w / \frac{1}{2}\rho_\infty U_\infty^2$; surface skin friction coefficient
C_H	$\dot{q}_w / \frac{1}{2}\rho_\infty U_\infty^3$; surface skin friction coefficient
D	constant in Parker potential (see App. C)
d	internuclear mass separation for diatomic molecule
d'	distance between repulsive force centres in Parker potential
E_{r_i}, E_{r_i}'	rotational energy of i^{th} particle before and after a binary collision
$\hat{E}_{r_i}$	$= E_{r_i}/kT$; nondimensionalised rotational energy
E'	potential well depth
f	distribution function
$\bar{f}_1, \bar{f}_2$	reduced distribution function; Eqs.(79) and (80)
$\underline{g}, \underline{g}'$	relative velocity before and after binary collision
g, g'	$= \underline{g} , \underline{g}' $ respectively
g^*	$= [mg^2/4kT]^{1/2}$; reduced relative velocity

g_c	critical value of g for orbiting
h_i	angular momentum of i^{th} particle
I	$= md^2/4$; moment of inertia of rigid rotor molecule
J_i	see Eqs.(60)
Kn	$= \lambda/L$; Knudsen number
L	length of flat plate; also typical flow dimension
m	molecular mass
M_∞	free stream Mach number
n, n'	general symbols for number density; variously used
n_k	density of simulated particles in cell k
N	sample number in flow property measurement; also number flux incident to plate surface
N_k	number of simulator particles instantaneously in cell k
p	conditional collision probability (see section 5.8.2 and App. A)
p_j	probability of diffuse reflection from j^{th} surface element
P	expression defined in Eq.(60B)
P_c	cavity pressure
P_n	normal surface pressure at wall
Q	expression defined in Eq.(60A); also general function of molecular properties [Eq.(3)]
$\bar{Q}$	mean value of Q [Eqs (4) and (28)]
$Q^{(2)*}$	collision integral (App. F)
$\underline{r}$	position vector in laboratory framework
R	distance between molecular centres in binary collision

R_0, R_1, R_2	zeroth first and second order R
R^*	$= R/\sigma$
$R_{AC}, R_{AD}, R_{BC}, R_{BD}$	distances between molecular repulsive centres (Fig.2A)
Re_x	$= \rho_\infty U_\infty x / \mu_\infty$; Reynolds number
S_∞	free stream speed ratio
$t, \hat{t}$	real and nondimensionalised physical time
t_c	time scale associated with molecular convection
t_i	relaxation time for i^{th} internal degree of freedom
t_m	mean free time for collisions
t_k	time counter for k^{th} cell
T	translational temperature
T_0	stagnation temperature; also initial translational temperature
T_{xx}, T_{yy}, T_{zz}	x, y and z components of T
T_R	rotational temperature
T_w	wall temperature
T_∞	equilibrium free stream temperature
T'	$= E'/k$ ($k \equiv$ Boltzmann's constant)
$\hat{T}_w$	$= T_w/T_\infty$
u_w	wall slip velocity
U_∞	free stream velocity
$\bar{v}, v$	mean (ensemble or time average) velocity and $ \underline{v} $
V_x, V_y, V_z	x, y and z molecular velocity
$\bar{V}$	$= M_\infty \sqrt{C^*/Re_x}$; rarefaction parameter
V	intermolecular potential

V_0, V_1, V_2	zeroth, first and second order V
x, y, z	rectangular laboratory fixed co-ordinates
x_i, y_i, z_i	non-rotating framework fixed to mass centre of i^{th} molecule in a binary collision
$\hat{x}, \hat{y}$	$= x/\lambda_\infty, y/\lambda_\infty$ respectively
$\hat{x}_f, \hat{y}_b$	$= x/\lambda_{fb}, y/\lambda_{bf}$ respectively
Z_i	collision number for i^{th} internal energy mode
Z_R	rotational collision number

Greek letters

α	range factor in Morse potential
α_j	energy accommodation coefficient for j^{th} surface segment
β	see Eq.(31)
β_i	polar orientation angle of i^{th} particle (see Fig.2A)
γ	ratio of specific heats
γ_i	see Eq.(17)
Γ	expression defined for Eqs.(60); also denotes external boundary of simulated region
Γ_i	$= \phi - \psi_i$; see Eqs.(9)
δ	expression defined for Eqs.(60)
δ_i	$= \gamma_i - \phi_0(0)$; see Eq.(35)
ΔE_{r_i}	rotational energy exchange in collision for i^{th} particle
Δt_m	time increment in Direct Simulation Method
$\Delta x, \Delta y$	physical cell dimensions
ϵ	perturbation parameter in potential expansion [see Eqs.(9)]; also collision plane azimuth angle

η	viscosity
θ	see Fig.2A
λ	general mean free path in Maxwellian gas
λ_{fb}	mean free path of free stream particle in a field of body reflected particles
λ_{bf}	mean free path of body reflected particle in the free stream
μ	$= m/2$; reduced mass of 2 particle system
v_i	$= \omega_i - \dot{\phi}_0(0)$; see Eq.(35)
ξ, ξ^*	see Eqs.(31) and (60) respectively
ρ	fluid mass density
$\bar{\rho}$	arbitrary ratio of real particle number density to simulator number density (App.A)
σ	potential zero point
Σ	denotes two-dimensional body surface
ϕ	polar orientation of line of centres for two particle system
ϕ_0, ϕ_1, ϕ_2	zeroth, first and second order ϕ
χ, χ_0	collision deflection angle; zeroth order χ
$\bar{\chi}$	$= M_\infty^3 \sqrt{C^*/Re_\chi}$; strong interaction parameter
ψ_i	aximuthal orientation of i^{th} molecule
$\psi_{i0}, \psi_{i1}, \psi_{i2}$	zeroth, first and second order ψ_i
ω_i	angular velocity of i^{th} particle
ω_k	denotes k^{th} cell of Ω
Ω	denotes region of physical space in simulated flow
Ω_i	denotes internal co-ordinates of i^{th} molecule
$\Omega^{(2,2)*}$	collision integral (see App. F)

Subscripts

fm refers to free molecule value

i = 1,2, refers to i^{th} particle in a binary collision

∞ refers to free stream value

0 zeroth order

1. INTRODUCTION

Interest in the theoretical study of nonequilibrium gas phenomena has continued at a high level in recent years with typical applications being the very high altitude flight of the proposed space shuttle vehicle and the solution of gas dynamic problems related to the production of nuclear power. For problems of practical interest, however, it is well known that the Boltzmann equation — which describes the time evolution of a dilute gas of neutral particles — has proved to be obstinately intractable to standard analytical or numerical solution techniques. Nevertheless one approach to the calculation of nonequilibrium gas flows that has enjoyed great practical success is the Direct-Simulation method Monte-Carlo method of G.A. Bird [15], in which analytic formulations of kinetic theory are bypassed in favour of a direct, probabilistic simulation of the full Boltzmann equation by the calculated motion of several thousand sample particles. Once a binary collision model and certain boundary conditions have been specified, the Bird technique may be used to simulate a wide range of complex rarefied gas flows providing detailed, albeit statistical estimates of all desired flow properties.

But while spherically symmetric monatomic collision models may be readily incorporated into the Direct Simulation method, great practical difficulties arise for exact, realistic models for polyatomic molecules, largely because of the formidable analytic character of the inelastic collision problem. Moreover, practice has shown that impulsive collision models [16][57] are not really suitable in simulation and although recently proposed phenomenological models [14][18] are simple and flexible, it is not clear that they offer an adequate description of the detailed energy transfer process which may have some importance for highly nonequilibrium flows such as the present leading edge problem. Consequently the first aim of the present study is to develop an approximate though realistic model

for binary collisions of rotationally excited molecules which might be utilised in diatomic gas simulations. The model considered is the classical soft molecule model of Parker which has been used by various authors [53][61][64] to successfully predict the temperature dependence of rotational collision numbers.

One of the most consistently studied rarefied gas flows is that of hypersonic flow past a two-dimensional flat plate aligned with the free stream. This problem, while being rather idealistic, none the less generates a wide variety of basic flow phenomena ranging from a highly nonequilibrium kinetic flow very near the leading edge, through the merged layer and strong interaction regimes to a classical boundary layer flow far downstream. Through intensive study, the character of the interaction and merged layer regimes are now well understood, but despite important contributions, there still appears to be some uncertainty regarding the fundamental structure of the initial kinetic flow. Basically there are two reasons for this state of affairs. On the one hand, great technical difficulties are associated with nonequilibrium gas flow measurements. On the other, while the majority of recent experimental studies such as those of Vidal and Bartz, [78], of Lewis [51] and of Uppington [76] has been for diatomic gases, the most extensive Direct Simulation calculations so far presented by Vogenitz et al. [80] have been for a monatomic gas. A discrete ordinate solution of a linearized kinetic equation for a diatomic gas leading edge flow has been obtained by Huang et al. [44] but this was for a much lower Mach number than has been used in many experiments.

The second aim of the present study then is to perform detailed Direct-Simulation calculations of the hypersonic leading edge flow of a rotationally excited diatomic gas and to undertake a comprehensive comparison of the results so obtained with a range of experimental data. Particular emphasis is placed on examining the structure of the flow in the kinetic regime in

terms of the kinetic length scales λ_{fb} and λ_{bf} (see notation) and on the subsequent transition to a merged layer flow. The gas surface interaction law assumed is that of diffuse molecular reflection with full accommodation of both translational and rotational energy modes.

In the following material, Chapters 2 and 3 present a survey of previous work in the areas discussed above. Chapter 2, which is concerned with the applied kinetic theory begins with a brief reference to general gas dynamic flows and continues with a discussion of the use of the Parker collision model in rotational relaxation studies. This is followed by a short account of the development of Monte-Carlo methods in kinetic theory -- with special reference to the Direct Simulation method -- which leads to a description of methods for extending these techniques to the treatment of polyatomic gases. Chapter 3 considers the physical nature of the leading edge problem, and surveys recent contributions on both the theoretical and experimental sides while Chapter 4 contains an account of the Direct Simulation method. The present form of Parker's inelastic collision model is developed in Chapter 5. This involves an approximate solution to the equations of motion for an inelastic binary collision using the "planar rotation" assumption employed originally by Parker [64], which results in a useful expression for the energy exchange in terms of the pre-collision dynamical parameters. A detailed description of the leading edge flow calculations together with a comprehensive comparison of the results obtained with experimental data is presented in Chapter 6. Concluding remarks and recommendations for future study are given in Chapter 7.

For the assumed gas-surface law, the physical picture of the leading edge flow obtained from the present investigation is summarized in Section 6.7. Briefly, the calculations indicate that the nonequilibrium kinetic regime extends to about $1.5 \lambda_{fb}$ downstream of the leading edge. The following transition to a merged layer flow is accompanied by maxima in the surface

properties before or near $x/\lambda_{fb} = 1.5$. Free molecule effects were detected near the leading edge but these do not appear to dominate the initial flow.

In addition to the flat plate flow, a calculation has been performed for the hypersonic flow past a plate with a forward facing step of height $4\lambda_\infty$ placed $48\lambda_\infty$ downstream of the leading edge. Due to present space limitations, a description of this case will be published elsewhere.

2. APPLIED KINETIC THEORY

To serve as a theoretical background for the present study, the present chapter will be concerned with reviewing some recent advances in the applied kinetic theory. Aerodynamic flows have been classified into various regimes depending on the degree of rarefaction as measured by the Knudsen number $Kn = \lambda/L$, where λ is the mean free path (inversely proportional to density) and L is a characteristic length scale for the flow field or subregion being considered. The detailed classification of particular flow fields is complicated and generally depends on body geometry, Mach number and Reynolds number. However, to appreciate our present point of interest in terms of the significance of the K_n scale, it is worthwhile outlining here some of its broader aspects. For more general and detailed discussions, see for example Tsein [75] or Probstein [65].

In the limit $\lambda/L \rightarrow 0$, collisions between molecules dominate over boundary interactions and the flow is said to be collision dominated and in thermal equilibrium. Here the distribution function is Maxwellian and the inviscid Euler equations are valid everywhere save near solid boundaries or in shockwaves. In these regions L must be interpreted either as a shock or boundary layer thickness δ in which case finite K_n effects are always important, but for moderate to high R_e , except very near a boundary (Knudsen layer) and for not too strong shocks, $\lambda/\delta \ll 1$ which means that departures from local equilibrium are generally small. The flow is still collision dominated and viscous and heat conduction effects may be represented by the transport coefficients in a Navier Stokes continuum flow description.

For the converse limit $\lambda/L \rightarrow \infty$, molecular encounters may be neglected compared with particle-body collisions. The flow is then regarded as free molecule and although the distribution function is generally

non-Maxwellian, it may be formally constructed from a knowledge of the initial and/or boundary conditions for a particular problem.

When $\lambda/L \sim 0(1)$ as for important flow regions considered in the present study, the flow is said to be rarefied. Another way of expressing this condition is to say that t_m the characteristic time scale for collisions is comparable with t_c that for molecular convection through L . In this case collisions are important but departures from thermal equilibrium may be large. The distribution function may then be highly non-Maxwellian and generally cannot be characterized by a few moments satisfying partial differential equations. Continuum flow descriptions must then be rejected in favour of a kinetic theory formulation involving a detailed description of molecular collisions. Thus a solution of the Boltzmann equation must be considered. For a general account of the significance of the Boltzmann equation in kinetic theory, see Grad [30] or Koga [48].

The presence of internal degrees of freedom for a polyatomic gas further complicates kinetic theory in that for inelastic collisions of such molecules, internal and translation energy may be exchanged. In general the importance of these effects in nonequilibrium flows depends strongly on the (usually complex) inelastic collision mechanics and hence indirectly on the relative time scales for energy transfer compared to t_m and t_c . A general discussion of relaxation processes in gases is given in Ref. [36] while Ref. [2] contains an interesting account of the general inelastic collision problem

2.1 Relaxation Processes

One of the simplest nonequilibrium gas phenomena is that of the homogeneous relaxation of an internal energy mode to equipartition with the translational mode. An investigation of this basic physical process provides a natural beginning to a study of internal nonequilibrium effects

in complex kinetic flows of polyatomic gases. At equilibrium, energy is exchanged between internal and translational energy modes in every collision but the average exchange is zero. If for some reason, however, the state of macroscopic equipartition is disrupted, then the average effect of the energy exchange per collision will operate so as to drive the particle ensemble towards some new state of equilibrium satisfying the principle of detailed balance.

A quantitative measure of the time scale of this adjustment process is given by the relaxation time t_i for a particular internal mode, or equivalently by the internal collision or relaxation number $Z_i = t_i/t_m$. This latter quantity may be thought of as the average number of collisions per particle required to relax the system to a quasi-equilibrium state.* Both t_i and Z_i are related to the efficiency of the energy exchange process in individual collisions. Thus if the exchange is accomplished easily, t_i may be only a few mean free times but if the exchange is difficult, t_i may be many thousands of mean free times.

The development of the transport theory of polyatomic gases by Wang Chang and Uhlenbeck [82] and also by Taxman [74] has led to formal relationships between t_i and the inelastic energy exchange. From a Chapman-Enskog type solution to a generalized Boltzmann equation, these authors showed that t_i could be related to the bulk viscosity and hence to the energy transfer through a complicated integral over all possible collisions. Hence to theoretically predict t_i , a solution to the inelastic collision problem is required which, for a realistic intermolecular potential, has proved to be quite formidable [2]. The various impulsive collision models that have therefore found application in the polyatomic transport theory will not be discussed here, but are well

* t_i is thus the "transient time" of an exponentially decaying process.

summarized in Ref. [39].

Note that in the foregoing discussion it has been tacitly assumed that each internal energy mode may be treated separately. Due to order of magnitude differences in either the t_i 's or characteristic excitation temperatures, this assumption is generally reasonable. Thus for a diatomic gas, rotational nonequilibrium may often be considered apart from the effects of vibration and other internal energy modes associated with electronic motion.

2.2 Rotational Relaxation

A diatomic gas has two degrees of freedom in rotation leading to equipartition rotational energies of kT per molecule. Since quantum effects should not be important in rotation at temperatures above the characteristic excitation temperature (2.9°K for N_2), classical collision models have proved adequate for the study of rotationally inelastic collisions at moderate temperatures. The first such model used successfully was that due to Parker [64]. Investigating relaxation processes in diatomic gases, Parker represented each molecule in a binary collision as a rigid rotor. The soft intermolecular potential was composed of long-range attractive and short-range repulsive components and included a small nonspherical part. In conjunction with the simplifying assumption that the rotation plane of each colliding particle was coincident with the collision plane (planar rotation), Parker expanded the appropriate equations of motion for a binary encounter in terms of a parameter representing the potential nonsphericity. From the first order equations of this scheme he obtained — for initially nonrotating molecules — an approximate expression for the inelastic energy exchange. The use of simple kinetic theory then led to predictions of the temperature variation of rotational relaxation numbers for a few

nonpolar gases including O_2 and N_2 . A similar analysis at higher collision energy yielded predictions of vibrational collision numbers.

The extension of Parker's analysis to initially rotating molecules was made by Nyeland [61] and more completely by Lordi and Mates [53], both of whom use Taxman's [74] polyatomic transport theory to calculate Z_R . Lordi and Mates also carried out calculations in which the complicated transport theory expressions were evaluated by Monte-Carlo integration, the post collision parameters in each trial being determined by full numerical integration of the equations of motion. However, they found this procedure to be rather time consuming, although on a rather small machine, obtaining only a few rather inconclusive results.

The main qualitative result which derives from the work discussed above is that for non-polar diatomic gases Z_R increases monotonically with temperature in contrast to the temperature independent result predicted by impulsive models such as loaded spheres. In particular the approximate theory of Lordi and Mates yields results which compare favourably with ultrasonic data [21], both theory and experiment yielding values of Z_R varying between 3 and 10 in the temperature range 200° - $1000^\circ K$. Although the planar rotation assumption represents a rather gross physical constraint on the two molecule system, the success of the approximate analyses used in Refs. [64], [61] and [53] in predicting $Z_R(T)$ suggests that the simplified model retains some of the physical features of the inelastic energy transfer process.

Other important transport theory studies are presently being carried out by Curtiss and co-workers. This group is using quantum mechanical methods to solve the inelastic collision problem for a general nonspherical potential [26]. Although explicit expressions for the rotational relaxation time [27] have been obtained, numerical evaluations of these for diatomic gases do not appear to have been published. However,

calculated results for relaxation in an Ar-N₂ mixture [68] have appeared in the literature.

2.3 The Solution of Practical Gas-Kinetic Problems

For most nonequilibrium kinetic flow situations of engineering interest, solutions of the appropriate Boltzmann equation cannot readily be obtained by either analytical nor finite difference numerical methods. This is, of course, because of the intractable nature of the multi-dimensional collision integral which is very complicated for monatomic gases and almost hopelessly so for polyatomic gases. Thus to facilitate the solution of practical problems various linearized kinetic equations such as those of the ellipsoidal-B-G-K type [4][40] have found wide application in kinetic theory. In the original B.G.K. equation for monatomic gases the Boltzmann collision integral was replaced by a linear approximation, involving, for the velocity space source term, a Maxwellian distribution characterized by the local lower order moments of the actual distribution function. An essential part of the simplest form of this model is the representation of the collision frequency, which generally depends on velocity, by a single appropriately chosen collision frequency or relaxation time. Applications of the B.G.K. equation have included the hyperthermal leading edge problem [43] for a monatomic gas.

Generalizations of the B G K scheme to polyatomic gases have been developed by Morse [59], by Holoway [40], and by Brau [19]. In these models additional linear terms representing internal degrees of freedom appear in the collision integral approximation. The extra phase space emission terms are chosen so as to yield the correct equations of change together with an appropriate description of the relaxation towards

equilibrium of the internal temperature. A single relaxation or inelastic collision frequency for each internal mode appears simply as a prespecified parameter to be determined experimentally or by some other means.

2.4 Monte-Carlo Methods in Kinetic Theory

While the linearized model equations are more tractable than the complete Boltzmann equation, considerable technical difficulties may still be encountered in their solution. These problems unfortunately tend to increase rapidly with the phase space dimensionality of the flow and also with the complexity of the boundary conditions involved. Thus, in recent years there has been increasing interest in the development of Monte-Carlo methods as an alternative practical approach to kinetic theory problems. Generally speaking, the great advantage of Monte-Carlo over deterministic numerical methods is that the scope and programming requirements of the former are somewhat more independent of system complexity than are those of the latter. The trade-off is two-fold. Firstly, Monte-Carlo "solutions" are statistical in nature, often with unknown error bounds. Secondly, convergence to acceptable accuracy levels is invariably slow which means long computing times. In an area such as kinetic theory where deterministic formulations are exceedingly complex, this compromise becomes very worthwhile in practical situations.

Derzko [28] has presented a comprehensive review of the three principal Monte-Carlo methods which have been used to date in kinetic theory. Of these, that of Nordsieck and Hicks [60] tackles the Boltzmann equation directly, employing a Monte-Carlo technique to evaluate a finite difference approximation to the collision integral. The method appears, however, to be confined to the treatment of simple problems. More in the spirit

of a simulation is the method of Haviland [34] in which an initially assumed "target distribution" is used to statistically generate the motions, including collisions, of a large number of test particles. The velocity distribution derived from the test particle motions is called the incident distribution. This eventually replaces the target distribution in an iterative cycle, convergent in the sense that after a time the two distributions tend to each other and presumably therefore, to a solution of the Boltzmann equation. But while a test particle approach is satisfactory where a natural division into incident and target particles exists, it is perhaps not so suitable for a system of identical strongly interacting particles. Moreover, core storage problems appear to limit this method to flows involving one space and two velocity dimensions.

2.5 G.A. Bird's Direct Simulation Method

Rather than considering special test particles, the Direct Simulation method of Bird [11][15] utilizes an approach in which the time evolution of a populous gasdynamic system is numerically simulated by the simultaneous motion of a many orders of magnitude smaller number of simulator particles. This is achieved by arranging that each sample particle has approximately the same collision probability as it would have as part of a real gas. Collisions are not, however, computed deterministically as in an early method due to Alder and Wainwright [1], but according to a statistical procedure which operates alternately with trajectory increments in a sequence of discretized time intervals. As each particle thus moves in random fashion through the system, its motion is followed concurrently with those of all other particles and its particular contribution to macro and micro flow properties in the vicinity of its flight path are monitored directly. The great advantage of the

Bird simulator is that the distribution function need not be considered explicitly, the phase space information being carried directly by the sample particles. Thus while estimates of the distribution function may be obtained as an outcome of the "numerical experiment", it is not a fundamental model entity.

Until recently, the precise relationship of the Direct Simulation method to the Boltzmann equation seemed to be somewhat uncertain. While the trajectory simulation is fairly self-evident, the method of calculating collisions requires some justification. Bird [15] however, has shown how the simulator collision selection procedure may be used to construct the gain and (by analogy) the loss terms of the Boltzmann collision integral, demonstrating that the correct collision frequency per simulator particle is obtained. Conversely, Borgnakke and Larsen [18] start from the Boltzmann equation for a polyatomic gas and obtain the general collision selection and calculation procedure for the ensemble of sample particles from consideration of the collision integral. But in spite of these contributions it is fair to say that a rigorous mathematical analysis of the Bird technique is still lacking. In this respect it may perhaps prove fruitful to consider the method from the point of view of nonequilibrium statistical mechanics rather than kinetic theory.

In any case the avoidance of the complex analytical apparatus of kinetic theory lends great practical flexibility to the Bird method and it is readily applicable to both steady and unsteady flows involving complex boundary conditions over a wide range of Knudsen number. Problems treated include a wide range of one-dimensional shock wave [7,9,12,13] and two-dimensional transition flow problems [8,80] and recently the method has been applied to three-dimensional flows [5]. General spherical molecular models are easily incorporated in to the technique, the simplest and most widely used being those for hard spheres and soft inverse power law molecules [39]. Also the modelling of gas mixtures of

widely differing constituent mass concentrations presents no difficulties [10]. A general description of the technique for two-dimensional flows is given in Chapter 4 of the present work.

2.6 The Treatment of Polyatomic Gases

principal

To date the applications of the Direct Simulation method have been to flows of monatomic gases for which elastic spherical molecular models are suitable. There is an obvious need to extend Monte-Carlo methods to molecules with internal energy. The difficulties of such an extension are similar to those encountered in a like extension of the transport theory, namely a satisfactory solution to the inelastic collision problem. Two distinct approaches have been tried. In the first, classical collision models developed originally for transport theory calculations have been incorporated into the Bird method. In the second local relaxation concepts have been used to model the energy exchange processes in individual collisions. The present approach falls into the first of these categories.

Impulsive classical models for rotationally excited gases have been tried by several authors. Bird [16] has adapted the rough sphere model for the simulation of one-dimensional flows. While this is a simple model for which the exact collision dynamics are known, in representing the behaviour of diatomic gases it has serious limitations which are discussed in Ref. [22]. Melville [57] has considered the loaded sphere model first proposed by Jeans. Unfortunately, Melville found that because of the loaded sphere asymmetry — a severe artificiality — a complex and time consuming collision procedure was necessary which appears to limit the use of the model for complex flows. Nevertheless, by neglecting some aspects of the wobbling motion of the loaded spheres,

Melville obtained good results in the simulation of a homogeneous relaxation problem and also for the one-dimensional plane shock problem.

Parker's [64] nonspherical soft molecule model which was discussed earlier has been used by Macpherson [54] in simulation studies of shock wave structure in O_2 and N_2 . Following the transport theory calculations of Lordi and Mates [53], Macpherson computed the post-collision dynamical parameters in individual collisions by full numerical solution of the equations of motion, an extremely time consuming procedure which is out of the question for complex flows. Macpherson performed two distinct sets of calculations, one in which Parker's planar rotation assumption was used and a second set in which molecular orientations were fully three-dimensional. Proper evaluation of Macpherson's shock profiles is not really possible since, due to prohibitive computing requirements, small particle samples were used resulting in large statistical fluctuations.

The principal disadvantages of the classical collision models are that they are either unacceptably artificial or that with a realistic representation of the energy exchange, excessive computing time is required. Alternative methods for the treatment of polyatomic gases which avoid altogether the complex inelastic collision dynamics have been proposed by Bird [14] and by Borgnakke and Larsen [18]. Both techniques combine the monatomic collision dynamics with phenomenological modelling of the energy transfer per collision.

In Bird's "Energy Sink" method, the energy exchange for each collision partner is assumed to be proportional to the difference between the precollision internal energy (of any kind) and a value characterized by the initial pair translational energy in the centre of mass framework. The constant of proportionality is itself inversely proportional to the prespecified constant value of Z_i . The energy exchange operates so as

to drive the pair internal and translational energies towards local equilibrium and averaged over large numbers of collisions this leads to macroscopic equilibrium but does not satisfy the principle of detailed balance. Essentially the Energy Sink method may be seen as an interpretation on a microscopic level, of an equation commonly used to model macroscopic relaxation processes. As such the representation of the energy exchange is somewhat gross and for this reason the model perhaps needs to be further tested.

Borgnakke and Larsen [18] have adapted the internal source term part of the analytical relaxation models discussed earlier into a form suitable for use in the Direct Simulation method. These authors apply the local equilibrium concept, which in the analytical models is applied to particle ensemble averages (moments) [19] to the outcome of individual binary collisions. The resulting probability density distributions for the post-collision dynamical parameters satisfy the conservation of energy and the principle of detailed balance, and may be interpreted statistically in Monte-Carlo simulation. However, while this model is simple and flexible, by virtue of its linear nature, it contains several somewhat artificial features. Firstly, individual collisions are either elastic or inelastic purely on the basis of a probability which depends on the prespecified Z_i . Secondly, the post-collision and pre-collision sets of dynamical parameters are essentially uncorrelated which means that the physical details of the inelastic exchange process are largely ignored. While these features are not important for small departures from equilibrium, it is not clear that this is the case for highly nonequilibrium situations such as exist for the present leading edge problem, in which the inelastic molecular model may have a substantial effect on the quantitative features of the flow structure.

We feel therefore, that until the phenomenological methods have been improved or further tested, it is worthwhile to continue investigating

the classical models.

The quantum mechanical inelastic collision models of Curtiss and co-workers [26] are very complicated and do not, at present, appear to be suitable for use in the Direct Simulation method

3. RAREFIED LEADING EDGE FLOWS

The present chapter is concerned specifically with the problem of rarefied hypersonic flow past the sharp leading edge of a two-dimensional flat plate the top surface of which is aligned with the free stream. We begin with a description of a qualitative physical model of leading edge flows built up through many notable contributions. This is followed by a review of the more recent of these on both the experimental and theoretical sides.

We consider the two-dimensional flow of a diatomic gas at very high Mach number past a flat plate. This is a complex problem involving the evolution of the flow from a purely kinetic rarefied one near the leading edge to a continuum flow dominated by continuum transport mechanisms far downstream. A schematic representation of the flow structure which has appeared widely in the literature [55] is shown in Fig. 1.

3.1 A Qualitative Description of the Flow

In the immediate vicinity of the leading edge, collisions between free stream and body reflected particles causes the initial disturbance away from a free-molecule convection dominated flow [51], generating the so-called "products of first collision". Through a collisional transfer of translational energy from directed to random motion, these particles have a more thermally agitated but less directed motion than free stream particles. Those moving downwards which strike the plate do so with an increased normal velocity component, the overall effect of which is to cause the surface properties, particularly the normal pressure and incident number flux, to rise above free-molecular values. In this initial kinetic regime, which may extend upstream of the leading edge [8],

body reflected particles penetrate large distances into the free stream and the highly nonequilibrium flow is thereby characterized by the strongly competing effects of molecule-molecule and molecule-body collisions. The distribution function is far from Maxwellian.

Farther downstream further molecule-molecule encounters produce secondary, tertiary, etc., products of collision while the effects of body molecules become confined to a subregion of the flow near the plate. The thermal motion of collision products saturates [51] causing the surface properties to maximize and then to decrease as the flow moves through a transition regime towards and into the merged layer.

Here a continuum of collisional classes develops through which the continuum transport mechanisms begin to operate, and the distribution function is more nearly Maxwellian. The initial flow disturbance now develops the dual features of a boundary layer next to the wall and a non-Rankine Hugoniot embryo shock [55] further out. Immediately adjacent to the wall a kinetic flow still exists as the collision products have not yet come into equilibrium with body molecules (slip flow). Values of the surface properties are rather less than is predicted by strong interaction theory as the transport processes are still affected by the shock structure and by the wall kinetic layer [55].

Eventually a more nearly equilibrium flow develops in the strong-interaction regime [35] where a region of inviscid but rotational flow separates the boundary layer from the now thin Rankine-Hugoniot shock type shock. At the flow boundaries the wall and shock kinetic layers are very thin and the slip at the wall vanishes. Even farther downstream the weak interaction regime develops with its accompanying weak shock and surface pressure gradient. Finally, the classical constant pressure boundary layer evolves while the shock degenerates to a Mach line.

3.2 Two Important Considerations

Lewis [51] points out that, among others, two very important mechanisms which influence the flow in the kinetic regime are firstly the gas-surface interaction and secondly the rotational degrees of freedom for diatomic molecules.

The gas-surface law determines the properties of reflected molecules and hence indirectly the very nature of the initial flow. There is some experimental evidence [50] for the commonly assumed completely diffuse fully accommodated model for low energy molecular reflection from "engineering" surfaces in which molecules are instantaneously re-emitted by the surface with a non-directed Maxwellian velocity distribution at the wall temperature. There appears to be little direct experimental evidence regarding the state of the internal modes of reflected particles although Lewis [51] has suggested that for diatomic molecules, the rotational mode is partly accommodated to the wall while the vibrational mode remains unaffected on re-emission.

As has been previously noted, internal degrees of freedom for a diatomic gas may have a large effect on the molecule-molecule collision dynamics. For hypersonic flow at moderate stagnation temperatures (to $< 2500^\circ\text{K}$), the effects of vibration, dissociation and ionization may be neglected. In the case of vibration, the relaxation time is very long [64]. Thus in experiments, this mode may be considered to be frozen at the stagnation temperature reached in the nozzle settling chamber. For dissociation and ionization the temperature quoted above is rather lower than the respective characteristic excitation temperatures [79]. The rotational modes, however, have relaxation times comparable with a particle transit time through the initial kinetic regime. Hence, through energy absorption in inelastic collisions, rotational excitation, with eventual equilibrium far downstream, may be expected to have a marked effect on the

flow properties. This has been observed experimentally by Hickman [37], Lewis and others and will be discussed more fully in Chapter 6 on the present calculations.

3.3 Review of Previous Work

3.3.1 Experimental Investigations

In the last decade a large number of experimental studies of hyperthermal leading edge flows have been presented from which Refs [3, 32, 37, 41, 46, 47, 51, 52, 55, 76-78] have been cited as those most relevant to the present work. With the effective scale expansion of the various flow regimes made possible by continual improvements in low density facilities, the general trend of experimental work has been to probe further into the nonequilibrium rarefied kinetic regimes near the leading edge. The test gas has usually been nitrogen but air, argon and helium have also been used. Results presented have often included density and lately rotational temperature profiles obtained using electron beam techniques, as well as measurements of surface properties such as heat transfer, skin friction, the component of the local pressure tensor normal to the wall and the incident number flux. In most cases experiments have been performed at approximately constant wall temperature.

An important experimental investigation of the merged layer was presented by McCroskey [55] who developed a physical model of the flow in this region briefly described earlier. McCroskey also confirmed that the rarefaction parameter $\bar{V} = M_\infty \sqrt{C^*/R_{ex}}$ introduced by Talbot [72], rather than the strong interaction parameter $\bar{\chi} = M_\infty^2 \bar{V}$ was the relevant parameter for the correlation of surface properties in the merged layer.

Early experiments in the kinetic regime led to an apparently inconsistent picture of the flow in this region. On the one hand, values of the surface

heat transfer and skin friction coefficients near the free molecular limit towards the leading edge were measured in a number of experiments [78]. Values of the normal surface pressure P_n [77,47], or the incident flux [41], however, did not seem to decrease towards the corresponding limit upstream of the observed maxima. With regard to P_n , it is widely recognized that there are great difficulties associated with the measurement of this quantity in the kinetic regime. In low density experiments, pressure is often measured with transducers connected to free molecular straight-walled tubes or sharp-lipped cavities embedded in the model surface. Unfortunately conditions existing in these orifices are very different to those in the flow immediately adjacent to their entrance planes. In the latter case the flow will be in a state of translational and internal nonequilibrium with, in particular the three diagonal components of the pressure tensor being unequal to each other (to first order) and to the pressure in the cavity P_c . A related problem is that the orifice geometry can have a critical effect [41] on the measured P_c .

It follows that P_c must be corrected to obtain estimates of P_n in the entrance plane and it is the choice of the appropriate correction scheme that has led to the large differences in the published results and to the current state of confusion regarding the surface pressure. The pressure measurements referred to above were for the most part corrected using a variety of semi-empirical methods which are discussed in Ref. [76]. All of these schemes predict that P_n exceeds the cavity pressure P_c for nonequilibrium flow which leads to the apparent non-free-molecular like behaviour of P_n near the leading edge. Unfortunately these methods lead to inconsistent results in the case of a genuinely free molecular flow [33].

A scheme which does give the appropriate corrections in both the equilibrium and free molecular limits has been presented by Harbour and Bienkowski [33]. This method is for pressures measured in sharp-lipped

cavities and is based on a two-stream two-sided free-molecule like model for the flow distribution function adjacent to the plate. Applying this scheme to a wide variety of published measurements, Harbour and Bienkowski found that substantial reductions in P_c resulted yielding near free-molecule values of P_n towards the leading edge in flat contradiction to the predictions of earlier methods. A strong case for the existence of free molecule conditions near the leading edge in an $M_\infty = 25$ stream has also been presented by Lewis [51]. In contrast to previous measurements [52], Lewis' density profiles display qualitatively free molecular behaviour close to the plate surface. Moreover, values of the incident number flux and also of P_n obtained using sharp-lipped cavities together with a correction scheme similar to that of Ref. [33] clearly approach the free-molecular limit towards the leading edge. The possibility exists, however, that the conclusions of Refs. [33] and [51] regarding P_n may be a consequence of the assumed free-molecule like flow model.

An objection to the small cavity approach to pressure measurement is that the correction $|P_{yy} - P_c|/P_c$ can be of order 50-100% which is very high for what are essentially approximate methods. These considerations led Uppington [76] to measure pressures in rather large straight walled tubes, which according to most theories require little or no correction. An objection to this method is that the orifice geometry may lead to sizable collisional interaction between the gas in the cavity and the flow adjacent to the wall. Uppington's estimates of P_n greatly exceed Lewis' results very near the leading edge more nearly resembling the earlier measurements of Vas and Allegre [77]. The interpretation of recent measurements obtained by Jeffery [46] at very rarefied conditions in blunt-lipped cavities of small orifice diameter depends on the correction scheme utilized.

As an alternative to measuring pressure in cavities, Vidal and Bartz [78] have made direct measurements of P_n using pressure transducers mounted

flush with the model surface. In the light of the previous discussion, the virtues of this method are obvious. The disadvantages are that firstly the transducers tend to be too large to obtain adequate resolution in many applications and secondly, they may have quite different surface characteristics to those of the plate model.

3.3.2 Theoretical Studies

A wide variety of continuum and kinetic theory methodologies have been applied in theoretical studies of the leading edge problem. In general the approach has been either to extend continuum methods towards their upstream limits which by definition lie somewhere in the transition region or to apply kinetic theory models downstream from the leading edge

Continuum Methods

A continuum treatment of the flow may be expected to be valid everywhere downstream of the transition regime save through the kinetic sublayer which exists adjacent to the wall in the merged layer. However, this sublayer is quite thin and can be incorporated into continuum treatments by including velocity slip and temperature jump conditions [69] at the wall as boundary conditions for the governing equations.*

In the interaction regimes, the classical no slip boundary conditions apply and the flow has been extensively studied using the well known weak and strong interaction theories [24,35]. These predict surface properties which depend primarily on $\bar{\chi}$ but lead to large negative pressure gradients upstream and to singularities at the leading edge. Clearly the interaction theories have an upstream limit which McCrockey [55] considers to lie roughly in the range $0.15 < \bar{V} < 0.20$.

* Unless otherwise stated, all merged layer studies referred to in this section include these conditions.

Early merged layer treatments were essentially extensions of interaction models retaining the notion of thin Rankine-Hugoniot shocks but including wall slip and fully viscous effects [62]. However, McCroskey's experimental work established that these concepts were inadequate and that an integrated theoretical treatment of viscous shock wave — boundary layer coupling was required in the merged layer. Consequently, Shorenstein and Probst [70] improved the earlier approach of Pan and Probst [63] replacing their thin shock assumption with that of a Navier Stokes type shock which is patched to the locally similar constant pressure boundary layer along a free boundary. This resulted in a reduction of calculated surface pressures compared with earlier predictions thus confirming the existence of a merged layer pressure plateau.

Two similar merged layer studies based on numerical solutions of simplified Navier Stokes equations have been presented by Rudman and Rubin [67] and by Cheng et al. [25]. These authors assume all layers are thin, neglecting streamwise compared to normal flow gradients. The Navier Stokes equations then reduce to a parabolic set which can be numerically integrated downstream using a marching technique requiring no special treatment of the shock. Initial conditions at the leading edge are taken to be the free stream conditions. In both the above studies the shock structure emerges naturally from the solution and is decidedly non-Rankine-Hugoniot. Both predict surface properties which are lower than the strong interaction values and which agree reasonably with experiment. However, Cheng et al. note a significant deviation upstream of $\bar{V} = 0.5$ which may well be due to kinetic flow effects in the tail of the kinetic/transition region.

Schaff and Chambré [69] consider that for hypersonic rarefied flow near a wall, the range of validity of a continuum description of the flow is given roughly by $M/\sqrt{Re} < 0.1$. But while this limit would seem to be somewhat stringent, at least for leading edge flow, there is no doubt that

a kinetic regime exists upstream of the merged layer in which continuum formulations are invalid. Nevertheless, several authors have obtained self-consistent numerical solutions of the complete Navier Stokes equations through the entire span of the interaction, merged layer and kinetic flow regimes.*

In an early approach of this kind, Butler [20] employed the fluid-in-cell and particle-in-cell solution techniques to compute a hypersonic flat plate flow but used a mesh size which was rather too coarse to adequately resolve the flow gradients near the leading edge. Tannehill et al. [73] overcome this difficulty by patching together differently scaled grids, a fine one being utilized in the kinetic regime. These authors obtain finite difference solutions to the time dependent Navier Stokes equations for which the steady flow evolves as that at large values of time. A very surprising result is that the surface properties, which asymptote to the strong interaction values far downstream, reduce quite naturally to near free-molecular values towards the leading edge. Moreover, the predicted flow in the kinetic regime compares quite reasonably qualitatively and in some instances quantitatively with experiment, and, for a monatomic gas, with the Monte-Carlo calculations of Vogenitz et al. [80]. However, the solutions of Ref. [73] were obtained at moderate Mach number. At higher M_∞ where translational and internal nonequilibrium effects** will be more pronounced it seems unlikely that a Navier-Stokes treatment would be adequate near the leading edge. In fact Tannehill et al. report that

* A numerical solution of the complete Navier Stokes equations in the merged layer interaction regimes has been presented by Hirschel [38] with the aim of studying the effects of the surface accommodation coefficients on the flow in the interaction region.

** Note that Tannehill et al. do not include bulk viscosity effects for a diatomic gas, which appears to be tantamount to neglecting internal non-equilibrium effects altogether.

for $M_\infty = 25$, there is a larger disagreement between calculation and experiment than for their published results.

The next step in a continuum treatment might perhaps be to consider the Burnett equations which may be obtained from a Chapman-Enskog type solution of the Boltzmann Equation valid formally to second order. But quite apart from the delicate questions of boundary conditions for these equations it has yet to be established that their range of validity extends further than does that of the Navier Stokes equations [69].

Kinetic Theory Methods

Kinetic theory descriptions of the flow should of course be valid globally. However, a direct numerical solution of the Boltzmann equation at present appears to be out of the question. Those kinetic theory treatments of the leading edge problem which have to date been presented may be broadly classified into three categories.

In the first of these several authors have through physical considerations analysed the initial kinetic flow in terms of a number of separate but collisionally interacting streams. In an early approach Charwat [23] considered first and second collisions between free stream and surface reflected molecules, estimating the effects of these collision products on the initial rise in the surface properties. Hamel and Cooper [31] divide the flow into an incident free stream, a body reflected (emitted) stream and a scattered stream representing the products of first collision. An analytical expansion of the Boltzmann equation based on this model then leads to predictions for the flow properties near the leading edge. The basis for this analysis is essentially the scaling of the flow in terms of Kogan's [49] scale length λ_{fb} , the mean free path of a free stream particle in a field of body emitted particles and the complementary scale λ_{bf} , the mean free path of body emitted particles in a sea of free stream molecules. While these and other [29] multi-stream theories have greatly increased the

understanding of the physics of leading edge flows, they cannot be expected to be quantitatively correct other than very near the leading edge. In the first place the treatment of molecular collisions is at best rudimentary. Secondly they appear to be unable to account for the possible effects of collisional flow disturbances forward of the leading edge.

The second kinetic theory approach referred to above is based on discrete ordinate solutions to the B.G.K./ellipsoidal type model equations. In the latest of a series of publications [42-44], Huang et al. [44] have presented the first kinetic theory treatment of the leading edge problem for a diatomic gas, using the Morse [59] - Holoway [40] - Brau [19] extension of the B.G.K. scheme for a gas with internal energy, to calculate the entire flow field at $M_\infty = 6.1$. Huang et al. find that the existence of rotational energy for the diatomic molecules has considerable effect on the flow field. The surface pressure is much lower for the flow of a diatomic gas than for that of a monatomic gas at similar conditions, but in neither case is the free-molecular limit reached near the leading edge. Furthermore the flow disturbance caused by the flat plate is stronger and more extensive in the normal direction in the monatomic case. Although the linearized approach has proved fruitful at moderate Mach numbers, it is not clear that this method is suitable for flows at very high M_∞ .

Finally the Direct Simulation method, which makes no simplification to the collision integral has been applied to the flat plate problem for a monatomic gas in a number of instances [8,80]. One notable feature of these calculations is that for long plates the flow very near the leading edge does not appear to be dominated by free-molecule effects. In fact, in computing the flow about short plates at moderate Mach number, Bird [8] concluded that there was no substantial free-molecule region for a plate greater than a few λ_∞ in length and further, that the first collision regime

appeared to extend upstream of the leading edge. Vogenitz et al. [80] present pressure distributions for a range of conditions, some at high Mach number. In all cases, pressures several times the free molecule value were obtained within a few λ_∞ of the leading edge although the actual limit tended to be somewhat obscured by statistical scatter. However, Vogenitz et al. also found that the gas-surface interaction law profoundly influenced the flow to distances of many λ_∞ downstream of the leading edge. The best comparison with experiment so far obtained with the Direct Simulation method is that of the calculated incident number flux with the helium data of Horstman [41].

It should be noted that both the B.G.K. and Monte-Carlo approaches are able to include the effects of forward disturbances from the leading edge.

From the preceding discussion we may conclude that a coherent experimental-theoretical picture of the flow in the kinetic regime at high M_∞ has not yet emerged. On the experimental side there are the difficulties of flow property measurement (particularly surface pressure) associated with the highly nonequilibrium nature of the flow. On the theoretical side, it is only recently that practical kinetic theory methods have been developed for polyatomic gases and it seems likely that the discrepancies between monatomic theory and diatomic data could be largely explained by the inclusion of internal degrees of freedom.

A further problem is the question of a scale parameter for the correlation of surface properties in the kinetic regime. The free stream mean free path does not provide a suitable scale length since this quantity is rather ill-defined at the very low free stream temperatures at which experiments are performed. Lewis [51] finds that x/λ_{fb} provides a good basis for the correlation of surface properties for a wide range of body temperature while Hamel and Cooper [31] present their results as functions of x/λ_{bf} . Vogenitz et al. [80] made no attempt to classify the flow into

different regimes and did not refer to λ_{fb} as a possible kinetic regime length scale but presented their results against x/λ_∞ and y/λ_∞ . The quantities λ_{fb} and λ_{bf} have two distinct advantages over λ_∞ as a kinetic length scale. Firstly they can be seen to have a physical significance in terms of a plausible model of the initial flow development. Secondly, they can be more clearly defined than λ_∞ . The present definitions are given in Section 6.2.

We return to specific consideration of the hypersonic leading edge problem in Chapter 6 where the present calculations are described and the flow properties obtained are compared with data on the basis of x/λ_{fb} and y/λ_{bf} . The principal object of these calculations is to provide a theoretical description of the leading edge flow of a diatomic gas at high M_∞ which might contribute towards a further understanding of this basic problem.

4. THE DIRECT SIMULATION TECHNIQUE

In this chapter we shall describe the main features of the Direct Simulation method as used in the calculation of general two-dimensional steady flows. Other general descriptions may be found in Refs. [11] and [28].

The real gas flow is to be simulated by what may be shown to be the statistically analogous motion of some thousands of simulator particles. Since the phase space information is to be carried by the particle ensemble, all flow properties of interest must be obtained by summing the contributions of individual particles, a process which is carried out concurrently with the dynamical simulation.

The two-dimensional region of the flow field to be simulated is denoted by Ω which is bounded externally by an imaginary boundary Γ and internally by the solid body surface Σ . At any time instant during simulation each molecule is defined by two spatial, three velocity components and a value of the internal (rotational) energy which are stored in six computer memory arrays. For the purposes of collision calculation and flow field sampling to be discussed, Ω is subdivided into a grid of contiguous two-dimensional spacial cells ω_k , $k=1,K$. Likewise Σ is divided into small segments σ_j , $j=1,J$ to gather molecule surface interaction information. The extent of the ω_k and σ_j must be such that adequate resolution of the flow is obtained, that is, across each the variation of the local flow properties must be small.

4.1 Initialization

An initial approximation to the ensemble flow is not required, a two-dimensional nonequilibrium steady flow being obtained as the asymptotic solution for the unsteady flow which results when Σ is instantaneously

inserted, at zero time into a uniform undisturbed flow. Initially then Ω is populated with a spacially uniformly distributed sample of simulator particles. The velocity and internal energy co-ordinates for each particle are obtained by sampling from the appropriate Maxwellian distributions for a gas in equilibrium moving with a specified mean velocity in the plane of Ω .

4.2 General Description

The dynamical simulation is discretized in time by introducing a small specified time interval Δt_m . Molecular collisions and convection are decoupled in this interval as follows: A group of labelled molecules m_ℓ , $\ell = L_{k-1}, L_k$ which happen to be in ω_k at the beginning of Δt_m are considered to comprise, during Δt_m , an isolated homogeneous sub-system of the overall particle ensemble. This is justified in the first place by recalling the restrictions on the extent of ω_k given previously. The group m_ℓ may then be regarded as a sample from the local distribution function. Secondly, Δt_m is chosen so as to be smaller than a typical convection time of a molecule across a cell, that is

$$v_i \Delta t_m / \Delta x_i < \delta \leq 1 \quad (1)$$

where v_i , $i = 1, 3$ are the components of the local mean velocity and Δx_i , $i = 1, 3$ represent the cell dimensions. As well as minimizing convective interaction between adjacent cells during Δt_m , the above condition reduces the probability of a molecule passing completely through a cell in Δt_m thus forgoing the possibility of collision.

With these assumptions collisions are calculated in each ω_k by disregarding molecular positions and by holding the molecules motionless. On completion of this process, a new set of dynamical co-ordinates for the group results. Each particle in Ω is then moved through Δt_m a distance

appropriate to its final instantaneous velocity and various boundary conditions are implemented. The Δt_m must also be small compared with a local mean free time so that trajectory distortions and slightly incorrect collision probabilities which result from the space and time discretization, are small. A quantitative expression of this condition is given by (A13) of Appendix A.

The above comprises an iteration which is repeated through a large number of Δt_m 's until eventually, after a time t_s the flow becomes steady and the total number of particles instantaneously in Ω is approximately constant. Sampling to determine flow field properties may then begin. The collision and movement modes of simulation may be regarded as analogous to the collision and convection terms in the Boltzmann equation.

4.3 Collision Calculation

The technique for numerically simulating binary collisions proposed by G.A. Bird lies at the heart of the Direct Simulation method. A justification for the collision calculation procedure is given in Appendix A where the method is shown to be consistent with the derivation of the collision term in the Boltzmann equation. Here we merely state the collision algorithm which is operated successively in each ω_k , $k = 1, K$ for each Δt_m . Let there be N_k particles currently in ω_k . Then collisions are computed as follows

1. Choose a pair of particles from the $\frac{1}{2}N_k(N_k - 1)$ possible pairs, each with equal probability.
2. Accept or reject the pair for collision with probability density proportional to $gb_0^2(g)$ in some prechosen range of g where $b_0(g)$ is the maximum impact parameter at the pair relative speed g .
3. If the pair is rejected choose another and repeat. If accepted, choose the impact parameter b and azimuthal angle ϵ (in the pair centre of

mass framework) in the distributions given in Appendix A and proceed to calculate the post-collision dynamical parameters according to the prescribed collision model.

4. Advance a time counter t_k for ω_k by an increment given by [Eq.(A9), Appendix A]

$$\Delta t_k = \frac{2}{N_k \bar{\rho} n_k g \pi b_0^2 (g)} \quad (2)$$

where $\bar{\rho}$ and n_k are defined in the Appendix.

Steps 1-4 are repeated until $t_k > M \cdot \Delta t_m$ where M is the number of Δt_m 's including the current one since the simulation was initiated. Any excess time $> M \cdot \Delta t_m$ is left in t_k as an initial time for the next sequence of collision calculations in ω_k .

4.4 Molecule Movement

Trajectory increments are computed by moving each molecule in Ω through a distance $|\underline{V}| \cdot \Delta t_m$ in the direction of $\underline{V}$, its instantaneous velocity. During these flight path elements, an individual particle may either cross Γ , in which case it is disregarded, or it may collide with the body surface in which case it is reflected according to the given surface interaction law. In the latter case the particle is moved through the remainder of the current Δt_m with its reflected velocity components. Particles remaining in Ω after the trajectory increment then take place in the next round of collisions.

4.5 Boundary Conditions

A. In the present work the boundary condition at the imaginary boundary

Γ is that of free molecule flow of the free stream. At the end of each Δt_m , an appropriate number of particles are entered into Ω along each segment γ_q , $q = 1, Q$ of Γ . The dynamical properties of entering particles are

sampled from the relevant distributions for free molecule flow of the free stream across γ_q . Their positions on entry are uniformly distributed along γ_q and the initial time of flight of each is given by $\xi \Delta t_m$ where ξ is a random number in (0,1). The property of the above boundary condition for the downstream boundary in the present calculations is discussed in Section 6.1.

B. The gas-surface interaction law used in the present work is taken to be a specified mixture of diffuse and specular reflection, both of which satisfy the reciprocity principle. Thus molecules striking the body are reflected diffusely with probability p_j or specularly with probability $1-p_j$. In diffuse reflection, particles are re-emitted with a Maxwellian distribution of dynamical properties (including internal energy) characterized by the energy accommodation coefficient α_j defined in the usual way [69] and the local wall temperature T_{w_j} . Specular reflection is elastic with the normal component of the incident momentum reversed and the tangential component unchanged. The p_j , α_j and T_{w_j} are taken as constant in segment σ_j but may vary from segment to segment.

4.6 Flow Properties

Flow properties being either local distribution function moments or histogram estimates of the distribution function f itself are obtained by averaging the contributions of individual particles. Thus the expectation value of some function $Q(\underline{V}, \underline{\Omega})$ of the velocity and internal co-ordinates

$$\langle Q \rangle = \iint Q(\underline{V}, \underline{\Omega}) f(\underline{V}, \underline{\Omega}, \underline{x}, t) d\underline{V} d\underline{\Omega} \quad (3)$$

is approximated by the average value

$$\bar{Q} = \frac{1}{N} \sum_{n=1}^N Q_n \quad (4)$$

over a sample of N independent particle observations. Hence $Q \equiv \bar{V}$ leads to mean velocity, $Q \equiv (\bar{V} - \bar{V})^2$ leads to translational temperature, $Q \equiv (V_i - \bar{V}_i)(V_j - \bar{V}_j)$ to the ij^{th} component of the pressure tensor, etc. The sampling falls into two categories

A. In spacial cells, samples of size N_k , are taken in each ω_k at regular time intervals Δt_s . Since for steady flow new particles are continuously flowing through the cells, a large number of successive samples may be accumulated to give an overall sample $N = \sum N_k$ for ω_k . To ensure non-correlation of successive samples, Δt_s is made rather larger than the mean convection time across some cell in an extreme case.

B. Successive molecule surface interactions are automatically independent. Thus sampling in each body segment for the determination of normal pressure, skin friction, number flux, etc., may be carried on continuously.

4.7 Statistical Fluctuations

In estimating statistical fluctuations it is usually assumed, following the central limit theorem that each $\bar{Q}$ is normally distributed with standard deviation $\bar{\sigma}$ proportional to $N^{-1/2}$. In general however, the constants of proportionality cannot be determined and hence it is often further assumed that

$$\frac{\bar{\sigma}}{\bar{Q}} = N^{-1/2} \quad (5)$$

as a guide to required sample sizes. Hence for 3% relative standard deviation — sufficient for engineering problems — samples of about 1000 are required which is the minimum aimed for in the present numerical calculations described in Chapter 6. A more extensive discussion of fluctuations and accuracy is given in Ref. [80].

4.8 Stability

A fundamental requirement for the practical success of any numerical method is that it be stable in its domain of application. To the author's knowledge, no systematic mathematical study of the Direct Simulation method has yet been published which might serve as the basis for a stability/accuracy analysis. Practice indicates that the method is inherently stable in the sense that estimates of flow quantities given by Eq.(4) appear to converge statistically with increasing N and with standard deviation decreasing roughly as given by Eq.(5). Bird [17] reports, however, that with certain somewhat artificial boundary conditions which have been used at an imaginary boundary, γ_j , local instabilities have resulted.

Borgnakke and Larsen [18] give inequality (1) in Section 4.2 of the present work as a stability criterion. Violation of this condition does not, however, appear to lead to an unstable simulation, but rather a stable but incorrect one in which the errors discussed in relation to (1) may be convected with the particles.

5. AN APPROXIMATE DIATOMIC COLLISION MODEL

In Section 4.3, it was seen that the final step in a collision calculation for the Direct Simulation method was the determination of the post-collision dynamical parameters from the specified collision model. In the present chapter we shall develop the approximate model employed for the above purpose in the present work.

As was indicated in Chapter 2, the classical elastic collision problem for general spherical potentials is quite straightforward. However, great analytical difficulties are encountered once any kind of internal energy is introduced [2]. Numerical solutions, on the other hand are feasible for general potentials, but even with modern computing machines, it is quite out of the question to repeat the numerical solution of the equations of motion for each of the, say, $O(10^6)$ encounters which might be needed for the simulation of a complex two-dimensional flow.

The present approach to include internal rotational energy in collisions of nonpolar diatomic molecules is to adapt an approximate form of Parker's classical model [64] for use in Monte-Carlo simulation. This model is appealing since as was discussed in Section 2.2, it has been used by numerous authors to successfully predict the temperature dependence of rotational collision numbers for various diatomic gases. In the course of this chapter, it will be seen that the adaptation of the Parker model involves an extension of the perturbation analysis of Lordi and Mates [53] resulting in an approximate analytical expression for the energy exchange in terms of the pre-collision dynamical parameters. Once the energy exchange is known, it remains a simple matter to determine the post-collision parameters from the various conservation conditions.

5.1 Parker's Classical Collision Model

We consider binary collisions of two identical homonuclear diatomic molecules under the assumption that rotation is the only active internal energy mode, that is, vibration and other internal modes associated with atomic structure are dormant. The intermolecular potential is that proposed by Parker [64]. Each molecule is represented as a rigid rotor, the force field of which consists of two short range centres of repulsion located symmetrically on the internuclear axis (but not necessarily co-incident with the mass centre of each atom) together with a longer range but weaker attractive force centre at the midpoint of the nuclear axis. The potential associated with each force centre is exponential in nature, i.e. of the form $e^{-\alpha r}$.

The initial velocities of the two molecules (long before collision) in a laboratory framework are $\underline{c}_i$ where $i = 1, 2$ for each particle respectively while the initial rotational energies are $E_{R_i} = \frac{1}{2} I \omega_i^2$. Equivalent quantities long after collision are $\underline{c}'_i$ and E'_{R_i} . The molecular mass is m and $I = \frac{1}{4} m d^2$ is the moment of inertia of each particle about its mass centre, d being the internuclear mass separation. Since no external forces or torques act on the system it is convenient to work in a co-ordinate framework fixed to the two-molecule mass centre which moves with constant velocity

$$\dot{\underline{r}}_g = \frac{1}{2}(\underline{c}_1 + \underline{c}_2) = \frac{1}{2}(\underline{c}'_1 + \underline{c}'_2)$$

during encounter. Conservation of linear momentum is then automatically satisfied. Furthermore, as is shown in Appendix B, the collision problem may be conveniently reduced to that of a rotating molecule with the pair reduced mass $\mu = m/2$ moving about a fictitious stationary rotating molecule.

Figure 2A shows the relative position and orientations (see the notation for definitions) of the two particles of the reduced system, at some point during the encounter. Molecule 1 is taken to be the fictitious stationary particle while molecule 2 is moving. The orientations of non-rotating axes

x_i, y_i, z_i are chosen such that long before collision the z_1 and z_2 axes point in the direction of the pair orbital angular momentum vector. The initial relative velocity vector $\mathbf{g} = \mathbf{c}_2 - \mathbf{c}_1$ lies in the x_1 - y_1 plane (henceforth called the "collision plane") and points in the negative x_1 direction.

For R much greater than the effective range of the intermolecular potential, the angular momentum vector of each particle is constant in time. During encounter each molecule is subject to a torque since the intermolecular force vector does not generally lie along the line of centres. This alters their respective rotational motions and may be thought of as constituting the "inelastic energy exchange mechanism".

The classical two particle problem described above contains seven co-ordinates in the centre of mass framework, namely the set $(R, \phi, \theta, \beta_1, \psi_1, \beta_2, \psi_2)$. A satisfactory solution to the appropriate equations of motion for this system would be very difficult. To the author's knowledge no such solution exists although Curtiss [26] has considered the equivalent quantum-mechanical case in relation to polyatomic transport theory calculations.

The complete classical problem for full three-dimensional molecular orientations is considered further in Appendix D where it is shown that a closed form solution for the inelastic energy transfer may be obtained to first order in a perturbation parameter. However, the result is very much more complicated than that for a simplified problem to be presently considered, and for reasons which may become apparent in Section 5.6, it seems likely that a second order result may be necessary for suitable adaptation to Monte-Carlo simulation. This appears to be much too difficult for the fully three-dimensional problem.

5.2 Planar Rotation Assumption

In view of the complexity of the general problem, Parker [64], Nyeland

[61] and Lordi and Mates [53] all introduced the simplifying assumption that the plane of rotation of each molecule is initially coincident with the collision plane, that is, the orbital and angular momentum vectors of the system are aligned. Examination of the general equations of motion reveals that if this condition is satisfied prior to collision, there is no subsequent out of plane motion, the entire interaction being confined to the x_1 - y_1 plane. The above assumptions lead to a tractable set of equations but as is noted by Macpherson [54], it appears to allow molecules only one degree of freedom in rotation rather than the required two. While the freedom to locate the repulsive potential centres at an arbitrary distance from the molecular mass centre goes some way to compensate for this limitation, it will nevertheless be seen to result in a collision model which is not entirely satisfactory for simulation in near equilibrium situations. However, in that the simplified model leads to the correct temperature dependence of Z_R , there is good reason to believe that it preserves some features of the microscopic energy exchange process which we feel to be necessary for a description of strongly inelastic collisions which will dominate highly nonequilibrium flows. Ad hoc measures for alleviating the above mentioned defects near macroscopic equilibrium are presented in Section 5.10 where the Parker model is further discussed.

The equations of motion for the planar rotation case can be obtained by putting

$$\beta_1 = \beta_2 = \theta = \pi/2$$

which reduces the number of free co-ordinates to four, viz: R , ϕ , ψ_1 and ψ_2 . Figure 2B shows the configuration of the simplified system at some point during collision. The initial relative speed g , the impact parameter or miss distance b and the initial molecular angular velocities ω_i are taken as known.

5.3 Perturbation Expansion of the Equations of Motion

Parker's nonspherical intermolecular potential described previously may be written as [64]

$$V(R, \phi, \psi_1, \psi_2) = \frac{K_1}{4} e^{\alpha D} \left\{ e^{-\alpha R_{AC}} + e^{-\alpha R_{AD}} + e^{-\alpha R_{BC}} + e^{-\alpha R_{BD}} \right\} - 2K_2 e^{-\frac{\alpha}{2}(R-D)} \quad (6)$$

where α is the range factor and D , K_1 and K_2 are arbitrary parameters.

The K_1 term in the above represents the overall action of the repulsive force centres located at A, B, C and D in Fig.2A while the K_2 term represents the effect of the attractive force centres located at P and O. The distances R_{AB} , R_{AD} , R_{BC} and R_{BD} are those between points A and B, A and D, etc., and $R = |PO|$. We denote the separation of the repulsive forces centres on each molecular axis by the fixed distance $d' = |AB| = |CD|$.

The Lagrangian form of the equations of motion are the most convenient. The Lagrangian for the planar rotation case is

$$L = \frac{1}{2}\mu\dot{R}^2 + \frac{1}{2}\mu(R\dot{\phi})^2 + \frac{1}{2}I(\dot{\psi}_1^2 + \dot{\psi}_2^2) - V(R, \phi, \psi_1, \psi_2) \quad (7)$$

from which the equations of motion may be derived in the usual way. These are*

$$\mu(\ddot{R} - R\dot{\phi}^2) = -\frac{\partial V}{\partial R} \quad (8A)$$

$$\mu \frac{d}{dt} (R^2 \dot{\phi}) = -\frac{\partial V}{\partial \phi} \quad (8B)$$

$$I\ddot{\psi}_i = -\frac{\partial V}{\partial \psi_i} \quad (8C)$$

$i = 1, 2$

Parker, Nyeland and Lordi and Mates solve Eqs.(8C) to first order by a perturbation method. This involves the expansion of R_{AB} , R_{AD} , etc., and hence of Eq.(6) for V in terms of a series containing powers of d'/R . This series is truncated past the first term and the resulting approximate form of V is itself expanded in terms of a perturbation parameter embodying the

*The dot and d/dt notation will be freely mixed.

potential non-sphericity. Details of this procedure are given in Appendix C of the present work. The results to second order are given by Eq. (C11) which we reproduce here as

$$V = V_0 + \epsilon V_1 + \epsilon^2 V_2 + O(\epsilon^3) \quad (9)$$

where

$$V_0(R) = E' \left\{ e^{-\alpha(R-D)} - 2e^{-\frac{\alpha}{2}(R-D)} \right\} \quad (9A)$$

$$V_1(R, \phi, \psi_1, \psi_2) = E' e^{-\alpha(R-D)} (\cos 2\Gamma_1 + \cos 2\Gamma_2) \quad (9B)$$

$$V_2(R, \phi, \psi_1, \psi_2) = E' e^{-\alpha(R-D)} \left\{ \cos 2\Gamma_1 \cos 2\Gamma_2 + \frac{1}{12} (\cos 4\Gamma_1 + \cos 4\Gamma_2) \right\} \quad (9C)$$

where $\Gamma_i = \phi - \psi_i$, $i = 1, 2$ and

$$\epsilon = \frac{2I_2(\alpha d'/2)}{I_0(\alpha d'/2)}$$

is the perturbation parameter which forms the basis of the V expansion, the I_0 and I_2 being modified Bessel functions of the zeroth and second order respectively.

The spherical zeroth order potential $V_0(R)$ may be identified with a Morse potential, E' being the potential well depth at $R = D$. A convenient alternative form of $V_0(R)$ is given by Eq. (C13) of Appendix C, viz:

$$V_0(R) = 4E' \left\{ e^{-a'(R/\sigma-1)} - e^{-a'/2(R/\sigma-1)} \right\} \quad (10)$$

where σ is given by $V_0(\sigma) = 0$ and $a' = \alpha\sigma$.

The Parker [64] solution is continued by expanding each of the co-ordinate variables in terms of ϵ , viz:

$$R = R_0 + \epsilon R_1 + \epsilon^2 R_2 + O(\epsilon^3) \quad (11A)$$

$$\phi = \phi_0 + \epsilon \phi_1 + \epsilon^2 \phi_2 + O(\epsilon^3) \quad (11B)$$

$$\psi_i = \psi_{i0} + \epsilon \psi_{i1} + \epsilon^2 \psi_{i2} + O(\epsilon^3) \quad (11C)$$

$i = 1, 2$

By substitution of Eqs. (9) and (11) into Eqs. (8) and by equating powers of ϵ , zeroth, first and second order equations of motion are obtained. We

include here the complete zeroth and first order set, but only the second order set for ψ_2 which are sufficient for our purposes. These are

$$\underline{\epsilon^0}, \quad \mu(\ddot{R}_0 - R_0 \dot{\phi}_0^2) = - \left(\frac{\partial V_0}{\partial R} \right)_0 \quad (12A)$$

$$\mu \frac{d}{dt} (R_0^2 \dot{\phi}_0) = 0 \quad (12B)$$

$$I \psi_{i0} = 0, \quad i=1,2 \quad (12C)$$

$$\underline{\epsilon^1}, \quad \mu(\ddot{R}_1 - R_1 \dot{\phi}_0^2 - 2R_0 \dot{\phi}_0 \dot{\phi}_1) = - \left\{ R_1 \left(\frac{\partial^2 V_0}{\partial R^2} \right)_0 + \left(\frac{\partial V_1}{\partial R} \right)_0 \right\} \quad (13A)$$

$$\mu \frac{d}{dt} (2R_0 R_1 \dot{\phi}_0 + R_0^2 \dot{\phi}_1) = - I(\ddot{\psi}_{11} + \ddot{\psi}_{21}) \quad (13B)$$

$$I \ddot{\psi}_{i1} = - \left(\frac{\partial V_1}{\partial \psi_i} \right)_0, \quad i=1,2 \quad (13C)$$

ϵ^3 (rotation only),

$$I \ddot{\psi}_{i2} = - \psi_{i1} \left(\frac{\partial^2 V_1}{\partial \psi_i^2} \right)_0 - \psi_{j1} \left(\frac{\partial^2 V_1}{\partial \psi_j \partial \psi_i} \right)_0 - \phi_1 \left(\frac{\partial^2 V_1}{\partial \phi \partial \psi_i} \right)_0 - R_1 \left(\frac{\partial^2 V_1}{\partial R \partial \psi_i} \right)_0 - \left(\frac{\partial V_2}{\partial \psi_i} \right)_0$$

$$i=1, j=2; i=2, j=1 \quad (14)$$

where in Eq.(13B) the condition of conservation of angular momentum has been used.

Conditions an infinite time before collision are given by

$$\left. \begin{array}{ll} \dot{R}_0 = -g & y_{01} = b \\ \phi_0 = 0 & \dot{\psi}_{i0} = \omega_i, \quad i=1,2 \end{array} \right\} \quad (15)$$

and all higher order quantities are zero. The origin of time $t = 0$ may now be defined as the point of closest approach for the zeroth order collision.

5.4 Zeroth Order Solution

Equations (12B) and (12C) may be simply integrated to give

$$\mu R_0^2 \dot{\phi}_0 = \mu g b \quad . \quad (16)$$

$$\psi_{i0}(t) = \omega_i t + \gamma_i \quad , \quad i=1,2 \quad (17)$$

where Eq.(16) expresses the constancy of the zeroth order orbital angular momentum. The γ_i are the zeroth order molecular orientations at $t = 0$ and the ω_i are the constant zeroth order angular velocities. Substitution of Eq.(16) into Eq.(12A) and integrating with respect to R_0 yields

$$\frac{1}{2} \mu \dot{R}_0^2 + \frac{1}{2} \frac{\mu g^2 b^2}{R_0^2} + V_0(R_0) = \frac{1}{2} \mu g^2 \quad . \quad (18)$$

For $V_0(R_0)$ given by Eq.(10), the above cannot be integrated analytically. Together with Eq.(16), it can, however, be used to obtain an integral expression for the zeroth order deflection angle χ_0 . The result is [39]

$$\chi_0(g,b) = \pi - 2b \int_{R_0(0)}^{\infty} \left\{ 1 - \frac{b^2}{u^2} - \frac{V_0(u)}{\frac{1}{2} \mu g^2} \right\}^{-\frac{1}{2}} \frac{du}{u^2} \quad (19)$$

In the above $R_0(0)$ is the point of closest approach given by the outer solution of

$$1 - b^2/R_0^2 = V_0(R_0)/\frac{1}{2} \mu g^2 \quad (20)$$

which is obtained from Eq.(18) by placing $\dot{R}_0 = 0$.

It is now convenient to introduce the reduced variables

$$R_0^* = R_0/\sigma$$

$$b^* = b/\sigma$$

$$g^{*2} = \frac{1}{2} \mu g^2 / kT'$$

where $T' = E'/k$ is a temperature measure of the potential well depth. Using the form of V_0 given by Eq.(10) and introducing the transformation

$$x^2 = \frac{u - R_0(0)}{u}$$

into Eq.(19), Eqs. (19) and (20) may be expressed as

$$\chi_0(g^*, b^*) = \pi - 4 \int_0^1 \left\{ (2-x^2) - \frac{R_0^{*2}(0)}{g^{*2}b^{*2}} \left[\frac{M(x^2) - M(0)}{x^2} \right] \right\}^{-\frac{1}{2}} dx \quad (21)$$

where $R_0^*(0)$ is given by the outer solution of

$$g^{*2} \left(1 - \frac{b^{*2}}{R_0^{*2}(0)} \right) - 4 \left[\exp \left\{ -a' (R_0^*(0) - 1) \right\} - \exp \left\{ -\frac{a'}{2} (R_0^*(0) - 1) \right\} \right] = 0 \quad (22)$$

In Eq.(21),

$$M(x^2) = 4 \left[\exp \left\{ -a' \left(\frac{R_0^*(0)}{1-x^2} - 1 \right) \right\} - \exp \left\{ -\frac{a'}{2} \left(\frac{R_0^*(0)}{1-x^2} - 1 \right) \right\} \right] \quad (23)$$

The integrand in Eq.(21) can be shown to be finite for all $x \in (0,1)$ for all b^{*2} provided g^{*2} is greater than a critical value g_c^{*2} . For each $g^{*2} \leq g_c^{*2}$ there exists a single value of b^{*2} such that the integral in Eq.(21) diverges. This corresponds to a physical situation in which the two colliding particles are mutually captured, each orbiting about the pair mass centre in a metastable orbital configuration [39]. The existence of orbital capture depends on the attractive part of the potential and does not arise for purely repulsive molecular models.

Note that χ_0 is a function of a two parameter family in contrast to the hard sphere - inverse power law models for which the deflection angle can be expressed as a function of a single variable [22].

5.5 Energy Exchange in Collisions

The rotational energy of each molecule is given by

$$E_{r_i} = \frac{1}{2} I \dot{\psi}_i^2, \quad i=1,2 \quad (24)$$

Using Eq.(11C) this may be expanded as

$$E_{r_i} = \frac{1}{2} I [\omega_i^2 + 2\epsilon \omega_i \dot{\psi}_{i1} + \epsilon^2 \{ \dot{\psi}_{i1}^2 + 2\omega_i \dot{\psi}_{i2} \} + O(\epsilon^3)] \quad (25)$$

from which the initial rotational energy is clearly

$$E_{r_i} = \frac{1}{2} I \omega_i^2 \quad (26)$$

The increase in rotational energy for each molecule is then

$$\Delta E_{r_i} = \epsilon I \omega_i \dot{\psi}_{i1}(\infty) + \frac{1}{2} I \epsilon^2 \{ \dot{\psi}_{i1}^2(\infty) + 2 \omega_i \dot{\psi}_{i2}(\infty) \} + O(\epsilon^3) \quad (27)$$

where the ∞ as argument refers to an infinite time after collision. We now assume that in collisions γ_1 and γ_2 are both uniformly distributed in $(0, \pi)$ and further that they are uncorrelated. These assumptions would seem to be consistent with that of molecular chaos used in deriving the Boltzmann equation. The range $(0, \pi)$ is appropriate since the molecules are homonuclear.

It is now convenient to average the energy exchange in collisions over γ_i , $i = 1, 2$. For some quantity Q , define an orientation averaged value as

$$\bar{Q} = \frac{1}{\pi^2} \int_0^\pi \int_0^\pi Q \, d\gamma_1 \, d\gamma_2 \quad (28)$$

Applying Eq.(28) to Eq.(27) we obtain the orientation averaged energy exchange per molecule, which we write as

$$\overline{\Delta E_{r_i}} = I \epsilon \omega_i \overline{\dot{\psi}_{i1}(\infty)} + \frac{1}{2} I \epsilon^2 \{ \overline{\dot{\psi}_{i1}^2(\infty)} + 2 \omega_i \overline{\dot{\psi}_{i2}(\infty)} \} + O(\epsilon^3) \quad (29)$$

Solution of Perturbation Equations

The closed form evaluation of Eq.(29) requires approximate solutions to Eqs. (13) and (14). This in turn requires an approximate solution for the zeroth order trajectory $R_0(t)$. Lordi and Mates [53] obtained such a solution by assuming that in Eq.(18), one may approximate

$$\frac{\mu g^2 b^2}{R_0^2(t)} \simeq \frac{\mu g^2 b^2}{R_0^2(0)} \quad (30)$$

in similar fashion to the analyses of Parker [64] and Nyeland [61]. The above can be justified by noting that the zeroth order collision is "sudden", most of the deflection taking place in the vicinity of $R(0)$, where the R_0^{-2} term in Eq.(18) varies much more slowly than $V_0(R_0)$.

Substitution of (30) into Eq.(18) and integrating yields [53]

$$e^{-\alpha[R_0(t)-D]} = \frac{\xi^4/\beta^4}{[(1+\xi^2/\beta^2)^{\frac{1}{2}} \cosh(\alpha\xi t/2) - 1]^2} \quad (31)$$

where $\beta^2 = \frac{2kT'}{\mu}$ and $\xi = g[1 - b^2/R_0^2(0)]^{\frac{1}{2}}$. In general $R_0(0) = f(g, b)$ obtained from a solution of Eq.(20). A reasonable approximation, however, is given by $R_0(0) \simeq \sigma$. This is reasonable for the Lennard Jones 6-12 potential and exact solutions to Eq.(20) indicate that it is also reasonable for the Morse potential with errors of order 10%.

To appreciate the subsequent analysis it is important to stress that the left-hand side of Eq.(31) is an even function of t which maximizes at $t = 0$ and which decreases as $\exp(-\alpha\xi|t|)$ for large $|t|$.

5.6 First Order Solution

Evaluating the right-hand side of Eq.(13C) using Eq.(9B), yields

$$I \ddot{\psi}_{i1} = 2E'e^{-\alpha(R_0-D)} \sin 2(\psi_{i0} - \phi_0) \quad (32)$$

Taking $\dot{\psi}_{i1}(-\infty) = 0$ and integrating with respect to t leads to

$$\dot{\psi}_{i1}(t) = \frac{2E'}{I} \int_{-\infty}^t e^{-\alpha(R_0-D)} \sin[2(\psi_{i0} - \phi_0)] du \quad (33)$$

An approximation to $\phi_0(t)$ near $t = 0$ is given by the first order Taylor series expansion.

$$\phi_0(t) = \phi(0) + \dot{\phi}(0)t + O(t^2) \quad (34)$$

which is consistent with the approximation (30) since $\dot{R}(0) = 0$. Substituting Eqs. (17), (31) and (34) into Eq. (33) one obtains an approximate solution for $\dot{\psi}_{i1}(t)$ valid near $t = 0$ as

$$\dot{\psi}_{i1}(t) = \frac{2E'}{I} \left(\frac{\xi}{\beta}\right)^4 \int_{-\infty}^t \frac{\sin(2\delta_i + 2v_i u) du}{[A \cosh(au) - 1]^2} \quad (35)$$

where

$$\delta_i = \gamma_i - \phi_0(0) , \quad v_i = \omega_i - \dot{\phi}_0(0)$$

$$A = (1 + \xi^2/\beta^2)^{\frac{1}{2}} , \quad a = \alpha\xi/2$$

and where we have neglected the $O(t^2)$ term in Eq.(34).

Setting the upper limit in Eq.(35) to ∞ , and expanding the trigonometric factor in the integrand yields an approximation for the first order increase in rotational velocity through a collision,

$$\dot{\psi}_{i1}(\infty) = \frac{2E'}{I} \left(\frac{\xi}{\beta} \right)^4 \sin(2\delta_1) L_1 . \quad (36)$$

where

$$L_1 = \int_{-\infty}^{\infty} \frac{\cos(2v_i u) du}{[A \cosh(au) - 1]^2}$$

Note that in obtaining Eq.(36) from Eq.(35), an integral of an odd function of time has vanished.

Application of Eq.(28) to Eq.(36) and to its square yields

$$\overline{\dot{\psi}_{i1}}(\infty) = 0 . \quad (37)$$

$$\overline{\dot{\psi}_{i1}^2}(\infty) = \frac{1}{2} \left\{ \frac{2E'}{I} \left(\frac{\xi}{\beta} \right)^4 \right\}^2 L_1^2 . \quad (38)$$

Hence it may be seen that the term of order ϵ in Eq.(29) vanishes and we are required to go to second order to obtain a non-zero value of $\overline{\Delta E_{Ri}}$.

Since $\overline{\dot{\psi}_i^2}(\infty)$ is necessarily positive, it can be seen from Eq.(29) that in the second order, this term can represent rotational excitations only. Parker considered the relaxation of initially non-rotating molecules for which all the ω_i are zero. In the polyatomic transport theory, for molecular models for which inverse collisions exist, the relaxation time depends (to first order) on the expectation $\langle \Delta E_R^2 \rangle$ over equilibrium distributions of the pre-collision dynamical parameters [53]. An examination of Eq.(27) in the light of Eqs. (37) and (38) then indicates that a first order rotation analysis is sufficient for a study of relaxation phenomena. In particular it turns out that $Z_R \sim \epsilon^{-2}$ times a monotonically increasing function of

temperature. However, for an adaptation of the Parker model suitable for the Direct Simulation method it is necessary to go to second order to include possible rotational de-excitations. This means that a solution to Eq.(14) to give $\dot{\psi}_{i2}(\infty)$ is required. The integral L_1 in Eq.(36) can be evaluated by contour integration (see Appendix E).

5.7 Incomplete Second Order Solution

Equation (14) contains two types of terms; those coupling first and zeroth order quantities and a single term derived from the second order potential. A complete solution to Eq.(14) would involve first a solution of Eqs.(13) for R_1 and ϕ_1 , which would at best be extremely complex and detailed. However, there is good reason to believe that the physical characteristics of a more complete second order solution and in particular a description of rotational de-excitation as well as excitation collisions, are retained if Eq.(14) is approximated by

$$I \ddot{\psi}_{i2} = - \psi_{i1} \left[\frac{\partial^2 V_1}{\partial \psi_i^2} \right]_0 - \left[\frac{\partial V_2}{\partial \psi_i} \right]_0 \quad (39)$$

that is, the R_1 and ϕ_1 terms are neglected. (The $\psi_{j1}(\partial^2 V_1 / \partial \psi_j \partial \psi_i)$ term can be shown to vanish from Eq.(9B).) Such an assumption cannot, of course, be justified a priori since by virtue of the ordering we would expect all terms to be of equal magnitude, but has primarily been introduced to lead to a tractable second order equation. Since Eqs. (12) and (13) for R_1 and ϕ_1 couple the rotational motion of the two particles, we may interpret the use of Eq.(39) for $\ddot{\psi}_{i2}$ as essentially equivalent to assuming that the energy exchange for each molecule depends only on its own rotational motion and not on that of its partner. Note that since the $\overline{\dot{\psi}_{i2}}(\infty)$ term in Eq.(29) is weighted by ω_i , it is probably less important than the $\overline{\dot{\psi}_{i1}^2}(\infty)$ term for rotational excitation collisions which we expect to be much more important

than de-excitation collisions for the leading edge problem (see Section 6.4.1).

Integration of Eq.(39) with respect to time yields

$$\dot{\psi}_{i2}(\infty) = -\frac{1}{I} \int_{-\infty}^{\infty} \psi_{i1} \left(\frac{\partial^2 V_1}{\partial \psi_i^2} \right)_0 dt - \frac{1}{I} \int_{-\infty}^{\infty} \left(\frac{\partial V_2}{\partial \psi_i} \right)_0 dt \quad (40)$$

Consider the second term in Eq.(40). Using Eq.(9C), this term becomes

$$-\int_{-\infty}^{\infty} \left(\frac{\partial V_2}{\partial \psi_i} \right)_0 dt = 2E' \int_{-\infty}^{\infty} e^{-\alpha(R-D)} \sin 2\Gamma_{10} (\cos 2\Gamma_{20} + \frac{1}{3} \cos 2\Gamma_{10}) dt \quad (41)$$

for molecule 1 together with an analogous equation for molecule 2. Here

$$\Gamma_{i0} = \phi_0(t) - \psi_{i0} = \phi_0(t) - \omega_i t - \gamma_i \quad (42)$$

$i=1,2$

Expansion of the trigonometric functions in Eq.(41) using Eq.(42) leads to a series of terms each of which contains trigonometric factors of argument $2n\gamma_i$. Application of operation (28) to Eq.(41) in this form then leads to the result

$$\int_{-\infty}^{\infty} \left(\frac{\partial V_2}{\partial \psi_i} \right)_0 dt = 0 \quad i=1,2 \quad (43)$$

as for the analogous first order term.

With this result we write Eq.(40) for the sake of brevity as

$$\dot{\psi}_{i2}(\infty) = -\frac{1}{I} \int_{-\infty}^{\infty} \psi_{i1} \left(\frac{\partial^2 V_1}{\partial \psi_i^2} \right)_0 dt + V_2 \text{ term} \quad (44)$$

where (43) can be used when we find it convenient to average the whole of Eq.(44) over the $t = 0$ orientation.

We now proceed to develop an approximate analytical expression for $\dot{\psi}_{i2}(\infty)$. Using Eq.(9B) for V_1 , Eq.(44) may be written

$$\dot{\psi}_{i2}(\infty) = \frac{4E'}{I} \int_{-\infty}^{\infty} \psi_{i1}(t) e^{-\alpha(R_0-D)} \cos[2(\phi_0 - \psi_{i0})] dt + V_2 \text{ term.} \quad (45)$$

Equations (17), (31), (34) and (42) may be now used to write this expression in a similar form to Eq.(36) as

$$\dot{\psi}_{i2}(\infty) = \frac{4E'}{I} \left(\frac{\xi}{\beta}\right)^4 \int_{-\infty}^{\infty} \frac{\psi_{i1}(t) \cos(2\delta_1 + 2v_1 t) dt}{[A \cosh(at) - 1]^2} + V_2 \text{ term.} \quad (46)$$

To approximate the integral in Eq.(36), the form of $\psi_{i1}(t)$, at least near $t = 0$, is required. To this end we may write Eq.(35) as

$$\dot{\psi}_{i1}(t) = \frac{2E'}{I} \left(\frac{\xi}{\beta}\right)^4 \int_{-\infty}^t g(u) du. \quad (47)$$

where
$$g(u) = \frac{\sin(2\delta_1 + 2v_1 u)}{[A \cosh(au) - 1]^2}$$

Integration of Eq.(47) with respect to t gives

$$\psi_{i1}(t) = \frac{2E'}{I} \left(\frac{\xi}{\beta}\right)^4 \int_{-\infty}^t \left\{ \int_{-\infty}^x g(u) du \right\} dx. \quad (48)$$

Equation (48) can be integrated by parts, the result being

$$\psi_{i1}(t) = \frac{2E'}{I} \left(\frac{\xi}{\beta}\right)^4 \left\{ t \int_{-\infty}^t g(u) du - \int_{-\infty}^t u g(u) du \right\}. \quad (49)$$

where in the integrated part the limit

$$\lim_{x \rightarrow -\infty} \left[x \int_{-\infty}^x g(u) du \right] \text{ can be shown to vanish.}$$

An approximation to $\psi_{i1}(t)$ near $t = 0$ is

$$\psi_{i1}(t) = \psi_{i1}(0) + \dot{\psi}_{i1}(0)t + O(t^2). \quad (50)$$

which is consistent with Eq.(34). The $\psi_{i1}(0)$ and $\dot{\psi}_{i1}(0)$ can be evaluated from Eqs. (47) and (49) respectively. The results may be written,

$$\psi_{i1}(0) = -\frac{2E'}{I} \left(\frac{\xi}{\beta}\right)^4 \int_{-\infty}^0 \frac{u \sin(2\delta_1 + 2v_1 u) du}{[A \cosh(au) - 1]^2}. \quad (51A)$$

$$\dot{\psi}_{i1}(0) = \frac{2E'}{I} \left(\frac{\xi}{\beta} \right)^4 \int_{-\infty}^0 \frac{\sin(2\delta_i + 2v_i u)}{[A \cosh(au) - 1]^2} du. \quad (51B)$$

Equation (50) may now be substituted into Eq.(46) resulting in an integrable approximation to $\dot{\psi}_{i2}(\infty)$,

$$\dot{\psi}_{i2}(\infty) = \frac{4E'}{I} \left(\frac{\xi}{\beta} \right)^4 \int_{-\infty}^{\infty} \frac{[\psi_{i1}(0) + \dot{\psi}_{i1}(0)t] \cos(2\delta_i + 2v_i t) dt}{[A \cosh(at) - 1]^2} + V_2 \text{ term.} \quad (52)$$

where we have neglected the $O(t^2)$ term.

By expanding the numerator in Eq.(52), one obtains

$$\begin{aligned} \dot{\psi}_{i2}(\infty) = \frac{4E'}{I} \left(\frac{\xi}{\beta} \right)^4 & \left\{ \psi_{i1}(0) \cos(2\delta_i) \int_{-\infty}^{\infty} \frac{\cos(2v_i t) dt}{[A \cosh(at) - 1]^2} \right. \\ & \left. - \dot{\psi}_{i1}(0) \sin(2\delta_i) \int_{-\infty}^{\infty} \frac{t \sin(2v_i t) dt}{[A \cosh(at) - 1]^2} \right\} + V_2 \text{ term.} \end{aligned} \quad (53)$$

where integrals of odd functions of time have vanished. It now remains to average Eq.(53) over the γ_i . This involves the substitution of Eqs. (51) into Eq.(53), the expansion of the trigonometric factors until trigonometric functions of argument $2\gamma_i$ result and finally the application of (28). After considerable manipulation one finally obtains

$$\overline{\dot{\psi}_{i2}(\infty)} = - \left[\frac{2E'}{I} \left(\frac{\xi}{\beta} \right)^4 \right]^2 \int_{-\infty}^{\infty} \frac{\cos(2v_i u) du}{[A \cosh(au) - 1]^2} \cdot \int_{-\infty}^{\infty} \frac{t \sin(2v_i t) dt}{[A \cosh(at) - 1]^2} \quad (54)$$

where of course the V_2 term vanishes by virtue of Eq.(43). Note that the first integral in the above is identical with L_1 in Eq.(36). We denote the second integral in Eq.(43) by L_2 . Both L_1 and L_2 may be evaluated by contour integration. The details are given in Appendix E, the result for L_1 being given by Eq.(E7) and that for L_2 being given by Eq.(E11).

We may now evaluate Eq.(29) to obtain an approximation to the second order energy exchange. Substituting Eqs. (38) and (54) into Eq.(29) for $\overline{\Delta E_{r_i}}$ leads to

$$\overline{\Delta E_{r_i}} = I\epsilon^2 \left[\frac{2E'}{I} \left(\frac{\xi}{\beta} \right)^4 \right]^2 L_1 (L_1/4 + \omega_i L_2) \quad i=1,2. \quad (55)$$

where we have dropped the $O(\epsilon^3)$ notation since our solution is not complete to second order.

The v_i appearing in L_1 and L_2 is given by $v_i = \omega_i - \dot{\phi}_0(0)$ as for Eq.(35). The $\dot{\phi}_0(0)$ can be obtained from Eq.(16) by writing $R(0) \approx \sigma$ as in Section 5.5. Hence

$$v_i \approx \omega_i - g \frac{b}{\sigma^2} \quad (56)$$

Since, as is indicated in Appendix E, $v_i L_1 L_2 < 0$, then the $\omega_i L_1 L_2$ in Eq.(55) will also be generally negative except when the gb/σ^2 term in the above dominates. An order of magnitude analysis indicates that this will be true only for ω_i near zero in which case we should expect $\overline{\Delta E_{r_i}} > 0$, that is an excitation collision. In most other cases $\omega_i L_1 L_2 < 0$ and thus the second term in Eq.(55) may be thought of as representing a "rotational de-excitation" process.

Equation (55) can be nondimensionalized by introducing a reference temperature T , (generally different to T') and by writing

$$\left. \begin{aligned} \hat{\Delta E}_{r_i} &= \overline{\Delta E_{r_i}}/kT \\ \hat{E}_{r_i} &= \frac{1}{2} I \omega_i^2 / kT \end{aligned} \right\} \quad i=1,2 \quad (57)$$

together with $\xi^* = \xi/\beta$, $\frac{1}{2} J_i^2 = \frac{1}{2} I v_i^2 / kT$ and the reduced variables of Section 5.4.

Substituting Eqs. (E7) and (E11) into Eq.(55) and applying (57), the final expression for the post-collision energy of molecule i is

$$\hat{E}'_{r_i} = \hat{E}_{r_i} + \hat{\Delta E}_{r_i} \quad (58)$$

where

$$\Delta \hat{E}_{r_i} = \frac{16\pi^2 \epsilon^2}{\alpha^2 d^2} \left(\frac{T'}{T} \right) Q \left\{ Q \pm (2\hat{E}_{r_i})^{\frac{1}{2}} \left(\frac{8}{\alpha d} \right) \sqrt{\frac{T}{T'}} P \right\} . \quad (59)$$

In Eq.(59), Q and P are given by (Appendix E)

$$Q = \left[\sinh \delta + \frac{\xi^*}{\pi} \Gamma \cosh \delta \right] / \sinh \Gamma \quad (60A)$$

$$P = \left[\cosh \delta (\sinh \Gamma - \Gamma \cosh \Gamma) + \delta \sinh \delta \sinh \Gamma + \frac{1}{\xi^*} (\mu \sinh \Gamma \cosh \delta - \pi \Gamma \sinh \delta) \right] / \sinh^2 \Gamma \quad (60B)$$

The arguments of the hyperbolic functions Γ and δ defined in Appendix E may be expressed in terms of the nondimensional pre-collision parameters as

$$\Gamma = \frac{4}{\alpha d} \sqrt{\frac{T}{T'}} \left(\frac{\pi J_i}{\xi^*} \right) , \quad \delta = \frac{4}{\alpha d} \sqrt{\frac{T}{T'}} \left(\frac{\mu J_i}{\xi^*} \right)$$

where in the above

$$\mu' = \pi/2 + a \tan(1/\xi^*) , \quad \xi^* = g^*(1-b^{*2})^{\frac{1}{2}}$$

and

$$J_i = \pm (2\hat{E}_{r_i})^{\frac{1}{2}} - \frac{4}{\alpha d} \sqrt{\frac{T'}{T}} g^* b^*$$

The $\pm$ signs appear above since we assume that for each molecule the rotational angular momentum points in the same or in the opposite direction as the pair orbital angular momentum with equal probability.

It can be seen that ξ^* becomes imaginary for $b^* > 1$, that is for $b > \sigma$. Lordi and Mates [53] use $b^* = 1$ as a cutoff in the b^* integration of the transport theory expression for Z_R . This was justified by exact numerical trajectory calculations which indicate that the integrated $\langle \Delta \hat{E}_T^2 \rangle$ for $b^* > 1$ is small resulting in a finite cross section for energy exchange. Hence we also choose $b^* = 1$ as an inelastic cutoff, those collisions for $b^* > 1$ being considered elastic. It is in fact possible to regard Eq.(59) as an inner solution for $\Delta \hat{E}_{r_i}$ and to develop an outer solution for $b^* > 1$ based on a straight line $R_0(t)$ approximation in place of Eq.(31) but this does not seem worthwhile.

5.8 Application of the Model to the Direct Simulation Method

The Direct Simulation procedure for the calculation of collisions was given in Section 4.3 and in Appendix A. From Eqs. (A6) and (A9) it can be seen that both the conditional collision probability p and the time counter Δt_k depend explicitly on the impact parameter cutoff b_0 or its nondimensional equivalent b_0^* . An implicit assumption in the analysis of Appendix A was that b_0^* could be chosen independently of the particle interval co-ordinates Ω_i . Since we will choose $b_0^* > 1$ and since $b^* = 1$ is an inelastic cutoff, then for the present model this assumption is reasonable. We may then refer to $b_0^*(g^*)$ as an elastic cutoff which can be determined from the zeroth order problem. For more complex polyatomic collision models which might involve strong inelastic coupling at large b^* , an overall cutoff of the form $b_0^* = b_0^*(g^*, \Omega_i)$ may be required.*

We further assume that even for $b^* < 1$, we may approximate $\chi \simeq \chi_0$ where χ_0 is given by Eq. (21), that is, inelastic trajectory corrections may be ignored. We justify this assumption by stating without proof that from a detailed analysis of Eqs. (13), it may be shown that $\overline{\phi_1(\infty)}$ (which represents first order χ corrections) vanishes as does $\overline{\psi_{i1}(\infty)}$ and that corrections first appear in the second order. This is consistent with observations made in Refs. [53] and [54] to the effect that in exact numerical calculations variations in Ω_i had little effect on χ except at low collision energies.

Thus in the present model inelasticity only affects collisions through the introduction of energy transfer superimposed on an otherwise spherical scattering process.

*For the loaded sphere model, because of the wobbling motion due to the mass asymmetry $p = p(g, \Omega_i)$. This also appears to be the case for most of the impulsive collision models and is the property that limits their use in the Direct Simulation method.

Once a set of pre-collision parameters g , E_{r_i} , and b have been selected (in appropriate non-dimensional form g^* , $\hat{E}_{r_i}$, etc.) as specified in Section 4.3 and in Appendix A, the calculation of the post-collision dynamical parameters proceeds as follows.

1. Calculate the post-collision rotational energy of each particle using Eqs. (58), (59) and (60) and also the deflection angle χ_0 from a table lookup as shown in the next section.

2. Determine the post-collision relative speed g' from the conservation of total energy as given by Eq.(B1.16) of Appendix B1, which we write here as

$$g'/g = \left\{ 1 - \frac{2kT}{\mu g^2} (\hat{\Delta E}_{r_1} + \hat{\Delta E}_{r_2}) \right\}^{\frac{1}{2}} \quad (61)$$

3. Calculate the post-collision particle velocities $\underline{c}_1'$ and $\underline{c}_2'$ in the laboratory framework, as shown in Appendix B2.

In certain situations it was found that the above scheme led to imaginary values of g'/g as given by Eq.(61) implying that rather too much energy had been transferred in a rotational excitation collision. Such anomalies occurred in a small number of collisions at very low translational energy for which it is likely that the various model approximations used in Sections 5.5-5.7 are least valid. For such cases g was set to zero and the available rotational energy divided between the two particles in the ratio of their calculated rotational energy.

5.8.1 Deflection Angle χ_0

Before presenting results for χ_0 and associated quantities, it is necessary to specify numerical values of the potential parameters employed. For Nitrogen these were taken as $\alpha = 4.02 \text{ \AA}^{-1}$, $\sigma = 3.681 \text{ \AA}$, $d' = 0.557 \text{ \AA}$ and $T' = 91.5^\circ\text{K}$, for which $\epsilon = 0.259$. Reasons for the above choice are given in Appendix C. The value of d is that quoted by Parker [64], $d = 1.094 \text{ \AA}$.

Lordi and Mates [53] consider that using a value of d' less than d is an effective means of averaging over molecular orientations precluded by the planar rotation assumption. For full three-dimensional orientations, a rather larger value of d' is necessary [54].

Convenient forms for the Lennard-Jones 6-12 potential V_{L-J} and for V_0 in matching form are given in Eqs. (10) and (C12). For the above parameters $a' = a\sigma$ in Eq. (10) has the value $a' = 14.80$. Figure 3A shows V_{L-J}/E' and V_0/E' versus R^* .

In the present work χ_0 was computed by numerical quadrature of Eq. (21) for $a = 14.80$. Figure 3B shows χ_0 plotted against b^{*2} for various values of g^{*2} . The negative χ_0 at large b^{*2} are due to the long range attractive force as of course are the singularities in χ_0 shown for $g^{*2} =$

1.0 and 0.4. For the exact inelastic problem, negative χ and mutual orbiting may also occur at low collision energies although as has been previously stated, in this range of g^* , there may be appreciable E_r dependence of the exact χ , not included in the present model. It can be seen from Fig. 3B that the effect of the attractive part of the potential diminishes rapidly for collision energies $\frac{1}{2}\mu g^{*2} > kT'$.

For the present calculations a table of values of χ_0 was stored in a two-dimensional array with equal increments in g^* and b^{*2} , i.e.*

$$\chi_{\ell,j} = \chi_0(g_{\ell}^*, b_j^{*2}) \quad \begin{matrix} \ell = 1 \dots L \\ j = 1 \dots J \end{matrix} \quad (62)$$

*The appearance of an absolute velocity scale in the functional dependence of χ_0 through $g^{*2} = mg^2/4kT'$ will mean that any other velocity scale introduced for convenience in simulation as in Appendix A must also be absolutely specified. For inverse power models, no such absolute scales are required. Furthermore, for these models χ_0 can be expressed as a function of a single parameter and may thus be tabulated as a one-dimensional array, resulting in a substantial core storage saving. We accept the disadvantages of the Parker potential in the above respects in the interests of utilizing a realistic collision model.

where $\hat{b}_j^{*2} = b_j^{*2}/b_0^{*2}(g_\ell^*)$. In simulation, for any g^*, b^{*2} , χ was determined by a simple 4-point interpolation formula.

5.8.2 Model Cutoff (Elastic)

The elastic cutoff $b_0^*(g_\ell^*)$ was determined from the conditions

$$\left. \begin{aligned} | \chi_{\ell,J} | &\leq \delta'(1-\delta'g_\ell^*), & g_\ell^* < 2 \\ | \chi_{\ell,J} | &\leq \delta'/g_\ell^* & \text{for } \ell \text{ such that } g_\ell^* > 2 \end{aligned} \right\} \quad (63)$$

which are applied in the range of negative increasing χ (see Fig.3B).

The parameter δ was chosen arbitrarily as $\delta' = 0.25$ in the belief that deflection angles smaller than those given by (63) contribute little to the transport properties. In computing the χ table and in the interpolation procedure, χ_0 singularities for $g^* < g_c^*$ were ignored which should cause little overall error in simulation. The g_1^* and g_L^* are prechosen estimates of the maximum and minimum relative speeds likely to be of physical importance for the particular problem being simulated. Values of the above parameters used for the present calculations were $L = 150$, $J = 100$, $g_1^* = 0.01$, $g_L^* = 10$. Figure 3C shows the effective collision cross section πb_0^{*2} and the cutoff value of $|\chi_0|$ as functions of g^* . These were obtained using Eq.(21) together with condition (63) above. The increase in πb_0^{*2} with decreasing g^* is due to the long range attractive part of V_0 .

Figure 3D shows the conditional collision probability $p = g^* b_0^{*2} / [g^* b_0^{*2}]_{\text{MAX}}$ for the present model with the above cutoff compared with the equivalent quantity for inverse power potentials of the form $V \sim R^{-\alpha}$. The cutoff for finite α for the inverse power models is $\chi_{\min} = \text{Const.}$, which leads to

$$p = (g^*/g_{\max}^*)^{(\alpha-4)/(\alpha-1)}$$

Figure 3D indicates that the present model is weighted to high collision energies compared with the well known result for inverse fourth power molecules

(Maxwell molecules) where p is independent of relative speed. It should be emphasized here that the g^* dependence of p depends entirely on the choice of a cutoff condition. We could for example in lieu of (63) define a cutoff in b^*-g^* space such that $p = \text{const}$, as for the Maxwell molecules. This would mean, however, the calculation of large numbers of collisions at low g^* and high b^* for which the set of post-collision dynamical parameters would differ negligibly from the pre-collision set.

5.9 Mean Free Path

For the sake of completeness the reduced collision integrals [39] $Q^{(2)*}(g^*)$ and $\Omega^{(2,2)*}(T/T')$ have also been calculated for the Morse potential and are shown graphically in Figs. 4A and 4B respectively compared with equivalent quantities [58] for the Lennard-Jones potential. The details of these calculations are given in Appendix F of the present work. We shall make use of both the above quantities in later sections. The $\Omega^{(2,2)*}$ appears in the monatomic transport theory where the first approximation for the viscosity $\eta(T)$ of a gas of spherical molecules is given by [39]

$$\eta(T) = \frac{5(\pi m k T)^{\frac{1}{2}}}{16\pi\sigma^2\Omega^{(2,2)*}(T/T')} \quad (64)$$

The monatomic transport theory has been successful in predicting the viscosity of many diatomic gases since, in the polyatomic theory η does not appear to depend strongly on internal energy [56] at least at moderate and high temperatures. For the above set of parameters, $\eta(T)$ for nitrogen given by Eq.(64) for the Morse potential, is shown in Fig.5 compared with the Lennard-Jones prediction [39]. At moderate and high temperatures the Morse result agrees quite well with the Lennard-Jones curve.

It is convenient to define here, for future reference, a nominal mean

free path based on viscosity in the usual way [79] as

$$\eta(T) = \frac{5\pi}{32} m n \bar{c} \lambda(T) \quad (65)$$

where $\bar{c} = (8kT/\pi m)^{1/2}$ is the mean speed in a Maxwellian gas. Using Eq.(64) for $\eta(T)$, Eq.(65) reduces to

$$\lambda(T) = \frac{1}{\sqrt{2} \pi \sigma^2 n \Omega^{(2,2)*}(T/T')} \quad (66)$$

at temperature T and number density n for a stationary gas in thermal equilibrium.

It should be emphasized that the above is not the actual mean free path experienced by molecules obeying the present collision model. By using simple kinetic theory this can be shown to be

$$\lambda_{\text{act}}(T) = \frac{1}{\sqrt{2} \pi \sigma^2 n I^*(T/T')} \quad (67)$$

$$\text{where } I^* = \frac{2}{(T/T')^2} \int_0^\infty g^{*3} b_0^{*2}(g^*) e^{-g^{*2}/(T/T')} dg^* .$$

The actual mean free path, of course, depends entirely on the choice of a cutoff. For hard spheres of radius σ , $b_0^{*2} = 1$, for which $\Omega^{(2,2)*} = I^* = 1$. Hence Eq.(66) and Eq.(67) agree which is a well known result for this model. The above is aimed at emphasizing the sense in which Eq.(66) represents a nominal mean free path independent of any cutoff.

5.10 Rotational Relaxation Test

The collision model was tested by simulating the rotational relaxation of Nitrogen. An ensemble of $N_0 = 2000$ particles was set up each with speed $(3kT_0/m)^{1/2}$ where T_0 is the initial translational temperature. The directions of the velocity vectors were distributed uniformly on the unit sphere. The initial rotational energy of each particle was set to zero, that is,

the rotational temperature of the ensemble is initially zero. No space-coordinates are assigned to the particles which may be regarded as representing a homogeneous isotropic mass of gas. Thus each of the $\frac{1}{2}N_0(N_0-1)$ particle pairs represents a possible collision pair in the collision calculation procedure. Time was normalized by the equilibrium mean free time at temperature T_0 , that is

$$\hat{t} = t \bar{c} / \lambda(T_0)$$

where $\bar{c} = (8kT_0/\pi m)^{1/2}$ and $\lambda(T_0)$ is given by Eq.(66). The time increment per collision for this case is given by Eq.(A11) for which the clarifying remarks made in Appendix A should be noted.

The simulation was initiated at $\hat{t} = 0$ by allowing the N_0 molecules to collide amongst themselves. Since we require two rotational degrees of freedom, it is to be expected that as $\hat{t} \rightarrow \infty$, the system should approach equilibrium with equipartition of energy at $T_{eq} = T = T_R = 0.6T_0$, and with Maxwellian speed and energy distributions.

Figures 6A and 6B show T_R/T_0 and T/T_0 (T here being the translational temperature at $\hat{t}$) versus $\hat{t}$ for relaxation from $T_0 = 500^\circ\text{K}$ and also from $T_0 = 1000^\circ\text{K}$. Although a steady state condition is reached at large $\hat{t}$, proper equipartition of energy is not achieved, T_R being rather lower than T . This effect can be attributed largely to the planar rotation assumption which evidently limits the mean rotational energy per molecule to less than kT_{eq} at "equilibrium". To alleviate the behaviour indicated in Fig.6A, it is necessary to weight the energy transfer more towards rotational excitation collisions* without substantially altering the relaxation rate.

To achieve this we introduce two ad-hoc modifications described below into the collision calculation procedure. The meaning and effect of these

* This cannot be achieved by altering c since this would merely influence $Z_R(T)$

modifications are subsequently discussed and improved ones for future use are suggested.

1. Collisions may be weighted towards excitation encounters by replacing the $\hat{E}_{R_i}$ argument in Eqs.(59) and (60) for $\hat{\Delta E}_{R_i}$ by $\lambda' \hat{E}_{R_i}$ where λ' is an arbitrary parameter. Hence

$$\hat{\Delta E}_{R_i}(g^*, b^*, \hat{E}_{R_i}) \rightarrow \hat{\Delta E}_R(g^*, b^*, \lambda' \hat{E}_{R_i})$$

By varying λ' near unity it was possible to modify the steady-state conditions of the simulation, without, as will presently be argued, altering the relaxation behaviour in terms of Z_R . The form of the functional dependence of $\hat{\Delta E}_{R_i}$ on the pre-collision dynamical parameters is largely preserved. Through trial and error it was found that the choice $\lambda' = 0.75$ improved the steady-state behaviour shown in Fig.6A to that in Fig.6B where for $T_0 = 500^\circ\text{K}$ and 1000°K , equipartition is very nearly achieved. Similar behaviour was obtained for $T_0 = 1500^\circ\text{K}$ and $T_0 = 2000^\circ\text{K}$. However, for the $T_0 = 200^\circ\text{K}$ curve shown in Fig.6B, there is a considerable overshoot of T_R which was generally the case when T_{eq} was of order T' . This effect, which also occurred for $\lambda' = 1$ (although it was less marked) probably arises because at low collision energies, the approximations used in the analysis leading to $\hat{\Delta E}_{R_i}$ are inaccurate [e.g. Eq.(31) for $R_0(t)$] or alternatively, because of strong rotational-translational coupling at low temperatures, the perturbation expansion fails to converge.

2. Thus the second ad-hoc modification was to introduce an elastic collision probability P_{el} such that $P_{el} = 0$ (inelastic collision) if the calculated $\hat{\Delta E}_{R_i}$ drives the collision pair towards a state of two-particle rotational-translational energy equipartition and $P_{el} = 1$ (elastic collision) otherwise.

Both of the above strategies are introduced primarily to drive the gas into a state of energy equipartition near equilibrium. Both should

have little effect on the averaged (macroscopic) energy transfer far from equilibrium and therefore should not greatly influence the results obtained in the present leading edge calculations since for the most part, the flow is highly nonequilibrium. However, in that they are artificial, they are somewhat unsatisfactory.

Figure 6C shows histogram estimates of the large $\hat{t}$ distributions of molecular speed and rotational energy for $T_0 = 500^\circ\text{K}$. The speed distribution is close to the equilibrium curve, but the E_r distribution is far from correct. This behaviour can be attributed to the loss, due to the assumptions and approximations used in the present model, of the reverse collision property retained by the fully 3-dimensional equations of motion. This property is necessary and sufficient to satisfy the principle of detailed balance at equilibrium [22] and, of course, is the fundamental reason for the generally poor behaviour of the model near equilibrium.

The model nevertheless retains an approximately correct description of $Z_R(T)$. The phenomenological equation commonly used to describe relaxation is given by

$$\frac{dT_R}{d\hat{t}} = \frac{T - T_R}{Z_R} \quad (68)$$

Interpreting this equation for individual binary collisions, estimates of Z_R were obtained by summing over the first N collisions such that $\sum_N \hat{\Delta t}_n > 1$ where $\hat{\Delta t}_n$ is the time increment for the n^{th} collision. An estimate of Z_R is then

$$Z_R \approx \frac{\sum_{n=1}^N (E_t - E_r)_n}{\sum_{n=1}^N \Delta E_R / \hat{\Delta t}_n} \quad (69)$$

where $E_r = E_{r_1} + E_{r_2}$ and $E_t = mg_n^2/4$. The results are shown in Fig. 6D where they may be seen to agree reasonably with the analytic results and with the data. Since the rotational modes were initially unexcited, Eq. (69) may be interpreted as the Monte-Carlo analog of Parker's analysis.

Note that the modifications given above have no effect on Eq.(69) since if $E_{r_i} = 0$ initially, ΔE_{r_i} is independent of λ' and all encounters are excitation collisions. Hence Parker's value of ϵ may be used.

It is useful here to list the assumptions and approximations used in the development of the collision model.

1. Assumption of planar rotation.
2. Mathematical approximations used to solve the perturbation equations.
3. Neglect of certain terms in solving the second order equations.
4. Ad-hoc modifications given above.

The phenomenological models are constructed in such a way that an ensemble of particles is driven into local equilibrium, at the expense of a rather gross representation of the energy transfer process. The idea behind the present approach was to start from the nonequilibrium limit and to formulate a model which drained energy from transitional modes in collisions at the correct rate while at the same time retaining a microscopic description of the energy exchange. Perhaps the most satisfactory approach would be to combine approximate classical models such as the present one with one or other of the phenomenological models. For example, modifications (1) and (2) above could be replaced by the following strategy.

(1) If the calculated $\hat{\Delta E}_{r_i}$ for each particle drives the pair towards two-particle energy equipartition, then proceed as in Section 5.8.

(2) If not, calculate the post-collision dynamical parameters using, say, the statistical model of Ref.[18]. This technique would then retain the advantages of both the classical and relaxation treatments.

6. NUMERICAL CALCULATIONS

We now describe the present Direct Simulation calculations of the hypersonic flow past sharp edged two-dimensional flat plates. For these calculations a FORTRAN IV programme embodying the Direct Simulation method with the present form of the Parker collision model was written to treat the flow about any two-dimensional body composed of straight line segments. This programme — which is not included in the present dissertation — was modelled on a Direct Simulation method programme described in Ref.[71], but has been designed for a somewhat different task.

What follows is a fairly detailed description of the present calculations in which the flow properties obtained are compared to a range of experimental data. A summary of the principal results of the present investigation, including a description of a physical picture of the leading edge flow, is given in Section 6.7.

6.1 Description of the Calculations

The calculations were performed for a number of two-dimensional flat plates for various flow conditions. These are summarized in Table I together with other relevant information including parameters specifying the principal features of body geometry. For a diatomic gas using the Parker collision model, the case for $M_\infty = 10.15$ matches the experimental conditions of Becker and Boylan [3] for air. The $M_\infty \approx 23$ conditions match closely those used by Jeffery [46] in recent experiments at Imperial College while the $M_\infty = 25$ case matches the nitrogen experiments of Lewis [51]. A single calculation at $M_\infty = 21$ using only the spherical part of the Parker potential was performed to study the effects of diatomicity on the flow structure.

Figure 7 shows a typical simulation configuration for the flat plate flow and also includes a body configuration for the forward facing step flat plate combination. A set of body fixed reference axes x - y have their origin at the body leading edge with the x axis aligned with the top surface of the plate. Each body was of finite length L and had a sharp leading edge with either a 10° or 0° undersurface angle. The free stream flow at M_∞ is in the positive x direction. The boundary of the simulated region was tailored to contain the leading edge flow disturbance, particularly forward propagation effects from both the upper surface and the wedge-like part of the lower surface insofar as this may affect the flow for $y > 0$. We regard this as important since experimental models have a finite undersurface angle, generally about 10° .

The incident boundary condition along each γ_i , $i = 1, 5$, was taken to be free molecule flow of the free stream. This will be incorrect along much of γ_3 and γ_4 but because of the high M_∞ , this should have little effect on most of the flow field and practically none on the flow near the plate. As can be seen from Table I, the nominal free stream temperatures — which must be specified for the present collision model — are very low and, for the high M_∞ cases, T_∞ is below the condensation point for N_2 , even at the rarefied experimental pressures employed. However, each experimenter considered that condensation had not occurred and that the free stream could be taken to be in translational-rotational equilibrium at T_∞ .

The gas surface interaction law is taken to be completely diffuse with complete energy accommodation for both translational and rotational modes, that is $p_j = \alpha_j = 1$ for all surface segments $j = 1, J$. Lewis [51] has suggested that the rotational modes may not be fully accommodated but in the absence of qualitative experimental values for α_j for rotation, we shall take it to be unity.

Since the Direct Simulation method should perhaps be most appropriately regarded as a "numerical experiment", the flow quantities obtained will

generally be presented graphically in the form of experimental data, each point representing a "measurement". No attempt at a serious assessment of statistical errors will be made apart from that given earlier in Section 4.7. In this respect it is worth repeating here that for estimates of surface and flow field properties, the minimum sample size was of the order 10^3 in the smallest cells. In larger cells or in regions of high density the sample was often of order $3-4 \times 10^3$ or higher. Perhaps the best idea of statistical scatter is obtained by observing fluctuations about a line of best fit drawn, say, through a set of points representing a flow property profile.

A short discussion relating to the choice of cell size Δt_m and the simulator particle number density is given in Appendix G.

6.2 Length and Time Scales

In the simulation, the unit of length was taken to be $\lambda(T_\infty)$ defined by Eq. (66). Hence

$$\lambda_\infty = \frac{1}{\sqrt{2} \pi \sigma^2 n_\infty \Omega^{(2,2)*}(T_\infty/T')} \quad (70)$$

where n_∞ is the real gas free stream number density. The units of velocity and time were taken to be $a_\infty = \sqrt{\gamma R T_\infty}$ and λ_∞/a_∞ respectively. For nondimensional quantities in these units we write

$$\left. \begin{aligned} \hat{x} &= x/\lambda_\infty, & \hat{y} &= y/\lambda_\infty \\ \hat{t} &= t \frac{a_\infty}{\lambda_\infty}, & \hat{V} &= V/a_\infty \end{aligned} \right\} \quad (71)$$

The expression for $\hat{\Delta t}_k$ scaled in the above units is given in Appendix A. The sense in which λ_∞ represents a purely nominal mean free path has been previously discussed. As can be seen from Fig. 4B, at low T_∞ , $\Omega^{(2,2)*}$ and hence λ_∞ is very sensitive to the molecular model. For this reason

λ_∞ should really be thought of as essentially a convenient length scale for simulation, related to the molecular model and in particular the molecular diameter σ . For each calculation $\Omega^{(2,2)*}(T_\infty/T')$ is determined from Fig.4B for the Morse potential.

More clearly defined length scales which have become widely used in hypersonic flow studies are the free paths λ_{fb} and λ_{bf} defined in the notation. The most general definitions of these quantities for a flat plate flow are [31]

$$\lambda_{fb} = \frac{\sqrt{T_w/T_\infty}}{n_\infty A_{fb}(g)} \quad (72)$$

$$\lambda_{bf} = \lambda_{fb}/S_\infty \quad (73)$$

where $S_\infty = \sqrt{\frac{\gamma}{2}} M_\infty$ is the speed ratio and $A_{fb}(g)$ a collision cross section for body-free stream particle collisions at relative speed g . A variety of definitions of A_{fb} have been used in the above. We shall use the general definition

$$A_{fb} = \pi \sigma^2 Q^{(2)*}(g^*) \quad (74)$$

We choose $Q^{(2)*}$ given by the Morse potential at values of g^* for collisions between free stream particles with velocity components $(U_\infty, 0, 0)$ and body particles with velocity components $(0, \bar{c}_b, 0)$ where $\bar{c}_b = \left(\frac{8}{\pi} RT_w\right)^{1/2}$. Then

$$g^{*2} = \frac{\gamma M_\infty^2}{4} \left(\frac{T_\infty}{T'}\right) + \frac{2}{\pi} (T_w/T') \quad (75)$$

where for cold walls ($T_w \ll T_0$), the second term is negligible compared with the first. Note from Fig.4A that at high g^* , $Q^{(2)*}$ is not very sensitive to molecular model and we could have easily chosen the Lennard-Jones value, or even the hard sphere value together with a slightly different value of σ .

Note that while λ_∞ refers to a reference framework moving with the free stream, λ_{fb} and λ_{bf} are defined in a body fixed framework. In the kinetic regime x/λ_{fb} and y/λ_{bf} represent scale parameters in the x and y directions

respectively [51].

6.3 Leading Edge Flows

The development of the flow in the kinetic regime near the leading edge in a hypersonic stream was qualitatively described in Section 3.1. Recall that emphasis was placed on the collisional interaction between free stream and body particles as the phenomenon which precipitates the rapid deceleration of the flow adjacent to the plate leading to the subsequent evolution of the kinetic layer. To appreciate the following discussion and interpretation of the present calculations of the surface and flow properties, it is perhaps helpful to reiterate here that the qualitative effect of first collisions is to produce particles with increased random or thermal motion at the expense of the highly directed momentum and energy of the free stream. In particular the y component of random motion will be greatly enhanced and since all surface properties involve a V_y moment of the distribution function at the wall, rapid changes in these quantities may be expected immediately downstream of the leading edge.

Since we are interested in the development of the kinetic flow away from a collisionless free-molecule flow, this limit represents a relevant point of reference for the present calculations. Table II shows free molecule values of the surface properties and also of the flow field properties immediately adjacent to the surface in nondimensional form for the various flow conditions. These were evaluated using Eqs. (H5)-(H12) of Appendix G for the free-molecule distribution function given by Eqs. (H1)-(H3).

6.4 Surface Properties

The surface properties obtained were the number flux N to the plate surface, the normal component of the pressure tensor at the surface P_{yy} henceforth referred to as the normal or surface pressure P_n , and the heat transfer $\dot{q}_w$ and skin friction τ_w at the wall. In the following text and in the figures these quantities will be presented in various nondimensional forms defined where convenient.

It is desirable that we test the present programme against previously published results. This is necessary since experience indicates that because of the inherent stability of the Direct Simulation method, a minor programming error can lead to quite plausible but erroneous results. Figure 9 shows P_n/P_{fm} against x/λ_∞ at $M_\infty = 12.9$ for a hard sphere monatomic gas compared with the similar calculations of Vogenitz et al. [80]. For a hard sphere of diameter σ , Eq.(21) is simply replaced by [39]

$$\chi(g,b) = 2 \arccos(b^*) \quad (76)$$

with $b_0^* = 1$. All collisions, of course, are elastic. As can be seen, the present calculations agree closely with those of Ref.[80]. The slight discrepancies may be attributed to the effects of cell size, Δt_m , etc. Other surface and flow field properties obtained also agree closely with those of Ref.[80]. Note that for hard spheres $\Omega^{(2,2)*} = 1$ in Eq.(70) for λ_∞ .

6.4.1 Incident Number Flux

Figure 10 shows the number flux N/N_{fm} , incident* to the plate surface for various conditions and different molecular models, plotted against x/λ_∞ . All of the curves show common characteristics. In each case the actual

* N_{fm} , P_{fm} represent free molecule values of number flux and normal pressure.

leading edge limit is somewhat obscured by statistical scatter and cell size effects, but it appears to be rather above the free molecular value. Immediately downstream of the leading edge the flux rises sharply to a maximum followed by a relatively gentle decline. Comparing the curves for a monatomic gas at high ($M_\infty = 21, 22.6$) and moderate ($M_\infty = 12.9$) Mach numbers indicates that the peak flux shows significant Mach number dependence. This seems reasonable in that N_{fm} is proportional to $\sqrt{T_\infty}$ while the energy available for conversion to thermal motion in initial collisions would depend strongly on the directed free stream energy density $\frac{1}{2}\rho_\infty a_\infty^2 M_\infty^2$.

The curves for N_2 at $M_\infty = 22.93$ and "monatomic N_2 " at $M_\infty = 21$ are for the same speed ratio $S_\infty \approx 19.2$, and illustrate the calculated effect of the internal degrees of freedom on the number flux.

The substantial difference in the peak flux may be ascribed to the fact that the rotational degrees of freedom of the diatomic gas absorb energy in initial high energy collisions near the leading edge. This essentially depletes the collision products of thermal energy thereby decreasing the local flux of molecular properties (including number) to the plate surface in comparison with the monatomic flow. Note that since the initial relative velocity vector in first collisions will very nearly point in the x-direction, then the correlation between inelastic energy exchange and the deflection angle in collisions [through the functional dependence of χ_0 and $\hat{\Delta E}_{r_i}$ on b in Eqs. (21) and (59)] can have a considerable effect on the y-component of the thermal motion of collision products and hence on the initial rise in the surface properties. The physics of the exchange process can thus be important in the kinetic regime of the flat plate flow.

The differences between the present monatomic calculation at $M_\infty = 21$ and those of Ref.[81] at $M_\infty = 22.6$ can be partly attributed to the M_∞ effect described above and partly to the effects of the different collision models employed.

Figure 11 shows N/N_{fm} plotted against x/λ_{fb} compared with Lewis's [51]* experimental data. The data represented by the hatching was obtained by measuring P_c in sharp lipped near free-molecular cavities in the model surface. The filled symbols represent data obtained by Lewis [51] by converting tube measured pressures from other experiments [32] into equivalent cavity pressures using a theory due to Hughes and De Leeuw [45]. It can be seen that the present calculations far exceed the data near the leading edge, although the discrepancy decreases further downstream. In particular, the present calculations indicate that the free molecular limit is not reached at the leading edge in contrast to the experimental trend.

In Fig.12 N/N_{fm} for the $M_\infty = 10.15$ case is shown compared to an envelope of the experimental results of Horstman [41]. Here the agreement is much better and in fact can be improved very near the leading edge by plotting data and theory against x/λ_{fb} . The present case for $M_\infty = 10.15$ was an early calculation and it is possible that the cell size used was rather too coarse near the leading edge. This may explain why the peak flux appears to exceed the experimental value at somewhat higher M_∞ .

Comparing Figs 11 and 12, it is peculiar that Lewis obtains about the same peak value $N/N_{fm} \simeq 2.8$ as that obtained by Horstman at much lower M_∞ , in contrast to the M_∞ dependence of the peak flux predicted by the calculation for monatomic and diatomic gases.

An analysis of the incident number flux for the $M_\infty = 25$ case using a scheme employed recently by Vogenitz and Takata [81] is presented in Fig.13.

* Lewis defines λ_{fb} in a formally similar manner to Eqs. (72) and (73) but employs a slightly different value of σ for a Lennard-Jones potential and in addition chooses $Q^{(2)*} = 1$. The present λ_{fb} can be related to Lewis's values roughly by $\lambda_{fb} = 1.3(\lambda_{fb})_{LEWIS}$ which has been used for converting experimental data.

Each molecule is labeled according to its collision history. Class I molecules are free stream particles which have not collided with any particle previously affected by the body. Class II particles have been reflected by the body while class III particles have been indirectly affected through collisions. Class I or III particles transfer to class II on surface reflection while class I particles become class III on collision with either class II or III particles. Once in class II molecules remain there. The flux of class I particles to the surface represents the effect of direct free molecular convection which may be seen to have vanished for $x/\lambda_{fb} \geq 0.8$. The combined flux of class II (scattered back to the surface) and class III molecules appears to be comparable with the free molecular flux even as $x/\lambda_{fb} \rightarrow 0$.

Since most particles which strike the surface near $x = 0$ do so with a positive x -velocity component (see Fig.27B together with discussion in Section 6.5.3) then it follows that the collisions producing them must occur upstream of the leading edge. We may then attribute the departure from a free molecule dominated leading edge flow to the effects of forward reflection from the leading edge and underside surface which leads to an appreciable collisional disturbance upstream of $x = 0$.

6.4.2 Surface Pressure

The effect of internal energy on P_n/P_{fm} is illustrated in Fig.14 where the peak pressure for the diatomic gas is about 25% below the monatomic peak. As for the number flux, the excitation of rotational energy modes is responsible for the lower pressures in the diatomic gas. The effect is somewhat larger for the surface pressure since this quantity has incident and reflected parts involving a V_y^2 moment of the distribution function whereas the flux involves only a V_y moment over the $V_y < 0$ half space.

In Figs. 15 and 16 P_n/P_{fm} is shown plotted against x/λ_∞ and x/λ_{fb}

respectively for the three high M_∞ cases. Both figures indicate that the behaviour of the normal pressure is qualitatively similar to the number flux. As $x \rightarrow 0$, P_n appears to be somewhat above the free molecular limit and both pressure and flux maximize at $x/\lambda_{fb} \approx 1.5$, thereafter decreasing further downstream presumably towards the continuum limit. As for the flux, that $P_n/P_{fm} > 1$ as $x \rightarrow 0$ may be attributed to collisional disturbance effects forward of the leading edge.

Lewis [51] finds that x/λ_{fb} provides a good scale parameter for the correlation of experimental surface properties over a wide range of T_w . Comparison of Figs. 15 and 16 indicates that the x/λ_{fb} plot does not provide a clearly superior correlation of the calculated pressure. However, Table I shows that while the relative scale changes $\lambda_\infty/\lambda_{fb}$ for the cases is significant, it is perhaps not large enough to distinguish systematic from statistical variations in P_n/P_{fm} near the leading edge. In this respect it would have been preferable to perform the high M_∞ calculations over a somewhat larger range of wall temperature.

Nevertheless, for $x/\lambda_{fb} \geq 1.0$ it is fair to say that a definite systematic wall temperature effect on P_n/P_{fm} is evident in the x/λ_{fb} plot and this is also the case in Fig. 11 for N/N_{fm} . This would be consistent with the conclusion that first collisions between free stream and body particles attenuate at about $x/\lambda_{fb} \approx 1$ due to mutual shielding by the developing secondary, tertiary, etc., collision products. The parameter λ_{fb} would then lose its physical significance in what is probably the beginnings of transition to a merged layer flow and the near surface flow could thus be expected to be strongly influenced by the properties of body reflected particles. This conclusion is supported by the free molecule flux curve (class I) in Fig. 13. Further evidence is presented in the remaining text. Both the N/N_{fm} and P_n/P_{fm} peaks occur at about $x/\lambda_{fb} = 1.5$ and this is probably the point at which the random or

thermal motion of the collision products saturates [51] marking the definite onset of transition.

In addition to the calculations listed in Table I, two more were performed for short plates of length $39\lambda_\infty$ and $50\lambda_\infty$ respectively. The first of these was to test for the influence of cell size and particularly simulator particle density on the calculated properties. Figure 17A shows P_n/P_{fm} for two cases at the same flow conditions, but for the shorter plate, the number density is more than double that for the longer plate. Any effect on the pressure can be seen to be within the statistical scatter of either set of points. Other surface and flow properties also showed negligible differences for the two cases. The pressure drop for the shorter plate near $x/\lambda_\infty \approx 40$ is a trailing edge effect.

The $L = 50\lambda_\infty$ calculation was performed for a plate with a $\theta = 0^\circ$ leading edge angle to investigate the influence of forward reflection from the undersurface angle in the $\theta = 10^\circ$ calculations. The effect on P_n/P_{fm} is shown in Fig. 17B. As $x/\lambda_\infty \rightarrow 0$, the pressure for the $\theta = 0^\circ$ case is discernably closer to (but appears to be still above) the free molecular limit than for the $\theta = 10^\circ$ case. Otherwise the effect is fairly small and decreases relatively with increasing x/λ_∞ as the flow becomes more collision dominated. Nevertheless, we should qualify earlier conclusions drawn relating to the influence of collision products created upstream of the leading edge on the surface (and flow field) properties near $x = 0$ by noting that the effect is partly due to forward reflection from the finite undersurface wedge angle. Since all experimental models have a finite leading edge angle this will only have bearing on comparison of the present results with data when this angle is not equal to 10° .

Comparison with Experiment

Comparison of the calculated normal pressure with experiment is somewhat complicated by the fact that the pressure P_c measured in tubular orifices or in sharp lipped cavities in the model surface is not generally equal to P_n . This is because of the nonequilibrium nature of the near surface flow and the resulting nonisotropy (to first order) of the pressure tensor. Various correction methods [76] have thus been devised to enable P_n to be estimated from P_c .

Harbour and Bienkowski [33], and also Lewis [51], have employed schemes in which the flow adjacent to the wall is modelled by a two stream two sided model for the distribution function. For a diffuse completely accommodating surface (as assumed by Lewis), the reflected stream is a half Maxwellian at T_w while the incident stream is characterized by parameters which can be determined from measured quantities. The application of the model to a number flux balance at the entrance plane of near free-molecular sharp lipped cavities leads to simple relationships between P_n and P_c . A feature of this model is that for a near free molecule flow, $P_c > P_n$.

Figure 18A shows estimates of P_n/P_{fm} obtained in the above manner by Lewis [51] together with mean curves faired by eye through the present results. There is substantial disagreement both qualitatively and quantitatively. As $x/\lambda_{fb} \rightarrow 0$, the experimental P_n/P_{fm} appears to approach unity in contrast to the calculations. Furthermore, the data maximizes to $P_n/P_{fm} \approx 7$ at $x/\lambda_{fb} \approx 6$ compared with the calculated peak of $P_n/P_{fm} \approx 9$ at $x/\lambda_{fb} \approx 1.5$. The leading edge angle for Lewis's model was 10° . Also shown in Fig. 18A is the data of Vidal and Bartz [78] obtained directly using pressure transducers mounted flush with the model surface. In this case the comparison is quite good and in particular the pressure peak is well predicted. However, in view of earlier comments it is likely

that the surface pressure near the leading edge was affected by the 30° undersurface angle of the C.A.L. model, although it is not clear to what extent the pressure peak was influenced.

Uppington [76] measured pressure in straight wall tubes of large diameter. The advantages and disadvantages of this method were outlined earlier in Section 3.3.1. Figure 18B indicates that Uppington's measurements substantially agree with the present calculations in the transition region and also with other data further downstream where the correction schemes employed are likely to be fairly reliable. Also shown in Fig.18B is the uncorrected data of Jeffrey [46] taken with blunt lipped orifices of much smaller diameter than Uppington's. Comparison of this data with the present results is not really meaningful until the corrections have been completed.

In Fig.19 the calculated P_n/P_∞ is plotted against $\bar{V}$ (see footnote) and is compared with a strong interaction result given by [24]

$$\left(\frac{P_n}{P_\infty}\right)_{SI} = \frac{\sqrt{3}}{2} \gamma \left(\frac{\gamma-1}{\gamma+1}\right) \left[0.664 + 1.73 \left(\frac{T_w}{T_0}\right)\right] \bar{x} \quad (77)$$

and also with the thin layer continuum calculations of Cheng et al. [25]. In Ref.[25] slip and temperature jump boundary conditions were included with a surface accommodation coefficient of unity. Other parameters were $Pr = 3/2$, $\gamma = 1.4$, $Re_{inch} = 10^4$ and $T_0 = 2000^\circ K$. The bulk viscosity was taken to be zero and hence rotational nonequilibrium effects were neglected. Figure 19 indicates that the present results are decreasing too rapidly for $\bar{V} < 0.3$ to properly approach the strong interaction limit

The rarefaction parameter $\bar{V}$ is given by

$$\bar{V} = M_\infty \sqrt{C^*/Re_x} \quad \text{where} \quad C^* = \frac{\eta(T'')T_\infty}{\eta(T_\infty)T''}, \quad Re_x = \frac{\rho_\infty U_\infty x}{\eta(T_\infty)}$$

and $T'' = T_0/6 + T_w/2$. Using Eq.(65), for η , $\bar{V}$ may be readily related to $\hat{x}$. Values of $\hat{x}\bar{V}^2 = \text{constant}$ for the various flow conditions are given in Table I.

if continued further downstream. This effect is manifest in the last three or four points in each case and may be attributed to the upstream effects of the flow expansion at the trailing edge.

The normal pressure for the $M_\infty = 10.15$ calculation is shown in Fig.20A compared with the air data of Becker and Boylan [3] at the same conditions and also with Horstman 's [41] air data at somewhat higher M_∞ . Becker and Boylan measured pressure in straight walled tubes and applied a semi-empirical correction scheme to account for heat transfer through the orifice opening while Horstman applied a similar correction to pressures measured in free molecular sharp lipped cavities. The comparison with Horstman 's data very near the leading edge can be improved significantly by plotting theory and experiment against x/λ_{fb} as shown in Fig.20B.

Comparison of Fig.20A with any of Figs. 15 and 16 shows that, as for the number flux the peak P_n/P_{fm} depends on M_∞ but not on T_w/T_∞ .

6.4.3 Heat Transfer and Skin Friction

The surface heat transfer and skin friction coefficients are shown in Fig.21. These quantities are essentially the $V_y(\frac{1}{2}mV^2 + E_R)$ and the mV_xV_y moments of the distribution function at the surface. Also shown is the data of Lewis [51] obtained by direct measurement and also using the two stream surface flow model together with an empirical form of C_F/C_H due to Vidal and Bartz [78]. There are several features of the C_F and C_H results which are in striking contrast to the number flux and pressure behaviour. Firstly as $x/\lambda_{fb} \rightarrow 0$, both C_H and C_F very nearly approach the free molecular limit in good agreement with the data. Secondly, C_F and C_H peaks are only about twice the free molecular limit compared with maximum values of $N/n_{fm} \approx 5$ and $P_n/P_{fm} \approx 9$. This behaviour may be understood by noting that the generic forms of the heat transfer and skin friction given above each contain V_xV_y products. Thus for small

x/λ_{fb} , the sharp increase in the V_y motion of incident particles is offset to some extent by the decrease in the V_x component. Since both the number flux and pressure do not explicitly depend on V_x , this effect does not arise for these quantities. Thus, as was suggested by Vidal and Bartz [78], near free-molecular values of C_F and C_H as $x/\lambda_{fb} \rightarrow 0$ does not necessarily accompany like behaviour of P_n/P_{fm} and N/N_{fm} . Note that the peak values of C_H and C_F occur near $x/\lambda_{fb} = 1.0$ (somewhat upstream of the pressure and flux peaks) and further that the x/λ_{fb} correlation definitely breaks down for $x/\lambda_{fb} \geq 1$. The C_H and C_F maxima may be associated with the combined and related attenuation of both direct free molecule convection to the surface and of first collisions.

6.5 Near Surface Properties

Estimates of moments representing macroscopic flow field properties were obtained in every cell in the simulated region.* Since the cells were of finite extent, it was not possible to obtain flow properties right at the plate surface. It is nevertheless interesting to examine the gas properties in cells adjacent to the plate surface. These cells were generally of height $\Delta y = \lambda_\infty/2$ although for $M_\infty = 25$, near $x = 0$, the first few cells were of height $\Delta y = \lambda_\infty/6$. Values of the gas properties at the plate surface for a purely free-molecule flow are tabulated in Table II (see Appendix H for formulae).

6.5.1 Tangential Velocity

Characteristic of the flow in the kinetic-transition-merged layer regimes are the well known phenomena of velocity slip and temperature jump

* Flow field properties will only be presented for the high M_∞ , $\gamma = 1.4$ calculations.

at the wall surface. The average x component of molecular velocity u/U_∞ for particles near the wall is plotted against x/λ_{fb} in Fig.22 for the three high M_∞ cases. For $x/\lambda_{fb} \lesssim 1.5$ the flow decelerates sharply from near the free molecular limit (see Table II) at $x/\lambda_{fb} = 0$. This, of course, is due to the loss of directed energy/momentum to thermal and internal energy of molecules in the initial collision regime. For $x/\lambda_{fb} \gtrsim 2$ the deceleration is much less marked. As with the surface properties, this change of flow character can be attributed to the onset of transition and the development of a wider class of collision products. Particles reaching the surface will then have suffered several collisions and will have little "memory" of their free stream or first collision history. The near surface flow then displays the slip-like features of the merged layer. Eventually, far downstream in the strong interaction regime, the body reflected particles will dominate the flow in the near surface Knudsen layer and the slip is of order $\lambda(T_w)/\delta$ where δ is the boundary layer thickness.

Also shown in Fig.22 are estimates of u_w/U_∞ inferred by Lewis [51] using the two stream model. These are much higher than the present results which is consistent with the near free-molecule picture of the kinetic flow presented in Ref.[51]. Note that the abrupt rise in u_w/U_∞ downstream for each case in Fig.22 is due to the flow expansion at the trailing edge.

6.5.2 Translational and Rotational Temperatures

The near surface translational and rotational temperatures T and T_R respectively are shown in Fig.23A normalized by T_w . In the kinetic regime, the translational temperature jump at the wall and the translational-rotational differential are both very high. Immediately downstream of the leading edge T rises sharply to a maximum that does not

correlate for the three conditions when normalized against T_w . This is reasonable since here the near surface flow may be considered to have a multi-stream (but not a two-stream) character. The translational temperature is then not a measure of the purely thermal motion of a group of particles with a near Maxwellian velocity distribution at say T_w , but reflects the highly nonequilibrium nature of the flow.

The rotational temperature on the other hand correlates quite well when plotted as T_R/T_w and T_R/T_w does not much exceed unity. For $x/\lambda_{fb} \geq 2$, the convergence of T and T_R towards equilibrium is slow since the convection effects of collision products created away from the surface are still substantial. Far downstream it is to be expected that both T/T_w and T_R/T_w should approach unity as the near surface flow comes into a state of quasi-equilibrium (Navier-Stokes flow) at T_w .

Lewis [51] measured rotational temperature directly throughout the flow field for $M_\infty = 25$, $T_w/T_\infty = 30$ using an electron beam technique. Surface values of these measurements obtained from Ref.[51] are shown in Fig.23A. As can be seen there is good agreement with calculations for $x/\lambda_{fb} \leq 2$. Thereafter the present results are somewhat lower than the data and this may well be due to the approximate form of the present collision model. Also shown are estimates of T obtained by Lewis from the two-stream model for $T_w/T_\infty = 30$. The peak value agrees quite well with the present results but it occurs rather further downstream than the calculated peak.

The translational temperature may be expressed as

$$\frac{T}{T_\infty} = \frac{1}{3} \left(\frac{T_{xx}}{T_\infty} + \frac{T_{yy}}{T_\infty} + \frac{T_{zz}}{T_\infty} \right) \quad (78)$$

where T_{xx} , T_{yy} and T_{zz} are the temperatures associated with the x , y and z motions respectively. Figure 23B shows near surface values of T_{xx}/T_∞ , T_{yy}/T_∞ , T_{zz}/T_∞ and T_R/T_∞ for the $M_\infty = 25$, $T_w/T_\infty = 30$ case. The nonequilibrium

effect between the translational temperature components is an order of magnitude near the leading edge and is a factor of two at $x/\lambda_\infty \approx 90$. The rotational temperature is close to T_{yy} and T_{zz} for the range of x/λ_{fb} shown. It might be conjectured that the translational nonequilibrium for large x could have been artificially induced by some spurious effect of the approximate inelastic collision model. For the present calculations $\gamma = 5/3$, however, nonequilibrium effects of similar magnitude to those in Fig.23B also occurred in the translational degrees of freedom. Note that since $P_{xx} = R\rho T_{xx}$, etc., Fig.23B also illustrates the non-isotropy of the pressure tensor near the wall.

6.5.2 Distribution Function Estimates

In addition to macroscopic flow properties, estimates of reduced forms of the distribution function were also obtained from the calculations.

These were of two kinds

1. The reduced distribution of x-velocities

$$\bar{f}_1(V_x, x, y) = \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty f \, dV_y dV_z dE_r \quad (79)$$

in a number of specified spacial cells.

2. The reduced distribution of x-velocities for particles striking specified surface segments,

$$\bar{f}_2(V_x, x) = \frac{n}{N} \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^0 V_y f \, dV_y dV_z dE_r \quad (80)$$

Note that $\bar{f}_2$ includes only incident particles, i.e. those with $V_y < 0$.

Figure 24A shows histogram estimates of $\bar{f}_2$ obtained in four cells adjacent to the body surface while Fig.24B shows like estimates of $\bar{f}_2$ for four nearby surface segments. Both figures illustrate the highly nonequilibrium character of the distribution function for the near surface

flow. For $x/\lambda_\infty = 1$, $\bar{f}_1$ in Fig.24A at first glance appears to be free molecule-like, with the tall narrow peak on the right representing the free stream and the squat peak near $\hat{V}_x = 0$ the body reflected particles. The small relative density of particles in the band $10 \lesssim \hat{V}_x \lesssim 20$ together with some particles for $\hat{V}_x < 10$ represent collision products. However, the corresponding $\bar{f}_2$ for $x/\lambda_\infty = 1$ indicates that the flux of collision products to the surface is high, as of course was shown in Fig.13. Evidently then, although the density of these particles is small, they have high V_y and therefore greatly influence the surface properties near $x = 0$. Note that collision products for $x/\lambda_\infty = 1$ generally have $V_y > 0$ which means that they must have been created upstream of this station. This supports comments made earlier in connection with the effects of forward propagation.

As the flow moves downstream the free stream peaks for both $\bar{f}_1$ and $\bar{f}_2$ shrink due to collisions. These maxima are quite strong for $x/\lambda_{fb} = 0.526$ and can be seen to have vanished at $x/\lambda_{fb} = 1.58$ for $\bar{f}_1$ in Fig.24A and at $x/\lambda_{fb} = 1.91$ for $\bar{f}_2$ in Fig.24B. This is consistent with the earlier conclusion that free stream-body particle collisions have become negligible for $x/\lambda_{fb} \gtrsim 1$. In Fig.24B the broad $\bar{f}_2$ curves for $x/\lambda_{fb} = 1.91$ and 3.44 shows that at these stations a wide spectrum of slowly evolving incident collision products has developed while Fig.24A clearly indicates the increasing importance of body reflected particles in the near surface flow. In particular the mixture of these and collision products is evident for $x/\lambda_{fb} = 1.58$ and 4.20.

6.6 Flow Field Properties

The gas properties in the flow field will generally be presented as families of profiles for constant x or constant y but in one case, density is presented in the form of contours. As with the surface properties,

where feasible, actual calculated values of the flow quantities will be plotted to give an indication of the statistical scatter in the results. Since it is difficult to present flow field quantities for different conditions on a single figure, a selection of the calculated results will be shown. Although we believe that λ_{fb} or λ_{bf} are not significant length scales for the flow past $x/\lambda_{fb} \approx 1$, they are still valuable as well defined parameters for the overall flow and will be used for the purposes of comparison of flow field properties with experiment.

6.6.1 Density

A set of calculated density profiles for constant x/λ_{fb} are shown in Figs. 25A and 25B for the $M_\infty = 25$ case compared with the measurements of Lewis to be discussed presently. The present calculated profiles are quite similar qualitatively to the monatomic profiles of Vogenitz et al. [80] and also to those presented for a diatomic gas at $M_\infty = 6.1$, by Huang et al. [44]. The initial rise in density away from the plate near the leading edge (Fig. 25A) can be attributed to the movement of surface reflected molecules and initial collision products into the free stream. Here both molecule-surface and molecule-molecule collisions are important in the flow field development although the effect of the latter is rapidly increasing. Further downstream (Fig. 25B) as molecule-molecule collisions begin to dominate the flow, the density profiles develop the characteristics of a boundary layer adjacent to the wall merged with a displaced shock wave developing further out. Under the influence of body molecules near the wall, n/n_∞ drops below unity presumably to approach a value of order T_∞/T_w very far downstream. The maximum n/n_∞ should correspondingly rise to approach the Rankine-Hugoniot value as the incipient merged layer shock focuses to a classical thin shock in the strong interaction regime. The transition from a kinetic to a merged

layer like density profile is just recognizable for $x/\lambda_{fb} = 1.29$ in Fig.25B and appears to be quite well developed for $x/\lambda_{fb} = 3.56$.

Several experimentalists have measured density in the kinetic and merged layer regimes using electron beam techniques. This is a delicate experiment in which a beam of electrons is passed through the gas. The intensity of light produced by electron-molecule collisions is a function of the gas density but various corrections including an important one for the secondary electron excitation have to be applied to enable the gas density to be evaluated throughout the flow field. Furthermore, due to the difficulties of measuring absolute light intensities, often only relative density measurements are made. The datum is taken to be the free stream value but because of axial and radial gradients that invariably exist in the flow, and because of the fluctuation in the primary beam and the secondary electron density, this is often difficult to locate accurately.

Gas density profiles obtained in the above manner by Lewis [51] are shown in Figs. 25. A striking feature of the comparison with the present results, particularly in Fig.25B, is that while the density peak appears to be well predicted, the experimental and calculated curves are displaced by an approximately constant amount. One possible reason for this systematic discrepancy is that the free stream datum had been incorrectly located in the experiment, perhaps for one or a combination of the reasons mentioned above.

Nearer the leading edge (Fig.25A) experiment and calculation compare reasonably away from the plate but towards the surface the calculated density is consistently larger than the measured value. In interpreting his near leading edge density profiles as evidence of a predominantly free-molecule flow, Lewis draws attention to the possible effect of the "shadow region" in the initial flow development, whereby a wedge-like

segment of the field defined roughly by $x/S_\infty \gtrsim y > 0$ is masked by the plate itself from the $V_y > 0$ half of the free stream distribution function. For a free molecule flat plate flow the effect certainly exists and for $T_w/T_\infty > 1$ leads to surface values of $\rho/\rho_\infty < 1$ (see Appendix H). It was not detected, however, in the monatomic calculations of Vogenitz et al. [80], although as Lewis points out, the near surface cell height $\Delta y \approx \lambda_{bf}$ used in Ref.[80] was too coarse to properly probe the shadow region. Hence for the present $M_\infty = 25$ case, the first few leading edge cells were of size $\Delta x = 2\lambda_{bf}$, $\Delta y = \lambda_{bf}/6$ which means that about 30% of the first, 70% of the second and all of the third near surface cells were within the shadow regime. Figure 25A indicates that for $x/\lambda_{fb} = 0.24$ (three cells from $x = 0$), the near surface ρ/ρ_∞ falls below unity*. Since Fig.13 shows that the free stream component of the near surface flow is still substantial at this station we conclude that the present calculations detect the remnants of the shadow effect but that it is soon obliterated by the incidence of collision products created near $x = 0$.

In Fig.26 density is shown in the form of contours for the $M_\infty = 22.9$, $T_w/T_\infty = 14.4$ case. The development of the shock and boundary layer regions of the flow past $x/\lambda_{fb} \approx 2$ is clearly evident. For this calculation the leading edge cell size was about $\Delta y = \lambda_{bf}/2$ in height and no shadow effect was detected. However we believe that this is only a local and quite small error in the density calculation that does not propagate downstream. From Fig.26 it can be seen that the flow disturbance intersects the upper boundary for $x/\lambda_\infty \gtrsim 50$, along which the incident free stream boundary condition used will be incorrect. There does not appear to be any discernible distortion in the density contours in this region and it would therefore seem that the effect is small and at most confined to a narrow

* Further downstream the near surface ρ/ρ_∞ drops below unity but this is a collision-dominated rather than a free-molecule effect.

wedge of the flow near the boundary. Note that the density disturbance extends some few λ_∞ upstream of the leading edge above the plate.

Figure 27 shows the influence of wall temperature on the density profiles at three stations. The same x/λ_∞ was chosen for comparison since one based on x/λ_{fb} showed systematic differences downstream of $x/\lambda_{fb} \approx 1$, as for the surface properties. Near the wall the density is lower for higher wall temperature which may easily be shown to be consistent with the strong interaction limit downstream. Further out the profiles appear to correlate quite well against y/λ_∞ and this seems reasonable since here body reflected molecules are not important and λ_∞ is the only available length scale.

The effect of diatomicity on the density is illustrated in Fig. 28. The disturbance is closer to the wall for the diatomic gas and this is related to the decreased thermal motion of the collision products for this case which inhibits the outward propagation of the flow disturbance.

6.6.2 Tangential and Normal Velocity

Families of tangential and normal velocity profiles are shown in Figs. 29 and 30 respectively. The tangential velocity profiles clearly show the growth of the boundary layer and the decrease in slip at the wall under the increasing influence of body molecules, but for large $\hat{x}$ they do not show any special characteristics in the shock formation region. The normal velocity profiles on the other hand exhibit shock and boundary layer features as the merged layer begins to form. Near the leading edge v/a_∞ is high quite close to the plate and this is due largely to the effects of outward moving body reflected particles. Further downstream v/a_∞ decreases near the wall in the developing boundary layer but increases in the region of the shock as the body disturbance is propagated outwards in the y -direction. Generally speaking the ρ/ρ_∞ and

v/a_∞ profiles show similar characteristics.

6.6.3 Translational and Rotational Temperature Profiles

Figure 31 shows a group of translational temperature profiles while Fig. 32 shows a slightly larger group of rotational temperature profiles. Note that all of Figs. 29-32 are for $M_\infty = 22.9$, $T_w/T_\infty = 14.4$. Some distance down stream of the leading edge, both the T/T_∞ and T_R/T_∞ profiles develop maxima which move away from the plate as the near surface value of these quantities tends towards T_w/T_∞ . Again this phenomenon is due to the influence of the plate through body reflected particles and may be associated with the transition to a merged layer type flow. The effect is somewhat delayed for the T_R/T_∞ profiles due to the presence of substantial translational-rotational nonequilibrium.

It may be observed from Figs. 29-32 that to the scale shown, forward propagation effects are not evident for $x/\lambda_\infty = -5$, but are strongly felt for $x/\lambda_\infty = -1$. The effect is particularly strong for $y < 0$ because of the larger forward component of reflection from the 10° undersurface leading edge angle. Note, however, that in terms of an increase in the flow properties, the forward disturbance is not necessarily due to collisions but is also present for a purely free-molecule flow.

To illustrate the high degree of nonequilibrium existing throughout much of the flow, T_{xx}/T_∞ , T/T_∞ and T_R/T_∞ profiles at three stations along the plate for $M_\infty = 22.9$, $T_w/T_\infty = 14.4$ are shown in Fig. 33. Far from the plate the approach to equilibrium is quite evident. Nearer the surface nonequilibrium effects are discernibly decreasing for increasing x/λ_∞ .

The flow field electron beam rotational temperature measurements of Lewis [51] are shown in Fig. 34 as the continuous lines and are compared with the present results at about the same x/λ_{fb} . Although these measurements are extremely difficult to do accurately, Lewis considers

that they were accurate to 2% for temperatures greater than about 100°K but that the error increases to about 40% at temperatures of order 10°K, the nominal freestream temperature for the experiment. Comparison between theory and experiment is good for $x/\lambda_{fb} \approx 0.24$ but becomes progressively worse further downstream. This could well be due to the approximate nature of the present collision model. However, there was almost certainly a decreasing free stream temperature along the tunnel in Lewis's experiment which might in part account for the large y/λ_{bf} discrepancy.

The influence of the internal energy on translational temperature profiles is shown in Fig.35. Reasons for the lower temperatures for the diatomic gas have been previously discussed. Very near the wall the discrepancy decreases because of the increasing dominance of body particles reflected with average translational energy $\frac{3}{2} kT_w$ for both cases.

6.6.4 Flow Distribution Functions

Histogram estimates of $\bar{f}_1$ as defined by Eq.(79) were obtained at various cells in the flow away from, as well as near to, the plate surface for the $T_w/T_\infty = 30$ calculation. These are shown graphically in Fig.36 at $x/\lambda_\infty = 33$ and $x/\lambda_\infty = 88$ for various values of y/λ_∞ as shown. At both x stations the departures from a Maxwellian (equilibrium) V_x distribution appear to decrease for increasing y/λ_∞ . It would be interesting to compare the reduced distribution functions obtained with Navier Stokes forms of $\bar{f}_1$ at the same points in the flow. These could be determined from the flow gradients from either the present calculations or from continuum calculations of the type presented in Refs. [25] and [67].

6.7 Summary and Discussion

The principal qualitative results obtained from the foregoing discussion of the present leading edge calculations may be summarized as follows

1. The collisional interaction between free stream and body reflected particles extends forward of the leading edge with the resulting collision products causing the incident number flux (Figs. 10-13) and the surface pressure (Figs. 14-16) to exceed the free molecule values as $x/\lambda_{fb} \rightarrow 0$. Figure 17 indicates that this phenomena may to some extent be attributed to the forward reflecting properties of the 10° undersurface angle, but that this leads to little overall effect on the developing flow. The heat transfer skin friction coefficients (Fig.21) appear to be close to the free molecular limit near the leading edge.

2. The kinetic regime in which molecule-molecule and molecule-surface interactions are equally important extends to about $1.5\lambda_{fb}$ downstream of the leading edge ($\bar{V} \approx 0.5$). The beginnings of transition to a merged-layer type flow appears to be associated with the attenuation of free-stream body particle encounters near $x/\lambda_{fb} \approx 1$ and the subsequent development of a wider spectrum of collision products (see Figs.24). Consequently the correlation of surface properties against x/λ_{fb} breaks down for $x/\lambda_{fb} \gtrsim 1$. The onset of transition is accompanied by maxima in the heat transfer and skin friction coefficients at $x/\lambda_{fb} \approx 1$ and in the incident number flux and normal surface pressure at $x/\lambda_{fb} \approx 1.5$.

3. The maximum values of N/N_{fm} and P_n/P_{fm} depend on M_∞ but not on T_w/T_∞ (see Figs. 10-12 and Figs. 16 and 20).

4. Merged layer characteristics seem to be quite well developed for $x/\lambda_{fb} \approx 4$. Near the wall the increasingly important role of body

reflected particles can be seen in the evolution of the macro and micro flow properties (Figs. 22-24). Further out the development of the shock is evident in the density and normal velocity profiles as shown in Figs.25 and Fig.30 respectively.

5. The internal rotational degrees of freedom introduce large quantitative but not qualitative changes in the flow structure when compared to the equivalent flow of a monatomic gas.

Comparison of the present results with experimental data was good for the heat transfer and skin friction (Fig.21) and reasonable for the rotational temperature (Fig.34). Some features of the measured density profiles were well predicted. Comparison with surface pressure and number flux data was reasonable with the notable exception of Lewis's [51] measurements (Figs. 11 and 18A). Here the discrepancy was of a qualitative nature in that Lewis concludes that there exists an essentially free molecule dominated region very near the leading edge in contrast to the present results. With regard to the normal pressure, the behaviour suggested by Lewis and by Harbour and Bienkowski [33] is not convincing since free molecule like conditions were implicitly assumed in the choice of the near surface flow model. No corrections or even assumptions about the gas-surface interaction law are required for the N/N_{fm} measurement and the large discrepancy in Fig.11 is therefore quite worrying.

Experiments on rarefied flows are extremely difficult to perform and the sources of error in the measurements are legion. Three-dimensional and conical flow effects in the undisturbed test flow, problems associated with the complex and sensitive instrumentation needed and large correction factors which have to be applied to most of the measurements all add to the uncertainty of the results (see cited Refs.).

In the light of this the agreement between calculation and experiment is considered most encouraging. Nevertheless the following criticisms of the theory may be important and could account for the discrepancies noted.

1. Approximate diatomic collision model. The present version of the Parker collision model is very approximate and involves many assumptions, the most unsatisfactory of which is that of planar rotation of collision partners. However, in that the rotational temperature appears to be reasonably well predicted, at least near the leading edge, there is good reason to believe that for the present calculations the model constitutes an adequate representation of rotational energy exchange. The difficulties and limitations of the model were discussed from a theoretical point of view in Section 5.10.

2. Leading edge singularity. For free-molecule flow past a mathematically sharp leading edge, the distribution function is not uniquely defined at the point of infinite curvature [66]. Hence as $x \rightarrow 0$ the macroscopic flow properties are multiple valued and the flow gradients are infinite, phenomena which are related to the shadow effect discussed by Lewis [51]. Richter [66], in presenting an integral method for the solution of the B.G.K. equation for the flow past a class of elliptical cylinders suggests that singular behaviour of this nature could well exist for a finite K_n flow. Apart from varying the cell size near $x = 0$ within fairly coarse limits we have taken no account of this effect.

Certainly in the present calculations even the smallest leading edge cells used were too coarse to properly resolve the large near surface normal flow gradients which exist near $x/\lambda_\infty \sim 0(1)$. Hence Lewis's criticism of the cell size used in Ref.[80] also applies to the present calculations in that we have neglected a possible leading edge singularity. However, while it is possible that resulting errors in the collision

simulation for cells very near the leading edge could propagate into the flow, it is difficult to see how this could occur on a scale large enough to seriously perturb the downstream flow. In this respect, the Direct Simulation technique has shown itself to be remarkably insensitive to cell size, even in very extreme cases.

Since the notion of a gas dynamic flow in a region of body curvature greater than $1/\sigma$ is unrealistic, a solution to the above problem would be as follows. Construct the leading edge with a radius of curvature R such that $\lambda_\infty \gg R \gg \sigma$. Cells near $x=0$ could then be consistently made of order R^2 in area.

3. Gas-surface Interaction Law. Vogenitz et al. [80] carried out monatomic gas Direct Simulation calculations for a 30% specular, 70% diffusely reflecting surface and found that this had a large effect on the flow for many λ_∞ downstream of the leading edge when compared with the flow past a fully diffuse surface. The maxima in the surface properties, particularly flux and pressure, were reduced in magnitude and occurred further downstream than for the fully diffuse case. It seems quite possible therefore that a specular component in the gas-surface interaction law could reduce the discrepancy between calculation and experiment evident in particular in Fig.11 for N/N_{fm} .

Although no calculations have been carried out for other than a fully diffuse completely accommodating surface, the effects of a fraction σ' of specular reflection on the flow structure can perhaps be qualitatively evaluated by observing that in this case λ_{fb} [Eq.(72)] would increase by a factor of $1/(1-\sigma')$. Since for $\sigma'=0$ the present calculations indicate that the kinetic regime extends to roughly $x/\lambda_{fb} \approx 1.5$, then for $\sigma' > 0$, it seems reasonable to suggest that it persists to $x/\lambda_{fb} \approx 1.5/(1-\sigma')$ where λ_{fb} is for a fully diffuse surface. The same arguments could be applied to the position of the maxima in the surface properties.

7. CONCLUDING REMARKS

The hypersonic flow of a diatomic gas past the sharp leading edge of a two-dimensional flat plate has been calculated using the Direct Simulation method. To include the effects of rotational nonequilibrium for a diatomic gas, an approximate form of Parker's classical inelastic collision method has been developed into a form suitable for Monte-Carlo simulation. In this model the assumption of planar rotation of the colliding rigid rotor molecules was used together with other assumptions introduced essentially to yield a tractable set of perturbation equations. An approximate solution of these equations along the lines of Lordi and Mates [53] led to a second order expression for the rotational-translational energy exchange, which used in conjunction with features of the zeroth order (spherical) collision dynamics forms the basis of the calculation of the post-collision dynamical parameters in simulation.

The present form of the Parker model has some unrealistic features in near equilibrium situations which appear to be associated with the difficulty of preserving, in the approximate analysis, the reverse collision property of the fully three-dimensional equations of motion. In particular the appropriate equilibrium distribution of internal energies is not achieved and at low temperatures special strategies are required to force the gas locally towards a state of rotational translational energy equipartition. Nevertheless, we believe that the physical validity of the model increases in the nonequilibrium limit. For this reason the above-mentioned defects are not thought to have a serious effect on the present calculations since for the most part, the gas is in a highly nonequilibrium state. It is concluded that accurate hybrid collision models could be constructed by combining the classical and phenomenological models as suggested in Section 5.10.

The majority of the leading edge flow calculations were performed for conditions chosen to match those used in recent nitrogen experiments at Mach numbers in the range 23-25. The development of the initial nonequilibrium flow has been studied and the characteristics of the kinetic regime and the transition to a merged layer flow have been identified with particular reference to the role of the length scale λ_{fb} in the kinetic flow. A physical picture of the leading edge flow obtained from the present calculations is summarized in Section 6.7. However, two important conclusions are perhaps worth reiterating. Firstly the calculated molecular flux and surface pressure appear to exceed the free molecular limit towards the leading edge in agreement with the earlier monatomic calculations of Bird [8] and Vogenitz et al. [80]. Secondly, a predominantly kinetic flow appears to exist for only about $1.5\lambda_{fb}$ downstream of the leading edge. Neither of these conclusions seem to be in qualitative agreement with the experimental flow model proposed by Lewis [51]. It should be strongly emphasized, however, that all of the present calculations were for a fully diffuse completely accommodating surface while most experimental measurements are independent of a specified gas-surface interaction. Since the results of the Monte-Carlo calculations are known to depend strongly on the properties of the surface reflected molecules [80] it is quite possible that a quite different picture of the flow may be obtained for a more realistic surface law.

It is recommended that further experimental work on gas-surface interactions for "engineering" surfaces is desirable with particular reference to low incidence collisions such as would be characteristic of molecule surface encounters in the kinetic regime of a hypersonic flow. Further Direct Simulation calculations for a mixture of diffuse and specular reflection are presently being performed using a hybrid inelastic collision model of the type mentioned above.

Appendix A

Time Counter and Collision Selection Procedure

In this Appendix, a derivation of the Direct Simulation collision selection procedure and time increment per collision is presented. The analysis is similar to that given in Ref.[18].

Consider binary collisions between a pair of molecules in the volume element $d\mathbf{x}$, with velocities in the range $(\mathbf{c}_1, \mathbf{c}_1 + d\mathbf{c}_1)$ and $(\mathbf{c}_2, \mathbf{c}_2 + d\mathbf{c}_2)$ respectively, internal co-ordinates in $(\Omega_1, \Omega_1 + d\Omega_1)$ and $(\Omega_2, \Omega_2 + d\Omega_2)$ and with mutual impact parameter and azimuthal angle in the ranges $(b, b + db)$ and $(\epsilon, \epsilon + d\epsilon)$ respectively. The probability per unit time of such collisions is given by an expression commonly used in the derivation of the Boltzmann equation, viz,

$$n'^2 f(\mathbf{c}_1, \Omega_1, \mathbf{x}, t) f(\mathbf{c}_2, \Omega_2, \mathbf{x}, t) d\mathbf{c}_1 d\mathbf{c}_2 d\Omega_1 d\Omega_2 g b db d\epsilon d\mathbf{x} \quad (A1)$$

where f is the distribution function, $g = |\mathbf{c}_2 - \mathbf{c}_1|$ is the relative speed and n' the local real gas number density. In the Direct Simulation method, the

$$f(\mathbf{c}_1, \Omega_1, \mathbf{x}, t) f(\mathbf{c}_2, \Omega_2, \mathbf{x}, t) d\mathbf{c}_1 d\mathbf{c}_2 d\Omega_1 d\Omega_2 d\mathbf{x}$$

factor in the above is generated simply by choosing partners, each with equal probability from a group known to be in ω_k in the interval Δt_m . This is justified by regarding ω_k as a local discretization of $d\mathbf{x}$ and also by the implicit assumption that dynamical information in the correct distribution is carried by the sample particles, that is, that they are a statistically representative sample from f . The usual assumption of molecular chaos is implicit in the independent choice of collision partners.

The conditional probability per unit time per unit volume of collisions at speed g may then be written as

$$p(g)p(b)db \, p(\epsilon)d\epsilon = g \, b \, db \, d\epsilon \quad (A2)$$

where $p(g)$, $p(b)$ and $p(\epsilon)$ are the unnormalized conditional probability densities for g , b and ϵ respectively, irrespective of $\underline{c}-\underline{\Omega}$ class.

The corresponding collision rate at relative speed g is

$$\frac{\delta N_{\text{coll}}}{\delta t} = \frac{1}{2} n'^2 V_k g \, b \, db \, d\epsilon \quad (A3)$$

where V_k is the volume of ω_k and the factor of $\frac{1}{2}$ has been introduced since in the implicit sum in simulation over all $\underline{c}-\underline{\Omega}$ space, each collision would otherwise be counted twice. Normalizing $p(b)$ and $p(\epsilon)$ such that

$$\int_0^{b_0(g)} p(b)db = 1, \quad \int_0^{2\pi} p(\epsilon)d\epsilon = 1$$

where $b_0(g)$ is the maximum allowed impact parameter (chosen in some way), then from Eq.(A2) we may write

$$p(b) = 2b/b_0^2(g), \quad b_0(g) > b > 0 \quad (A4)$$

$$p(\epsilon) = 1/2\pi, \quad 2\pi > \epsilon > 0 \quad (A5)$$

Integrating Eq.(A2) over b and ϵ in the above ranges and normalizing $p(g)$ to unity at its maximum value leads to

$$p(g) = gb_0^2(g)/[gb_0^2(g)]_{\text{max}}, \quad g_{\text{max}} > g > g_{\text{min}} \quad (A6)$$

for the conditional probability density of accepting a pair of relative speed g for collision, irrespective of b and ϵ . A similar integration of Eq.(A3) yields the total collision rate at speed g ,

$$\left(\frac{\delta N_{\text{coll}}}{\delta t} \right)_{\text{tot}} = \frac{1}{2} n'_k{}^2 V_k g \pi b_0^2(g) \quad (A7)$$

Now let $\bar{\rho}$ be the arbitrary ratio of the actual local particle density to the local simulator density n_k . Then

$$n' = \bar{\rho} \, n_k, \quad N_{\text{coll}} = \bar{\rho} \, N_{\text{coll},k} \quad (A8)$$

where $N_{\text{coll},k}$ is the simulated number of collisions in ω_k . Putting $\delta N_{\text{coll},k} = 1$ and substituting relations (A8) into Eq.(A7) leads to the real time increment per simulated collision

$$\Delta t_k = \frac{2}{N_k \bar{\rho} n_k g \pi b_0^2(g)} \quad (\text{A9})$$

where $N_k = V_k n_k$ is the number of simulator particles in ω_k .

Equation (A6) for $p(g)$ is satisfied by accepting/rejecting a pair at relative speed g for collision accordingly as

$$p(g) \leq R_1$$

where R_1 is a random number in $(0,1)$. From Eqs. (A4) and (A5), b and ϵ may be chosen as

$$b = b_0(g) \sqrt{R_2}, \quad \epsilon = 2\pi R_3$$

where R_2 and R_3 are random numbers in $(0,1)$.

Note that in the above we have considered only the sink or absorption term in the Boltzmann collision integral given in infinitesimal form in expression (A1). However, as Bird points out [15], as long as the sink term is adequately simulated through the appropriate collision selection procedure, the source or emission term arises automatically as the outcome of the dynamical collision calculation.

Nondimensionalization

The development from expression (A1) to Eq.(A9) implies that each simulator particle will have the same collision probability and hence statistically the same collision rate as it would have as part of a real gas. However, Eq.(A9) still contains $\bar{\rho}$. This quantity can be eliminated by a suitable choice of time unit. Put

$$\hat{t} = t \cdot \bar{c} / \lambda(t) \quad (\text{A10})$$

where $\lambda(T)$ is the mean free path at some reference temperature T and $\bar{c}$ is

a reference speed. Then using Eq.(66) of the main text and substituting Eq.(A10) into Eq.(A9) yields

$$\hat{\Delta t}_k = \frac{2\sqrt{2} \Omega^{(2,2)*} (T/T')}{N_k \hat{n}_k \hat{g} b_0^{*2}} \quad (\text{A11})$$

where $b_0^* = b_0(g)/\sigma$

$$\hat{g} = g/\bar{c}$$

and $\hat{n}_k = n_k/n_0$, $n_0 = \bar{\rho} n$

The quantity n_0 is a reference simulator particle density. For the simulation of a homogeneous zero dimensional relaxation problem, $\hat{n}_k$ may be taken as unity. For a problem involving one or more physical space dimensions, $\hat{n}_k$ is taken as the best estimate of the relative density in ω_k , n_0 being chosen, say, as the free stream density.

Equation (A11) is for any molecular model. For hard spheres of radius σ for example, $b_0^* = 1$ and $\Omega^{(2,2)*} = 1$. Hence

$$\hat{\Delta t} = \frac{2\sqrt{2}}{N_k \hat{n}_k \hat{g}} \quad (\text{A12})$$

Note that the elimination of $\bar{\rho}$ implies that the collision simulation can be performed with an arbitrary number of simulator particles. An obvious lower limit is $N_k = 2$ particles per cell since at least two particles are required for a collision.

The condition that Δt_m be less than the local mean free path may now be more explicitly stated. If $\hat{g}'$ is the maximum relative speed at which collisions are expected to be important on physical grounds, then from Eq.(A9) the above condition may be more rigorously expressed as

$$\hat{\Delta t}_m = \Delta t_m \frac{\bar{c}}{\lambda} < \frac{\sqrt{2} \Omega^{(2,2)*} (T/T')}{\hat{n}_k \hat{g}' b_0^{*2}(\hat{g}')} \quad (\text{A13})$$

Appendix B

The Two Particle System

B1 Equations of Motion

We investigate the interactive motion of two particles labeled $i = 1$ and 2 respectively, each of mass m . Since each particle consists of a rigid structure, its motion may be separated into the translational motion of its mass centre and the rotational motion of the structure about the mass centre. The forces and moments acting on each particle are taken to be entirely due to the effect of the intermolecular potential.

If $\underline{r}_i$ denotes the position vector of particle i in the laboratory framework, the equations of motion of the system may be written as

$$m \ddot{\underline{r}}_1 = \underline{F}_{12} \quad , \quad m \ddot{\underline{r}}_2 = \underline{F}_{21} \quad (B1.1)$$

$$\dot{\underline{h}}_1 = \underline{T}_{12} \quad , \quad \dot{\underline{h}}_2 = \underline{T}_{21} \quad (B1.2)$$

where $\underline{h}_i$ is the rotational angular momentum of particle i about its mass centre and $\underline{F}_{12}$, $\underline{F}_{21}$, $\underline{T}_{12}$ and $\underline{T}_{21}$ are the forces and moments acting on the particles. The position of the centre of gravity of the system is given by

$$\underline{r}_g = \frac{1}{2}(\underline{r}_1 + \underline{r}_2) \quad (B1.3)$$

Using Eqs.(B1) it is easily seen that

$$\begin{aligned} 2m \ddot{\underline{r}}_g &= m(\ddot{\underline{r}}_1 + \ddot{\underline{r}}_2) \\ &= \underline{F}_{12} + \underline{F}_{21} \\ &= 0 \end{aligned} \quad (B1.4)$$

since no external forces are acting. Hence

$$\underline{F}_{21} = - \underline{F}_{12} \quad (B1.5)$$

Integrating Eq.(B1.4) yields

$$\dot{\underline{r}}_g = \text{constant} \quad (B1.6)$$

Writing $\underline{r}_{12} = \underline{r}_2 - \underline{r}_1$, then using Eq.(B1.3)

$$\underline{r}_1 = \underline{r}_g - \frac{1}{2} \underline{r}_{12} \quad (\text{B1.7A})$$

$$\underline{r}_2 = \underline{r}_g + \frac{1}{2} \underline{r}_{12} \quad (\text{B1.7B})$$

From Eqs.(B1.1) and (B1.5) the relative motion of the two particles can be expressed as

$$\mu \ddot{\underline{r}}_{12} = - \underline{F}_{12} \quad (\text{B1.8})$$

Equations (B1.2) and (B1.8) indicate that the equations of motion for the two particle system can be reduced to those of a single rotating particle of mass $\mu = m/2$ and position vector $\underline{r}_{12}$ moving about a fictitious rotating stationary particle. The reduced system automatically preserves conservation of linear momentum of the original system since by virtue of Eqs.(B1.7)

$$m(\dot{\underline{r}}_1 + \dot{\underline{r}}_2) = 2m\dot{\underline{r}}_g = \text{constant} \quad (\text{B1.9})$$

It is easily shown that the total angular momentum and energy of the reduced system are invariant. The angular momentum in the laboratory framework may be written

$$\underline{r}_1 \times m\dot{\underline{r}}_1 + \underline{r}_2 \times m\dot{\underline{r}}_2 + \underline{h}_1 + \underline{h}_2 = \underline{M} \quad (\text{B1.10})$$

and is constant since no external torques are acting. Substituting Eqs.(B1.7) into the above yields

$$\underline{r}_{12} \times \mu \dot{\underline{r}}_{12} + \underline{h}_1 + \underline{h}_2 = \underline{M} - 2m\underline{r}_g \times \dot{\underline{r}}_g \quad (\text{B1.11})$$

which is constant by virtue of Eq.(B1.6).

The total energy in the laboratory framework is

$$\frac{1}{2}m(\dot{\underline{r}}_1^2 + \dot{\underline{r}}_2^2) + \underline{h}_1^2/2I + \underline{h}_2^2/2I = E_t \quad (\text{B1.12})$$

Substituting Eqs.(B1.7) into Eq.(B1.12) leads to

$$\frac{1}{2}\mu \dot{\underline{r}}_{12}^2 + \underline{h}_1^2/2I + \underline{h}_2^2/2I = E_t - m\dot{\underline{r}}_g^2 \quad (\text{B1.13})$$

which is constant.

The relative speeds before and after collision may be related through Eq.(B1.13). Put

$$\underline{g} = \dot{\underline{r}}_{12} , \quad E_{r_i} = h_i^2/2I , \quad i=1,2 \quad (B1.14)$$

evaluated as $t \rightarrow -\infty$ (long before collision) and denote by $\underline{g}'$, E'_{r_i} , the corresponding quantities as $t \rightarrow \infty$, long after collision. The right hand side of Eq.(B1.13) may then be eliminated to yield

$$\frac{1}{2} \mu g^2 + E_{r_1} + E_{r_2} = \frac{1}{2} \mu g'^2 + E'_{r_1} + E'_{r_2} \quad (B1.15)$$

from which we obtain

$$g'/g = \left\{ 1 - \frac{2}{\mu g^2} (\Delta E_{r_1} + \Delta E_{r_2}) \right\}^{\frac{1}{2}} \quad (B1.16)$$

where $\Delta E_{r_i} = E'_{r_i} - E_{r_i}$, $i=1,2$

B2 Transformation of Pre- and Post-Collision Velocities

If the particle velocities prior to collision are denoted by $\underline{c}_i = \dot{\underline{r}}_i(-\infty)$ and those long after collision by $\underline{c}'_i = \dot{\underline{r}}_i(\infty)$, $i=1,2$, then from Eqs.(B1.7) it follows that

$$\underline{c}'_1 = \underline{c}_1 + \frac{1}{2}(\underline{g} - \underline{g}') \quad (B2.1A)$$

$$\underline{c}'_2 = \underline{c}_2 - \frac{1}{2}(\underline{g} - \underline{g}') \quad (B2.1B)$$

which clearly satisfies the conservation of linear momentum. Denote the components of $\underline{g}$ and $\underline{g}'$ by g_k and g'_k , $k=1,3$ respectively. Referring to Fig.B2 below and remembering that for the case of planar rotation, the collision is confined to the initial collision plane,* the g'_i can be

*The collision plane is normal to the vector $\underline{r}_{12} \times \dot{\underline{r}}_{12}$ and is the x_1 - y_1 plane of Fig.2A.

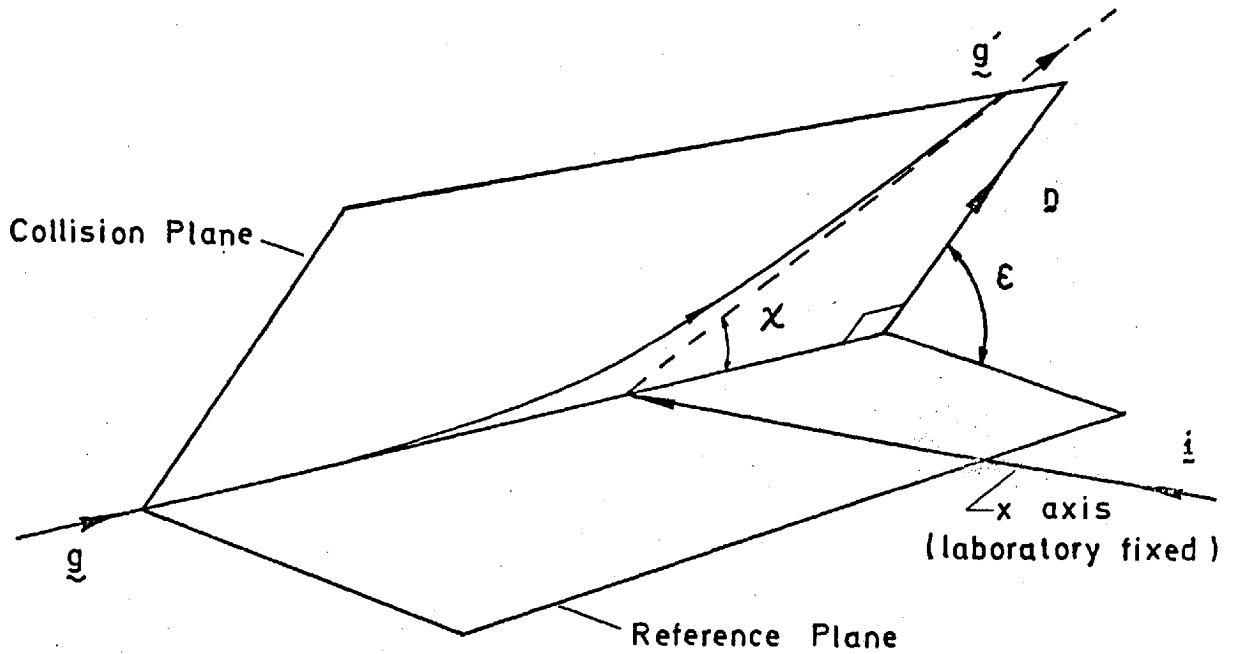


Fig.B2 Pre and Post Collision Relative Velocity

determined from g_i , the deflection angle χ and the azimuthal angle measured as shown from a reference plane normal to $\underline{g} \times \underline{i}$ where $\underline{i}$ is a unit vector in the x direction.

If n_k are the components of a unit vector $\underline{n}$ in the collision plane normal to $\underline{g}$ as shown in Fig.B2 then

$$g'_k = g' \cos \chi \left(\frac{g_i}{g} \right) + g' \sin \chi n_k \quad (\text{B2.2})$$

Writing

$$n_k = n_{k\parallel} \cos \epsilon + n_{k\perp} \sin \epsilon \quad (\text{B2.3})$$

where $\parallel$ and $\perp$ refer to parallel to and normal to the reference plane respectively, then it can be shown that

$$\underline{n}_{\perp} = \frac{\underline{g} \times \underline{i}}{|\underline{g} \times \underline{i}|} = \frac{g}{g_t} \underline{j} - \frac{g}{g_t} \underline{k} \quad (\text{B2.4A})$$

and

$$\underline{n}_{\parallel} = \frac{\underline{g} \times \underline{n}_{\perp}}{|\underline{g} \times \underline{n}_{\perp}|} = -\frac{g_t}{g} \underline{i} + \left(\frac{g_1}{g} \cdot \frac{g_2}{g_t} \right) \underline{j} + \left(\frac{g_1}{g} \cdot \frac{g_3}{g_t} \right) \underline{k} \quad (\text{B2.4B})$$

where $g_t = (g_1^2 + g_2^2)^{1/2}$ and $\underline{j}$ and $\underline{k}$ are unit vectors in the y and z directions respectively.

Substituting the components of $\underline{n}_\perp$ and $\underline{n}_\parallel$ in Eqs.(B2.4) into Eq.(B2.3) and the result into Eq.(B2.2) leads to

$$g_1 - g'_1 = g_1 \left(1 - \frac{g'}{g} \cos \chi \right) + g_t \frac{g'}{g} \sin \chi \cos \epsilon \quad (\text{B2.5A})$$

$$g_2 - g'_2 = g_2 \left(1 - \frac{g'}{g} \cos \chi \right) - \frac{g'}{g} \sin \chi \left(g_1 \frac{g_2}{g_t} \cos \epsilon + g \frac{g_3}{g_t} \sin \epsilon \right) \quad (\text{B2.5B})$$

$$g_3 - g'_3 = g_3 \left(1 - \frac{g'}{g} \cos \chi \right) - \frac{g'}{g} \sin \chi \left(g_1 \frac{g_3}{g_t} \cos \epsilon - g \frac{g_2}{g_t} \sin \epsilon \right) \quad (\text{B2.5C})$$

The post-collision velocities in the laboratory framework may now be obtained from Eq.(B2.1) and Eqs.(B2.5) above.

Appendix C

Potential Expansion

The Parker potential is given by

$$V(R, \phi, \psi_1, \psi_2) = K_1 \frac{e^{\alpha D}}{4} \left\{ e^{-\alpha R_{AC}} + e^{-\alpha R_{AD}} + e^{-\alpha R_{BC}} + e^{-\alpha R_{BD}} \right\} - 2K_2 e^{-\frac{\alpha}{2}(R-D)} \quad (C1)$$

where the R_{AC} , R_{AD} , R_{BC} and R_{BD} are the distances between the respective points A, B, C and D shown in Fig.(2A). For the sake of brevity it is convenient to relable these distances as R_i , $i=1, \dots, 4$ respectively.

From simple geometrical considerations, it can be shown that

$$R_i = R \left\{ 1 + A_i \left(\frac{d'}{R} \right) + B_i \left(\frac{d'}{R} \right)^2 \right\}^{\frac{1}{2}} \quad i=1, \dots, 4 \quad (C2)$$

where

$$\begin{aligned} A_1 &= \cos \Gamma_1 - \cos \Gamma_2, & B_1 &= \frac{1}{2}(1 - \cos \Delta) \\ A_2 &= \cos \Gamma_1 + \cos \Gamma_2, & B_2 &= \frac{1}{2}(1 + \cos \Delta) \\ A_3 &= -A_2, & B_3 &= B_2 \\ A_4 &= -A_1, & B_4 &= B_1 \end{aligned}$$

and

$$\Gamma_i = \phi - \psi_i, \quad \Delta = \psi_2 - \psi_1$$

For small d'/R , the Taylor series expansion of Eqs.(C2) leads to

$$R_i = R \left\{ 1 + \frac{1}{2} A_i \left(\frac{d'}{R} \right) + E_i \left(\frac{d'}{R} \right)^2 + O \left(\frac{d'}{R} \right)^3 \right\}, \quad i=1, 4 \quad (C3)$$

where $E_i = \frac{1}{2}(B_i - A_i^2/4)$.

Substitution of Eqs.(C3) into Eq.(C1) and expansion of the factor $\exp[-\alpha d' E_i \left(\frac{d'}{R} \right)]$ gives

$$\begin{aligned} V &= K_1 e^{-\alpha(R-D)} \left\{ \frac{1}{4} \sum_{i=1}^4 e^{-\frac{\alpha d'}{2} A_i} - \frac{\alpha d'}{4} \left(\frac{d'}{R} \right) \sum_{i=1}^4 E_i e^{-\frac{\alpha d'}{2} A_i} + O \left(\frac{d'}{R} \right)^2 \right\} \\ &\quad - 2K_2 e^{-\frac{\alpha}{2}(R-D)} \end{aligned} \quad (C4)$$

Terms of $O\left(\frac{d'}{R}\right)$ and higher in Eq.(C4) are somewhat difficult to handle in terms of Parker's expansion. We therefore redefine V by truncating the series in braces in Eq.(C4) at the first term. Such a redefinition is implied in Ref.[64] by neglecting terms of higher order than d'/R in Eq.(C3). The new form of V is then

$$V = K_1 e^{-\alpha(R-D)} \cdot \frac{1}{4} \sum_{i=1}^4 e^{-\frac{\alpha d'}{2} A_i} - 2K_2 e^{-\frac{\alpha}{2}(R-D)} \quad (C5)$$

The summed factor in the first term of the above can be written as

$$\frac{1}{4} \sum_{i=1}^4 e^{-\frac{\alpha d'}{2} A_i} \equiv \cosh\left(\frac{\alpha d'}{2} \cos \Gamma_1\right) \cosh\left(\frac{\alpha d'}{2} \cos \Gamma_2\right) \quad (C6)$$

Each hyperbolic cosine in the above may now be written as

$$\cosh\left(\frac{\alpha d'}{2} \cos \Gamma_i\right) = I_0 \left\{ 1 + \frac{2I_2}{I_0} \cos 2\Gamma_i + \frac{2I_4}{I_0} \cos 4\Gamma_i + \dots \right\} \quad (C7)$$

where I_0 , I_2 and I_4 are modified Bessel functions [83] each of argument $\Lambda = \alpha d'/2$. The zeroth and first order terms of the potential expansion were obtained by Parker by introducing the parameter

$$\epsilon = \frac{2I_2(\Lambda)}{I_0(\Lambda)} \simeq \frac{\Lambda^2}{4 + \Lambda^2} \quad (C8)$$

Past the first order, however, ϵ is no longer a natural expansion parameter in Eq.(C7). Nevertheless, for the third term of Eq.(C7) we may write

$$\frac{2I_4(\Lambda)}{I_0(\Lambda)} = c_1 \epsilon^2, \quad (C9)$$

$$\text{where } c_1 = \frac{1}{2} \frac{I_4 I_0}{I_2^2} = \frac{1}{12} \left[1 + O\left(\frac{\Lambda^2}{4}\right) \right] \simeq \frac{1}{12}$$

since c_1 is a relatively weak function of Λ for $\Lambda \sim O(1)$. Hence Eq.(C7) may be approximated as

$$\cosh\left(\frac{\alpha d'}{2} \cos \Gamma_i\right) \approx I_0 \left\{ 1 + \epsilon \cos 2\Gamma_i + \frac{\epsilon^2}{12} \cos 4\Gamma_i + \dots \right\} \quad (C10)$$

Substituting the above into Eq.(C6) and the result into Eq.(C5), and choosing $K_1 I_0^2 = E'$ and $K_2 = E'$ then leads to

$$V = V_0(R) + \epsilon V_1(R, \phi, \psi_1, \psi_2) + \epsilon^2 V_2(R, \phi, \psi_1, \psi_2) + \dots \quad (C11)$$

where

$$\begin{aligned} V_0 &= E' \left\{ e^{-\alpha(R-D)} - 2e^{-\frac{\alpha}{2}(R-D)} \right\} \\ V_1 &= E' e^{-\alpha(R-D)} \left\{ \cos 2\Gamma_1 + \cos 2\Gamma_2 \right\} \\ V_2 &= E' e^{-\alpha(R-D)} \left\{ \cos 2\Gamma_1 \cos 2\Gamma_2 + (\cos 4\Gamma_1 + \cos 4\Gamma_2)/12 \right\} \end{aligned}$$

The zeroth order potential $V_0(R)$ is spherically symmetric and can be reduced to a form matching the Lennard-Jones 6-12 potential

$$V_{L-J}(R) = 4E' \left\{ \left(\frac{\sigma}{R} \right)^{12} - \left(\frac{\sigma}{R} \right)^6 \right\} \quad (C12)$$

by requiring that $V_0(R)$ vanish for $R = \sigma$. This leads to

$$D = \sigma + \frac{2}{\alpha} \ln 2$$

Substituting into the expression for $V_0(R)$ yields

$$V_0(R) = 4E' \left\{ \exp[-a'(R/\sigma - 1)] - \exp[-a'/2(R/\sigma - 1)] \right\} \quad (C13)$$

where $a' = \alpha\sigma$. In the above $E' = kT'$ represents the potential well depth which occurs at $R=D$ for V_0 while $R=\sigma$ is clearly the zero point for both V_0 and V_{L-J} .

Choice of Potential Parameters

We use the same values for the potential parameters α , σ , d' and T' used by Lordi and Mates for nitrogen. In Ref.[53], the value of the range factor α was chosen by matching an exponential type repulsion law

to virial coefficient data. The matching forms of Eqs. (C12) and (C13) allow the quantities T and σ to be chosen as those for the Lennard-Jones potential which has been used successfully in predicting the viscosity of both monatomic and diatomic gases. The Lennard-Jones values obtained from viscosity data and listed in Ref.[39] may then be used. For the value of d' we use that value which Parker determined by matching experimental values of the vibrational collision number to his theory at high temperatures.

For N_2 the complete set of parameters is

$$\begin{array}{ll} \alpha = 4.02 \text{ \AA}^{-1} & d' = 0.557 \text{ \AA} \\ \sigma = 3.681 \text{ \AA} & T' = 91.5^\circ\text{K} \end{array}$$

Hence $\Lambda = \alpha d^*/2 = 1.12$ and $\epsilon = 0.259$. The maximum value of d'/R will be of order $d'/\sigma \simeq 1/7$.

Appendix D

Three-Dimensional Rotations

For fully three-dimensional rotations it may be shown that Eq.(C11) is still a valid approximation to V , but that for this case

$$\cos \Gamma_i = \cos \theta \cos \beta_i + \sin \theta \sin \beta_i \cos(\phi - \psi_i) \quad (D1)$$

Hamilton's equations are the most suitable for the three-dimensional case.

The Hamiltonian is

$$H = \frac{P_R^2}{2\mu} + \frac{P_\theta^2}{2\mu R^2} + \frac{P_\phi^2}{2\mu R^2 \sin^2 \theta} + \sum_{j=1}^2 \frac{1}{2I} (P_{\beta_j}^2 + P_{\psi_j}^2 / \sin^2 \beta_j) + V \quad (D2)$$

from which the equations of motion can be derived in the usual manner as

$$\dot{R} = P_R, \quad \dot{P}_R = \frac{P_\theta^2}{R^3} + \frac{P_\phi^2}{R^3 \sin^2 \theta} - \frac{\partial V}{\partial R} \quad (D3A)$$

$$\dot{\theta} = \frac{P_\theta}{R^2}, \quad \dot{P}_\theta = \frac{P_\theta^2 \cos \theta}{R^2 \sin^2 \theta} - \frac{\partial V}{\partial \theta} \quad (D3B)$$

$$\dot{\beta}_i = \frac{1}{I} P_{\beta_i}, \quad \dot{P}_{\beta_i} = \frac{1}{I} \frac{P_{\psi_i}^2 \cos \beta_i}{\sin^3 \beta_i} - \frac{\partial V}{\partial \beta_i} \quad (D4A)$$

$$\dot{\psi}_i = \frac{1}{I} \frac{P_{\psi_i}}{\sin^2 \beta_i}, \quad \dot{P}_{\psi_i} = - \frac{\partial V}{\partial \psi_i} \quad (D4B)$$

Expanding each co-ordinate and conjugate momentum in terms of ϵ in Eqs.(D3) and (D4) as in Section 5.3, one obtains zeroth and first order sets of equations. The zeroth order solutions for R and ϕ are the same as those given in Section 5.4 for the planar rotation case. Zeroth order solutions for θ , β_i and ψ_i may be readily shown to be

$$\theta_0 = \pi/2 \quad (D5A)$$

$$\cos \beta_{i0}(t) = A \cos(J_i t + \hat{\delta}) \quad (D5B)$$

where $\cos \hat{\delta} = \cos \beta_{i0}(0)/A, \quad A = \sqrt{1 - \sin^2 \beta_{i0}(0) \sin^2 \eta_i}$

$$\sin \hat{\delta} = \cos \eta_i \sin \beta_{i0}(0)/A$$

$$\text{also } \psi_{i0}(t) = \text{atan} \left\{ \frac{F \sin(J_i t) + G \cos(J_i t)}{D \sin(J_i t) + E \cos(J_i t)} \right\} \quad (\text{D5C})$$

where

$$F = \sin \psi_{i0}(0) \cos \beta_{i0}(0) \cos \eta_i + \cos \psi_{i0}(0) \sin \eta_i$$

$$G = \sin \psi_{i0}(0) \sin \beta_{i0}(0)$$

$$D = \cos \psi_{i0}(0) \cos \beta_{i0}(0) \cos \eta_i - \sin \psi_{i0}(0) \sin \eta_i$$

$$E = \cos \psi_{i0}(0) \sin \beta_{i0}(0)$$

and where $J_i = |\underline{J}_i|$ is the magnitude of the angular velocity vector prior to collision, $\psi_{i0}(0)$ and $\beta_{i0}(0)$ are the zeroth order orientation angles at $t=0$ and η_i measures the direction of $\underline{J}_i$ in a plane normal to the molecular axis at $t=0$.

The rotational energy of each molecule is

$$E_{r_i} = \frac{1}{2I} \left\{ p_{\beta_i}^2 + \frac{p_{\psi_i}^2}{\sin^2 \beta_i} \right\} \quad (\text{D6})$$

Differentiating and using Eqs.(D4) we find that

$$\frac{dE_{r_i}}{dt} = -\frac{1}{I} \left\{ p_{\beta_i} \frac{\partial V}{\partial \beta_i} - \frac{p_{\psi_i}}{\sin^2 \beta_i} \frac{\partial V}{\partial \psi_i} \right\} \quad (\text{D7})$$

Writing $E_{r_i} = E_{r_{i0}}(0) + \epsilon E_{r_{i1}} + 0(\epsilon^2)$ and expanding the right hand side of Eq.(D7) in powers of ϵ , yields

$$\frac{dE_{r_{i1}}}{dt} = -\frac{1}{I} \left\{ p_{\beta_{i0}} \left(\frac{\partial V_1}{\partial \beta_i} \right)_0 - \frac{p_{\psi_{i0}}}{\sin^2 \beta_{i0}} \left(\frac{\partial V_1}{\partial \psi_i} \right)_0 \right\} \quad (\text{D8})$$

Integrating Eq.(D8) gives the first order rotational energy exchange for each particle as

$$E_{r_{i1}}(\infty) = \frac{1}{I} \int_{-\infty}^{\infty} \left\{ p_{\beta_{i0}} \left(\frac{\partial V_1}{\partial \beta_i} \right) - \frac{p_{\psi_i}}{\sin^2 \beta_{i0}} \left(\frac{\partial V_1}{\partial \psi_i} \right) \right\} dt \quad (\text{D9})$$

Using Eq.(C11) for V_1 with Γ_i given by Eq.(D1) and using Hamilton's

equations (D4), the above can be written as

$$E_{r_{i1}}(\infty) = 2E' \int_{-\infty}^{\infty} \{ \dot{\psi}_{i0} \sin^2 \beta_{i0} \sin[2(\phi_0 - \psi_{i0})] - \dot{\beta}_{i0} \sin 2\beta_{i0} \cos^2(\phi_0 - \psi_{i0}) \} e^{-\alpha(R-D)} dt \quad (D10)$$

It is easily verified that for the planar rotation case ($\beta_{i0} = \pi/2$), Eq.(D10) reduces to Eq.(27) of the main text and that Eq.(D5C) reduces to $\psi_{i0} = J_i t + \psi_{i0}(0)$ as for Eq.(17). An approximate analytical expression for $E_{r_{i1}}(\infty)$ could be obtained in much the same way as for the planar rotation case. Near $t=0$, Eqs.(D5) could be approximated by a first order Taylor expansion as for Eq.(34) of the main text. However, an expansion to $O(t)$ for $\dot{\psi}_{i0}$ and $\dot{\beta}_{i0}$ would also be required since for the three-dimensional case, these quantities are not constant. This could be obtained from Eqs. (D5B) and (D5C) but would be complicated. When the appropriate expressions were substituted into Eq.(D10), an integrable but complex closed form result would be obtained. While this would not be suitable for Monte-Carlo simulations of bulk fluid flows, it might nevertheless be useful in detailed calculations of the transport properties of diatomic gases.

A formal expression for the second order (or n^{th} order) energy exchange can be obtained but appears to be hopelessly complicated.

Appendix E

Contour Integrations

The integrals appearing in Eqs. (36) and (54), namely

$$L_1 = \int_{-\infty}^{\infty} \frac{\cos(2v_i t) dt}{[A \cosh(at) - 1]^2} \quad (E1)$$

and

$$L_2 = \int_{-\infty}^{\infty} \frac{t \sin(2v_i t) dt}{[A \cosh(at) - 1]^2} \quad (E2)$$

may be readily evaluated by contour integration in the z plane, where

$z = t + iS$. In the above

$$a = \alpha \xi / 2, \quad A = (1 + \xi^2 / \beta^2)^{\frac{1}{2}}$$

and ξ and β are as for Eq.(31).

Firstly for the integral (E1), consider the contour integral

$$J = \int_C \frac{\cos(2v_i z) dz}{[A \cosh(az) - 1]^2} \quad (E3)$$

where C is the rectangle ABCD in the $z = t + iS$ plane as shown in Fig.E1.

Writing

$$J = J_{AB} + J_{BC} + J_{CD} + J_{DA} \quad (E4)$$

where each term on the right hand side of the above refers to that part of J evaluated along the appropriate sement of C . It may be readily shown that as $T \rightarrow \infty$

$$J_{AB} \rightarrow L_1, \quad J_{BC} \rightarrow 0$$

$$J_{CD} \rightarrow -L_1 \cosh(4\pi v_i / a), \quad J_{DA} \rightarrow 0$$

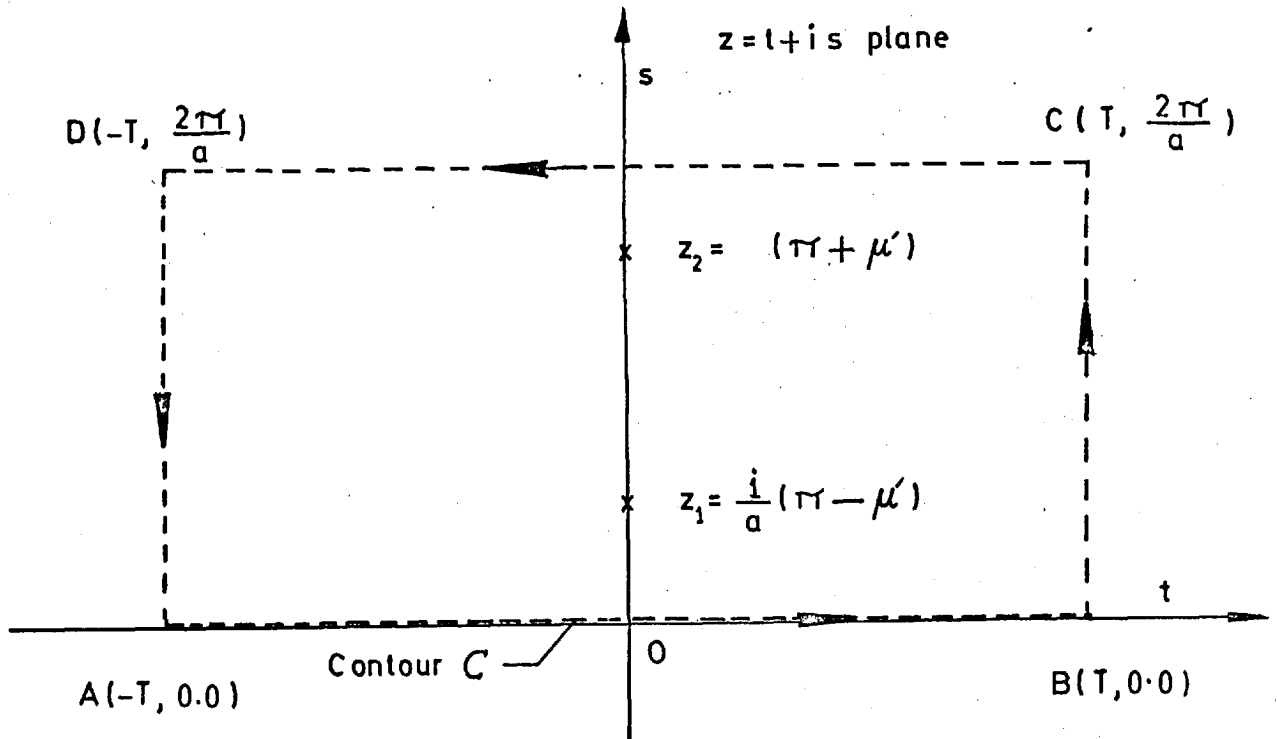


Fig. E1 Contour in $z = t + is$ Plane for
Contour Integration

Thus from Eq. (E4) as $T \rightarrow \infty$

$$L_1 = \frac{J}{[1 - \cosh(4\pi v_1/a)]} \quad (\text{E5})$$

The integral J may be evaluated from Cauchy's Residue theorem as there are two poles falling within C at

$$z_1 = \frac{i}{a} (\pi - \mu'), \quad z_2 = \frac{i}{a} (\pi + \mu')$$

where $\mu' = \pi/2 + \text{atan}(\beta/\xi)$.

The residue at these may be obtained by expanding the integrand in a Laurent series about the appropriate pole. The residue R_ℓ at pole z_ℓ turns out to be

$$R_\ell = - \frac{\left[2v_i \sin(2v_i z_\ell) + a \cos(2v_i z_\ell) \frac{\cosh(az_\ell)}{\sinh(az_\ell)} \right]}{[A a \sinh(az_\ell)]^2} \quad \ell = 1, 2 \quad (\text{E6})$$

Thus R_1 and R_2 may be evaluated, yielding from the Residue theorem and Eq.(E5)

$$L_1 = \frac{2\pi}{a} \left(\frac{\beta}{\xi} \right)^3 Q \quad (E7)$$

where $Q = \left[\sinh \delta + \frac{2v_i}{a} \cosh \delta \right] / \sinh \Gamma$

and $\delta = \frac{2\mu v_i}{a}$, $\Gamma = \frac{2\pi v_i}{a}$

The above result agrees with that given by Lordi and Mates [53].

The integral L_2 may be obtained in an exactly analogous manner by considering the integral

$$K = \int_C \frac{z \sin(2v_i z)}{[A \cosh(az) - 1]^2} dz \quad (E8)$$

around the contour C defined previously. In this case, it may be readily verified that in the limit $T \rightarrow \infty$

$$L_2 = \frac{\left[K - \frac{2\pi}{a} L_1 \sinh\left(\frac{4\pi v_i}{a}\right) \right]}{\left[1 - \cosh\left(\frac{4\pi v_i}{a}\right) \right]} \quad (E9)$$

The residue of the integrand in Eq.(E8) is obtained in a similar manner to that for Eq.(E3), the result being, at pole $z = z_\ell$

$$R_\ell = \frac{\left[\sin(2v_i z_\ell) + 2v_i z_\ell \cos(2v_i z_\ell) - a \frac{\cosh(az_\ell)}{\sinh(az_\ell)} z_\ell \sin(2v_i z_\ell) \right]}{[A a \sinh(az_\ell)]^2} \quad (E10)$$

The evaluation of the above at z_1 and z_2 leads to an expression for K using the Residue theorem. Equation (E7) may then be used for L_1 together with this result for K to evaluate the right hand side of Eq.(E9). After considerable algebra one finally obtains

$$L_2 = - \left(\frac{2\pi}{a^2} \right) \left(\frac{\beta}{\xi} \right)^2 P \quad (E11)$$

where

$$P = \left[\cosh \delta (\sinh \Gamma - \Gamma \cosh \Gamma) + \delta \sinh \Gamma \sinh \delta \right. \\ \left. + \left(\frac{\beta}{\xi} \right) \{ \mu \sinh \Gamma \cosh \delta - \pi \cosh \Gamma \sinh \delta \} \right] / \sinh^2 \Gamma$$

A detailed examination of expressions (E7) and (E11) shows that L_1 is an even function of v_i , positive for all v_i , while L_2 is an odd function of v_i , positive for all $v_i < 0$. The product $v_i L_2$, then, is always negative as is $v_i L_1 L_2$.

Appendix F

Collision Integrals

The reduced collision integrals relevant to the coefficient of viscosity of a single component simple monatomic gas are [39]

$$Q^{(2)*}(g^*) = 3 \int_0^\infty \sin^2 \chi \, b^* \, db^* \quad (F1)$$

$$\Omega^{(2,2)*}(T/T') = \frac{1}{3(T/T')^4} \int_0^\infty g^{*7} Q^{(2)*}(g^*) e^{-g^{*2}/(T/T')} \, dg^* \quad (F2)$$

where $\chi(g^*, b^*)$ is given by Eq.(21) of the main text. For a hard sphere gas both the above quantities are unity. Tables of $Q^{(2)*}$ and $\Omega^{(2,2)*}$ for the Lennard-Jones 6-12 potential may be found in Ref.[58].

For the Morse potential given by Eq.(10) of the main text, the reduced collision integrals were calculated over ranges of g^* and T/T' respectively, for $a = 14.80$. To obtain values of $Q^{(2)*}$, a suitable transformation of b^* was used to reduce the integral in Eq.(F1) to one over a finite range. The resulting integral was then segmented into a number of smaller ones in such a way that the singularity in χ at low g^* was isolated. Integrals not containing a singularity were each evaluated numerically using Gauss-Laguerre 12 point quadrature, values of χ being obtained by 16 point G-L quadrature of Eq.(21) in the main text. The integral containing the singularity was treated in similar fashion to that for an equivalent singularity for the Lennard-Jones potential in Ref.[58].

In this way some 300 values of $Q^{(2)*}$ were obtained for 300 values of g^* in the range $(10^{-3}, 10^4)$. Best fit curves of the form

$$A \, g^{*n} \sum_{m=1}^N C_m T_m(g^{*2})$$

where A , n and C_m , $m=1,N$, are constants and T_m is a Chebychev polynomial of order m , were then fitted to the 300 values of $Q^{(2)*}$ in each of 10 appropriately chosen segments of the above g^* range. For a range of values of T/T' , the contribution to the integral in Eq.(F2) in each of the 10 segments were obtained using a Gauss-Laguerre 10 point formula and the results summed to give $\Omega^{(2,2)*}(T/T')$.

Values of $Q^{(2)*}$ and $\Omega^{(2,2)*}$ so obtained are shown in Figs 4A and 4B compared with values for the Lennard-Jones potential. The procedure described above was tested by computing a few values of $Q^{(2)*}$ for the L-J potential. At high g^* , these agreed to four figures with the results of Ref.[58] while at low $g^* < g_c^*$, the agreement was to the third significant figure.

Appendix G

Coarse Graining

The questions of cell size, choice of Δt_m and the simulator particle number density are briefly discussed in this Appendix under the above general title.

G1 Cell Size

Typically the simulated region was divided into 600-700 rectangular cells which varied in size depending on the expected local flow gradients indicated by experiment. Figure 8 shows typical cell structuring in various parts of the flow field.* Immediately downstream of $x = 0$, near the plate surface, cells were of size $\Delta x = \lambda_\infty$, $\Delta y = \lambda_\infty/2$ for most runs. However, to investigate the shadow region which Lewis [51] claims has an important bearing on the initial flow, somewhat thinner cells of size $\Delta x = 2\lambda_\infty$, $\Delta y = \lambda_\infty/6$ were used for the $M_\infty = 25$ calculation. Away from the immediate vicinity of the plate flow gradients are smaller (provided the shock remains fairly thick) and rather larger cells, typically $\Delta x = 4\lambda_\infty$, $\Delta y = \lambda_\infty$, may be used.

G2 Choice of Δt_m

The general requirements for Δt_m were given in Section 4.2. A condition of particular importance for leading edge flows is that Δt_m should be less than the free times of order λ_{fb}/U_∞ and $\lambda_{bf}/\bar{c}_b$ associated

* Included in Fig. 8 is an illustration of the cell structuring near the step for a flat plate-step calculation that has been performed but which is not described in the present dissertation.

with free stream body particle first collisions. Vogenitz et al. [80] suggest that $\Delta t_m \leq t_m/M_\infty$ for flow near a wall, which from Eq.(A13) of Appendix A (with $\hat{g}' = M_\infty$), may be shown to satisfy the above conditions. Hence $\hat{\Delta t}_m \approx 1/M_\infty$ was generally chosen for the present calculations although a somewhat smaller value of $1/2M_\infty$ was employed for the $M_\infty = 25$ case in which the leading edge cell size $\Delta y = \lambda_\infty/6$ was rather small. This is to satisfy Eq.(1) for the convection condition for body emitted particles.

G3 Simulation Particle Number Density

As is indicated in Appendix A, the simulation should not depend, in a systematic manner, on the number of simulator particles per cell in the flow at any given instant. Derzko [28] has shown that the computing time required per independent sample particle observation for data acquisition is roughly independent of the instantaneous number of particles in the flow, or in a cell. Hence from the point of view of core storage, a small overall number is desirable. There are, however, lower limits on N_k which should be avoided. For example, if N_k is such that mean values of $\hat{\Delta t}_k$ are of order $\hat{\Delta t}_m$ then because of the time discretization, a statistically inadequate collision increment to the local particle ensemble per Δt_m may result [15]. Bird [17] suggests that for this reason N_k should not be smaller than about six. In the present calculations this constraint was applied to the smallest cells with the larger ones containing typically 10-15 particles at a given instant. To keep N_k approximately constant in cells of widely differing areas, a weighting factor scheme [28] was employed whereby the relative values of $\bar{\rho}$ are different in various regions of the flow.

In general the choice of Δt_m , Δx , Δy and N_k for a particular problem require some experience with the Direct Simulation method. However,

provided certain constraints such as those discussed above are observed, a wide range of choice is generally available through which the calculated results show remarkably little variation. The sensitivity of the present calculations to the choice of the above quantities is discussed in various sections of the main text.

In a typical simulation for the high M_∞ cases there were about 8000 sample particles in the flow field at any one instant. The simulations were run for about 1200-1500 Δt_m 's and involved the calculation of $O(10^6)$ collisions. Steady state conditions were assumed to exist at about 300 Δt_m after which the flow field properties were sampled, say every 8 Δt_m 's. A typical calculation required 25-30 minutes on a CDC-7600 machine. While this is very long by any standards, it is felt that we have been conservative in the coarse graining (in the interests of accuracy) and that by using larger cells, etc., reasonable results could have been obtained in considerably shorter computing times.

Appendix H

Free Molecule Flow for the Flat Plate Problem

The distribution function for the flow adjacent to a wall can be written as

$$f = \frac{n_r^+ f_r^+ + n_i^- f_i^-}{\frac{1}{2}(n_r^+ + n_i^-)} \quad (H1)$$

where f_r^+ and f_i^- are the half space distribution functions for reflected particles ($V_y > 0$) and for incident particles ($V_y < 0$) respectively. The n_r^+ and n_i^- are the reflected and incident half space particle number densities. For free molecule flow past a flat plate at zero incidence, f_i^- is one half of the free stream distribution function, viz,

$$f_i^- = \left(\frac{m}{2\pi k T_\infty} \right)^{3/2} \exp[-((V_x - U_\infty)^2 + V_y^2 + V_z^2)/2kT_\infty] \cdot \frac{1}{kT_\infty} \exp(-E_r/kT_\infty) \quad (H2)$$

$V_y < 0$

and $n_i^- = n_\infty/2$.

For a translationally and rotationally completely accommodating surface at temperature T_w , f_w^+ can be written as

$$f_w^+ = \left(\frac{m}{2\pi k T_w} \right)^{3/2} \exp\left[\frac{-(V_x^2 + V_y^2 + V_z^2)}{2kT_w} \right] \frac{1}{kT_w} \exp\left(\frac{-E_r}{kT_w} \right) \quad (H3)$$

$V_y > 0$

The n_r^+ can be obtained from a number flux balance at the surface and may be readily shown to be

$$\frac{n_r^+}{n_\infty} = \frac{1}{2} \sqrt{\frac{T_\infty}{T_w}} \quad (H4)$$

The specification of f is then complete.

The various moments of f representing free molecular number flux, normal pressure, etc., may be easily obtained. In nondimensional form

these are

Number Flux

$$N/n_{\infty} U_{\infty} = \frac{1}{M_{\infty} \sqrt{2\pi\gamma}} \quad (H5)$$

Normal Pressure

$$P_n/P_{\infty} = \frac{1}{2}(1 + \sqrt{T_w/T_{\infty}}) \quad (H6)$$

Heat Transfer

$$C_H = \dot{q}/\frac{1}{2}\rho_{\infty} U_{\infty}^3 = \frac{1}{M_{\infty} \sqrt{2\pi\gamma}} \left[1 + \frac{6}{\gamma M_{\infty}^2} \left(1 - \frac{T_w}{T_{\infty}} \right) \right] \quad (H7)$$

Skin Friction

$$C_F = \tau_w/\frac{1}{2}\rho_{\infty} U_{\infty}^2 = \frac{1}{M_{\infty} \sqrt{\pi}} \left(\frac{2}{\gamma} \right)^{\frac{1}{2}} \quad (H8)$$

In addition free molecule values of density, velocity and temperature at the surface may also be found;

$$n/n_{\infty} = \frac{1}{2}(1 + \sqrt{T_{\infty}/T_w}) \quad (H9)$$

$$u/a_{\infty} = M_{\infty}/(1 + \sqrt{T_{\infty}/T_w}) \quad (H10)$$

$$T_{xx}/T_{\infty} = \sqrt{\frac{T_w}{T_{\infty}}} \left[1 + \gamma M_{\infty}^2 \left(\frac{T_{\infty}}{T_w} \right) (1 + \sqrt{T_{\infty}/T_w})^{-2} \right] \quad (H11)$$

$$T_{yy}/T_{\infty} = T_{zz}/T_{\infty} = T_R/T_{\infty} = \sqrt{T_w/T_{\infty}} \quad (H12)$$

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M_∞	S_∞	T_∞ (°K)	T_w/T_∞	T_w/T_0	γ	COLLISION MODEL	$\lambda_\infty/\lambda_{fb}$	$\lambda_\infty/\lambda_{bf}$	$\hat{x} \bar{V}^2$	LEADING EDGE ANGLE °	L/λ_∞
12.9	11.8	-	4.51	0.08	1.67	HARD SPHERE	0.33	3.9	3.68	0	60
21.0	19.2	20	14.4	0.097	1.67	MORSE POTENTIAL	0.073	1.40	6.94	10	96
10.15	8.49	139	2.16	0.10	1.4	PARKER POTENTIAL	0.31	2.62	5.60	0	60
22.9	19.2	20	14.4	0.136	1.4	"	0.073	1.40	8.24	10	96
23.4	19.6	13.5	21.5	0.195	1.4	"	0.061	0.990	7.34	10	114
25.0	20.9	10	30.0	0.238	1.4	"	0.048	1.00	7.10	10	102

Flow Conditions and Details of Body Geometry

TABLE I

M_∞	T_w/T_∞	γ	n/n_∞	P_n/P_∞	$N/\frac{1}{2}\rho U_\infty$	C_H	C_F	u/a_∞	T_{xx}/T_∞	T_{yy}/T_∞ T_{zz}/T_∞ T_R/T_∞
12.9	4.51	1.67	0.735	1.56	0.0239	0.0221	0.0478	8.77	62.6	2.12
21.0	14.4	1.67	0.632	2.40	0.0147	0.0131	0.0294	16.62	125.3	3.79
10.15	2.16	1.4	0.840	1.23	0.0332	0.0316	0.0664	6.04	36.2	1.46
22.9	14.4	1.4	0.632	2.40	0.0147	0.0131	0.0294	18.15	125.3	3.79
23.4	21.5	1.4	0.608	2.82	0.0144	0.0121	0.0288	19.24	116.5	4.64
25.0	30.0	1.4	0.591	3.24	0.0135	0.0108	0.0270	21.14	119.7	5.48

Free Molecule Values of Surface Properties

TABLE II

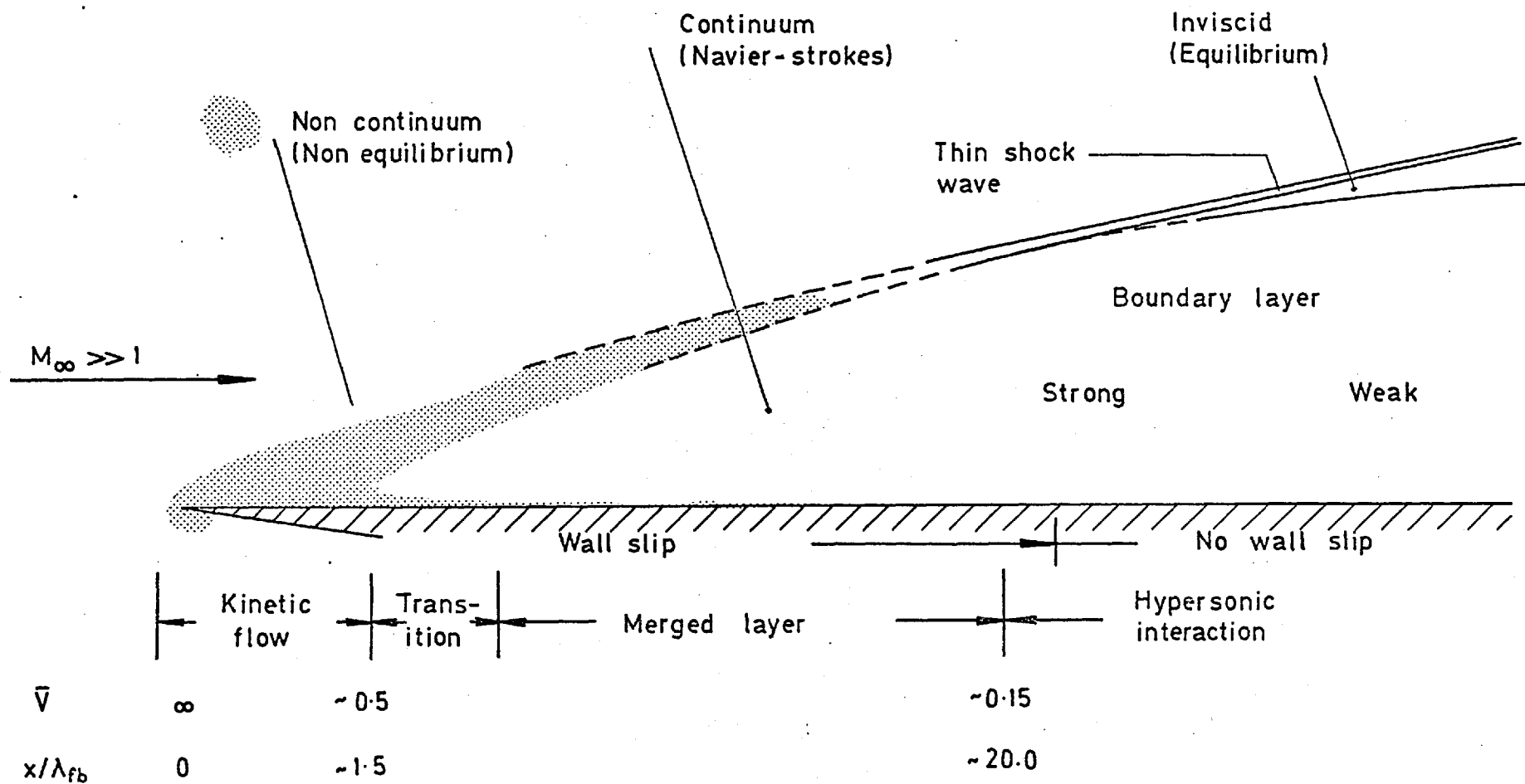


FIG. 1. SCHEMATIC MODEL OF LEADING EDGE FLOW.

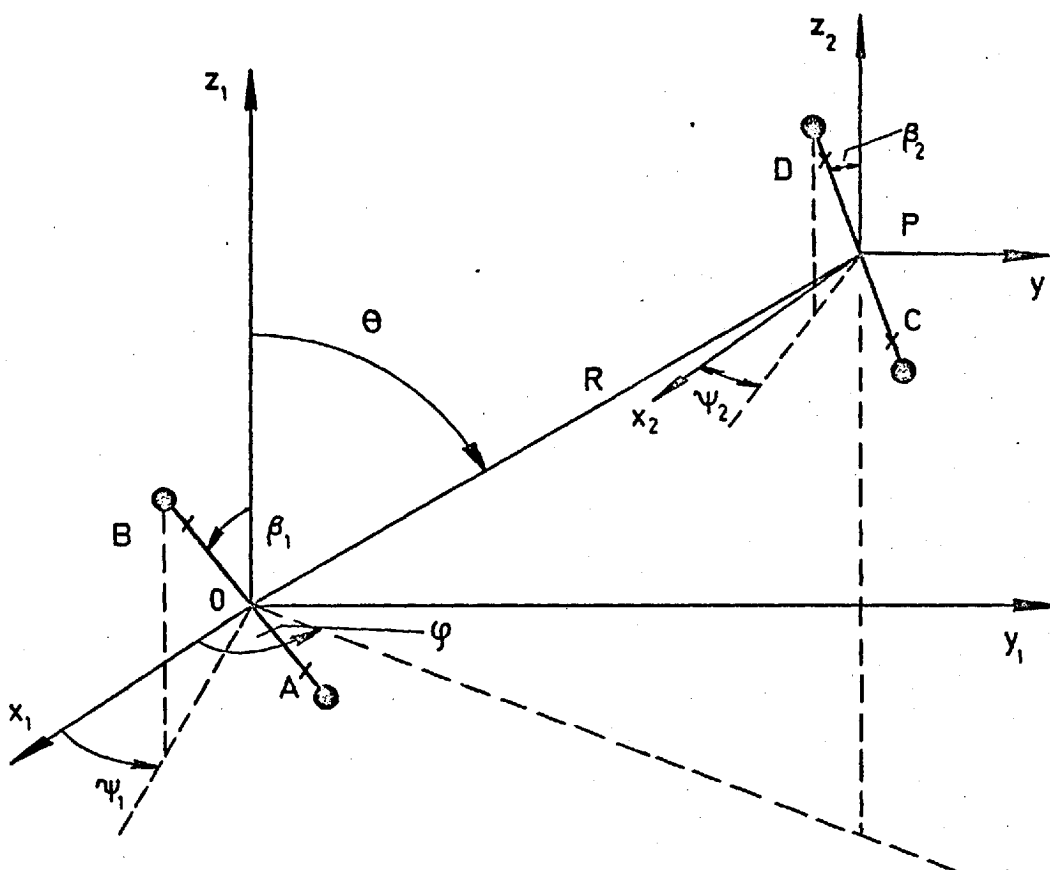


FIG. 2A MOLECULAR ORIENTATIONS FOR 3-DIMENSIONAL ROTATIONS.

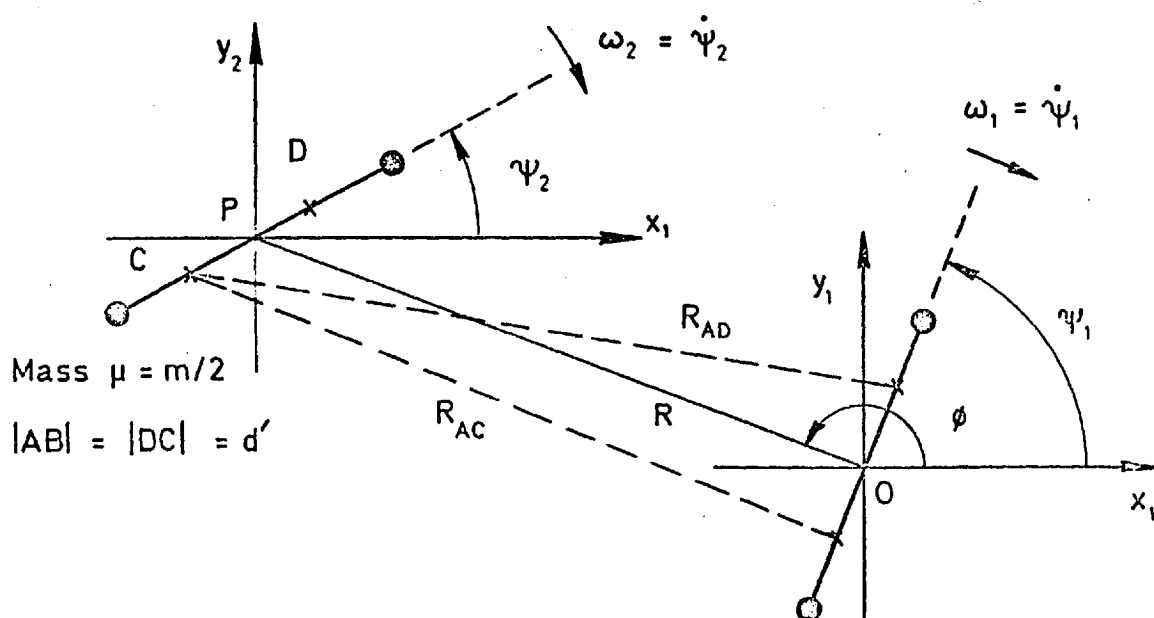


FIG. 2B MOLECULAR ORIENTATION FOR PLANAR ROTATION.

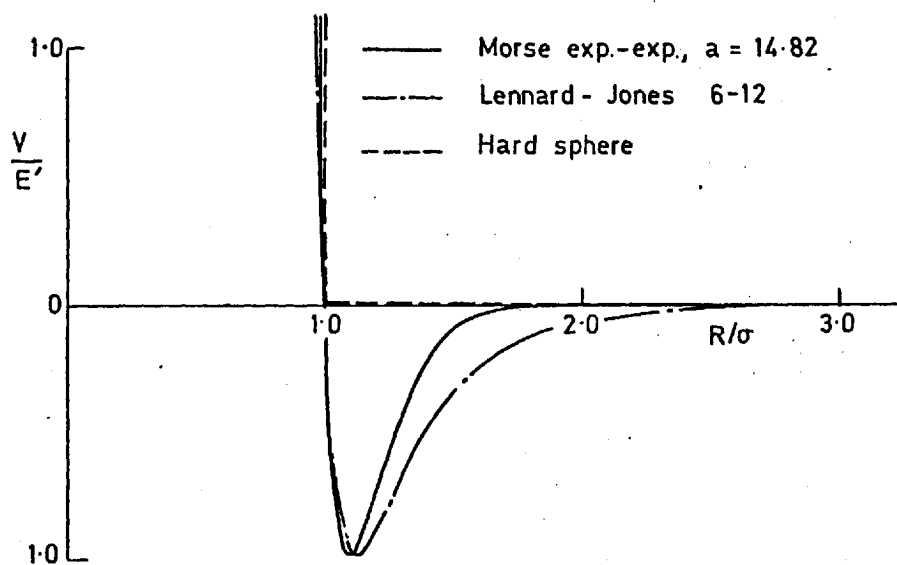


FIG. 3A INTERMOLECULAR POTENTIAL (ZEROTH ORDER).

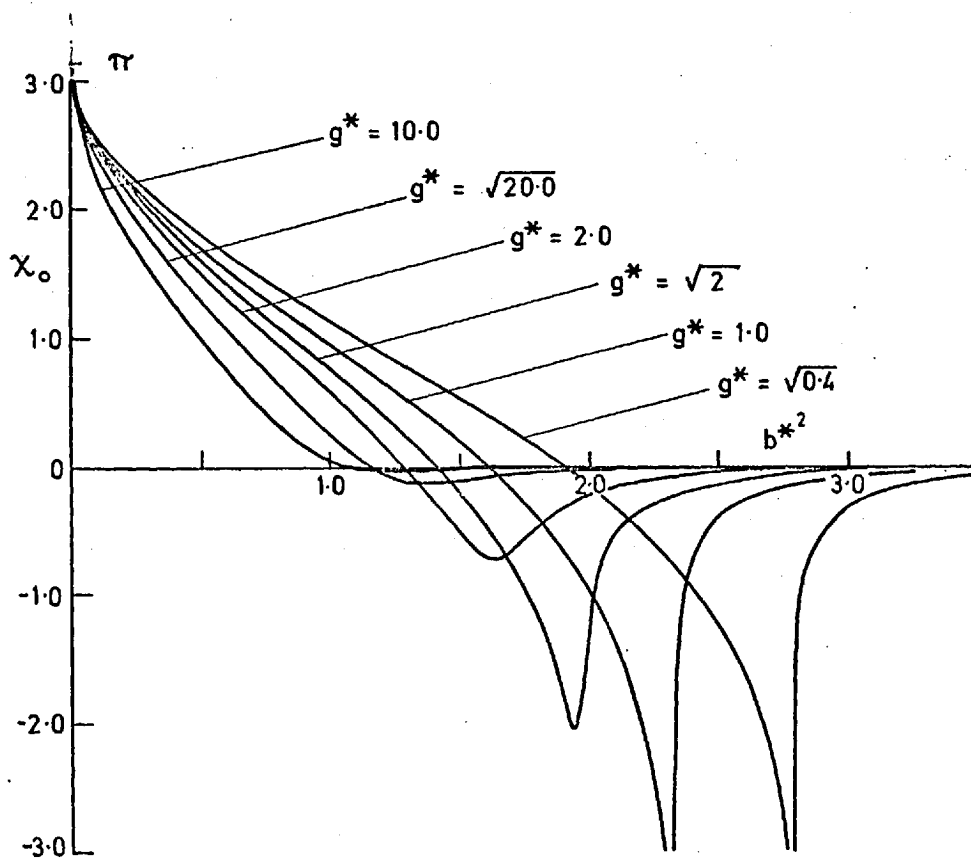


FIG. 3B ZEROTH ORDER DEFLECTION ANGLE (MORSE POTENTIAL).

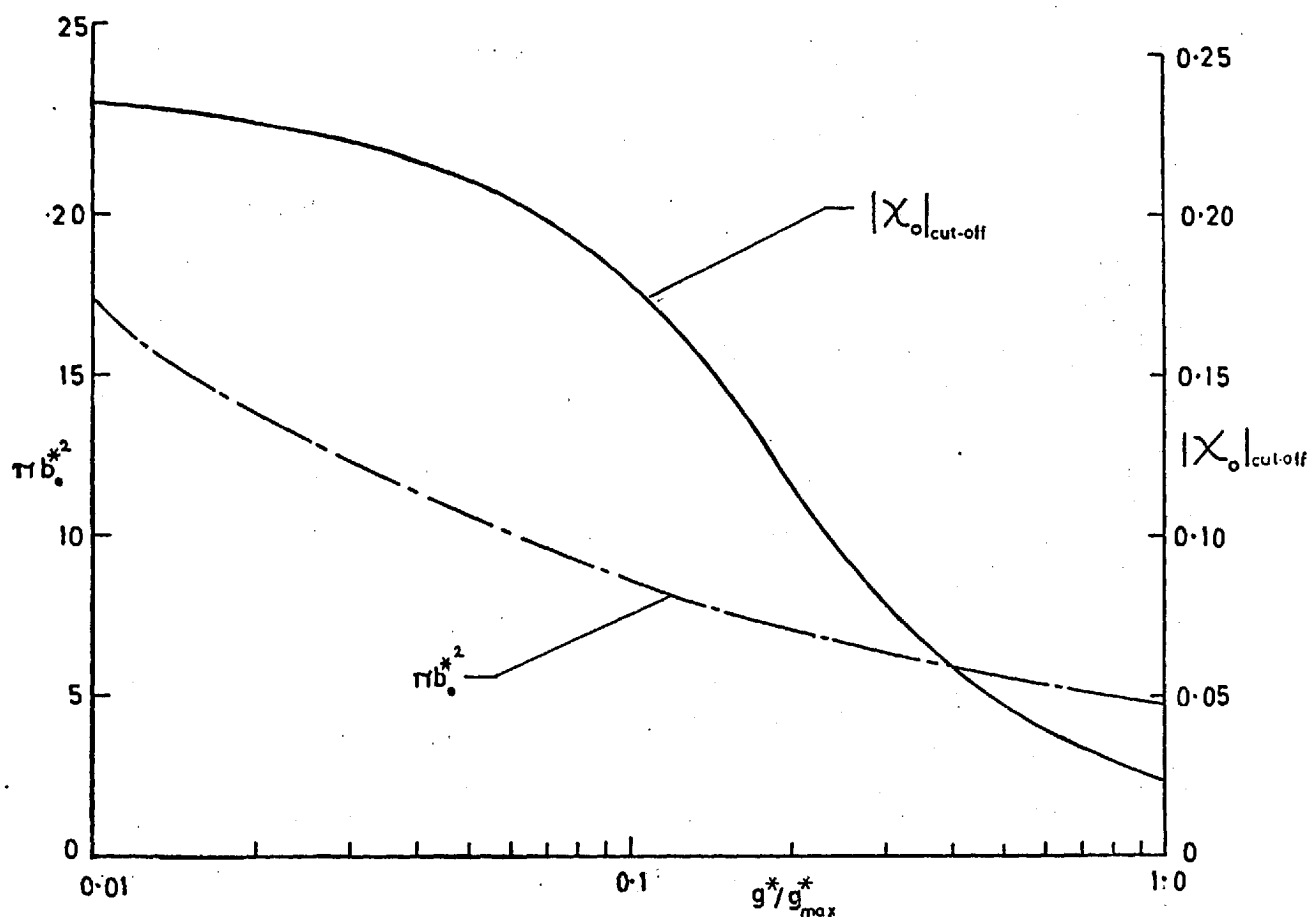


FIG. 3C COLLISION CROSS SECTION AND CUT-OFF DEFLECTION ANGLE

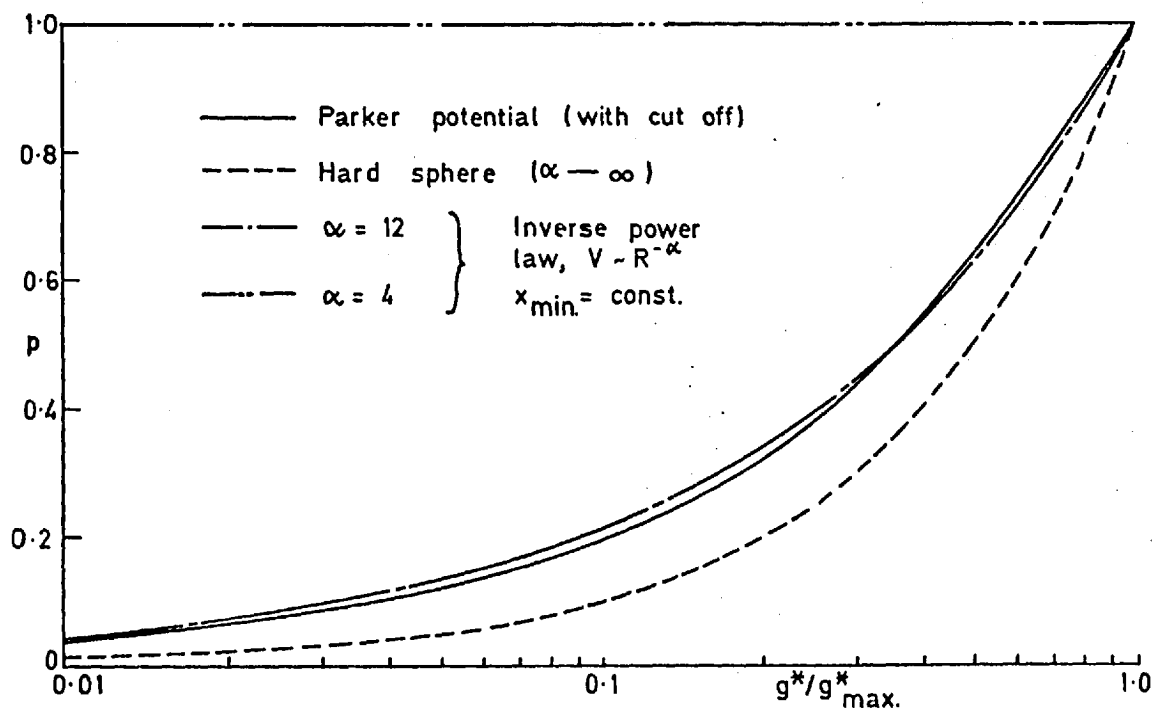
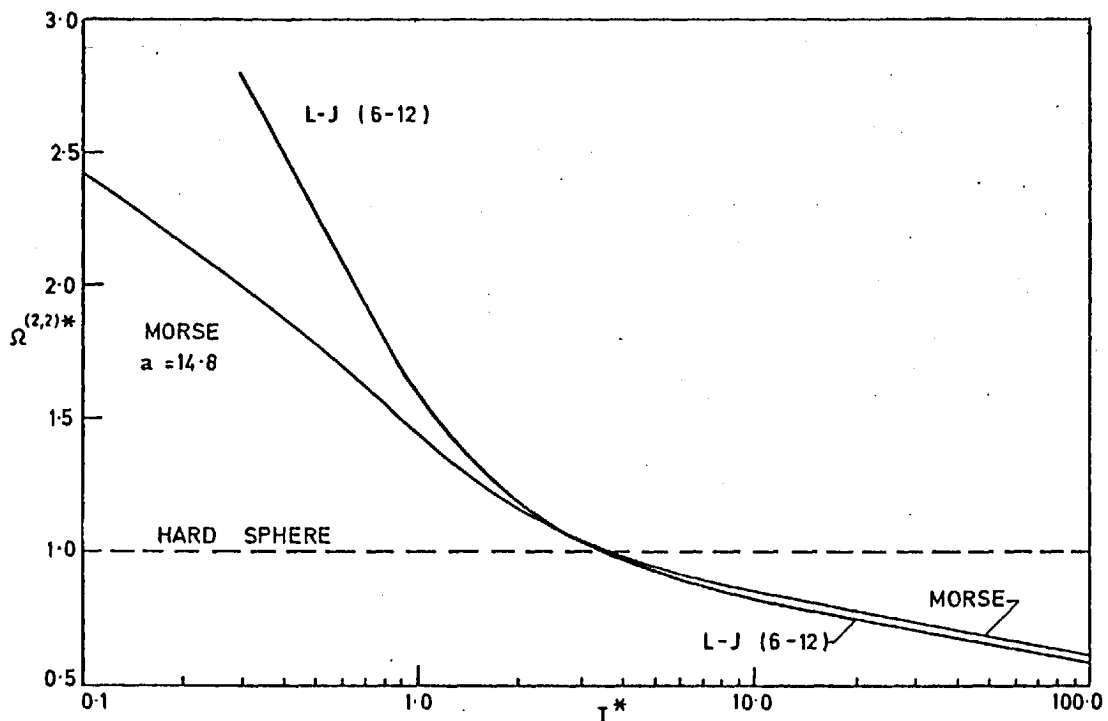
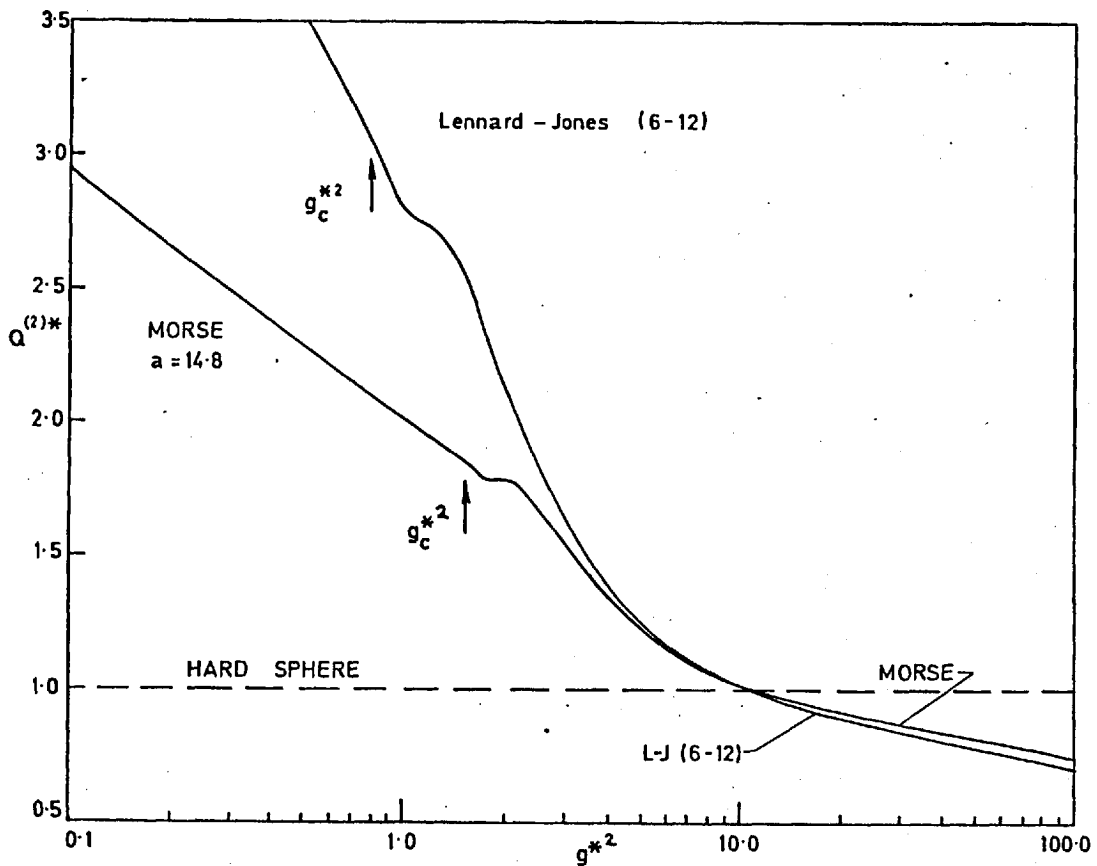


FIG. 3D CONDITIONAL COLLISIONAL PROBABILITY.



REDUCED COLLISION INTEGRALS $Q^{(2)*}(g^{*2})$ AND $\Omega^{(2,2)*}(T^*)$.

FIGS. 4A(top) and 4B

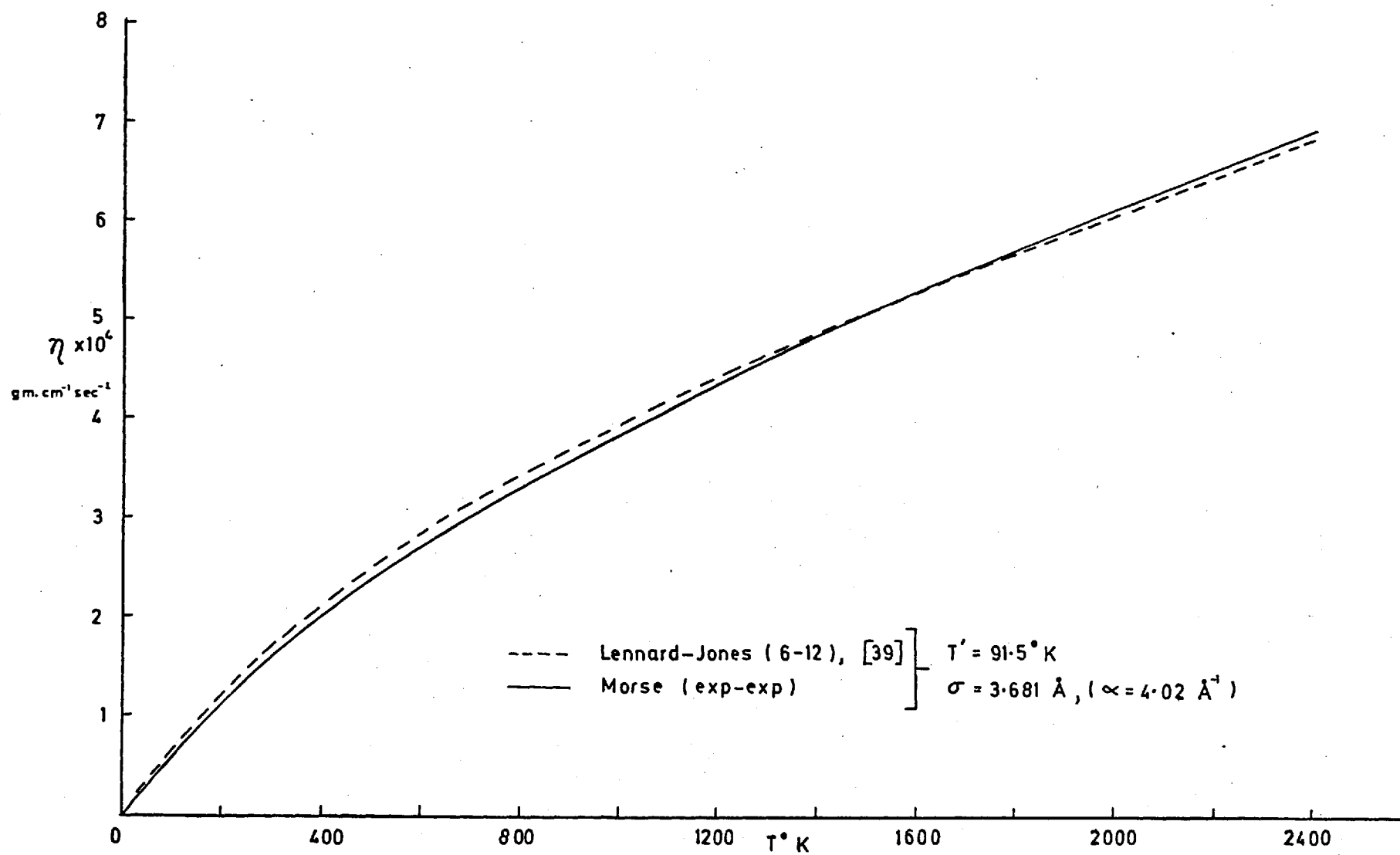


FIG.5 VISCOSITY OF NITROGEN.

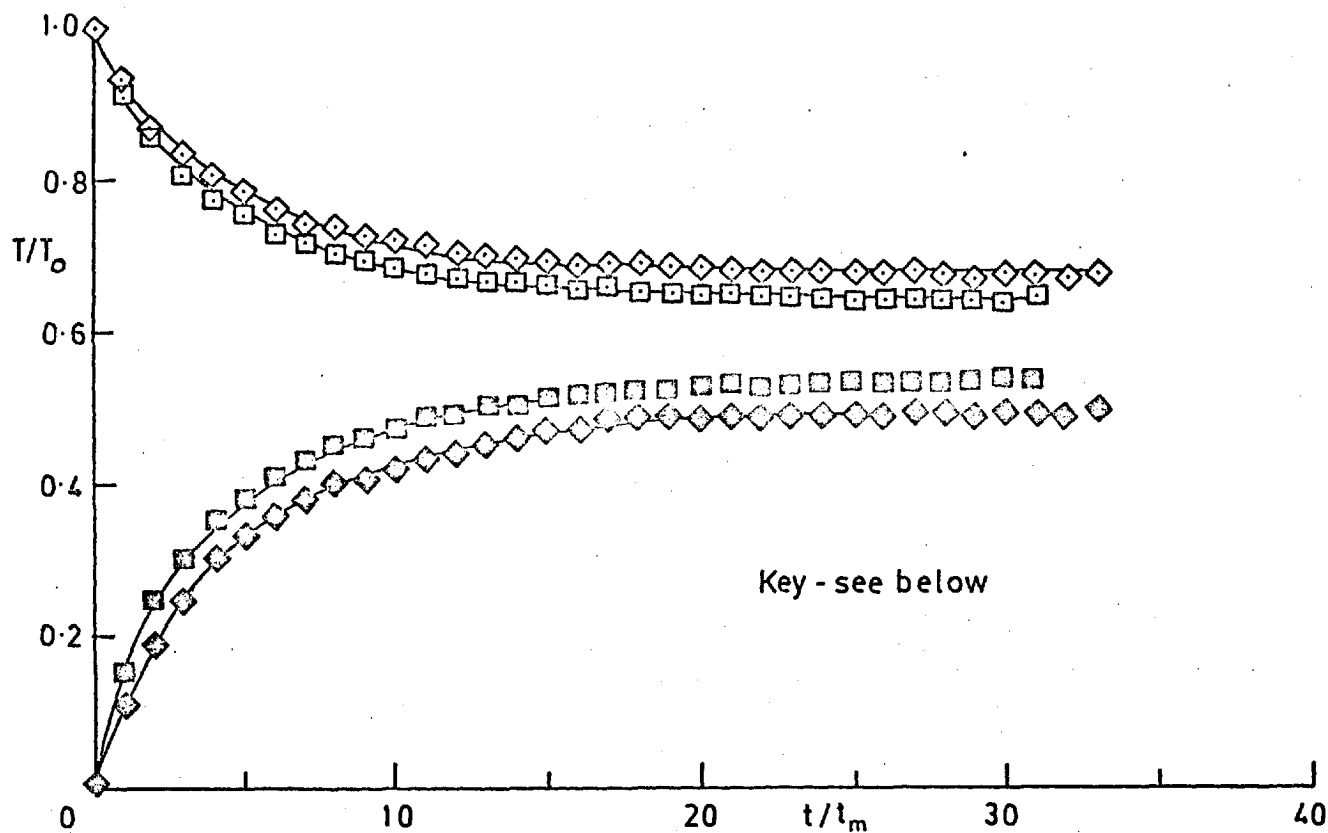


FIG. 6A ROTATIONAL RELAXATION IN NITROGEN, $\dot{\lambda} = 1.0$

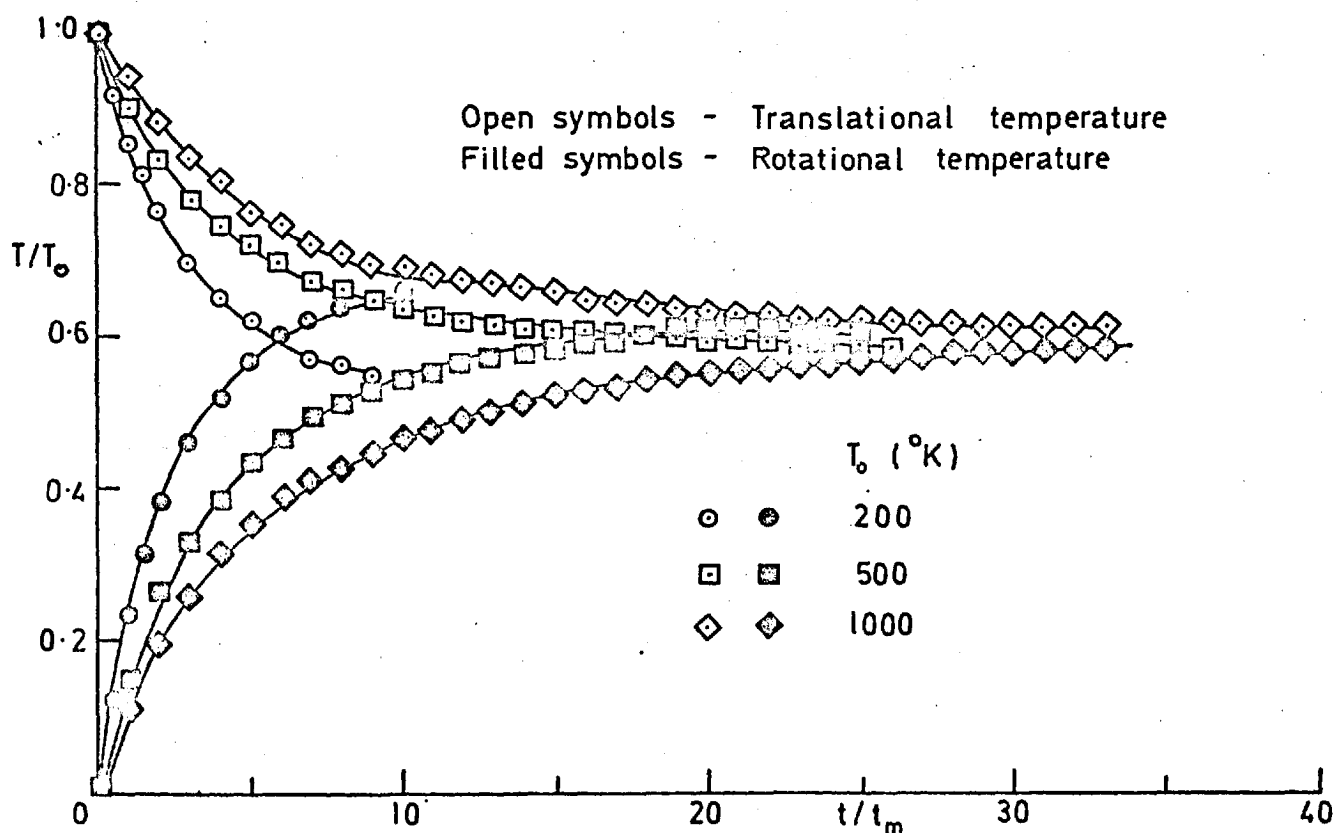
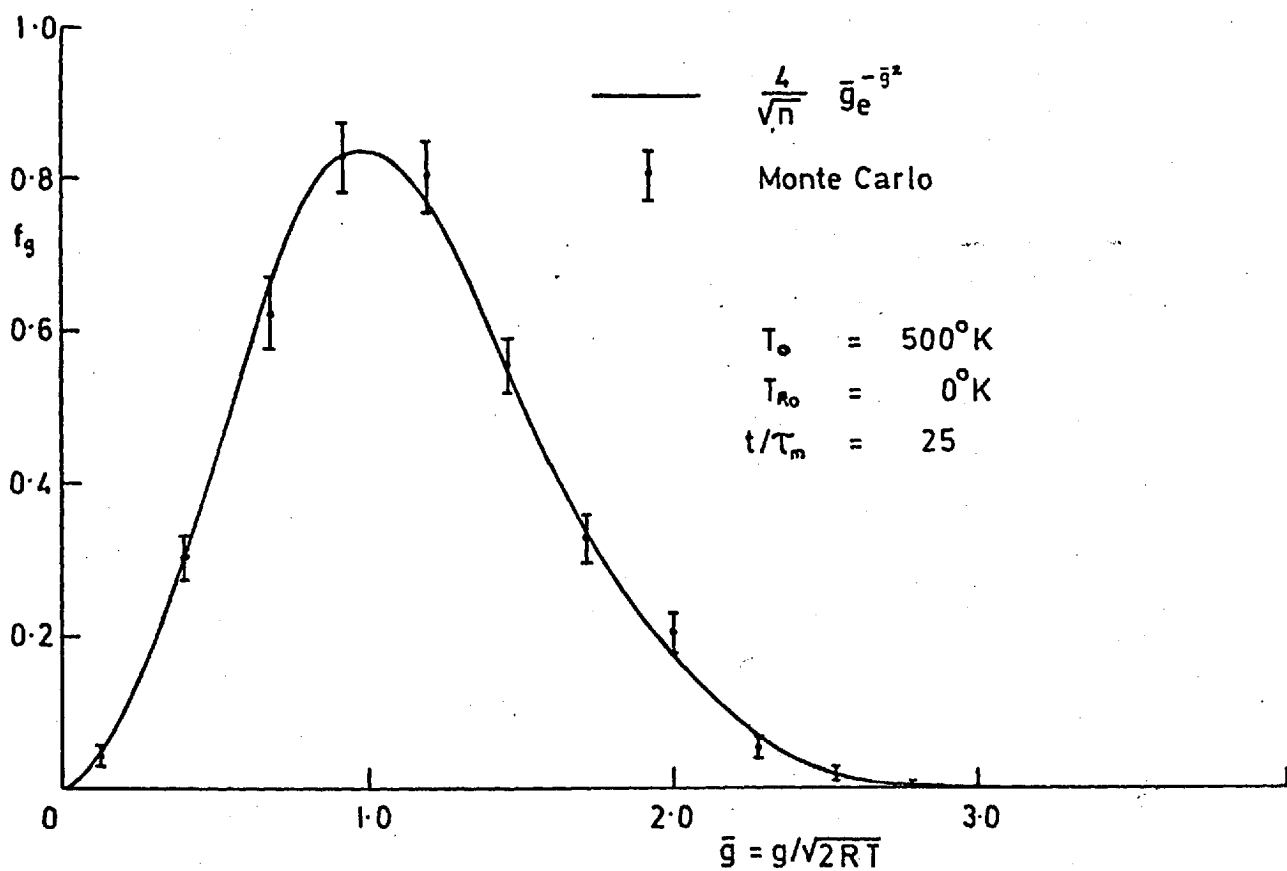


FIG. 6B ROTATIONAL RELAXATION IN NITROGEN, $\dot{\lambda} = 0.75$



SPEED DISTRIBUTION, $T \approx 300^\circ\text{K}$.

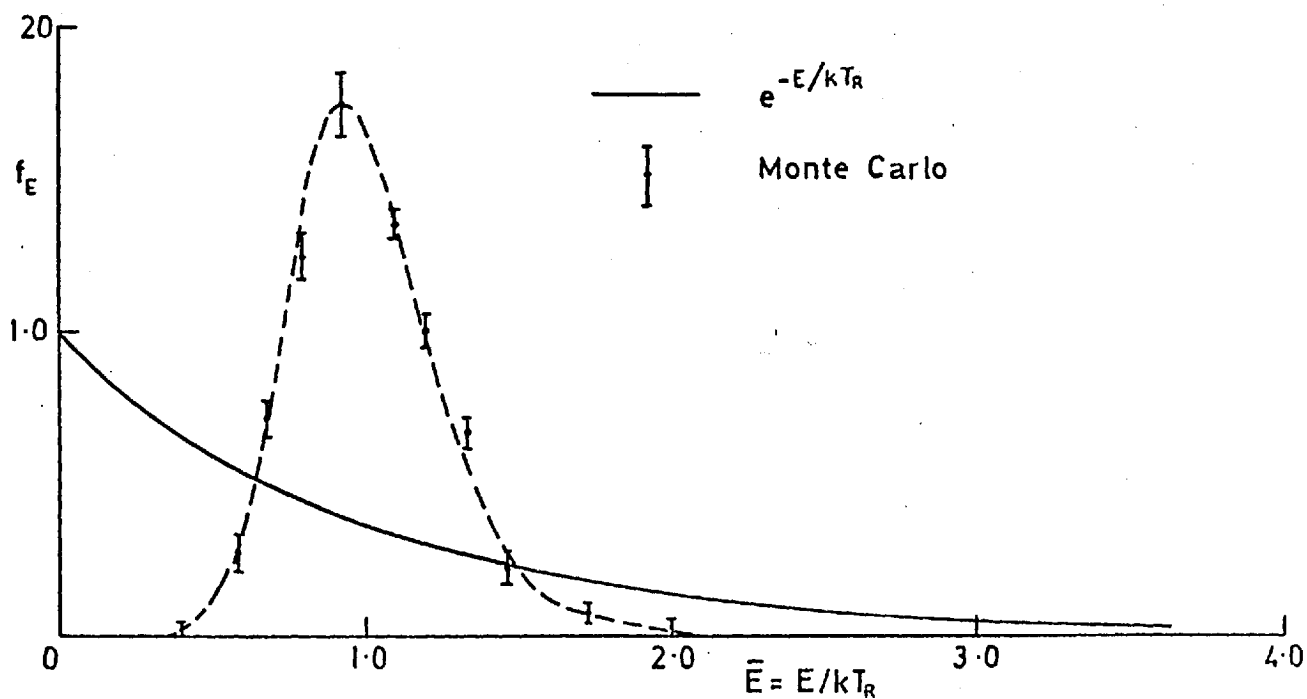


FIG. 6C ROTATIONAL ENERGY DISTRIBUTION, $T_R \approx 300^\circ\text{K}$

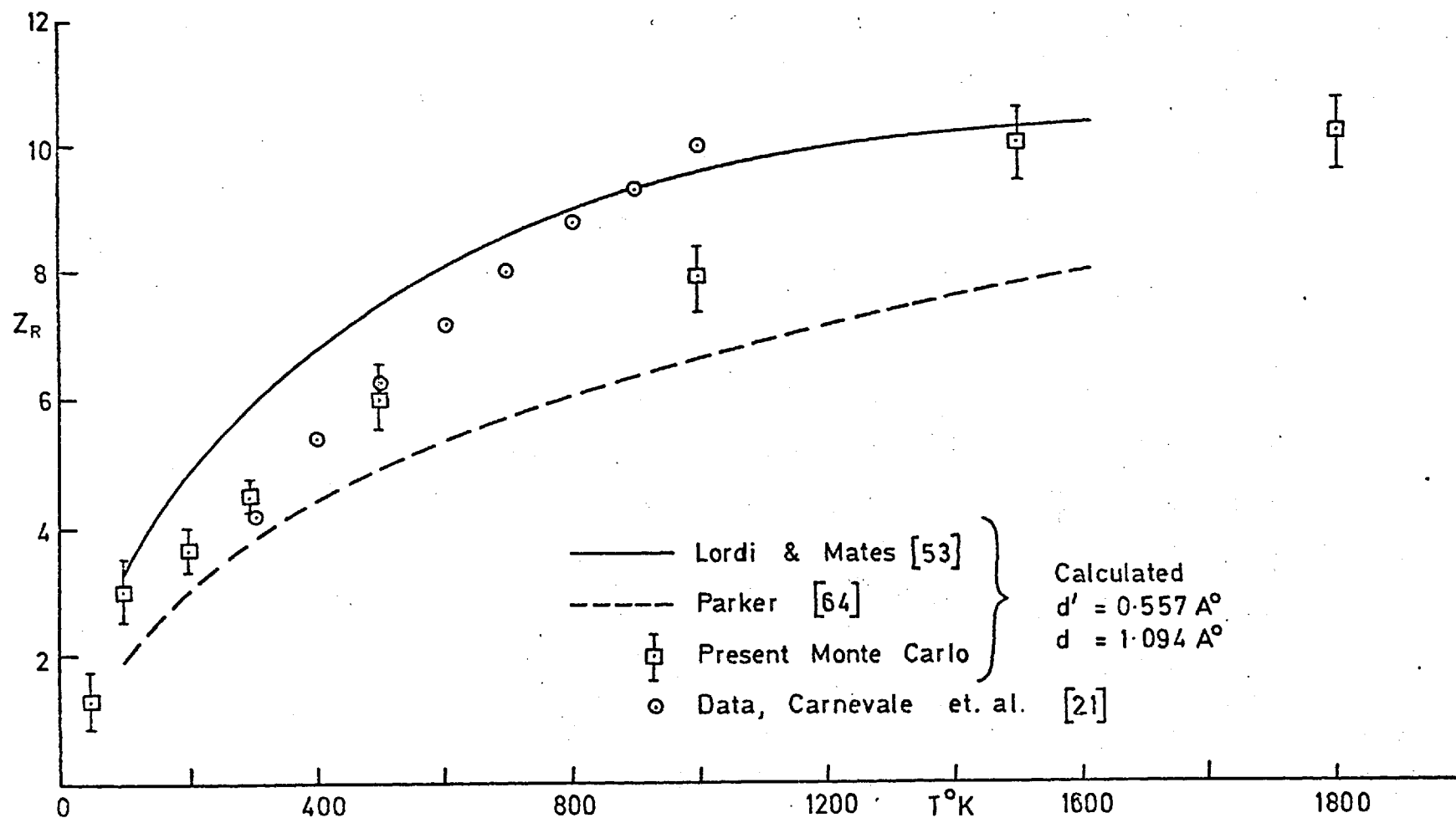


FIG. 6D ROTATIONAL COLLISION NUMBER FOR NITROGEN.

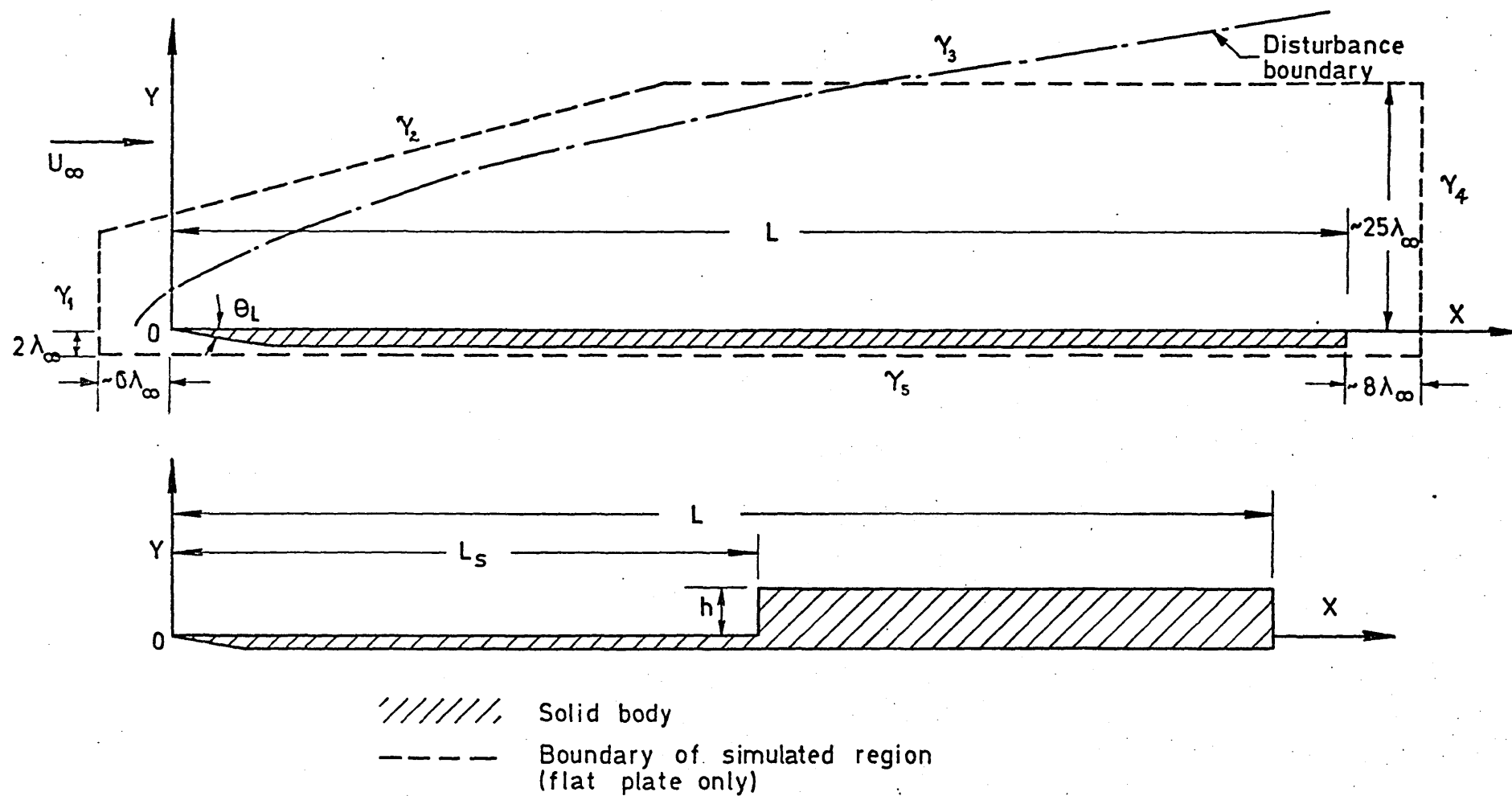


FIG.7 GEOMETRICAL CONFIGURATION FOR FLOW SIMULTATION.

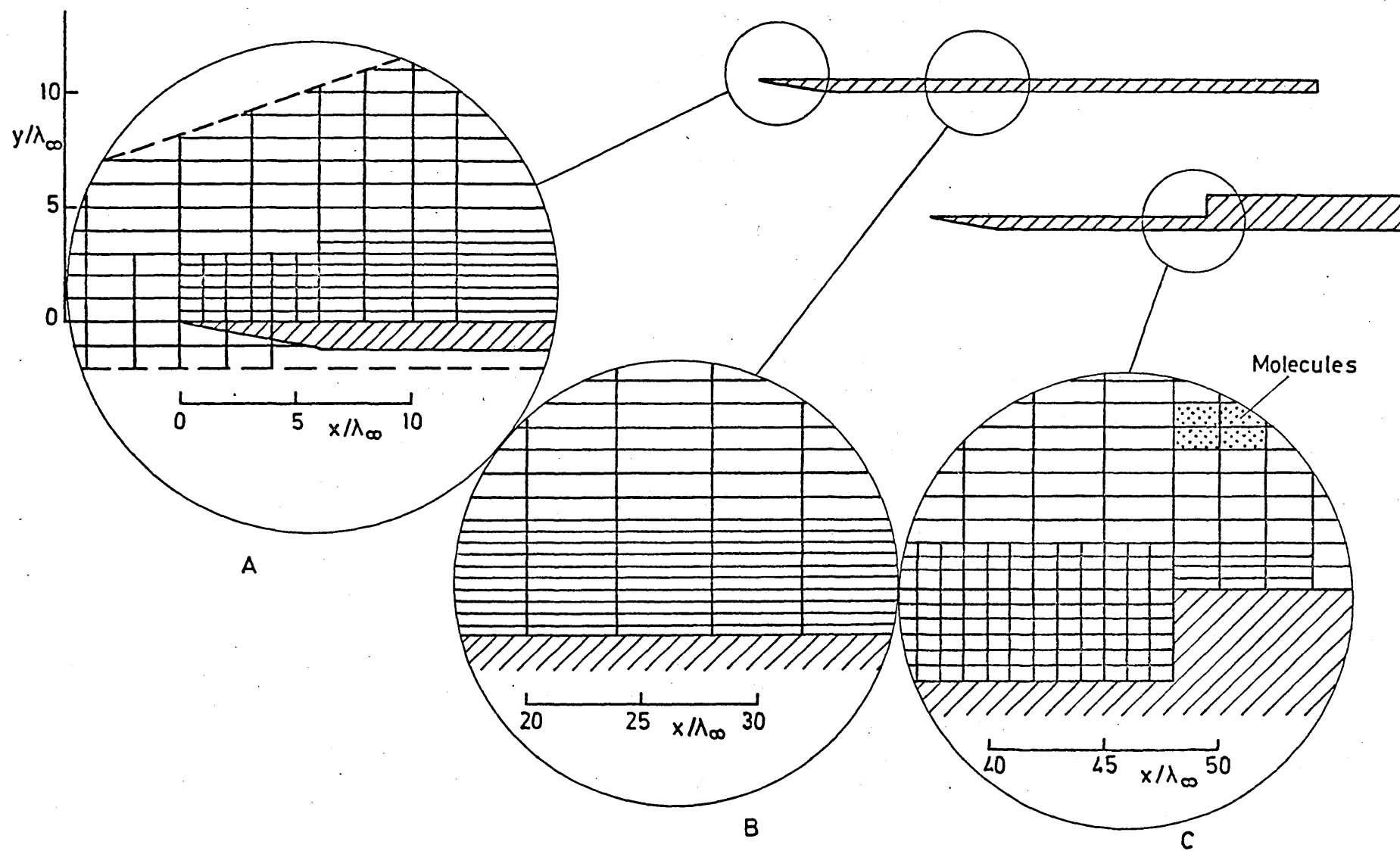


FIG. 8 TYPICAL CELL STRUCTURE

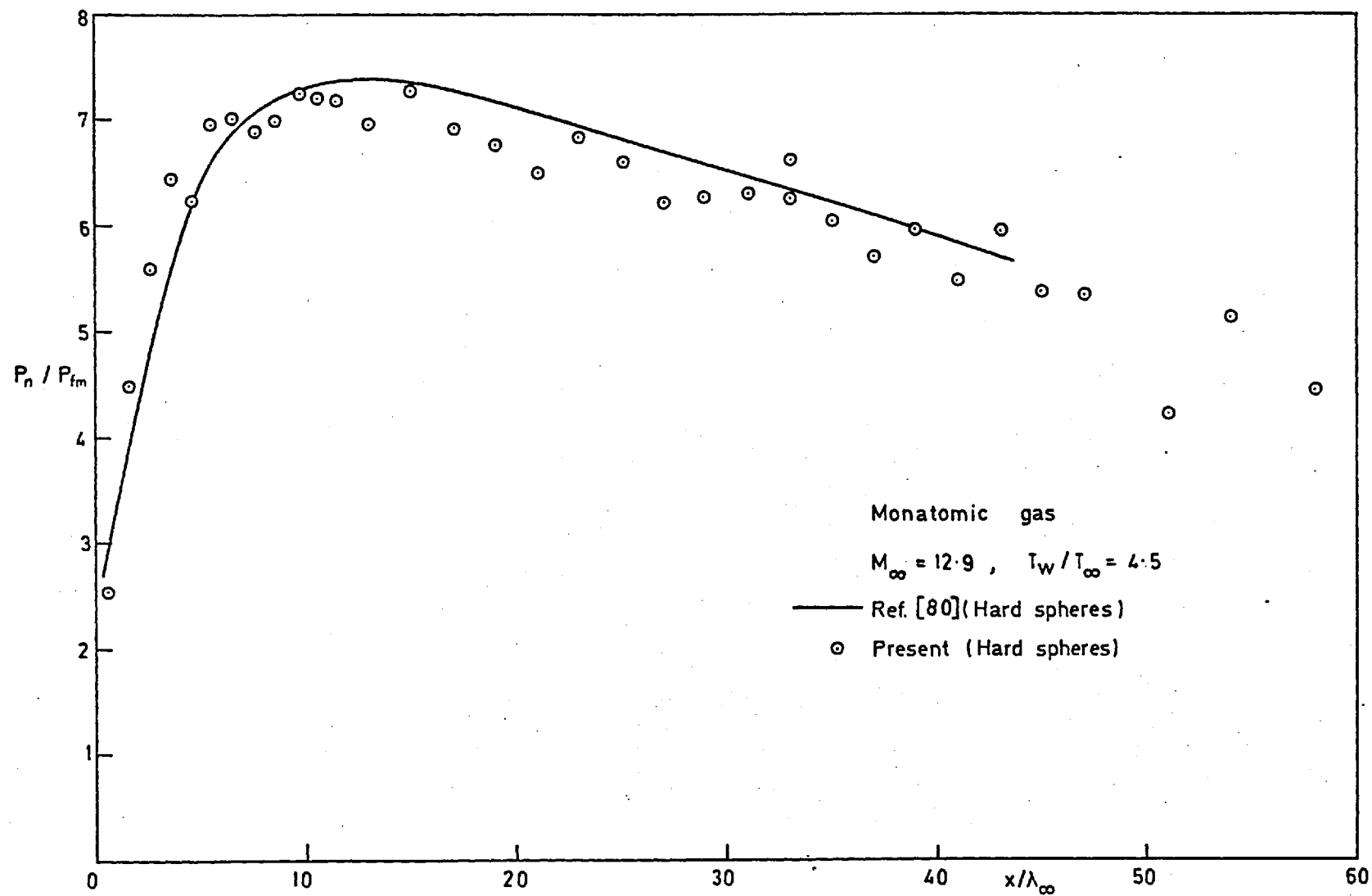


FIG. 9 SURFACE PRESSURE AT $M_{\infty} = 12.9$

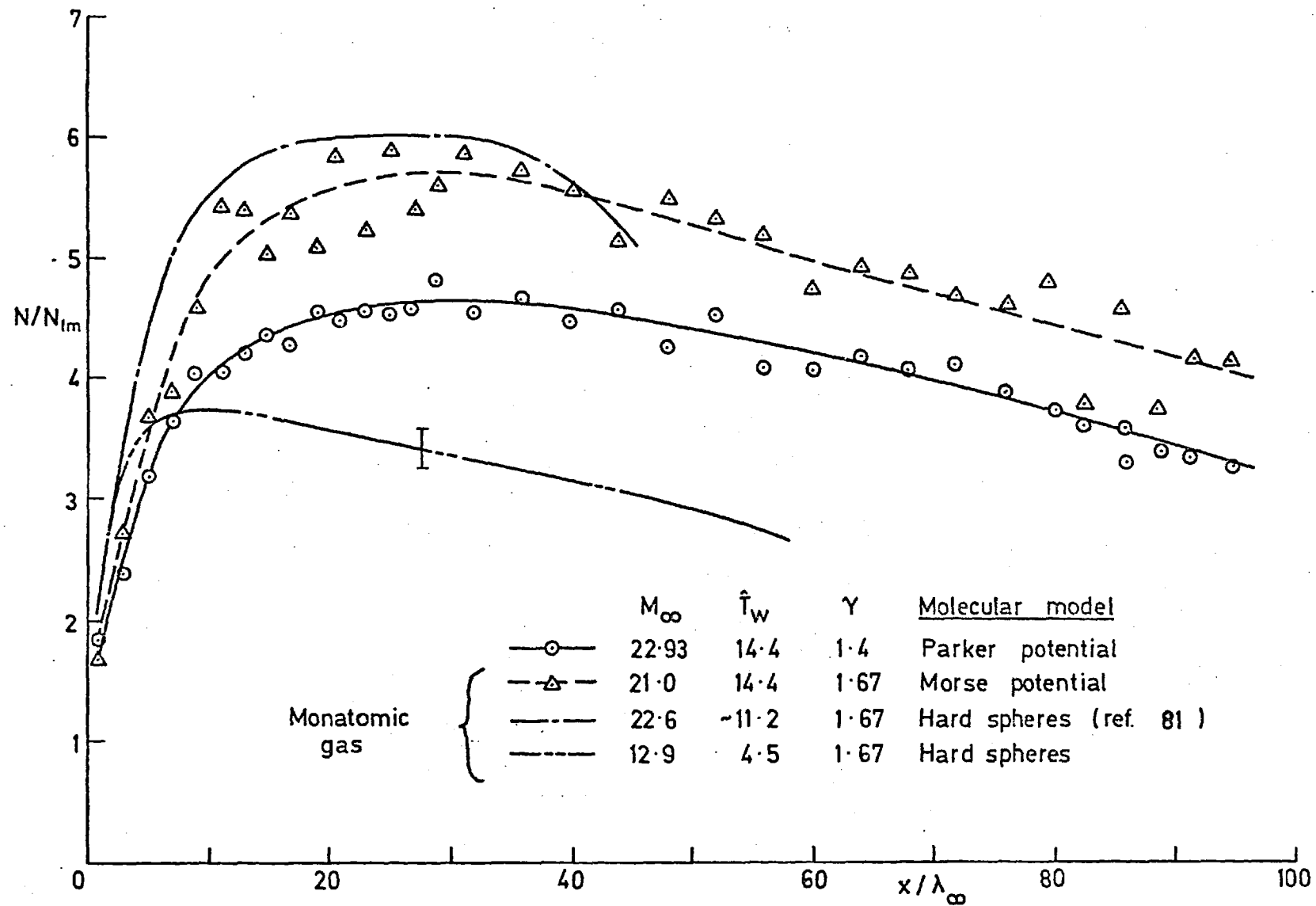


FIG. 10 NUMBER FLUX TO SURFACE FOR VARIOUS CONDITIONS.

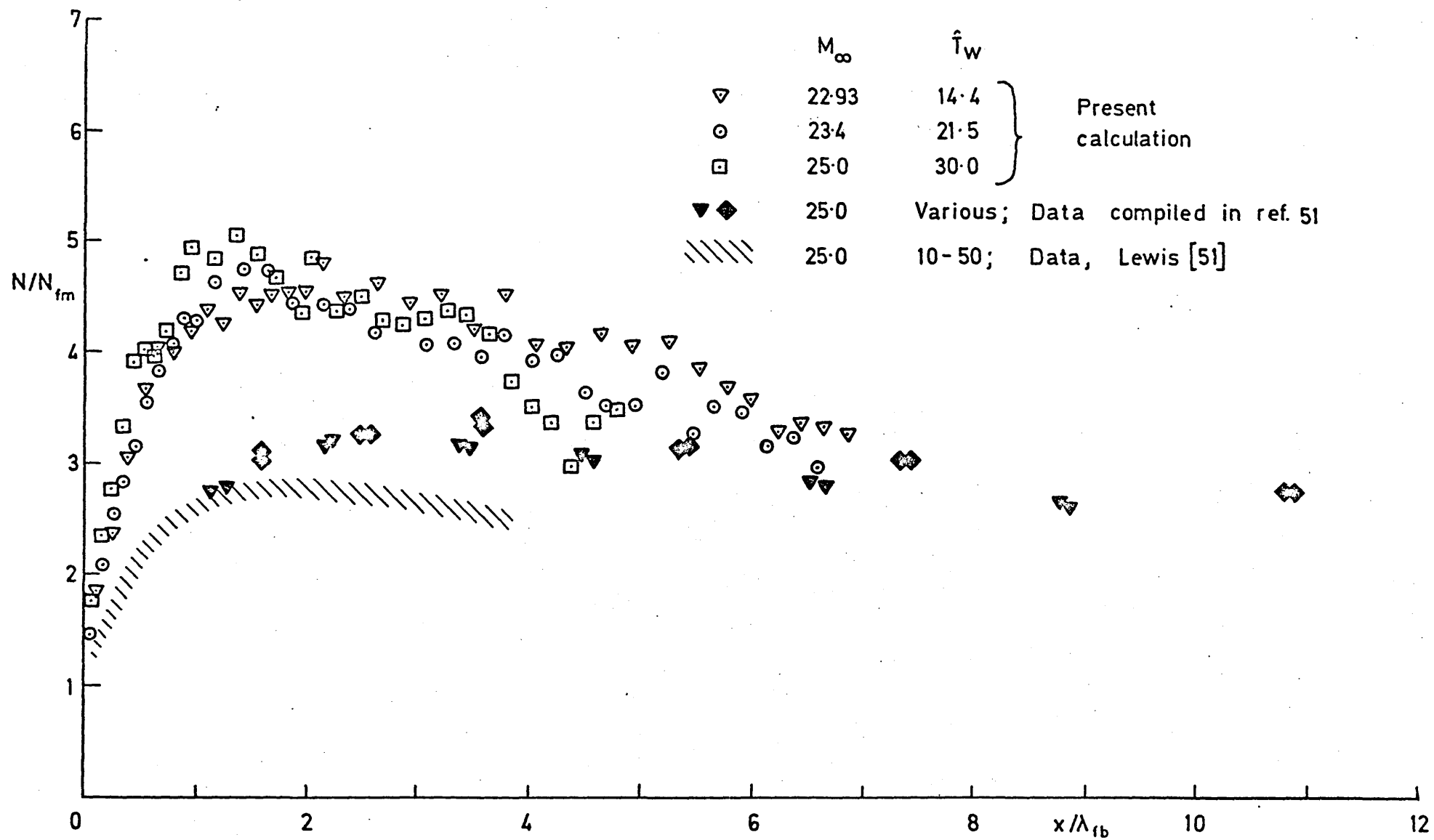


FIG.11 NUMBER FLUX TO SURFACE. AT HIGH M_∞ Vs. x/λ_{fb}

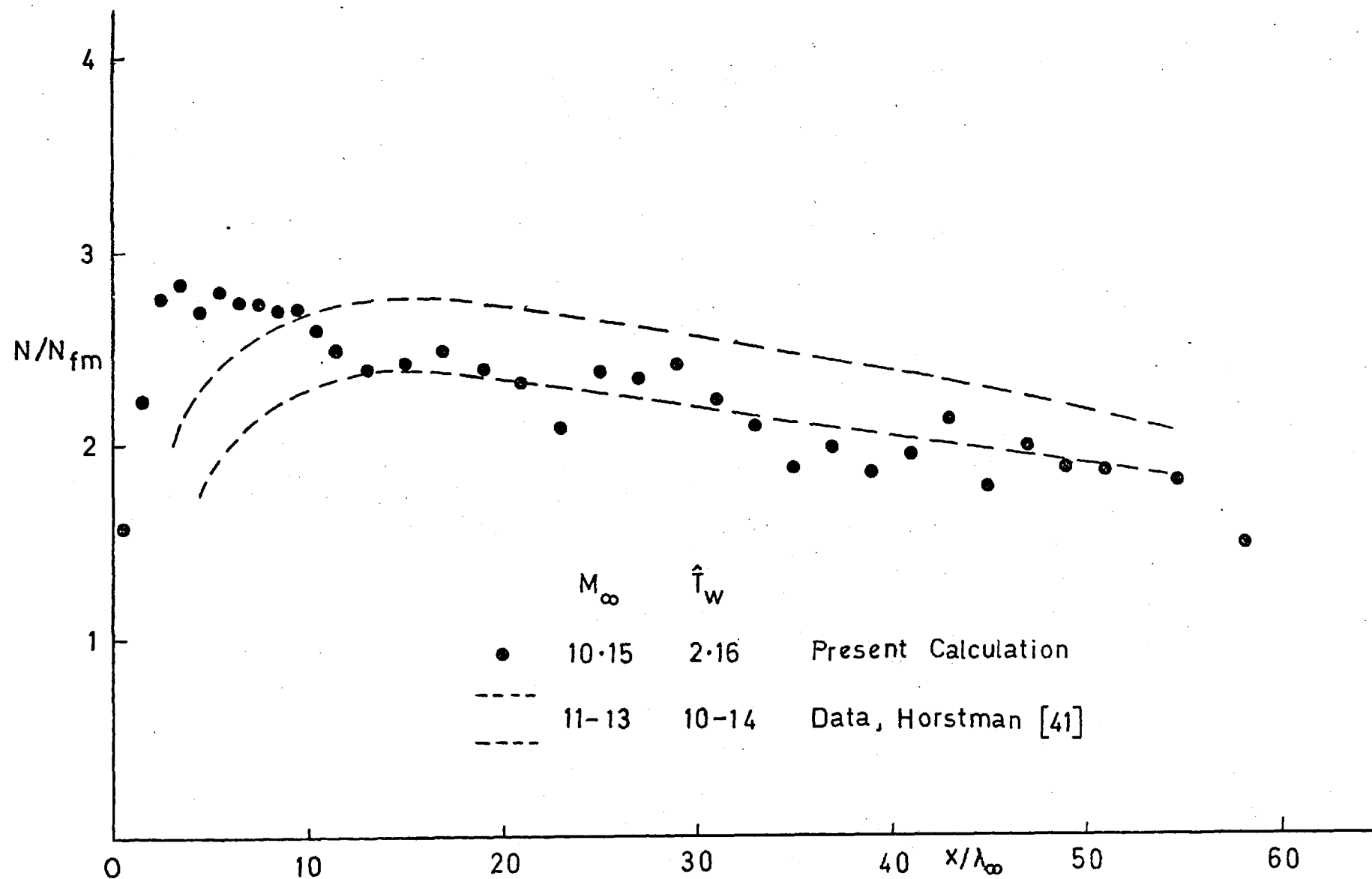


FIG.12 NUMBER FLUX AT MODERATE M_∞ Vs. x/λ_∞

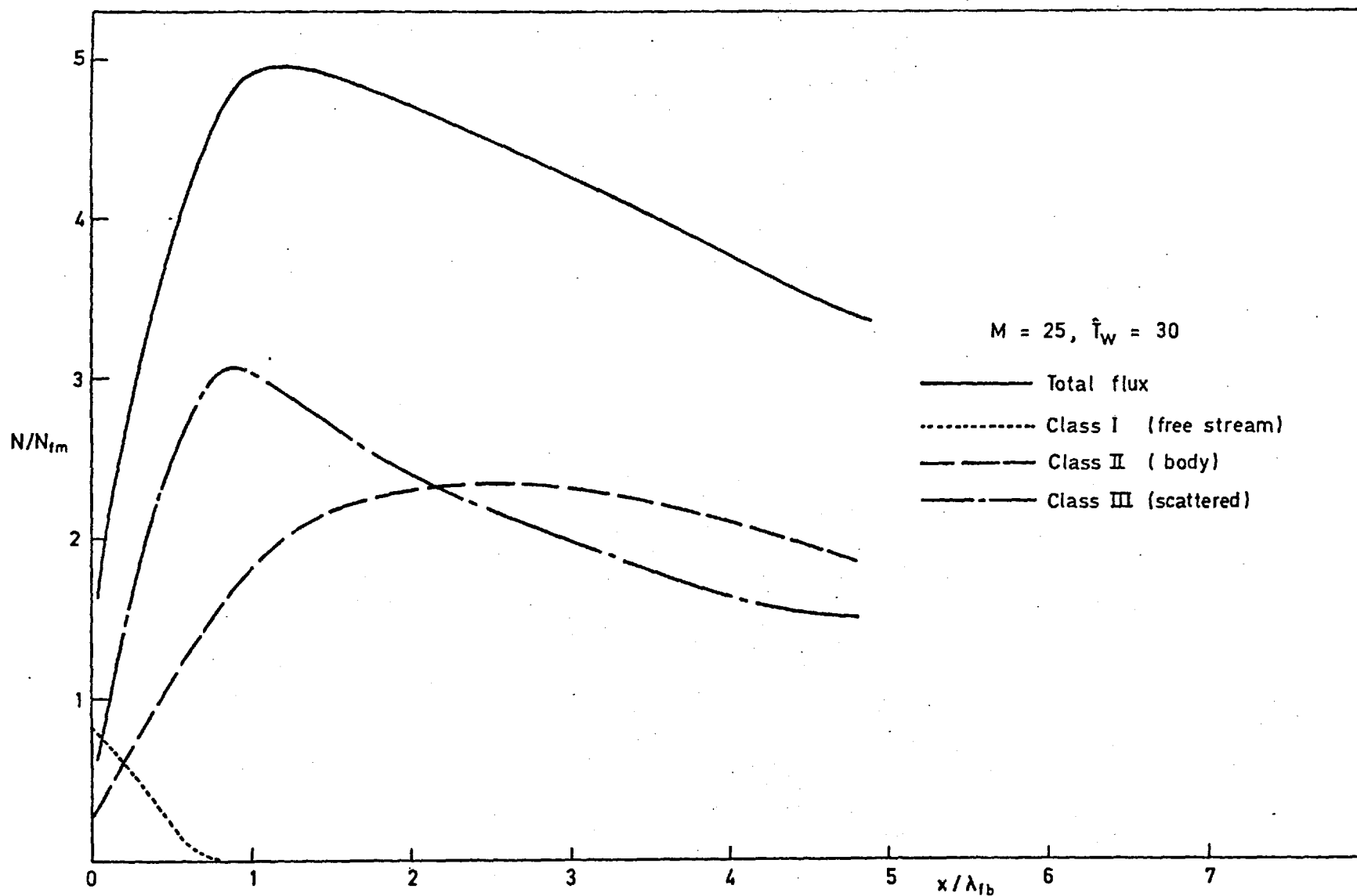


FIG.13 NUMBER FLUX TO SURFACE

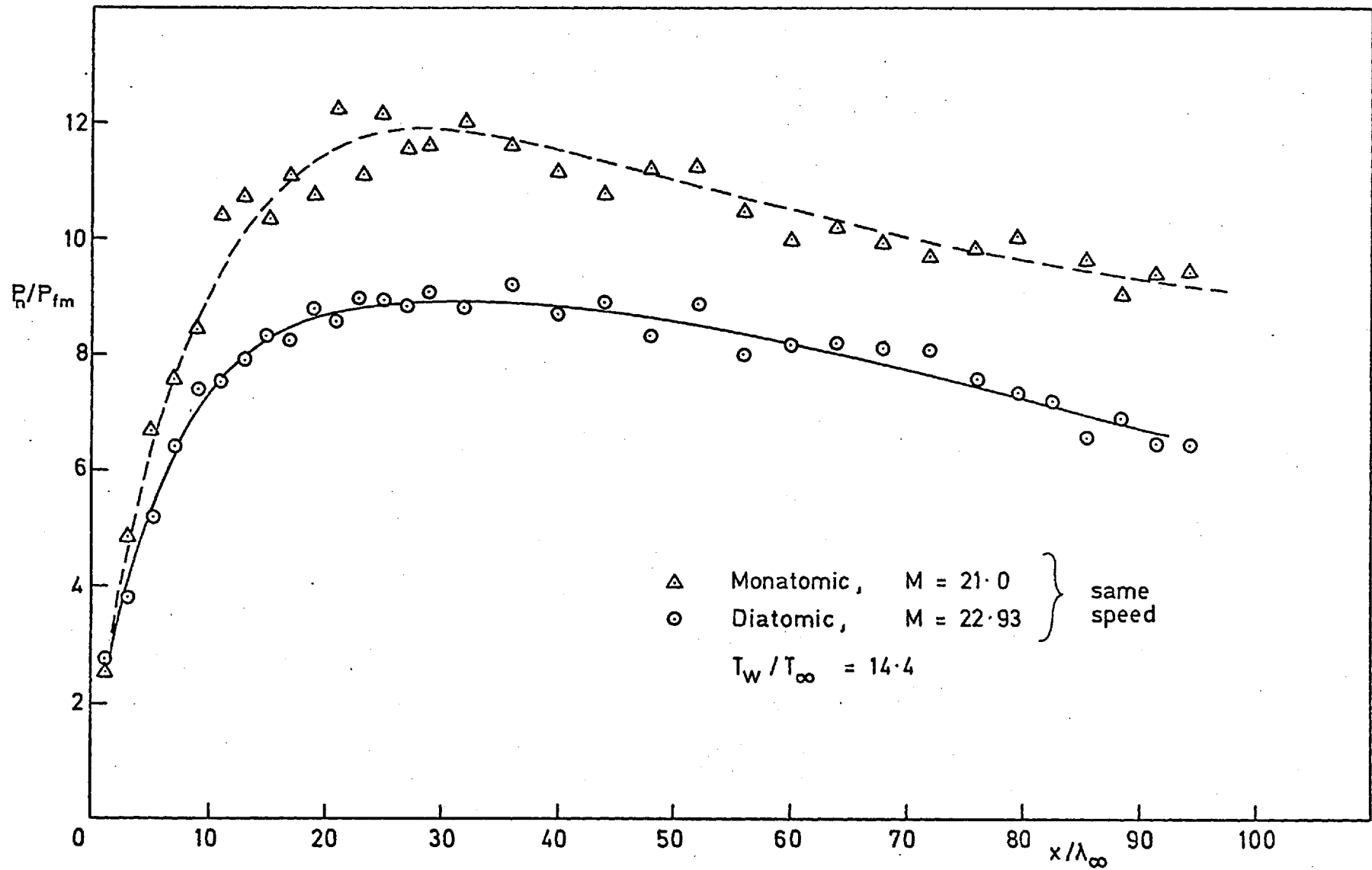


FIG 14 EFFECT OF DIATOMICITY ON SURFACE PRESSURE.

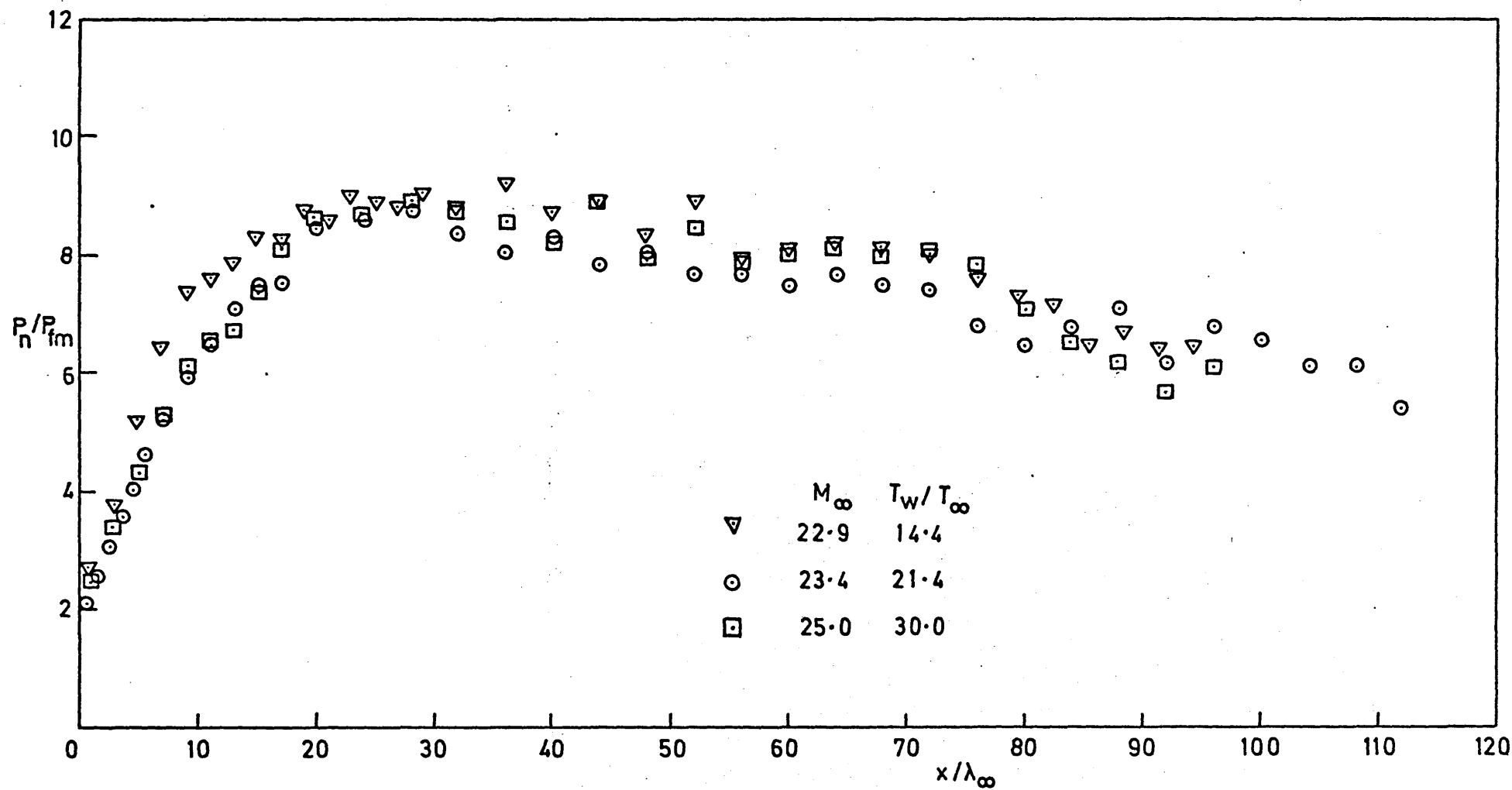


FIG. 15 P_n/P_{fm} vs. x/λ_∞

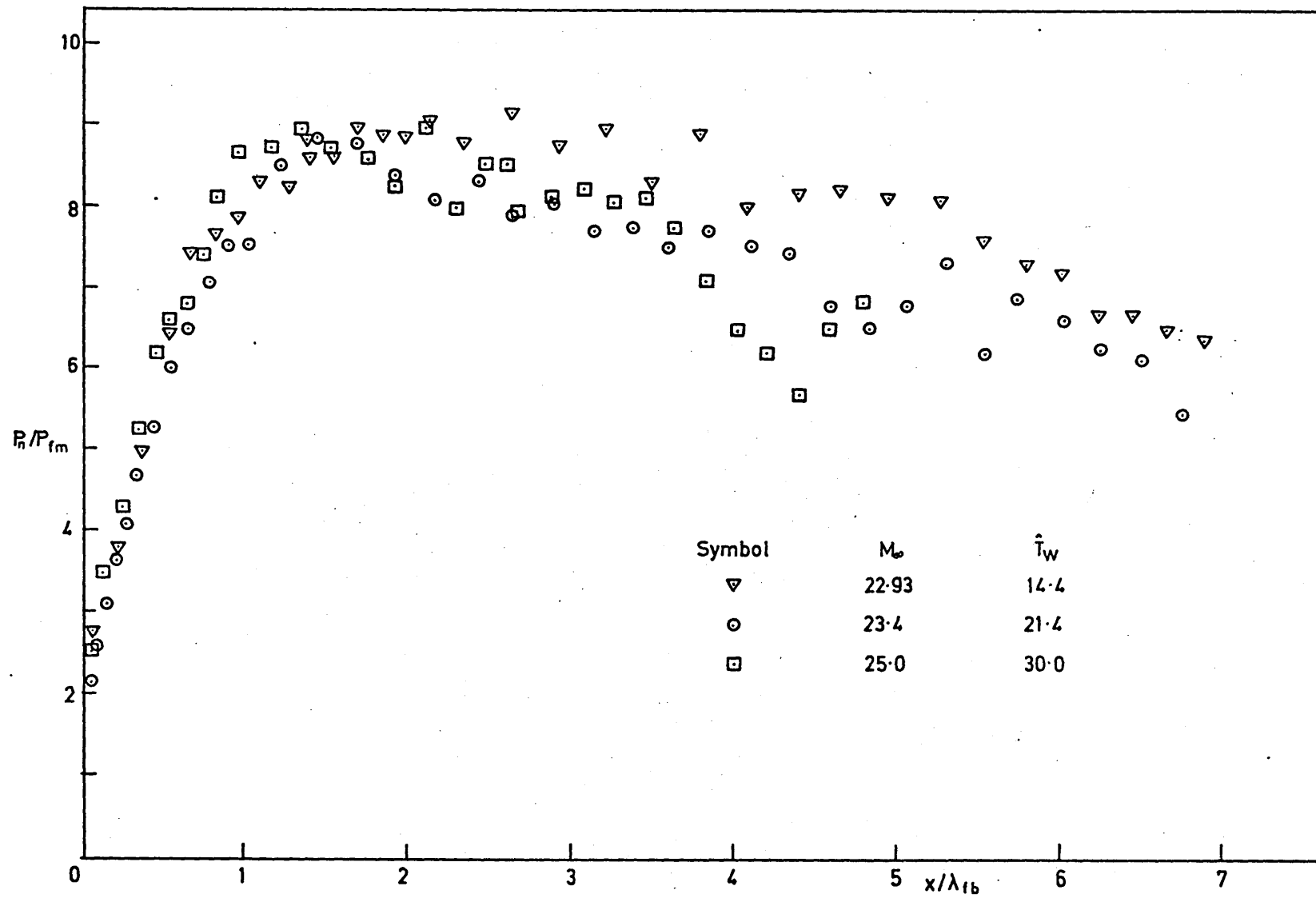


FIG. 16 SURFACE PRESSURE vs. x/λ_{fb}

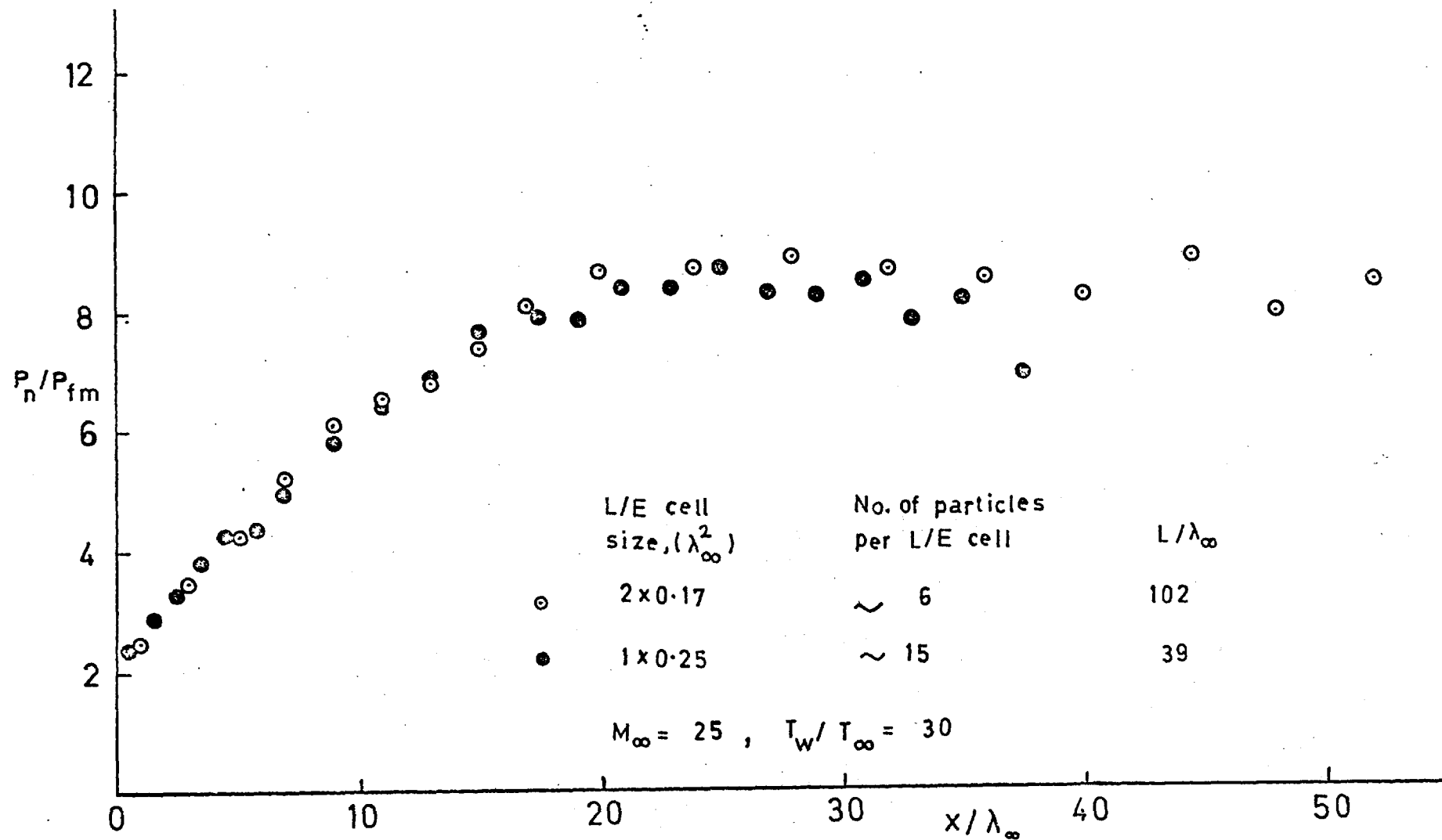


FIG. 17A EFFECT OF CELL SIZE AND PARTICLE DENSITY ON SURFACE PRESSURE

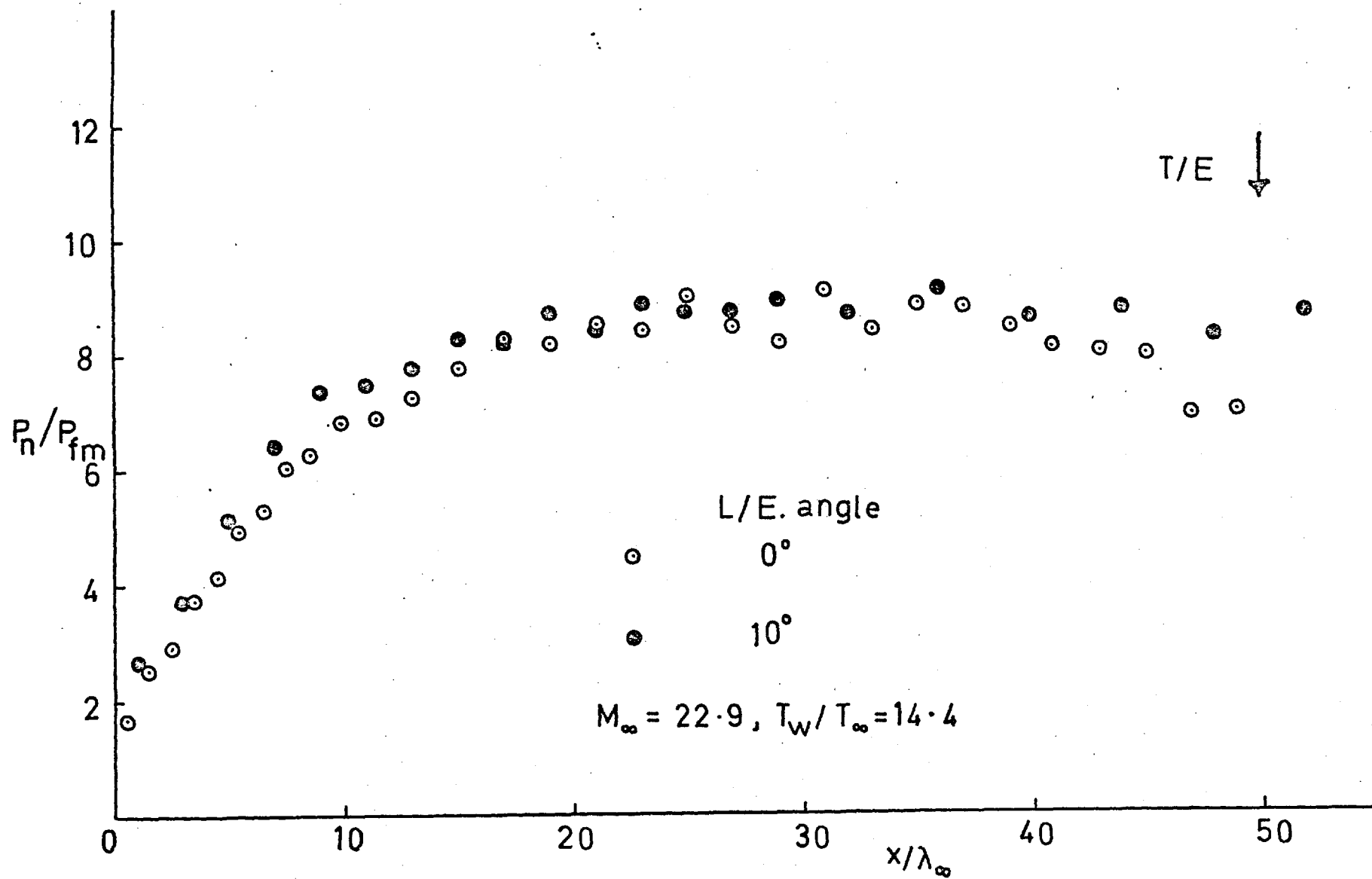


FIG.17B. EFFECT OF LEADING EDGE ANGLE ON SURFACE PRESSURE

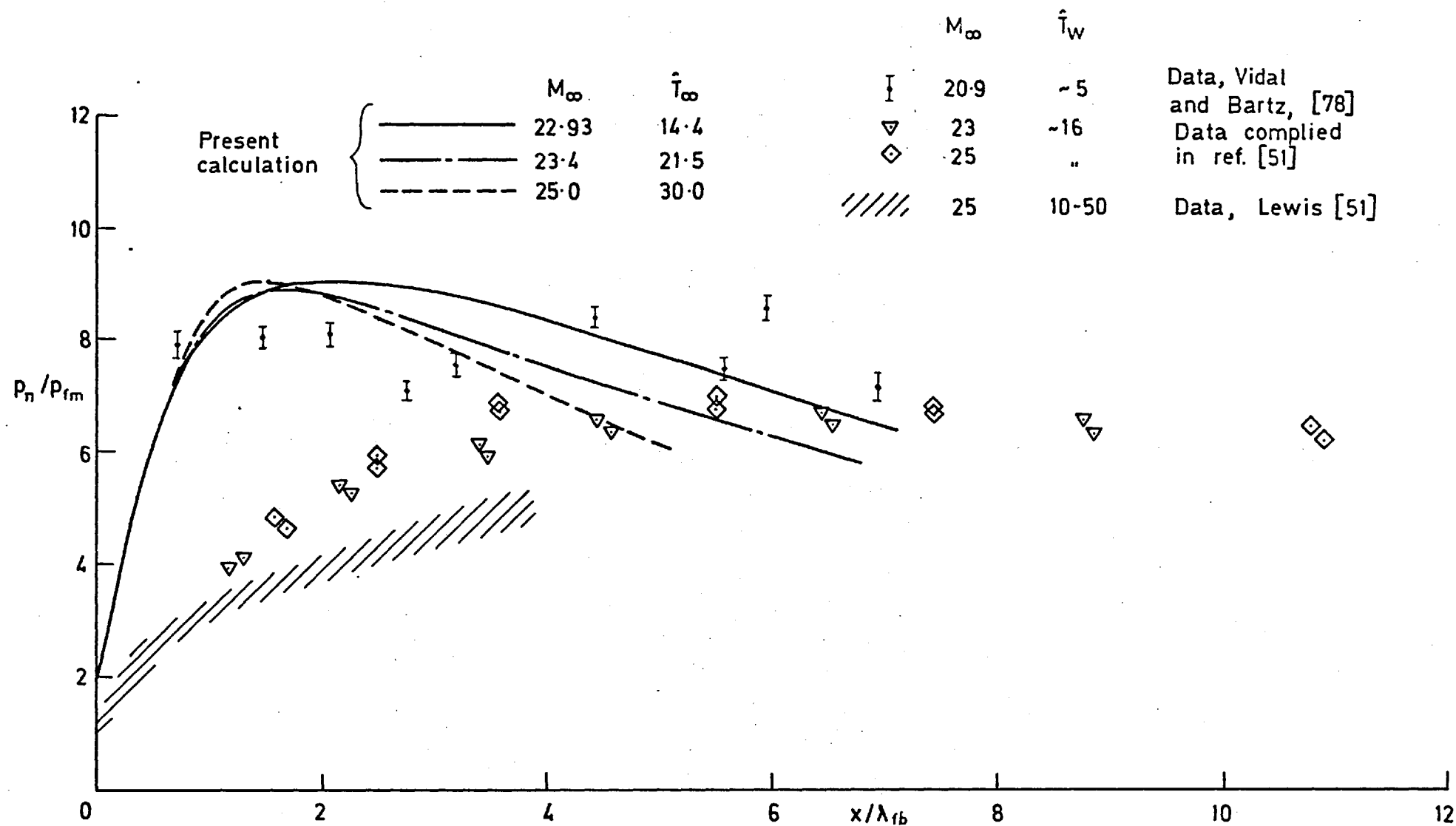


FIG. 18 A SURFACE PRESSURE

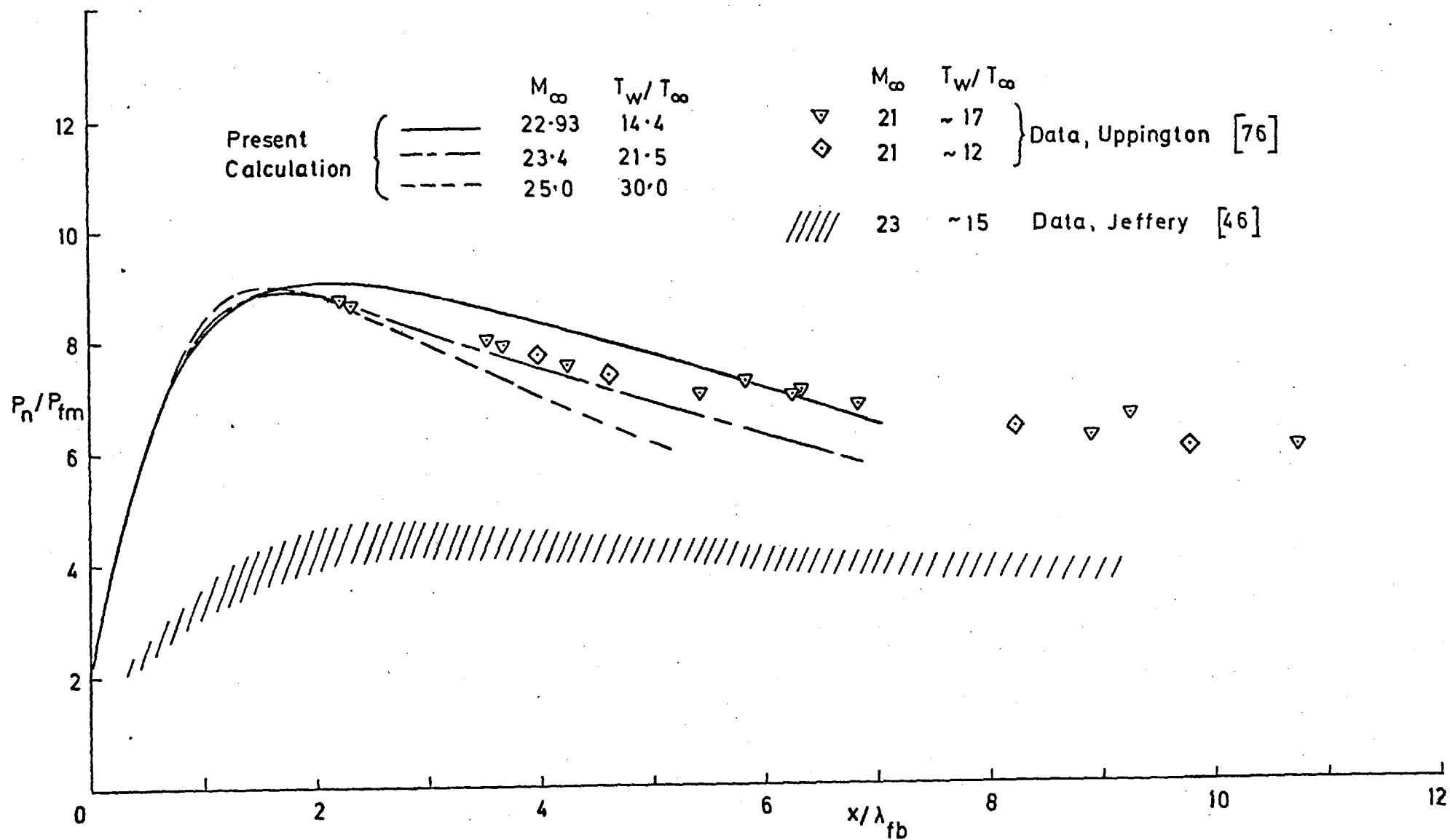


FIG.18B SURFACE PRESSURE ; COMPARISON WITH DATA

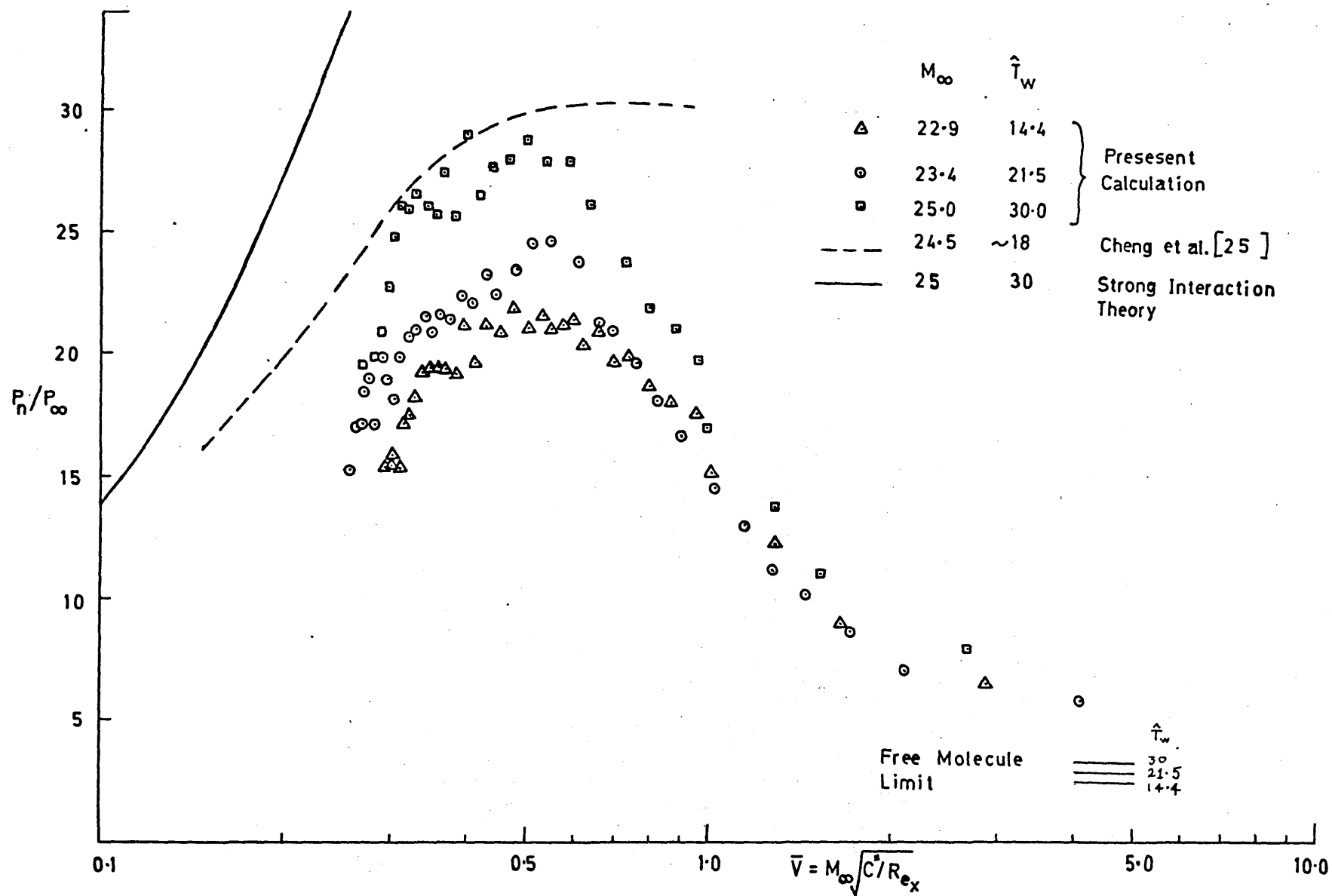


FIG. 19 SURFACE PRESSURE Vs. THE RARIFACTION PARAMETER

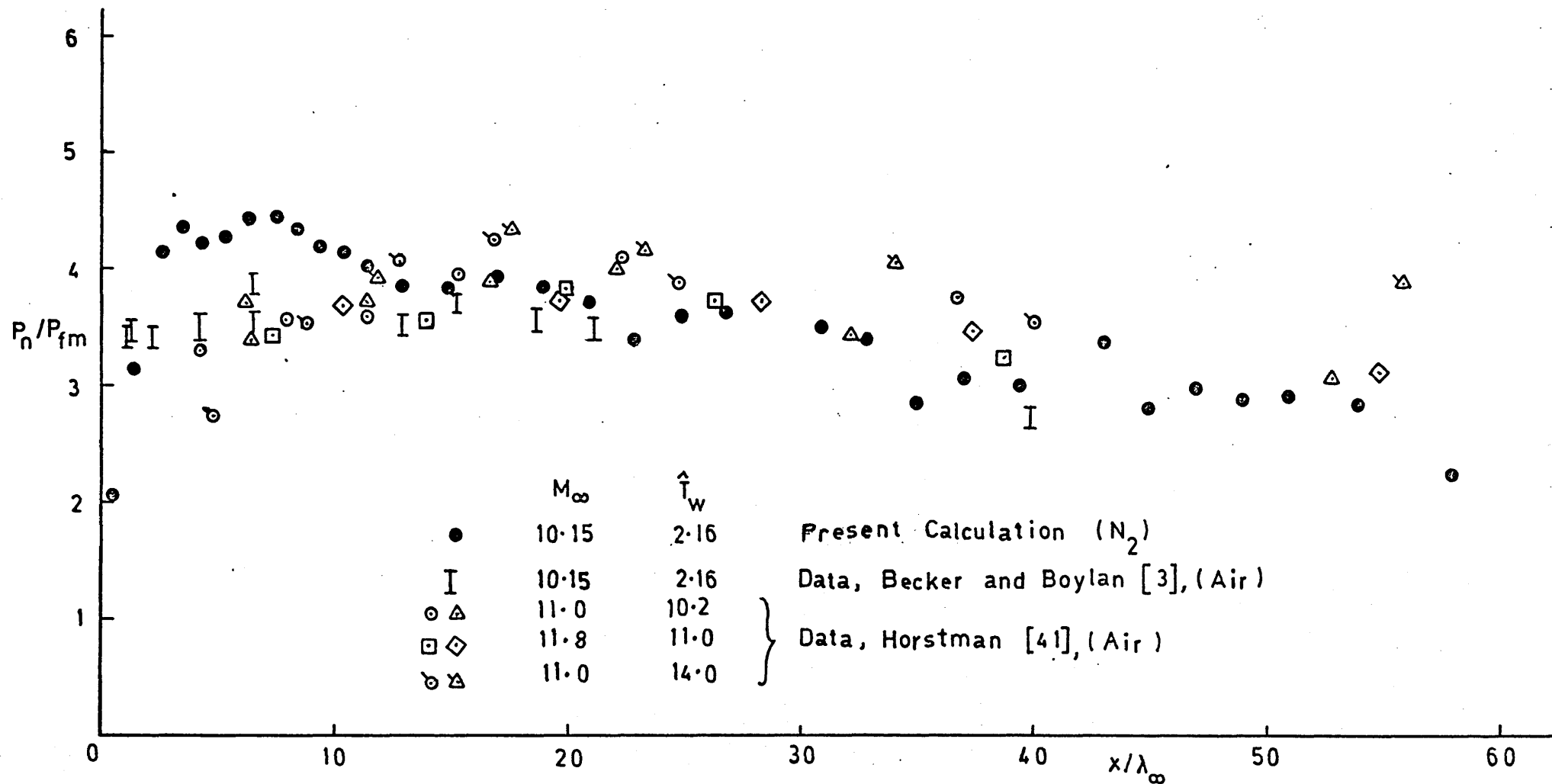


FIG-20 A SURFACE PRESSURE AT MODERATE M_∞ Vs. x/λ_∞

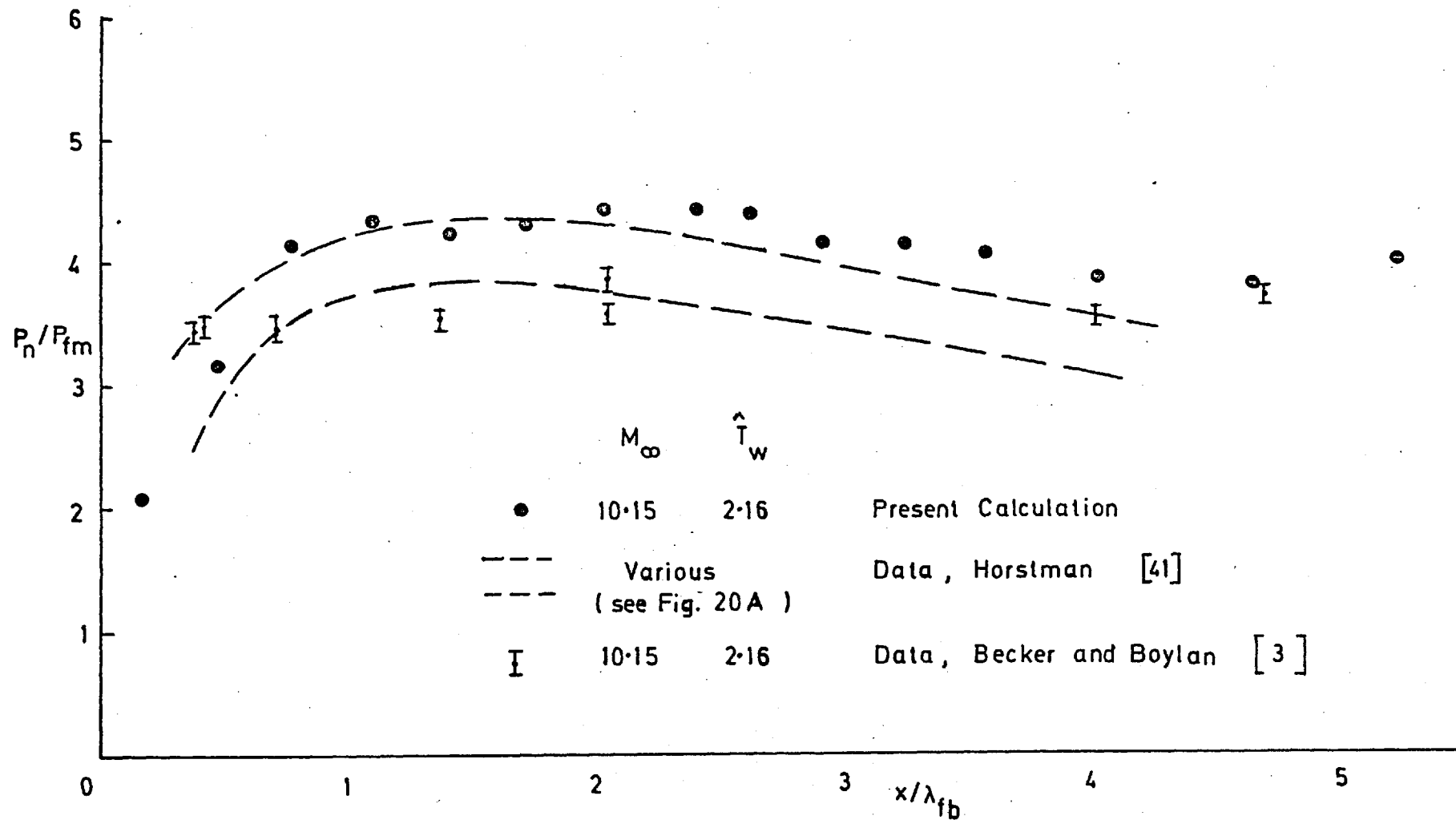


FIG. 20 B SURFACE PRESSURE AT MODERATE M_∞ Vs. x/λ_{fb}

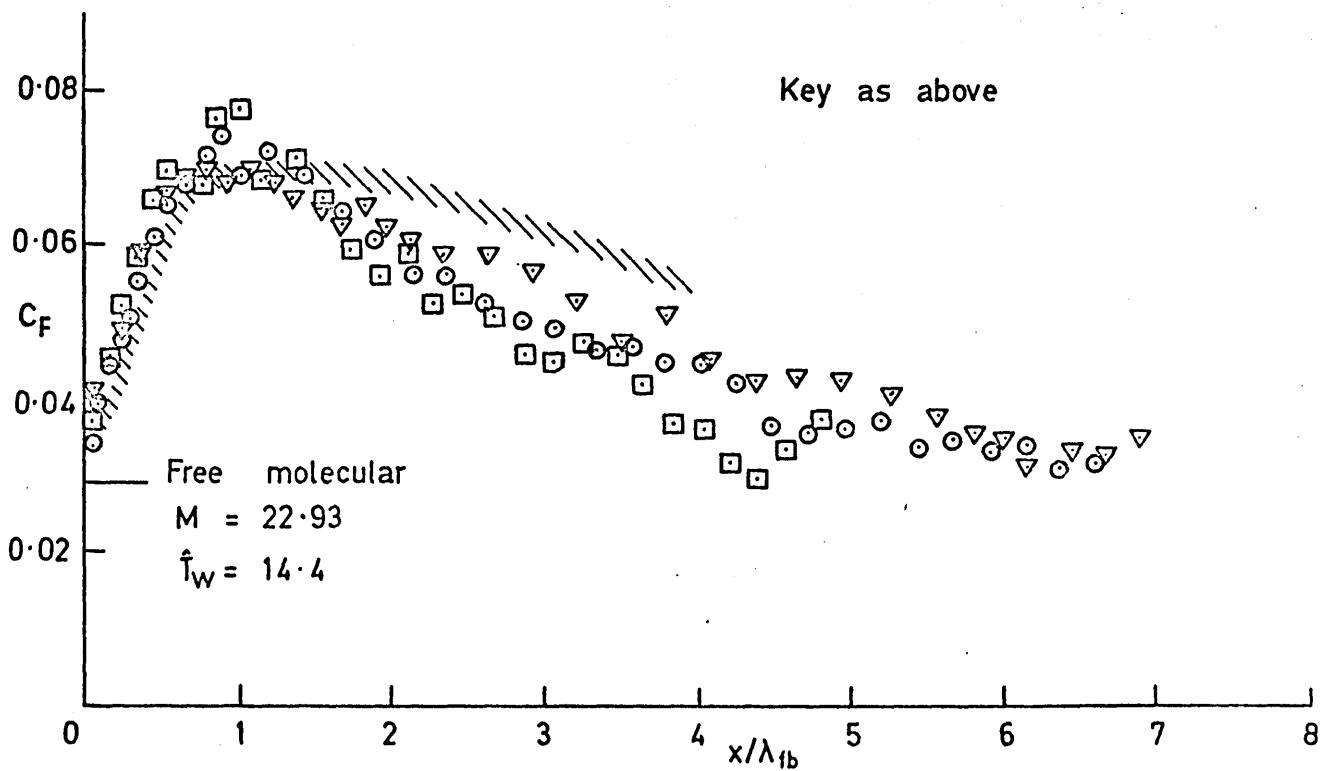
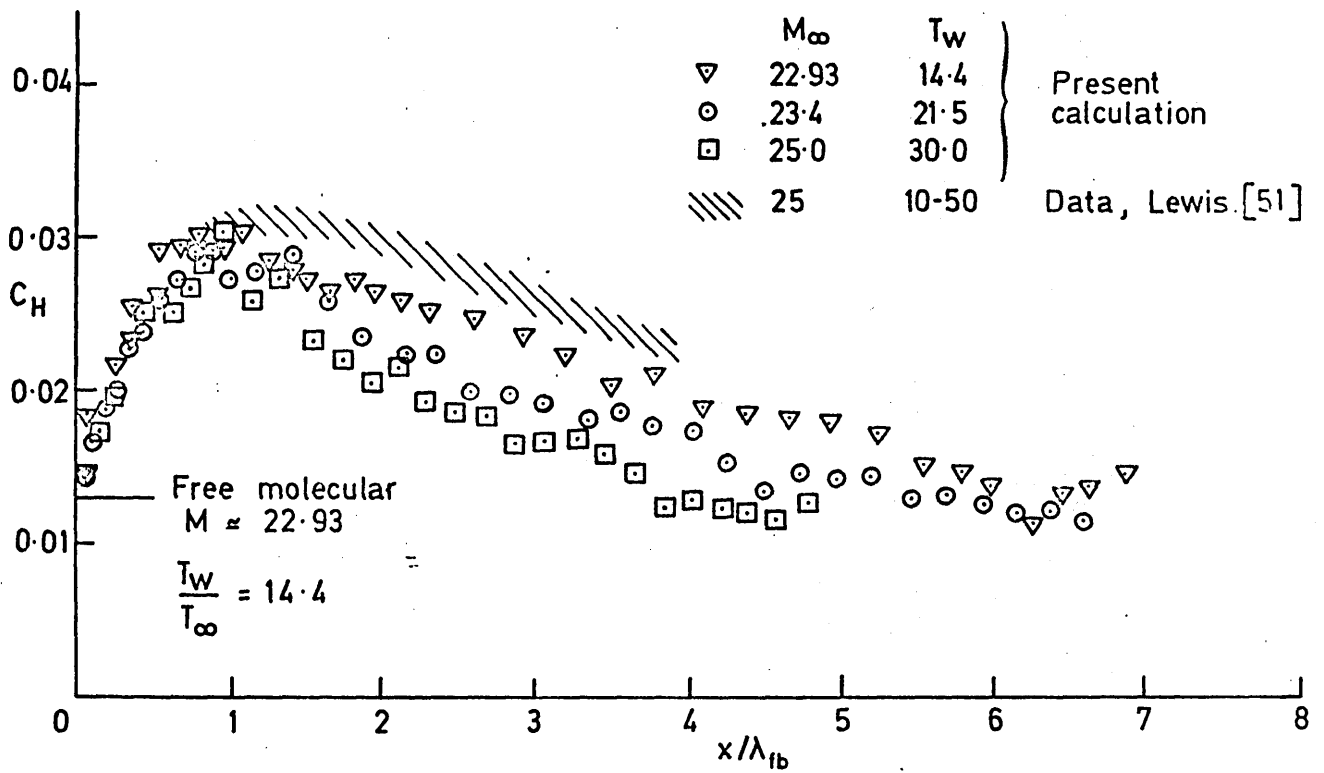


FIG. 21 HEAT TRANSFER AND SKIN FRICTION COEFFICIENTS.

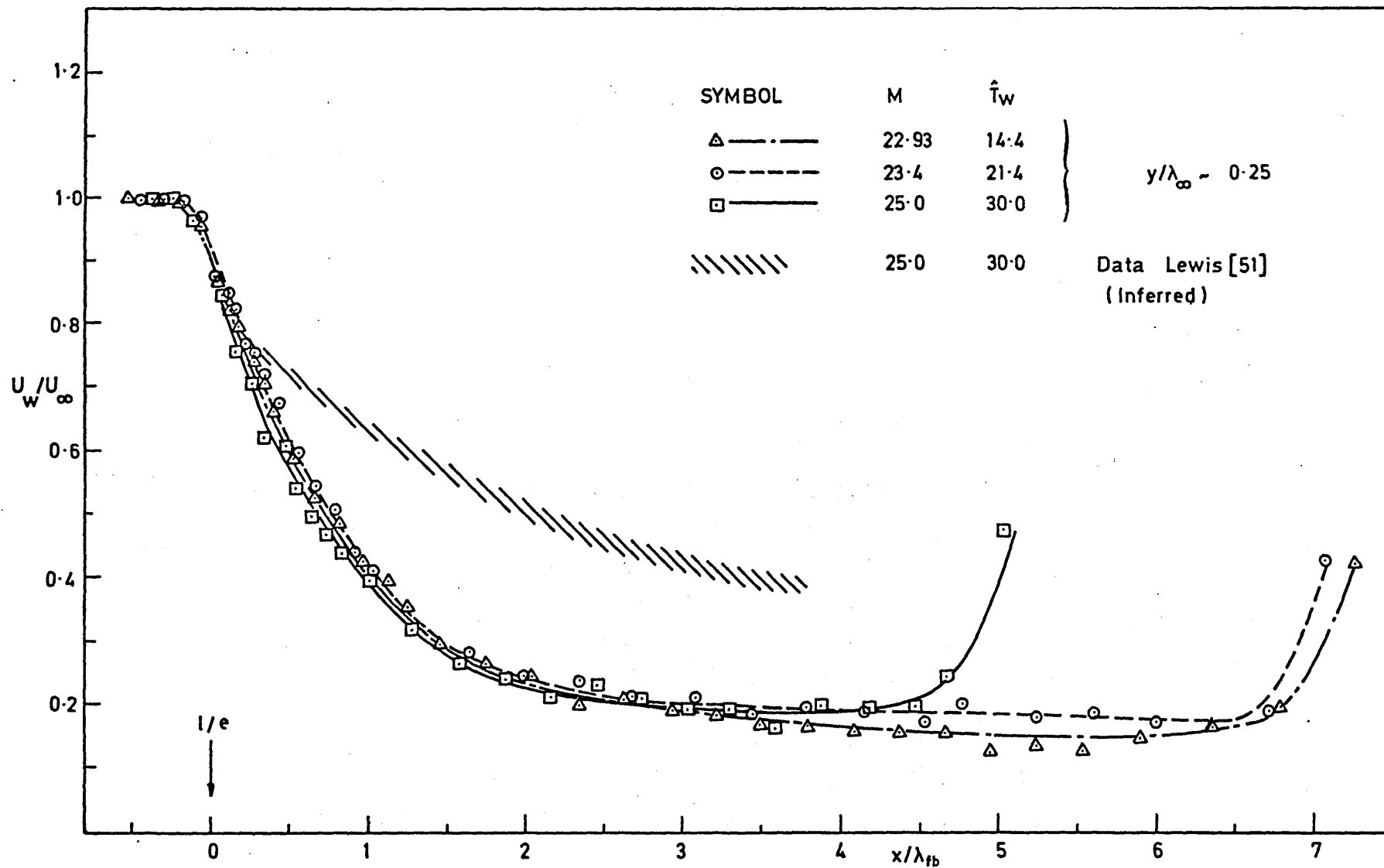


FIG. 22 TANGENTIAL VELOCITY NEAR WALL

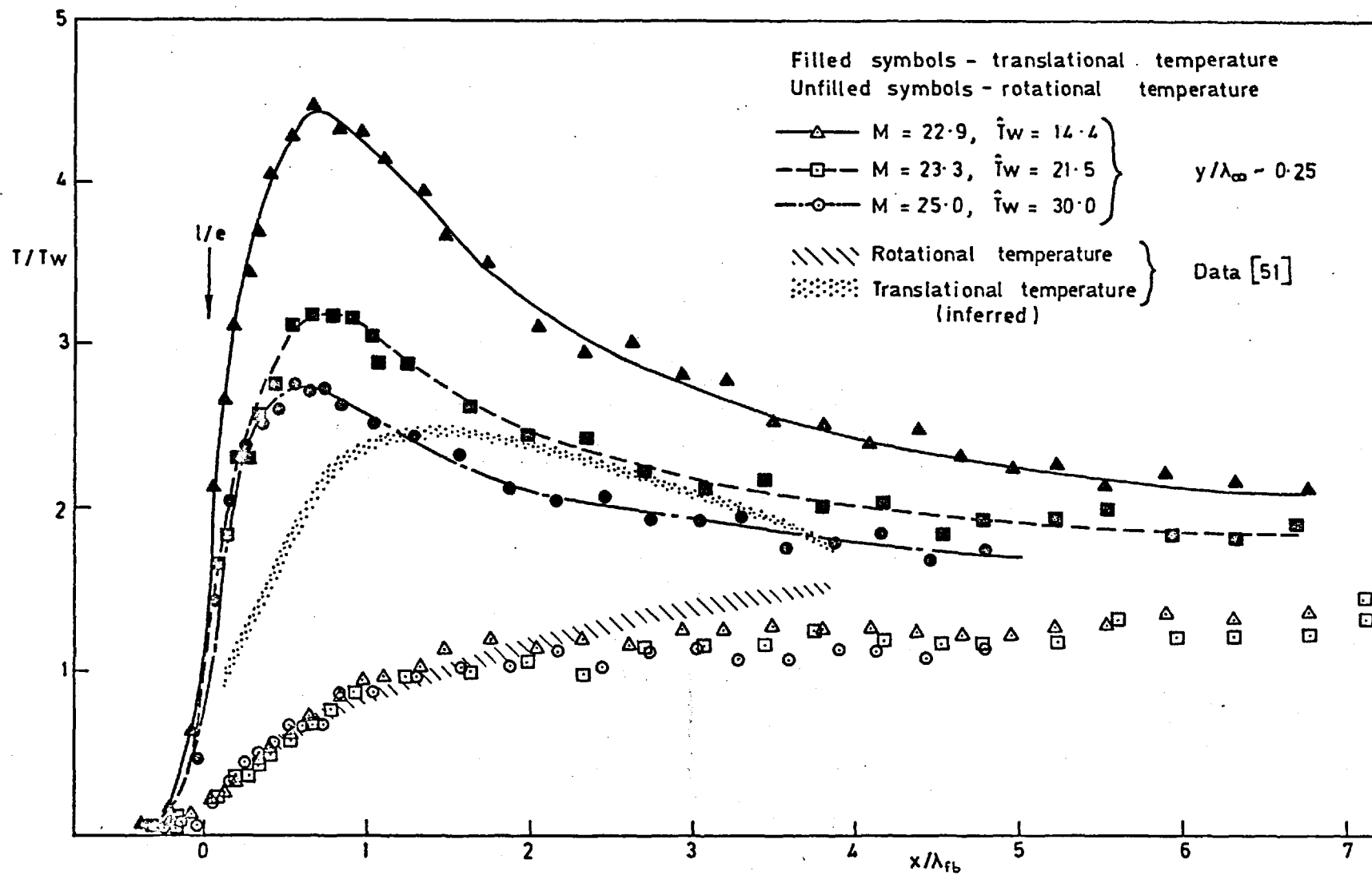


FIG. 23A TRANSLATIONAL AND ROTATIONAL TEMPERATURE NEAR WALL.

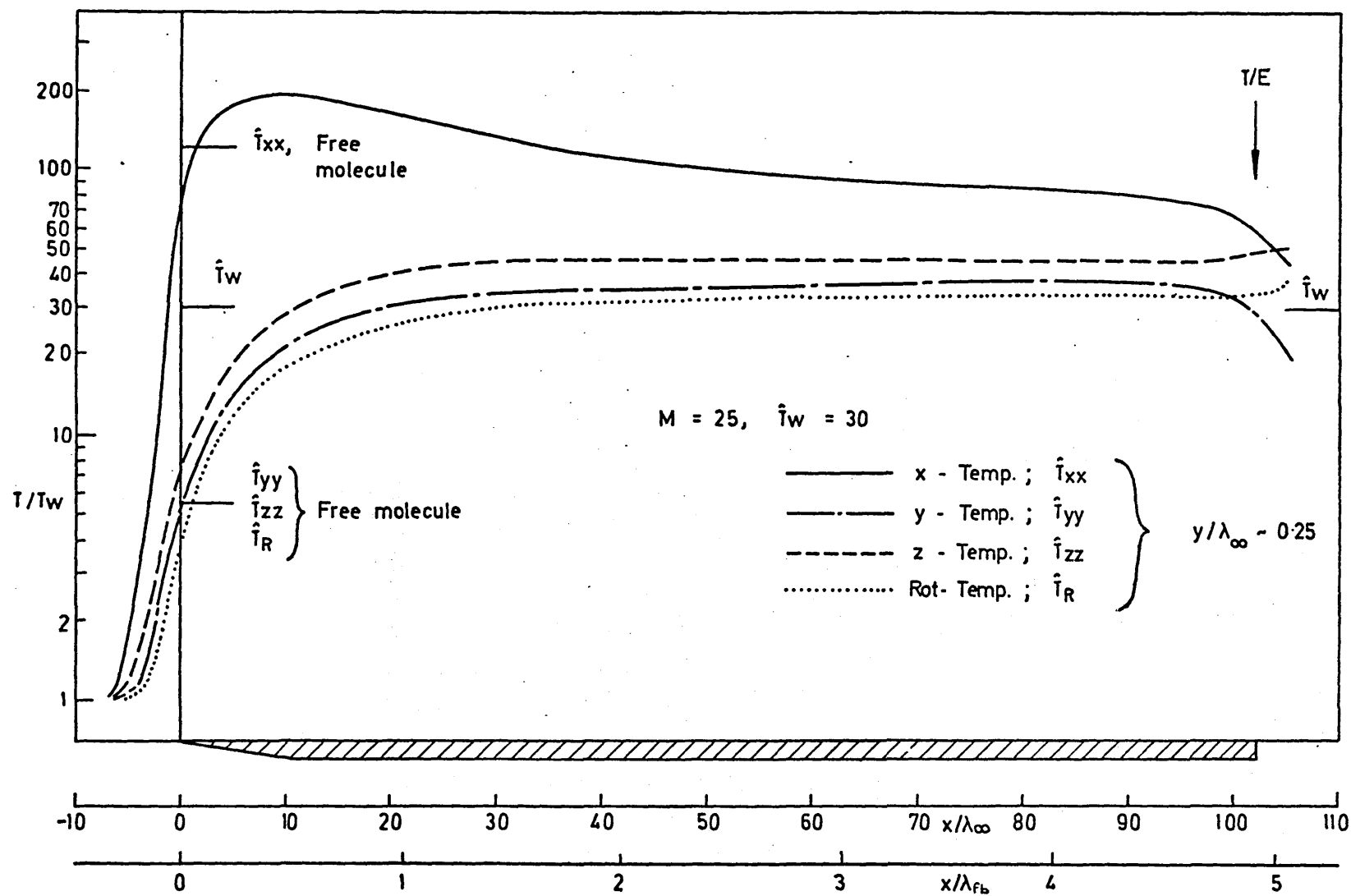


FIG 23 B x, y, z AND ROTATIONAL TEMPERATURES NEAR WALL.

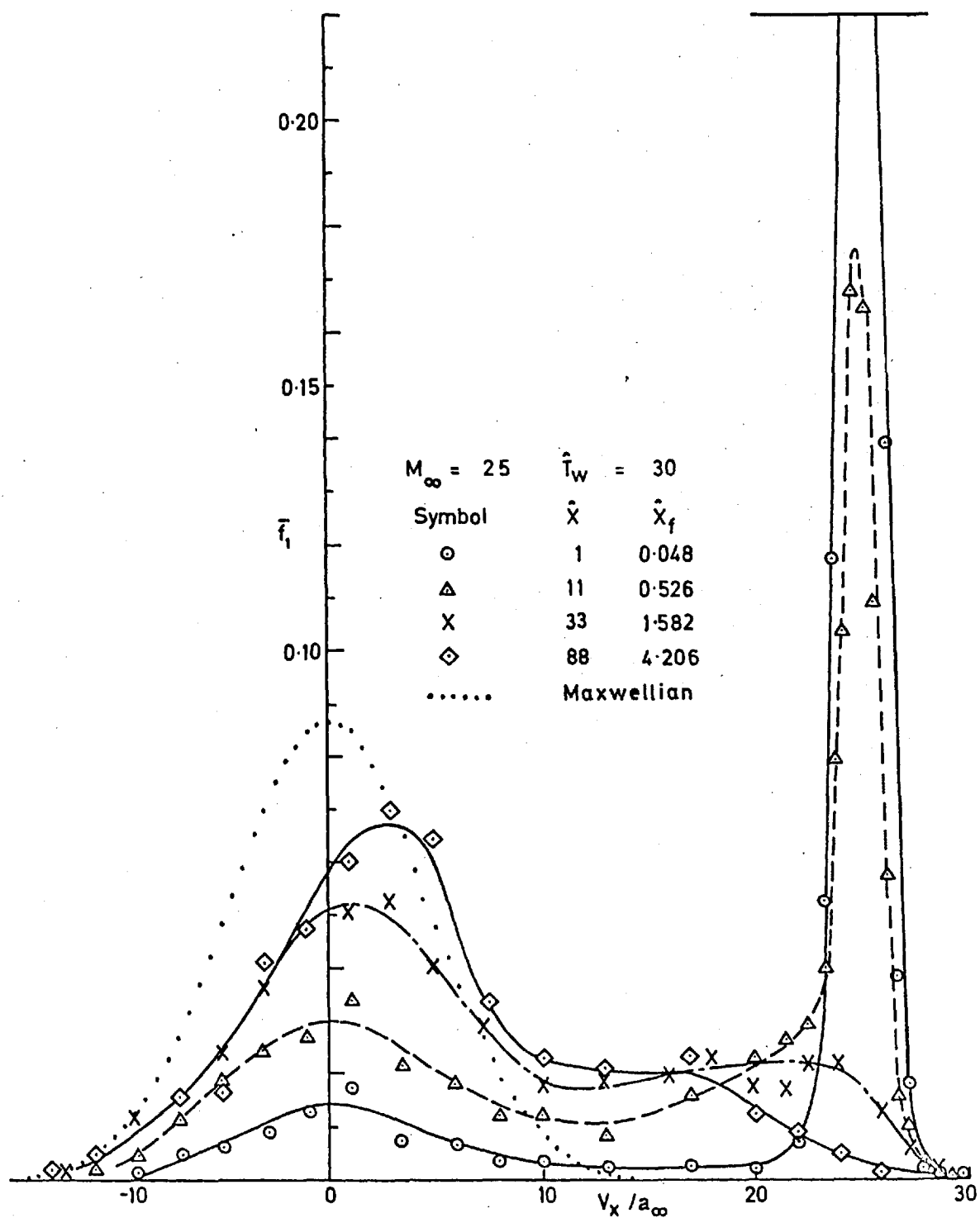


FIG. 24 A V_x DISTRIBUTION NEAR WALL.

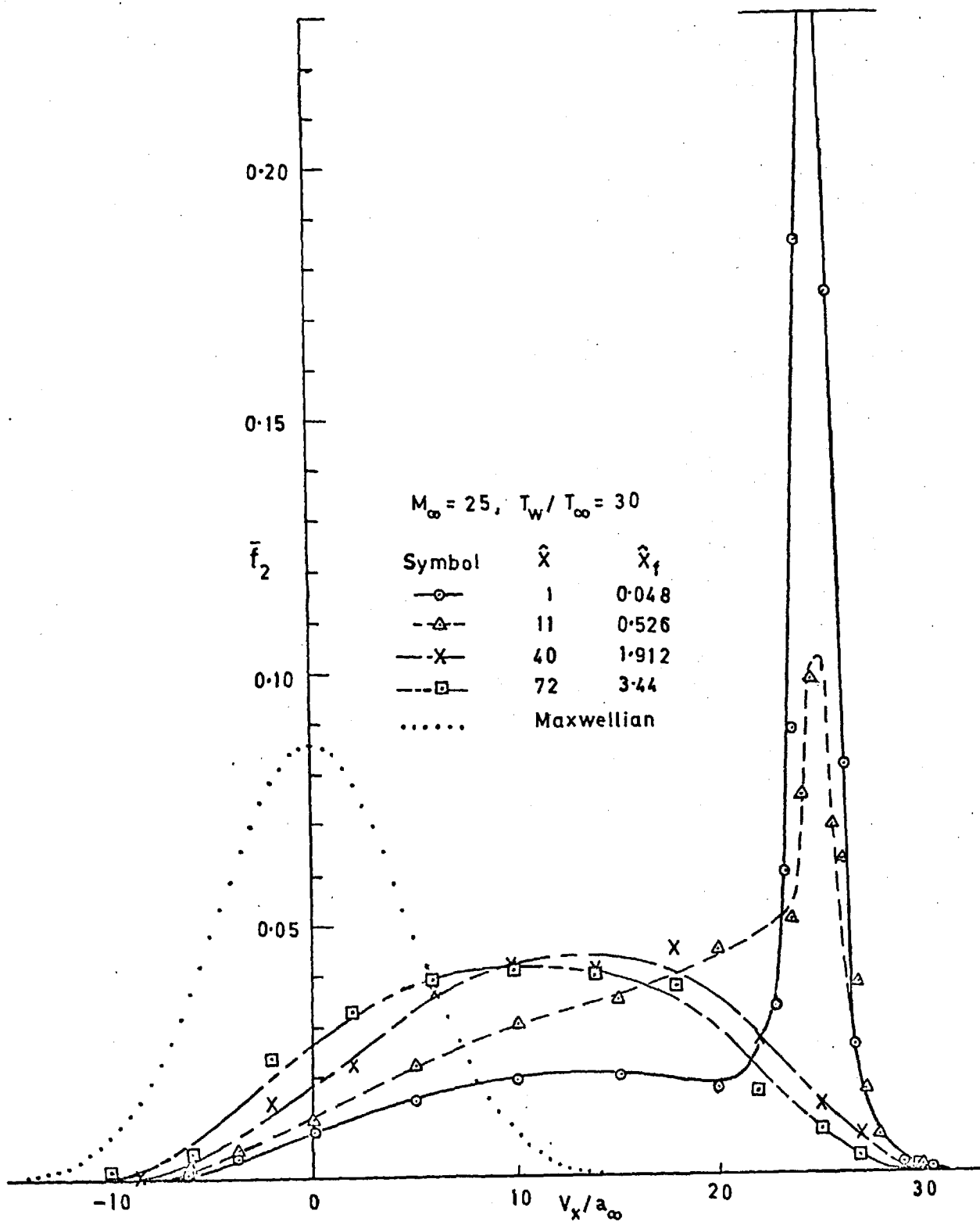


FIG. 24B V_x DISTRIBUTION FOR INCIDENT PARTICLES

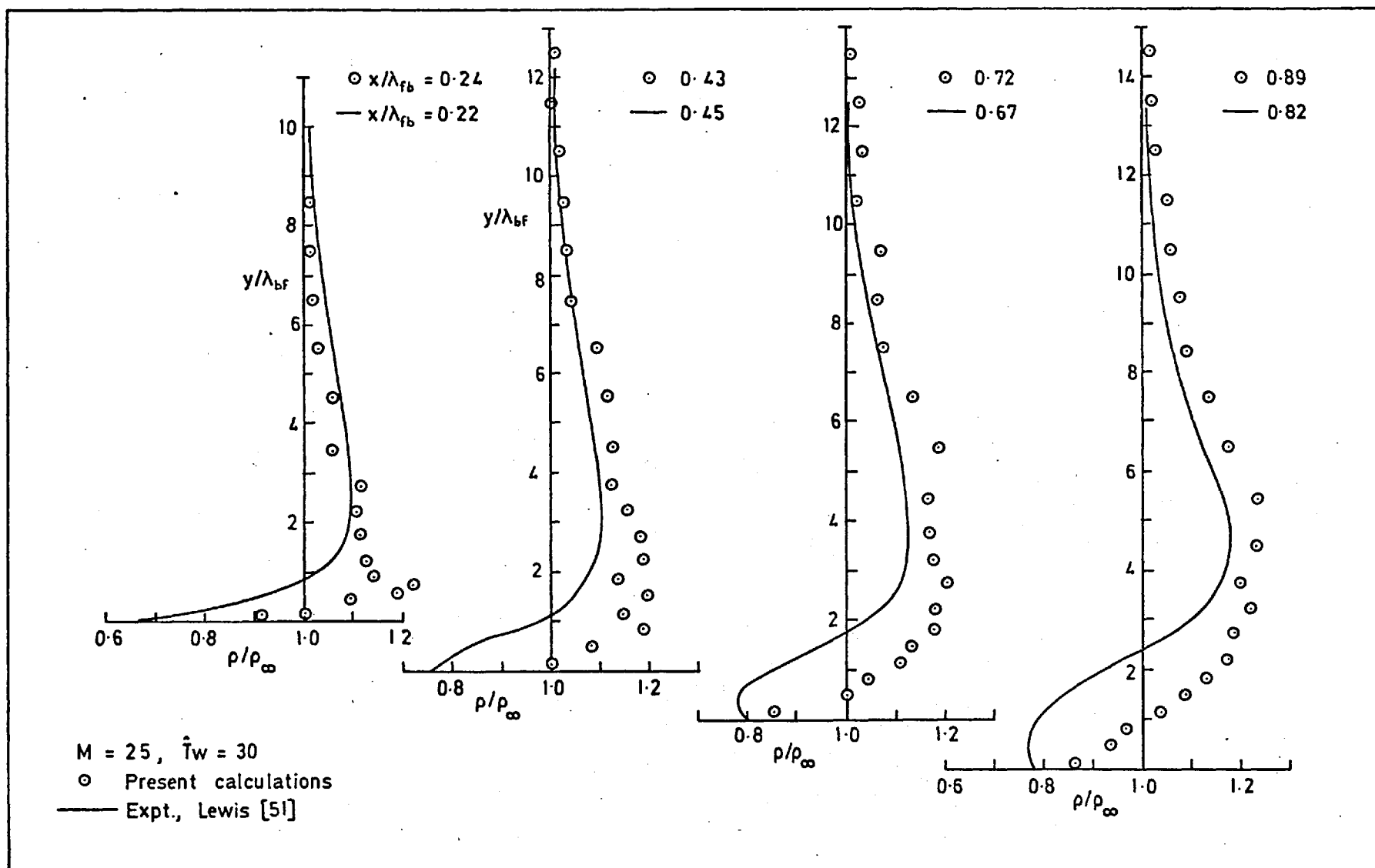


FIG. 25A COMPARISON OF DENSITY PROFILES WITH EXPERIMENT.

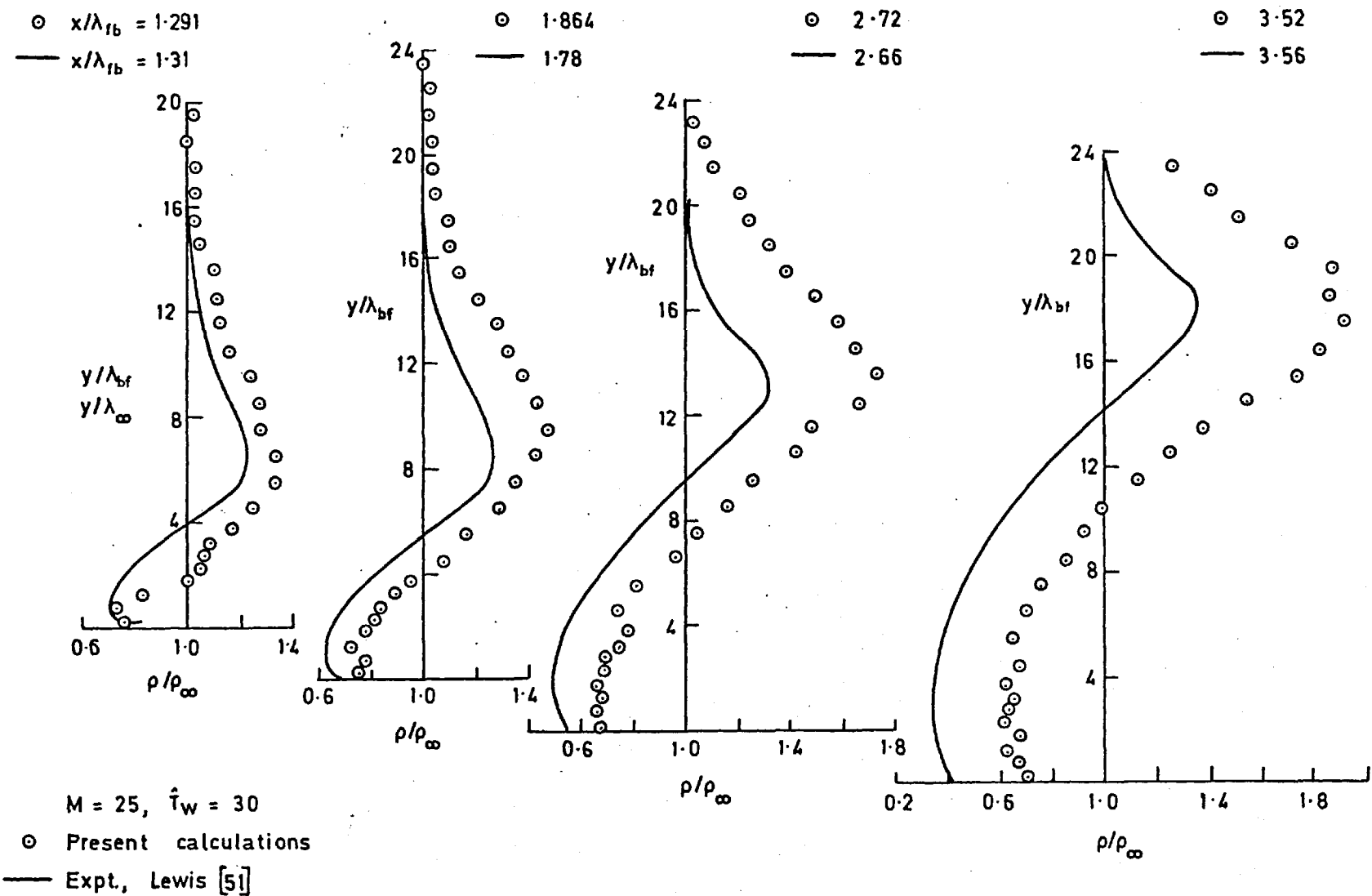


FIG. 25B COMPARISON OF DENSITY PROFILES WITH EXPERIMENT.

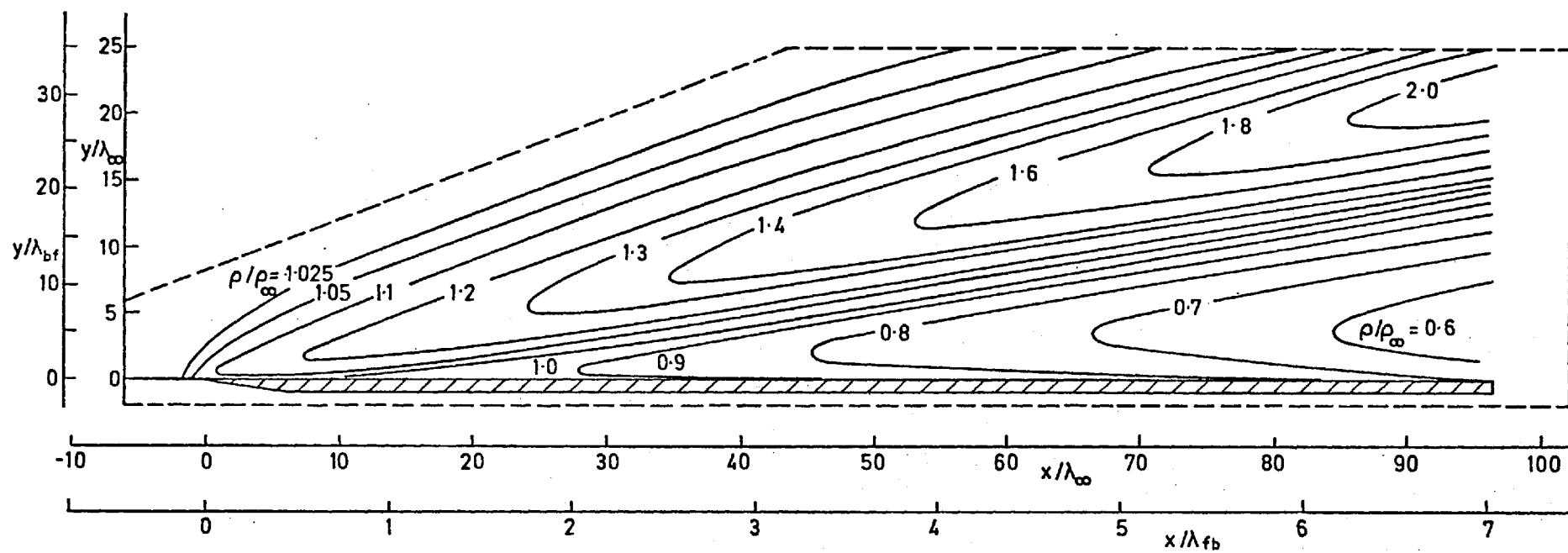


FIG 26 DENSITY CONTOURS $M = 22.93$; $T_w / T_\infty = 14.4$.

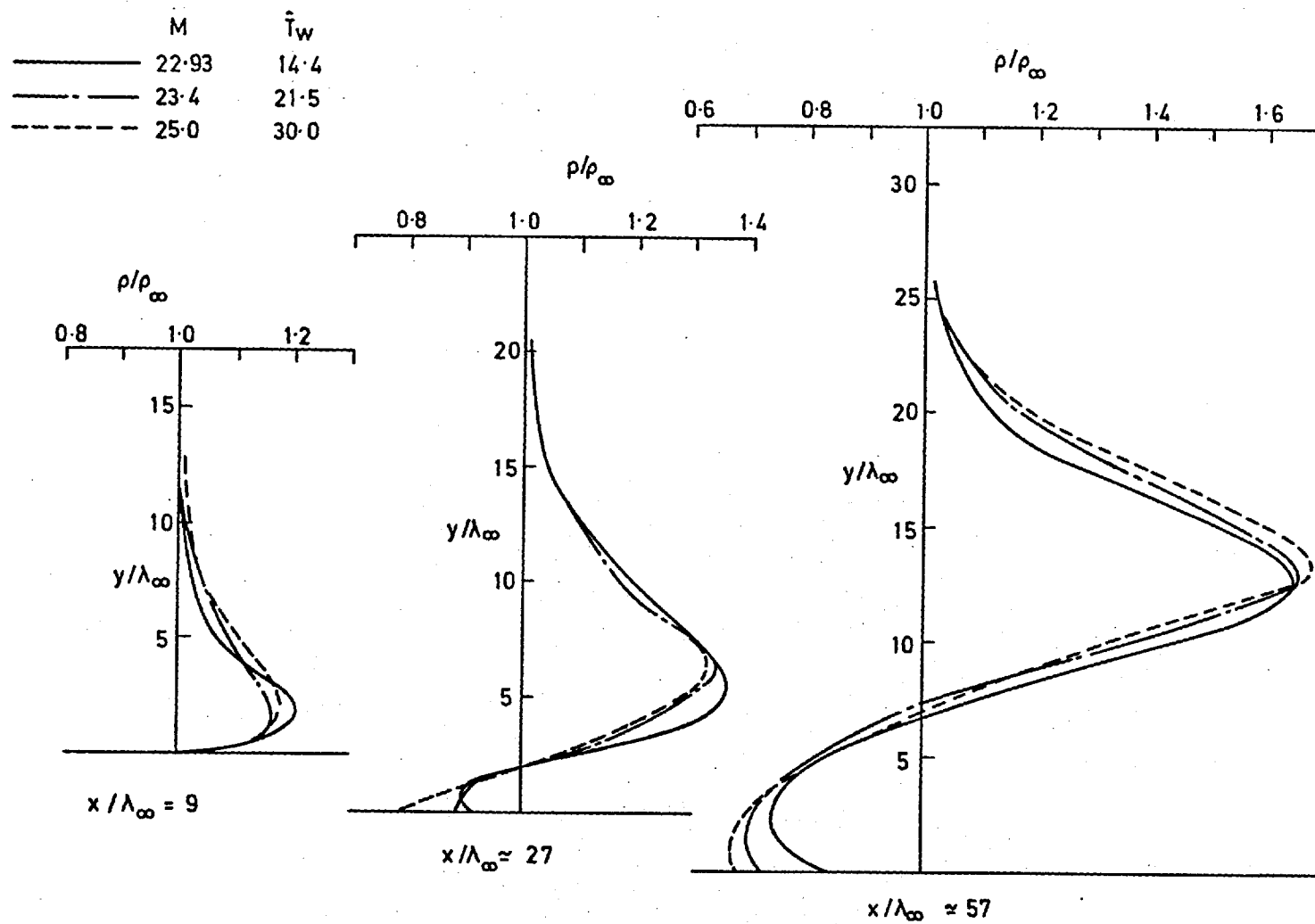


FIG. 27 EFFECT OF WALL TEMPERATURE ON DENSITY.

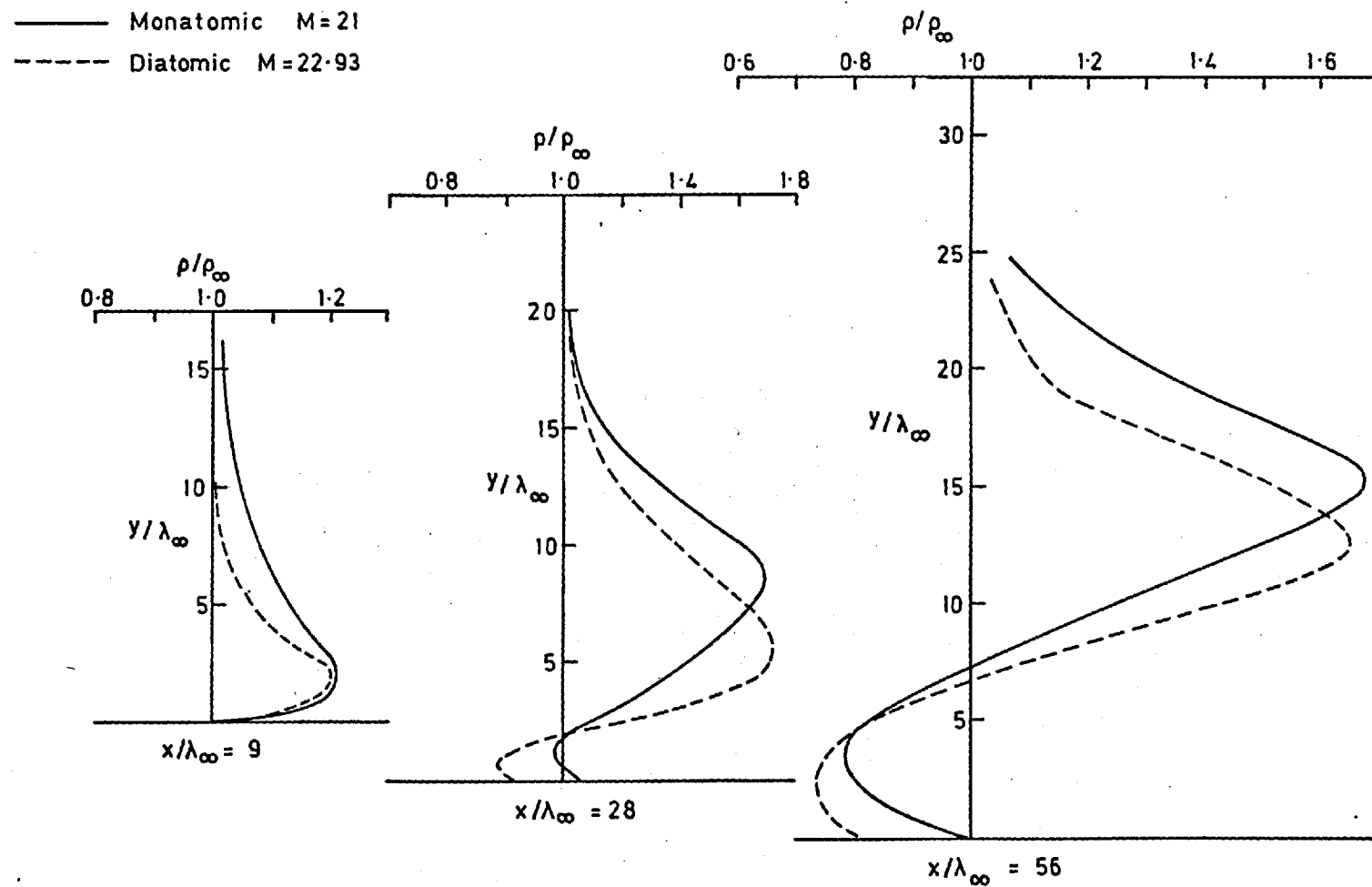


FIG. 28 EFFECT OF DIATOMICITY ON DENSITY, $T_w/T_\infty = 14.4$.

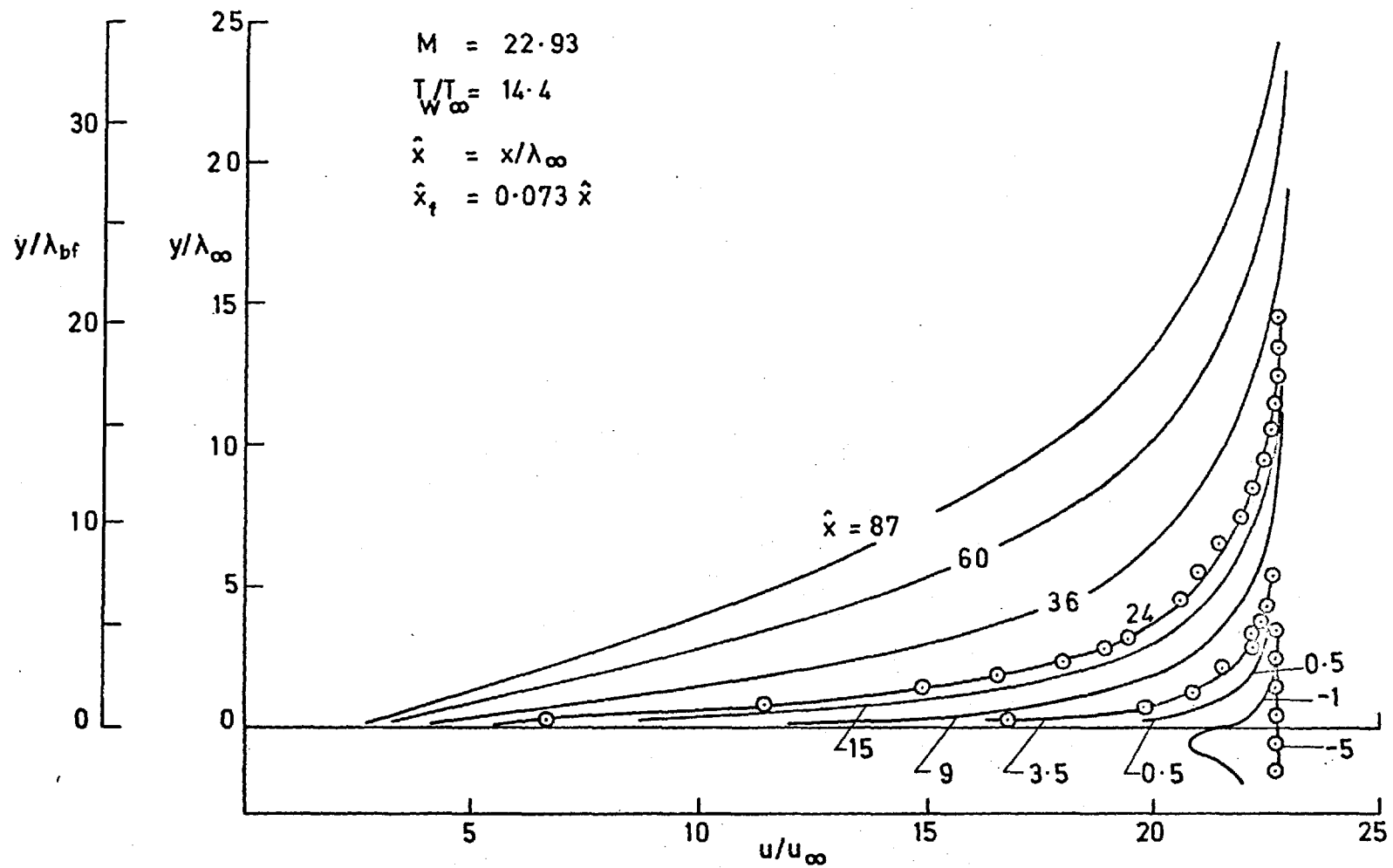


FIG. 29 FLAT PLATE X-VELOCITY PROFILES.

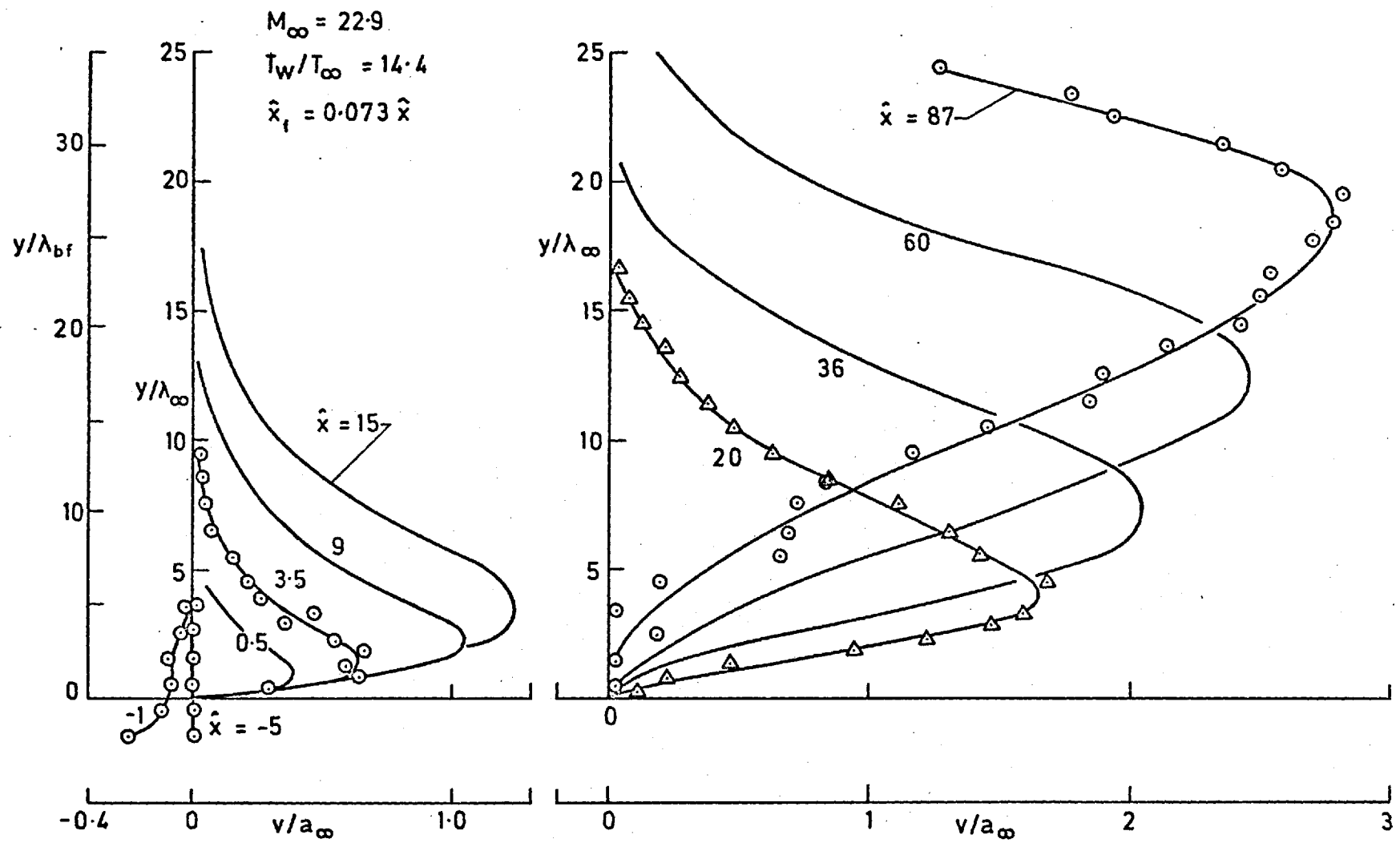


FIG. 30 FLAT PLATE Y VELOCITY PROFILES.

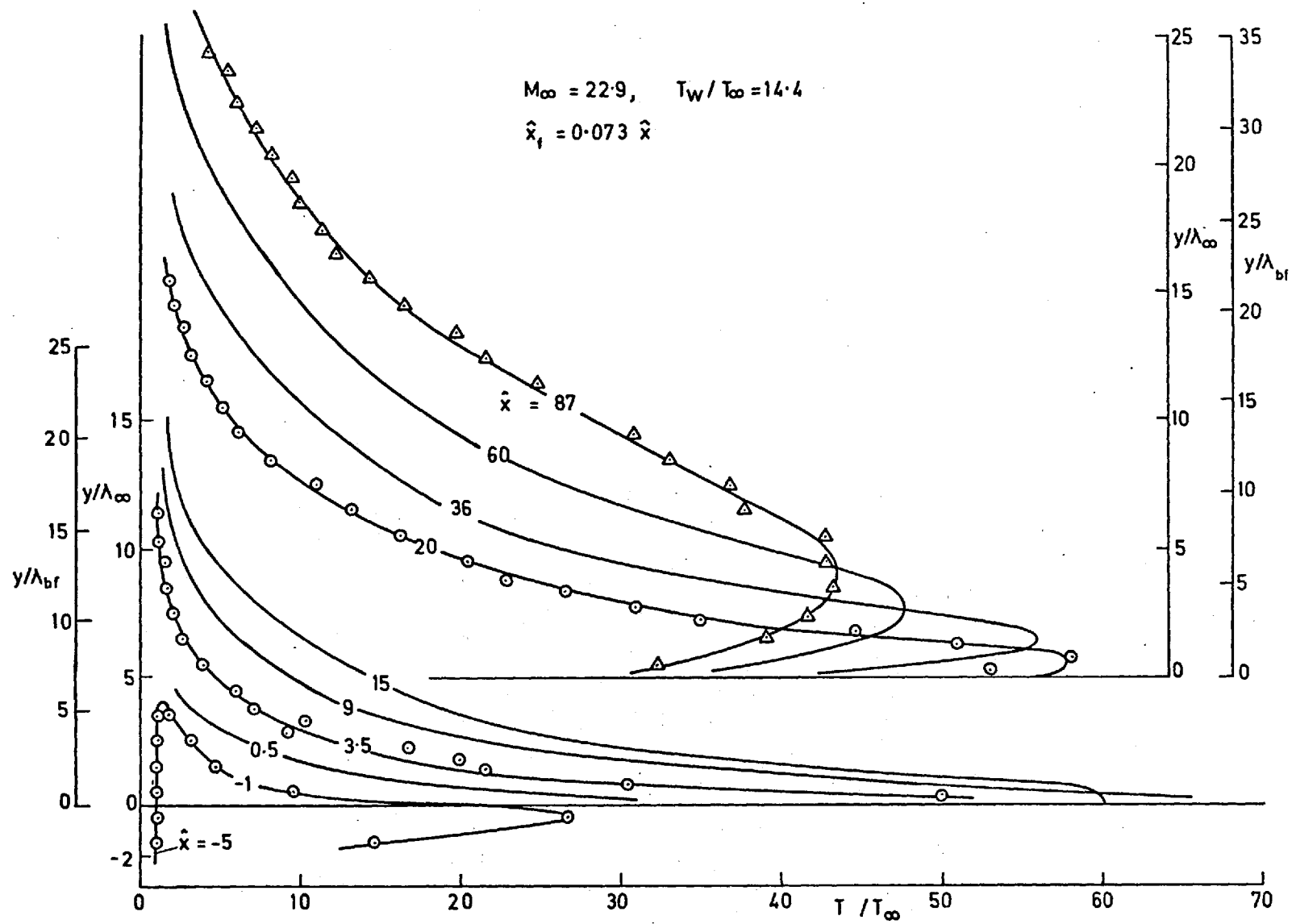


FIG. 31 TRANSLATIONAL TEMPERATURE PROFILES.

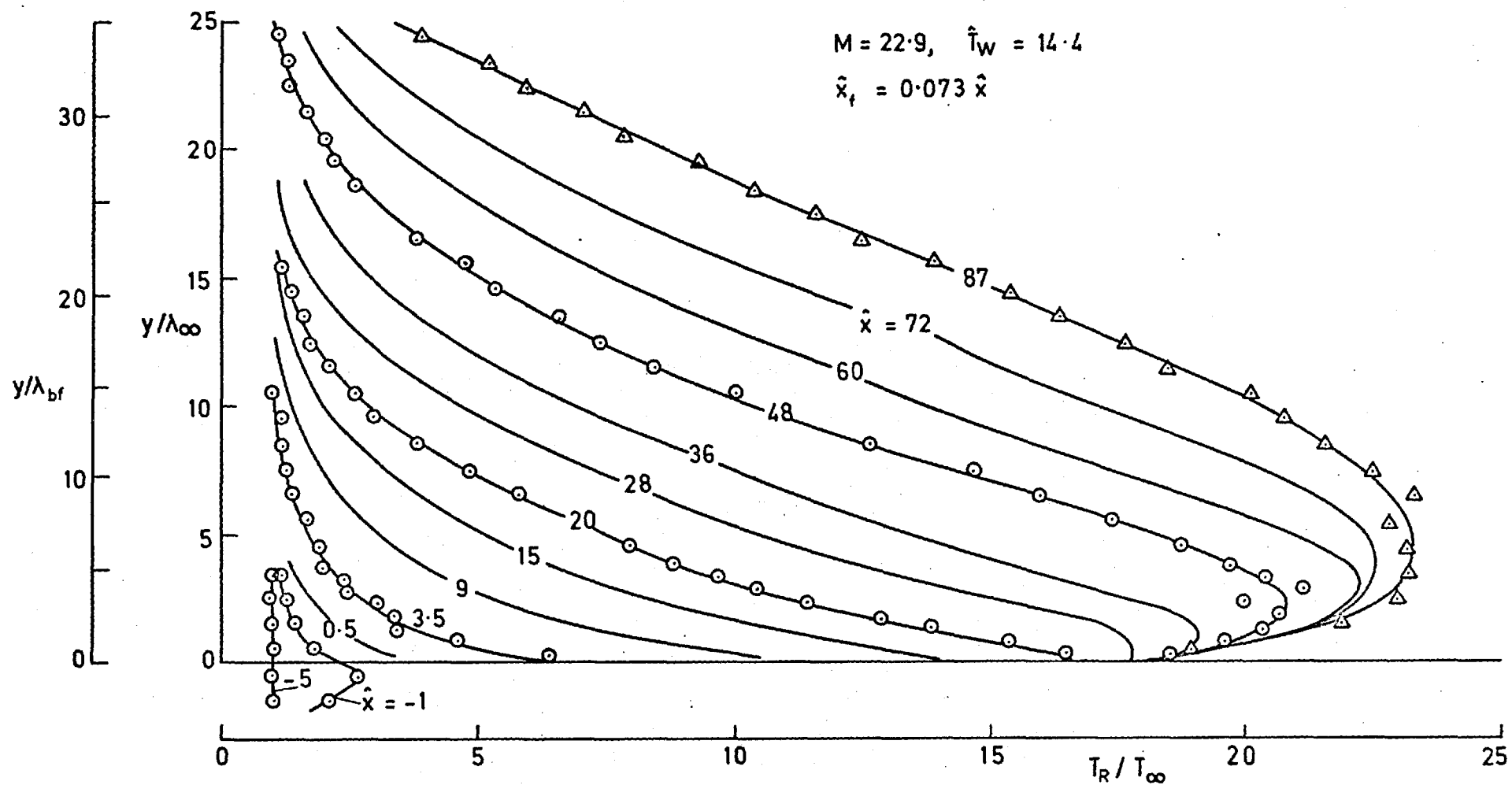


FIG. 32 ROTATIONAL TEMPERATURE PROFILES.

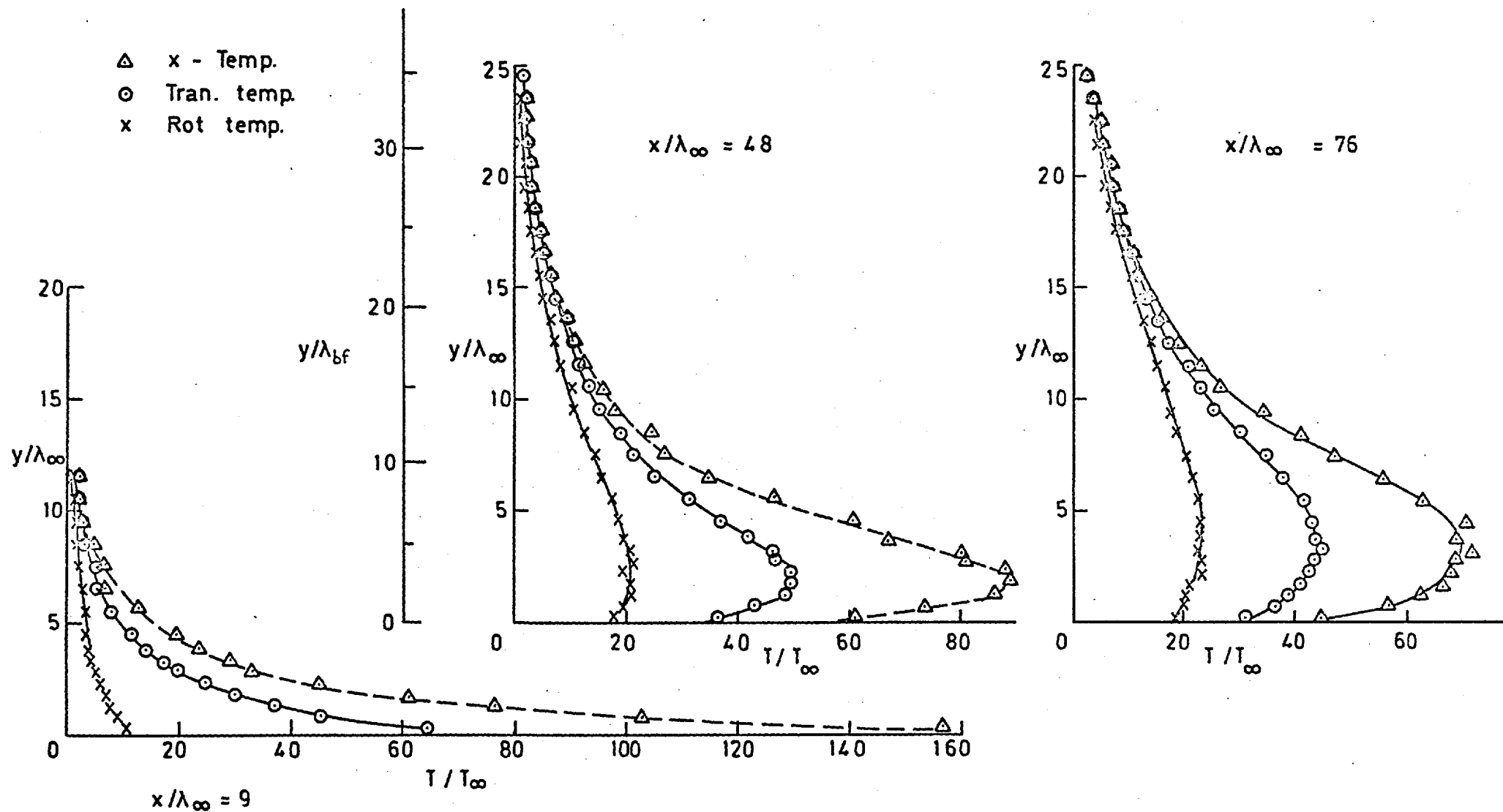


FIG 33 FLAT PLATE TEMPERATURE PROFILES. $M = 22.93$, $\hat{i}_w = 14.4$.

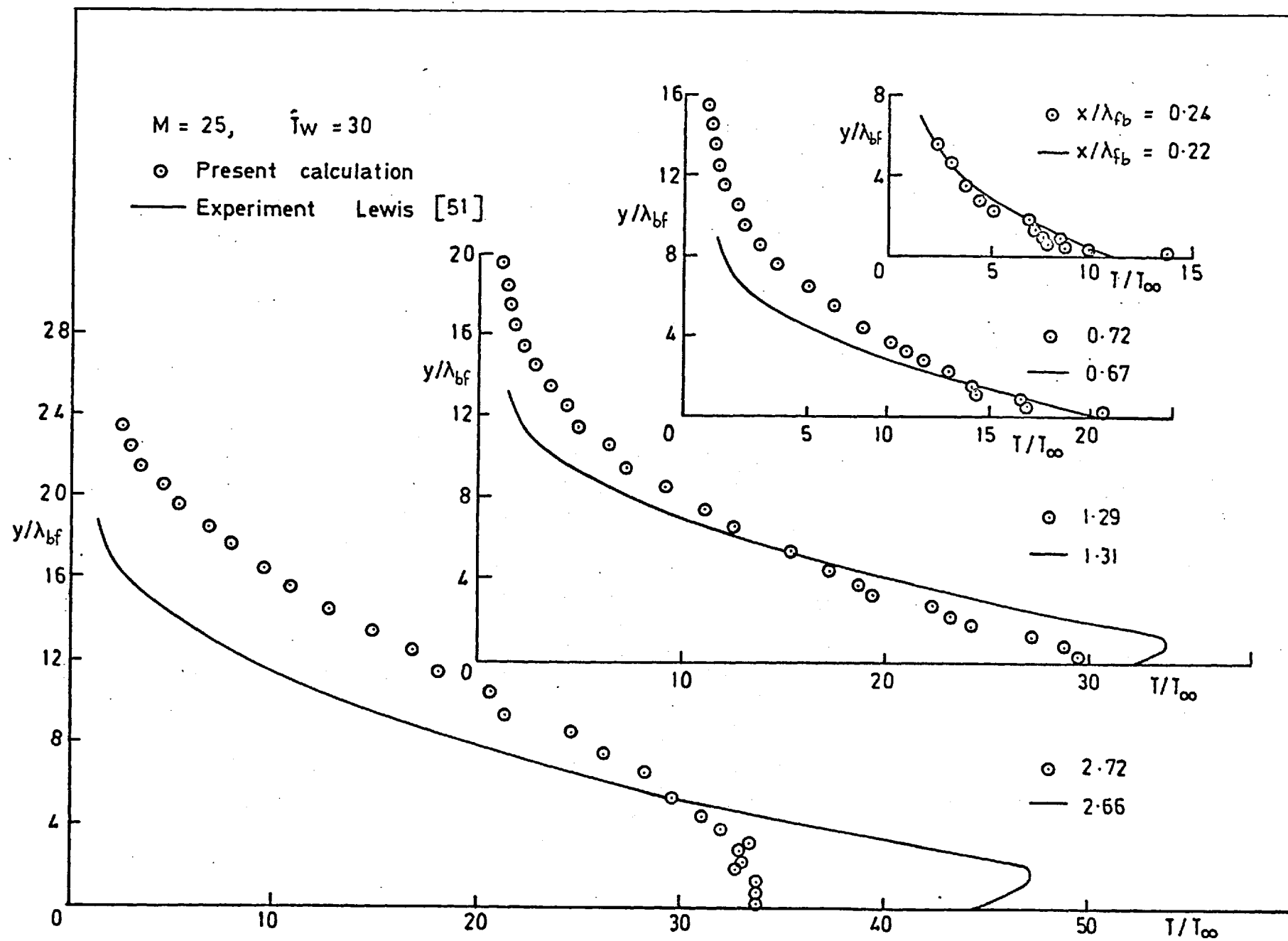


FIG.34 COMPARISON OF ROTATIONAL TEMPERATURE PROFILES WITH EXPERIMENT.

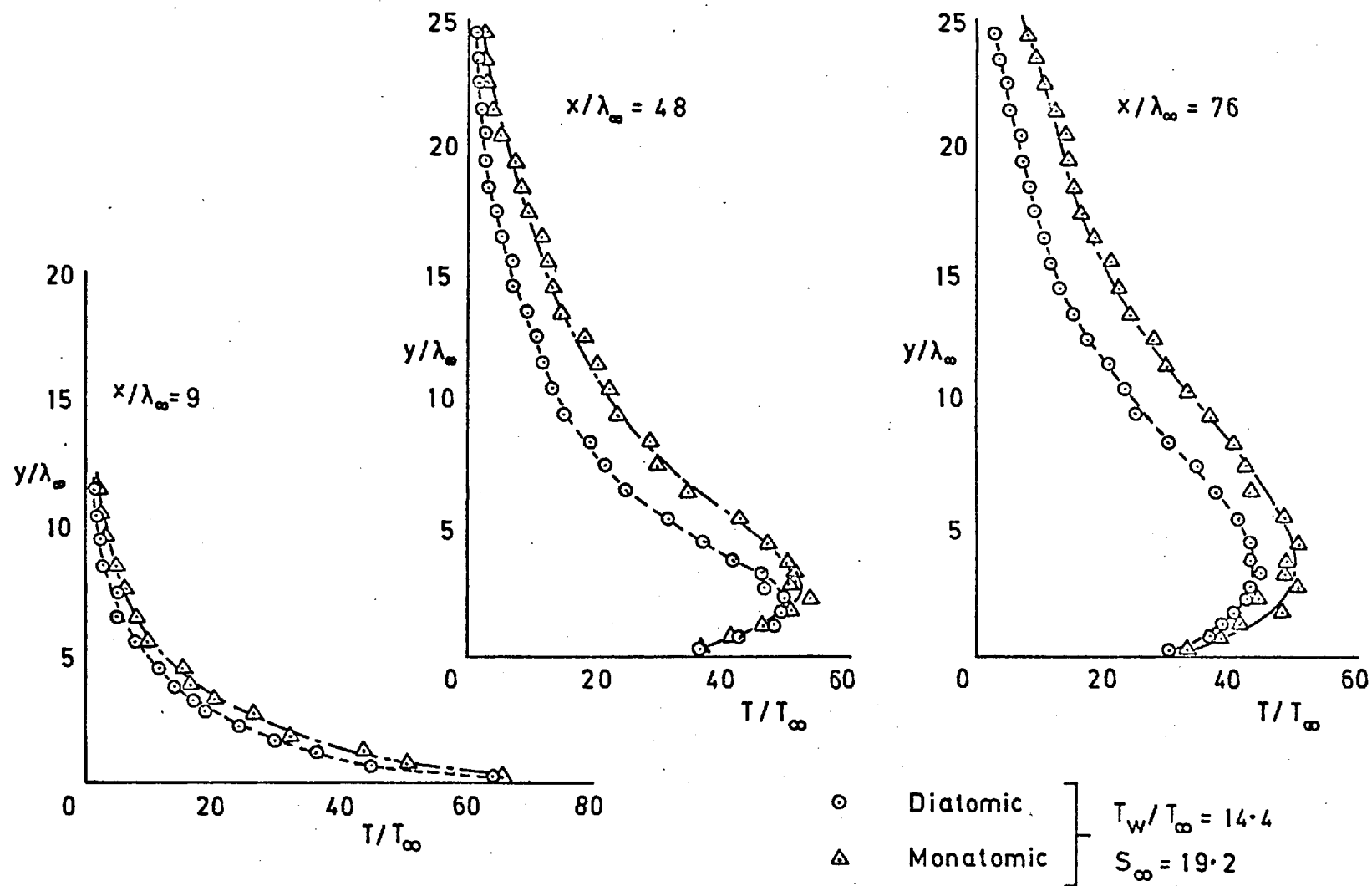


FIG.35 EFFECT OF INTERNAL DEGREES OF FREEDOM ON TRANSLATIONAL TEMPERATURE

