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LOW DISCREPANCY METHODS
FOR THE BOLTZMANN EQUATION

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Abstract

As an alternative to the commonly used Monte Carlo Simulation methods for solving the Boltzmann equation we have developed a new code with certain important improvements. We present results of calculations on the reentry phase of a space shuttle. One aim was to test physical models of internal energies and of gas-surface interactions.

1. Introduction

Simulation methods are the most important tool to solve the Boltzmann equation in realistic settings. In the past, a number of so-called Direct Simulation Monte Carlo Schemes have been developed (see Nanbu's review[1]). The most popular standpoint for their derivation was: Imitate the behavior of real gas molecules, but in a reduced particle system. One step beyond this interpretation has been done by Nanbu when deriving his scheme from the Boltzmann equation. This scheme is now quite well understood (from a physical as well as a

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rigorous mathematical point of view[1], and it has been proven to yield approximations of solutions of the Boltzmann equation provided a sufficiently large number of test particles[2,3]. However, also this method can be interpreted as to imitate a physical situation: the motion of particles in a fixed background gas[4].

For the derivation of a powerful simulation code, we propose to forget about the physical situation and instead to search for a mathematical model yielding results as close to the Boltzmann equation as possible. Such a code (called Low Discrepancy Code) has been developed by our group. The philosophy behind it is completely different from that of Monte Carlo schemes, since it replaces the purely random "microscopic" behavior by one which is as regular as possible in order to cut down fluctuations. Our code - as far as it is by now - shows essential improvements compared with all Monte Carlo schemes in use. It
- imitates two particle collisions and thus satisfies
strictly the conservation laws (in contrast to Nanbu's);
- is highly vectorizable (in contrast to Bird's), even in the
   treatment of internal energies and boundary conditions;
- has reduced fluctuations and thus allows to reduce particle
   numbers.

The main application for our scheme have been calculations on the reentry phase of the European Space Shuttle Hermes. In order to obtain results for two and three dimensional test cases we had to develop an efficient adaptive grid, applicable

to all geometries of interest, which allows for the reconstruction even of high gradients (shocks) within reasonable calculation times. Details are described in section 3.

We have carefully studied problems of modelling physical effects like internal degrees of freedom and gas surface interactions. The usual way of treating these is to apply robust models which are easy to implement and which produce plausible results. The commonly used models are the Larsen-Borgnakke model for internal energies and diffuse reflection with accomodation coefficient for the gas surface interaction. In order to test their physical relevance we have also implemented alternative models which seem to be better motivated from a physical point of view. The results are shown in the sections 4 and 5. (Calculations concerning gas mixtures and chemical reactions are on progress and cannot be presented here.)

All calculations have been performed on the vector calculator Fujitsu VP 100.

2. The idea of Low Discrepancy

In order to explain the main idea of Low Discrepancy we choose a situation as simple as possible. Therefore, in this section we only consider the space homogeneous Boltzmann equation

$$\frac{\partial}{\partial t} f(v) = J[f,f](v) = \iint k \cdot \{f(v')f(w') - f(v)f(w)\} d\eta dw$$

(η unit vector, $v' = v - \eta \langle v-w, \eta \rangle$, $w' = w + \eta \langle v-w, \eta \rangle$)

and its time discretization

$$f_{j+1}(v) = f_j(v) + \Delta t \cdot J[f_j, f_j](v)$$

$$= (1 - \Delta t \cdot \iint k f_j(w) d\eta dw) f_j(v) + \Delta t \cdot \iint k f_j(v') f_j(w') d\eta dw.$$

Multiplying a test function ϕ and integrating with respect to v one can compress this formula to the following weak version[2]:

$$\int \phi(v) f_{j+1}(v) dv = \int \phi(\psi(v,w,b)) d^2 b f_j(v) dv f_j(w) dw$$

with impact parameter b and

$$\psi(v,w,b) = \begin{cases} v' & \text{if b indicates "collision"} \\ v & \text{if b indicates "no collision".} \end{cases}$$

This version is appropriate for our aims since it can be interpreted as follows:

> If f_j is the velocity distribution at the j-th time step then with probability
> $$d^2 b f_j(v) dv f_j(w) dw$$
> the velocity at the (j+1)st time step is
> $\psi(v,w,b)$.

This motivates the following general simulation scheme:

General scheme: (one time step)

1st step: Start with an N point approximation

$$(v_i(0))_{i \leq N} = (v_1(0), \ldots, v_N(o))$$

of $f_o(0)dv$.

2nd step: Select for each $v_i(0)$

- a "collision partner" $w_i(0) = v_{n(i)}(0)$

- and an "impact parameter" b_i

such that

$$(b_i, v_i(0), w_i(0))_{i \leq N}$$

is a good approximation of $d^2b \; f_o(v)dv f_o(w)dw$

("factorization property" of selection mechanism).

3rd step: Define new velocities

$$v_i(1) = \psi(v_i(0), w_i(0), b_i).$$

(If the collection of pairs $(i, n(i))$ is "symmetric", i.e.

$$n(i) = j \quad <=> \quad n(j) = i,$$

and if $b_i = b_{n(i)}$, then the scheme satisfies the conservation laws.)

Taking the Monte Carlo version of this scheme (this is equivalent to Nanbu's) one has to choose b_i and $n(i)$ as independent random numbers. In this case one can show that the simulation result is a good approximation of the solution of the Boltzmann equation, if N is large enough[2]. (A similar statement is true in the space dependent case[3].)

In order to construct a Low Discrepancy version one has to find a selection algorithm with an optimal factorization property. The following simple example should clarify this a

little bit: Suppose f_j depends only on $|v|$, and the veloc-
ities are arranged as follows:

$$|v_1| \angle \ldots \angle |v_N| \, .$$

Then the best approximation of $f_j(v)dv f_j(w)dw$ by pairs
(v_i, w_i) is that for which the pairs $(i, n(i))$ are spread over
$\{1, \ldots, N\} \times \{1, \ldots, N\}$ as uniformly as possible. Figure 1 shows
a Monte Carlo and a Low Discrepancy choice for $(i, n(i))$.
In this simple one dimensional case it is possible to find a
practicable strategy which is almost optimal. In higher
dimensional cases a practicable alternative is to find
sequences of pseudo-random numbers with a good factorization
property (such as Hammersley sequences, etc.).

The idea of Low Discrepancy is not restricted to the approx-
imation of $d^2 b f_j(v)dv f_j(w)dw$. It may also be applied (in an
obvious manner) in order to treat initial and boundary condi-
tions, internal energies, etc.

3. GENERATION OF ADAPTIVE GRID STRUCTURES

Recall that the collision operator of the Boltzmann-Equation
is local in the space coordinates. In simulations it is
therefore necessary to homogenize the density function with
respect to the space coordinates. This homogenization proce-
dure is done according to a cell structure which is influ-
enced by the properties of the flow field. Therefore the cell
structure may vary from time to time.

To be acceptable in a simulation a given grid must fulfill
three conditions:

- the approximate homogeneity of the density function over
  each cell must be guaranteed,
- it must be easy to refind the particles in the cells after
  the free flow,
- the number of cells must yield a reasonable computer
  storage.

Until now several criteria have been given to refine or to
coarsen an existing grid. Widely used are physically moti-
vated ones which are based e.g. on the particle density or on
gradients of the macroscopic quantities. Instead of those we
have chosen a mathematical criterion which is based on a
requirement of the proof of convergence of Babovsky and
Illner:

We have to ensure that

$$(1) \qquad \text{ess sup} |f(t,x+\Delta x,v) - f(t,x,v)| \exp(\alpha v^2) \leq B \Delta x$$
$$ {}_{t,x,v}$$

for some $\alpha > 0$, $B > 0$ and all spatial displacements Δx.

To perform this requirement we use the following algorithm:

For each time step

- divide the domain of computation into rectangular cells
  (2D) or cubes (3D) of fixed shape;
- divide each rectangle (cube) into smaller rectangles
  (cubes) until (1) is satisfied.

It is clear that this algorithm allows the indexing of the particles in a straightforward way (the only things you have to do are modulo operations and reorderings!).

As a first testcase for the performance of the algorithm we have chosen the problem of the calculation of the flowfield around a 2D ellipse. The input data were the following:

- flow velocity: Mach 20
- wall temperature: 1000 <k
- gas temperature: 194 <k
- mean free path: 0,13 m
- ellipse axes: 6,85 m; 2,055 m
- angle of attack: 40°

Fig. 2a and 2b show the initial coarse grid and the refined grid in the stationary state at the end of the simulation. We have plotted the midpoints of the cells.

4. GAS-SURFACE-INTERACTION LAWS

Usually the structure of a solid boundary is by far to complicated to compute the interaction potential between the surface and the incoming particles. Even if this were possible the incomplete knowledge of the state of the surface (roughness, chemical reactions etc.) made such a calculation impossible.

Therefore the description of gas-surface-interaction phenomena is done by simple models which are motivated by phenomenological reasoning and which have some disposable parameters. These parameters have to be fitted on experimental results. The usual mathematical description of these models can be done in the frame of scattering kernels yielding an integral equation of the form:

$$|v \cdot n| f(x,v,t) = \int_{v' \cdot n < 0} R(v' \longmapsto v, \cdot x,t) f(x,v',t) |v' \cdot n| dv .$$

Here n is the inner normal at the boundary point x and $R(v' \longmapsto v, \cdot x, t)$ is the scattering kernel. The probabilistic interpretation of R is: Rdv is the probability that a particle which hits the wall at x with velocity v' leaves the wall with a velocity in the volume element around v.

Beside the simple models

- specular reflection (no parameters)

- diffuse reflection (the wall temperature can be considered as parameter)

- Maxwell boundary (parameters: wall temperature and accomodation coefficient)

we have implemented the Cercignani-Lampis model[5]. This model treats the normal component v_n and the tangent component v_t

of the scattered velocity in different ways.

The features of the Cercignani-Lampis-model are:

- scattering in the tangent space and in the normal direction are independent

- specular reflection and diffuse reflection are special cases of this model

- the scattering kernel satisfies the reciprocity condition[5]

- good agreement with scattering experiments can be achieved by suitable choice of the accomodation coefficients.

Another advantage of the model is the easy implementation in the simulation procedure. The algorithm is as follows:

A) Scattering in tangent space:

- choose random numbers r_1, r_2

$$s \longleftarrow \sqrt{-\alpha_t(2-\alpha_t)\log(1-r_1)}$$

$$v_t^{(1)} \longleftarrow (1-\alpha_t)v_t^{'(1)}-s*\cos(2\pi r_2)$$

$$v_t^{(2)} \longleftarrow (1-\alpha_t)v_t^{'(2)}-s*\sin(2\pi r_2)$$

Here $v_t^{'(1)}$, $v_t^{'(2)}$ are the two components of the incoming velocity in the tangent space.

B) Scattering in normal direction, Polya-Aeppli-distribution algorithm:

- Generate Poisson $(\dfrac{1-\alpha_n}{\alpha_n} \cdot v_n^{'2})$ random variable z

- Generate Gamma (1+z) random variable G

$$v_n' \longleftarrow \sqrt{\alpha_n G}$$

It should be noticed that in this way of implementing the

gas-surface-interaction procedure is completely vectorized
and therefore not time consuming.

As testcase for gas surface models we have selected the heat
transfer problem in one dimension. Fig. 4.1 shows the temper-
ature profile of a monoatomic hard sphere gas between two
infinite walls. At the left boundary we have a temperature of
180 K and at the right boundary a temperature of 220 K.

As can be seen by comparison of fig. 3b and fig. 3c the
results are the same for the diffuse reflection model and
Cercignani-Lampis model. Fig. 3a shows that the profile
becomes more flat if the accomodation coefficients are lower
than 1.0. So we are able to adjust our results to measure-
ments by fitting the parameters. But to get some guess about
the right values we need measurements of the temperature
profile in this simple case.

5. TREATMENT OF CLASSICAL INTERNAL DEGREES OF FREEDOM

Because of the temperatures which arise in the simulation of realistic gas flow problems the internal states of the gas molecules have to be considered. In many cases we deal with linear molecules (e.g. N_2, O_2) for which the rotations of the molecules are of particular importance.

Whereas there is little doubt about the right kinetic equation for monoatomic gases a generalization to polyatomic molecules is not quite straightforward (one has to decide, for example, whether to treat the internal degree of freedom by means of quantum mechanics or not).

In this paper we report about classical internal degrees of freedom. To save computer storage and time we calculate the distribution of the internal energy only. The kinetic equation we use was described by Pullin[6]:

$$(\frac{\partial}{\partial t} + v \cdot \nabla_x) f(t,x,v,\varepsilon) =$$

$$= \int_{R^3} \int_0^\infty \int_{\Delta_E} \int_{S^2} \|v-w\| \sigma(E; \varepsilon, \varepsilon_1; \varepsilon', \varepsilon_1'; \eta, \eta') \times$$

$$\times \{f'f_*' - f \cdot f_*\} dw(\eta) d^2\varepsilon' d\varepsilon_1' d^3w \tag{1}$$

with

$$E = \frac{m}{4} \|v-w\|^2 + \varepsilon + \varepsilon_1 = \frac{m}{4} \|v'-w'\|^2 + \varepsilon' + \varepsilon_1'$$

$$f = f(t,x,v,\varepsilon), \quad f_* = f(t,x,w,\varepsilon_1)$$

$$f' = f(t,x,v',\varepsilon') \quad f_*' = f(t,x,w',\varepsilon_1')$$

$$\Delta_E = \{(\varepsilon', \varepsilon_1') : 0 \leq \varepsilon', 0 \leq \varepsilon_1', \varepsilon' + \varepsilon_1' \leq E\} .$$

It is clear that different models of the exchange of internal and translational energy are characterized by the particular form of the scattering cross section $\sigma(E; \varepsilon, \varepsilon_1; \varepsilon', \varepsilon_1'; \eta \cdot \eta')$.

A widely used model is that proposed by Larsen and Borgnakke[7]. For this model the scattering cross section reads:

$$\sigma(E; \varepsilon, \varepsilon_1; \varepsilon', \varepsilon_1'; \eta \cdot \eta') =$$

$$Z(E) \sigma_o(\|v-w\|) h(\eta \cdot \eta') \delta(\varepsilon - \varepsilon') \delta(\varepsilon_1 - \varepsilon_1') +$$

$$+ (1-Z(E)) \sigma_o(\|v-w\|) R(E; \varepsilon, \varepsilon_1; \varepsilon', \varepsilon_1') h(\eta \cdot \eta') \qquad (2)$$

$$\text{with:} \quad \int_{S^2} h(\eta \cdot \eta') dw(\eta') = 1$$

$$R = \sigma_o(\|v'-w'\|) \|v'-w'\|^2 (\varepsilon' \cdot \varepsilon_1')^{\chi/2-1} N(E)$$

$$\int_{\Delta_E} R \, d^2\varepsilon' = 1 .$$

The features of this model are:
- The total cross section depends on $\|v-w\|$ only.
- A part of the collisions is elastic. The ratio of elastic to inelastic collisions is controlled by the total colli- sional energy.
- The "energy scattering kernel" does not depend on ε and ε_1; it is determined by the total cross section σ_o.

According to this model we have the following simulation algorithm to perform the collision process:

1) Define the collision partners in such a way that the pairs $((v_i, \varepsilon_i), (w_i, \tilde{\varepsilon}_i))$ are a good approximation of the product density function.

2) For each pair $((v, \varepsilon), (w, \tilde{\varepsilon}))$

$P_{coll} \leftarrow \vert \; n \cdot \sigma_o(\Vert v-w \Vert) \cdot \Vert v-w \Vert \Delta t'.$

If $(1-r) \leq P_{coll}$

$E \leftarrow \vert \; \frac{m}{4} \Vert v-w \Vert + \varepsilon + \tilde{\varepsilon}; \quad \varepsilon_t \leftarrow \vert \; \frac{m}{4} \Vert v-w \Vert^2$

If $(\tilde{r} \geq Z(E))$

    generate r·v. μ_t, μ_1 according to P_t, P_1

    generate r·v. η' according to $h(\eta \cdot \eta')$

    $\varepsilon_t \leftarrow \vert \; \mu_t E$

    $\varepsilon \leftarrow \vert \; (1-\mu_1)(1-\mu_t)E$

    $\tilde{\varepsilon} \leftarrow \vert \; \mu_1(1-\mu_t)E$

End if

$$\binom{v}{w} \leftarrow \vert \; \frac{1}{2} \; [\,(v+w) \; {\overset{+}{\underset{-}{}}} \; \eta' \sqrt{\frac{4}{m} \varepsilon_t} \;]$$

Here we have

$$P_t(\mu_t) = N(E) \sigma_o(\mu_t E) \mu_t (1-\mu_t)^{\chi-1}$$

$$P_1(\mu_1) = C_2(\mu_1(1-\mu_1))^{\chi/2-1}$$

where C_2 is chosen in a way to ensure that $\int_0^1 P_1(\mu_1) d\mu_1 = 1$.

It should be noticed that this simulation procedure is completely vectorizable because there is no need for the use of a time counter (remember that the introduction of time counters causes recurrence which avoids the possibility of vectorization).

To study the influence of the parameters we have calculated a 1D shock wave of gases with 2 internal degrees of freedom. In all our calculations the initial distribution was given by

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a Maxwellian with different parameters upstream respectively
downstream with a jump at zero. The downstream values are
determined from the upstream values by the Rankine-Hugoniot
relations. Equilibrium at infinity is assumed. In fig. 4 we
show the results obtained by using a hard sphere total cross
section, in fig. 4 those obtained with the help of the VHS
scattering cross section of I. Kuscer[8]:

$$\sigma_O(\|v-w\|) = \sigma_\infty \cdot \left[1 + \frac{6KT_S}{m\|v-w\|^2} \right].$$

Here T_S is the Sutherland temperature of the gas molecules
which are to be simulated and σ_∞ is a constant which has to
be adapted on the measured viscosity (notice that the viscos-
ity calculated with the help of this scattering cross section
obeys the Sutherland formula). In the results shown the
function $Z(E)$ has been kept constant at the values 0.9 and
0.6 respectively. As can be seen by comparison of the various
results both the temperature and the density profiles are
influenced by the choice of the scattering cross section and
the ratio of elastic collisions. Therefore by comparison of
calculated with measured shock profiles it should be possible
to make a decision about the interaction law which is
suitable for a given gas type.

6. SUMMARY AND CONCLUSIONS

We have developed a new code for the simulation of Boltzmann's Equation which is based on the LD-method. Because of the structure of this algorithm the vectorization of the code is straightforward. This vectorization property yields reasonably short computation times: to calculate the flow field around a 2D ellipse we needed about 18 CPU minutes on the Fujitsu VP 100.

Also, the LD ideas are very appropriate for simulating boundary conditions. In this field we implemented the Cercignani-Lampis model which has, to our opinion, enough parameters to fit on experimental results.

The consideration of internal energies is also straight-forward because the LD method is based on binary collisions. This property of the method has been demonstrated by the calculation of a 1D shock wave of gases with 2 internal degrees of freedom.

The most important property of our algorithm is, to our opinion, the proof of convergence. This proof shows that the LD method is based on a good mathematical ground and does not rely on heuristics (as e.g. Bird's scheme). This ground work allows further consideration of the scheme as e.g. its behaviour when the number of simulation particles is very small. The study of this behaviour will be one of our main research topics in the future.

Figure Captions

Fig. 1: Selection of N points from N^2 points
  a) Monte Carlo
  b) Low Discrepancy

Fig. 2: Midpoints of the coarse and the refined grid for the flow around a 2D ellipse

Fig. 3: Temperature profile of the heat transfer problem
  a) C-L model with $\alpha_n=.3$, $\alpha_t=.1$
  b) diffuse reflection
  c) C-L model with $\alpha_n=1.$, $\alpha_t=1.$

Fig. 4: Profiles of reduced density and temperatures for a shock wave of molecules with 2 internal degrees of freedom at upstream temperature of 200 K. Hardsphere model
  a) Z = 0.9
  b) Z = 0.6
  curves 0: density profile
      X: internal temperature
      *: translational temperature

Fig. 5: Profiles of reduced density and temperatures for a shock wave of molecules with 2 internal degrees of freedom at upstream temperature of 200 K. Kuscer model ($\sigma_\infty = 3\cdot10^{-19}$ m^2, $T_s = 107$ K)
  a) Z = 0.9
  b) Z = 0.6
  curves 0: density profile
      X: internal temperature
      *: translational temperature

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D-6750 Kaiserslautern, FRG
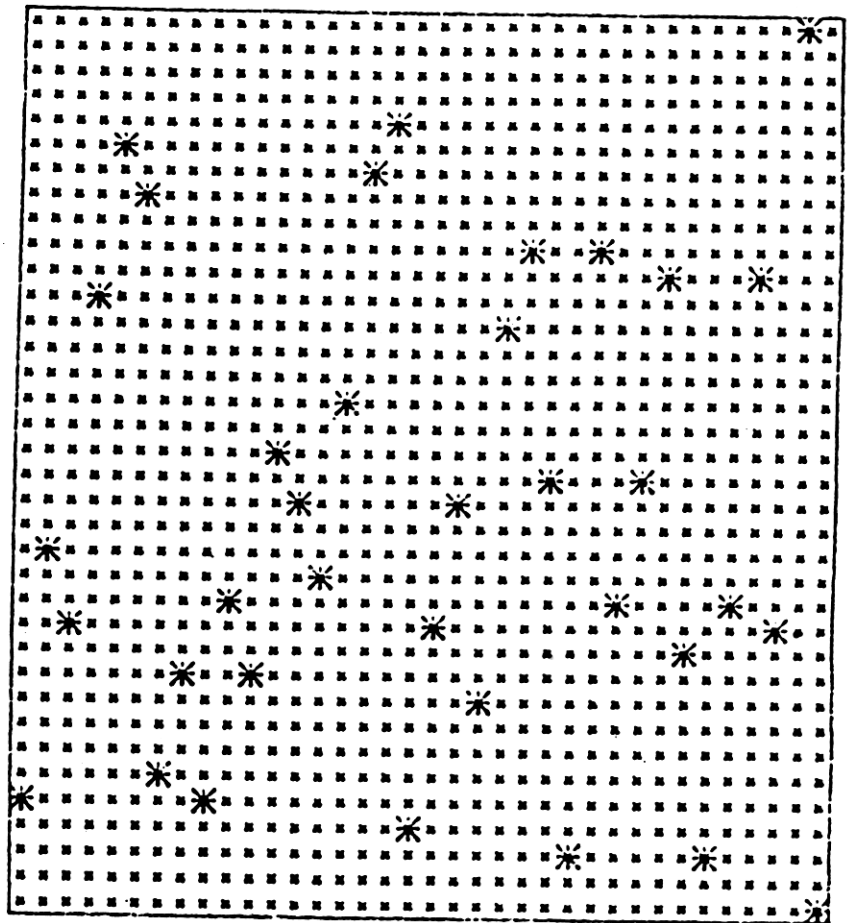
Figure 1a

MC-METHOD

SELECTION

OF

COLLISION

PARTNERS
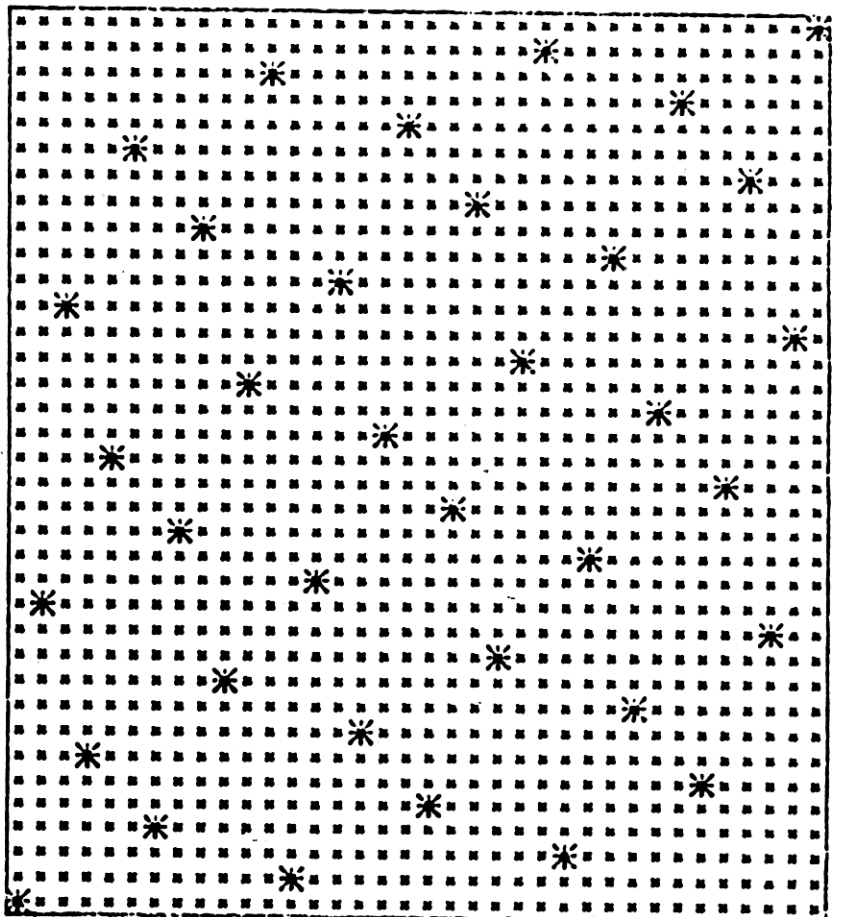

Figure 1b
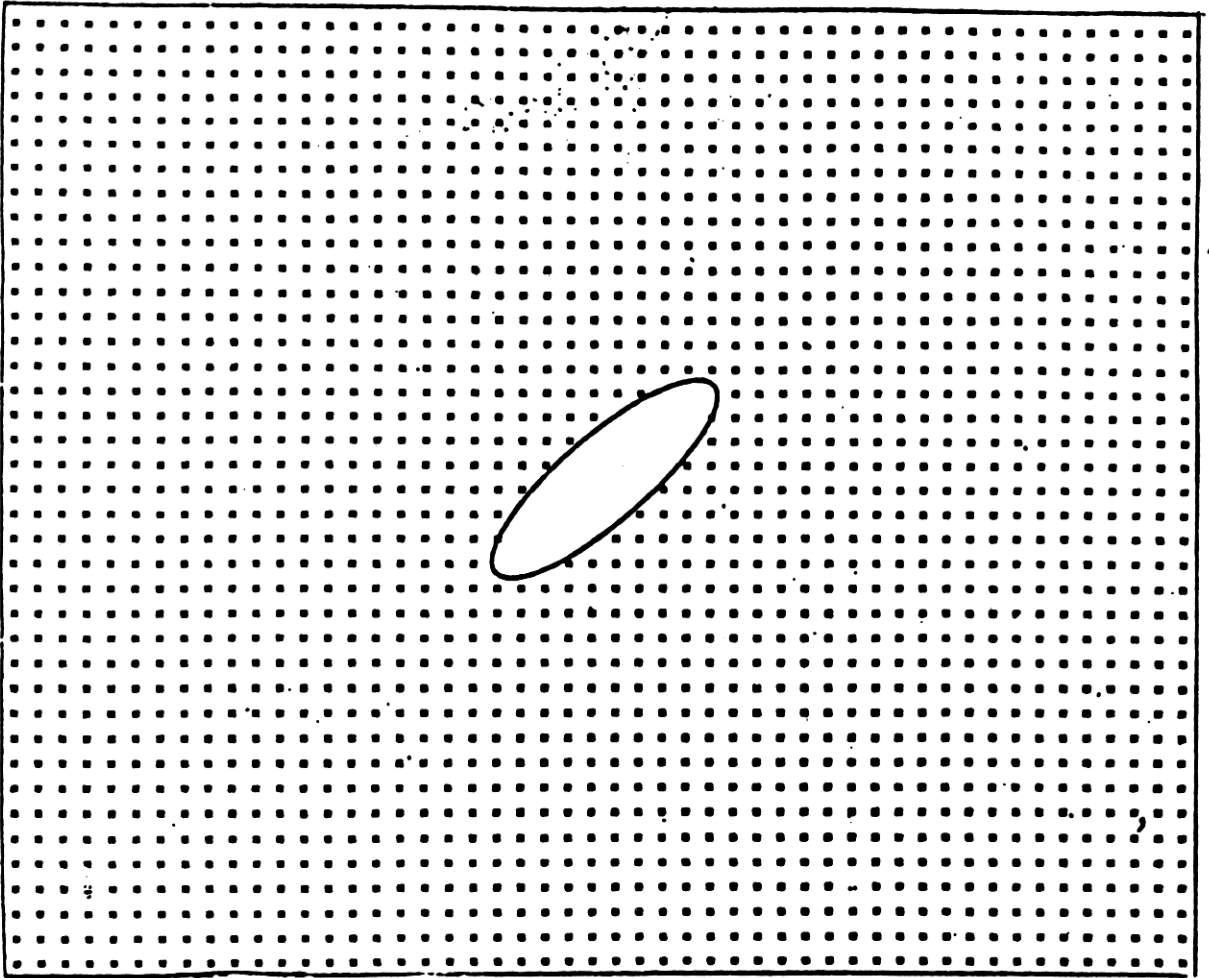
LD-METHOD
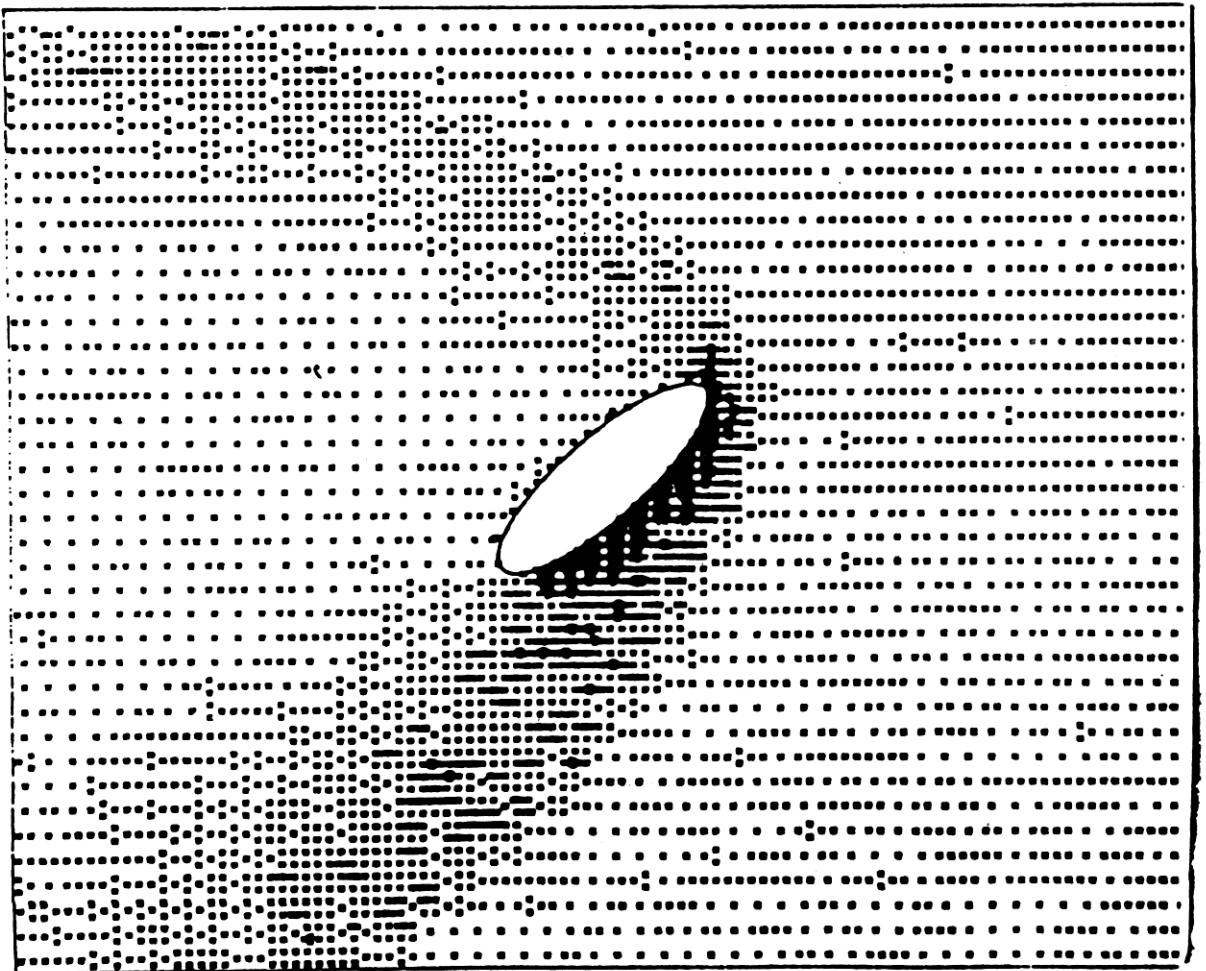
SELECTION

OF

COLLISION

PARTNERS

Fig. 2a

Fig. 2b

Figure 3

LD-METHOD

SIMULATION OF HEAT TRANSFER

PARAMETER :

CELL SIZE - 0.1 M

MEAN FREE PATH - 0.05 M

PART/CELL - 2000

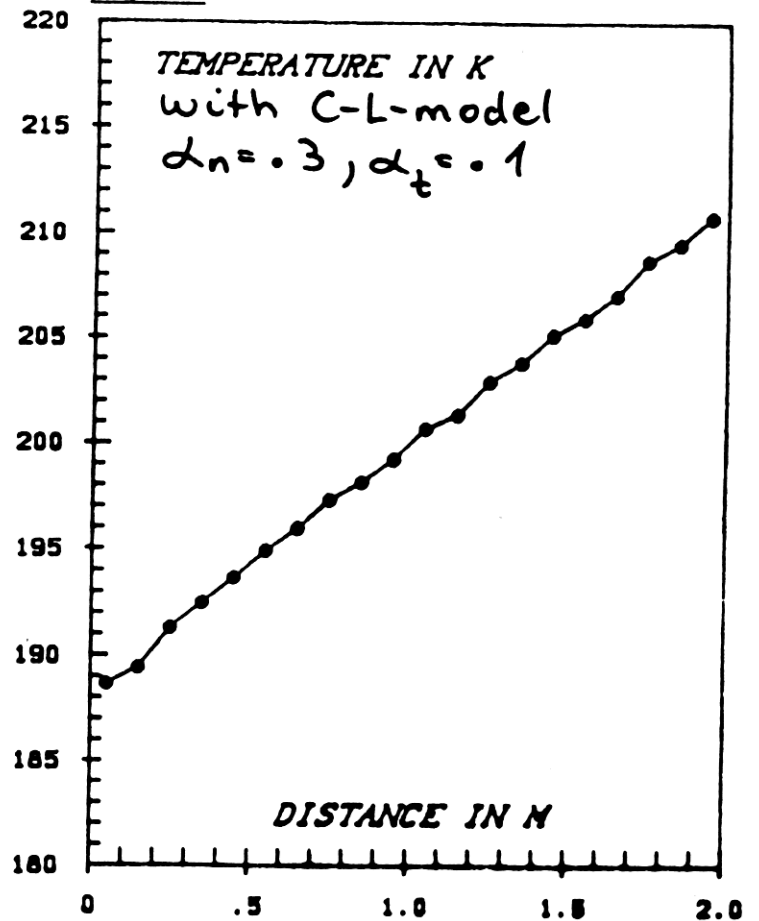*TEMP LEFT - 180 K*

TEMP RIGHT - 220 K

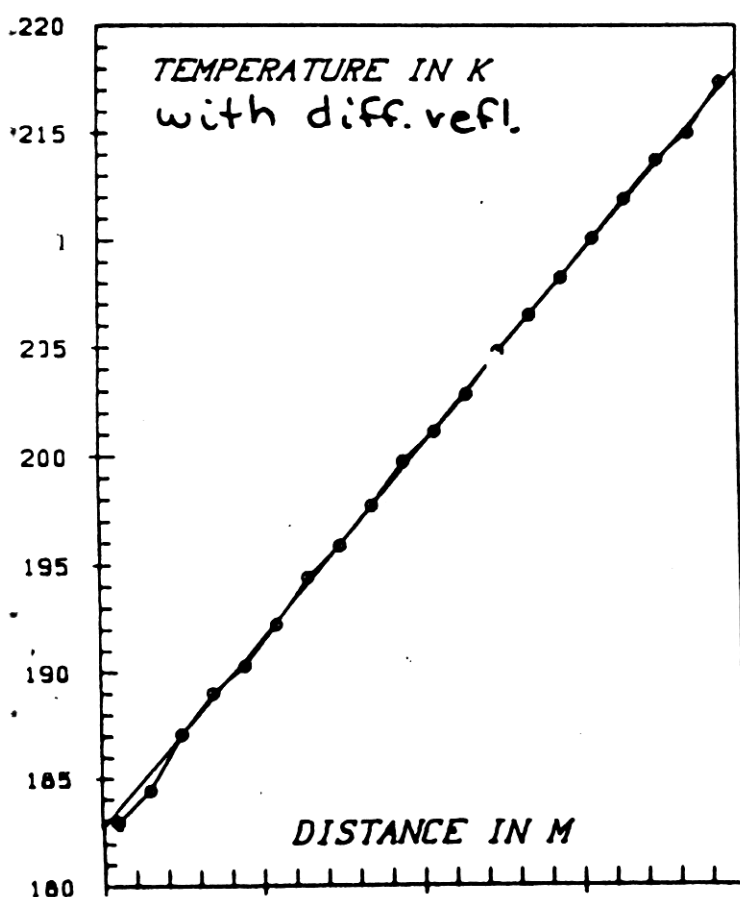Fig. 3a

TEMPERATURE IN K with C-L-model $\alpha_n = .3, \alpha_t = .1$

DISTANCE IN M

Fig. 3b

TEMPERATURE IN K with diff. refl.

DISTANCE IN M

Fig. 3c

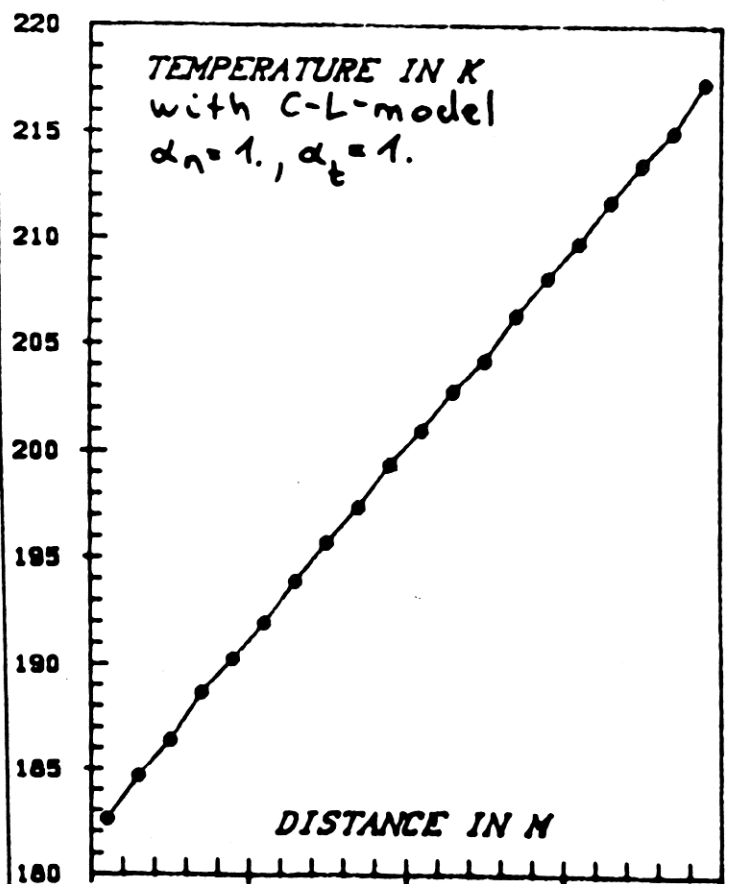*TEMPERATURE IN K* with C-L-model $\alpha_n = 1., \alpha_t = 1.$

DISTANCE IN M

Figure 4a

LD-METHOD

SIMULATIUN OF A SHOCK

PARAMETER :

UPSTREAM VEL=2900.0 M/SEC

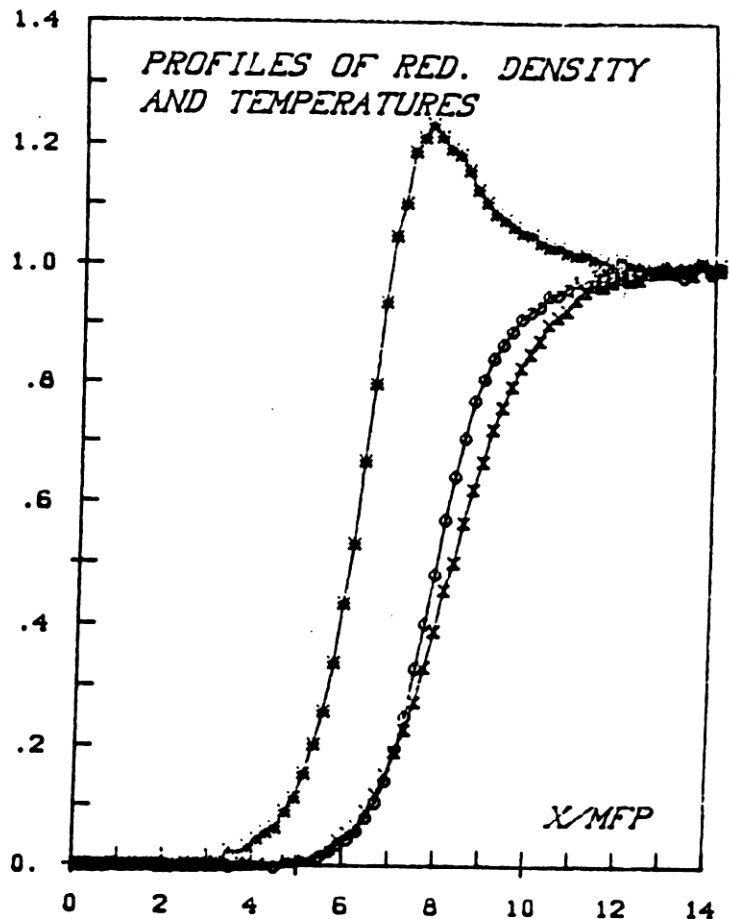MEAN FREE PATH = 0.12 M

COLL RATIO = 0.90

TEMPERATURE = 200 K

PROFILES OF RED. DENSITY AND TEMPERATURES

X/MFP

Figure 4b

LD-METHOD

SIMULATION OF A SHOCK

PARAMETER :

UPSTREAM VEL=2900.0 M/SEC

MEAN FREE PATH = 0.12 M

COLL RATIO = 0.60

TEMPERATURE = 200 K
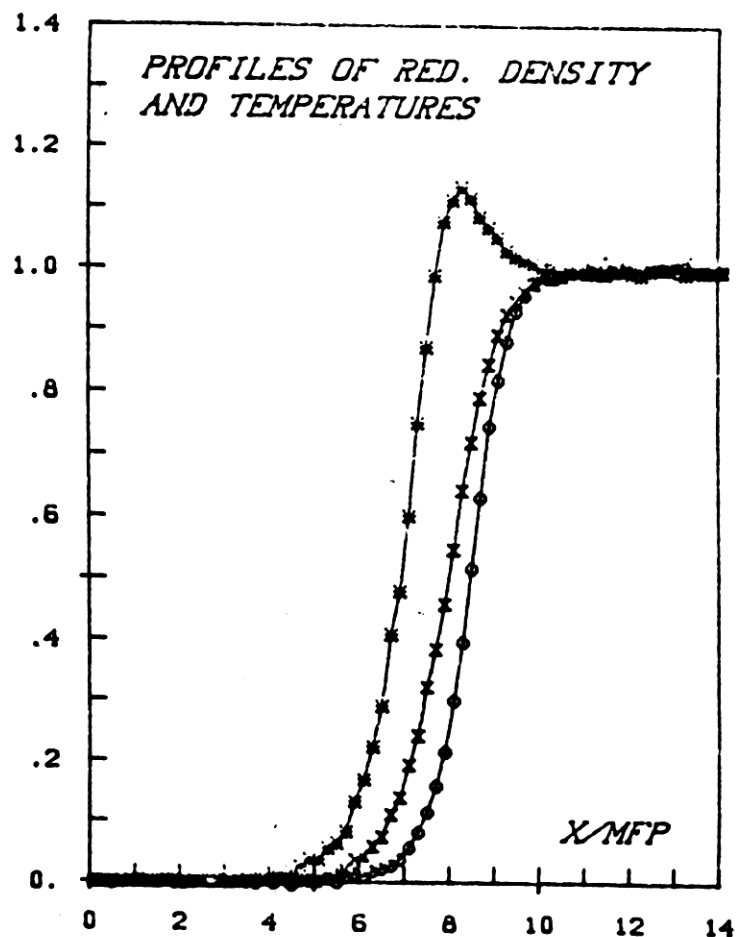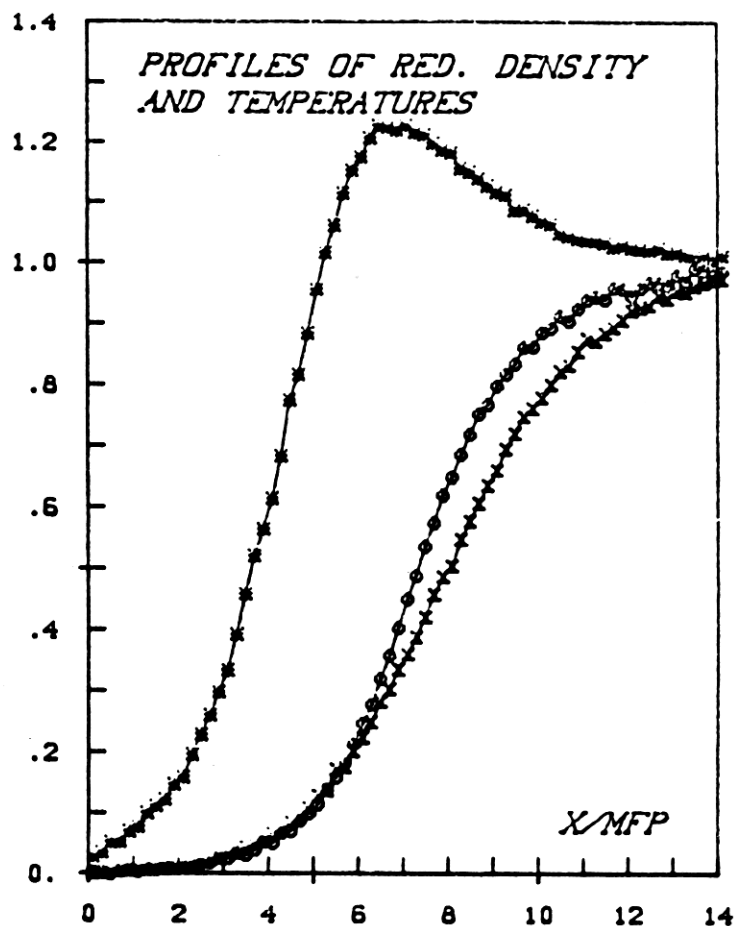
PROFILES OF RED. DENSITY AND TEMPERATURES

X/MFP

Figure 5a

LD-METHOD

SIMULATION OF A SHOCK

PARAMETER :

UPSTREAM VEL=2300.0 M/SEC

MEAN FREE PATH = 0.12 M

COLL RATIO = 0.90

TEMPERATURE = 200 K

PROFILES OF RED. DENSITY AND TEMPERATURES
X/MFP

Figure 5b

LD-METHOD

SIMULATION OF A SHOCK

PARAMETER :

UPSTREAM VEL=2900.0 M/SEC

MEAN FREE PATH = 0.12 M

COLL RATIO = 0.60

TEMPERATURE = 200 K

PROFILES OF RED. DENSITY AND TEMPERATURES
X/MFP