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**Natural Co-ordinates And High Speed Flows
A Numerical Method For Reactive Gases**

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Abstract

A new high resolution, space marching, numerical method, based on operator splitting, for high speed, steady, planar two dimensional, Inviscid, chemically reacting (real gas) flow fields is described. A simple model for chemical non-equilibrium was used based on Lighthill's *ideal dissociating gas model* for diatomic Oxygen. The method is formulated within the natural co-ordinate space consisting of streamlines and their normals. Boundaries are treated exactly and the variation of the chemistry shown to be along the streamline co-ordinate. Operator splitting is used to split the full problem up into two consisting of wave and chemical contributions. We use the Riemann problem based Random Choice Method (RCM) for solving the homogeneous Euler equations with frozen initial data for the wave contribution. The definition of the Riemann problem for the natural co-ordinate space is described. The RCM does not suffer from numerical smearing or spurious oscillations like other methods and this will be a positive advantage for chemical non-equilibrium due to the sudden rise in temperature across a shock wave. The flow field changes due to the chemical non-equilibrium are included by solving numerically a system of *stiff* ordinary differential equations. This was done using the stiff solver LSODE.

The algorithm is first validated for inert flow fields. This is done by making comparisons between theoretical and experimental results for several classic high speed configurations. The method is then validated for chemical non-equilibrium by making comparisons with results from other numerical methods. Finally, the qualitative effect of these real gas effects on the aerodynamic characteristics of a simple re-entry profile (modelling the Space Shuttle) was investigated.

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Nomenclature

A_α	Abbreviation for chemical formula for species α .
$A(U), B(U), C(U)$	Jacobian Matrices.
a_f	Frozen speed of sound.
a_e	Equilibrium speed of sound.
c_a	Coefficient for axial force.
c_d	Coefficient for drag force.
c_L	Coefficient for lifting force.
c_m	Coefficient for moment about leading edge.
c_n	Coefficient for normal force.
c_α	Mass fraction of α species $\equiv \rho_\alpha / \rho$.
$c_{v\alpha}$	Specific heat capacity at constant volume for species α .
$c_{p\alpha}$	Specific heat capacity at constant pressure for species α .
c_v	Specific heat capacity at constant volume.
c_p	Specific heat capacity at constant pressure.
$c_f^{(r)}$	Forward reaction rate coefficient for r-th reaction.
$c_b^{(r)}$	Backward reaction rate coefficient for r-th reaction.
C_+	Left Characteristics.
C_-	Right Characteristics.
dS	Elemental surface area.
D	Dissociation energy per mole.
Da	Damkhöler number.
dV	Elemental control volume.
dv	Elemental change in angle between Simple Waves.
dr	Elemental change in r .
dx_j	Elemental change in co-ordinate x_j .
$d\xi_j$	Elemental change in co-ordinate ξ_j .
d_k	Directional derivative defined by equation (2.47).
$\underline{e}_1, \underline{e}_2$	Basis vectors for Natural co-ordinates.
e_α	Specific energy for α species.
f	Arbitrary function.
g_α	Specific Gibbs free energy for species α .
g	Total specific Gibbs free energy.
h_α	Specific Enthalpy for α species.
h	Total specific enthalpy.
h	Plank's Constant.
i, j	Co-ordinates of nodal points.
I	Identity Matrix.
J	Transformation Jacobian.
$J_\pm(\chi_\pm)$	Riemann invariants.
k	Boltzmann constant.
k_1	Curvature of streamline co-ordinate.
k_2	Curvature of normal co-ordinate.
$k_f^{(r)}$	Forward reaction rate constant for r-th reaction.
$k_r^{(r)}$	Reverse reaction rate constant for r-th reaction.
K_α	Total mass production per unit volume per unit time for species α .
$K_\alpha^{(r)}$	Mass rate production for the r-th chemical reaction per unit volume per unit time for species α .

$K_e^{(r)}$	Equilibrium constant for r-th reaction.
$\underline{l}_1, \underline{l}_2$	Basis vectors for Cartesian co-ordinates.
L	Matrix of left Eigenvectors.
L^k	k-th left Eigenvector.
$m(\xi_2)$	Defined by equation (2.28).
M_f	Frozen Mach number.
M_e	Equilibrium Mach number.
N_A	Avogadro's number.
$\underline{n}$	Normal component pointing outwards from surface (positive sense).
p_α	Partial pressure.
Q_α	Partition function for species α .
$Q(U)$	Modified chemical source term $= A(U)^{-1} S(U)$.
q	Measure of the degree of non-equilibrium.
q	Magnitude of velocity vector $ \underline{V} $.
R	Universal gas constant.
R_α	Specific gas constant for species α .
$R^{(r)}$	Rate of progress of r-th reaction.
$\underline{r}$	Positional vector.
$S(U)$	Chemical source Term.
S_α	Specific entropy for species α .
S	Total Entropy.
T	Absolute Temperature.
U	Column vector of primitive/dependent variables.
$\underline{V}$	Flow velocity vector.
s, n	Natural Co-ordinates. Streamline and normal distances respectively.
W	Total molar weight for mixture.
W_α	Molar weight for species α .
x_1, x_2	Cartesian Co-ordinates.
x, y	Cartesian Co-ordinates.
x_{cp}	Position of centre of pressure from leading edge along body surface.
β_f	Frozen oblique shock angle.
β_e	Equilibrium oblique shock angle.
γ	Ratio of specific heat capacities.
$\underline{\zeta}$	Vorticity.
η_s	Similitude.
θ	Angle subtended by streamline with respect to x_1 .
$\theta_{\alpha\alpha}$	Characteristic rotational temperature.
$\theta_{v\alpha}$	Characteristic vibrational temperature.
$\theta_f^{(r)}$	Characteristic forward activation temperature for r-th reaction.
$\theta_b^{(r)}$	Characteristic backward activation temperature for r-th reaction.
θ_d	Lighthill's characteristic dissociation temperature.
λ_k	k-th Eigenvalue.
μ_f	Frozen Mach angle.
$\mu_\alpha^{(r)}$	Specific chemical potential for r-th reaction.
$\hat{\mu}_\alpha^{(r)}$	Molar chemical potential for the r-th reaction.
$v(M_f)$	Prandtl-Meyer relation.
v	Specific volume.
v_{CFL}	CFL number.
$v_\alpha^{(r)}$	Stoichiometric coefficient for reactants of r-th reaction.
$v_\alpha^{(r)''}$	Stoichiometric coefficient for products of r-th reaction.
ξ_1, ξ_2	Computational natural Co-ordinates.
ρ_α	Partial density.

ρ	Total density.
ρ_d	Lighthill's characteristic density.
σ_1	Scaling factor for the ξ_1 co-ordinate.
σ_2	Scaling factor for the ξ_2 co-ordinate.
$\sigma_{1,i}$	σ_1 for flow region i.
$\sigma_{2,i}$	σ_2 for flow region i.
$(\sigma_1)_{i,j}$	Value of σ_1 at grid co-ordinates (i,j).
$(\sigma_2)_{i,j}$	Value of σ_2 at grid co-ordinates (i,j).
χ	Characteristic surface.
χ_+, χ_-	Distances measured along the C_- and C_+ characteristics.
v	Control volume.
v	Specific Volume.
v_α	Specific Volume for species α ($\equiv 1 / \rho_\alpha$).
Ω_2	Van der Corput series (2,1).
Ω_A	Anderson's series.
ω	$\theta + \mu$

Subscripts

e	Equilibrium state.
f	Frozen state.
L	Left state.
R	Right state.
$*$	Centred state.
α	Species number.
∞	Freestream conditions.

Superscripts

el	Electronic degree of freedom.
r	Reaction number.
ref	Reference Conditions.
rot	Rotational degree of freedom.
tr	Translational degree of freedom.
vib	Vibrational degree of freedom.

Acronyms

CPU	Central Processing Unit.
CP	Centre of Pressure.
CFL	Courant-Friedrich-Lewy stability condition.
MoC	Method of Characteristics.
RCM	Random Choice Method.
RP	Riemann problem.

Some notation which is used infrequently is labelled within the main body of the text.

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Chapter 1

Introduction

During hypersonic flight through the upper Earth's atmosphere the field of flow about the vehicle is governed by high temperature, real gas effects. These are due to the presence of shock waves across which the freestream temperature is observed to rise suddenly. If this rise is high enough the intermolecular collisions between gas particles will become strong enough to excite the internal degrees of freedom. For molecules these are the vibrational and electronic modes, while for atoms it is just the electronic modes. By increasing the collisional energy further the molecules will be observed to dissociate and finally ionization will ensue. The duration over which these reactions and energy modes re-adjust to a new equilibrium state will be the relaxation time. Where the gas density is low these times will not be negligible. This non-equilibrium behaviour will have a significant affect on the behaviour of the flow field as compared to an inert flow. The review article by Anderson[5] gives an excellent account of these details and all other phenomena associated with hypersonic flight. The recent texts by Anderson[6] and Park[72] are also invaluable within this area.

The real gas phenomena was much evident on the American's Space Shuttle STS-1 maiden flight at the approximate altitude of 74km. Woods et al[102] has shown that the effect of the Shuttle's control surfaces was significantly reduced by these real gas effects. One of the difficulties was that the original aerodynamic data was generated from conventional high speed wind tunnels, see Liepmann and Roshko [59, pages 136-137] for details. The high Mach numbers were correctly simulated but the temperatures were too low to produce any real gas phenomena. Hence, the experimental data was only valid for an inert flow field. These problems have now been addressed by Stalker[88] and other workers using shock tube tunnels. However, these have other difficulties such as very small experimental times and small model size due to the dimensions of the tube.

The development of the digital computer and subsequent rise to fame of Computational Fluid Dynamics (CFD) has gone a long way to alleviating the problems encountered experimentally. In essence, the computer simulation of the flow field will not have the same hazards and problems associated with the experimental arrangement. CFD's greatest successes are in the realm of inert flow fields, but there are numerical difficulties with them near discontinuities. We give a description of the various methods and their weakness in the next section.

During hypersonic flight where non-equilibrium is prevalent inert calculations do not paint a true picture of reality; which was determined the hard way during the flight of STS-1. With the development around

the world of the next generation of space transportation[34,55], CFD has been turned to this new area of hypersonic research; this is particularly because of the ease of use of these algorithms as compared with the great difficulties experienced with the experimental arrangement. Generally these numerical methods are time dependent schemes. However, if steady state conditions are only required it will take a large amount of CPU time to reach it. The design of steady state CFD methods using a space marching approach is then desirable. Particular examples for inert flow fields is ZEUS[94]. It is the intention of this thesis to describe a new space marching numerical method, based on the Random Choice Method and formulated within the natural co-ordinate space, for high speed, steady, planar, two dimensional, reactive flow fields.

1.1 Background

Because of CFD's success the number of different numerical methods has increased greatly. The underlining strategy for each of them is the ability to be able to calculate as accurately as possible the flow field for a given configuration with the minimum of computational work. For non-equilibrium phenomena two numerical strategies have been adopted. The first technique is to solve the full set of equations which include the fluid dynamic and chemical contributions. These are known generally as *fully coupled systems*. The numerical method must consider the different time/convection scales over which the fluid and chemical reactions changes. Generally the chemical changes will occur quicker than those in the fluid. This difference poses problems for numerical schemes. They are known technically as *stiff* systems[57]. The numerical scheme must base any temporal/spatial incremental step on the quickest changes. For explicit schemes the numerical step will usually be too small for practical computations, but is necessary for convergence of the method. To overcome this an implicit method can be used which is unconditional convergent. However, the accuracy of results depends on the different scales. This problem has been investigated by Chiang and Hoffmann[17]. Another strategy is to split the equations up into contributions due to the changes in the fluid and those due to the reactions. These *loosely coupled systems* have the advantage that each part making up the system is better understood numerically than the coupled problem. There is a vast body of literature dealing with numerical methods for frozen/inert flow fields, their successes, and numerical problems. The chemical equations are solved by numerical methods specially designed for the problem of stiffness in mind. A review of these is given by Byrne and Hindmarsh[14]. Because of these underlining advanced techniques it is hoped that the combined result should be better behaved. The reader should consult Park[72] for a more detailed account of both these methods. In this thesis we shall adopt the latter approach using the method of Fractional steps by Yanenko[104].

Traditional numerical methods, such as finite difference and finite volume, for inert flows suffer from numerical difficulties close to discontinuities. These will effect the strength of the chemical contributions

and the position at which they start within the flow field. We briefly review these methods, their difficulties, and the development of new methods to overcome them. We then describe the birth and development of a novel method, known as the Random Choice Method (RCM), which does not have these problems and which we shall use in the thesis.

1.1.1 Traditional Numerical Methods

The numerical methods of old used linear finite differences to integrate the Euler equations for inviscid fluid flow. Typical methods are the Lax-Wendroff and MacCormack schemes which are described in Hirsch[49,50]. However, these *shock capturing methods* were un-successful with spurious oscillations being observed in the vicinity of shock waves. The numerical difficulty lies in the fact that the Euler equations can admit discontinuous solutions which are monotone. It is an important consequence of Godunov's theorem, described within Roe[78], that a linear difference scheme with accuracy greater than first order is non-monotonicity preserving. That is first order schemes are monotonicity preserving but those with greater accuracy are not and produce spurious oscillations. If these are not removed they will have the effect of perturbing an equilibrium flow field. If they are upstream of discontinuity, i.e. in the freestream, the disturbance of the freestream would be un-physical since the shock acts as a natural barrier between the upstream and downstream (thus what happens downstream does not get communicated upstream past the shock).

One way to overcome these problems is to track the discontinuities. Where there are no discontinuities the flow is solved in the usual way but at the discontinuities the appropriate jump conditions are applied. This *shock fitting method* has been used by Moretti[64]. However, for a large number of discontinuities the book keeping can be enormous. Hence *shock capturing methods* are easier to implement but troublesome at discontinuities.

Through the actions of heat conduction and viscosity a real fluid does not admit a true discontinuity. These shock waves have a physical thickness at sea level of approximately 10^{-7} m. For practical circumstances no computational mesh could resolve the internal structure. It was argued by von Neumann and Richtmeyer[99] that the physical coefficients of heat conduction and viscosity could be artificially increased to smear the shocks to the point where they could be resolved by the computational mesh but without significantly changing the whole flow. From these ideas has spored *artificial viscosity methods* which are typified by the work by Jameson et al[53]. A discussion of these methods for external hypersonic flows can found in the work by Yoon and Kwak[106]. Essentially, for a high order numerical method extra terms are added. In smooth parts of the flow these do not affect the profile. However, where discontinuities occur the *artificial viscosity correction* smooths out the oscillations producing a smeared or monotone shock profile. One of the weaknesses of these methods is that a parameter must be tuned for each specific problem to add the *right* amount of *artificial viscosity*. Note, for reactive gases the smearing

of the shock profile will again influence the effect of the chemical source term.

To overcome the problem of smearing numerical schemes have been developed which combine first and higher order methods. Essentially, within smooth regions the higher order method is used to resolve the flow. However, about discontinuities the lower order method is used, stopping the formation of spurious oscillations. These methods are known as *linear-hybridized* or Flux Corrected Transport (FCT) schemes, see Boris and Book[13]. However, their draw back is that the resolution is limited by the lower order scheme. These perform better than *artificial viscosity methods*.

Recently, the development of high resolution¹ based schemes which are *Total Variational Diminishing* (TVD) and are monotonicity preserving have been developed by Harten[46], see also Hirsch[50]. These new difference methods are non-linear in character with a term which corrects the numerical flux near discontinuities. Essentially, the *flux limiter* reduces the order of scheme to first order near discontinuities. These methods offer one solution to the problem of numerical oscillations and smearing. They appear to give good accuracy for the problem considered by Yee & Harten[105]. Widhopt & Wang[100] have applied the method to an unsteady two dimensional reactive gas problem with apparently good accuracy.

A radically different approach to the numerical solution of flow fields was suggested by Godunov[44]. He assumed that the flow is represented by a series of piecewise constant states. This representation closely approximates the true solution near discontinuities. The numerical flow solution is then evolved by the non-linear interactions between neighbouring states. Each pair of states represents a Riemann problem. The non-linear interactions arising from the Riemann problem can be calculated exactly. The results from the Riemann problems are then averaged to find the updated flow solution. Godunov's method results in an accurate and well behaved treatment of shock waves because much of the essential physics is contained within the Riemann problem. However, the method losses a lot of its power in the averaging process; because of this the method is first order accurate and is very diffusive. Advances on this method is the piecewise parabolic method (PPM) by Collela & Woodward[26] and the weighted average flux (WAF) method by Toro[92].

All the above methods have been computed on fixed computational meshes. However, more recently the development of ultra high resolution methods employing Roe's method[76] together with local adaptive mesh refinement about discontinuities has proved extremely successful, see Quirk[74].

There are many other methods which we have not described here but are equally important. We have tried to give a general flavour of the available numerical methods for inert flows, their inherent difficulties, and apparent fixes. These numerical problems if not properly controlled or removed will compromise the accuracy of the flow fields for reactive gas based methods. The TVD and Riemann problem based schemes appear to offer a way forward with these problems. For a review of other methods we refer the reader to the articles by Boris[12], Moretti[65], Woodward & Colella[103], Sod[86], Roe[77,78],

¹ A numerical scheme is termed a high resolution method if a discontinuity is smeared over 1-2 cells.

Anderson, Tannehill, & Pletcher[1], and Hirsch[49,50].

1.1.2 The Random Choice Method

The Random Choice Method is a high resolution method which is similar to the Godunov method. However, the updated solution is not averaged but sampled randomly from the exact solutions from the local Riemann problems. This method does not suffer from any smearing or oscillations near discontinuities but does have lower than first order accuracy. In essence, RCM has the following advantages over other methods

1. Discontinuities as shocks or contacts surfaces suffer no numerical diffusion or oscillations.
2. Shock waves are resolved with infinite resolution.

As discussed earlier the last feature is particularly important when these waves will cause non-equilibrium phenomena to begin. The position where these effects will begin must be resolved correctly.

The undesirable features of the method are that the profile of a rarefaction wave is not computed smoothly due to randomness inherent within the method, but on the average the solution is close to the exact solution. The location of discontinuities at any position are not exact but their average positions are.

RCM is different from the usual methods above because it is based on an existence proof, set out by Glimm[42], for solutions to systems of non-linear, hyperbolic, one dimensional, unsteady equations. Chorin[18,19] developed it many years later into a practical numerical method. The accuracy of the method is controlled by the choice of quasi random number series used. Colella[25] improved on the original accuracy by using the Van der Corput series[95]. Since then many researchers, such as Glimm et al[43], Gottlieb[45], Saito and Glass[79,80], Sod[85], Takano[90], and Toro[91], have developed it further into a powerful numerical tool.

The governing equations for steady, planar, supersonic, two dimensional flow fields have analogous properties with those for the one dimensional unsteady equations. Because of these similarities the RCM has been developed in this direction independently by, the present author[32,33], Honma et al[51], Marshall and Plohr[62], Oliver and Grönig[67], and Shi and Gottlieb[83] into a numerical method for Cartesian co-ordinates. More recently the method has been developed within a Lagrangian frame of reference by Loh and Hui[61]. It has been apparent that the RCM for two dimensional problems has not been developed as extensively as for the one dimensional case. For the latter it has been extended to consider reactive gases, see Takano[90], and detonation problems, see Singh and Clarke[84]. This disinterest could be due to its limitation to supersonic steady two dimensional flow fields. We address the imbalance within this thesis.

It became apparent from the literature review that the number of numerical methods employing a true *natural* type co-ordinate space (streamline and normals) was surprisingly small. There is, however, a vast body of literature concerning numerical methods employing transformation techniques using curvilinear co-ordinates; which is not the same. We refer the reader to Anderson, Tannehill, & Pletcher[1] for these details. It was also clear that the natural co-ordinate space was frequently referred to, particularly in the development of the Method of Characteristics (MoC), but numerical methods employing it never referenced. This was true of Emanuel[37]. However, for the benefit of the reader I break with the tradition of other authors and list some numerical methods found employing the natural or similar formulation: Verhoff & Stookesberry[96,97], Nacem & Barren[69], and Barger & Brooks[9].

The lack of available literature for the natural co-ordinate space suggests that the numerical method developed within this thesis is more original than was first thought.

1.2 Motivation For Work

We are concerned within this thesis with the development of the a highly original space marching numerical algorithm designed for predicting the behaviour of steady, high speed, planar, two dimensional, reacting gas flow fields. Shock waves must be captured as accurately as possible if the position where chemical non-equilibrium behaviour starts is to be treated correctly. For this purpose the Random Choice Method is ideal because it does not have the dissipation/smearing and spurious oscillations associated with other methods. Waves are captured with infinite resolution.

The natural co-ordinate system was chosen to simplify the governing equations so that there was no ambiguities in the use of operator splitting[104] when incorporating the chemical source term. The chemical contribution can be included in just one step due to its dependence only on the streamline direction. Physical boundaries are also captured with greater accuracy because the streamlines are the natural boundaries within the flow with no mass flux crossing them. Therefore no special procedures, such as mesh refinement, around them will be necessary. By choosing natural co-ordinates, boundaries and especially the chemistry are treated much more accurately.

With these motivations in mind it was first necessary to familiarize ourselves with the RCM for one dimensional unsteady problems, see Dawes[32]. From this the RCM was developed for supersonic, planar, two dimensional flow fields within a Cartesian framework[32]. Earlier results from the original algorithm *2DRCMXY* (two dimensional RCM in Cartesian space) was compared with others from similar developments elsewhere. There was good agreement. The RCM for inert flow fields within the natural co-ordinate space was briefly described within the report by the present author[33].

The work contained within this thesis is motivated towards describing the full numerical method for reactive gases and the results generated from it.

1.3 Thesis Outline

The thesis has two clear aims. Firstly, to explain the original development of the RCM, fractional step based numerical method for reactive high speed flows within the natural co-ordinate space. A full description of the Riemann problem and the positioning of the waves within it will be of particular interest as the former has only been briefly touched upon in the literature, see Clarke[23]. There appears to be no mention of it anywhere else. Secondly, we describe the validation of the method for both frozen and chemically reacting flow fields against results from other numerical and analytic methods. It is this last stage which will demonstrate the power of the new method.

We first derive the governing equations within *chapter two* for a general mixture of chemically reacting perfect gases. The natural co-ordinate system is described using general principals pertaining to a generalized orthogonal curvilinear co-ordinate space. We then describe a simple two component (atom and diatomic Oxygen) gas model for chemical non-equilibrium based on Lighthill's[60] *ideal dissociating gas* for dissociation. Finally, the equations are non-dimensionalized.

We proceed within *chapter three* to describe the principles and complex parts contained within the numerical algorithm *2DRCMSNCH* (Two dimensional RCM for natural co-ordinate space with chemistry). The algorithm was validated in two stages. Firstly, we neglect chemical non-equilibrium and concentrate on validating the method for frozen flow fields. There is a vast body of theoretical results available to choose from to make a direct comparison against. This is done within *chapter four*. Secondly, we consider the full problem of chemical non-equilibrium within *chapter five*. We first look at the problem of a cusped body supporting an oblique shock wave. Given the shock angle and initial conditions the body supporting the shock can be calculated numerically. This boundary data was read in during execution of *2DRCMSNCH* and the numerical and analytic solutions compared. We next consider the effects of non-equilibrium on a wedge with positive and negative deflection angles for different initial conditions. We make a direct comparison with results from other numerical methods and *2DRCMSNCH*. We finally explore qualitatively the effects of chemical non-equilibrium on the aerodynamic characteristics of a simple hypersonic re-entry configuration.

Finally, within *chapter six*, we make various observations and conclusions based on the results. We then discuss the aspect of future work.

Chapter 2

Basic Equations

The purpose of this chapter is to derive the governing equations for a planar, two dimensional, inviscid, flow field, composed of a mixture of perfect gases undergoing finite rate chemical reactions. The following, additional, assumptions are also made:

1. The local frozen Mach number remains greater than unity.
2. The field of flow is isoenergetic.
3. All transport phenomena, such as diffusion, are neglected.

The equations are first written in vector integral conservation law form from which the equations for two dimensional planar flow fields are derived in a straightforward way. For regions where the flow field variables and their derivatives are continuous functions of position the governing equations are reduced to a system of non-linear partial differential equations best known as the Euler equations modified with chemical source term. These are expanded for the natural co-ordinate space comprised of streamlines and normals. For surfaces across which the flow field variables change discontinuously jump conditions are derived.

Finally, we describe a thermodynamic model for chemical non-equilibrium based on Lighthill's 'ideal dissociating gas' model[60] for a symmetric diatomic gas.

2.1 Integral Conservation Laws

The equations for fluid motion in which transport processes are neglected can be written in vector integral conservation law form as

$$-\int_S \rho \underline{Y} \cdot \underline{n} dS = 0 \quad (2.1)$$

$$-\int_S [(\rho \underline{Y}) \underline{Y} \cdot \underline{n} + p \underline{n}] dS = 0 \quad (2.2)$$

$$-\int_S \rho \underline{Y} h_s \cdot \underline{n} dS = 0 \quad (2.3)$$

where

$$h = e + \frac{p}{\rho} ; h_s = h + \frac{1}{2} \underline{Y} \cdot \underline{Y} \quad (2.4)$$

Derivations for these equations can be found in any good text introducing fluid mechanics. See for example the book by Anderson[3,4]. Equations (2.1)-(2.3) are global conservation laws and are independent of the thermodynamic and chemical state of the gas. They represent conservation of mass, momentum, and total specific energy. Here ρ , p , e , h , h_s , and $\underline{Y}$ are local values for the total density, pressure, specific intrinsic energy (per unit mass), specific enthalpy, specific stagnation enthalpy, and mass averaged velocity¹ respectively within the elemental volume dv . v is the control volume specified within the fluid which has surface area S . $\underline{n}$ is the unit normal pointing outwards from the volume surface (positive sense). The inclusion of the minus sign in the above equations was for clarity only; the flux by definition entering the control volume must be positive. We drop the sign from now on.

The intrinsic energy for the mixture will be a function of any two state variables² together with the variable q which is a measure of the degree of local non-equilibrium present within the flow field. Thus $e = e(p, T, q)$. For chemically reactive gases q is replaced by the mass fractions for each species which are defined by $c_\alpha = \rho_\alpha / \rho$. Therefore $e = e(p, T, c_1, c_2, \dots, c_{n-1})$. ρ_α is the density the species α would have if it alone occupied the control volume v . The total density is then just the sum of all the densities for the components. Whence

¹ The mass averaged velocity appears naturally in the Boltzmann equation. We refer the reader to the text by Clarke and McChesney[21], chapter five, for the details.

² We use the two state variables pressure and temperature unless told otherwise.

$$\rho = \sum_{\alpha=1}^n \rho_\alpha \quad (2.5)$$

with the sum of the mass fractions given by

$$\sum_{\alpha=1}^n c_\alpha = 1 \quad (2.6)$$

Due to the chemical reactions, conservation equations must be specified for $(n-1)$ species since the n -th can be found by using equation (2.6). Hence

$$\int_S \rho c_\alpha \underline{Y} \cdot \underline{n} dS = \int_v K_\alpha dv ; \alpha = 1, 2, \dots, n-1 \quad (2.7)$$

where K_α is the mass rate of production for species α per unit volume per unit time. We discuss its analytic form later on. The fluid is homogeneous and there must be no mass created or destroyed within the fluid. Whence

$$\sum_{\alpha=1}^n K_\alpha = 0 \quad (2.8)$$

2.2 Continuous Solutions

If the flow variables and their derivatives are continuous functions of position equations (2.1)-(2.3) and (2.7) are reducible, by application of Gauss' divergence theorem and vector identities (appendix A), to the form

$$\nabla \cdot (\rho \underline{Y}) = 0 \quad (2.9)$$

$$\nabla(V^2/2) - \underline{Y} \wedge \underline{\zeta} + v \nabla p = 0 \quad (2.10)$$

$$\rho \underline{Y} \cdot \nabla h_s = 0 \quad (2.11)$$

$$\rho \underline{Y} \cdot \nabla c_\alpha = K_\alpha ; \alpha = 1, 2, \dots, n-1 \quad (2.12)$$

where $\underline{\zeta} (= \nabla \wedge \underline{Y})$ is the vorticity. These are best known as the Euler equations modified with chemical source term.

2.2.1 The Natural Co-ordinate System

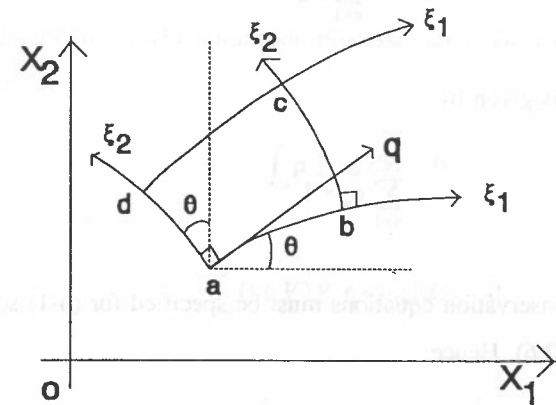


Figure 2.1 Natural co-ordinates with respect to Cartesian co-ordinates.

The formulae derived for the natural co-ordinate system was developed from the concepts belonging to those for a generalized orthogonal curvilinear co-ordinate system described in the text by Spiegel[87].

Natural co-ordinates for the field of flow consists of a network of orthogonal curvilinear co-ordinates composed of streamlines ξ_1 ($\xi_2 = \text{constant}$) and normals to them ξ_2 ($\xi_1 = \text{constant}$) respectively³. They are related to the rectangular Cartesian co-ordinates (x_1, x_2) with fixed normalized basis vectors $(\underline{e}_1, \underline{e}_2)$ through the equations

$$\begin{aligned}\xi_1 &= \xi_1(x_1, x_2) \\ \xi_2 &= \xi_2(x_1, x_2)\end{aligned}\quad (2.13)$$

If the Jacobian $J = \partial(x_1, x_2)/\partial(\xi_1, \xi_2)$ remains finite and non-zero there exists the unique transformation

$$\begin{aligned}x_1 &= x_1(\xi_1, \xi_2) \\ x_2 &= x_2(\xi_1, \xi_2)\end{aligned}\quad (2.14)$$

Changes in the positional vector $\underline{r}$ are given by

$$d\underline{r} = \sum_{j=1}^2 \underline{e}_j dx_j = \sum_{j=1}^2 \sigma_j \underline{e}_j d\xi_j \quad (2.15)$$

with physical distances invariant thus

$$|d\underline{r}|^2 = d\underline{r} \cdot d\underline{r} = \sum_{j=1}^2 dx_j^2 = \sum_{j=1}^2 (\sigma_j d\xi_j)^2 \quad (2.16)$$

where $ds = \sigma_1 d\xi_1$ and $dn = \sigma_2 d\xi_2$ are the infinitesimal distance measured along the respective co-ordinate direction ξ_1 and ξ_2 . Changes along these co-ordinates have the physical distances given by

$$\begin{aligned}s &= \int \sigma_1 d\xi_1 \\ n &= \int \sigma_2 d\xi_2\end{aligned}\quad (2.17)$$

The velocity vector $\underline{V}$ for the flow field is by definition tangential to the streamlines ($\xi_2 = \text{constant}$). Whence

$$\underline{V} = q \underline{e}_1 \quad (2.18)$$

The normalized basis vectors $(\underline{e}_1, \underline{e}_2)$, which are tangential to and in the direction of increase of the co-ordinates ξ_1 and ξ_2 respectively are given in terms of the Cartesian system as

$$\underline{e}_i = \frac{1}{\sigma_i} \sum_{j=1}^2 \frac{\partial x_j}{\partial \xi_i} \underline{e}_j \quad ; i=1,2 \quad (2.19)$$

where σ_1 and σ_2 are the local scaling factors⁴ used to normalize the basis vectors. Because the basis vectors are orthogonal the scales have the form

$$\sigma_i^2 = \sum_{j=1}^2 \left(\frac{\partial x_j}{\partial \xi_i} \right)^2 \quad ; i=1,2 \quad (2.20)$$

with the metrics for the flow field of the form

$$\begin{aligned}\frac{\partial x_1}{\partial \xi_1} &= \sigma_1 \cos \theta \quad ; \quad \frac{\partial x_1}{\partial \xi_2} = -\sigma_2 \sin \theta \\ \frac{\partial x_2}{\partial \xi_1} &= \sigma_1 \sin \theta \quad ; \quad \frac{\partial x_2}{\partial \xi_2} = \sigma_2 \cos \theta\end{aligned}\quad (2.21)$$

For the Cartesian co-ordinate space the scales are both constant and equal to unity. However, the natural co-ordinates does not possess this unique property and are functions of the co-ordinates. They must be calculated at each point within the flow field. The local change of the scales can be determined from the local curvatures of the streamlines and normals. They are given by the geometric, partial differential,

³ These are in reality computational co-ordinates. They do not represent physical distances.

⁴ σ has been used instead of h (this symbol is used in texts describing Differential Geometry, and Vector Analysis) to avoid confusion with the specific enthalpy.

relations thus

$$\begin{aligned} k_1 &= \frac{1}{\sigma_1 \sigma_2} \frac{\partial \sigma_1}{\partial \xi_2} = -\frac{1}{\sigma_1} \frac{\partial \theta}{\partial \xi_1} \\ k_2 &= \frac{1}{\sigma_1 \sigma_2} \frac{\partial \sigma_2}{\partial \xi_1} = \frac{1}{\sigma_2} \frac{\partial \theta}{\partial \xi_2} \end{aligned} \quad (2.22)$$

where k_1 and k_2 are the local curvatures of the streamlines and normals respectively and θ is the angle subtended by the streamline with respect to the rectangular co-ordinate x_1 , see Figure 2.1. For further details we refer the reader to the text by Emanuel[37] who gives an excellent account of these matters. The scales are determined by integrating equations (2.22) as

$$\begin{aligned} \sigma_1(\xi_1, \xi_2) &= -\int_0^{\xi_2} \sigma_2 \frac{\partial \theta}{\partial \xi_1} d\xi_2 + \sigma_1(\xi_1, \xi_2=0) \\ \sigma_2(\xi_1, \xi_2) &= \int_0^{\xi_1} \sigma_1 \frac{\partial \theta}{\partial \xi_2} d\xi_1 + \sigma_2(\xi_1=0, \xi_2) \end{aligned} \quad (2.23)$$

where the right hand side of each of the integrals are the initial/boundary conditions which must be specified. We discuss the choice of these within the next chapter.

The transformation Jacobian has the simple form $J = \sigma_1 \sigma_2$ which remains finite and non-zero; it therefore preserves the uniqueness of the transformation between the two co-ordinate systems. This property will be used later on when translating from the computational space defined by the natural co-ordinates to physical space.

2.2.2 Euler Equations for Natural Co-ordinates

The Euler equations are expanded, using the definitions for grad, div, and curl (see appendix A) to yield

$$\frac{1}{\sigma_1} \frac{\partial(\rho q \sigma_2)}{\partial \xi_1} = 0 \quad (2.24)$$

$$\mathbf{e}_1 : \frac{\rho q}{\sigma_1} \frac{\partial q}{\partial \xi_1} + \frac{1}{\sigma_1} \frac{\partial p}{\partial \xi_1} = 0 \quad (2.25)$$

$$\mathbf{e}_2 : \frac{\rho q^2}{\sigma_1} \frac{\partial \theta}{\partial \xi_1} + \frac{1}{\sigma_2} \frac{\partial p}{\partial \xi_2} = 0 \quad (2.26)$$

$$\frac{1}{\sigma_1} \frac{\partial h_s}{\partial \xi_1} = 0 \quad (2.27)$$

$$\frac{\rho q}{\sigma_1} \frac{\partial c_\alpha}{\partial \xi_1} = K_\alpha ; \alpha = 1, 2, \dots, n-1 \quad (2.28)$$

Equations (2.24), (2.25), (2.27), and (2.28) are dependent on the single characteristic direction ξ_1 . Further, equations (2.24) and (2.27) can be integrated immediately to give the algebraic relations

$$\rho q \sigma_2 = m(\xi_2) ; h_s = h + \frac{1}{2} q^2 = H_s(\xi_2) \quad (2.29)$$

which are both functions of the normal ξ_2 co-ordinate only. Given any one of the streamlines ($\xi_2 = \text{constant}$) the mass and total enthalpy remain fixed with the constants defined by the initial conditions specified along the data line $\xi_1 = 0$.

The enthalpy is a function of any two state variables⁵ and the species mass fractions. Equation (2.27) can be expanded as

$$\left(\frac{\partial h}{\partial p} \right)_{p, c_\alpha} \frac{1}{\sigma_1} \frac{\partial p}{\partial \xi_1} + \left(\frac{\partial h}{\partial p} \right)_{p, c_\alpha} \frac{1}{\sigma_1} \frac{\partial p}{\partial \xi_1} + \frac{q}{\sigma_1} \left(\frac{\partial q}{\partial \xi_1} \right)_{p, p, c_\alpha} + \frac{1}{\rho q} \sum_{\alpha=1}^{n-1} h_c K_\alpha = 0 \quad (2.30)$$

where

$$h_c = \left(\frac{\partial h}{\partial c_\alpha} \right)_{p, p, c_\beta} \quad (2.31)$$

and the subscripts refer to the variables held constant, with c_α all the values of c_α that are constant and c_β all the c_α except c_α itself are held constant. By substituting equations (2.24), (2.25) and (2.28) we obtain

$$\frac{M_f^2 - 1}{\rho q^2 \sigma_1} \frac{\partial p}{\partial \xi_1} + \frac{1}{\sigma_2} \frac{\partial \theta}{\partial \xi_2} = K \quad (2.32)$$

with

$$K = \frac{1}{\rho^2 q h_p} \sum_{\alpha=1}^{n-1} h_c K_\alpha ; h_p = \left(\frac{\partial h}{\partial p} \right)_{p, c_\alpha} \quad (2.33)$$

where M_f is the local frozen Mach number $M_f = q/a_f$ and a_f is the frozen sound speed.

⁵ For convenience we use density and pressure.

Thus equations (2.24)-(2.28) together with the geometric equations (2.22) constitute the system of equations to be solved. It is worth pointing out the above equations can also be derived from an equivalent approach using the principles described by Viviand and Vinokur[1, pages 252-255] for preserving the strong conservation law form for a general orthogonal curvilinear co-ordinate system.

We note that Oswatitsch[68, pages 249-255] as early as 1956 using a co-ordinate transformation based on streamlines and surfaces of equipotential has produced a similar set of equations and scaling factors. However, the scaling factors for his system are the direct inverse of ours.

2.2.3 Compatibility Equations and Characteristics

To determine the compatibility equations and characteristics for the system, the Euler equations are written in quasi-linear form⁶

$$A \frac{\partial U}{\partial \xi_1} + B \frac{\partial U}{\partial \xi_2} = S(U) \quad (2.34)$$

where U , A , B , and S are the column matrix for primitive variables, the Jacobian Matrices, and the column matrix for the source terms respectively are given by

$$U = \begin{pmatrix} \rho \\ q \\ p \\ \theta \\ c_1 \\ \vdots \\ c_{n-1} \end{pmatrix}; A = \begin{pmatrix} \frac{q}{\sigma_1} & \frac{p}{\sigma_1} & 0 & 0 & 0 & \cdots & 0 \\ 0 & \frac{\rho q}{\sigma_1} & \frac{1}{\sigma_1} & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \frac{\rho q^2}{\sigma_1} & 0 & \cdots & 0 \\ 0 & 0 & \frac{M_f^2 - 1}{\sigma_1 \rho q^2} & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \frac{\rho q}{\sigma_1} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & \frac{\rho q}{\sigma_1} \end{pmatrix} \quad (2.35)$$

and

⁶We follow a similar procedure to that given by Hirsch[49].

$$B = \begin{pmatrix} 0 & 0 & 0 & \frac{\rho q}{\sigma_2} & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & \frac{1}{\sigma_2} & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \frac{1}{\sigma_2} & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}; S(U) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ K \\ K_1 \\ \vdots \\ K_{n-1} \end{pmatrix} \quad (2.36)$$

Provided the local Frozen Mach number does not become sonic the Jacobian matrix A can be inverted to give

$$\frac{\partial U}{\partial \xi_1} + C \frac{\partial U}{\partial \xi_2} = Q(U) \quad (2.37)$$

where the modified Jacobian Matrix C and source term $Q(U)$ are written

$$C = A^{-1}B = \begin{pmatrix} 0 & 0 & 0 & \frac{\sigma_1 \rho M_f^2}{\sigma_2 (M_f^2 - 1)} & 0 & \cdots & 0 \\ 0 & 0 & 0 & -\frac{\sigma_1 q}{\sigma_2 (M_f^2 - 1)} & 0 & \cdots & 0 \\ 0 & 0 & 0 & \frac{\sigma_1 \rho q^2}{\sigma_2 (M_f^2 - 1)} & 0 & \cdots & 0 \\ 0 & 0 & \frac{\sigma_1}{\sigma_2 \rho q^2} & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}; Q = A^{-1}S = \begin{pmatrix} \frac{\sigma_1 \rho K}{M_f^2 - 1} \\ \frac{\sigma_1 q K}{M_f^2 - 1} \\ \frac{\sigma_1 \rho q^2 K}{M_f^2 - 1} \\ 0 \\ \frac{\sigma_1 K_1}{\rho q} \\ \vdots \\ \frac{\sigma_1 K_{n-1}}{\rho q} \end{pmatrix} \quad (2.38)$$

By defining the characteristic surface $\chi(\xi_1, \xi_2) = \text{constant}$, any incremental change along it will be zero, thus:

$$d\chi = \sum_{k=1}^2 \chi_k d\xi_k = \nabla\chi \cdot d\mathbf{r} = 0; \chi_k = \frac{\partial\chi}{\partial\xi_k} \quad (2.39)$$

therefore

$$\left(\frac{d\xi_2}{d\xi_1} \right)_x = -\frac{\chi_1}{\chi_2} = -\frac{n_1}{n_2} \quad (2.40)$$

where n_1, n_2 are the components of the normal vector $\underline{n} = \nabla\chi$. Thus the system of equations transforms as

$$\left(\frac{\partial U}{\partial \xi_1} \right)_x + \left(\frac{n_1}{n_2} I + C \right) \frac{\partial U}{\partial \xi_2} = Q \quad (2.41)$$

where I is the identity matrix. We now operate on both sides of this equation using the set of left eigenvectors L

$$L \left(\frac{\partial U}{\partial \xi_1} \right)_x + L \left(\frac{n_1}{n_2} I + C \right) \frac{\partial U}{\partial \xi_2} = LQ \quad (2.42)$$

where L has the form for the system

$$L = \begin{pmatrix} 1 & 0 & -\frac{1}{a_f^2} & 0 & 0 & \cdots & 0 \\ 0 & 1 & \frac{1}{\rho q} & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 1 & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 \\ 0 & 0 & \frac{\sqrt{M_f^2-1}}{2\rho q^2} & \frac{1}{2} & 0 & \cdots & 0 \\ 0 & 0 & -\frac{\sqrt{M_f^2-1}}{2\rho q^2} & \frac{1}{2} & 0 & \cdots & 0 \end{pmatrix} \quad (2.43)$$

Each row corresponds to a different left eigenvector for the system L^k ($k = 1, 2, \dots, n+3$).

The characteristic surface will exist if the system can be reduced to the form

$$L \left(\frac{\partial U}{\partial \xi_1} \right)_x = LQ \quad (2.44)$$

such that

$$L \left(C + \frac{n_1}{n_2} I \right) = 0 \quad (2.45)$$

This is an eigenvalue problem with non-trivial solutions defined by

$$\det |C - \lambda I| = 0; \lambda = -\frac{n_1}{n_2} \quad (2.46)$$

where λ are the eigenvalues; there are $(n+3)$ of them. They can be shown to be $\lambda_k = 0$ ($k=1, 2, \dots, n+1$) which from equation (2.40) implies that these are parallel with the streamline directions. Also there are two additional eigenvalues

$$\lambda_k = \pm \frac{\sigma_1 \tan(\mu_f)}{\sigma_2} = \pm \frac{\sigma_1}{\sigma_2} \frac{1}{\sqrt{M_f^2-1}}; k=n+2, n+3 \quad (2.47)$$

where we have used the local frozen Mach angle μ_f defined via the relation $M_f \sin \mu_f = 1$. We immediately notice from the last equation that provided the flow field remains supersonic $M_f > 1$ the characteristics are all real with the system of equations of Hyperbolic type. The three characteristic directions are represented schematically by Figure 2.2.

Because $L^k C = \lambda_k L^k$ the compatibility equations for the system are defined in terms of a directional derivative thus

$$L^k d_k(U) = L^k Q \quad (2.48)$$

with the directional derivative operator for the k -th eigenvalue given by

$$d_k = \frac{\partial}{\partial \xi_1} + \lambda_k \frac{\partial}{\partial \xi_2} \quad (2.49)$$

where we have removed the bracketed terms for convenience. It is now a simple matter to expand the equations. For $\lambda_k = 0$ the directional derivative operator reduces to $\partial/\partial \xi_1$ and equation (2.49) becomes

$$\begin{aligned}\frac{\partial \rho}{\partial \xi_1} - \frac{1}{a_f^2} \frac{\partial p}{\partial \xi_1} &= -\sigma_1 \rho K \\ \frac{\partial q}{\partial \xi_1} + \frac{1}{\rho q} \frac{\partial p}{\partial \xi_1} &= 0 \\ \frac{\partial c_\alpha}{\partial \xi_1} &= \frac{\sigma_1 K_\alpha}{\rho q} ; \alpha=1,2,\dots,n-1\end{aligned}\quad (2.50)$$

For the eigenvalues defined by equation (2.47) the compatibility equations reduce to

$$\frac{\cot \mu_f}{\rho q^2} \frac{dp}{d\chi_+} \pm \frac{d\theta}{d\chi_+} = \sigma_1 K \tan \mu_f \quad (2.51)$$

where we have redefined the directional derivative operator as

$$\frac{d}{d\chi_+} = \frac{\partial}{\partial \xi_1} \pm \frac{\sigma_1 \tan \mu_f}{\sigma_2} \frac{\partial}{\partial \xi_2} \quad (2.52)$$

where χ_- varies only along the C_+ characteristic and χ_+ varies only along the C_- characteristic respectively.

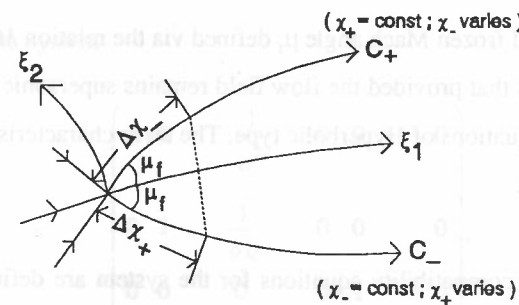


Figure 2.2 Characteristic Directions.

2.2.4 Similitudes

The work presented within this subsection is essentially that described within the paper by Clarke[23]; it was felt necessary to include it here, with a few additions, for clarity.

We investigate whether, with a chemical source term, solutions in terms of the similarity parameter η_s for the natural co-ordinate space exists. Here

$$\eta_s = \frac{\xi_2 - (\xi_2)_0}{\xi_1 - (\xi_1)_0} \quad (2.53)$$

The bracketed terms are chosen as the co-ordinates for the origin. For an arbitrary function $f = f(\eta)$ the differential operator equation (2.52) becomes

$$\frac{df}{d\chi_+} = \frac{1}{\xi_1 - (\xi_1)_0} \left(-\eta_s \pm \frac{\sigma_1 \tan \mu_f}{\sigma_2} \right) \frac{df}{d\eta} \quad (2.54)$$

where the term $1/(\xi_1 - (\xi_1)_0)$ will become a problem at the origin. However, if the source term is some function divided by the term $\xi_1 - (\xi_1)_0$ (which will generally not be the case) or identically zero the problem can be removed by *multiplying* the offending term out. Indeed for frozen flow the source term will be identically zero and at equilibrium the equation (2.51) reduces to

$$\frac{M_\infty^2 - 1}{\sigma_1 \rho q^2} \frac{\partial p}{\partial \xi_1} + \frac{1}{\sigma_2} \frac{\partial \theta}{\partial \xi_2} = 0 \quad (2.55)$$

as the source term is absorbed into the equation for the speed of sound at equilibrium.

By choosing η_s equal to

$$\eta_s = \pm \frac{\sigma_1 \tan \mu_f}{\sigma_2} \quad (2.56)$$

equation (2.54) is identically zero. Therefore the function f remains constant along the characteristics. Because of this η_s must be constant also, since the scales are dependent on the flow conditions. Thus the flow remains constant along rays if and only if the source term is identically zero or at equilibrium.

2.2.5 Riemann invariants

For frozen/inert flow fields equation (2.51) can be represented by the integral equation

$$\int \frac{\cot \mu_f}{\rho q^2} dp \pm \theta = J_\pm(\chi_\pm) \quad (2.57)$$

where $J_\pm(\chi_\pm)$ are constants of integration and remain fixed along the characteristics. The integral has the closed form solution in terms of the Mach number for irrotational flow

$$v(M_f) = \int \frac{\cot \mu_f}{\rho q^2} dp = \frac{1}{k} \tan^{-1} \left\{ k \sqrt{M_f^2 - 1} \right\} - \tan^{-1} \left\{ \sqrt{M_f^2 - 1} \right\}; k = \sqrt{\frac{\gamma - 1}{\gamma + 1}} \quad (2.58)$$

where $v(M_f)$ is the Prandtl-Meyer relation. Whence

$$v(M_f) \mp \theta = J_*(\chi_*) \quad (2.59)$$

These are the Riemann invariants for the flow field domain. For equilibrium the task of evaluating the integral becomes a little more tricky because the speed of sound is now directly dependent on the equilibrium mass fractions through *the law of mass action*. However, the equation can be solved numerically. We refer the reader to appendix B for an account of the procedures necessary for solving a system of equations defined for an equilibrium expansion wave using Lighthill's 'ideal dissociating gas' model[60].

The characteristic directions can themselves be used to define a co-ordinate system for supersonic flows along which the Riemann invariants remain constant. The technique is known as the Method of Characteristics (MoC) and is described in the texts by Liepmann and Roshko[59] and Zucrow & Hoffman[107,108].

2.3 Discontinuous phenomena

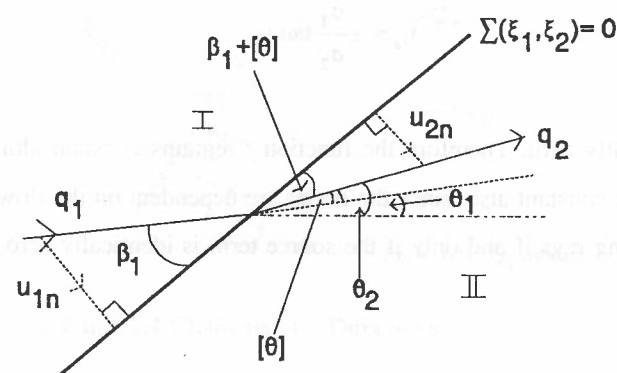


Figure 2.3 Parameters for the discontinuous surface $\Sigma(\xi_1, \xi_2)=0$.

At the point where the flow variables become discontinuous the Euler equations fail to provide an accurate description of the flow field. By defining a surface $\Sigma(\xi_1, \xi_2) = 0$ across which the flow variables are discontinuous, jump relations can be derived from the integral conservation equations (see Hirsch[49]).

Whence for frozen or chemical non-equilibrium

$$\begin{aligned} [\rho u_n] &= 0 \\ [\rho u_n^2 + p] &= 0 \\ [\rho u_n u_t] &= 0 \\ [\rho u_n h_s] &= 0 \\ [\rho u_n c_n] &= 0 \end{aligned} \quad (2.60)$$

where $[f]$ represents the jump in the function f across the surface from region one to two: $[f] \equiv f_2 - f_1$. These are the Rankine-Hugoniot relations for the surface. The normal and tangential velocity components to the surface Σ (subscripts n and t respectively) can best be written in terms of the surface inclination angle β_1 with respect to the freestream and the change in flow angle across the wave $[\theta]$ as

$$\begin{aligned} u_{1n} &= q_1 \sin(\beta_1) ; u_{1t} = q_1 \cos(\beta_1) \\ u_{2n} &= q_2 \sin(\beta_1 - [\theta]) ; u_{2t} = q_2 \cos(\beta_1 - [\theta]) \end{aligned} \quad (2.61)$$

The equations have the following solutions

2.3.1 Contact Surfaces

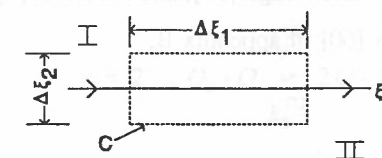


Figure 2.4 Contour around contact surface.

Contact surfaces are those surfaces which have a zero mass flux through them: $\rho_1 u_{1n} = \rho_2 u_{2n} = m = 0$ which implies that $\beta_1 = 0$ and $[\theta] = 0$. The jump relations become

$$[\rho] \neq 0; [u_i] \neq 0; [c_\alpha] \neq 0; [p] = 0; [h_\alpha] = 0 \quad (2.62)$$

remembering that the flow is isoenergetic. A further relation can be found by writing the integral conservation equation for momentum in terms of the natural co-ordinates

$$\int_C \{(\rho q^2 + p \sigma_2) e_1 \sigma_2 d\xi_2 + p e_2 \sigma_1 d\xi_1\} = 0 \quad (2.63)$$

where C is the path of integration defined by Figure 2.4. In the limit as $\Delta\xi_2$ tends to zero ($\Delta\xi_2 \rightarrow 0$) we obtain the condition that

$$[p\sigma_1] = 0 \quad (2.64)$$

since the basis vector $\underline{e}_1$ is constant across the contact surface. This implies that $[\sigma_1] = 0$ because $[p] = 0$ by equation (2.62). Therefore the scaling factor for the streamline must remain constant across the contact surface.

2.3.2 Oblique Shock Waves

Oblique shock waves are solutions of the jump relations with non-zero mass flux through the surface: $m \neq 0$. The jump relations become

$$[\rho] \neq 0; [p] \neq 0; [u_t] = 0; [h_t] = 0; [c_a] = 0 \quad (2.65)$$

Across an oblique shock wave the mass fractions remain constant. However, for equilibrium conditions there is a discontinuous change in them across the surface. The Rankine-Hugoniot relations are supplemented with equations for the 'law of mass action' and solutions are usually found by solving the system of equations numerically. Examples of such procedures can be found in the excellent texts by Clarke and McChesney[21,22], Vincenti and Kruger[98], and Anderson[6]. We apply our own procedure using Lighthill's 'ideal dissociating gas'[60] in appendix B.

2.4 Thermodynamic Model

The field of flow is composed of a mixture of two perfect gases; which are respectively atomic and diatomic Oxygen. Initially the mixture is in thermodynamic equilibrium and either it is in chemical equilibrium or is chemically frozen. Any perturbations, such as a change in flow deflection angle, will cause non-equilibrium behaviour to develop. To analyze the system⁷ we define that locally there is thermodynamic equilibrium but chemical non-equilibrium (unless frozen conditions are specified throughout). The rotational, vibrational, and electronic energy modes are in equilibrium with the translational degrees of freedom. The governing thermodynamic equations are complex in character and are simplified using the model purposed by Lighthill[54], known as the *ideal dissociating gas*.

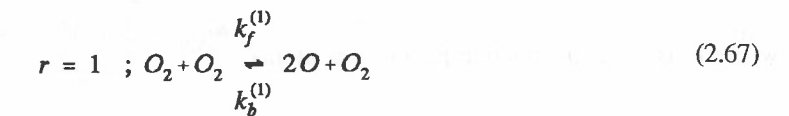
The degree of chemical non-equilibrium can be represented by the similarity parameter Da as

⁷The properties of a mixture of chemically reacting perfect gases are well documented. We refer the reader to appendix F for a summary of general thermodynamic principles.

$$Da = \frac{\tau_c}{\tau_f} \quad (2.66)$$

which is the Damkhöler number. τ_c and τ_f are the characteristic chemical reaction time and characteristic flow time respectively. For frozen flows the characteristic chemical time is very much bigger than that for the fluid; Thus $Da \gg 1$. For equilibrium the characteristic chemical time is very much smaller than that for the fluid; Thus $Da \ll 1$. For non-equilibrium the characteristic times are of the same order of magnitude; Thus $Da \approx 1$.

Chemical non-equilibrium will cause the system to relax back to a new chemical equilibrium state. During this process finite rate chemical reactions will occur. These are represented by the dissociation and recombination reactions



and



where r is the reaction number. These reactions can be represented concisely by the chemical equation as



where A_{α} ($\alpha = 1, 2$) represents the chemical formula (here $A_1 = O$, $A_2 = O_2$). $v_{\alpha}^{(r')}$, $v_{\alpha}^{(r'')}$ are the stoichiometric coefficients for reactants and products respectively. Here $v_1^{(1'')} - v_1^{(1')} = 2$, $v_2^{(1'')} - v_2^{(1')} = -1$, and $v_1^{(2'')} - v_1^{(2')} = 2$, $v_2^{(2'')} - v_2^{(2')} = -1$. $k_f^{(r)}$, $k_b^{(r)}$ are the forward and backward reaction rate constants respectively and are functions of the absolute temperature only. Their general form are given in appendix F.

The reverse reaction rate constant will be used in deriving the rate equation for chemical non-equilibrium. Values for the coefficients for the recombination reactions can be found in Baulch[8]. However, there is a wide spread, and error, in measuring these coefficients experimentally. In keeping with our qualitative study of chemical non-equilibrium we make the simplifying assumption that both reverse

reaction rates are equal and constant (unless told otherwise). Thus $k_b = k_b^{(1)} = k_b^{(2)}$, with the coefficients having the values

$$c_b = 1000 \text{ m}^6 \text{ mol}^{-2} \text{ s}^{-1}, \eta_b = 0.0, \theta_b = 0.0$$

where c_b , η_b , and θ_b are defined in appendix F. Whence

$$k_b = 1000 \text{ m}^6 \text{ mol}^{-2} \text{ s}^{-1}$$

2.4.1 Mixture of Perfect Gases

The equation of state for the mixture (using equation (F.5)) is

$$p = \rho(1 + c_1) \frac{R}{W_2} T \quad (2.70)$$

where c_1 is the mass fraction for Oxygen atoms.

The specific intrinsic energy for atomic Oxygen e_1 will depend on the translational and electronic degrees of freedom

$$e_1 = e_1^{tr} + e_1^{el} + e_1^{ref} \quad (2.71)$$

while for diatomic Oxygen there are additional contributions from the rotational and vibrational modes

$$e_2 = e_2^{tr} + e_2^{rot} + e_2^{vb} + e_2^{el} + e_2^{ref} \quad (2.72)$$

The different energy modes are measured with respect to their zero point energies at absolute zero and e_α^{ref} is a reference energy from which measurements are made. For our purposes we make all measurements with respect to the ground state of diatomic Oxygen. The ground state of atomic Oxygen will exist at the higher energy level with respect to the diatomic Oxygen ground state due to the energy required to dissociate diatomic Oxygen. Each atom has one half of the total dissociation energy in addition to its normal energy modes. Thus $e_1^{ref} = D/W_2$ (where D is the energy required to dissociate completely a Mole of diatomic Oxygen into atomic Oxygen) and e_2^{ref} equals zero. The partition functions for atomic and diatomic Oxygen are defined as

$$\begin{aligned} Q_1 &= Q_1^{tr} Q_1^{el} Q_1^{ref} \\ Q_2 &= Q_2^{tr} Q_2^{rot} Q_2^{vb} Q_2^{el} \end{aligned} \quad (2.73)$$

The atomic species is observed to have a lower probability of occurring with respect to the diatomic

species. Whence

$$Q_1^{ref} = \exp\left(-\frac{D}{2RT}\right) = \exp\left(-\frac{\theta_d}{2T}\right) \quad (2.74)$$

where θ_d is the characteristic dissociation temperature. The translation partition functions are given by equation (F.11) for $(\alpha = 1, 2)$ as

$$Q_\alpha^{tr} = v \left(\frac{2\pi m_\alpha kT}{h^2} \right)^{3/2} \quad (2.75)$$

where m_α is the mass of an Oxygen atom ($\alpha = 1$) or molecule ($\alpha = 2$). For diatomic Oxygen the rotational and vibrational partition functions are given by equation (F.11) and (F.12) as

$$Q_2^{rot} = \frac{1}{2} \left(\frac{T}{\theta_{r2}} \right); \quad Q_2^{vb} = \frac{1}{1 - \exp(-\theta_{v2}/T)} \quad (2.76)$$

where θ_{r2} and θ_{v2} have values given in Table 2.1. Typical values for the electronic partition functions are

$$\begin{aligned} Q_1^{el} &= 5 + 3e^{-228/T} + e^{-327/T} \\ Q_2^{el} &= 3 + 2e^{-11,300/T} \end{aligned} \quad (2.77)$$

where terms of order $e^{-23,000/T}$ have been neglected.

Table 2.1

α	A_α	$\theta_{r\alpha}$	$\theta_{v\alpha}$	θ_d	W_α
1	O	----	----	----	16Kg
2	O ₂	2.1K	2,270K	59,000K	32Kg

2.4.2 Local Equilibrium And Law Of Mass Action

Locally the pressure and temperature are equal to their equilibrium values even though chemical non-equilibrium exists. However, the density and mass fractions are not equal to their equilibrium values, but are related, using equation (2.70), as

$$\frac{\rho_e}{\rho} = \frac{1+c_1}{1+c_{1e}} \quad (2.78)$$

Using the law of mass action Equilibrium constants for both reactions can be derived. It can be shown that they are both equal. Written in terms of the partition functions they have the form

$$K_e = \frac{c_{1e}^2}{1-c_{1e}} = \frac{m_1}{2\rho v} \frac{Q_1^2}{Q_2} \exp(-\theta_d/T) \quad (2.79)$$

which when written out in full

$$\frac{c_{1e}^2}{1-c_{1e}} = \frac{\exp(-\theta_d/T)}{\rho} \left[m_1 \left(\frac{\pi m_1 k}{h^2} \right)^{3/2} \theta_{v2} \sqrt{T} (1 - \exp(-\theta_{v2}/T)) \frac{(Q_1^e)^2}{Q_2^e} \right] \quad (2.80)$$

reveals that the right hand side has the units of density and is a function of T only.

2.4.3 Lighthill Ideal Dissociating Gas Model

Lighthill[60] noted that the right hand side of equation (2.80), in the temperature range 1000 to 7000K, was small. Calculated values for the factor in units of gm/cm³ are given for Oxygen in the following table taken from Lighthill's work:

T, K	1000	2000	3000	4000	5000	6000	7000
	145	170	166	156	144	133	123

The variation is seen to be small, especially when compared with the enormous variation of the exponential term over the same range. Lighthill therefore suggested that the factor in brackets should be taken constant and have the value 150 gm/cm³. He calls it the *characteristic density for dissociation*, denoted ρ_d . The law of mass action for the resulting ideal dissociating gas is therefore

$$\frac{c_{1e}^2}{1-c_{1e}} = \frac{\rho_d}{\rho} \exp(-\theta_d/T) \quad (2.81)$$

Setting the bracketed term in equation (2.80) equal to a constant is equivalent to making an approximation in the temperature dependence of the partition functions. Thus a consistent approximation must be made in the other equations for the gas. The specific energy for the mixture will be given by

$$e = T^2 \left(R_1 c_1 \frac{\partial \ln Q_1}{\partial T} + R_2 c_2 \frac{\partial \ln Q_2}{\partial T} \right) + c_1 \frac{1}{2} \frac{D}{W_1} \quad (2.82)$$

By comparing equations (2.79) and (2.81) we note that

$$\frac{m_1 Q_1^2}{2v Q_2} = \rho_d = \text{constant} \quad (2.83)$$

from which it follows by differentiation that

$$\frac{\partial \ln Q_2}{\partial T} = 2 \frac{\partial \ln Q_1}{\partial T} \quad (2.84)$$

Whence

$$e = 2R_2 T^2 \frac{\partial \ln Q_1}{\partial T} + R_2 \theta_d c_1 \quad (2.85)$$

In the temperature range of interest the variation of Q_1 is given solely by the translational term with a negligible contribution from the electronic term. By setting Q_1^e to unity, Q_1 can be written as

$$Q_1 = Q_1^e = \text{constant} \times v T^{3/2} \quad (2.86)$$

Thus the total specific energy (2.85) becomes

$$e = 3R_2 T + R_2 \theta_d c_1 \quad (2.87)$$

The specific enthalpy for the mixture is given by

$$h = e + p/\rho = (4+c_1)R_2 T + R_2 \theta_d c_1 \quad (2.88)$$

With these approximations the system is equivalent, where the electronic energy modes are neglected, to a system where the vibrational modes of diatomic Oxygen are frozen and half excited. Thus the specific heat capacities at constant volume and pressure are

$$\begin{aligned} c_v &= 3R_2 \\ c_p &= (4+c_1)R_2 \end{aligned} \quad (2.89)$$

with the ratio of specific heat capacities given by

$$\gamma = \frac{c_p}{c_v} = \frac{4+c_1}{3} \quad (2.90)$$

For no dissociation $\gamma = 4/3$ and for full dissociation $\gamma = 5/3$.

Anderson[7] has studied the Lighthill model in detail using a diverging nozzle. He has shown that the error in ignoring the variation of the vibrational energy modes is small. This is due to the balanced between the increase in the vibrational energy with temperature and loss of the molecules to the atomic state, i.e. the number of molecules with the higher vibrational temperature goes down.

2.4.4 Rate Equation For Chemical Non-Equilibrium

Using equation (F.34) the atomic Oxygen rate of production per unit volume for the first reaction has the form

$$K_1^{(1)} = \frac{2\rho W_1(1-c_1)}{\tau_1^{(1)}} (K^{(1)}(1-c_1) - c_1^2) \quad (2.91)$$

and for the second reaction

$$K_1^{(2)} = \frac{2\rho W_1 c_1}{\tau_1^{(2)}} (K^{(2)}(1-c_1) - c_1^2) \quad (2.92)$$

where

$$\tau_1^{(1)} = \frac{W_2^3}{4k_b \rho^2} ; \quad \tau_1^{(2)} = \frac{1}{2} \tau_1^{(1)} \quad (2.93)$$

and

$$K^{(1)} = K^{(2)} = \frac{\rho_e c_{1e}^2}{\rho (1-c_{1e})} \quad (2.94)$$

where ρ_e and c_{1e} are the local equilibrium values for density and mass fractions respectively. $\tau_1^{(1)}$ and $\tau_1^{(2)}$ have the units of time and are proportional to the time taken for a small deviation from equilibrium to fall to e^{-1} of its original value as a result of the first and second reactions. The total atomic Oxygen rate of production per unit volume is the sum over both reactions. Using the Lighthill law of mass action, equation (2.81), the total rate becomes

$$K_1 = \frac{\rho}{\tau_1} \left((1-c_1) \frac{\rho_d}{\rho} \exp(-\theta_d/T) - c_1^2 \right) \quad (2.95)$$

where we re-define the characteristic reaction time to be

$$\tau_1 = \frac{W_2^2}{4k_b \rho^2 (1+c_1)} \quad (2.96)$$

Freeman[39], using a different approach, has derived an equivalent rate equation

$$K_1 = C \rho^2 T^{-s} \left((1-c_1) \exp(-\theta_d/T) - \frac{\rho}{\rho_d} c_1^2 \right) \quad (2.97)$$

where s and C are constants with the latter having the dimensions of [(temperature)^s / (density) / time]. Comparison between equations (2.95) and (2.99) reveals that C , in terms of Clarke's rate equation, has the form

$$C = \frac{4k_b T^s \rho_d (1+c_1)}{W_2^2} \quad (2.98)$$

With all these results equation (2.33) can be shown to have the form

$$K = \frac{1}{4+c_1} \left(\frac{3}{1+c_1} - \frac{\theta_d}{T} \right) \frac{K_1}{\rho q} \quad (2.99)$$

2.4.5 Entropy Production and Crocco's Theorem For Rotational Flow

The First Law of Thermodynamics can be written in terms of the grad operator ∇ as

$$T\nabla S = \nabla h - v\nabla p - (\mu_1 - \mu_2)\nabla c_1 \quad (2.100)$$

upon substitution of the momentum equation (2.10) the first law can be written in terms of flow field vorticity

$$-\nabla \wedge \zeta = T\nabla S - \nabla h_s + (\mu_1 - \mu_2)\nabla c_1 \quad (2.101)$$

This is Crocco's equation modified for the presence of chemical reactions. The vorticity, which is due to

the entropy gradients, is also generated where there are regions where the species are non-uniform. By taking the scalar product between the velocity vector and equation (2.100) the entropy production along a streamline ($\xi_2 = \text{constant}$) can be shown, using equation (F.40), to be

$$\frac{\partial S}{\partial \xi_1} = -\frac{\sigma_1 R_2 K_1}{\rho q} \ln \left[\frac{c_1^2}{1-c_1^2} \frac{1-c_{1e}^2}{c_{1e}^2} \right] \quad (2.102)$$

and along the normal direction the first law has the expanded form

$$\frac{\partial S}{\partial \xi_2} = \frac{\sigma_2 q \zeta}{T} - \frac{\mu_1 - \mu_2}{T} \frac{\partial c_1}{\partial \xi_2} \quad (2.103)$$

remembering that the flow is isoenergetic. ζ is the sole surviving vorticity component given by

$$\zeta = -\frac{1}{\sigma_1 \sigma_2} \frac{\partial(\sigma_1 q)}{\partial \xi_2} \quad (2.104)$$

We observe for inert flow fields, with uniformly distributed c_1 , that⁸

$$\ln(\sigma_1 q) = -\int \frac{T}{q^2} \frac{\partial S}{\partial \xi_2} d\xi_2 + f(\xi_1) \quad (2.105)$$

and where there are no entropy gradients (irrotational flow)

$$\ln(\sigma_1 q) = f(\xi_1) \quad (2.106)$$

which remains constant along the normal co-ordinate ($\xi_1 = \text{constant}$). This can also be derived from equations (2.10), (2.22), and (2.26).

2.4.6 Sound Speeds

The Frozen sound speed for the mixture can be shown, using equation (F.42) and (F.43), to be

$$a_f^2 = \frac{4+c_1}{3} \frac{p}{\rho} \quad (2.107)$$

and the ratio of frozen to equilibrium sound speeds is given by

⁸ With regard to our earlier discussion this equation is equivalent to Oswatitsch's result for rotational flows[68, page 255].

$$\left(\frac{a_f}{a_e} \right)^2 = 1 + \frac{c_{1e}(1-c_{1e})}{3} \frac{\left[\left(1 + \frac{\theta_d}{T} \right) (1+c_{1e}) - (4+c_{1e}) \right]^2}{\left(1 + \frac{\theta_d}{T} \right)^2 c_{1e}(1-c_{1e}) + 8 + 2c_{1e}} \quad (2.108)$$

2.5 Non-Dimensionalization

The flow variables are non-dimensionalized with respect to the freestream flow conditions in the following manner,

$$\begin{aligned} \bar{p} &= \frac{p}{\rho_\infty q_\infty^2} & \bar{\rho} &= \frac{\rho}{\rho_\infty} & \bar{q} &= \frac{q}{q_\infty} & \bar{T} &= \frac{R_2 T}{q_\infty^2} \\ \bar{e} &= \frac{e}{q_\infty^2} & \bar{h} &= \frac{h}{q_\infty^2} & \bar{S} &= \frac{S}{R_2} & \bar{\tau}_1 &= \frac{\tau_1}{\tau_{1\infty}} \\ \bar{\sigma}_1 &= \frac{\sigma_1}{L} & \bar{\sigma}_2 &= \frac{\sigma_2}{L} & \bar{s} &= \frac{s}{L} & \bar{n} &= \frac{n}{L} \end{aligned} \quad (2.109)$$

where the overbar denotes the non-dimensionalized variables, the subscript ∞ the freestream conditions, R_2 is the specific gas constant for diatomic Oxygen, species $\alpha = 2$, and L is a characteristic reference length used in the freestream Damkhöler number

$$Da_\infty = \frac{q_\infty \tau_{1\infty}}{L} \quad (2.110)$$

where

$$\tau_{1\infty} = \frac{W_2^2}{4k_b \rho_\infty^2 (1+c_{1\infty})} \quad (2.111)$$

With this non-dimensionalization the equations, without sources terms, remain unchanged in form. However, those with sources terms are modified by the presence of the freestream and local Damkhöler numbers. Thus we observe that

$$\frac{\partial c_1}{\partial \xi_1} = \frac{1}{Da_\infty} \frac{\bar{\sigma}_1}{\bar{\rho} \bar{q}} \bar{K}_1 \quad (2.112)$$

$$\bar{K}_1 = \frac{\bar{p}}{\tau_1} \left((1-c_1) \frac{\bar{p}_d}{\bar{p}} \exp(-\bar{\theta}_d/\bar{T}) - c_1^2 \right) \quad (2.113)$$

$$\frac{\partial \bar{S}}{\partial \xi_1} = -\frac{1}{Da_\infty} \frac{\bar{\sigma}_1}{\bar{p} \bar{q}} \bar{K}_1 \ln \left[\frac{c_1^2}{1-c_1^2} \frac{1-c_{1e}^2}{c_{1e}^2} \right] \quad (2.114)$$

and

$$\bar{K} = \frac{1}{4+c_1} \left(\frac{3}{1+c_1} - \frac{\bar{\theta}_d}{\bar{T}} \right) \frac{\bar{K}_1}{\bar{p} \bar{q}} \quad (2.115)$$

The system of equations for the ideal dissociating gas becomes

$$\frac{\partial \bar{U}}{\partial \xi_1} + \bar{C} \frac{\partial \bar{U}}{\partial \xi_2} = \frac{1}{Da_\infty} \bar{Q} \quad (2.116)$$

with

$$\bar{U} = \begin{pmatrix} \bar{p} \\ \bar{q} \\ \bar{\theta} \\ c_1 \end{pmatrix}; \quad \bar{C} = \begin{pmatrix} 0 & 0 & 0 & \frac{\bar{\sigma}_1 \bar{p} M_f^2}{\bar{\sigma}_2 (M_f^2 - 1)} & 0 \\ 0 & 0 & 0 & -\frac{\bar{\sigma}_1 \bar{q}}{\bar{\sigma}_2 (M_f^2 - 1)} & 0 \\ 0 & 0 & 0 & \frac{\bar{\sigma}_1 \bar{p} \bar{q}^2}{\bar{\sigma}_2 (M_f^2 - 1)} & 0 \\ 0 & 0 & \frac{\bar{\sigma}_1}{\bar{\sigma}_2 \bar{p} \bar{q}^2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}; \quad \bar{Q} = \begin{pmatrix} \frac{\bar{\sigma}_1 \bar{p} \bar{K}}{M_f^2 - 1} \\ -\frac{\bar{\sigma}_1 \bar{q} \bar{K}}{M_f^2 - 1} \\ \frac{\bar{\sigma}_1 \bar{p} \bar{q}^2 \bar{K}}{M_f^2 - 1} \\ 0 \\ \frac{\bar{\sigma}_1 \bar{K}_1}{\bar{p} \bar{q}} \end{pmatrix} \quad (2.117)$$

Chapter 3

Numerical Method For Natural Co-ordinates

3.1 Introduction

We seek solutions to the initial/boundary value problem defined by the Euler equations, repeated here for clarity, as

$$\frac{\partial \bar{U}}{\partial \xi_1} + \bar{C} \frac{\partial \bar{U}}{\partial \xi_2} = \frac{1}{Da_\infty} \bar{Q} \quad (3.1)$$

with the geometric equations (2.22) together with prescribed initial data along the normal co-ordinate ξ_2 (say for $\xi_1 = 0$)

$$\bar{U}(\xi_2) = \bar{U}(0, \xi_2) \quad (3.2)$$

and

$$\bar{\sigma}_2(\xi_2) = \bar{\sigma}_2(0, \xi_2) \quad (3.3)$$

for $0 \leq \xi_2 \leq 1$, and along some chosen boundary⁹

$$\begin{aligned} \theta_b &= \theta(\xi_1, \xi_2 = \text{constant}) \\ \bar{\sigma}_{1b} &= \bar{\sigma}_1(\xi_1, \xi_2 = \text{constant}) \end{aligned} \quad (3.4)$$

In general there are no analytic solutions to these equations for practical situations and an approximate numerical solution must be calculated. For this purpose we have developed a space marching, high resolution, cell centred, numerical method based on the method of Fractional steps[104].

We first perform a space discretization of the continuous two dimensional natural co-ordinate space¹⁰ (ξ_1, ξ_2). The ξ_2 co-ordinates are divided up into N equally spaced cells, plus two half cells, with nodal point representing the cell centre defined by j . Its position from the lower boundary $\xi_2 = 0$ is then $\xi_{2j} =$

⁹ It will become apparent that θ and σ_1 must be known along a particular streamline/boundary ($\xi_2 = \text{constant}$) if a solution downstream of the initial data line is to be calculated.

¹⁰ It should be remembered that these computational co-ordinates do not represent physical distances. Physical distances are calculated using equation (2.17).

$(j-1/2)\Delta\xi_2$ with $j = 0, 1, \dots, N+1$. The spacing between the cell centres is equal to $\Delta\xi_2 = 1/N$ with the field of flow chosen for convenience to be bounded between $0 \leq \xi_2 \leq 1$. The two half cells at the positions $j = 0$ and $j = N+1$, which are outside the flow domain, are pseudo cells and are used for providing the boundary conditions for the flow field domain. We discuss this aspect in more detail later on. Each cell will have its own boundaries defined by $j \pm 1/2$ with positions $\xi_{2,j} \pm \Delta\xi_2/2$, see Figure 3.1. The incremental step size between nodes along any streamline $\Delta\xi_{1,i} = \xi_{1,i+1} - \xi_{1,i}$ ($i = 0, 1, 2, \dots, M$) is variable and is determined from the stability requirement defined by the Courant-Friedrich-Lewy (CFL) condition to be discussed later on. Because of this the number of computational steps M needed to compute the flow field to a given position downstream (say at position $\xi_1 = 1$) of the initial data line will not be known in advance. The streamline co-ordinate ξ_1 will have position given by the sum of the step sizes thus

$$\xi_{1,i+1} = \xi_{1,0} + \sum_{s=1}^i \Delta\xi_{1,s} \quad (3.5)$$

since $\xi_{1,0} = 0$.

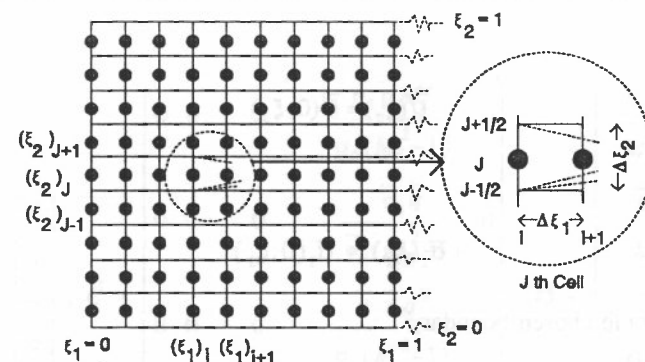


Figure 3.1 Numerical Grid Layout.

The exact initial data is approximated by a set of piecewise constant states which are calculated by averaging the initial data within each cell using the formula

$$\bar{U}(0, \xi_{2,j}) = \bar{U}_{0,j} = \frac{1}{\Delta\xi_2} \int_{\xi_{2,j-1/2}}^{\xi_{2,j+1/2}} \bar{U}(\xi_2) d\xi_2 \quad (3.6)$$

It is seen that this data remains constant within each cell but is discontinuous at the cell interfaces, see Figure 3.2. Whence we can define left and right states such that

$$\begin{aligned} \bar{U}_L &= \bar{U}_{i,j+1} ; \xi_2 > \xi_{2,j+1/2} \\ \bar{U}_R &= \bar{U}_{i,j} ; \xi_2 < \xi_{2,j+1/2} \end{aligned} \quad (3.7)$$

together with the geometric conditions σ_{1L} , σ_{1R} , σ_{2L} , and σ_{2R} where

$$\xi_{2,j+1/2} = j \Delta\xi_2 \quad (3.8)$$

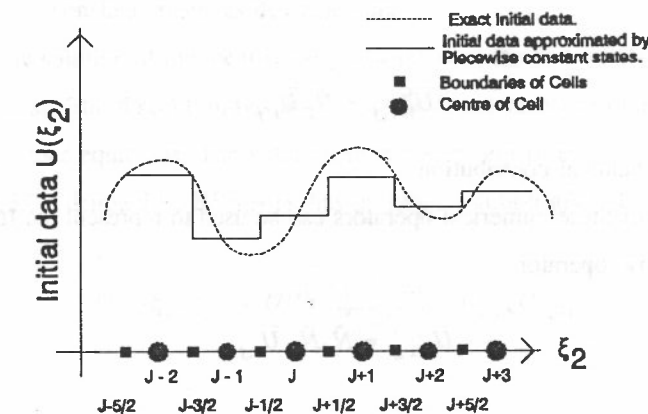


Figure 3.2 Approximate Initial data.

From this initial data we wish to calculate the numerical solution downstream at the new spatial position $\Delta\xi_1$ and subsequently further on. This can be accomplished by the numerical operation written explicitly as

$$\bar{U}_{i+1,j} = \hat{N} \bar{U}_{i,j} \quad (3.9)$$

where $\hat{N}$ represents a numerical non-linear operator which models the non-homogeneous Euler equations. The method of Fractional steps of Yanenko[104] can be used to replace the single operation by a number of simpler intermediate steps. This has the effect of splitting up the operator, containing all the essential physics, into many which are in general less complicated than the original system but each will model some essential aspect of the flow. In this way the flow field can be built up in stages.

Two subsystems can be identified. The first will be due to the influence on the flow field by wave interactions. These are modeled by the homogeneous Euler equations written as

$$\frac{\partial \bar{U}}{\partial \xi_1} + \bar{C} \frac{\partial \bar{U}}{\partial \xi_2} = 0 \quad (3.10)$$

which can be written concisely in operator notation as

$$\bar{U}_{i+1,j}^W = \hat{N}_W \bar{U}_{i,j} \quad (3.11)$$

where W represents the wave contribution. The other contribution will be due to the influence of the chemical reactions on the field of flow modelled approximately through the system of ordinary differential

equations as

$$\frac{d\bar{U}}{d\xi_1} = \frac{1}{Da_-} \bar{Q} \quad (3.12)$$

and in operator notation

$$\bar{U}_{i+1,j}^C = \hat{N}_c \bar{U}_{i,j} \quad (3.13)$$

where C represents the chemical contribution.

Various combinations of these numerical operators can be used to represent the full system. The most popular are the asymmetric operator

$$\bar{U}_{i+1,j} = \hat{N}_c \hat{N}_w \bar{U}_{i,j} \quad (3.14)$$

the symmetric operator

$$\bar{U}_{i+1,j} = \frac{1}{2} (\hat{N}_c \hat{N}_w + \hat{N}_w \hat{N}_c) \bar{U}_{i,j} \quad (3.15)$$

and that identified by Strang[89]

$$\bar{U}_{i+1,j} = \hat{N}_w \hat{N}_c \hat{N}_w \bar{U}_{i,j} \quad (3.16)$$

where the subscript $W/2$ represents half a spatial step.

We shall use only the asymmetric operator. For piecewise constant initial data predicted values are first calculated by solving for the wave contributions equation (3.11) for frozen conditions. For chemical non-equilibrium these values are used as the starting conditions for the chemical or corrector step equation (3.13). The procedure is repeated until the desired position downstream is reached. For convenience we now drop the bar over the symbols denoting non-dimensional values and use, unless told otherwise, these values throughout.

3.2 Random Choice Method For Natural Co-ordinates

The solution of the homogeneous Euler equations for the wave contributions was performed using the Random Choice Method (RCM) which is similar to the Godunov type method[44]. There are important differences which will be highlighted later on. However, both methods share the following property. Starting from piecewise constant initial data at $\xi_{1,i}$ the evolution of the flow downstream at the next spatial step $\xi_{1,i+1}$ results from the wave interactions originating at the cell boundaries between adjacent cells, see figure 3.1. The cell interfaces separate two different fluid states U_L and U_R defined by equation (3.7). The

resulting local interaction can be exactly resolved since the solution of the homogeneous Euler equations together with the initial data equation (3.7) corresponds locally to a Riemann problem (RP). The whole solution at the next spatial level is then the sum of all the interactions between the different RP.

The RCM, like the Godunov method, is based on a three stage procedure. *Step one:* Approximate the initial data by piecewise constant states, as described above.

Step two: Determine the solution of the local Riemann problem at the cell interfaces. This is the physical step to the whole process. The discontinuities at the interfaces are resolved in a superposition of waves satisfying locally the Euler equations. The solution to the Riemann problem in the interval $j, j+1$ with initial data equation (3.7), denoted by $RP(j,j+1)$, has an exact solution given by

$$U^{(e)}(\xi_1, \xi_2) = U^{(e)}\left(\frac{\xi_2 - \xi_{2,j+1/2}}{\xi_1 - \xi_{1,i}}; U_{i,j}, U_{i,j+1}\right) \quad (3.17)$$

for $\xi_{2,j} < \xi_2 < \xi_{2,j+1}$.

Step three: Calculate the solution at the next spatial position. At this stage the Godunov method and RCM differ. We refer to Hirsch[50] for a description of the Godunov step.

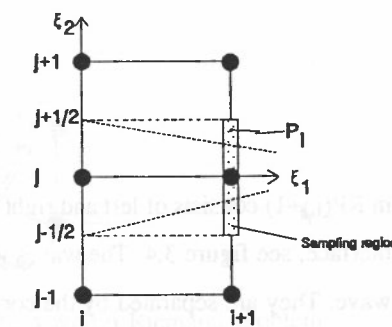


Figure 3.3 Sampling Region.

Consider the j -th cell with waves propagating outwards from its interfaces. The CFL condition stops the waves from interacting with each other by limiting the spatial step size $\Delta\xi_1$. To calculate the vector of primitive variables at the new spatial point $U_{i+1,j}$ the waves are sampled downstream between the cell boundaries, see figure 3.3. The point P_i is chosen randomly within the interval $\xi_{2,j-1/2} \leq \xi_2 \leq \xi_{2,j+1/2}$ using the equidistributed quasi-random number series $\theta_i \in [0,1]$ discussed further on. However, this value must remain constant for each normal $\xi_{1,i}$. The sampling point has the co-ordinates, taken from the bottom interface, given by

$$P_i = \{\xi_{1,i} + \Delta\xi_1, \xi_{2,j-1/2} + \theta_i \Delta\xi_2\} \quad (3.18)$$

The solution $U_{i+1,j}$ is given by the calculated conditions at the sampling point thus

$$U_{i+1,j} = U^{(e)}(P_i) \quad (3.19)$$

However, the sampling region lies within two RP's. Whence for $\theta_i < 1/2$ the sampling point lies within RP(j-1,j) with solution vector given by

$$U_{i+1,j} = U^{(e)}\left(\frac{\theta_i \Delta\xi_2}{\Delta\xi_1}; U_{i,j-1}, U_{i,j}\right) \quad (3.20)$$

and for $\theta_i > 1/2$ the sampling point lies within RP(j,j+1) with solution vector given by

$$U_{i+1,j} = U^{(e)}\left(\frac{(\theta_i - 1) \Delta\xi_2}{\Delta\xi_1}; U_{i,j}, U_{i,j+1}\right) \quad (3.21)$$

Thus the random sampling produces the interaction between the waves from the different RP's. The last two results will be used later on. With the basic Random Choice Method described we proceed to elaborate on steps two and three.

3.2.1 Riemann Problem

The solution of the Riemann problem RP(j,j+1) consists of left and right waves propagating outwards from the initial discontinuity at the cell interface, see figure 3.4. The waves w_1 and w_3 can either be an oblique shock or Prandtl-Meyer expansion wave. They are separated by the contact surface w_2 which is along the streamline direction ξ_1 . The region downstream of the waves is uniform and will be known as the centred or * state. The left and right centred states downstream are labelled by U_{L*} and U_{R*} , respectively.

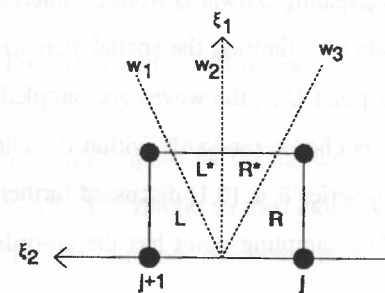


Figure 3.4 Solution of Riemann Problem RP(j,j+1).

Four permutations of these waves are possible consisting of either two elemental oblique shock waves, two expansions, shock and expansion, or expansion and shock. These are represented schematically by figure 3.5, where the different flow field regions are numbered.

The flow deflection angle downstream of the left wave can be written in terms of the initial deflection angle and the jump in the deflection across the wave thus

$$\theta_{L*} = \theta_L + [\theta]_L \quad (3.22)$$

and similarly for the right wave

$$\theta_{R*} = \theta_R + [\theta]_R \quad (3.23)$$

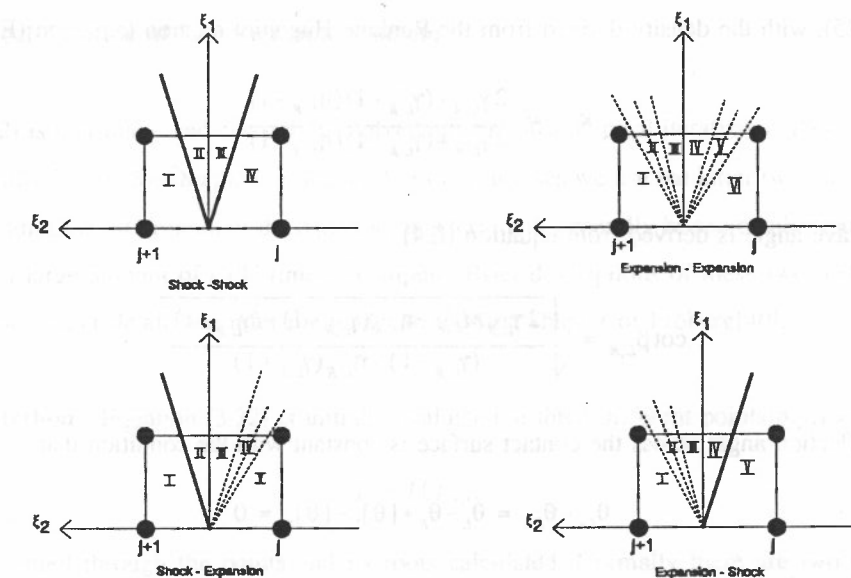


Figure 3.5 Wave permutations within Riemann problem.

For left and right running expansion waves the change in the flow deflection across them is related to the change in the Prandtl-Meyer function, through the Riemann invariants equation (2.59), by

$$[\theta]_{L,R} = \mp [v]_{L,R} \quad (3.24)$$

The frozen Mach number downstream can be written in terms of the pressure changes across the wave thus

$$M_{L,R*} = \sqrt{\frac{2}{\gamma_{L,R} - 1} \left(\frac{\kappa_{L,R}}{\eta_{L,R}} \left(1 + \frac{\gamma_{L,R} - 1}{2} M_{L,R}^2 \right) - 1 \right)} \quad (3.25)$$

where $\eta_{L,R} = p_* / p_{L,R}$. Note p_* is constant across the contact surface by equation (2.62). The density is

calculated using the isentropic relation

$$\kappa_{L,R} = \frac{\rho_{L,R*}}{\rho_{L,R}} = (\eta_{L,R})^{\frac{1}{\gamma_{L,R}}} \quad (3.26)$$

The flow deflection across an oblique shock wave can be shown from the Rankine Hugoniot relations (appendix E) to be

$$[\theta]_{L,R} = \pm \frac{\cot \beta_{L,R} (\eta_{L,R} - 1)}{\gamma_{L,R} M_{L,R}^2 - (\eta_{L,R} - 1)} \quad (3.27)$$

where $\beta_{L,R}$ is the left and right shock wave angle. The change in the frozen Mach number is given by equation (3.25), with the density derived from the Rankine-Hugoniot relation (equation (E.2))

$$\kappa_{L,R} = \frac{2\gamma_{L,R} + (\gamma_{L,R} + 1)(\eta_{L,R} - 1)}{2\gamma_{L,R} + (\gamma_{L,R} - 1)(\eta_{L,R} - 1)} \quad (3.28)$$

The shock wave angle is derived from equation (E.4)

$$\cot \beta_{L,R} = \sqrt{\frac{2\gamma_{L,R} M_{L,R}^2 - \eta_{L,R} (\gamma_{L,R} + 1) - (\gamma_{L,R} - 1)}{(\gamma_{L,R} - 1) + \eta_{L,R} (\gamma_{L,R} + 1)}} \quad (3.29)$$

The flow deflection angle across the contact surface is constant with the condition that

$$\theta_{L*} - \theta_{R*} = \theta_L - \theta_R + [\theta]_L - [\theta]_R = 0 \quad (3.30)$$

By making the substitution

$$\chi_{L,R} = \mp [\theta]_{L,R} \quad (3.31)$$

we obtain an equation which is more useful for numerical purposes, i.e. easier to program, as

$$f(p_*; U_L, U_R) = \theta_L - \theta_R - \chi_L - \chi_R = 0 \quad (3.32)$$

Grouping the above equations they can be written in a more concise form

$$\kappa_{L,R} = \begin{cases} (\eta_{L,R})^{\frac{1}{\gamma_{L,R}}} & ; \eta_{L,R} \leq 1 \\ \frac{2\gamma_{L,R} + (\gamma_{L,R} + 1)(\eta_{L,R} - 1)}{2\gamma_{L,R} + (\gamma_{L,R} - 1)(\eta_{L,R} - 1)} & ; \eta_{L,R} > 1 \end{cases} \quad (3.33)$$

and

$$\chi_{L,R} = \begin{cases} [\nu]_{L,R} & ; \eta_{L,R} \leq 1 \\ -\frac{\cot \beta_{L,R} (\eta_{L,R} - 1)}{\gamma_{L,R} M_{L,R}^2 - (\eta_{L,R} - 1)} & ; \eta_{L,R} > 1 \end{cases} \quad (3.34)$$

with the Mach number given by equation (3.25).

It is observed that equation (3.32) is only dependent on the pressure downstream within the centred state p_* . However, no closed form solutions exist for the two dimensional RP and it must be solved numerically¹¹. Once the pressure has been calculated all the other flow conditions within the left and right centred states follow.

3.2.2 Numerical Solution of The Riemann Problem

Equation (3.32) is non-linear and can only be solved numerically. Typical iterative methods are Newton-Raphson's, Muller's, and *Regula falsi* or Secant. For our purposes we use the latter two methods because they do not require the differential of the equation; this term will generally be too cumbersome to manage and will take a large amount of CPU time to compute. Brief descriptions of these two methods will be given here. For further details we refer the reader to the first chapter of Fröberg[40].

Muller's Method : Equation (3.32) is initially evaluated at three different points $p_{*,i}$ ($i = 1, 2, 3$) thus

$$f_i = f(p_{*,i}) \quad (3.35)$$

A parabola is fitted through the points and its roots calculated. Normally there are two of them. We choose the smallest positive root $p_{i,4}$ which corresponds to the weak oblique shock wave solution. The strong shock solution is undesirable because the flow downstream is subsonic. Equation (3.32) is re-evaluated for the new point. If f_4 lies outside a certain tolerance the first point is removed and a new parabola fitted through the remaining points. The procedure is repeated until the required convergence is reached. Starting conditions for the method, from Shi and Gottlieb[83], are chosen

$$p_{*,1} = 0.95 p_{*} ; p_{*,2} = 1.05 p_{*} ; p_{*,3} = p_{*}$$

where p_{*} is a seed/starting value to be determined.

Regula Falsi : Equation (3.32) is initially evaluated at the two different positions

$$p_{*,1} = p_{*} ; p_{*,2} = 1.001 p_{*}$$

¹¹ For the one dimensional unsteady Riemann problem there exists a closed form solution to a flow field with two rarefaction waves, see Toro[91].

from which a third point can be calculated from the equation

$$p_{*,i+1} = \frac{f_i p_{*,i-1} - p_{*,i} f_{i-1}}{f_i - f_{i-1}} \quad (3.36)$$

Equation (3.32) is re-evaluated using the new point. As before if its value is outside a certain tolerance the procedure is repeated until convergence is reached.

Any numerical iterative method, must begin from some starting or seeding conditions. If they are far away from the desired solution the numerical method may take a large number of iterative steps and CPU time before convergence is achieved. The type of seeding values may even cause the method to fail completely by crashing the algorithm (such as square root of negative number i.e. pressure). Usually when the absolute of the difference of the new and old functional values has gone below a certain tolerance (say 10^{-6}) it is assumed to have converged. If the function has to be solved a large number of times, particularly for our problem, then the seed values must be chosen as close to the solution as possible therefore minimizing the effort. We have used the following seeding conditions for the iterative scheme based on approximations of the governing equations themselves.

For low frozen supersonic Mach numbers (we use the range $1 < M_t < 5$) the pressure change across a left and right running waves can be linearized in terms of the change in flow deflection angle [82, pages 561-563]. This change expanded to two terms¹² has the form

$$\eta_{L,R} = 1 + \frac{\gamma M_{L,R}^2}{2} (c_{1L,R} [\theta]_{L,R} + c_{2L,R} [\theta]_{L,R}^2) \quad (3.37)$$

where $\eta_{L,R} = p / p_{L,R}$ and

$$c_{1L,R} = \pm \frac{2}{\sqrt{M_{L,R}^2 - 1}} ; \quad c_{2L,R} = \frac{(M_{L,R}^2 - 2)^2 + \gamma M_{L,R}^4}{2(M_{L,R}^2 - 1)^2} \quad (3.38)$$

we have taken equation (3.37) to two terms because in general the change in deflection angle will not be small. The pressure equations are coupled through the pressure in the centred state. We could solve the resulting equation numerically for θ , but this would defeat our effects to reduce the CPU time. Thus we define as a first shot that

¹² For two terms it is independent of the wave type.

$$\begin{aligned} \theta_* &= \frac{1}{2}(\theta_L + \theta_R) \\ \gamma &= \frac{1}{2}(\gamma_L + \gamma_R) \end{aligned} \quad (3.39)$$

From which

$$p_{s*} = \frac{1}{2}(p_L \eta_L + p_R \eta_R) \quad (3.40)$$

For Hypersonic conditions ($M_t \geq 5$) the basic equations for oblique shock wave and expansion waves can be simplified without to much error [6, pages 33-44]. For oblique shock waves we use the limiting shock angle given by

$$\beta_{L,R} = \pm \frac{\gamma + 1}{2} [\theta]_{L,R} \quad (3.41)$$

where we have used equation (3.39) for γ . The pressure jump is derived from the usual Rankine Hugoniot relation equation (E.1)

$$\eta_{L,R} = 1 + \frac{2\gamma}{\gamma + 1} (M_{L,R}^2 \sin^2 \beta_{L,R} - 1) \quad (3.42)$$

For expansion waves the pressure equation can be approximated for large Mach numbers as

$$\eta_{L,R} = \left(1 - \frac{\gamma - 1}{2} M_{L,R} [\theta]_{L,R} \right)^{\frac{2\gamma}{\gamma - 1}} \quad (3.43)$$

Applying the conditions that the left and right waves are expansions if $[\theta]_L \leq 0$ or $[\theta]_R \geq 0$ and oblique shock waves if $[\theta]_L \geq 0$ or $[\theta]_R \leq 0$ respectively, and by using equation (3.39) for θ_* , the centre state pressure can be calculated using equation (3.40).

With these seeding conditions and a tolerance of 10^{-6} , Muller's method was found to be the most robust of the two methods used. However, even though it has a faster convergence rate to the regula falsi it will take slightly more CPU time per iterative step due to the solution of a quadratic equation at each stage and deciding which root is the smallest. Therefore it would be desirable to improve on the accuracy of the seeding conditions and use the regula falsi method. But because of this in-accuracy Muller's method should be used for reliability.

3.2.3 Determination of the Wave Positions

Before the Riemann problems can be sampled the position of the waves within them must be known. These positions are not needed for the solution of the Riemann problem; it depends on the type of waves

but not where they are in space. Since we are dealing with a similarity solution the wave positions will be given by the parameter, equation (2.56), for left and right waves

$$\frac{\xi_2 - \xi_{2,j \pm 1/2}}{\Delta \xi_1} = \pm \frac{\sigma_1}{\sigma_2} \tan \{\phi_{L,R}\} \quad (3.44)$$

where $\phi_{L,R}$ are the left and right wave angles.

It is clear from this equation that the scaling factors σ_1 and σ_2 must be known if we are to position the waves within each cell. That is the effective streamline length and its area must be given. σ_2 is defined along the initial data line $\xi_2 = 0.0$. From the mass conservation equation (2.29) it can be determined downstream. σ_1 on the other hand is only defined along some boundary. Its behaviour along a normal can be determined from equation (2.23) as long as the change in $\partial\theta/\partial\xi_1$ along the normal is known. For isentropic flows, i.e. across expansion waves, equation (2.23) is equivalent to equation (2.106) derived from Crocco's Theorem. Whence

$$\sigma_1 q = f(\xi_1) \quad (3.45)$$

Therefore along any normal the scaling factor along the streamline will be inversely proportional to the magnitude of the velocity.

For an oblique shock wave there are the geometric conditions, see figure 3.6, for the uniform initial upstream state

$$\frac{\Delta n}{\Delta s} = \frac{\sigma_2 \Delta \xi_2}{\sigma_1 \Delta \xi_1} = \tan \{\beta\} \quad (3.46)$$

and for the uniform conditions downstream i.e. in centred state region *

$$\frac{\Delta n}{\Delta s} = \frac{\sigma_{2*} \Delta \xi_2}{\sigma_{1*} \Delta \xi_1} = \tan \{\beta - \delta\} \quad (3.47)$$

Because the mass between the streamlines ξ_2 and $\xi_2 + \Delta \xi_2$ remains fixed it can be shown that

$$\sigma_1 q = \sigma_{1*} q_* \quad (3.48)$$

This is equivalent to the condition that the velocity tangential to the shock be constant across it. Also σ_1 remains constant across the contact surface by equation (2.64)

Thus we observe that along a normal $\xi_1 = \text{constant}$ equations (3.45) and (3.48) are equivalent and can be written

$$[\sigma_1 q] = 0 \quad (3.49)$$

However, across contact surfaces this is not true

$$[\sigma_1 q] \neq 0 \quad (3.50)$$

by virtue of $[q] \neq 0$.

Using equation (3.49), together with the solutions from the Riemann problems for velocity, σ_1 can be calculated at the cell centres along the normal from its boundary value. Also, its value within the centred state can now be determined. These values are only valid along the normal on which they are calculated.

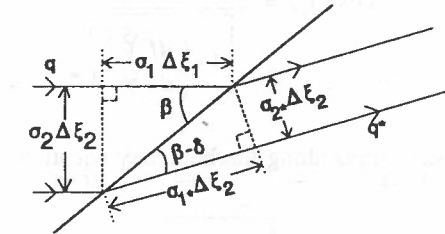


Figure 3.6 Oblique shock wave position.

3.2.4 Boundary Conditions

In addition to the initial data specified along $\xi_1 = 0.0$, to determine the flow field downstream of this data line we need to know the behaviour of θ and σ_1 along a particular boundary i.e. θ_b and σ_{1b} . Thus the equation for a boundary must be known and will usually be specified along a solid or free boundary. If it has the functional form $y = f(x)$ and is twice differentiable then its deflection angle is

$$\theta_b = \theta_b(x) = \tan^{-1} \left(\frac{df}{dx} \right) \quad (3.51)$$

with curvature

$$\frac{\partial \theta_b}{\partial s} = \frac{\frac{d^2 f}{dx^2}}{\left(1 + \left(\frac{df}{dx} \right)^2 \right)^{3/2}} \quad (3.52)$$

From these results we have to determine their behaviour with respect to ξ_1 i.e. or equivalently find the functional form of x in terms of ξ_1 . Since the boundary is by definition a streamline we have the condition along it $\xi_2 = \text{constant}$ or more importantly $d\xi_2 = 0.0$. This result together with equation (2.21) yields

$$dx = \sigma_{1b} \cos(\theta_b) d\xi_1 \quad (3.53)$$

where $\sigma_{1b} = \sigma_1$ ($\xi_1, \xi_2 = \text{constant}$). Whence

$$x = \int \sigma_{1b} \cos(\theta_b) d\xi_1 \quad (3.54)$$

Now

$$\cos(\theta_b) = \frac{1}{\sqrt{1 + \left(\frac{df}{dx}\right)^2}} \quad (3.55)$$

By assuming that σ_1 is constant (say unity) along the boundary equation (3.54) yields

$$\xi_1 = \int \sqrt{1 + \left(\frac{df}{dx}\right)^2} dx \quad (3.56)$$

If the boundary is a linear function of x then by integrating equation (3.56) x can be written in terms of ξ_1 . However, for quadratic functions no easy inversion of the integral is possible. By imposing the more profitable condition

$$\sigma_{1b} = \sqrt{1 + \left(\frac{df}{dx}\right)^2} \quad (3.57)$$

equation (3.54) yields

$$x = \xi_1 \quad (3.58)$$

where the constant of integration is zero since $x = \xi_1 = 0$ at the origin.

Thus the equation for the boundary can be re-written as $y = f(\xi_1)$. From which the functional forms for θ_b and σ_{1b} can be derived satisfying the requirement set down in equation (3.4). Note, within the freestream the streamlines remains un-deflected and without loss of generality the deflection angle is zero throughout. Hence $f(x) = \text{constant}$. From equation (3.57) σ_1 is unity within this region.

We describe the procedures necessary to impose boundary conditions at the lower ($\xi_2 = 0.0$) and upper ($\xi_2 = 1.0$) positions within the flow field domain using the pseudo or half cells at $j = 0$ and $j = N+1$ respectively. For the most part the lower boundary will be taken solid and the upper a free boundary.

3.2.4.1 Solid Boundary Conditions

Given the flow field conditions within the cell $j = 1$ (left state) we need to impose conditions within the pseudo cell $j = 0$ (right state) such that the streamline along $\xi_2 = 0.0$ satisfies the behaviour of the body deflection angle. This system defines a Riemann problem with left and right states

$$\begin{aligned} U_L &= U_{i,1} ; \xi_2 > 0 \\ U_R &= U_{i,0} ; \xi_2 < 0 \end{aligned} \quad (3.59)$$

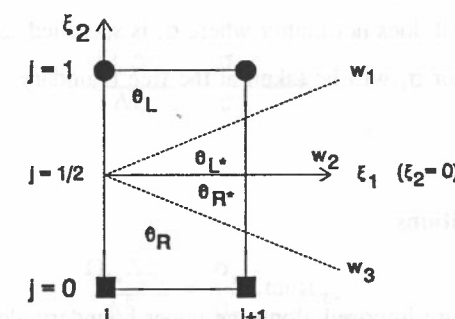


Figure 3.7 Riemann problem for solid boundary.

The solid boundary will have deflection angle equation (3.51). If w_1 within cell $j = 1$, figure 3.7, represents the physical wave generated due to the change in body angle then we have the condition

$$\theta_b = \theta_* = \theta_L + [\theta]_L \quad (3.60)$$

where θ_* is the flow deflection in the centred state. The mirror image of this wave w_3 will be created within the pseudo cell. Whence

$$\theta_b = \theta_R + [\theta]_R \quad (3.61)$$

Because the waves are symmetrical about the boundary or contact surface we have the condition

$$[\theta]_L = -[\theta]_R \quad (3.62)$$

Thus θ at the pseudo cell centre must have the value

$$\theta_R = 2\theta_b - \theta_L \quad (3.63)$$

In addition to this we must impose

$$\begin{aligned} \rho_L &= \rho_R & p_L &= p_R & q_L &= q_R \\ \sigma_{2L} &= \sigma_{2R} & S_L &= S_R & c_{\alpha L} &= c_{\alpha R} \end{aligned} \quad (3.64)$$

Because the waves are symmetric and regardless of the wave type we have the additional condition that

$$\sigma_{1L} = \sigma_{1R} \quad (3.65)$$

By choosing to specify σ_1 along the boundary σ_{1R} can be calculated using equation (3.49) thus

$$\sigma_{1R} = \frac{\sigma_{1b} q_{R*}}{q_R} \quad (3.66)$$

In a similar way one can also impose that we know σ_1 at the pseudo cell centre ($j = 0$) and calculate σ_{1b} . It is important to note that it does not matter where σ_1 is specified so long as we can do so. For most purposes the boundary value for σ_1 will be taken at the free boundary.

3.2.4.2 Free Boundary Conditions

The free boundary conditions are imposed along the upper boundary along $\xi_2 = 1.0$. They are modelled using the following conditions within the upper pseudo cells $j = N+1$.

$$\begin{aligned} \rho_L &= \rho_R & p_L &= p_R & q_L &= q_R & \theta_R &= \theta_L \\ \sigma_{2R} &= \sigma_{2L} & S_L &= S_R & c_{\alpha L} &= c_{\alpha R} \end{aligned} \quad (3.67)$$

The subscripts L and R corresponds to the left and right states with cell centres $j = N+1$ and $j = N$ respectively. By choosing to specify σ_1 along the boundary we impose the simplifying assumption that it is constant defined by $\sigma_{1b} = 1.0$. The Riemann problem for this boundary produces no waves. Thus because of these uniform conditions we have $\sigma_{1L} = \sigma_{1R} = \sigma_{1b}$.

3.2.5 Sampling The Riemann Problem

For the frozen initial data all the Riemann problems are first solved. Using these solutions together with σ_1 defined along some boundary, σ_1 can be calculated along the normal from the boundary. Considering the initial data equation (3.7) and σ_1 known within the right state then by equation (3.49) we have the conditions

$$\begin{aligned} q_L \sigma_{1L} &= q_{L*} \sigma_{1*} \\ q_R \sigma_{1R} &= q_{R*} \sigma_{1*} \end{aligned} \quad (3.68)$$

since σ_1 is constant across the contact surface we have for the left state

$$\sigma_{1L} = \sigma_{1R} \frac{M_R}{M_{R*}} \frac{M_{L*}}{M_L} \sqrt{\frac{\eta_L \kappa_R}{\eta_R \kappa_L}} \quad (3.69)$$

The reverse of this is true if σ_1 had been specified along the free boundary. The positions of the waves within each RP can now be determined. Consider the j -th cell, figure 3.3, with waves propagating outwards. If $\theta_i < 1/2$ then the sampling point, equation (3.18), lies within RP($j-1,j$). For an expansion wave, figure 3.8, the head and tail of the fan is bounded by the points Ω_L and Ω_{L*} , which are fractions of $\Delta \xi_2$, defined by

$$\frac{\Omega_L \Delta \xi_2}{\Delta \xi_1} = \frac{\sigma_{1L}}{\sigma_{2L}} \tan \mu_{fL} \quad (3.70)$$

and

$$\frac{\Omega_{L*} \Delta \xi_2}{\Delta \xi_1} = \frac{\sigma_{1L*}}{\sigma_{2L*}} \tan \mu_{fL*} \quad (3.71)$$

If $\Omega_L \leq \theta_i$ the sampling point lies within the initial left state. The solution vector is therefore $U_{i+1,j} = U_L$ by equation (3.20).

If $\Omega_{L*} \geq \theta_i$ the sampling point lies within the left centred state. The solution vector is therefore $U_{i+1,j} = U_{L*}$. However, if $\Omega_{L*} < \theta_i < \Omega_L$ then the sampling point lies within the fan itself. The flow conditions at this point can be determined from the similarity equation

$$\frac{\theta_i \Delta \xi_2}{\Delta \xi_1} = \frac{\sigma_1}{\sigma_2} \tan \mu_f = \frac{\sigma_1 q}{\rho q \sigma_2} \rho_L \kappa_L \tan \mu_f \quad (3.72)$$

By using equations (3.25) and (3.26) this equation can be solved numerically in terms of pressure since $\sigma_1 q$ and $\rho q \sigma_2$ are constants. From the pressure all other values follow. Therefore $U_{i+1,j}$ will be equal to these solution values.

For an oblique shock wave, figure 3.8, the wave is bounded by Ω_L given by

$$\frac{\Omega_L \Delta \xi_2}{\Delta \xi_1} = \frac{\sigma_{1L}}{\sigma_{2L}} \tan \beta_L \quad (3.73)$$

If $\Omega_L \leq \theta_i$ the sampling point lies within the initial left state. The solution vector is therefore $U_{i+1,j} = U_L$. If $\Omega_L > \theta_i$ the sampling point lies within the left centred state. The solution vector is therefore the shocked conditions downstream thus $U_{i+1,j} = U_{L*}$.

If $\theta_i > 1/2$ then the sampling point, equation (3.18), lies within RP($j,j+1$). For an expansion wave, figure

3.9, the head and tail of the fan is bounded by the points Ω_R and Ω_{R*} which are defined by

$$\frac{\Omega_R \Delta \xi_2}{\Delta \xi_1} = -\frac{\sigma_{1R}}{\sigma_{2R}} \tan \mu_{fR} \quad (3.74)$$

and

$$\frac{\Omega_{R*} \Delta \xi_2}{\Delta \xi_1} = -\frac{\sigma_{1R*}}{\sigma_{2R*}} \tan \mu_{fR*} \quad (3.75)$$

If $\Omega_R \geq \theta_i - 1$ the sampling point lies within the initial right state. The solution vector is therefore $U_{i+1,j} = U_R$ by equation (3.21).

If $\Omega_{R*} \leq \theta_i - 1$ the sampling point lies within the right centred state. The solution vector is therefore $U_{i+1,j} = U_{R*}$.

However, if $\Omega_R < \theta_i - 1 < \Omega_{R*}$ then the sampling point lies within the fan itself. The flow conditions at this point can be determined from the similarity equation

$$\frac{(\theta_i - 1) \Delta \xi_2}{\Delta \xi_1} = \frac{\sigma_1}{\sigma_2} \tan \mu_f \equiv \frac{\sigma_1 q}{\rho q \sigma_2} \rho_R \kappa_R \tan \mu_f \quad (3.76)$$

By using equations (3.25) and (3.26) this equation can be solved numerically in terms of pressure since $\sigma_1 q$ and $\rho q \sigma_2$ are constants. From the pressure all other values follow. Therefore $U_{i+1,j}$ will be equal to these solution values.

For an oblique shock wave, figure 3.9, the wave is bounded by Ω_R given by

$$\frac{\Omega_R \Delta \xi_2}{\Delta \xi_1} = -\frac{\sigma_{1R}}{\sigma_{2R}} \tan \beta_R \quad (3.77)$$

If $\Omega_R \geq \theta_i - 1$ the sampling point lies within the initial right state. The solution vector is therefore $U_{i+1,j} = U_R$.

If $\Omega_R < \theta_i - 1$ the sampling point lies within the right centred state. The solution vector is therefore the shocked conditions downstream thus $U_{i+1,j} = U_{R*}$.

The vector of primitive variables for frozen conditions has now been updated for the new point downstream. We now must update the scaling factors. For σ_2 this is easily done by using the data from the sampled point together with the equation for mass conservation (2.29). However, σ_1 can not be updated so easily. To calculate it we must know the behaviour of $\partial \theta / \partial \xi_1$ along the new initial data line. This can only be done (ignoring finite difference techniques) by solving the RP's along the new initial data line.

For frozen flow field problems there is no problem since they are solved anyway in the next computational step. However, for chemical non-equilibrium, where a chemical step is performed before the next wave step, this can cause a problem. We discuss this aspect within the next section.

It will be apparent that even though cell centres are fixed within the computational space (ξ_1, ξ_2) they appear to move within physical space (s, n) or (x, y) . This is due to the position of the sampling point and the values of the scales at that point.

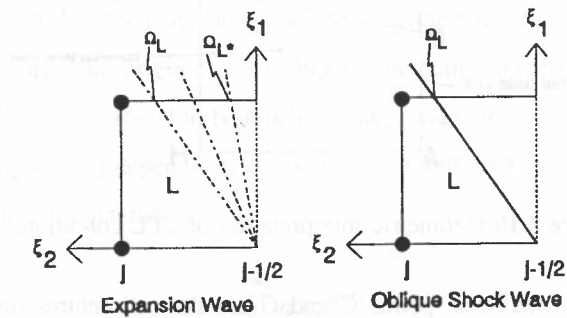


Figure 3.8 Sampling RP(j-1,j).

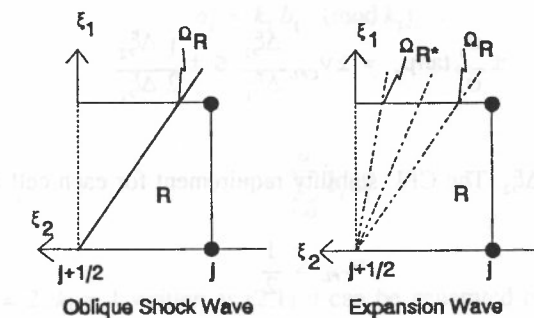


Figure 3.9 Sampling RP(j,j+1).

3.2.6 Courant-Friedrich-Lewy Condition For Stability

The CFL condition[29]¹³ for hyperbolic systems is the requirement that the domain of dependence of any numerical scheme, region AEG of figure 3.10, must contain the domain of dependence of the differential equations defined by region BDG. That is the Mach waves for the differential equations must have Mach angles which are less than or equal to the calculated Mach angles for the numerical scheme. Written mathematically as

¹³ English translation of original paper.

$$(\eta_s)_{\text{differential}} \leq (\eta_s)_{\text{numerical}} \quad (3.78)$$

where $\eta_s = \xi_2 / \xi_1$.

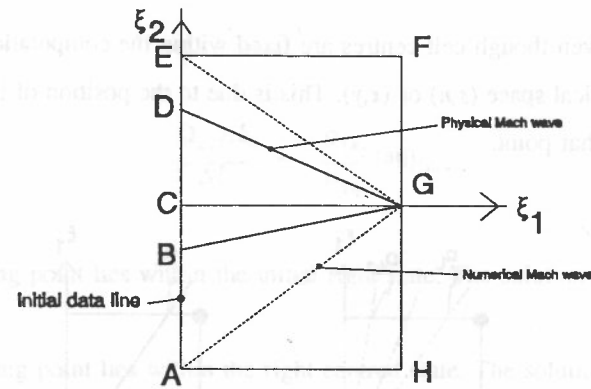


Figure 3.10 Geometric interpretation of CFL condition.

If AH, EF are the cell interfaces, points C and G are the cell centres then the above statement is equivalent to the requirement that waves emanating from the interfaces do not interact or cross each other downstream. Because $GF = +0.5 \Delta \xi_2$, $GH = -0.5 \Delta \xi_2$, $AH = EF = \Delta \xi_1$, and by using equations (3.78) and (2.56) we have the condition for each cell

$$\pm \frac{\sigma_1}{\sigma_2} \tan \mu_f = \pm v_{CFL} \frac{\Delta \xi_2}{\Delta \xi_1} \leq \pm \frac{1}{2} \frac{\Delta \xi_2}{\Delta \xi_1} \quad (3.79)$$

where v_{CFL} is some fraction of $\Delta \xi_2$. The CFL stability requirement for each cell is

$$v_{CFL} \leq \frac{1}{2} \quad (3.80)$$

The values for the scaling factors and Mach angle are based on the values at the cell centres and also those values calculated within the centred state. The maximum step size is given by

$$\Delta \xi_1 = v_{CFL} \Delta \xi_2 \frac{\sigma_2}{\sigma_1} \cot \mu_f \quad (3.81)$$

Because there are $N+2$ cell centres and $N+1$ RP's with generally different centred states the step size must be the minimum value based on all of them. For consistency we have included the conditions within the centred state because in various instances, such as shock waves, the Mach waves will have angles greater than those for the nodes. Whence

$$\Delta \xi_1 = v_{CFL} \Delta \xi_2 \min \left\{ \frac{\sigma_2}{\sigma_1} \cot \mu_f \right\} \quad (3.82)$$

3.2.7 Quasi-Random Number Series

The accuracy of the Random Choice Method can be controlled by the type of quasi-random number series used in the sampling procedure. The original quasi random (random numbers generated by computer) numbers used by Chorin[18,19] were found to be much less accurate than for Van der Corput series used by Colella[25]. The series $\theta_n \in [0,1]$ depends on the two prime numbers k_1 and k_2 such that $k_1 > k_2 > 0$. It can be defined in the following manner

$$\theta_n = \sum_{i=0}^m a_i k_1^{-(i+1)} \quad (3.83)$$

where

$$a_i = k_2 b_i \pmod{k_1} \quad (3.84)$$

and

$$n = \sum_{i=0}^m b_i k_1^i \quad (3.85)$$

For the binary series $k_1 = 2$, $k_2 = 1$ written as (2,1) it can be generated by the recursive relation

$$\Omega_2(n) = \begin{cases} \frac{1}{2} \Omega_2(n/2) & \text{for } n \text{ even,} \\ \Omega_2(n-1) + \frac{1}{2} & \text{for } n \text{ odd.} \end{cases} \quad (3.86)$$

with $\Omega_2(1) = 1/2$.

Anderson et al[2] has claimed to produce a new quasi-random series which improves on the accuracy of the Van der Corput series. The series can be generated by the recursive relation

$$\Omega_A(n) = \begin{cases} \frac{1}{2} \Omega_A(n/2) & \text{for } n \text{ even,} \\ 1 - \Omega_A(n-1) & \text{for } n \text{ odd.} \end{cases} \quad (3.87)$$

where $\Omega_A(1) = 1/2$. We test the claim later on in chapter four by performing a series of numerical tests and comparing the results to an analytic solution.

3.3 Solution of ODE's For Chemistry Step

For chemical non-equilibrium the calculated vector of primitive variables at each cell centre, using the RCM step, are the initial conditions for the chemical step equation (3.12). However, we also require knowledge of the distance over which these reactions are to take place. That is the effective streamline length. This distance will be very much dependent on the sampling point chosen within each RP of the wave step. To see this consider the example of a Prandtl-Meyer expansion fan within the RP, see figure 3.11. If the sampling point was placed at point B then the streamline will have a different length to that if it had been placed at point C. That is $\Delta s_{AB} \neq \Delta s_{AC}$. The streamline distance is given by equation (2.17) which can be approximated by the Trapezoidal rule as

$$\Delta s = \frac{1}{2}((\sigma_1)_{i,j} + \sigma_{1,p})\Delta\xi_1 \quad (3.88)$$

From this equation we observe that we need to know the predicted value of σ_1 , $\sigma_{1,p}$, at the new spatial position in addition to the predicted primitive variables; which we know. However, as we have seen earlier this means solving the RP's. This is going to be computationally expensive since we would need to solve two RP's, per cell, for each new spatial step downstream. To reduce this expense we purpose not to solve this additional RP, but assume that the predicted value of σ_1 is the same as its initial value. Therefore the streamline distance becomes

$$\Delta s = (\sigma_1)_{i,j}\Delta\xi_1 \quad (3.89)$$

The ordinary differential equations (3.12) are generally chemically *stiff*[57,75]. That is the distance over which chemical reactions take place will generally be very much smaller than the distance over which the flow field changes. This is represented by the Damkhöler number Da defined earlier. To integrate these equations numerically using an explicit scheme for convergence the step size must be based on the smallest distance i.e chemical distance. These schemes are conditionally convergent. If this distance is very small then the number of computational steps needed to reach a given point within the flow field can be extremely large. To overcome this an implicit numerical method can be used. These are unconditionally convergent. However, the accuracy of the scheme will be dependent on the coarseness of the mesh with respect to the smallest chemical distance. The solution of *stiff* equations goes back to Curtiss and Hirschfelder[31].

We use the numerical package LSODE[75] to solve these equations which has been developed from the highly successful method by GEAR, see Lambert[57, pages 112 and 242] for details, for stiff ODE problems. With these equations solved we repeat the above procedures until the desired position downstream is reached.

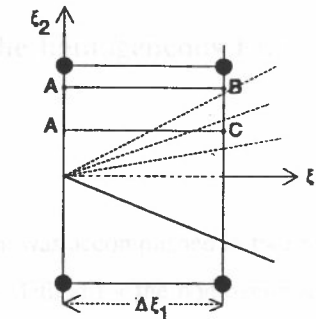


Figure 3.11 Two streamlines with different distances.

3.4 Co-ordinate Transformations

We have computed the flow field to the chosen point downstream ($\xi_1 = 1$) from the original initial data line at $\xi_1 = 0$. Therefore with solutions within computational space, in the form $f = f(\xi_1, \xi_2)$, we wish to convert these solutions to solutions in Cartesian co-ordinates $f = f(\xi_1(x, y), \xi_2(x, y)) = g(x, y)$. This can easily be done if the scaling factors and flow angle are known. To see this we integrate two of the metrics, equation (2.21), for (ξ_1, ξ_2) space as

$$\begin{aligned} x(\xi_1, \xi_2) &= \int_0^{\xi_1} \sigma_1 \cos \theta d\xi_1 + x(\xi_2) \\ y(\xi_1, \xi_2) &= \int_0^{\xi_1} \sigma_1 \sin \theta d\xi_1 + y(\xi_2) \end{aligned} \quad (3.90)$$

where we have assumed that $x(\xi_2)$ and $y(\xi_2)$ are calculated along the initial data line $\xi_1 = 0.0$. These equations can be written in discretized form

$$\begin{aligned} x_{i,j} &= x(\xi_1, \xi_2) = \int_0^{\xi_{1,i}} \sigma_1 \cos \theta d\xi_1 + x_{0,j} \\ y_{i,j} &= y(\xi_1, \xi_2) = \int_0^{\xi_{1,i}} \sigma_1 \sin \theta d\xi_1 + y_{0,j} \end{aligned} \quad (3.91)$$

with zero initial streamline angle within the freestream the right hand side of each of these equations have

Validation and Results for the homogeneous Euler Equations

Validation of the numerical algorithm was accomplished in two stages. The first, which we describe here, was to validate the Random Choice Method for the homogeneous Euler equations. This is equivalent to investigating chemically inert or frozen flow fields where the Damköhler number is negligible. The second stage, to be described in the next chapter, was the validation of the full numerical algorithm for the chemically modified Euler equations incorporating Lighthill's 'ideal dissociation gas' model for chemical non-equilibrium.

Where ever possible results are presented within the Cartesian co-ordinate space. However, where extra clarity becomes necessary the results are also presented within the natural co-ordinate space. The regions within which contour plots are presented have an aspect ratio of unity i.e. a square. This may create the illusion, where the true physical aspect ratio of the Cartesian space is $y/x < 1$, that the co-ordinate lines are non-orthogonal. The lines are indeed orthogonal throughout. Solution of the RP's was achieved using Mullers method with a tolerance of 10^{-6} throughout.

4.2 Validation of the Random Choice Method

$$N_w U = 0 \quad (4.1)$$

Four numerical tests were used to validate the method. The first three tests were based around the centred Prandtl-Meyer expansion wave and oblique shock wave. These two wave systems are fundamental to any inert high speed flow field and must be resolved accurately by the numerical method. Their

physical properties are such that there are exact analytic solutions from which to compare the numerical results. The fourth test was used to investigate the effectiveness of the non-reflecting boundary conditions. Finally, the numerical algorithm was tested against more complex configurations where exact/approximate analytic solutions exist but can only be generated from the governing equations numerically. These are described, and results given.

4.2.1 Centred Prandtl-Meyer Expansion Wave (Continuous solution)

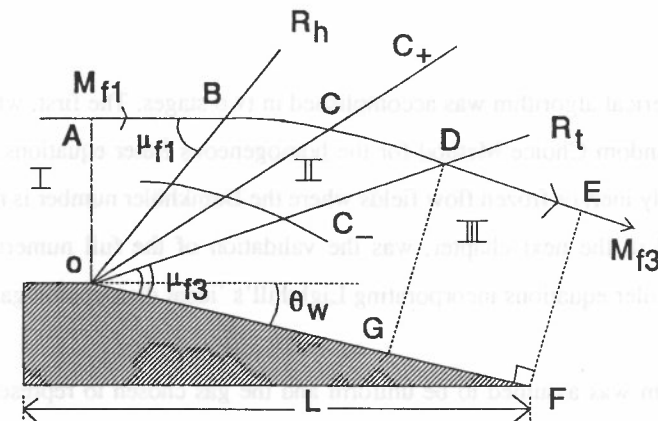


Figure 4.1 Centred Prandtl-Meyer Expansion Wave.

A Prandtl-Meyer expansion wave will be generated when ever a high speed flow passes over a sharp downward sloping wedge. Three regions can be identified, see figure 4.1. Region one is the un-disturbed freestream flow which is bounded by the head of the expansion wave R_h . Region two is where the flow field is expanded and region three is the final uniformly expanded state bounded by the tail of the expansion wave R_t . The downstream Mach number for region three can be calculated by solving (by numerical iteration) the C_- Riemann invariant (defined earlier). It is now a simple matter to calculate the pressure and density from the equation for conservation of total enthalpy along a streamline together with the equation of state for isentropic flow.

For region two $M_t \in [M_{f1}, M_{f3}]$ and for a given Mach number within this interval the flow variables can be determined using the above principles. However, the corresponding position along the streamline BD inside the fan remains unknown. The location can be calculated using equation (C.12) derived in appendix C. By using this equation the streamline positions for the corresponding flow variables can be calculated and are represented in tabular form as:

Point	Pressure	Density	Mach number	Streamline distance
A	p_1	ρ_1	M_{f1}	0.0
B	p_1	ρ_1	M_{f1}	AB
B→D	$p_3 \leq p \leq p_1$	$\rho_3 \leq \rho \leq \rho_1$	$M_{f1} \leq M \leq M_{f3}$	AB+Δs
D	p_3	ρ_3	M_{f3}	AD
E	p_3	ρ_3	M_{f3}	AD+OF-OG

where Δs is the streamline distance through the fan, OF is the length of the wetted surface downstream of wave. AD is just AB plus the result of Δs evaluated between the limits of M_{f1} and M_{f3} , and finally

$$AB = r_1 \cot(\mu_{f1}) ; OG = r_3 \cos(\mu_{f3}) \quad (4.2)$$

where from appendix C the radius for the tail of the expansion wave can be related to the head (region one) by:

$$\frac{r_3}{r_1} = \left[\frac{5 + M_{f3}^2}{5 + M_{f1}^2} \right]^3 \quad (4.3)$$

4.2.1.1 Validation #1

As was discussed in the last chapter the accuracy of the RCM can be controlled by the choice of quasi-random number series used. Due to the finite extent of the expansion wave one would expect to produce the greatest numerical fluctuations in the numerical solution within the expansion fan. The first validation was chosen to determine what affect the binary Van der Corput series (2,1) and the new series, starting at different integer values within each, had on the accuracy of the numerical solutions. To make an assessment of the error we define an error measurement based on the absolute of the error in streamline position (abbreviated APE) for fixed Mach number given by

$$APE = |s_n - s_a| \quad (4.4)$$

where the subscripts n and a refer to numerical and analytic solutions respectively. Through the expansion fan and for a given streamline ($\xi_2 = \text{constant}$) there corresponds an exact distance along the streamline for a given Mach number. By choosing the numerical Mach number and its corresponding numerical position

an exact analytic position can be calculated from equation (C.12) and the APE determined.

We choose four tests which were a combination of the frozen Mach numbers $M_{f1} = 2$ and 5 and flow deflection angles of $\theta_w = -10^\circ$ and -30° respectively. For each test we used both the binary Van der Corput and new series at different starting positions. The grid was fixed at 100 cells along ξ_2 and the CFL number at 0.4.

The boundary value for σ_1 was chosen to be unity along the upper boundary $\xi_2 = 1$, so that it would be unity within the freestream. Analytic values for the pressure, density, Mach number etc for region three were calculated and are given by:-

$$M_{f1} = 2 ; \theta_w = -10^\circ$$

$$p_3 / p_1 = 0.54797 ; \rho_3 / \rho_1 = 0.65072 ; M_{f3} = 2.3849 ; \sigma_{1,3} = 0.91387 ; \sigma_{2,3} = 1.4044$$

$$M_{f1} = 2 ; \theta_w = -30^\circ$$

$$p_3 / p_1 = 0.12387 ; \rho_3 / \rho_1 = 0.22497 ; M_{f3} = 3.3683 ; \sigma_{1,3} = 0.80019 ; \sigma_{2,3} = 3.5569$$

$$M_{f1} = 5 ; \theta_w = -10^\circ$$

$$p_3 / p_1 = 0.24848 ; \rho_3 / \rho_1 = 0.36989 ; M_{f3} = 6.2974 ; \sigma_{1,3} = 0.96871 ; \sigma_{2,3} = 2.618929$$

$$M_{f1} = 5 ; \theta_w = -30^\circ$$

$$p_3 / p_1 = 3.6179E-03 ; \rho_3 / \rho_1 = 0.018032 ; M_{f3} = 12.021747 ; \sigma_{1,3} = 0.928527 ; \sigma_{2,3} = 51.494129$$

Results for the numerical runs can be viewed in figures 4.11 - 4.34. A careful inspection of them reveals that the new series does not produce any marked improvement in the accuracy of all the results through the wave positions and flow field profiles. Like the Van der Corput series the starting position within the series has a clear affect on the apparent accuracy of the results generated. Therefore by choosing the starting point carefully one can get the *best* results for the specific problem. This effect can be viewed in figures 4.35 - 4.36 where four different starting positions within the Van der Corput series have been used to highlight this aspect. A similar study for the one dimensional unsteady RCM was performed by Toro[93].

One should mention that Δn , the physical distance between cell centres, does not remain fixed but depends on σ_2 through $\Delta n = \sigma_2 \Delta \xi_2$. Through the expansion fan adjacent streamlines move apart with the physical spacing between cells Δn becoming larger and the mesh coarser. This will have the affect of reducing the accuracy of the numerical results within these regions. In the most severe of the tests investigated ($M_{f1} = 5$, $\theta_w = -30^\circ$) the adjacent streamlines close to the wall move apart by over 51 times their original value. One must base any measurement on the accuracy of the numerical results on the coarsest part of the computational mesh or where σ_2 is the largest!

4.2.1.2 Validation #2

The four test cases were again used, together with the series producing the most accurate results, to investigate to what extent the numerical mesh needs to be refined to obtain *good* results. The term *good* is used to mean that the results match the analytic solution closely. The CFL number was again fixed at 0.4 throughout. The meshes used to resolve the flow field features and the time taken for completion of each run (stopped at the value $\xi_1 = 1$) are preserved in table 4.2.

Table 4.2

$M_{f1}=2$	Grid $\xi_1 \times \xi_2$		CPU Time h:m:s		Maximum no. of cells within region 3	
	Coarse	Fine	Coarse	Fine	Coarse	Fine
$\theta_w = -10^\circ$	162x100	803x500	0:0:52.9	0:19:58.7	30	150
$\theta_w = -30^\circ$	210x100	1,043x500	0:1:36.1	0:37:19.1	7	35
$M_{f1}=5$						
$\theta_w = -10^\circ$	55x100	269x500	0:15.1	0:4:04.5	6	30
$\theta_w = -30^\circ$	953x1,500	2,857x4,500	0:51:10.2	7:21:10.6	2	7

The numerical results are to be found in figures 4.37 - 4.42. It is clear that by increasing the Mach number for a fixed flow deflection angle, the mesh must be refined to resolve the flow field features. This is because the angular extent of the fan diminishes (i.e. closes up). The tail of the fan shifts towards the downstream boundary $\xi_2 = 0$ with a subsequent loss in the number of cells resolving it in region three. For the coarse meshes used for $M_{f1} = 2$ and 5 and deflection $\theta_w = -10^\circ$, the maximum number of cells within region three is seen to reduce from thirty to six for the increase in the Mach number. The coarse mesh is seen to resolve the field of flow for case of $M_{f1} = 2$ and deflection $\theta_w = -10^\circ$ accurately, figure 4.37, while we need to use a finer mesh for $M_{f1} = 5$ with the same deflection angle, figure 4.39. The finer mesh increases the maximum number of cells within region three to thirty with the flow field now resolved. However, the penalty for this increase in accuracy was an increase in the CPU time by over sixteen times.

For a fixed Mach number and by increasing the flow deflection angle the tail of the expansion fan moves towards the downstream boundary due to the increase in the frozen Mach number and a subsequent reduction in the frozen Mach angle. The distance between adjacent streamlines increases due to the decrease in the density of the gas. The increase has the effect of making the effective computational mesh

coarser downstream. This has the undesirable feature of reducing the maximum number of cells to be found in region three. It can be clearly seen from table 4.2 that for $M_{f1} = 2$ with the deflections of $\theta_w = -10^\circ$ and $\theta_w = -30^\circ$ the number of cells has been reduced, for the coarse mesh, from thirty to seven respectively. For the most severe of the test cases good resolution was only achieved using a mesh of 4,500 cells with the CPU time well in excess of seven hours! This is due to the tail of the expansion fan being very close to the downstream boundary with the frozen Mach angle $\sim 4.77^\circ$ and more importantly the streamlines close to the wall had increased by over fifty one times there original value!

From the results we conclude that for combinations of either large Mach numbers and/or large flow deflections the field of flow can only be resolved at the expense of an increase in the CPU time due to the fineness of the meshes used. One must look towards some adaptive mesh refinement where the distance between adjacent streamlines becomes large.

Finally the numerical boundaries of the expansion wave, using the fine meshes, are compared with their analytic counterpart in figures 4.43 - 4.44. The randomness present in the method can be seen in the numerical results with the solution fluctuating about the analytic solution. However, there is generally good agreement for all the cases considered.

4.2.2 Oblique shock Wave (Discontinuous Solution)

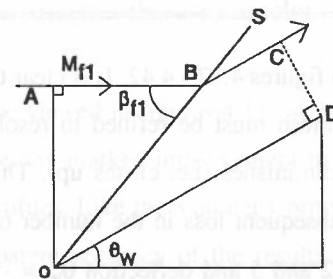


Figure 4.2 Frozen oblique shock wave.

Where ever there is a sharp, discontinuous deflection of a high speed flow field an oblique shock wave is generated across which the flow variables increase discontinuously. For an inert, polyatomic gas the conditions downstream of the wave are determined using the Rankine-Hugoniot relations, see appendix E. For a given height above the wedge OA, shock wave angle β_{f1} , flow deflection angle θ_w , and the boundary length OD, the streamline distances AB, BC can be calculated. An analytic solution to the problem can be formulated and is represented in tabular form as

Table 4.3

Point	Pressure	Density	Mach number	Streamline distance
A	p_1	ρ_1	M_{f1}	0.0
B	p_1	ρ_1	M_{f1}	AB
B	p_2	ρ_2	M_{f2}	AB
C	p_2	ρ_2	M_{f2}	AC

where

$$AB = OA \cot(\beta_{f1}) \quad (4.5)$$

and

$$AC = OD + OA \left(\cot(\beta_{f1}) - \frac{\cos(\beta_{f1} - \theta_w)}{\sin \beta_{f1}} \right) \quad (4.6)$$

4.2.2.1 Validation #3

As with validation #1 we investigate the effect of the two quasi-random number series' on the accuracy of the numerical results generated for an oblique shock wave. We choose as the tests a positive flow deflection angle of 30° produced by a wedge and four different initial freestream Mach numbers ranging from supersonic up to hypersonic ($M_{f1} = 3, 5, 10$ and 25 respectively). The boundary value for σ_1 was again chosen to be unity along the upper boundary. Typical analytic values for pressure, density, oblique shock wave angle etc for the different freestream Mach numbers are:

$$M_{f1} = 3$$

$$p_2 / p_1 = 6.3558 ; \rho_2 / \rho_1 = 3.1673 ; M_{f2} = 1.4059 ; \sigma_{1,3} = 1.5064$$

$$\sigma_{2,3} = 0.4756 ; \beta_{f1} = 52.014^\circ ; \Delta S = 0.5883$$

$$M_{f1} = 5$$

$$p_2 / p_1 = 13.0667 ; \rho_2 / \rho_1 = 4.16434 ; M_{f2} = 2.1364 ; \sigma_{1,3} = 1.32124$$

$$\sigma_{2,3} = 0.31727 ; \beta_{f1} = 42.340^\circ ; \Delta S = 1.4322$$

$$M_{f1} = 10$$

$$p_2 / p_1 = 45.0785 ; \rho_2 / \rho_1 = 5.31478 ; M_{t2} = 2.7156 ; \sigma_{1,3} = 1.2644$$

$$\sigma_{2,3} = 0.23791 ; \beta_{t1} = 38.520^\circ ; \Delta S = 3.6743$$

$$M_{t1} = 25$$

$$p_2 / p_1 = 269.118 ; \rho_2 / \rho_1 = 5.87278 ; M_{t2} = 2.9592 ; \sigma_{1,3} = 1.2480$$

$$\sigma_{2,3} = 0.21251 ; \beta_{t1} = 37.420^\circ ; \Delta S = 7.7917$$

The computational grid was fixed at a hundred cells and the CFL number remained at 0.4 throughout. The number of nodes needed to reach the end of the wedge surface OD ($\xi_1 = 1$), see figure 4.2, and the time taken for completion of each run can be found in table 4.4 below. It is apparent from the table that for the higher Mach numbers the CPU time has increased considerable. This is because the numerical step size $\Delta \xi_1$ has been reduced by the CFL condition; see earlier definition. The step size is inversely proportional to the Tangent of the largest Mach angle subtended by the Mach waves in the (ξ_1, ξ_2) co-ordinate space. By increasing the freestream Mach number the downstream Mach angle increases, due to the decrease in the Mach number, with a subsequent decrease in the numerical step size and increase in CPU time.

Comparison between the numerical and analytic shock wave positions together with the absolute of the shock wave positional error are shown in figures 4.45 - 4.50. The analytic and numerical flow variable profiles are compared for one specific streamline position ($\xi_2 = 0.195$) in figures 4.51 - 4.56. As for the expansion wave the choice of series and starting position within it will have an overall effect on the numerical results. For the four cases considered Anderson's series starting at $n = 1$ produced the best matching shock wave positions and lowest positional error, figure 4.45. Upon inspection of the corresponding flow field profiles the values are found to be in excellent agreement, and this is apparent for all the profiles no matter which series was used. This should not come as a complete surprise since we are using, locally within each cell, an exact Riemann solver and its solution will not be affected by the choice of the series.

TABLE 4.4

M_{t1}	ξ_1 nodes	CPU h:m:s
3	540	0:2:52.7
5	416	0:4:29.7
10	1,967	0:17:22.8
25	3,560	0:31:28.1

4.2.3 Validation #4

The last validation was used to determine the effectiveness of the upper boundary conditions used by letting either an expansion or oblique shock wave impinge onto them and observing the effect on the downstream flow field. The first test was to use an expansion wave generated from a freestream Mach number of $M_{t1} = 3$ deflected by angle $\theta_w = -10^\circ$. The full wave, head and tail, was allowed to encroach the boundary. The pressure history for the numerical experiment can be viewed as a three dimensional surface contour plot in figure 4.3. One can immediately pin point the freestream where the pressure is constant and non-dimensional value unity, the head and tail for the expansion wave between which the pressure diminishes, and the downstream uniform state. The presence of any secondary waves would cause the downstream contours to ripple and this is not evident from the figure.

An oblique shock wave, generated from a freestream Mach number of $M_{t1} = 3$ and deflection angle $\theta_w = 10^\circ$, was allowed to impinge onto the boundary. The numerical results for the experiment can be found in figure 4.4. The step between the two regions can be seen. Again there is no evidence for any secondary waves coming off the boundary.

From the two tests considered the boundary conditions appear to be non-reflecting and are adequate for the inert field of flow.

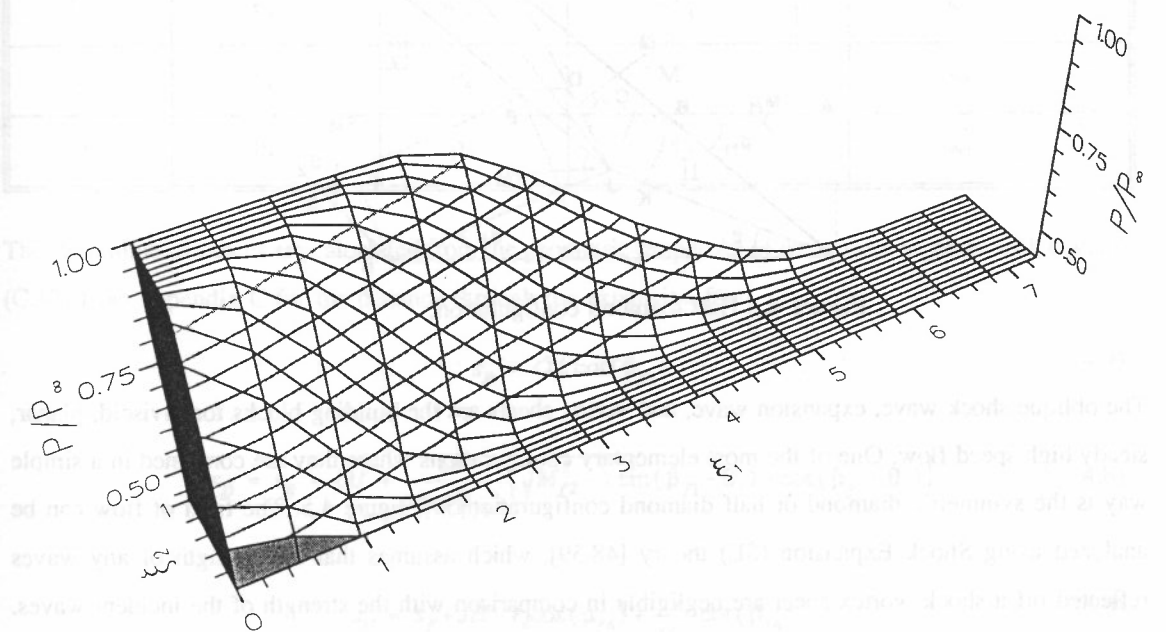


Figure 4.3 Expansion wave impinging onto the upper boundary.

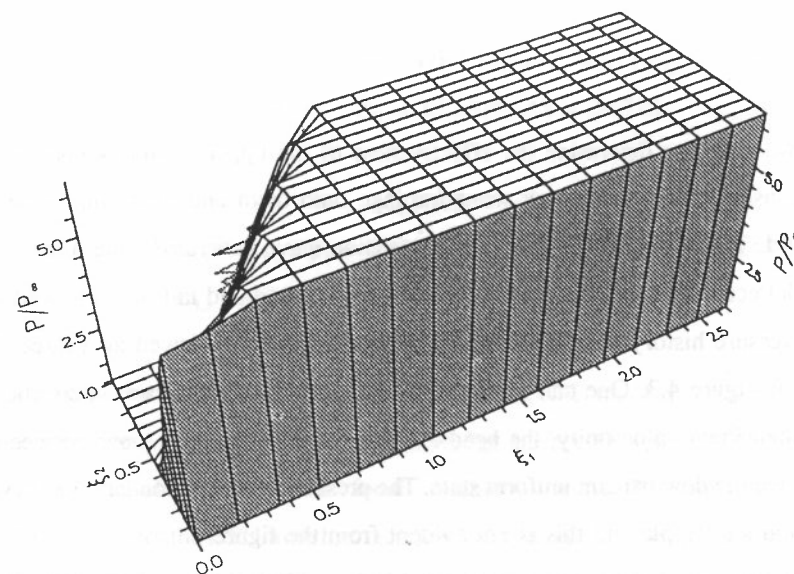


Figure 4.4 Oblique Shock Wave impinging onto the upper boundary.

4.3 Half Diamond Configuration

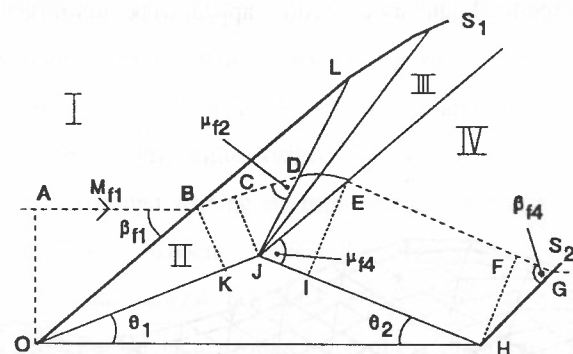


Figure 4.5 Half diamond configuration.

The oblique shock wave, expansion wave, and vortex sheets are the building blocks for inviscid, planar, steady high speed flow. One of the most elementary configurations where they are combined in a simple way is the symmetric diamond or half diamond configuration[59], figure 4.5. The field of flow can be analyzed using Shock Expansion (SE) theory [48,59], which assumes that the strength of any waves reflected off a shock, vortex sheet are negligible in comparison with the strength of the incident waves. An approximate analytic solution for the configuration can be calculated, numerically, in a straight forward way. The accuracy of the solution will be very much dependent on the strength of any reflected waves present within the flow field. One of the main sources of such waves will come from the interaction of the expansion wave with the leading oblique shock wave. The interaction will cause the shock wave to weaken with a small percentage of the incident wave reflecting back towards the body surface. A local reflection coefficients R_s at the leading shock wave, defined as the ratio of the pressure difference across

the reflected wave to the difference across the incident wave, can be calculated and this was used to give an indication of the strength of the actual waves reflected from the leading shock, see Eggers et al[35]. A algorithm was written to calculate these coefficients for several different Mach numbers and flow deflection angles. These are plotted in figure 4.7. As a first approximation we assume that the strength of the reflected waves at the leading shock wave are negligible from which an analytic solution can be derived and is written in tabular form as:

Table 4.5

Point	pressure	density	Frozen Mach number	Streamline distance
A	p_1	ρ_1	M_{f1}	0.0
B	p_1	ρ_1	M_{f1}	s_B
B	p_2	ρ_2	M_{f2}	s_B
D	p_2	ρ_2	M_{f2}	s_D
D→E	$p_4 \leq p \leq p_2$	$\rho_4 \leq \rho \leq \rho_2$	$M_{f4} \leq M_f \leq M_{f2}$	$s_D + \Delta s$
E	p_4	ρ_4	M_{f4}	s_E
G	p_4	ρ_4	M_{f4}	s_G
G	p_5	ρ_5	M_{f5}	s_G

The streamline distances are calculated from the geometric properties of the system together with equation (C.12) from appendix C for the distance through the expansion fan:

$$s_B = OA \cot(\beta_{f1}) \quad (4.7)$$

$$s_D = s_B + OJ + \frac{OA}{\sin(\beta_{f1})} \left\{ \sqrt{M_{f2}^2 - 1} \sin(\beta_{f1} - \theta_1) - \cos(\beta_{f1} - \theta_1) \right\} \quad (4.8)$$

$$s_G = s_E + JH - r_4 \cos(\mu_{f4}) + \frac{r_4}{M_{f4}} \cot(\beta_{f4}) \quad (4.9)$$

$$\frac{r_4}{r_2} = \left(\frac{1 + \frac{\gamma-1}{2} M_{f4}^2}{1 + \frac{\gamma-1}{2} M_{f2}^2} \right)^{\frac{\gamma+1}{2(\gamma-1)}}; r_2 = \frac{OA M_{f2} \sin(\beta_{f1} - \theta_1)}{\sin \beta_{f1}} \quad (4.10)$$

where OJ, JH, and OH are the lengths of the front, back and base of the diamond respectively. The former two are equal and have the value $\{2 \cos(\theta_1)\}^{-1}$, while the latter has the value of unity. β_{f1} and β_{f4} can be calculated by solving the two equations

$$\tan(\theta_1) = 2 \cot \beta_{f1} \left(\frac{M_{f1}^2 \sin^2 \beta_{f1} - 1}{M_{f1}^2 (\gamma + \cos(2\beta_{f1})) + 2} \right) \quad (4.11)$$

$$\tan(\theta_2) = 2 \cot \beta_{f4} \left(\frac{M_{f4}^2 \sin^2 \beta_{f4} - 1}{M_{f4}^2 (\gamma + \cos(2\beta_{f4})) + 2} \right) \quad (4.12)$$

respectively. The Mach numbers M_{f2} and M_{f5} are calculated from the oblique shock wave relations, and M_{f4} by solving the Riemann invariant for the C_- characteristic together with M_{f2} and the deflection angle $(\theta_1 - \theta_2)$. From these values the pressures and densities for the respective regions follow. The calculation of the wave positions bounding the uniform regions can now be calculated from the above information. Beyond point L, figure 4.5, where the expansion first interacts with the leading shock wave, the shock wave loses its simple linear positional variation due to its weakening. The shock wave angle will now be a function of position $\beta_n = \beta_n(x)$ and its profile $y = f(x)$ will generally not be known in advance. By using SE theory an approximate profile can be determined using a number of piecewise linear functions. Thus in the interval $x \in [x_i, x_{i+1}]$ we have the functional form

$$\left. \begin{aligned} \beta_i &= \beta_{f1}(x) \\ y &= f_i(x) = x \tan \beta_i + c_{s,i} \end{aligned} \right\} i=0, 1, \dots, N \quad (4.13)$$

where N is the total number of functions used in the interval $[x_0, x_N]$ (the distance x_N is unknown), β_i and $c_{s,i}$ are unknown for $i \geq 1$, with $c_{s,i}$ a constant.

The functions are not independent of each other. For a typical point x_{i+1} we have the condition

$$y_{i+1} = f_i(x_{i+1}) = f_{i+1}(x_{i+1}) \quad (4.14)$$

we must also specify a starting point from which to begin the calculation. Since the leading shock wave begins at the point $x_0 = y_0 = 0$ and has initial shock angle $\beta_0 = \beta_n$ we can define the starting condition $c_{s,0} = 0$.

To determine the discrete shock wave angles β_i we make the simplifying assumption that both the pressure and the flow deflection angle δ remains constant along the C_+ characteristics. Therefore the characteristics are un-deflected by the presence of the entropy layer caused by the weakening of the shock, figure 4.6. A local reflection coefficient R_v can be defined[48] and is found only to be positive with the effect that the waves remain of the same type upon reflection. One should note that by including these reflections and ultimately the deflection of the transmitted waves the shock wave would be found to be

weaker than that calculated using the above approximations.

A general equation for the leading characteristics with appropriate boundary conditions can be written as

$$y = (x-1/2) \tan(\delta_i + \mu_{f3,i}) + 1/2 \tan \theta_1 \quad (4.15)$$

where $\delta_i \in [\theta_2, \theta_1]$, $\mu_{f3,i} \in [\mu_{f2}, \mu_{f4}]$ with the starting conditions $\delta_0 = \theta_1$ and $\mu_{f3,0} = \mu_{f2}$.

Combining this equation with equation (4.13) yields an equation for the new x co-ordinate x_{i+1} in terms of the old co-ordinates and wave angles

$$\left. \begin{aligned} x_{i+1} &= \frac{1}{2} \frac{(\tan \omega_i - \tan \theta_1) + y_i - x_i \tan \beta_i}{\tan \omega_i - \tan \beta_i} \\ \omega_i &= \delta_i + \mu_{f3,i} \end{aligned} \right\} i \geq 0 \quad (4.16)$$

where, for the Mach number $M_{f3,i} \in [M_{f2}, M_{f4}]$, the deflection angle δ_i was derived from the C_- Riemann invariant

$$\delta_i = \theta_1 + v(M_{f2}) - v(M_{f3,i}) \quad (4.17)$$

and the pressure along each C_+ characteristic from

$$\frac{p_{3,i}}{p_1} = \frac{p_2}{p_1} \left(\frac{1 + \frac{\gamma-1}{2} M_{f2}^2}{1 + \frac{\gamma-1}{2} M_{f3,i}^2} \right)^{\frac{\gamma}{\gamma-1}} \quad (4.18)$$

with the starting condition $p_{3,0} = p_2$. The leading shock wave angle can be calculated from the pressure using the shock wave relation:

$$\beta_i = \sin^{-1} \left(\frac{\sqrt{\left(\frac{p_{3,i}}{p_1} - 1 \right) \frac{\gamma+1}{2\gamma}} + 1}{M_{f1}} \right) \quad (4.19)$$

By substituting equations (4.17) to (4.19) into (4.16) and for a known value of $M_{f3,i}$, x_{i+1} can be calculated from equation (4.16) and finally y_{i+1} from the equation

$$y_{i+1} = (x_{i+1} - x_i) \tan(\beta_i) + y_i ; i \geq 0 \quad (4.20)$$

The calculation proceeds until the desired distance x_N has been reached.

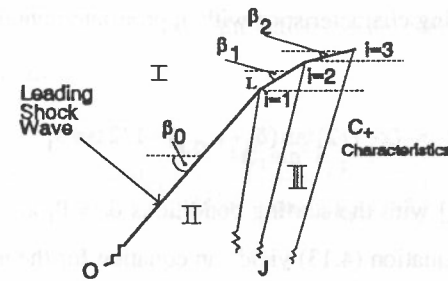


Figure 4.6 Approximate Shock Profile.

Numerical tests were designed to determine the usefulness of SE theory when the strength of the reflected waves becomes large. Two freestream Mach numbers were chosen ($M_\infty = 5, 15$) to produce respectively small and large local leading shock wave reflection coefficients with the half diamond deflection angles of $\theta_1 = 10^\circ$ and $\theta_2 = -10^\circ$.

Coarse and fine meshes were used to demonstrate the extent of grid fineness and CPU time required to resolve the essential flow field features, see table 4.6. The numerically generated profiles are compared with their corresponding analytic counterpart in figures 4.57 - 4.60. As was stated earlier the position along which the boundary condition for σ_1 can be specified was arbitrary. To confirm this assumption we purpose two further numerical tests by specifying the boundary condition for σ_1 at two different positions within the flow field. Thus the numerical data in figures 4.57 - 4.58 was calculated using the boundary condition for σ_1 chosen to have a value of unity along the solid boundary at $\xi_2 = 0$, and for those in figures 4.59 - 4.60, it was specified to have the value unity along the upper boundary at $\xi_2 = 1$ (table 4.5 applies to this case only). It is clear from the four figures that for the coarser meshes used the choice does have an affect on positional accuracy of the numerical flow variable profiles. One would expect that as the mesh is refined this discrepancy disappears and earlier assumption confirmed. This is indeed confirmed when the results for the fine meshes are examined. However, there is a clear difference between the profiles calculated for σ_1 . For figures 4.59 - 4.60, σ_1 appears to diminish after the trailing shock wave. Because σ_1 is calculated, downwards, from the position $\xi_2 = 1$ it first increases from unity across the leading shock wave. Passing through the expansion wave it decreases and then, finally, increases again across the trailing shock wave. However, the weakening of the leading shock wave subsequently influences the final outcome of σ_1 downstream of the trailing shock wave causing it to decrease.

Finally a comparison was made between the numerical and analytic solutions for the spatial wave positions and leading shock wave strengths, see figures 4.61 - 4.62. For $M_\infty = 5$, figure 4.61, there is excellent agreement between the numerical and analytic wave positions. The analytic leading shock wave strength appears to be stronger initially than the numerical shock strength. This confirms that the incident waves are indeed reflected off the entropy layer. Thus the numerical shock strength is initially weaker than the analytical solution as we have ignored these reflections. The numerical shock strength is observed to increase past the analytic value. From figure 4.7 the local reflection coefficient for $M_\infty = 5$ is observed

to be low and negative for $\theta_1 = 10^\circ$ with the effect that the incident expansion wave is reflected as a compression wave of very low strength. Due to the increase in the pressure across the reflected waves the true leading shock wave strength will be observed to increase and become stronger than that calculated using SE theory. This is observed in figure 4.61. The increase is small confirming the smallness of the strength of the reflected waves. In this instance SE theory clearly provides an accurate description of the flow field.

For $M_\infty = 15$ the numerical leading shock position is observed to deviate upwards after interacting with the expansion wave, implying that it is becoming stronger, from that calculated using SE theory, see figure 4.62. On inspection of figure 4.7 it is observed that the local reflection coefficient for $\theta_1 = 10^\circ$ is negative but magnitude much larger than for the earlier case. Therefore the influence of the reflected compression waves will be much greater causing the true leading shock wave strength to deviate greatly from that calculated using SE theory. This is clearly confirmed in figure 4.62. Hence in this instance the usefulness of SE theory has diminished.

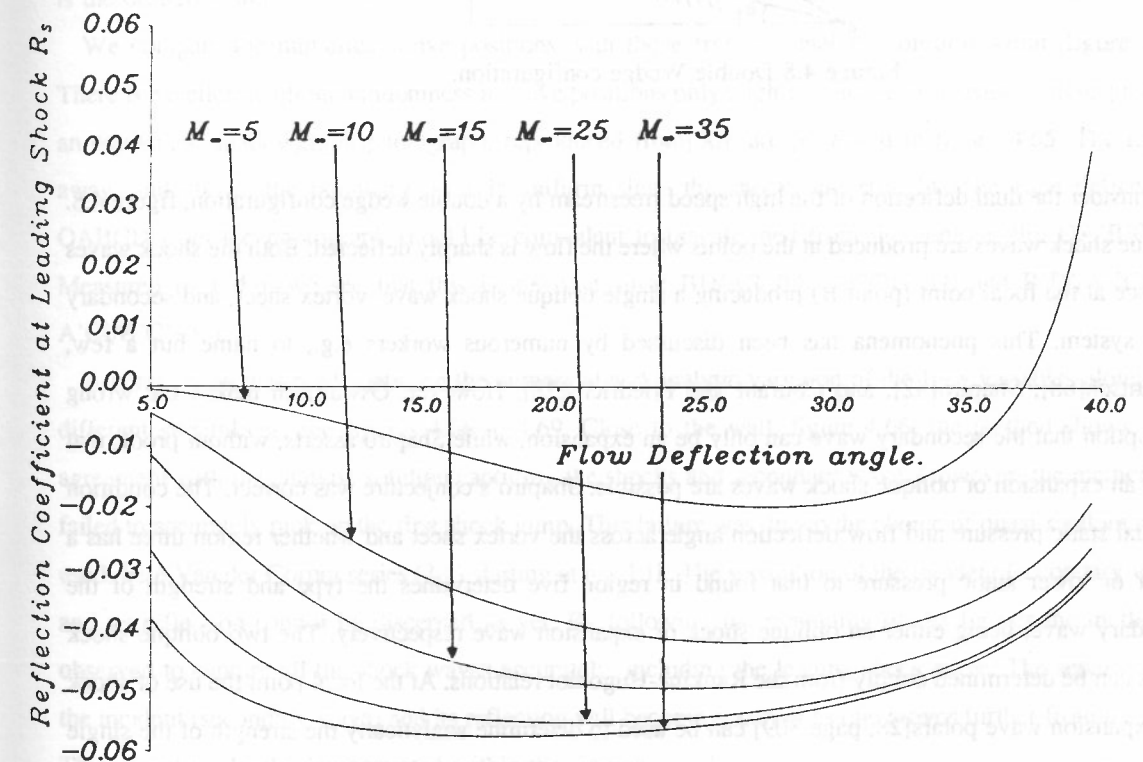


Figure 4.7 Calculated reflection coefficients for $\gamma = 1.4$

TABLE 4.6

M_{f1}	Grid $\xi_1 \times \xi_2$	CPU h:m:s	Grid $\xi_1 \times \xi_2$	CPU h:m:s
5	824x100	0:9:33	4,111x500	3:50:45
15	2,683x500	2:31:51	8,110x1,500	22:54:55

4.5 Double Wedge

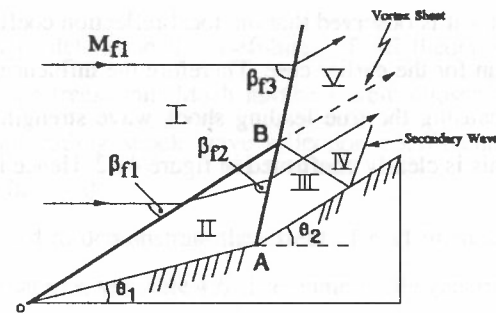


Figure 4.8 Double Wedge configuration.

We consider the dual deflection of the high speed freestream by a double wedge configuration, figure 4.8. Oblique shock waves are produced at the points where the flow is sharply deflected. Both the shock waves coalesce at the focal point (point B) producing a single oblique shock wave, vortex sheet, and secondary wave system. This phenomena has been discussed by numerous workers e.g., to name but a few, Oswatitsch[68], Shapiro[82], and Courant and Friedrichs[28]. However, Oswatitsch makes the wrong assumption that the secondary wave can only be an expansion, while Shapiro asserts, without proof, that either an expansion or oblique shock waves are possible. Shapiro's conjecture was correct. The condition of equal static pressure and flow deflection angle across the vortex sheet and whether region three has a higher or lower static pressure to that found in region five determines the type and strength of the secondary wave; being either an oblique shock or expansion wave respectively. The two oblique shock waves can be determined simply from the Rankine-Hugoniot relations. At the focal point the use of shock and expansion wave polars[28, page 309] can be used to determine analytically the strength of the single oblique shock wave and the type of the secondary wave. It is interesting to note the successful application of the double wedge into supersonic engine intakes[81]. Also under special circumstances during re-entry of the space shuttle into the Earth's atmosphere the flow interacts with the wing and fuselage to produce the above two shock phenomena[11].

We choose the flow deflection angles of $\theta_1 = 8^\circ$, $\theta_2 = 19^\circ$ with the initial Mach number $M_{f1} = 7.4$. These conditions are taken from the experimental investigation of the double wedge by Crane and Woodley[30].

The number of cells was fixed at 200 and CFL number at 0.4. The number of ξ_1 nodes was 2526 and CPU time approximately 47 Minutes 27 Seconds. The base of the double wedge was chosen to be unity with the second flow deflection occurring half way along it from the leading edge. The CPU time was found to be 132 seconds. Shock wave polars are calculated for the two oblique shocks, see left hand plot in figure 4.63. The first polar, labelled S_1 , was calculated using the initial freestream conditions. For the first flow deflection the pressure downstream of the leading shock wave can easily be read off the polar. This was then used as the starting condition for the second polar, labelled S_2 . For the second flow deflection, the pressure downstream of the second shock wave can be read off. It is clear that the pressure increase across the two shock waves is greater than that for a single shock wave for the same flow deflection. Thus across the secondary wave, which must be an expansion wave, there must be a pressure drop to the pressure downstream of the single shock wave. The line AB, figure 4.63, is the expansion wave polar connecting the two shock polars; where point A is the initial pressure within region three and point B the pressure across the expansion wave and single shock wave for the same flow deflection, which is the desired result.

We compare the numerical wave positions with those from an analytic solution within figure 4.64. There is excellent with the randomness in wave positions only slightly evident. A density contour plot and an equivalent shadowgraph photograph, reproduced from[30], are presented in figure 4.65. The region away, and above, the boundary layer is uniform since the shocks are straight. The zone defined by OABCD from the photograph should be equivalent to that defined from the contour plot OA'B'C'D'. Measured to 1 d.p. we see that this is the case since $BD/AB \sim 0.8$, $AC/BC \sim 3.0$ and $B'D'/A'B' \sim 0.8$, $A'C'/B'C' \sim 3.0$.

A comparison was made between the numerical and analytic variation of the flow variables along four different streamlines, see figures 4.66 to 4.69. Close to the wall, figure 4.66, the method shows good agreement with the analytic solution capturing the shocks and secondary wave. However, the method has failed to accurately pick up the first shock jump. This failure was due to the choice of quasi-random series used; here Van der Corput series (2,1) starting at $n = 101$. The separation of the incident (secondary wave) and its reflection cannot be discerned as yet. By following the remaining of the figures the method is observed to capture all the shock waves accurately, including the leading shock wave. The separation of the incident (secondary wave) and its reflection will become apparent as one moves further from the wall. This aspect is clearly demonstrated within the figures.

4.6 Compressive Surface

We investigate the behaviour of the flow field when it is compressed continuously, up to some predetermined deflection angle, by a smooth compressive turn. The flow is isentropic near the wall with the Mach waves (C_+ characteristics) propagating outwards which gradually coalesce forming an oblique

shock wave. The locus of the points representing the interaction of the characteristics defines an envelope with cusp specifying the point where the shock is born with zero strength. The characteristics can be represented in parametric form[28] by the expression

$$y = x \tan\{\omega(\beta)\} + \xi(\beta), \quad \omega(\beta) = \theta(\beta) + \mu_f(\beta) \quad (4.21)$$

where $\omega \in [\omega_{f1}, \omega_{f3}]$. At the envelope the derivative of y with respect to β vanishes so that

$$x = -\frac{d\xi}{d\omega}, \quad y = \xi - \omega \frac{d\xi}{d\omega} \quad (4.22)$$

here ω has been used instead of β as the parameter as long as $\omega_p \neq 0$. If the functional form for the compressive turn is known, i.e. $y = f(x)$, and its first and second derivatives are defined and continuous, an expression for the envelope can simply be derived in terms of the co-ordinates for the local body surface $(x_b, y_b = f(x_b))$, from equation (4.21), as

$$x_e = \frac{2}{\gamma+1} \frac{M_f^2 - 1}{M_f^4 \theta_x} \left\{ \sqrt{M_f^2 - 1} - \tan\theta \right\} \cos(2\theta) + x_b, \quad y_e = (x_e - x_b) \tan(\omega) + f(x_b) \quad (4.23)$$

where θ, θ_x are the respective local values for the flow deflection angle and curvature of the body surface. The flow field variables and Mach angles are calculated for the local body position by solving the Riemann invariant for the C_- characteristics. At the leading edge where $\theta = 0, x_b = y_b = 0$ equation (4.23) reduces to the simple form

$$x_e = \frac{2}{\gamma+1} \frac{(M_f^2 - 1)^{3/2}}{M_f^4 \theta_x}, \quad y_e = x_e \tan(\omega_1) \quad (4.24)$$

which is the result obtained by Johannesen[54].

For our investigation we choose the freestream Mach number $M_{f1} = 5$ and maximum flow deflection angle $\theta_w = 10^\circ$. σ_1 was again unity within the freestream with its boundary value specified along $\xi_2 = 1$. The analytic values for the flow field variables close to the body surface for this isentropic compressive turn (region 3) are given by :-

$$p_3 / p_1 = 3.10368, \quad \rho_3 / \rho_1 = 2.24564, \quad M_{f3} = 4.08733, \quad \sigma_{1,3} = 1.04055, \quad \sigma_{2,3} = 0.46336$$

The compressive turn was specified to have the functional form

$$f(x_b) = \frac{x_b^3}{2} (2 - x_b) \tan\theta_w \quad (4.25)$$

which has the properties that it has zero curvature at its front and back ($x_b = 0$ and $x_b = 1$ respectively) with maximum curvature at its centre ($x_b = 1/2$). Thus the interaction between the characteristics is

observed to decrease from infinity to some minimum at the cusp where $\omega = \omega_0$, with co-ordinates (x_c, y_c) , and increase again to infinity.

The Van der Corput series (3.2) was used starting at $n = 728$. The computational grid had 100 cells along ξ_2 and 1532 ξ_1 nodes where needed to reach the point where $x = 2.0$. The CFL number was fixed at 0.4 and CPU time found to be 16 minutes 42 seconds. The results to the investigation can be found in figures 4.70 to 4.74.

For figure 4.70, 18 Frozen Mach wave contours have been plotted, with an equal incremental value between regions 1 and 3, within both the natural and Cartesian co-ordinate spaces. The characteristics are clearly observed to converge to the point where the shock wave develops. The concentration of contours representing the shock wave. The region close to where the shock wave was created has been magnified, see figure 4.71. The envelope and cusp, calculated by solving iteratively equation (4.23) together with the C_- Riemann invariant, are plotted as a thin dotted line and solid dot respectively; The envelope and the functional behaviour of x with respect to ω are plotted in figure 4.72. It is clear from the magnified region that the Mach waves converge and focus at the cusp with the shock wave growing from it. As expected the shock is observed to lie between the two branches of the envelope. Within figure 4.73 and 4.74 the variation of the flow field variables along several different streamlines and normals are plotted. An indication of the strength of the shock wave can be found in the entropy. Close to the body surface there is zero entropy production. (One will note that there is indeed some entropy production close to the body. This is due to the approximation, within the local Riemann problems, of the compression waves by an oblique shock wave causing a small but noticeable entropy production to occur over a large distance). Further away from the body surface the entropy increases indicating a strengthening shock wave. The difference in pressures between the body surface and downstream of the shock wave (higher at body surface) causes a secondary wave system to be generated tending to equalize them out. This is observed in the pressure profiles along ξ_2 with ξ_1 positions furthest downstream. The entropy layer downstream of the wave system can be clearly identified with the non-uniformity due to the secondary wave system.

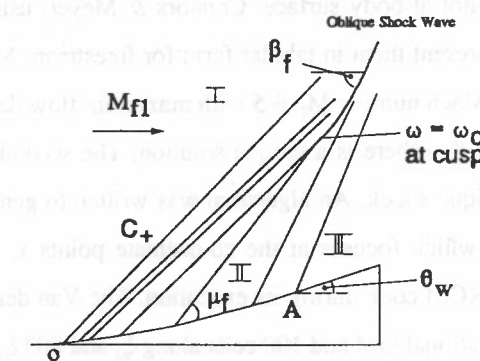


Figure 4.9 Compressive surface.

4.7 Focusing Compressive Surface

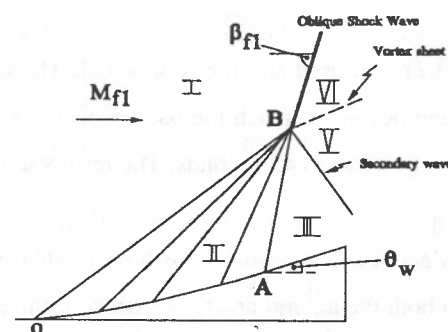


Figure 4.10 Surface producing focused compression waves.

We further investigate the compressive turn with a surface producing focused compression waves. The problem is similar to the double wedge such that at the focal point (point B) an oblique shock, vortex sheet, and secondary wave are created. One of the first practical investigations of this type of problem was by Connors and Meyer[27] as part of their study of external high speed engine intakes. This type of surface has been used as part of external engine intake on the Anglo-French Concorde supersonic plane, see Seddon and Goldsmith[81]. More recently Emanuel[36,37] has investigated the effect of the surface inclination angle on the number of valid solutions, i.e. the strength and type of primary and secondary waves generated, at the focal point or 'near field'. The study revealed that for small deflection angles there is a unique solution. However, by increasing the angle the number of valid solutions increases until there are no real solutions possible.

The surface supporting the focused compression waves was not known analytically in advance but can be calculated approximately by solving the governing equations derived by Emanuel. Essentially the equations are the Prandtl-Meyer expansion wave relations reversed for a compressive turn with singularity occurring within the flow and not at body surface. Connors & Meyer, using a different approach, have calculated these contours and present them in tabular form for freestream Mach numbers up to $M_{f1} = 4.0$.

We consider the freestream Mach number $M_{f1} = 5$ with maximum flow deflection of $\theta_w = 10^\circ$. For these conditions Emanuel has shown that there is a unique solution; The secondary wave being an expansion wave with a weak primary oblique shock. An algorithm was written to generate the approximate surface supporting a compression fan which focuses at the co-ordinate points $x_c = 0.490$ and $y_c = 0.100$. The surface data was read into the RCM code during its execution. The Van der Corput series (3,2) was used starting at $n = 728$. The computational grid had 100 cells along ξ_2 and 803 ξ_1 nodes where needed to reach the point where $x = 1.0$. The CFL number was fixed at 0.4 and CPU time found to be 8 minutes 58 seconds. Frozen Mach wave contours are plotted within the natural and Cartesian co-ordinate spaces, figure 4.75. The convergence of the compression waves are clearly observed to focus around the focal

point and oblique shock created, figure 4.76. The calculated variation of the flow field through the fan and shock are presented in figures 4.77 to 4.78. It is observed that the change in the flow increases much more quickly than for the earlier compressive surface. The shock is observed to jump to its full strength suddenly. There is a noticeable rise in the entropy close to the boundary. The reasoning for this is the same as above. Because the compression wave is stronger the shocks within each of the Riemann problems, modelling it, will also be stronger. This strength is clearly observed in the pressure increases close to the boundary. These are significantly higher than for the other compressive surface. By considering the variation along the normals the contact surface is clearly discerned, figure 4.78. There is a smoothly varying entropy layer brought about by the error in the entropy. In reality there should a jump in the entropy at the point where the normals crosses the contact surface.

Validation (Inert) : Prandtl-Meyer Expansion wave.

The effect of quasi random number series on numerical solution.

Anderson's series with $n=1$, CFL = 0.4, $\xi_s=100$ cells.

$$M_\infty = 2, \delta_r = -10^\circ, \gamma=1.4$$

Key :-

— Analytic Solution for $\xi_s=0.115$

□ Numerical Solution.

○ Errors.

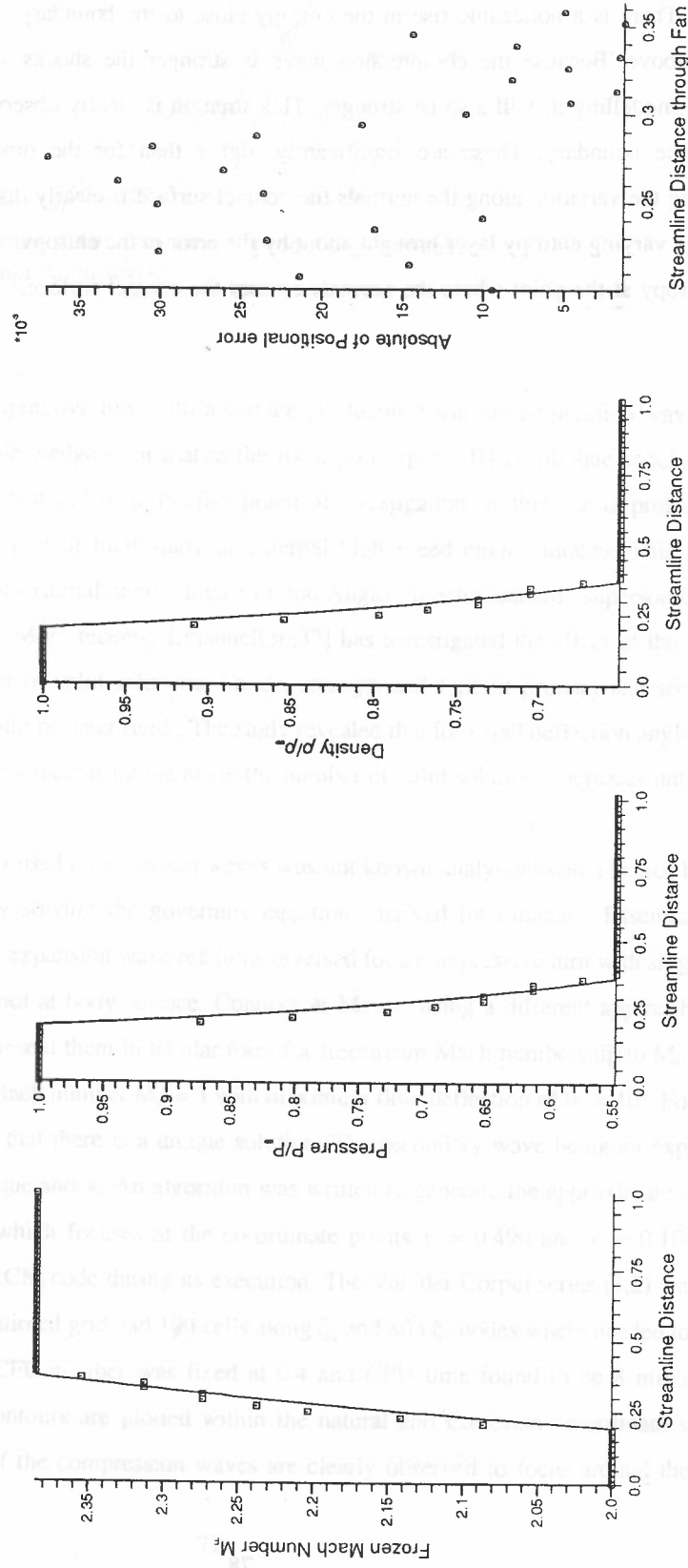


Fig. 4.11

Validation (Inert) : Prandtl-Meyer Expansion wave.

The effect of quasi random number series on numerical solution.

Van der Corput series $k_1=2, k_2=1, n=1$, CFL = 0.4, $\xi_s=100$ cells.

$$M_\infty = 2, \delta_r = -10^\circ, \gamma=1.4$$

Key :-

— Analytic Solution for $\xi_s=0.115$

□ Numerical Solution.

○ Errors.

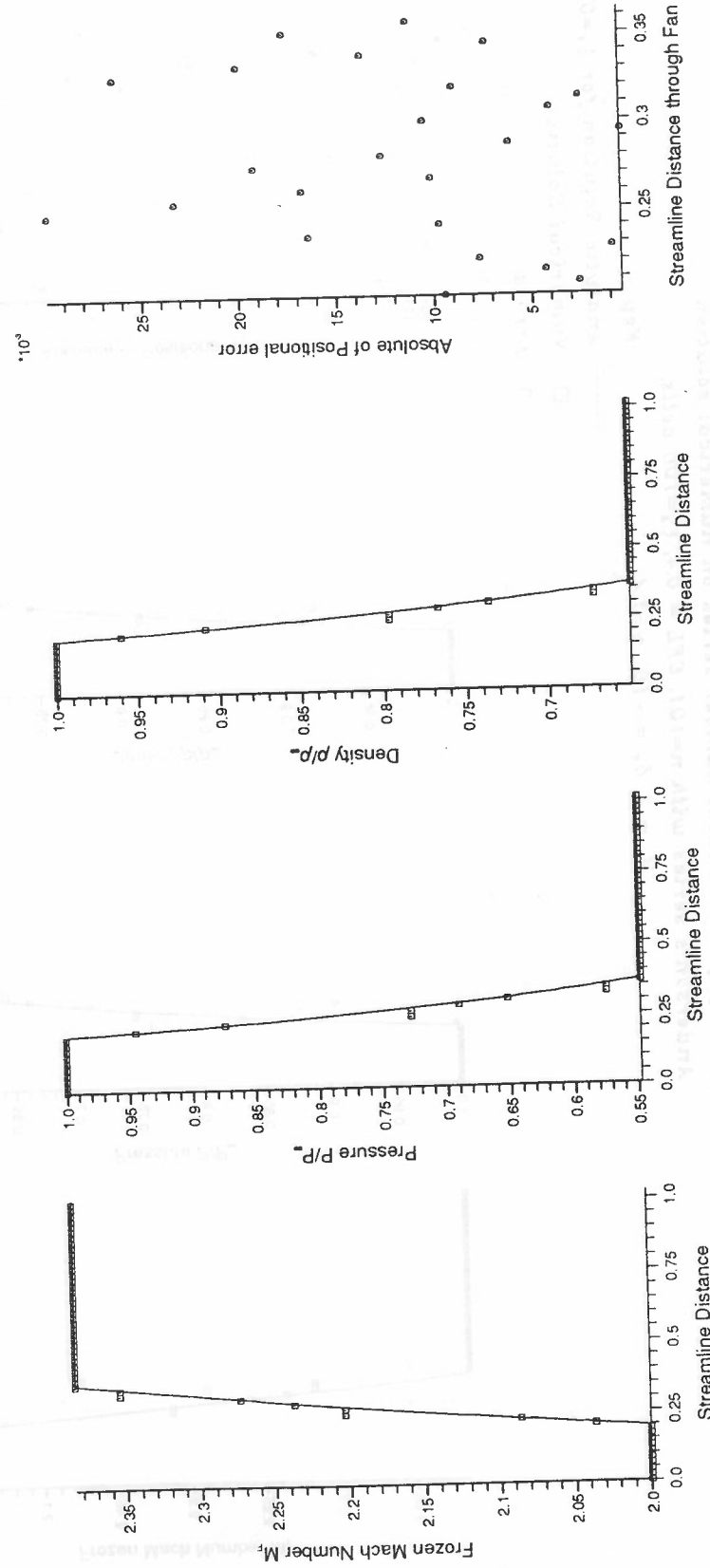


Fig. 4.12

Validation (Inert) : Prandtl-Meyer Expansion wave.
The effect of quasi random number series on numerical solution.
Anderson's series with $n=101$, $CFL = 0.4$, $\xi_s=100$ cells.

$$M_\infty = 2, \delta_r = -10^\circ, \gamma=1.4$$

Key :-

- Analytic Solution for $\xi_s=0.115$
- Numerical Solution.
- Errors.

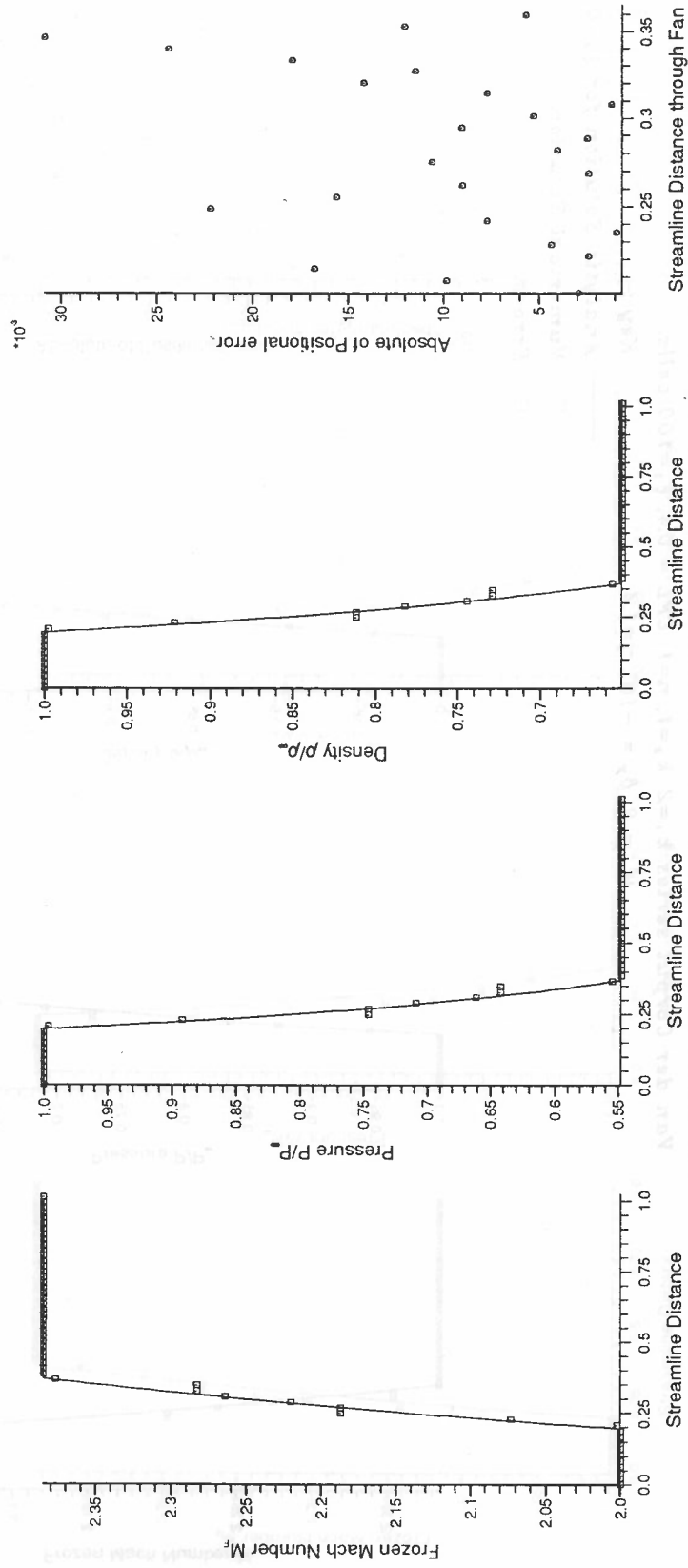


Fig. 4.13

Validation (Inert) : Prandtl-Meyer Expansion wave.
The effect of quasi random number series on numerical solution.
Van der Corput series $k_1=2, k_2=1, n=101$, $CFL = 0.4$, $\xi_s=100$ cells.

$$M_\infty = 2, \delta_r = -10^\circ, \gamma=1.4$$

Key :-

- Analytic Solution for $\xi_s=0.115$
- Numerical Solution.
- Errors.

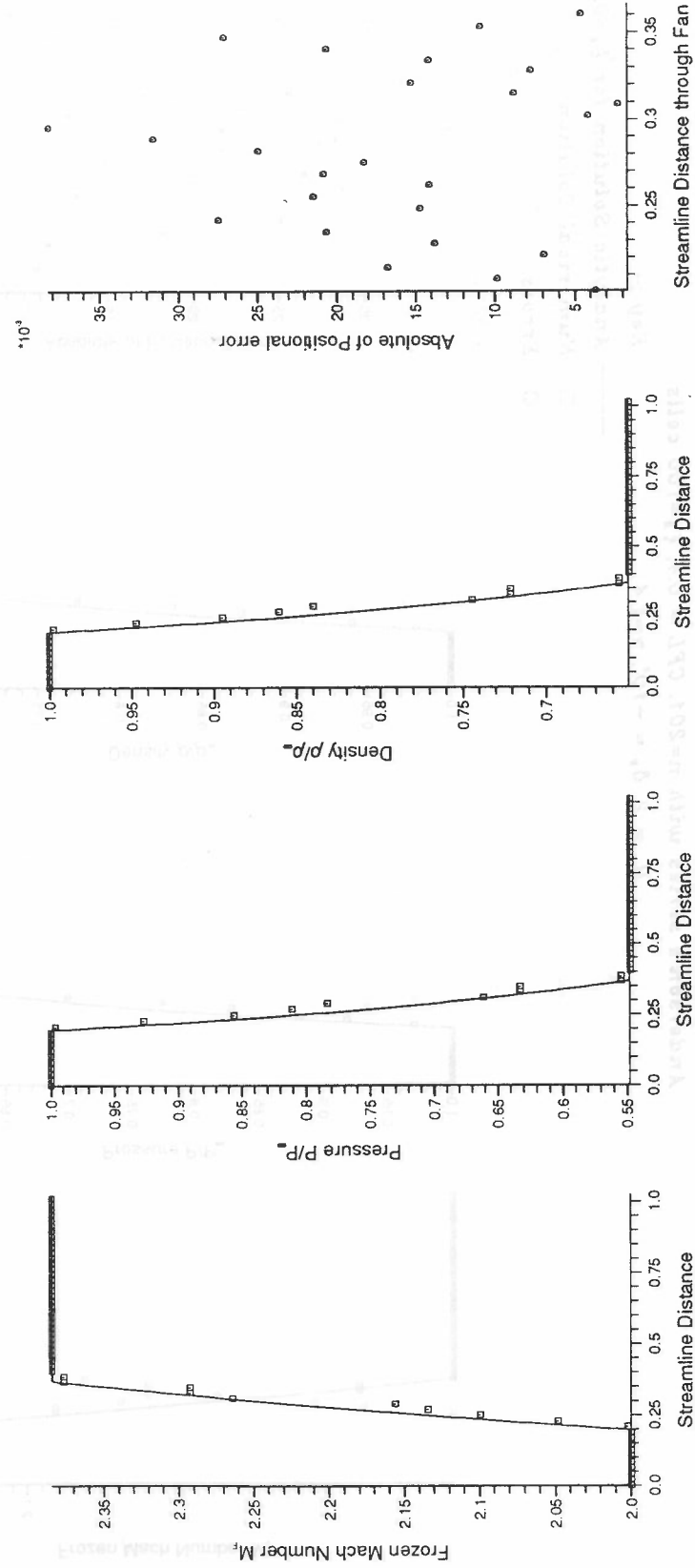


Fig. 4.14

Validation (Inert) : Prandtl-Meyer Expansion wave.

The effect of quasi random number series on numerical solution.

Anderson's series with $n=201$, $CFL = 0.4$, $\xi_s=100$ cells.

$M_\infty = 2$, $\delta_r = -10^\circ$, $\gamma=1.4$

Key :-

— Analytic Solution for $\xi_s=0.115$

□ Numerical Solution.

○ Errors.

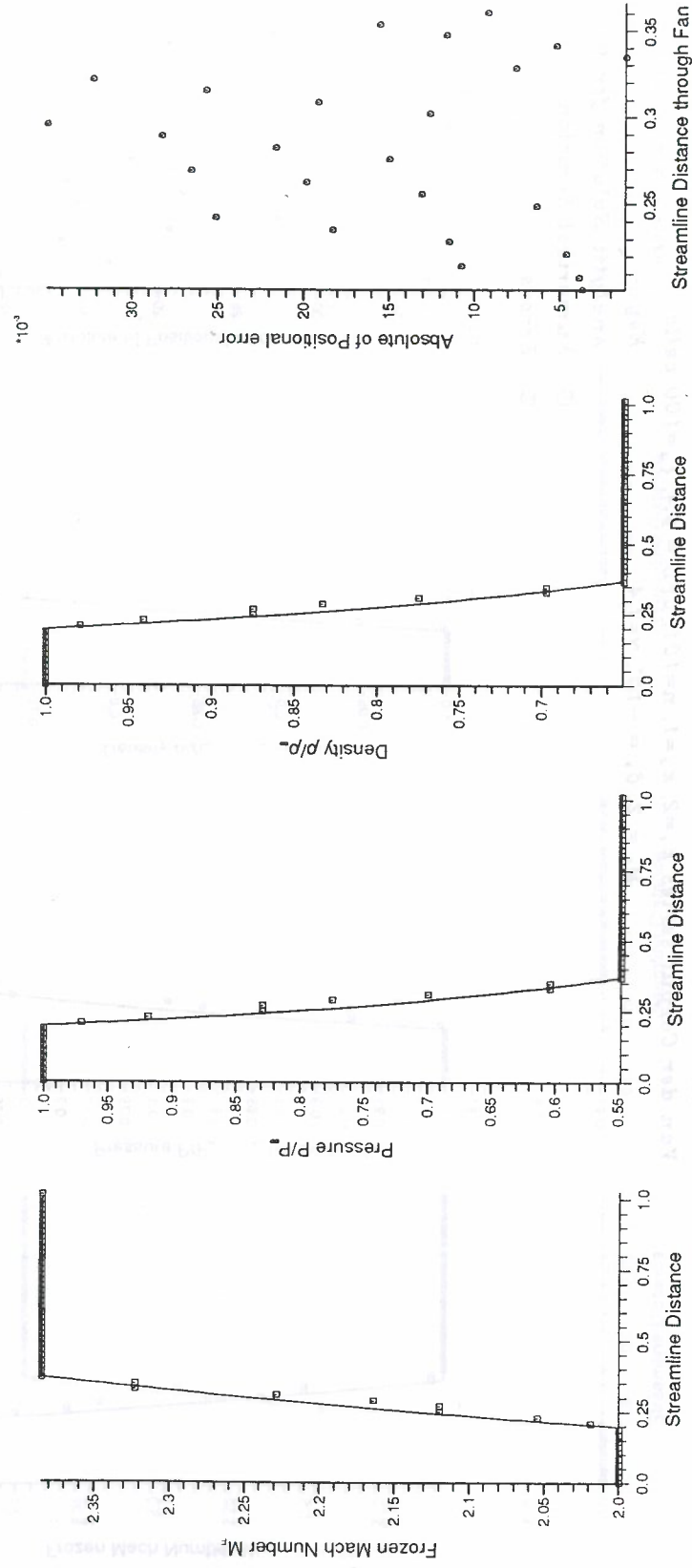


Fig. 4.15

Validation (Inert) : Prandtl-Meyer Expansion wave.

The effect of quasi random number series on numerical solution.

Van der Corput series $k_1=2$, $k_2=1$, $n=201$, $CFL = 0.4$, $\xi_s=100$ cells.

$M_\infty = 2$, $\delta_r = -10^\circ$, $\gamma=1.4$

Key :-

— Analytic Solution for $\xi_s=0.115$

□ Numerical Solution.

○ Errors.

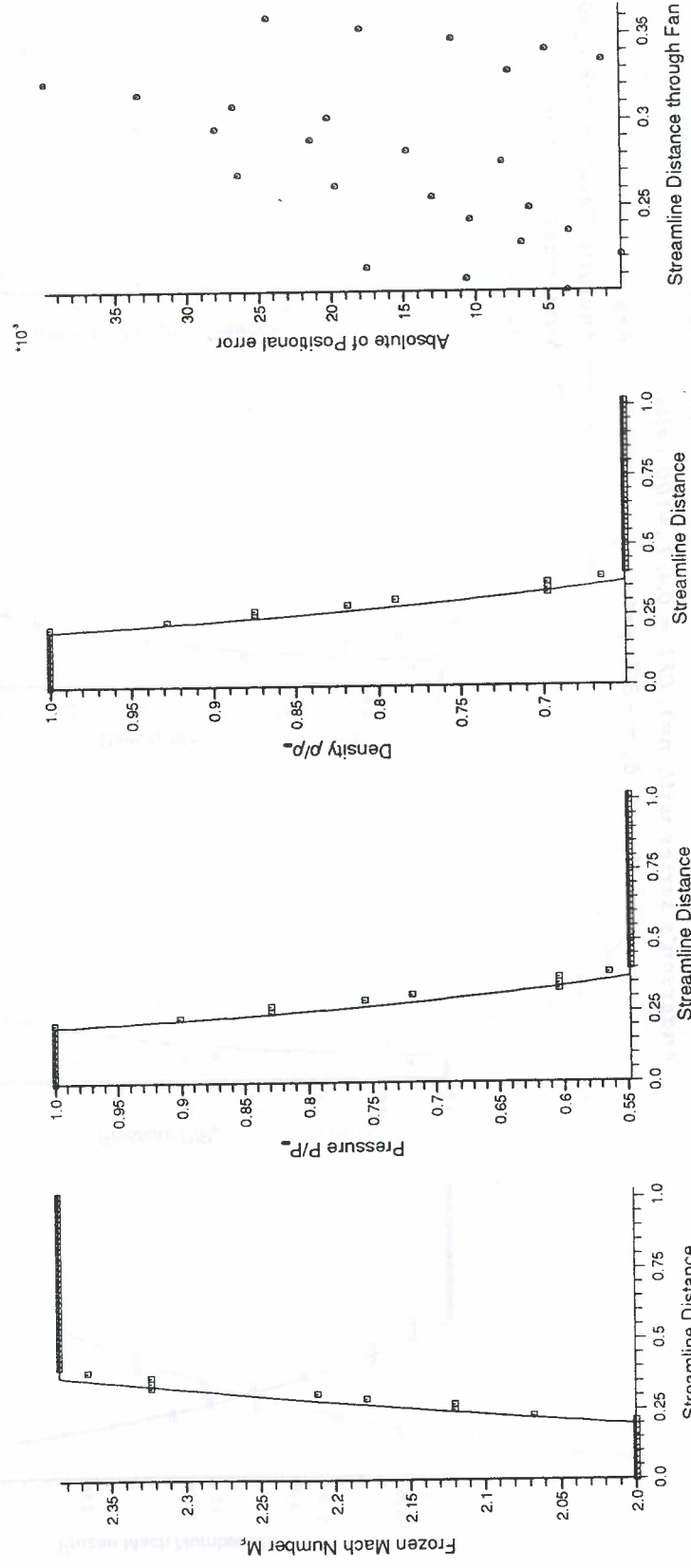


Fig. 4.16

Validation (Inert) : Prandtl-Meyer Expansion wave.

The effect of quasi random number series on numerical solution.

Anderson's series with $n=1$. CFL = 0.4, $\xi_z=100$ cells.

$M_\infty = 2$, $\delta_r = -30^\circ$, $\gamma=1.4$

Key :-

— Analytic Solution for $\xi_z=0.045$

□ Numerical Solution.

○ Errors.

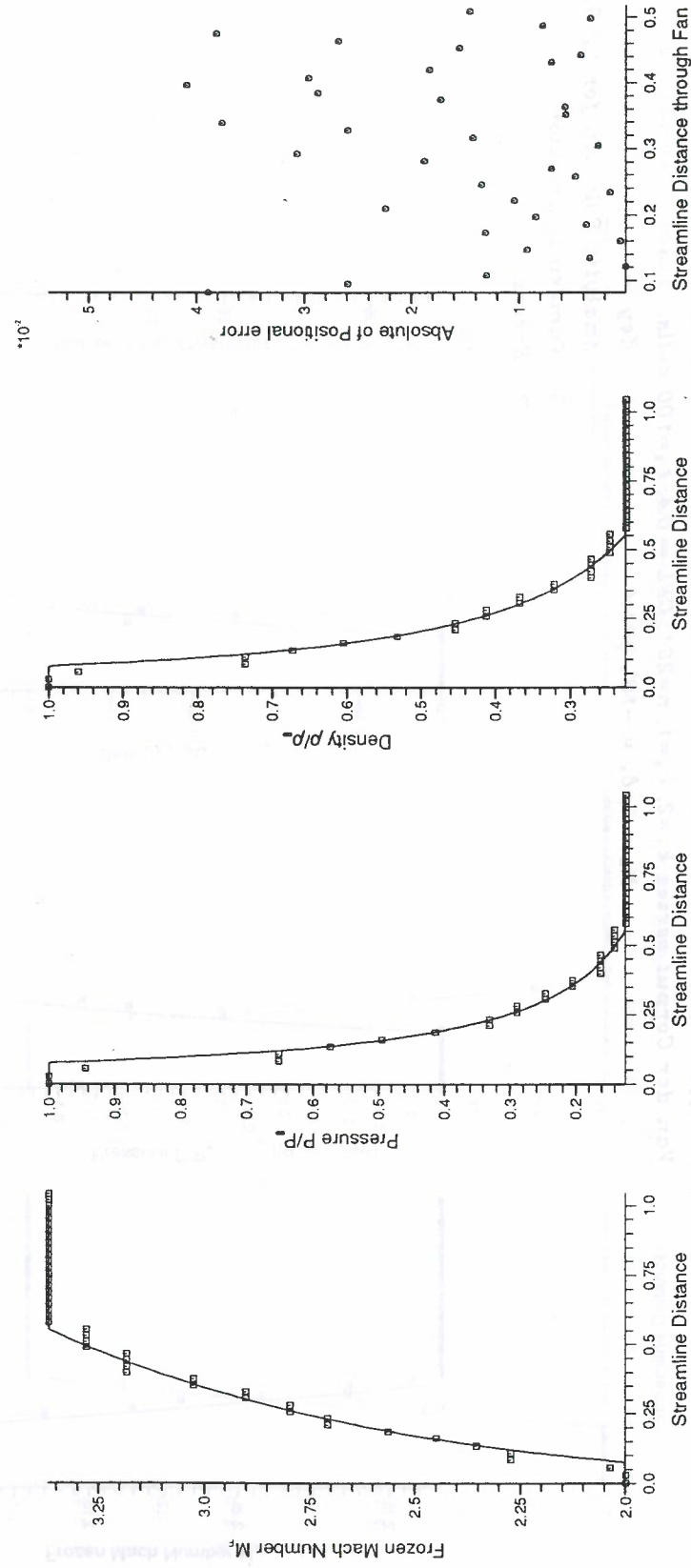


Fig. 4.17

Validation (Inert) : Prandtl-Meyer Expansion wave.

The effect of quasi random number series on numerical solution.

Van der Corput series $k_1=2$, $k_2=1$, $n=1$. CFL = 0.4, $\xi_z=100$ cells.

$M_\infty = 2$, $\delta_r = -30^\circ$, $\gamma=1.4$

Key :-

— Analytic Solution for $\xi_z=0.045$

□ Numerical Solution.

○ Errors.

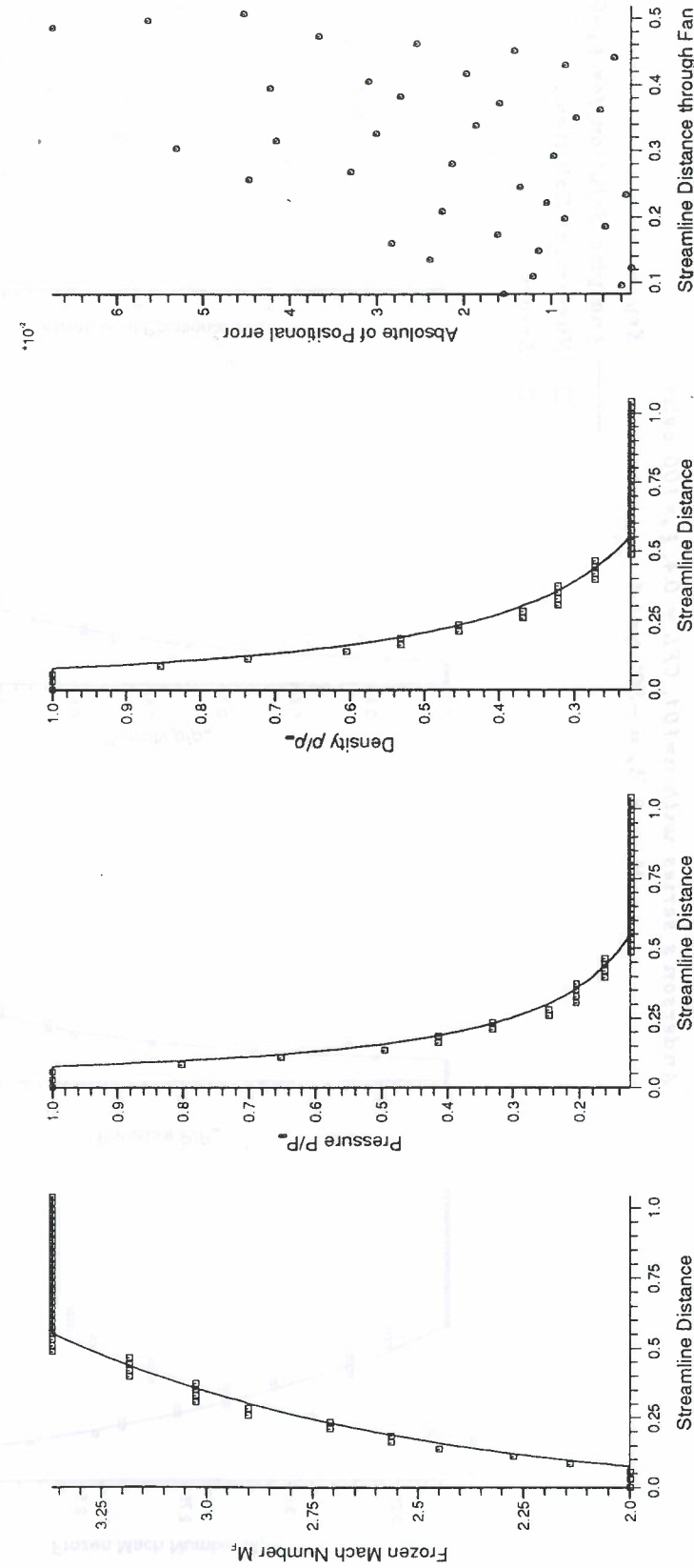


Fig. 4.18

Validation (Inert) : Prandtl-Meyer Expansion wave.

The effect of quasi random number series on numerical solution.

Anderson's series with $n=101$. CFL = 0.4, $\xi_s=100$ cells.

$M_\infty = 2$, $\delta_r = -30^\circ$, $\gamma=1.4$

Key :-

— Analytic Solution for $\xi_s=0.045$

□ Numerical Solution.

○ Errors.

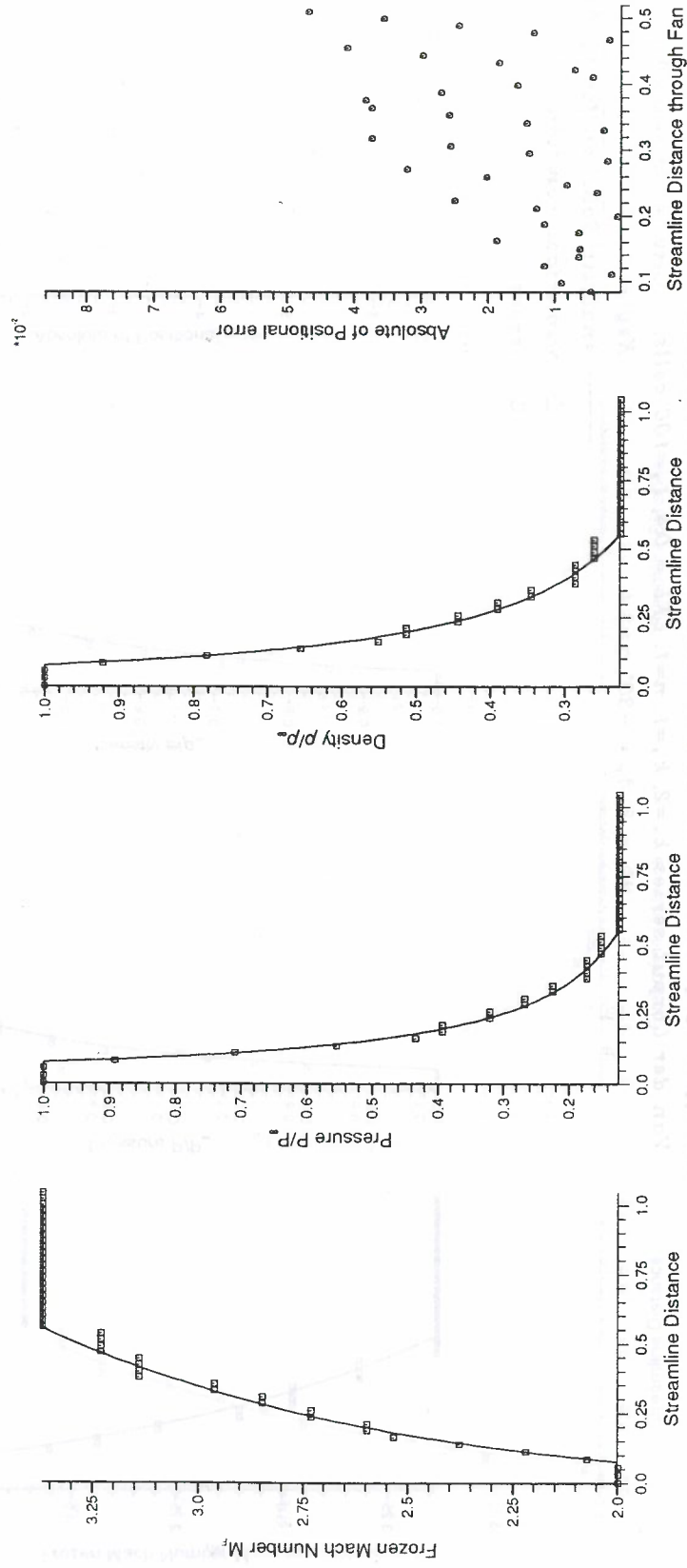


Fig. 4.19

Validation (Inert) : Prandtl-Meyer Expansion wave.

The effect of quasi random number series on numerical solution.

Van der Corput series $k_1=2$, $k_2=1$, $n=101$. CFL = 0.4, $\xi_s=100$ cells.

$M_\infty = 2$, $\delta_r = -30^\circ$, $\gamma=1.4$

Key :-

— Analytic Solution for $\xi_s=0.045$

□ Numerical Solution.

○ Errors.

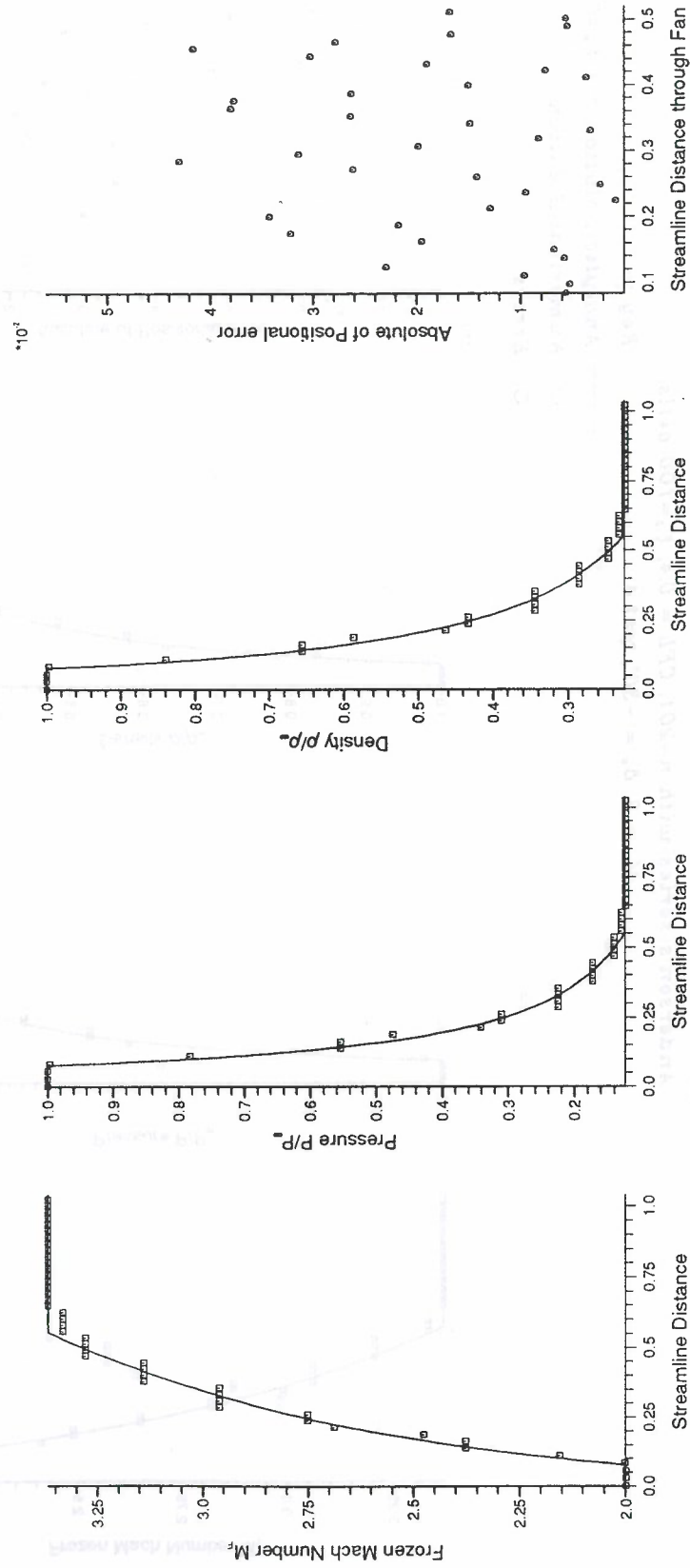


Fig. 4.20

Validation (Inert) : Prandtl-Meyer Expansion wave.

The effect of quasi random number series on numerical solution.

Anderson's series with $n=201$. CFL = 0.4, $\xi_s=100$ cells.

$M_\infty = 2$, $\delta_r = -30^\circ$, $\gamma=1.4$

Key :-

— Analytic Solution for $\xi_s=0.045$

□ Numerical Solution.

○ Errors.

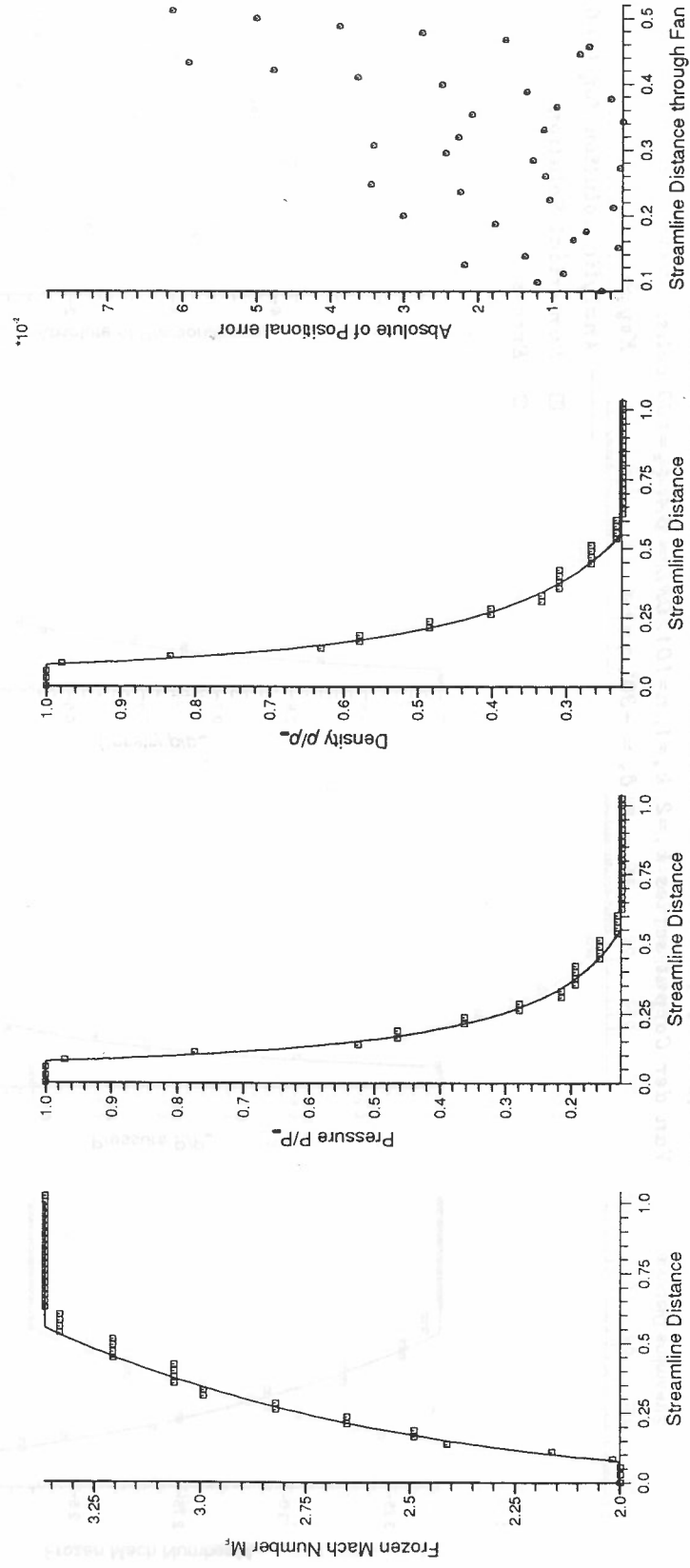


Fig. 4.21

Validation (Inert) : Prandtl-Meyer Expansion wave.

The effect of quasi random number series on numerical solution.

Van der Corput series $k_1=2$, $k_2=1$, $n=201$. CFL = 0.4, $\xi_s=100$ cells.

$M_\infty = 2$, $\delta_r = -30^\circ$, $\gamma=1.4$

Key :-

— Analytic Solution for $\xi_s=0.045$

□ Numerical Solution.

○ Errors.

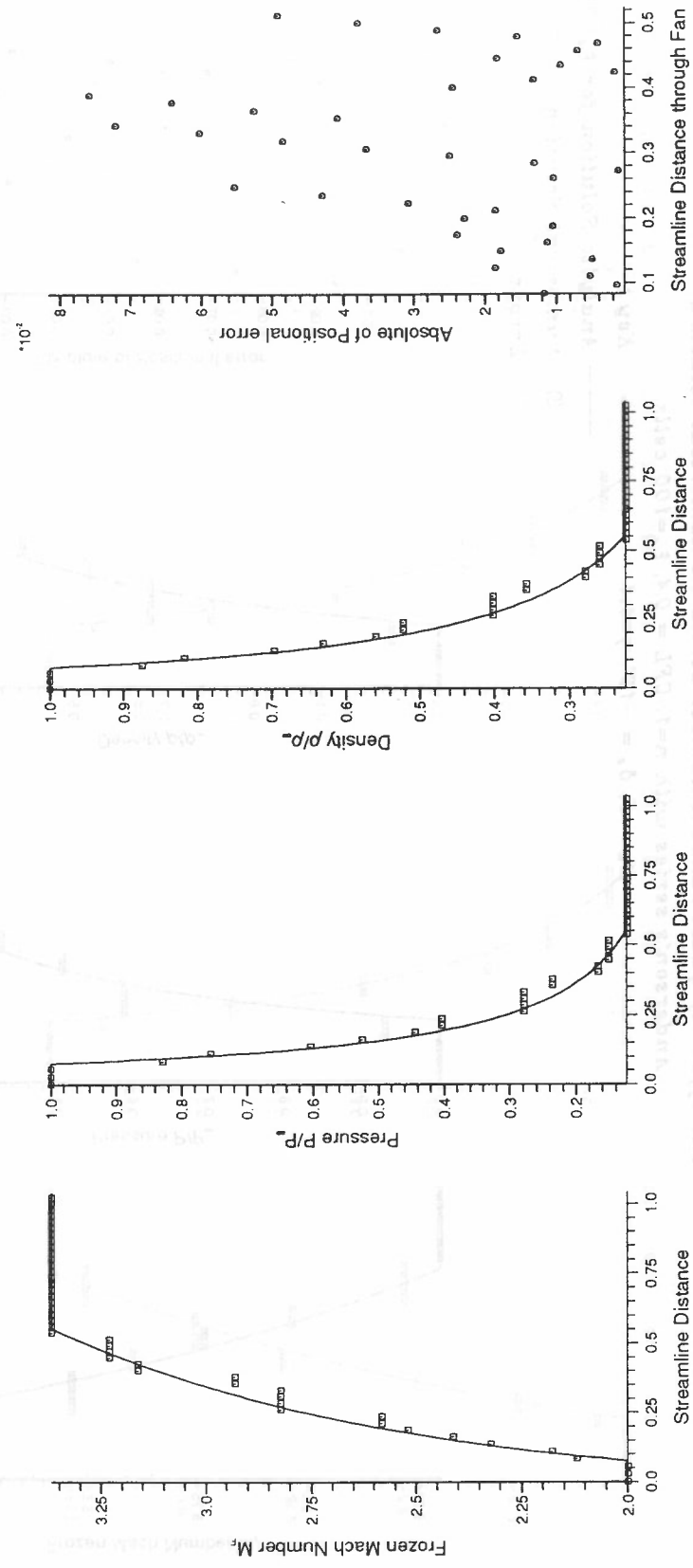


Fig. 4.22

Validation (Inert) : Prandtl-Meyer Expansion wave.

The effect of quasi random number series on numerical solution.

Anderson's series with $n=1$. $CFL = 0.4$, $\xi_s = 100$ cells.

$M_\infty = 5$, $\delta_r = -10^\circ$, $\gamma = 1.4$

Key :-
Analytic Solution for $\xi_s = 0.045$

□ Numerical Solution.

○ Errors.

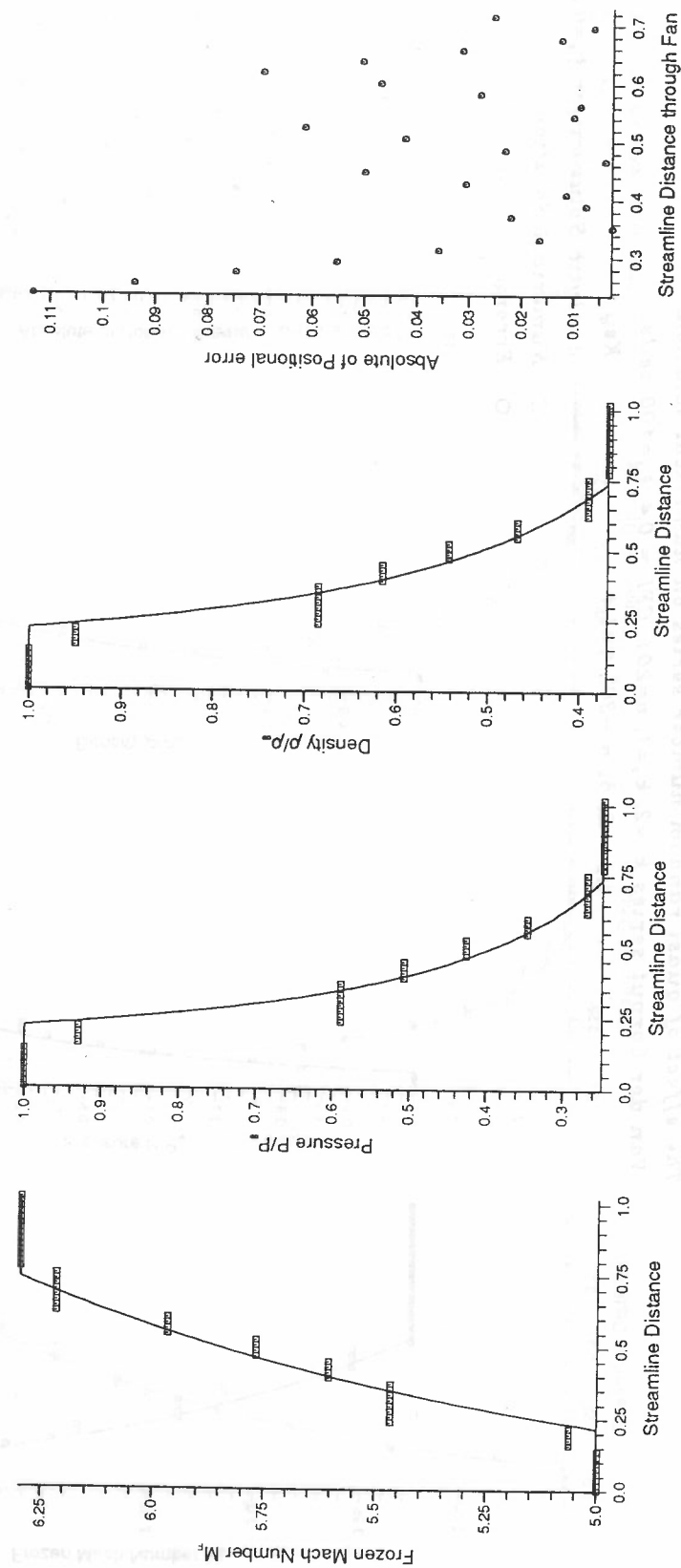


Fig. 4.23

Validation (Inert) : Prandtl-Meyer Expansion wave.

The effect of quasi random number series on numerical solution.

Van der Corput series $k_1=2$, $k_s=1$, $n=1$. $CFL = 0.4$, $\xi_s = 100$ cells.

$M_\infty = 5$, $\delta_r = -10^\circ$, $\gamma = 1.4$

Key :-

Analytic Solution for $\xi_s = 0.045$

□ Numerical Solution.

○ Errors.

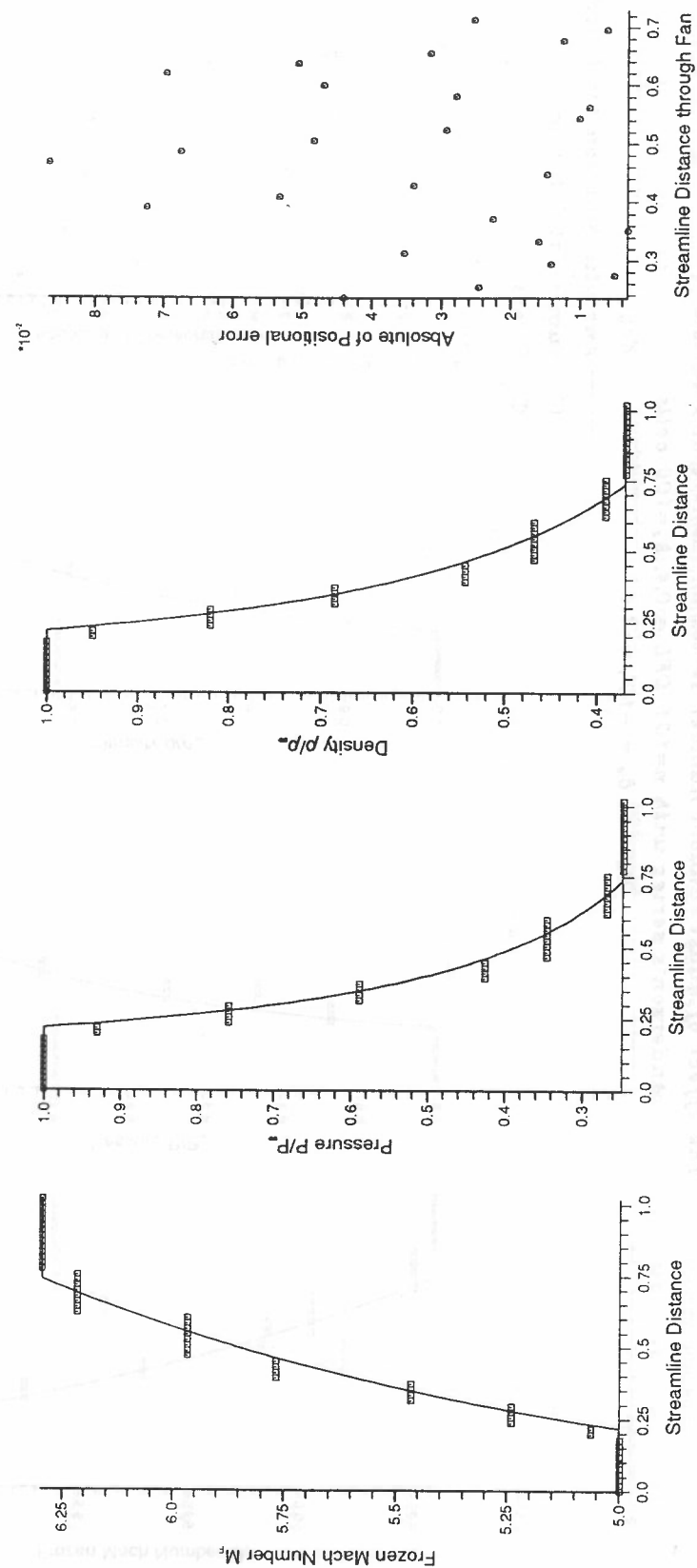


Fig. 4.24

Validation (Inert) : Prandtl-Meyer Expansion wave.
The effect of quasi random number series on numerical solution.
Anderson's series with $n=101$. CFL = 0.4, $\xi_s=100$ cells.

$$M_\infty = 5, \delta_r = -10^\circ, \gamma=1.4$$

Key :-

- Analytic Solution for $\xi_s=0.045$
- Numerical Solution.
- Errors.

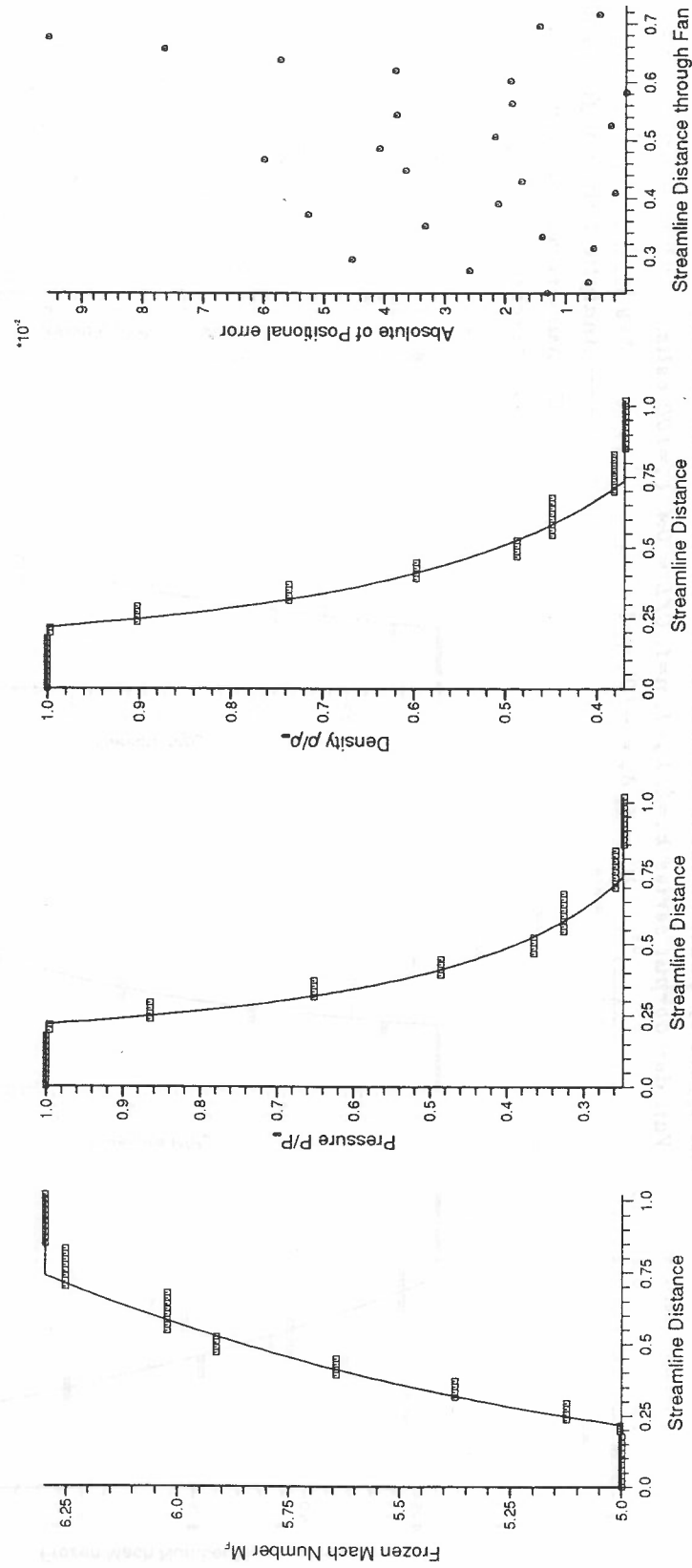


Fig. 4.25

Validation (Inert) : Prandtl-Meyer Expansion wave.
The effect of quasi random number series on numerical solution.
Van der Corput series $k_1=2, k_2=1, n=101$. CFL = 0.4, $\xi_s=100$ cells.

$$M_\infty = 5, \delta_r = -10^\circ, \gamma=1.4$$

Key :-

- Analytic Solution for $\xi_s=0.045$
- Numerical Solution.
- Errors.

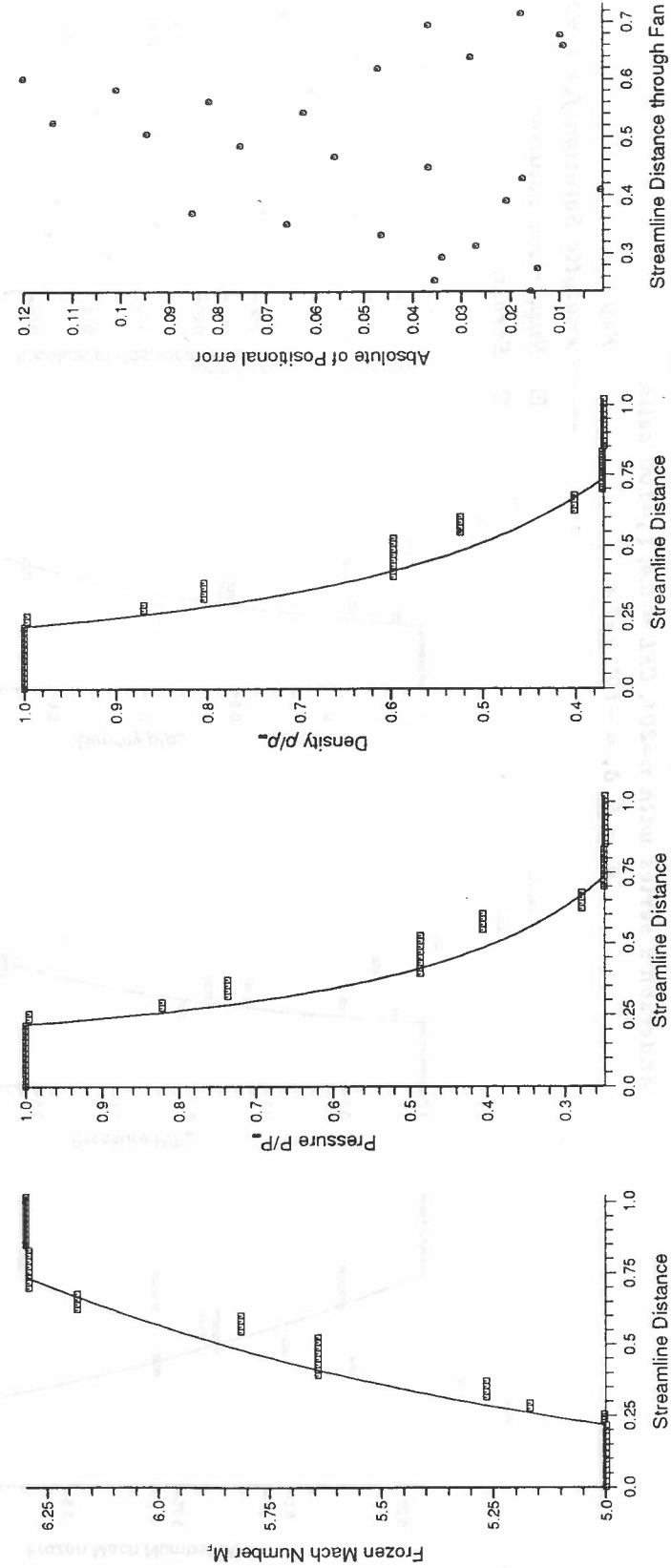


Fig. 4.26

Validation (Inert) : Prandtl-Meyer Expansion wave.
 The effect of quasi random number series on numerical solution.
 Anderson's series with $n=201$, $CFL = 0.4$, $\xi_s=100$ cells.
 $M_\infty = 5$, $\delta_r = -10^\circ$, $\gamma=1.4$

Key :-
 — Analytic Solution for $\xi_s=0.045$
 □ Numerical Solution.
 ○ Errors.

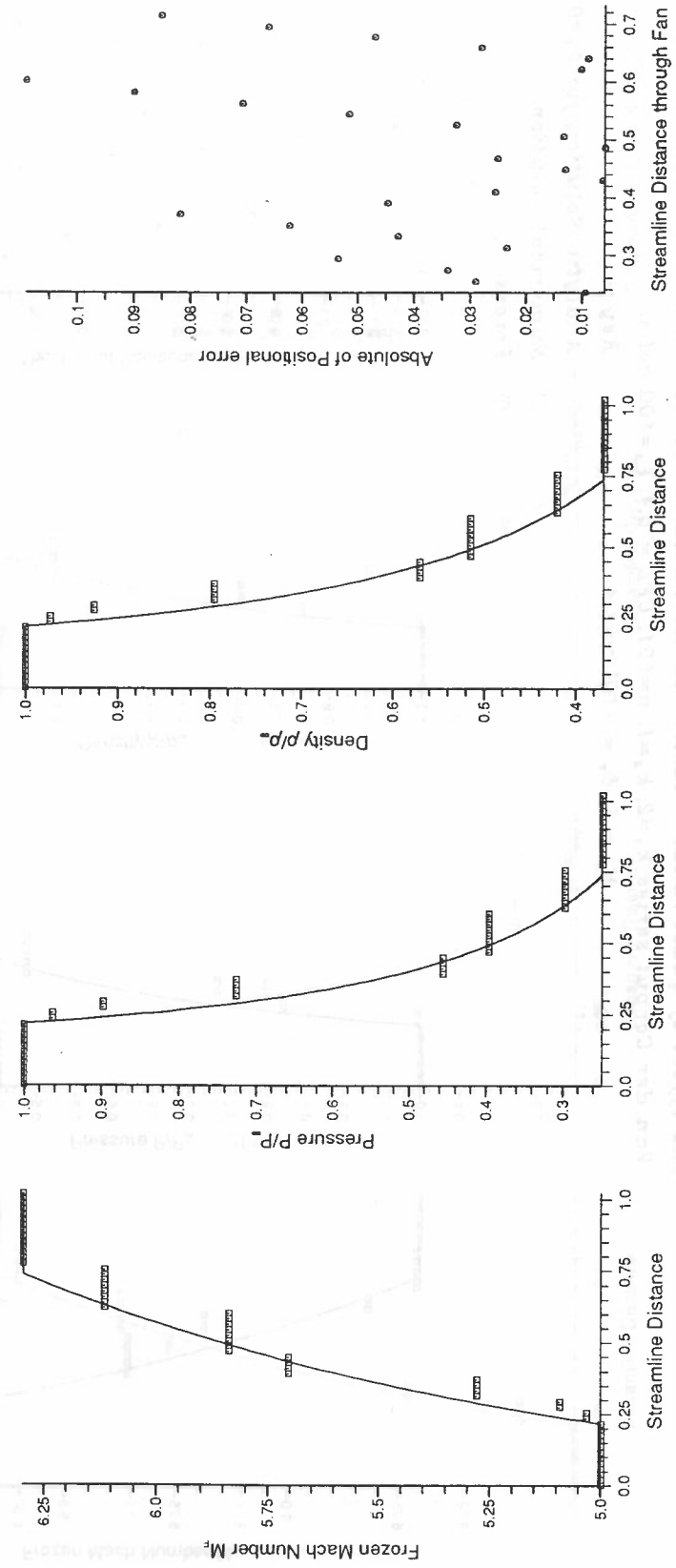


Fig. 4.27

Validation (Inert) : Prandtl-Meyer Expansion wave.
 The effect of quasi random number series on numerical solution.
 Van der Corput series $k_1=2$, $k_2=1$, $n=201$, $CFL = 0.4$, $\xi_s=100$ cells.
 $M_\infty = 5$, $\delta_r = -10^\circ$, $\gamma=1.4$

Key :-
 — Analytic Solution for $\xi_s=0.045$
 □ Numerical Solution.
 ○ Errors.

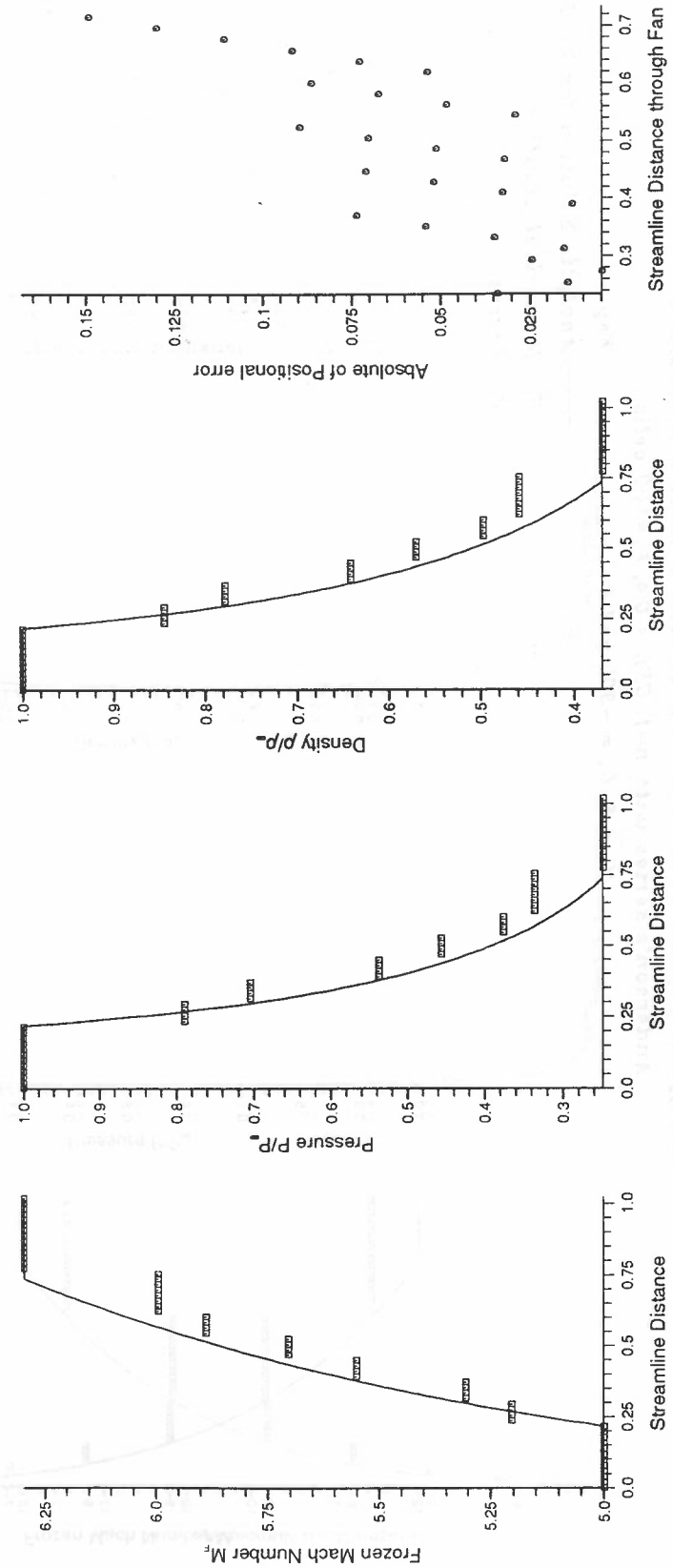
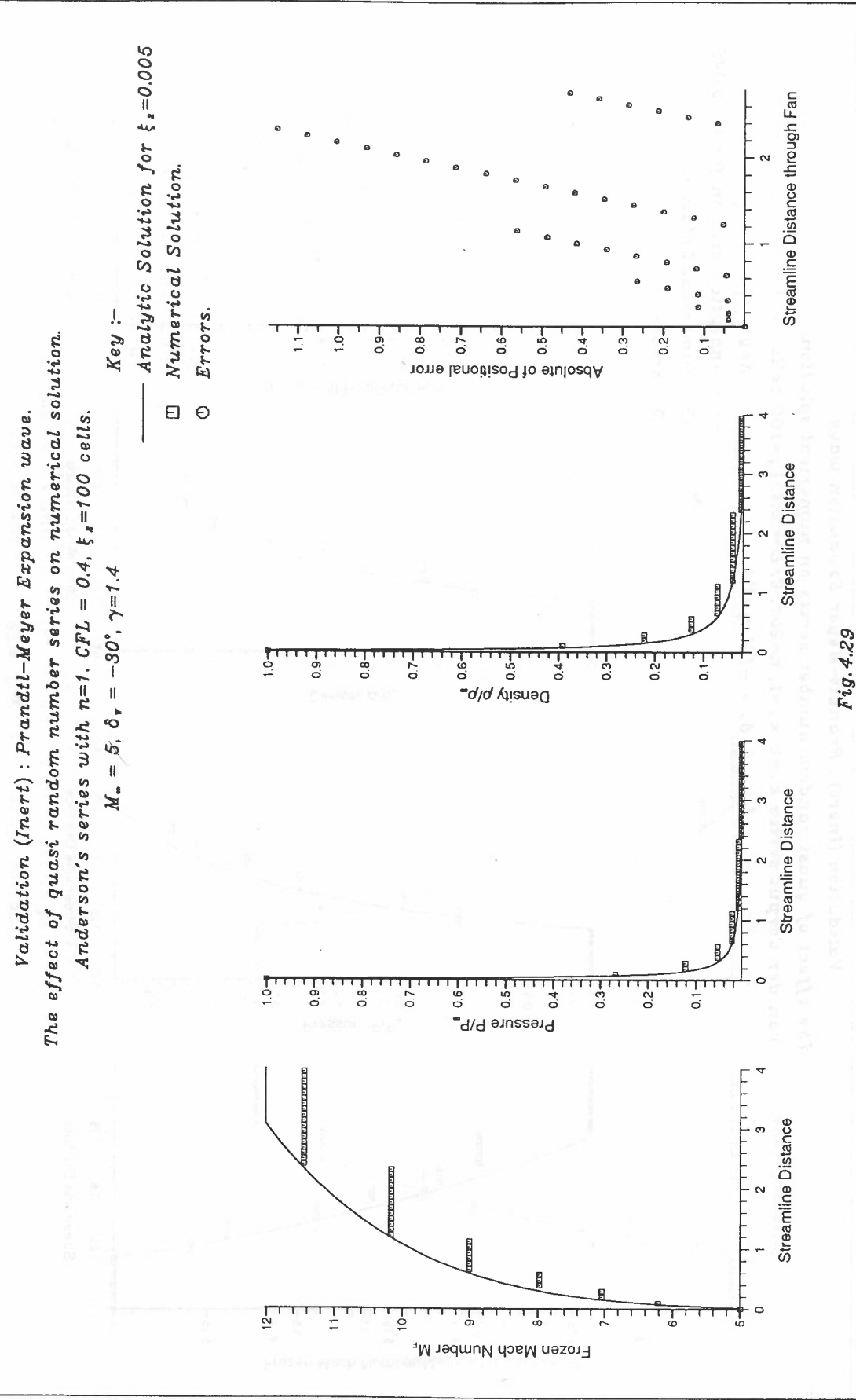
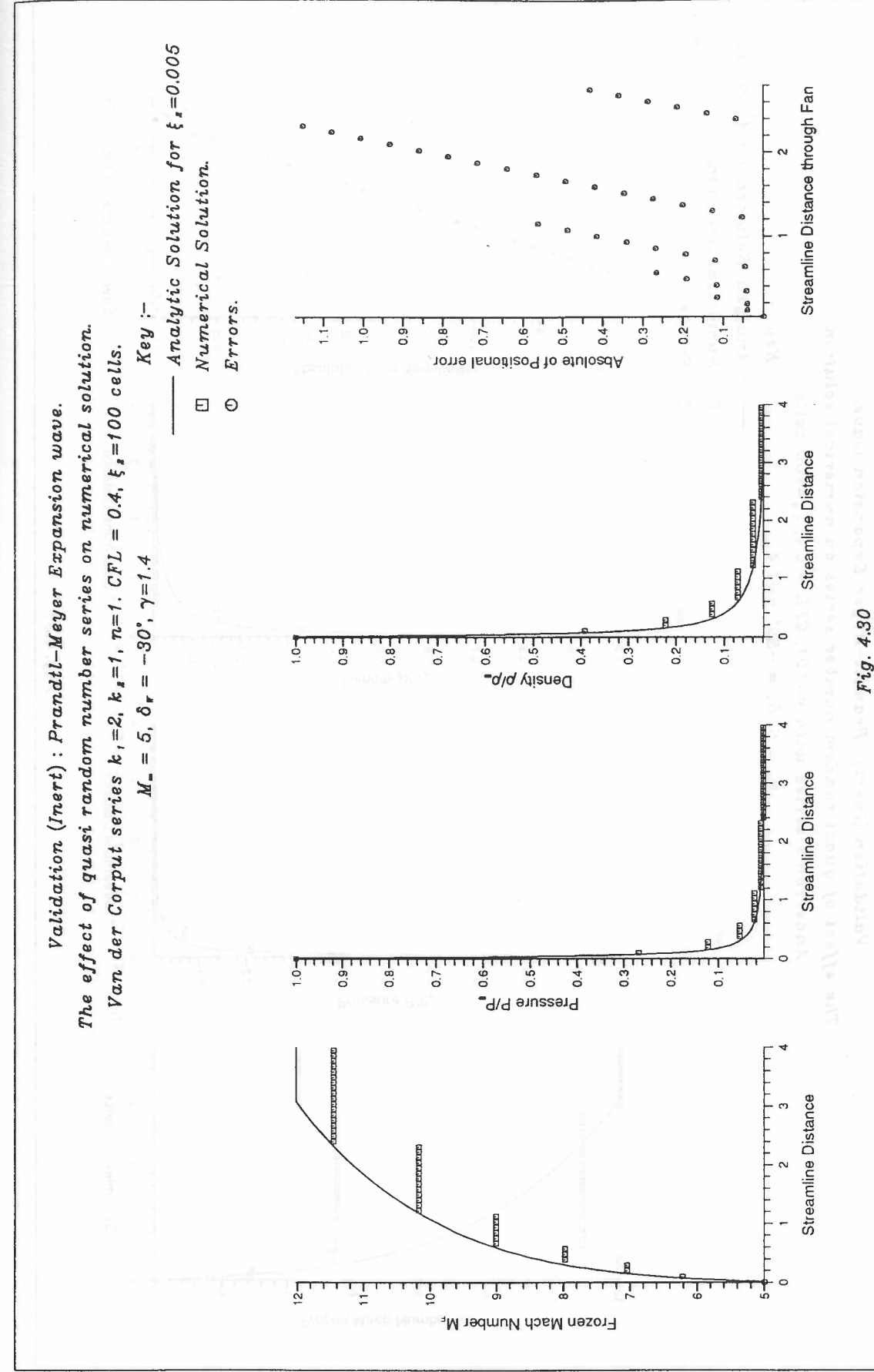


Fig. 4.28



Validation (Inert) : Prandtl-Meyer Expansion wave.

The effect of quasi random number series on numerical solution.

Anderson's series with $n=101$. CFL = 0.4, $\xi_s=100$ cells.

$M_\infty = 5$, $\delta_r = -30^\circ$, $\gamma=1.4$

Key :-

— Analytic Solution for $\xi_s=0.005$

□ Numerical Solution.

○ Errors.

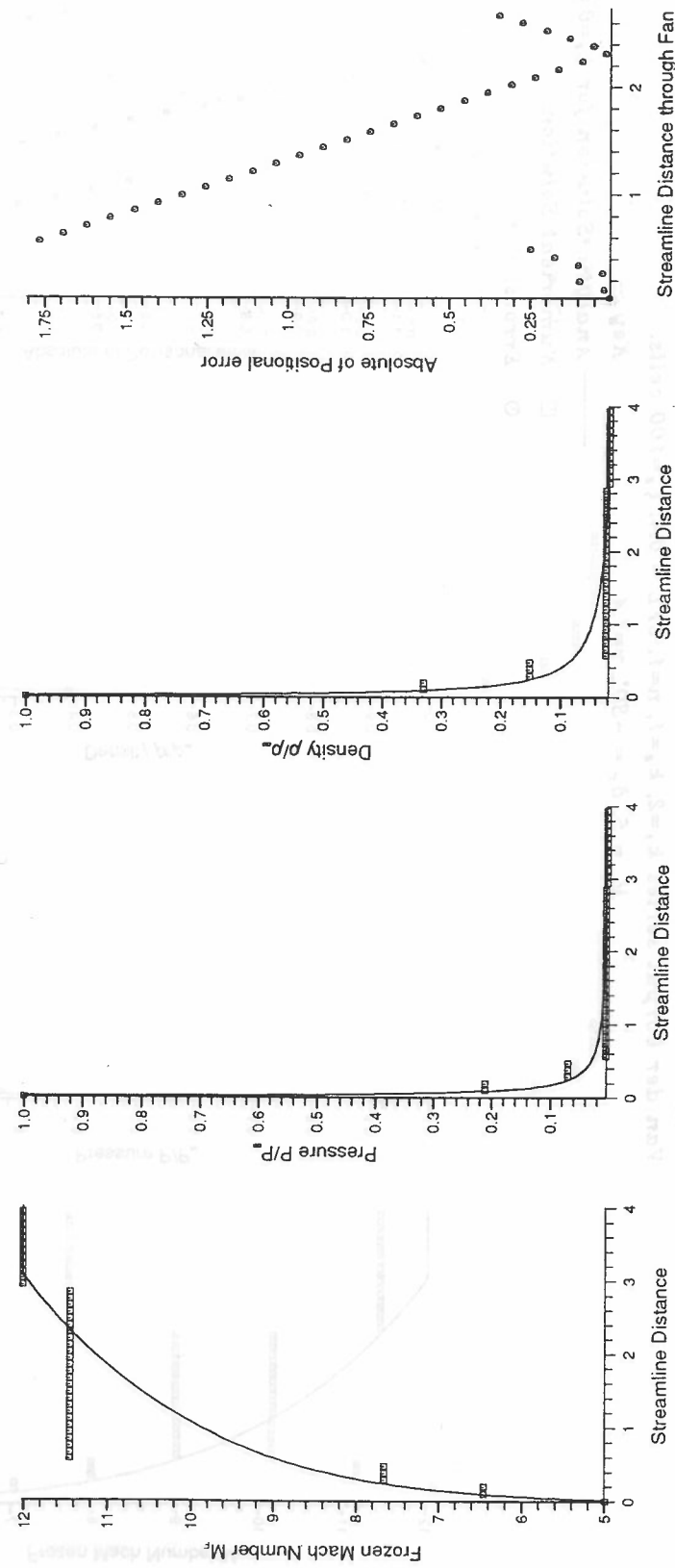


Fig. 4.31

Validation (Inert) : Prandtl-Meyer Expansion wave.

The effect of quasi random number series on numerical solution.

Van der Corput series $k_1=2$, $k_2=1$, $n=101$. CFL = 0.4, $\xi_s=100$ cells.

$M_\infty = 5$, $\delta_r = -30^\circ$, $\gamma=1.4$

Key :-

— Analytic Solution for $\xi_s=0.005$

□ Numerical Solution.

○ Errors.

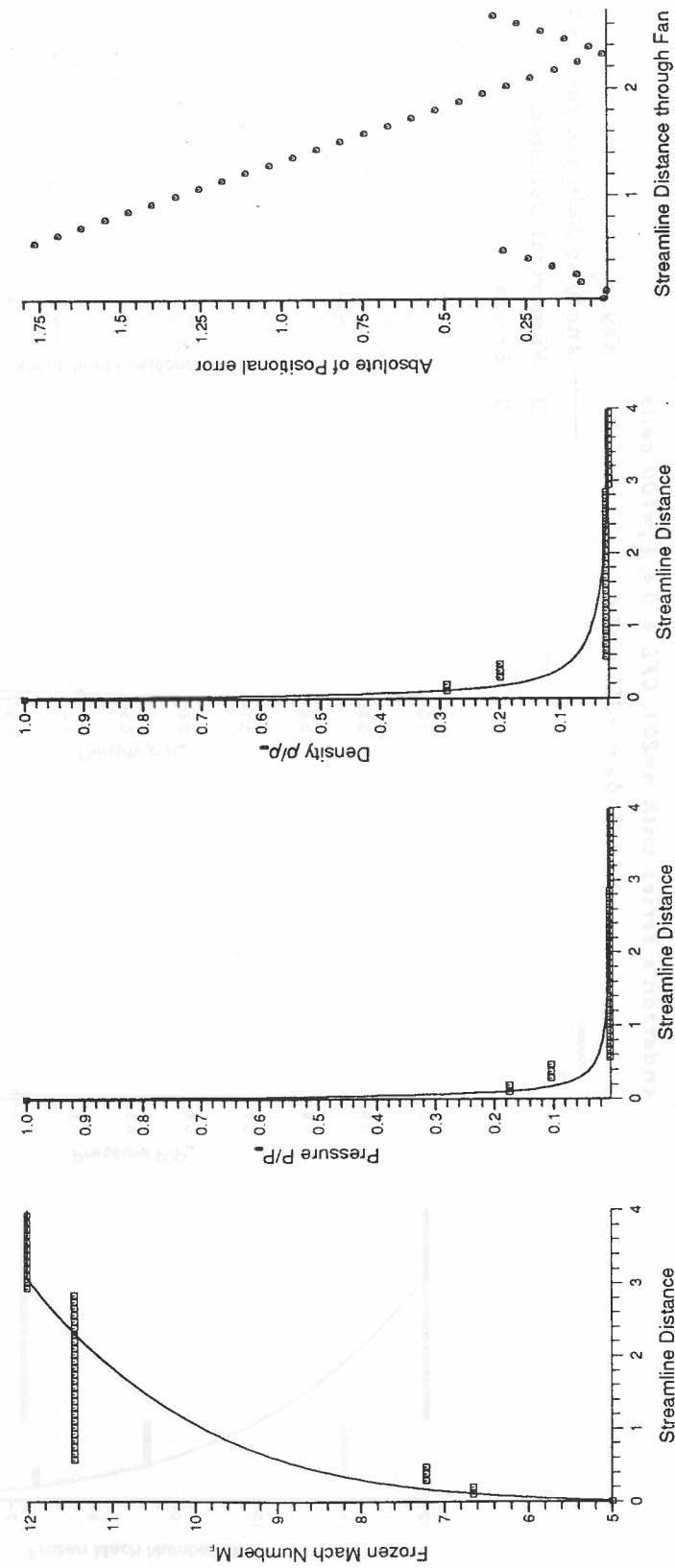


Fig. 4.32

Validation (Inert) : Prandtl-Meyer Expansion wave.
 The effect of quasi random number series on numerical solution.
 Anderson's series with $n=201$. CFL = 0.4, $\xi_s=100$ cells.
 $M_\infty = 5$, $\delta_r = -30^\circ$, $\gamma=1.4$

Key :-
 — Analytic Solution for $\xi_s=0.005$
 □ Numerical Solution.
 ○ Errors.

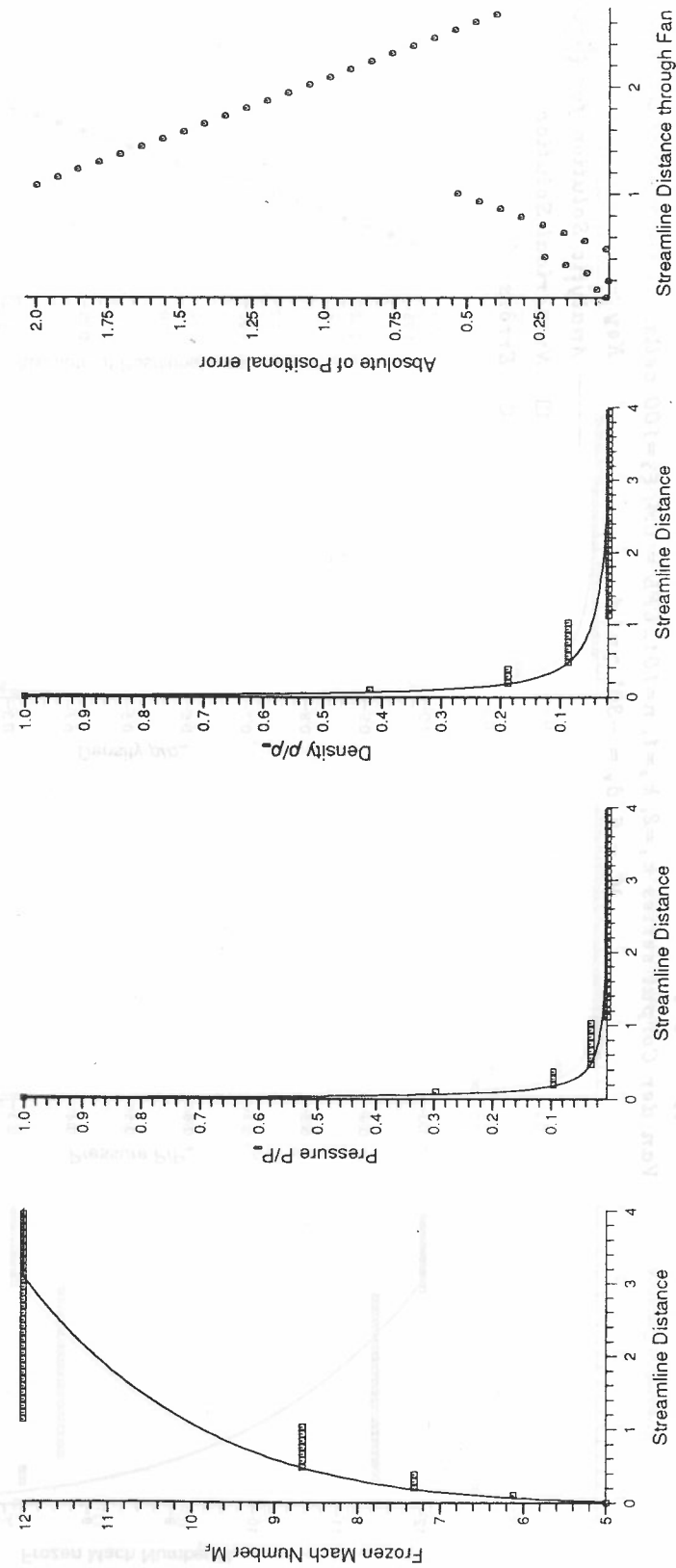


Fig. 4.33

Validation (Inert) : Prandtl-Meyer Expansion wave.
 The effect of quasi random number series on numerical solution.
 Van der Corput series $k_1=2$, $k_2=1$, $n=201$. CFL = 0.4, $\xi_s=100$ cells.
 $M_\infty = 5$, $\delta_r = -30^\circ$, $\gamma=1.4$

Key :-
 — Analytic Solution for $\xi_s=0.005$
 □ Numerical Solution.
 ○ Errors.

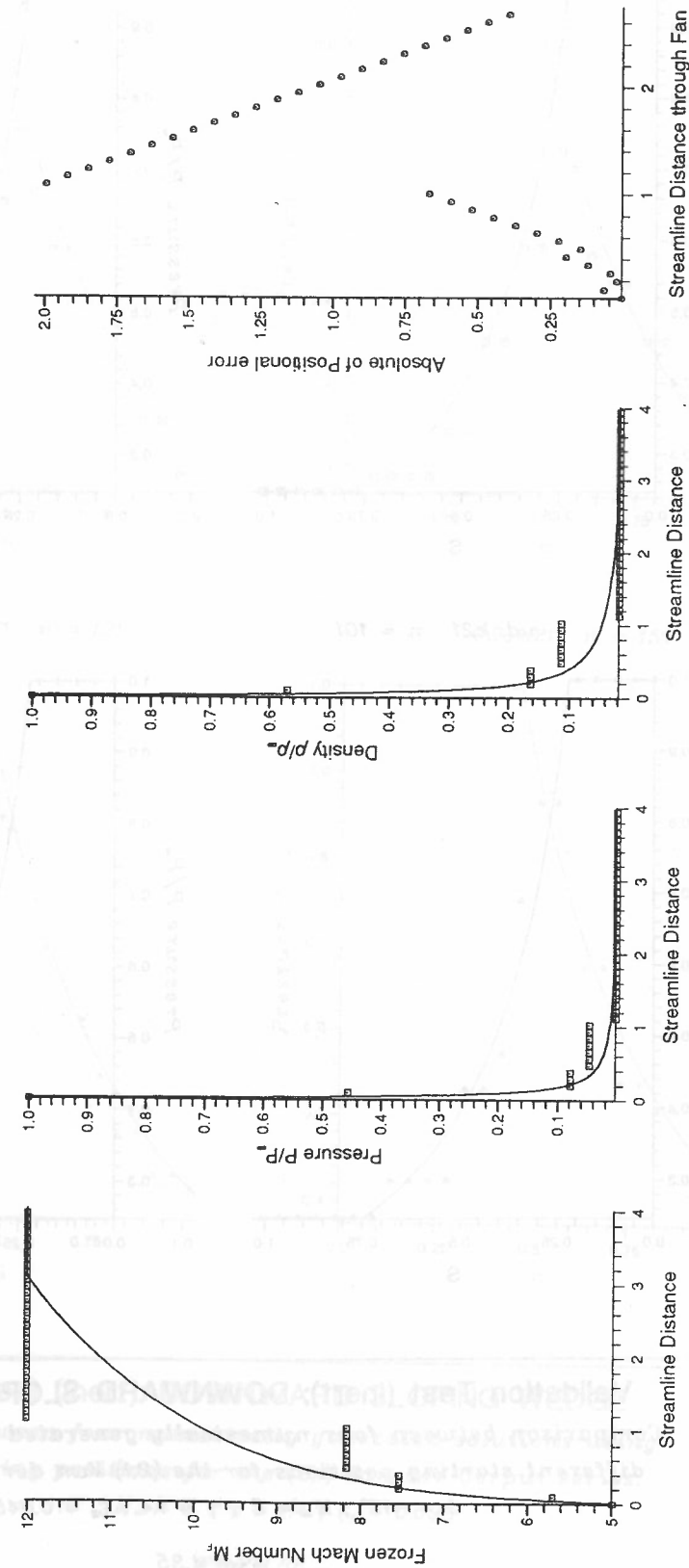
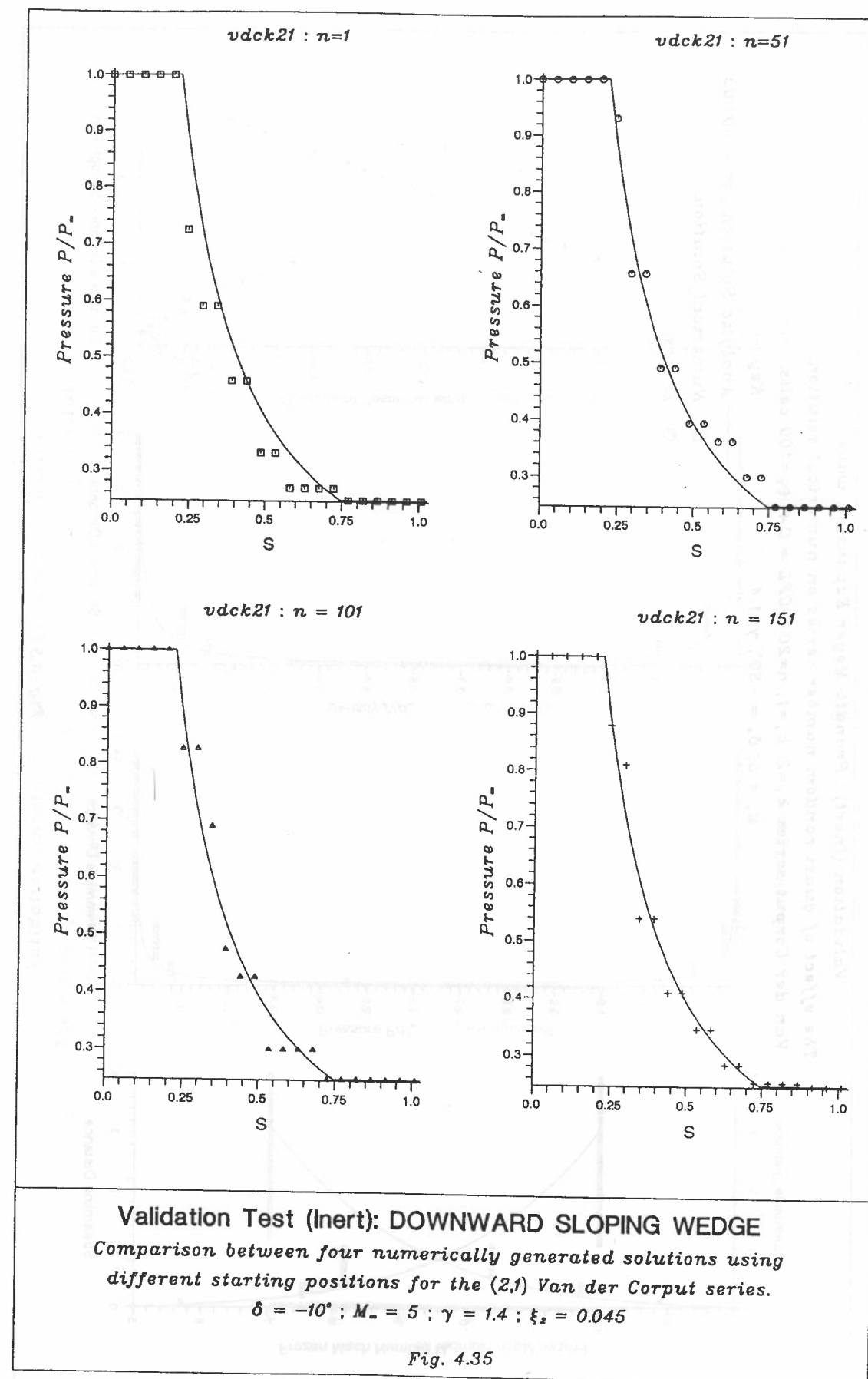
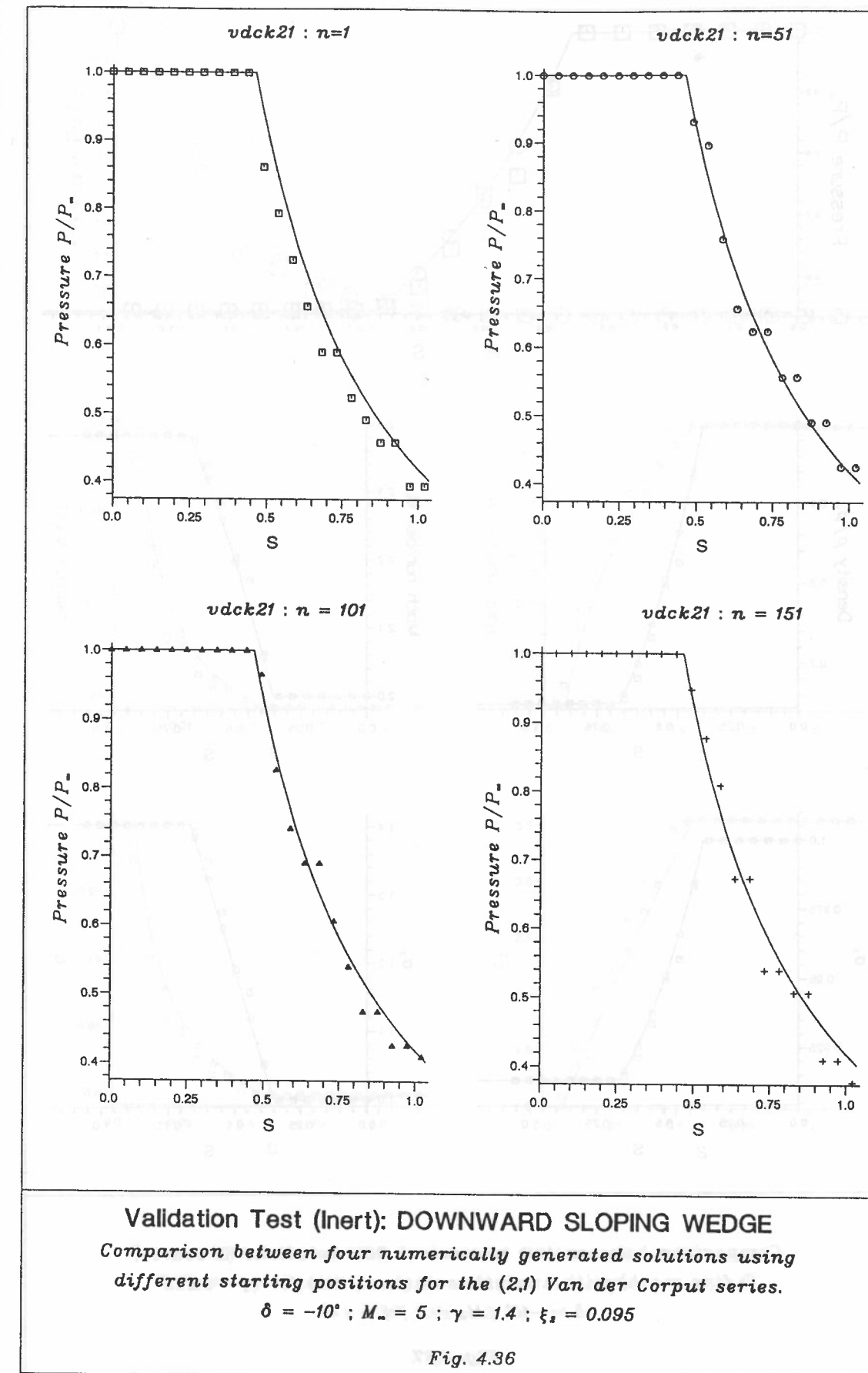
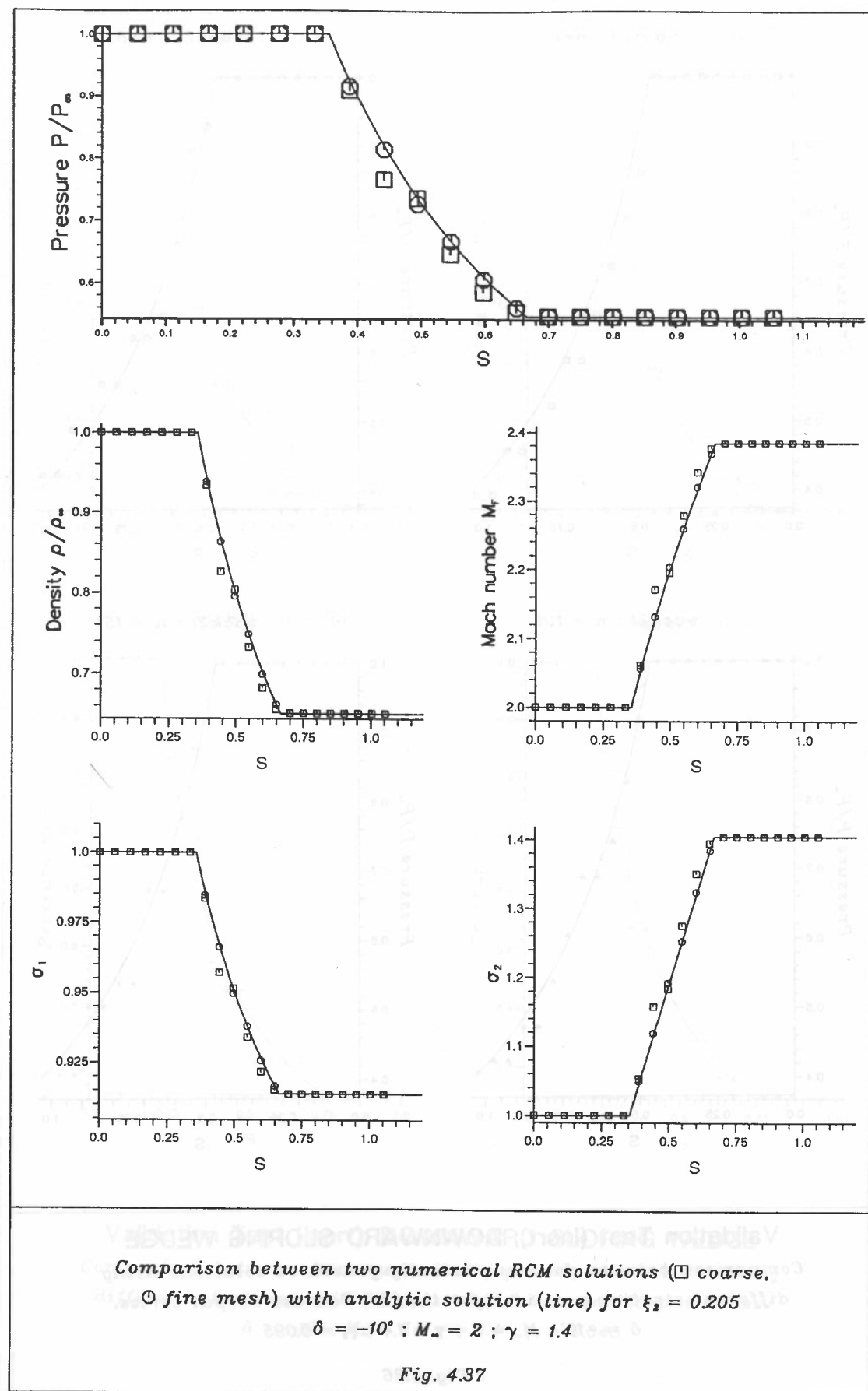
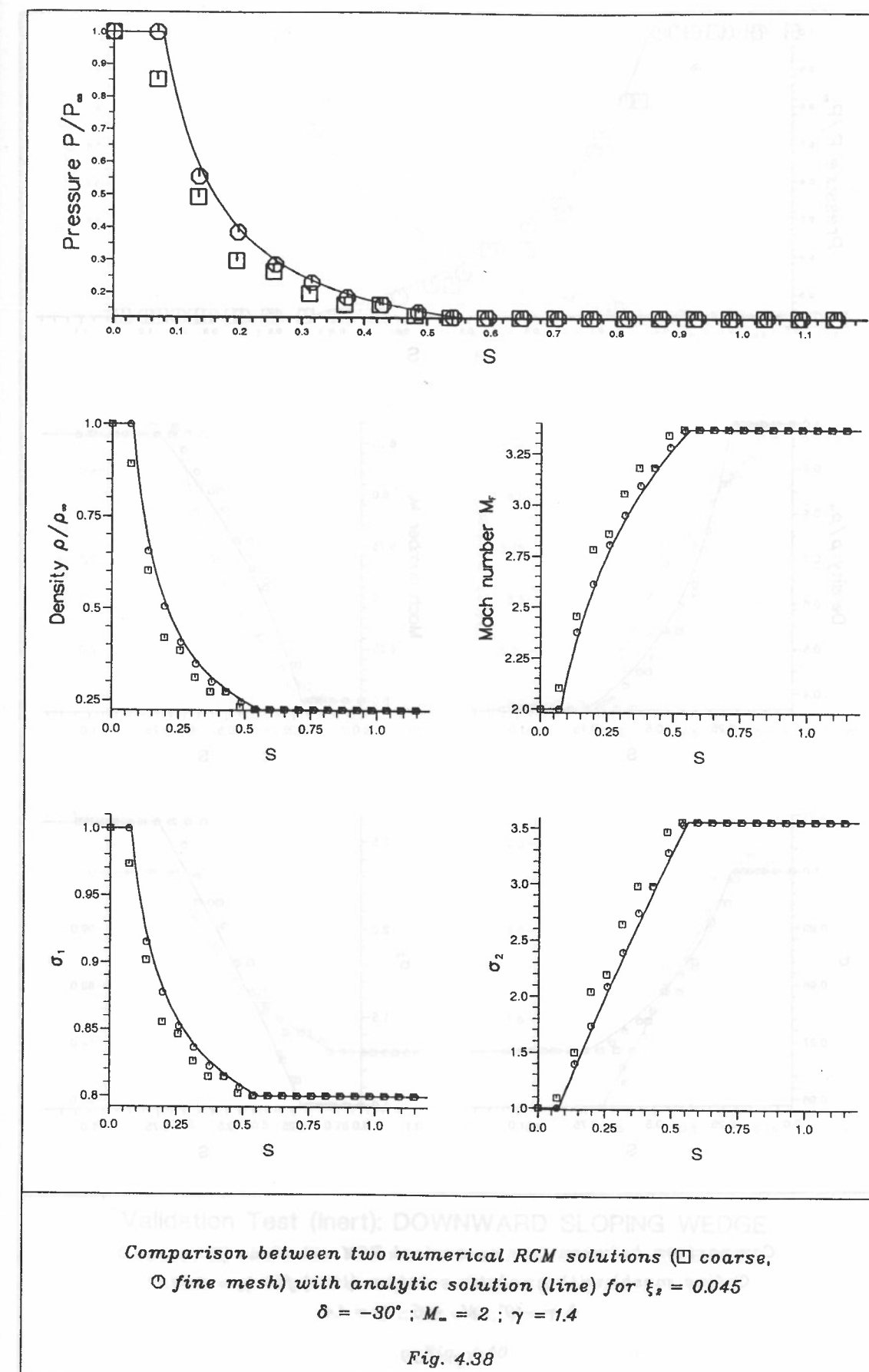
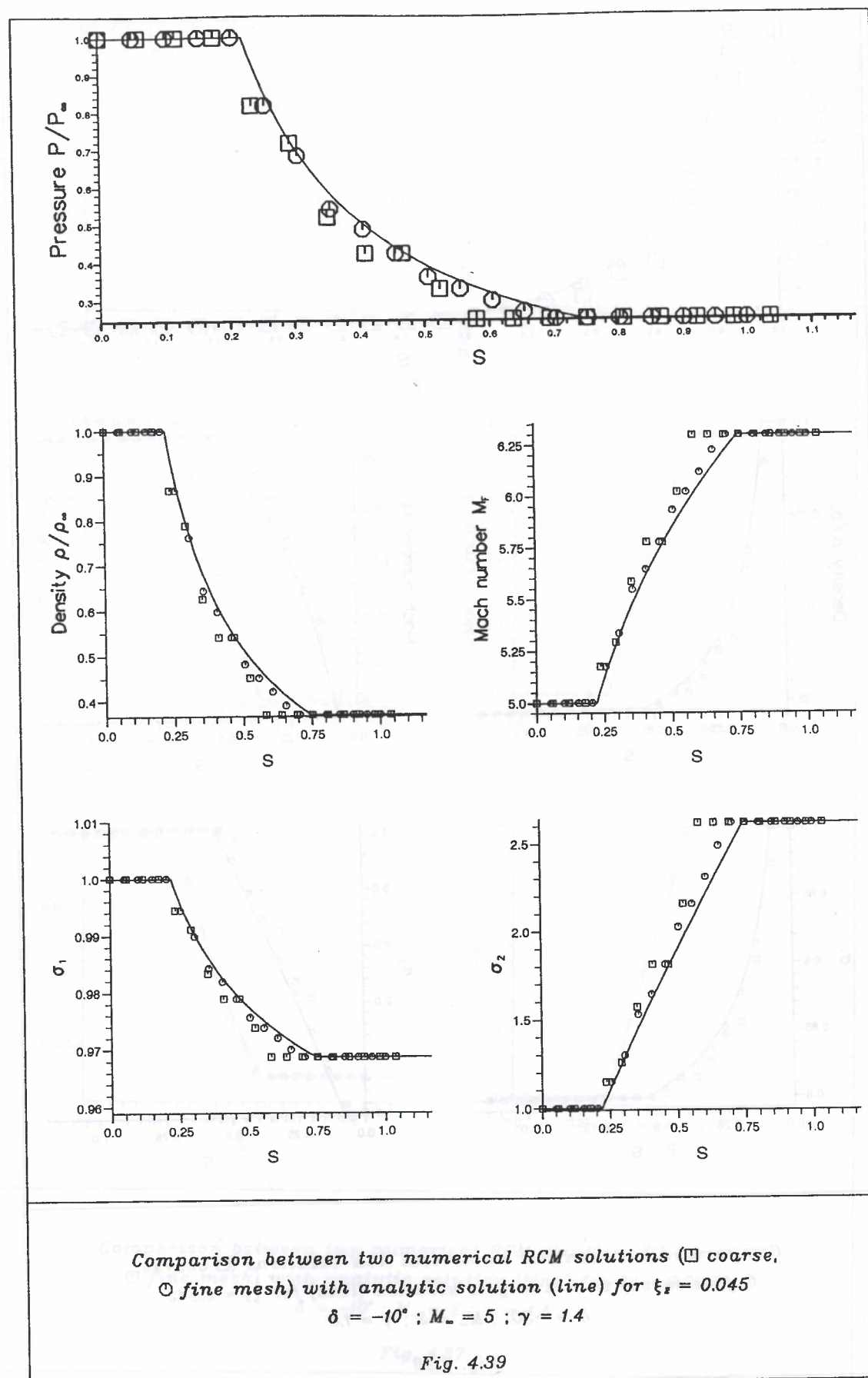
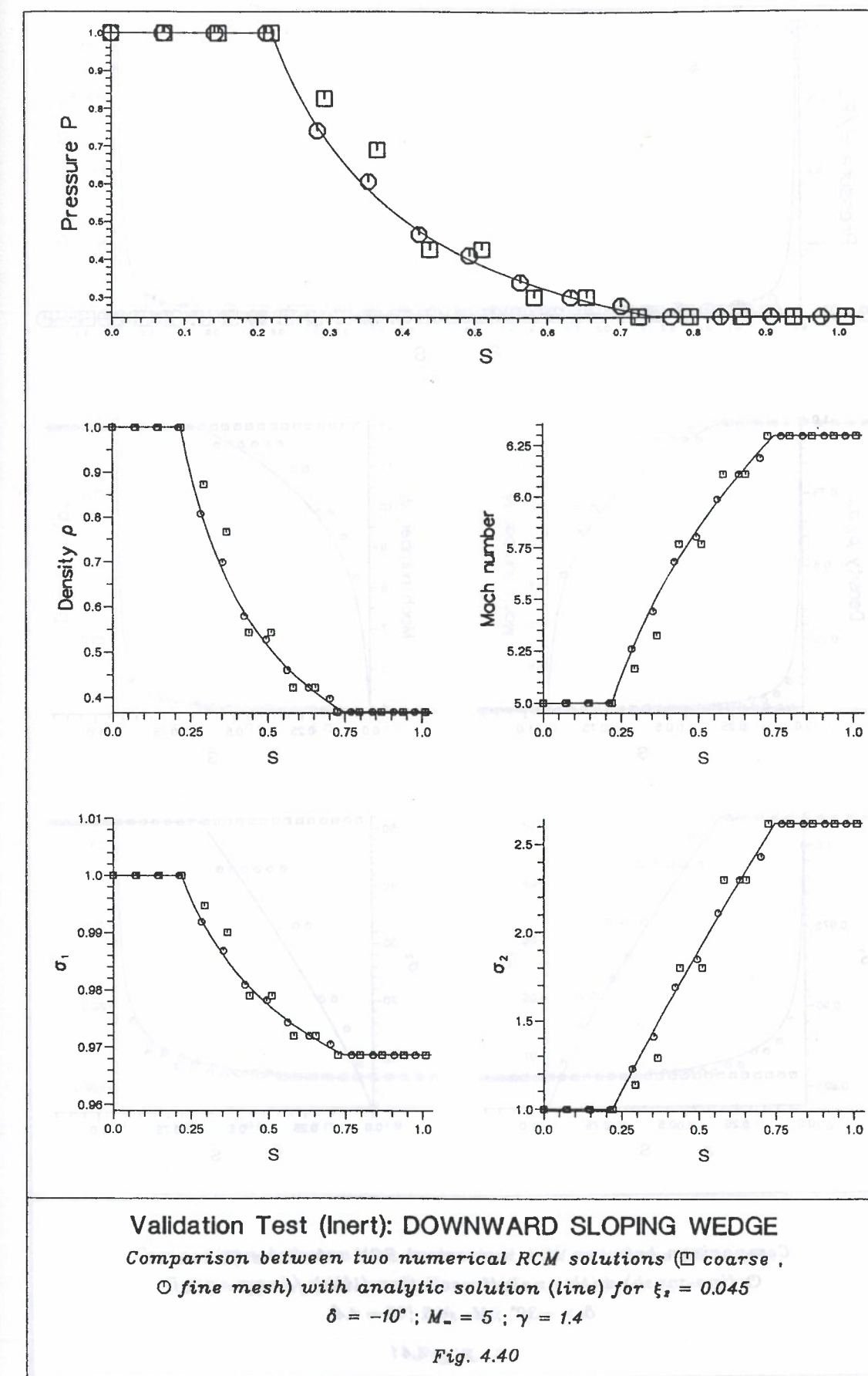
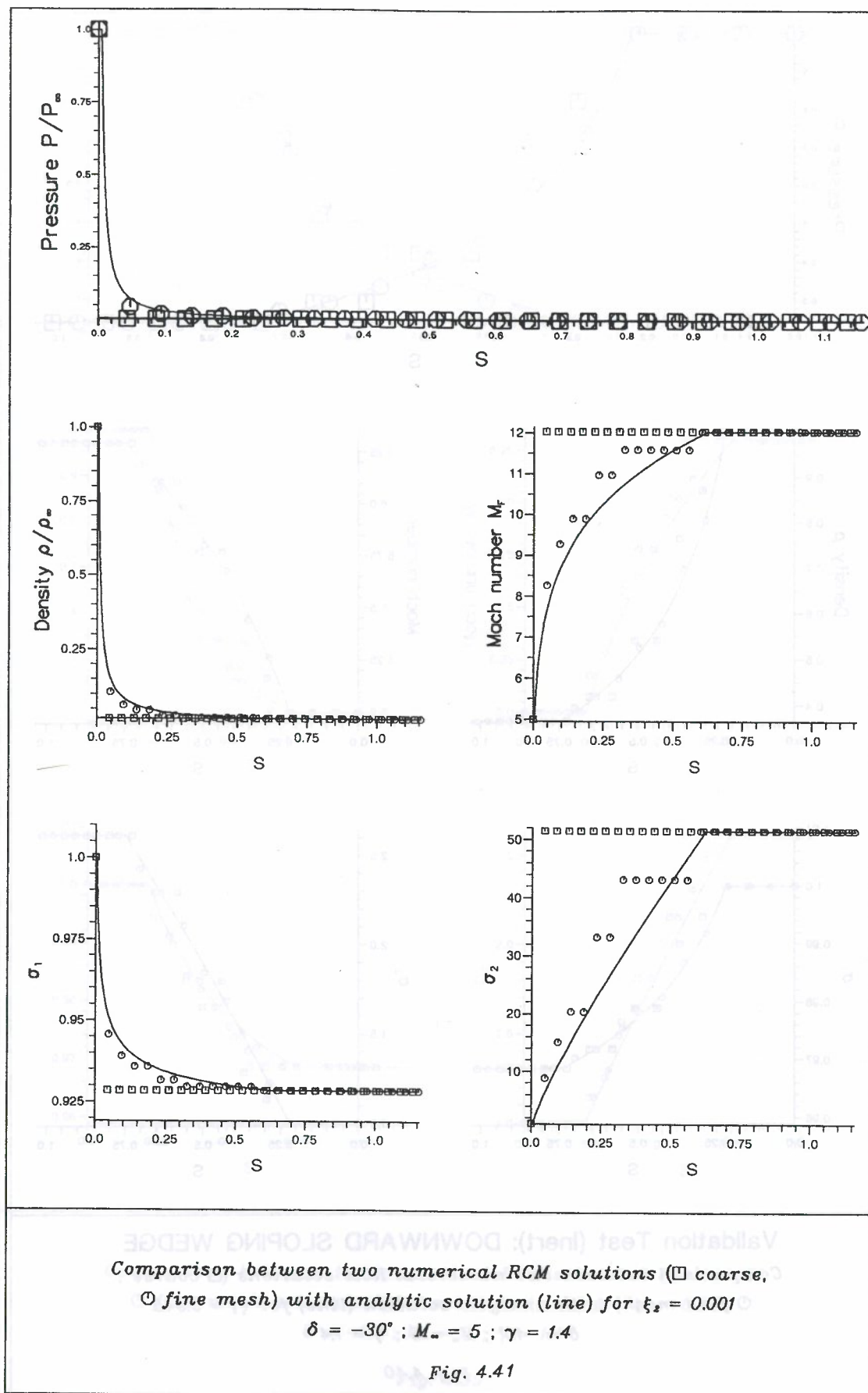
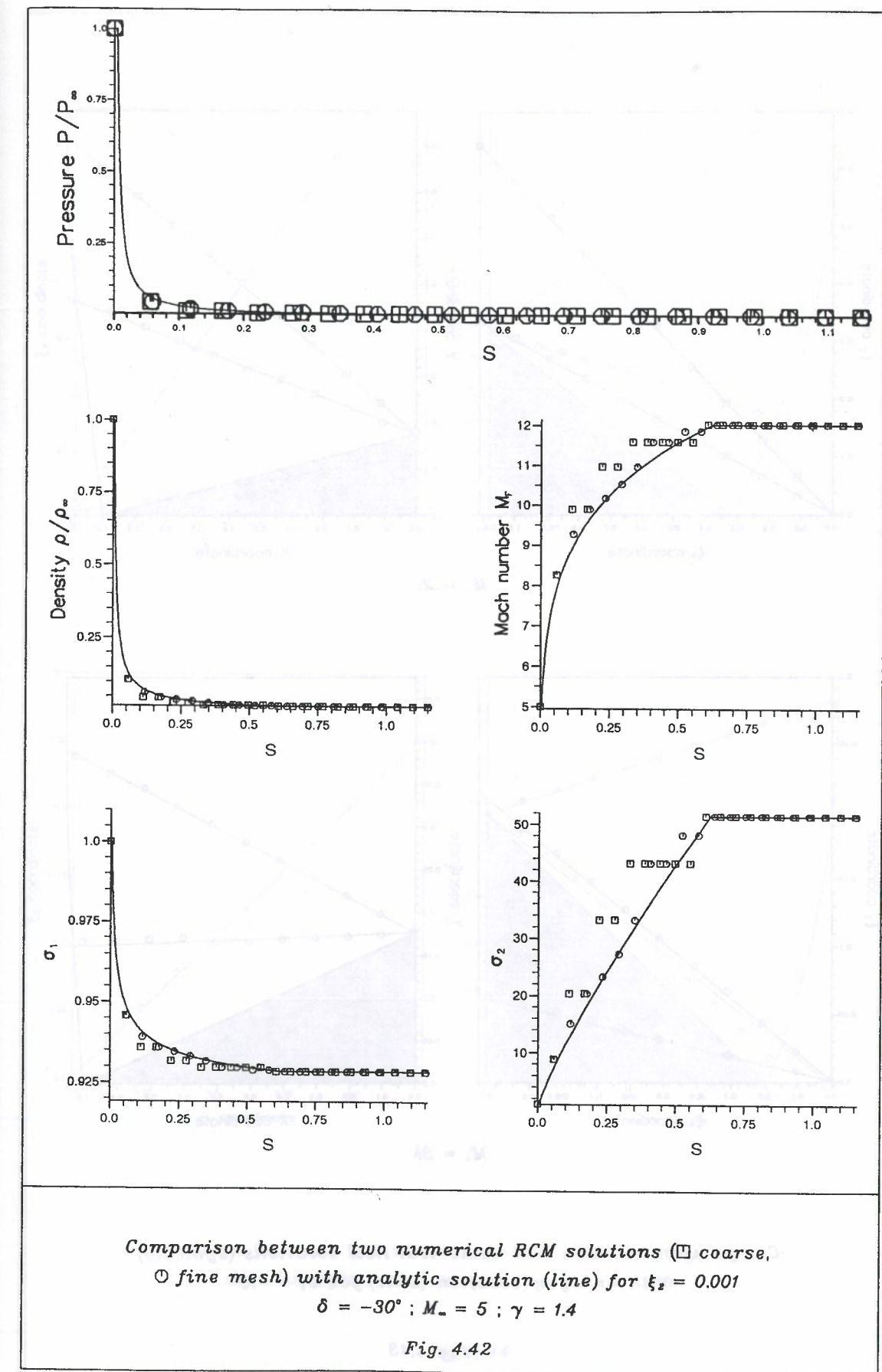


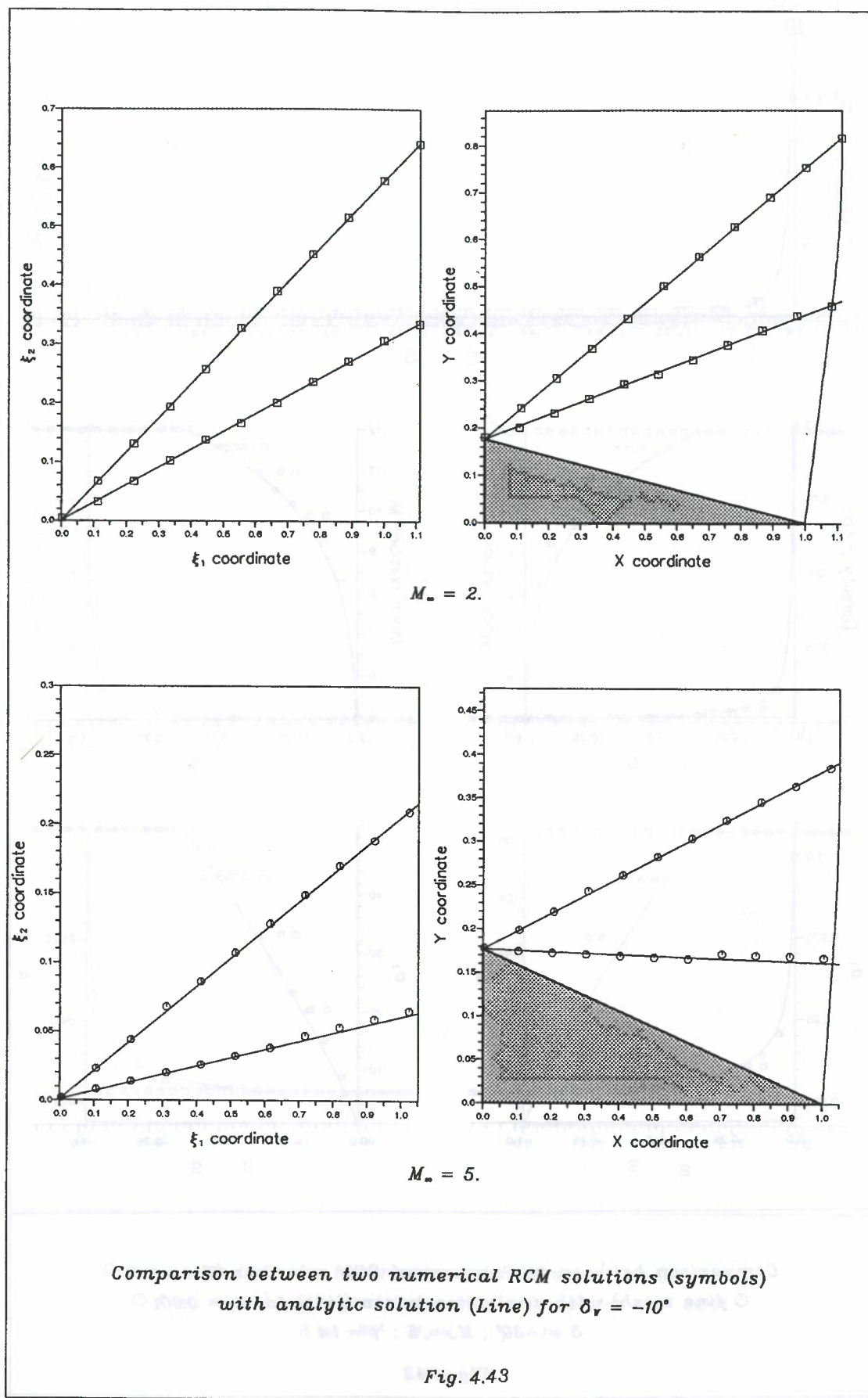
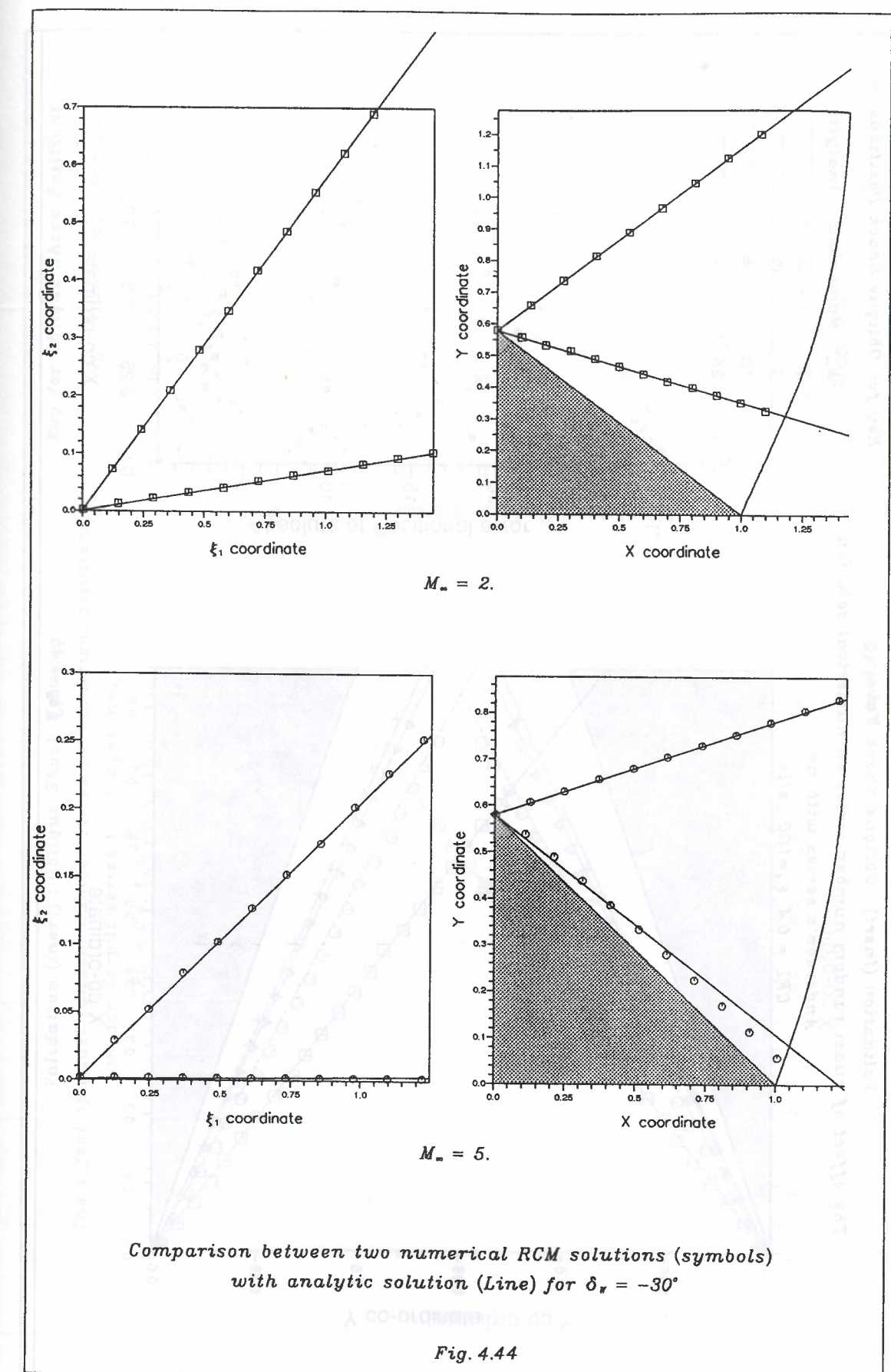
Fig. 4.34











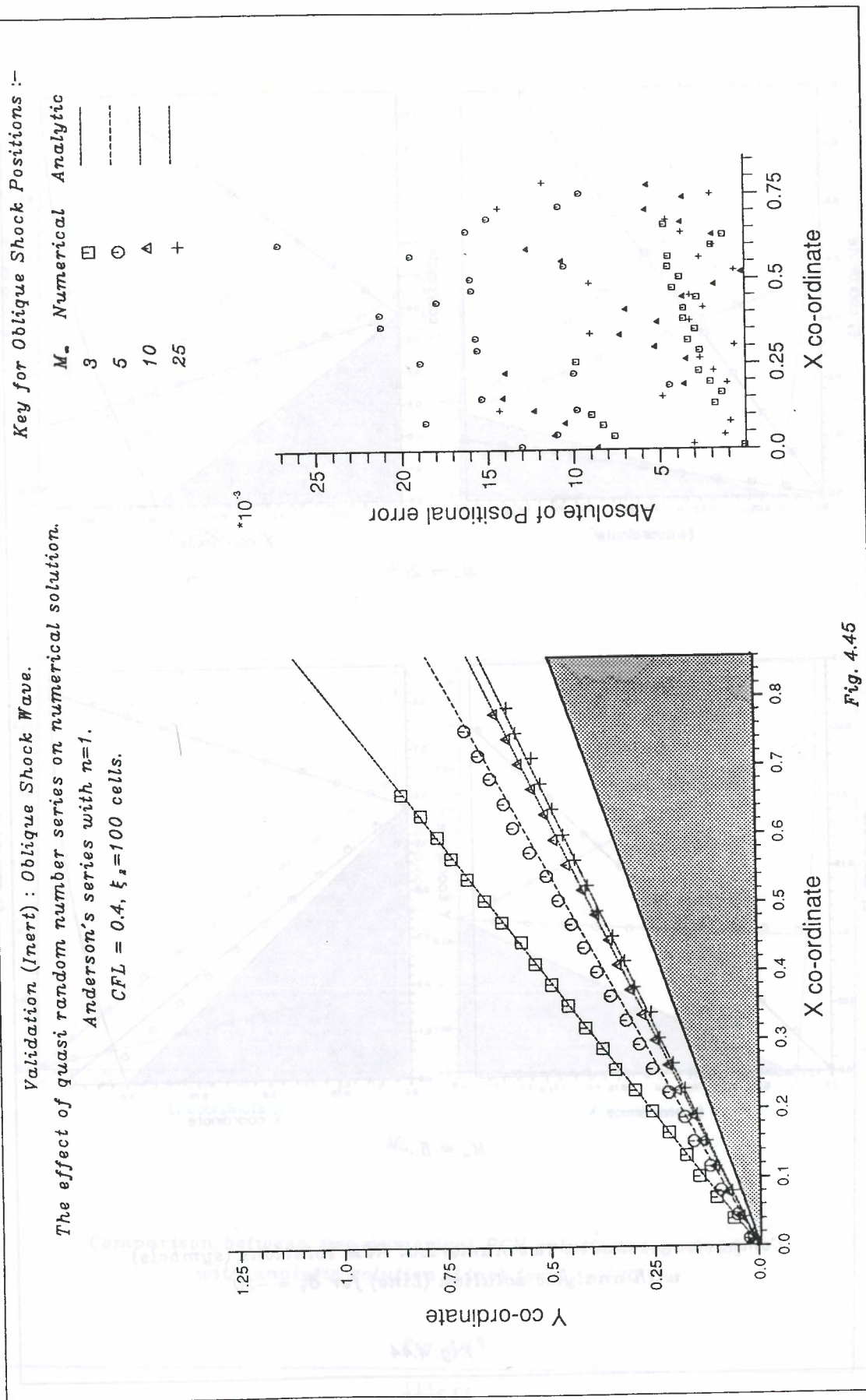


Fig. 4.45

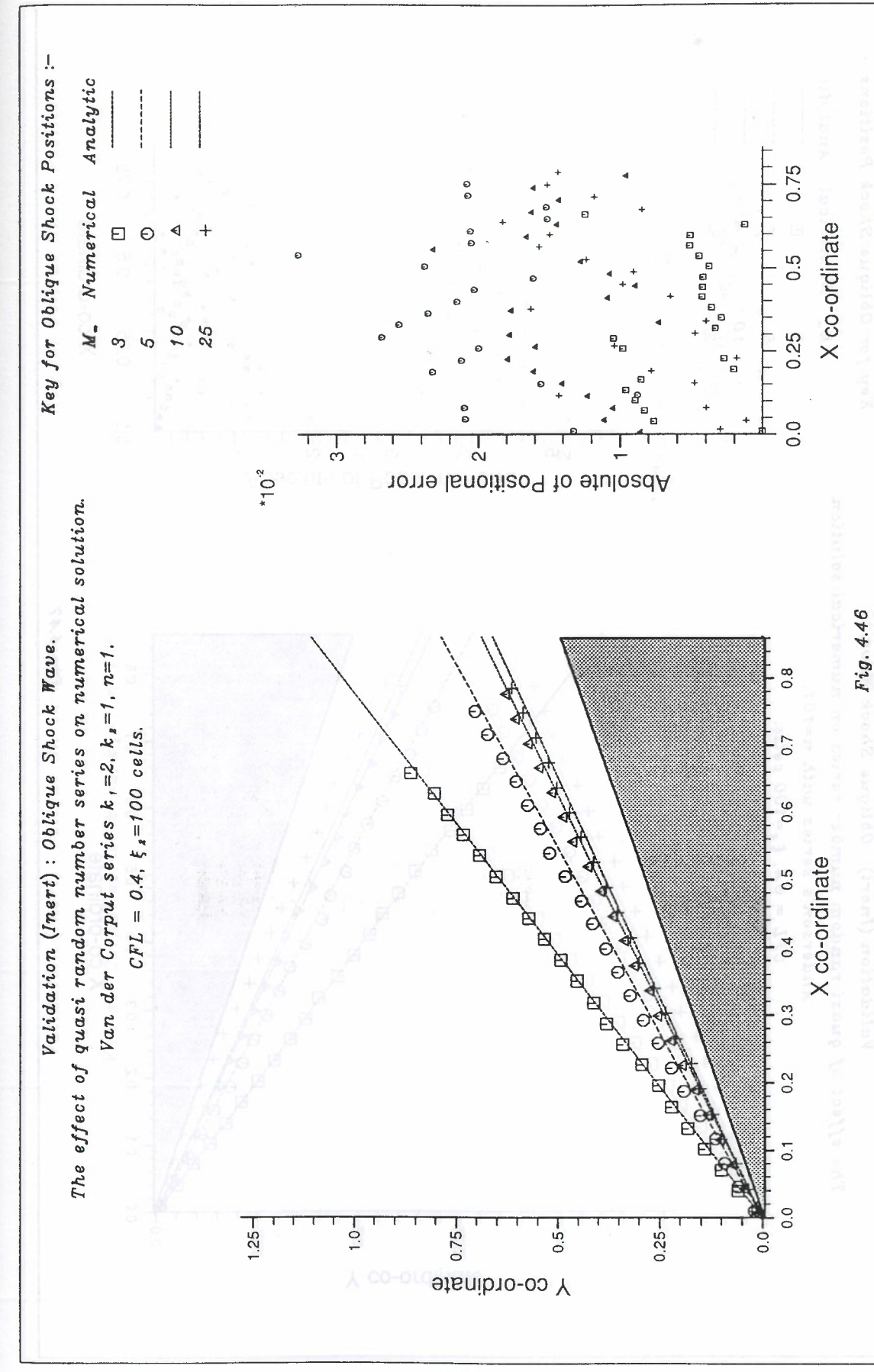
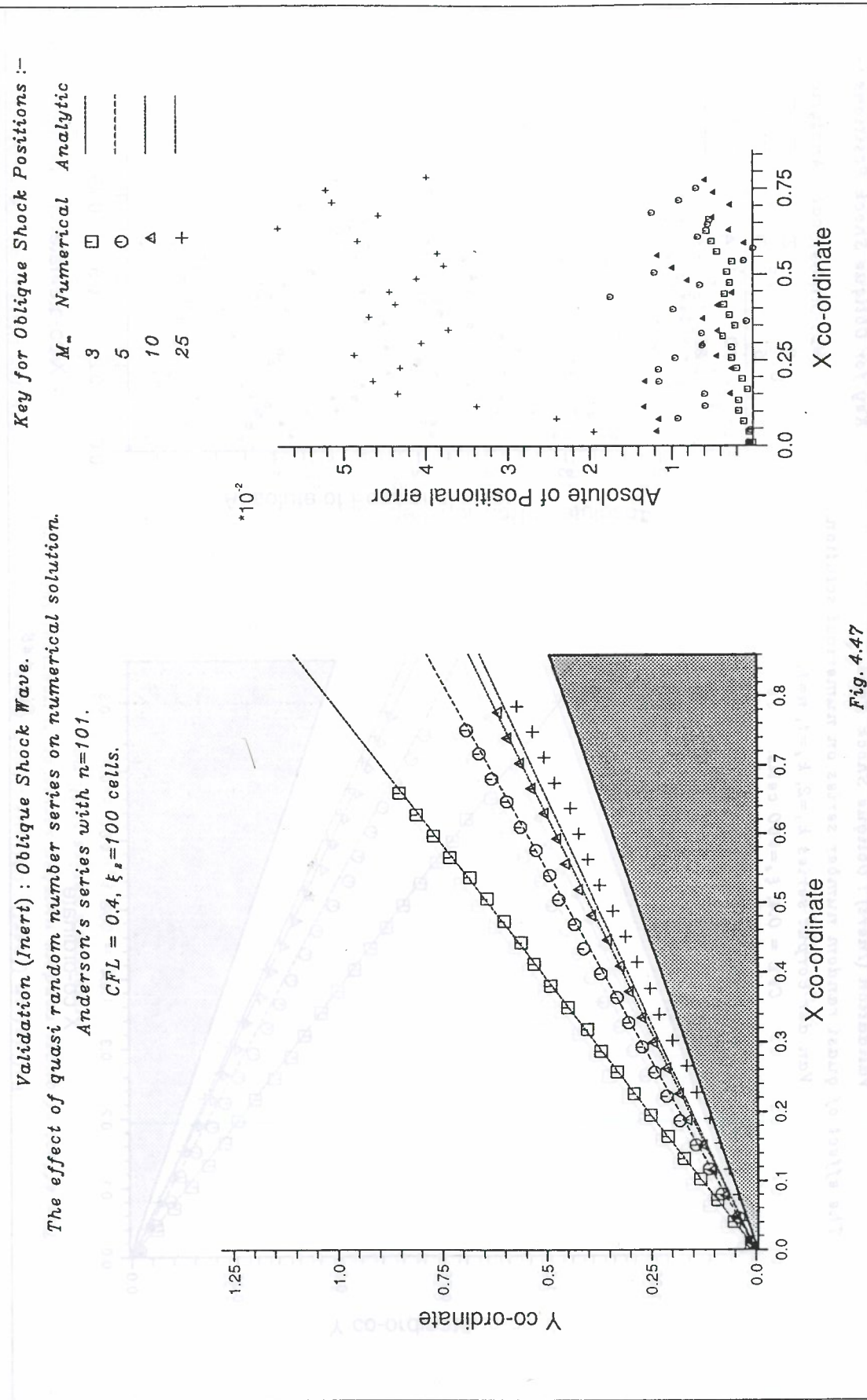
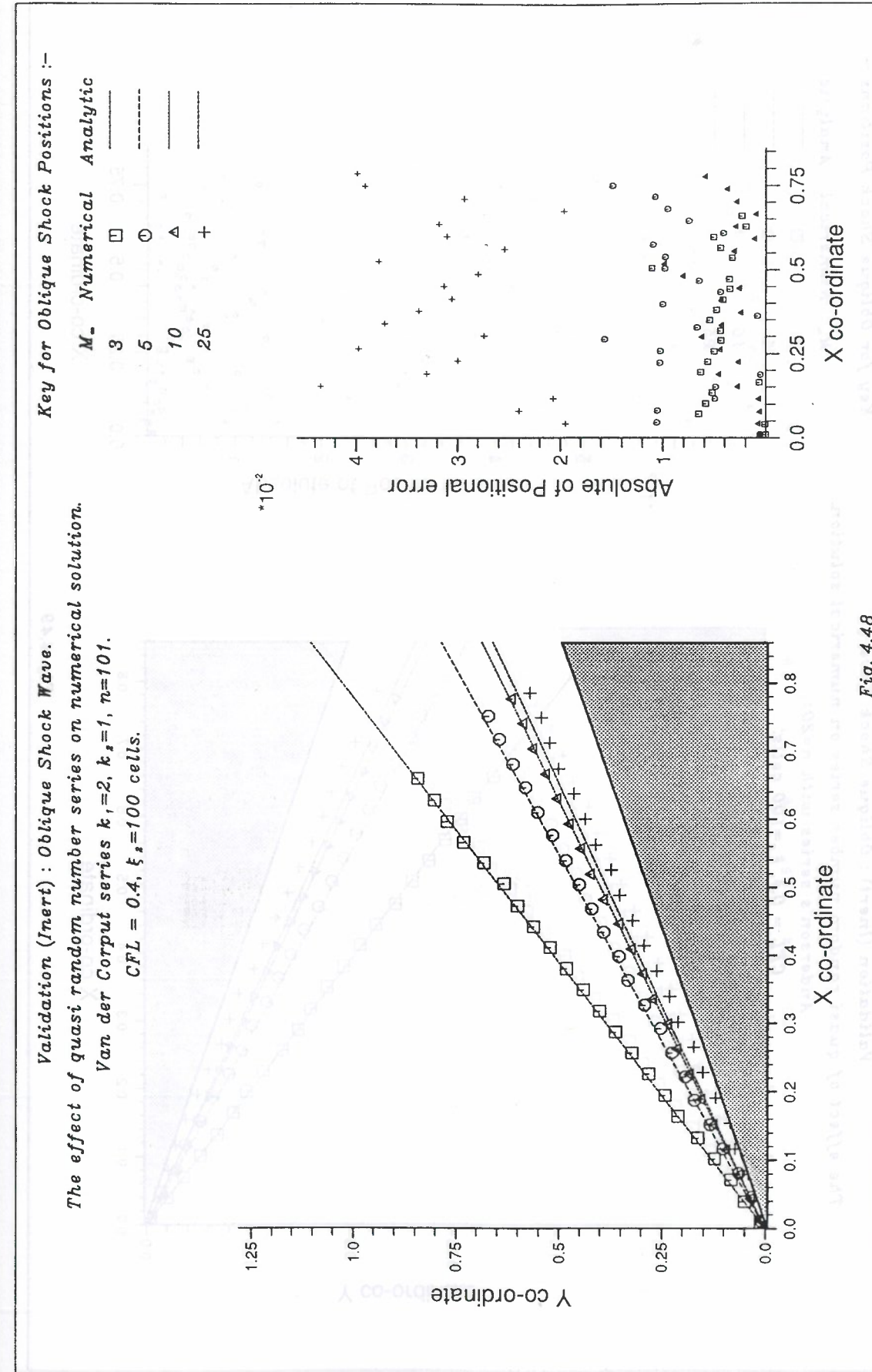


Fig. 4.46



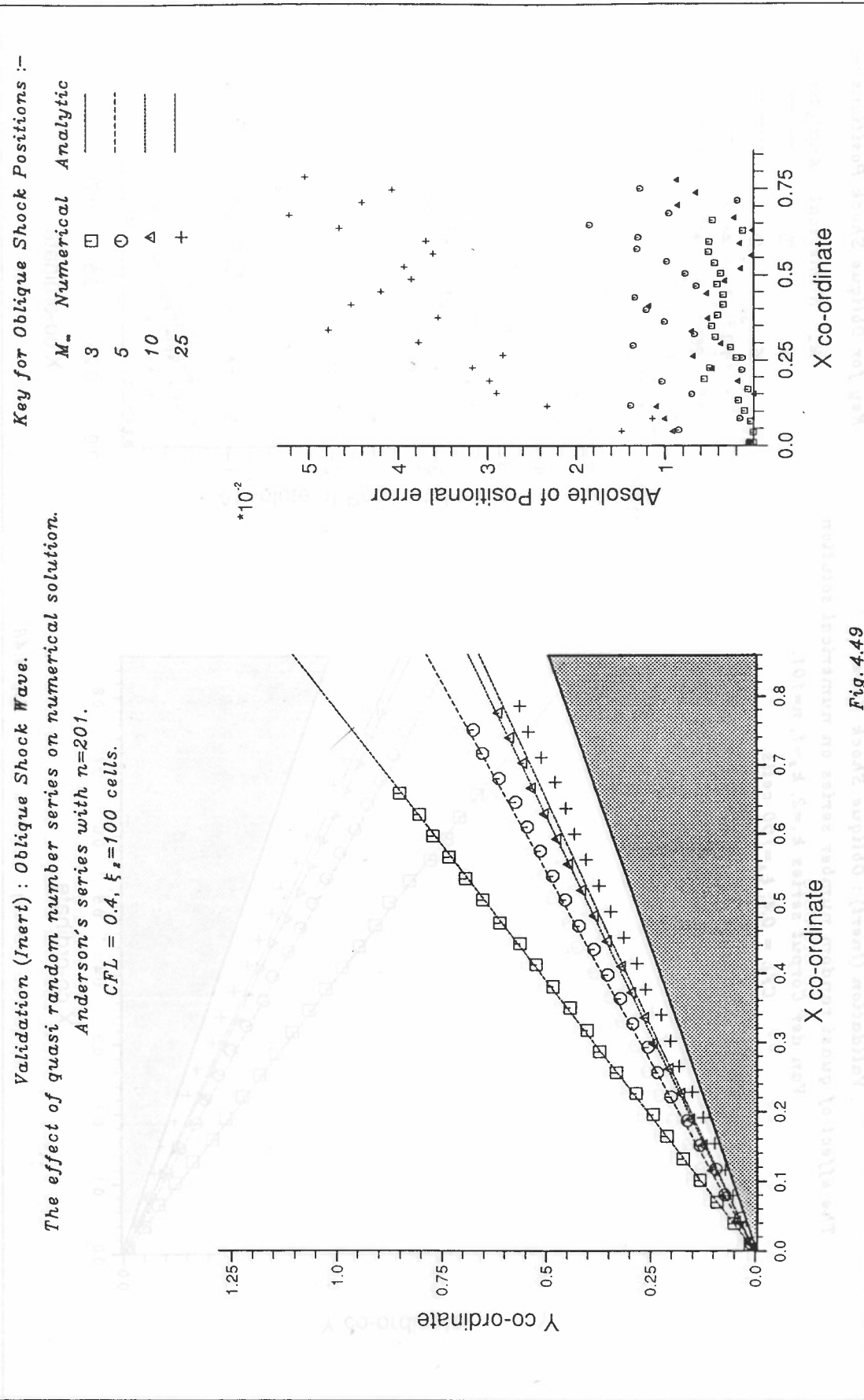


Fig. 4.49

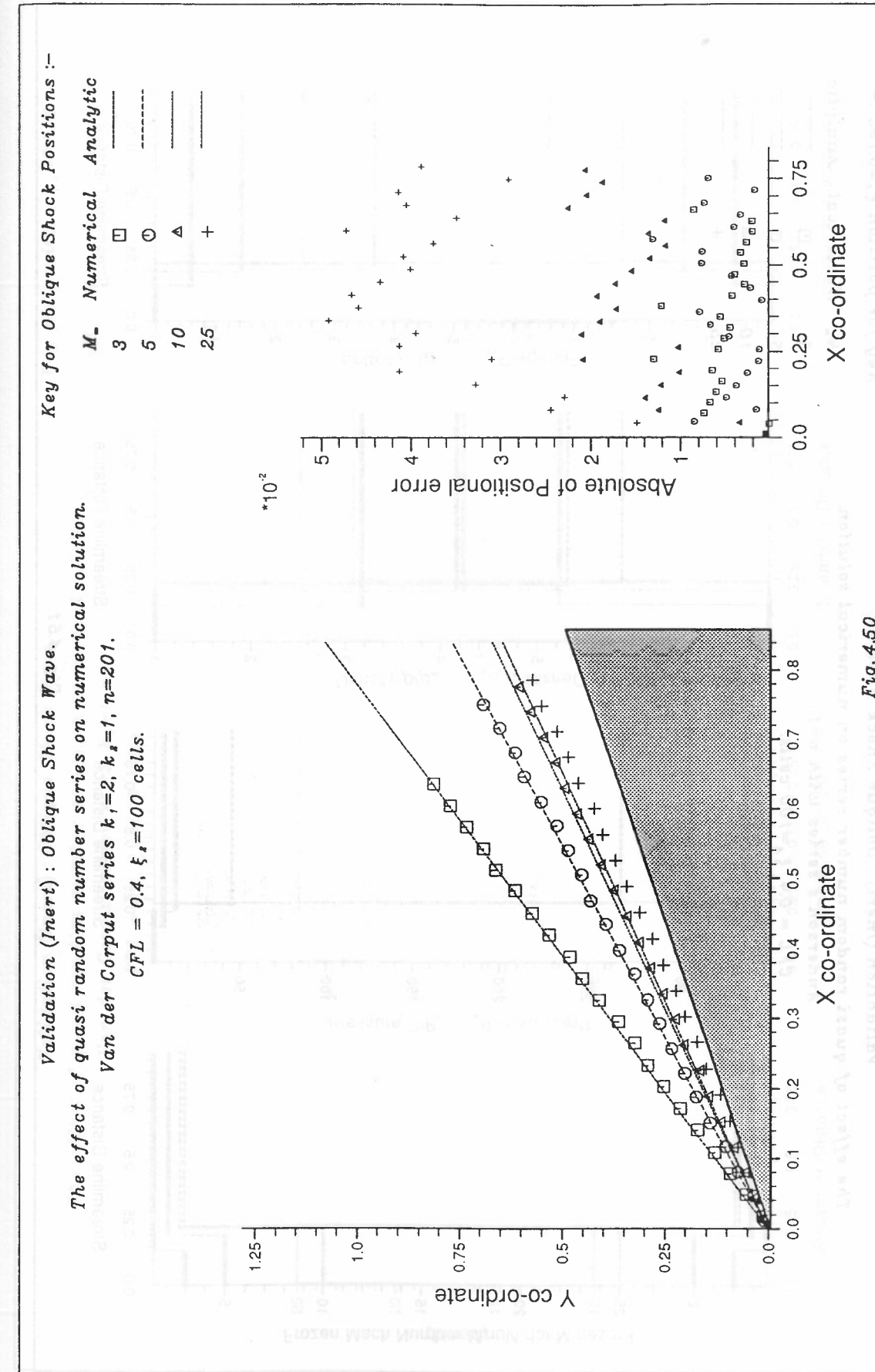
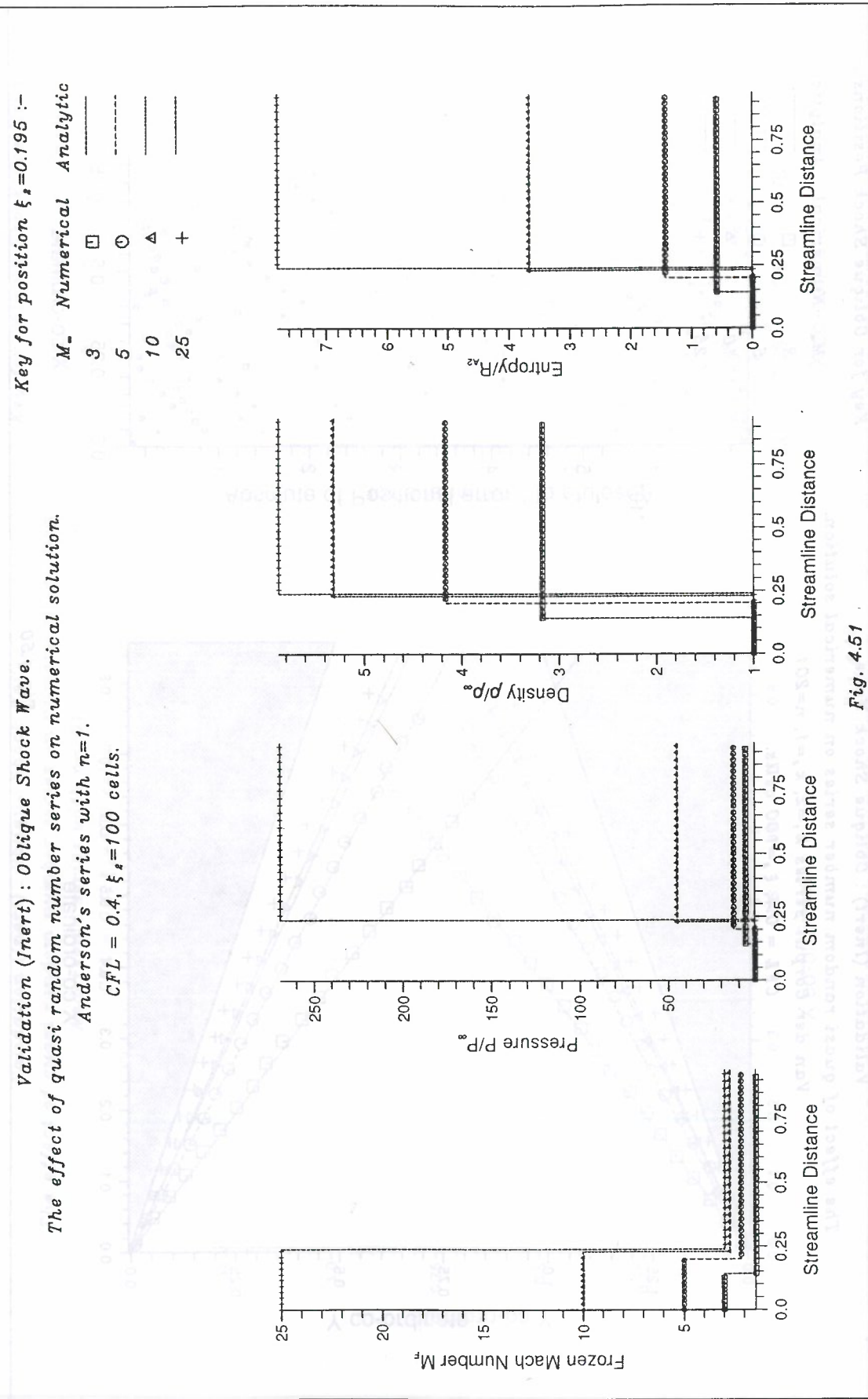
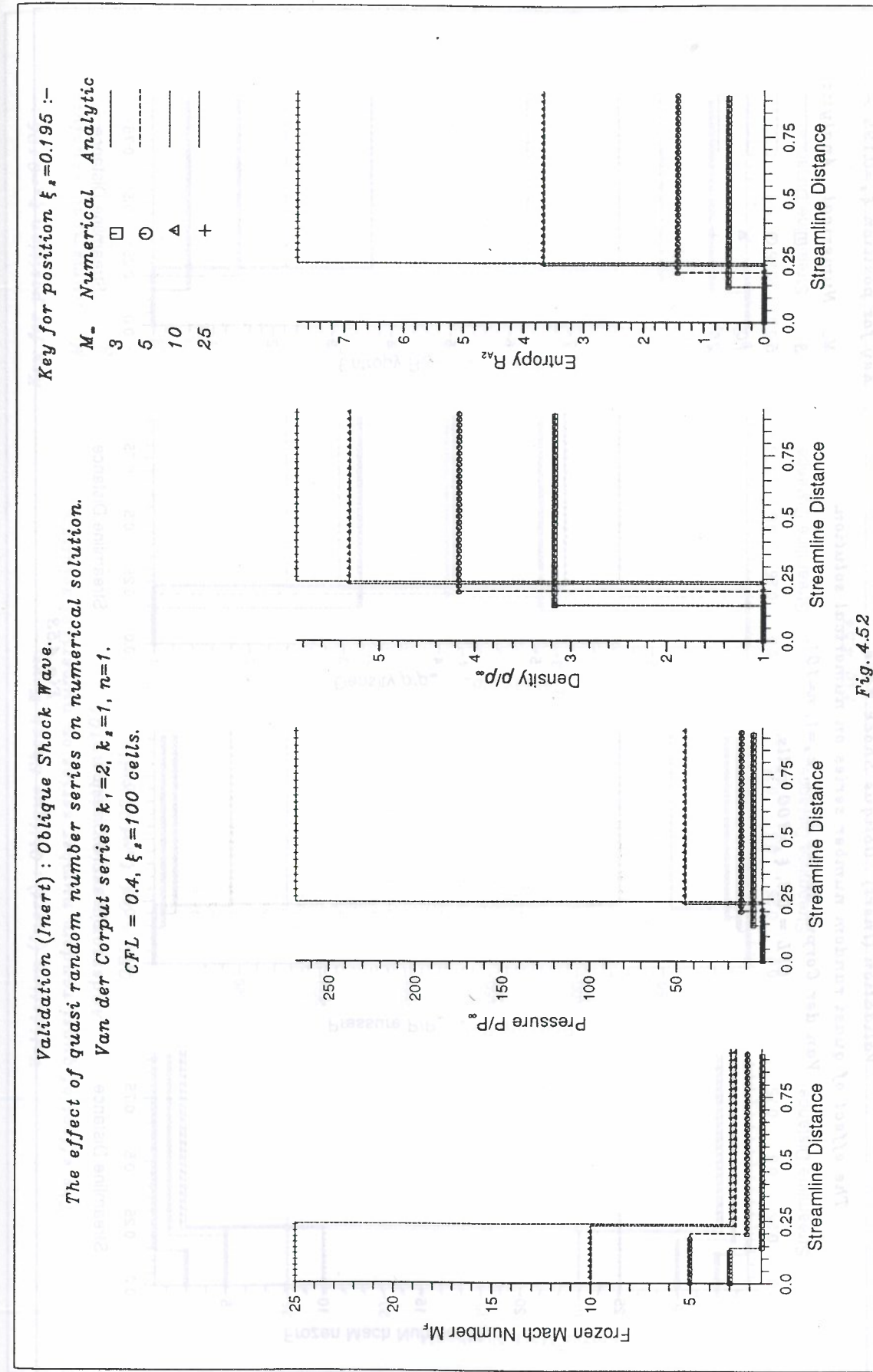


Fig. 4.50



Validation (Inert) : Oblique Shock Wave.
 The effect of quasi random number series on numerical solution.
 Van der Corput series $k_1=2, k_2=1, n=101$.
 $CFL = 0.4, \xi_s=100$ cells.

Key for position $\xi_s=0.195$:-

M_∞	Numerical	Analytic
3	□	-----
5	○	-----
10	△	-----
25	+	-----

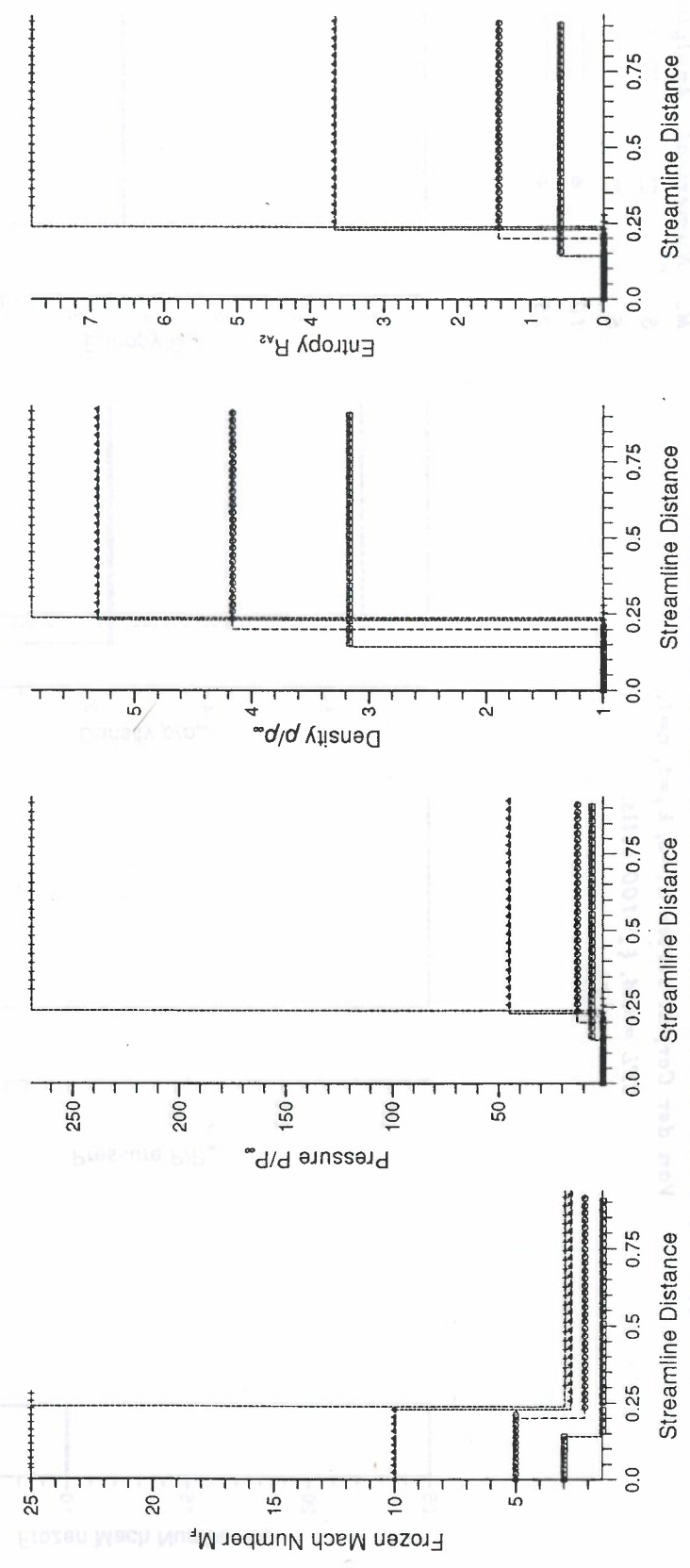


Fig. 4.53

Validation (Inert) : Oblique Shock Wave.
 The effect of quasi random number series on numerical solution.
 Anderson's series with $n=101$.
 $CFL = 0.4, \xi_s=100$ cells.

Key for position $\xi_s=0.195$:-

M_∞	Numerical	Analytic
3	□	-----
5	○	-----
10	△	-----
25	+	-----

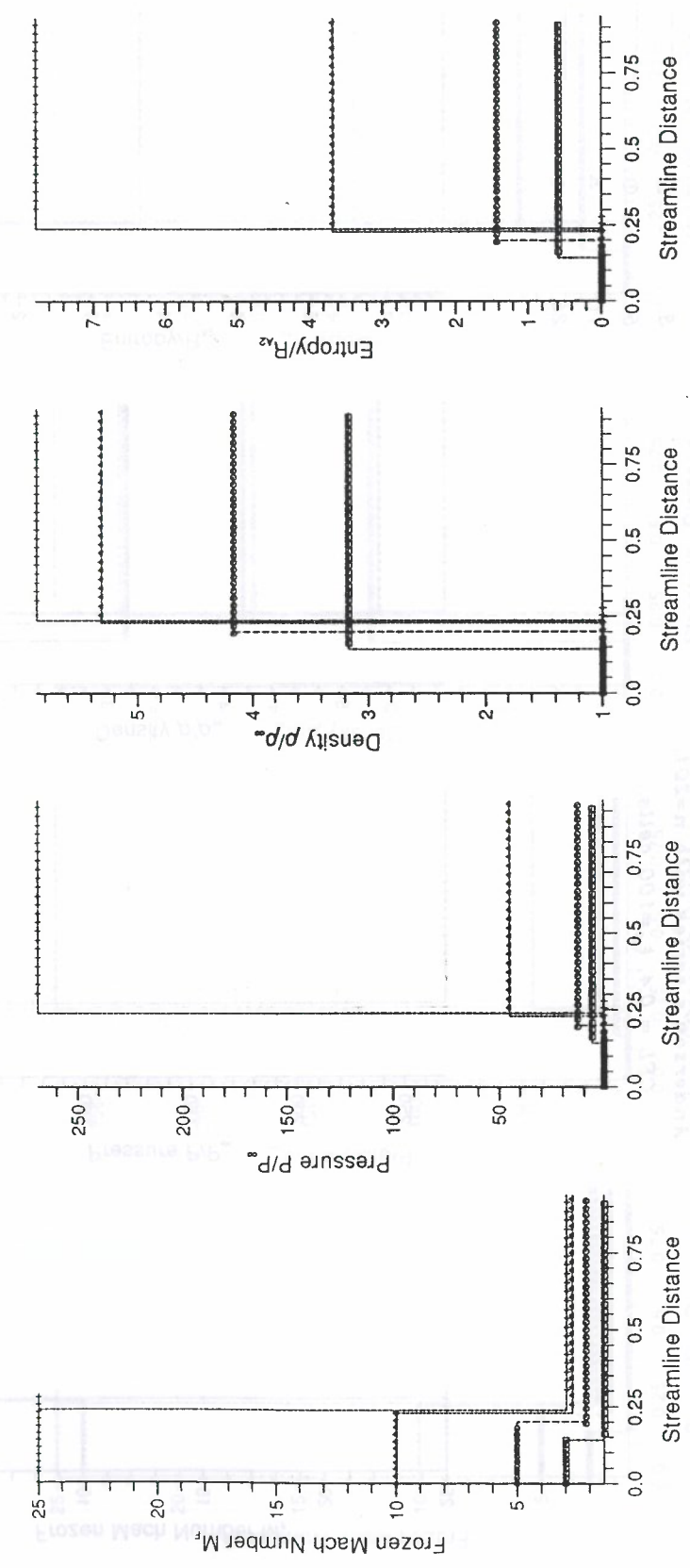
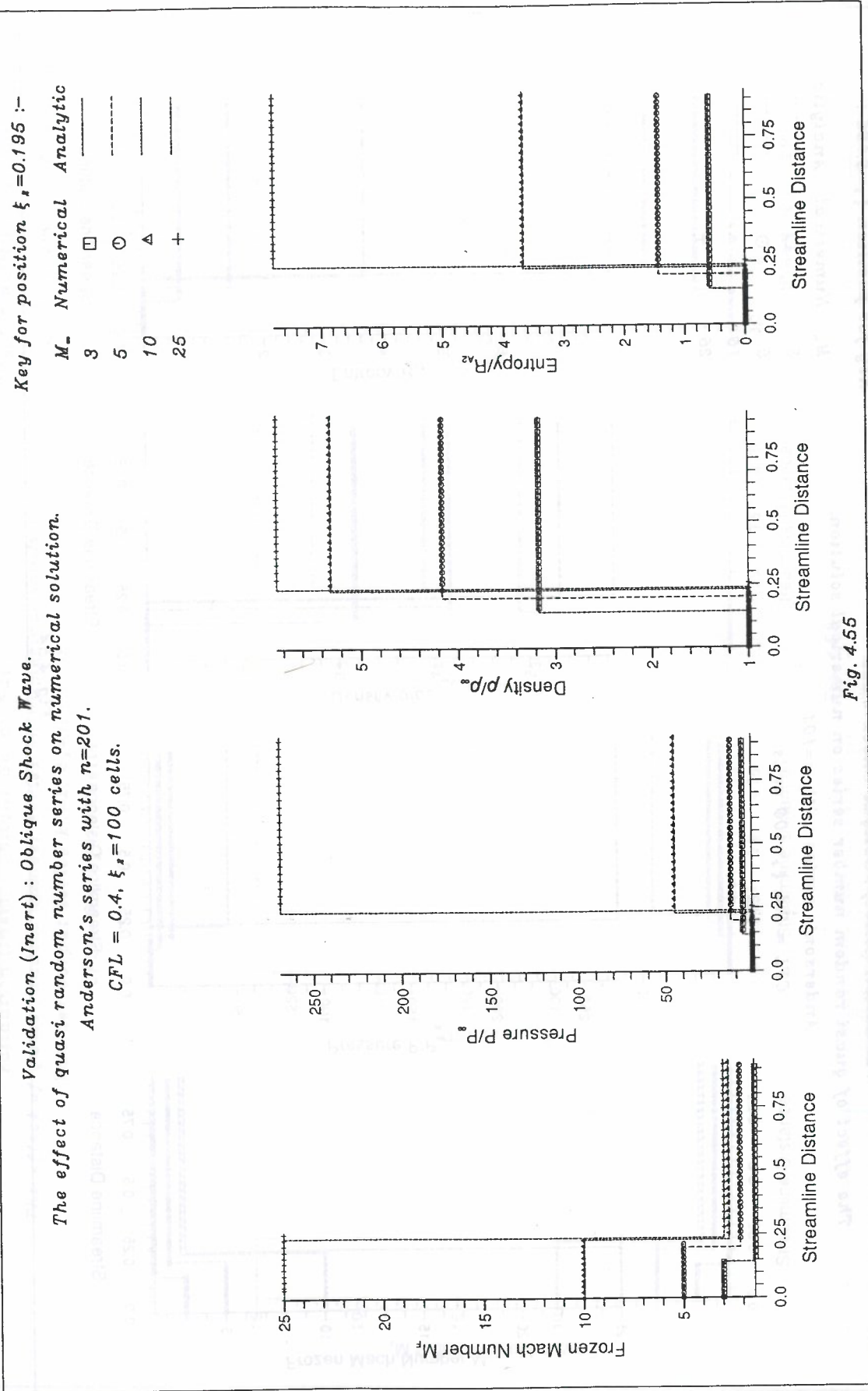
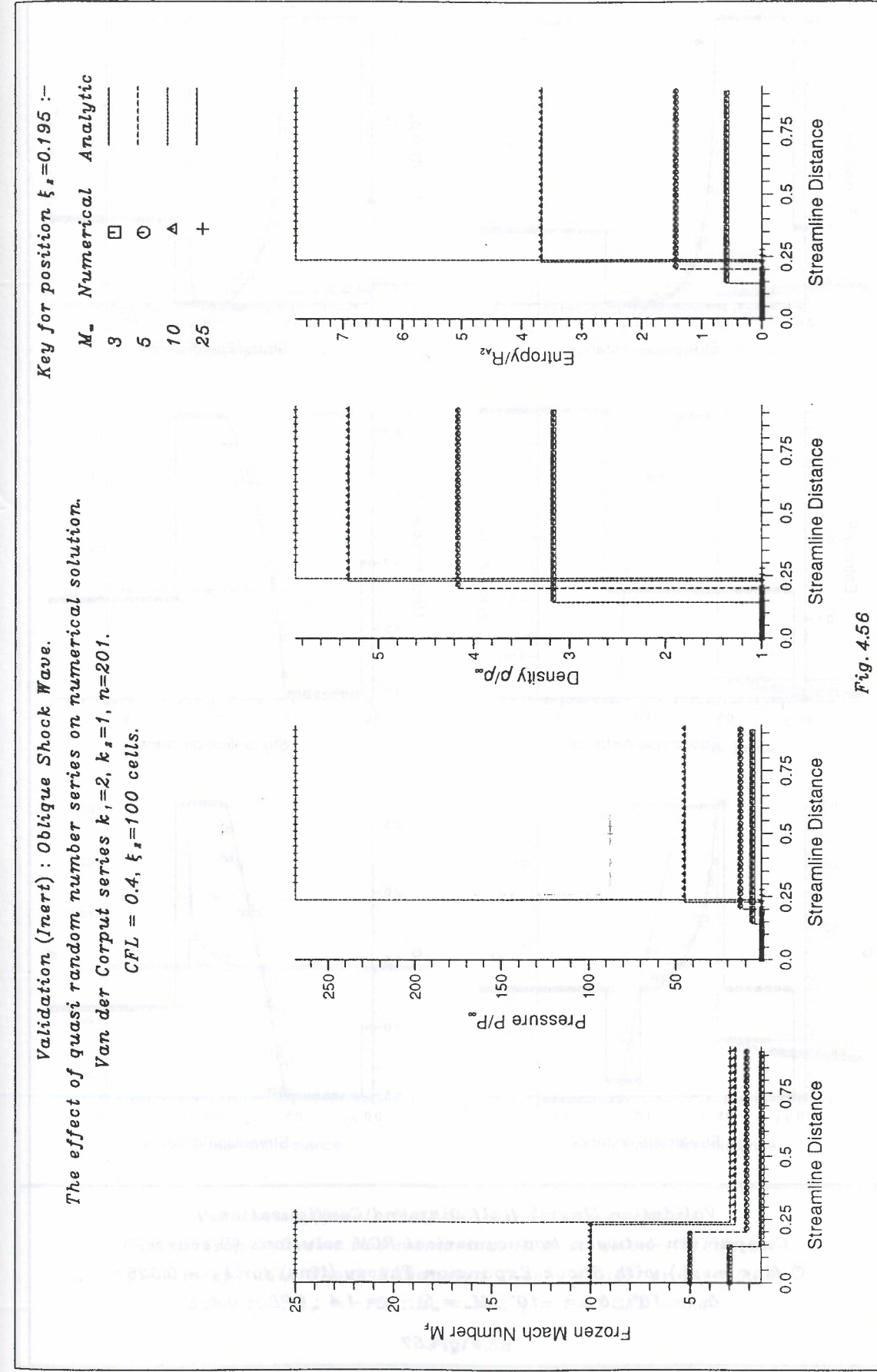
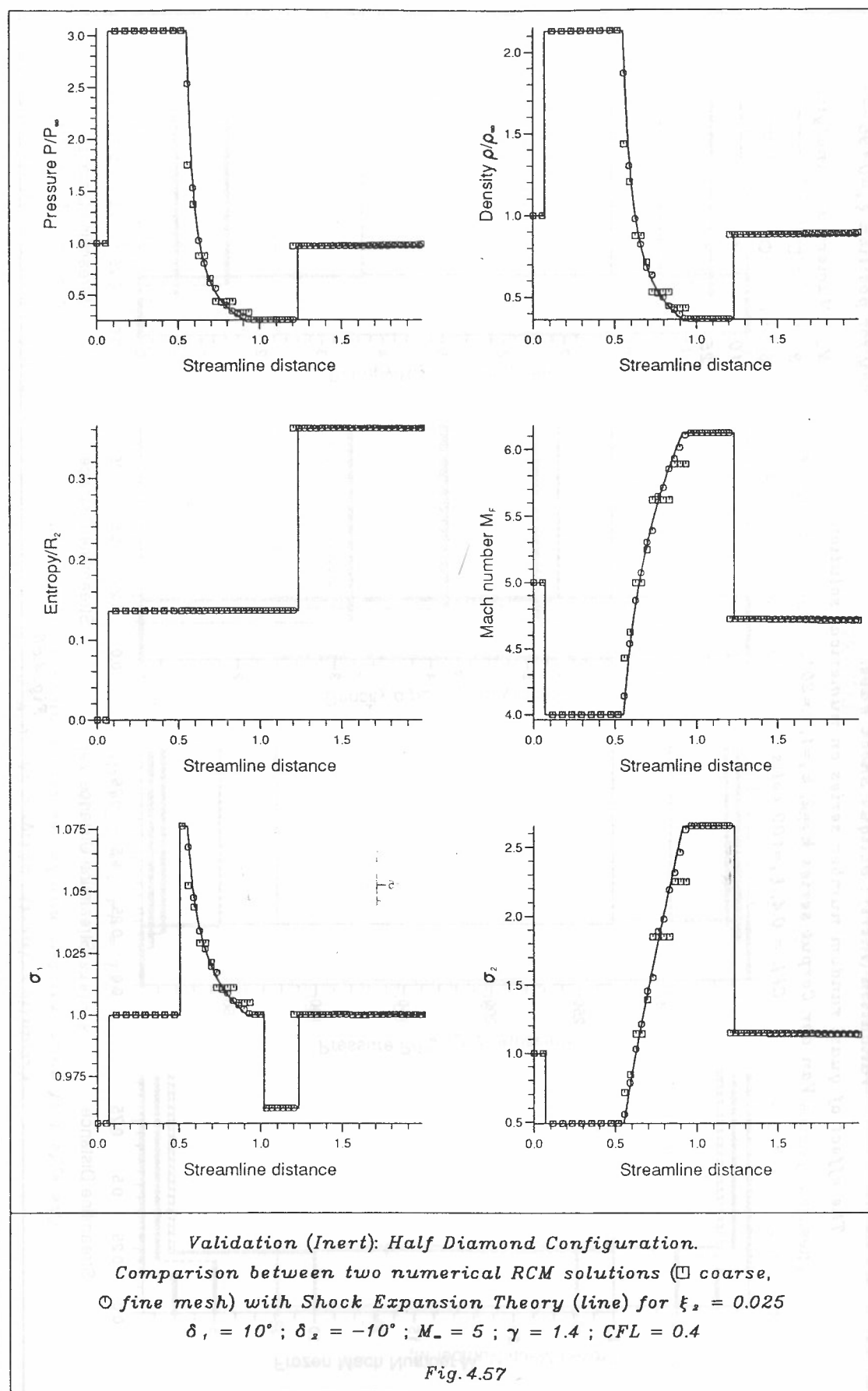
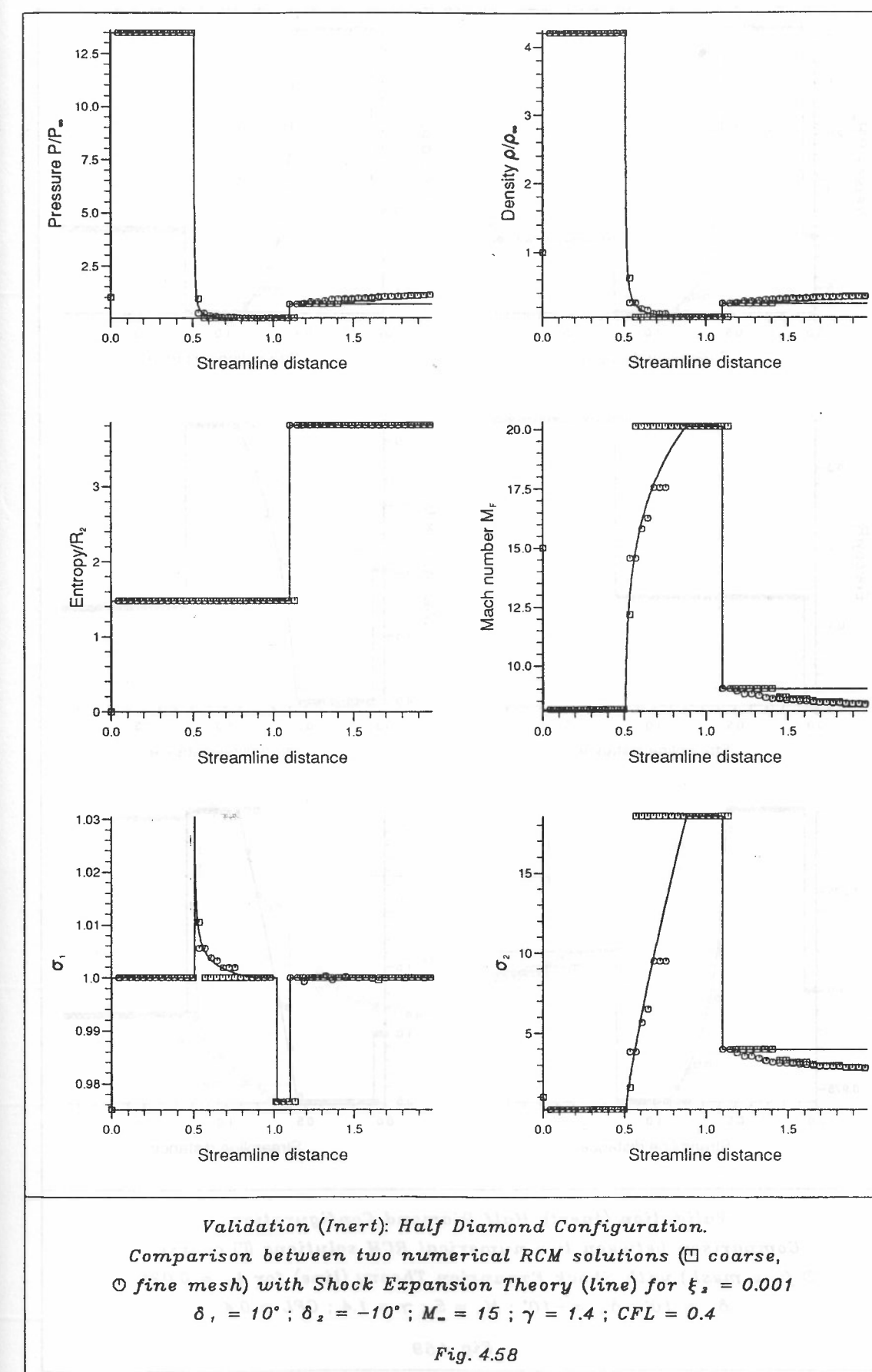
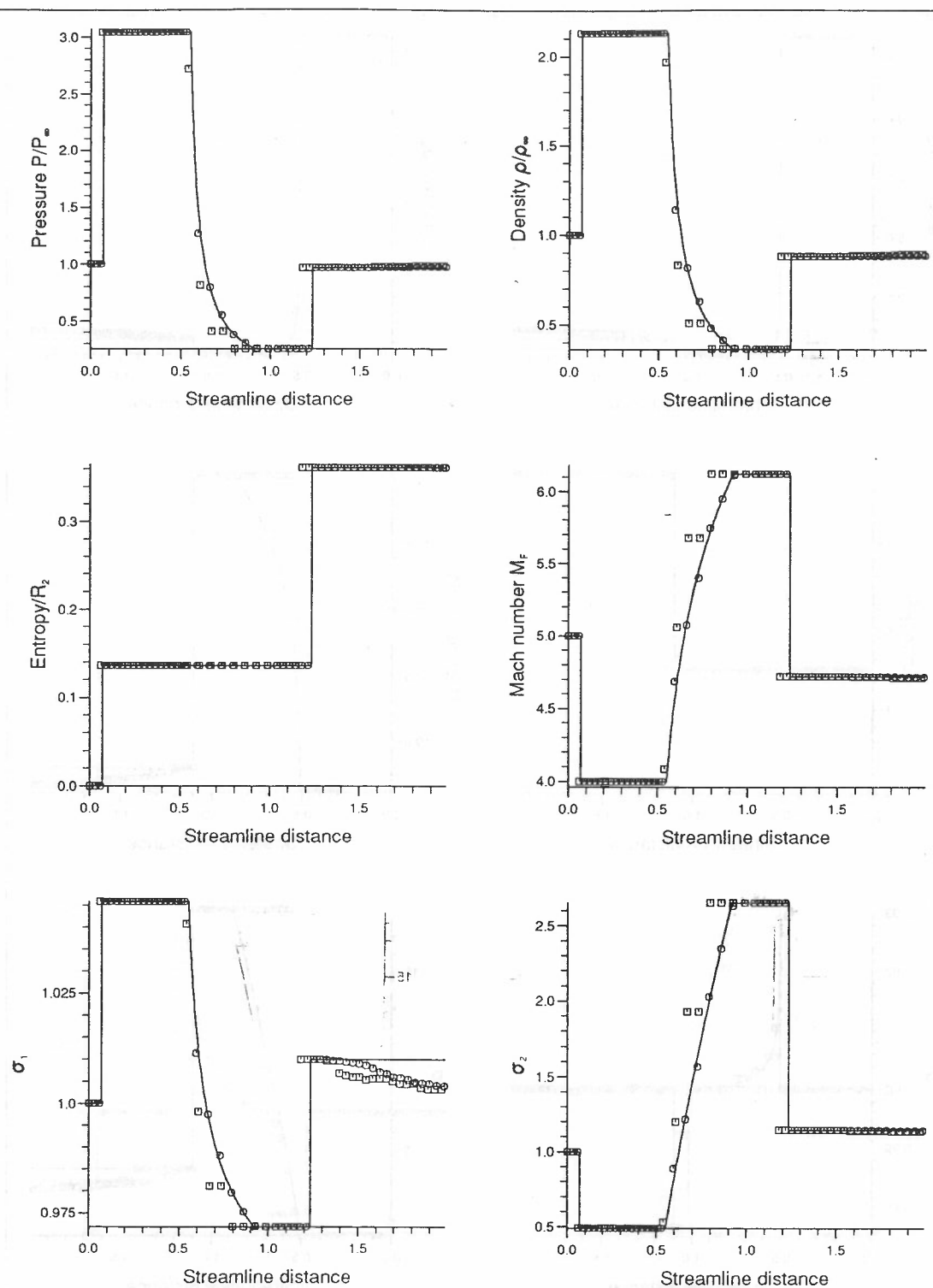


Fig. 4.54

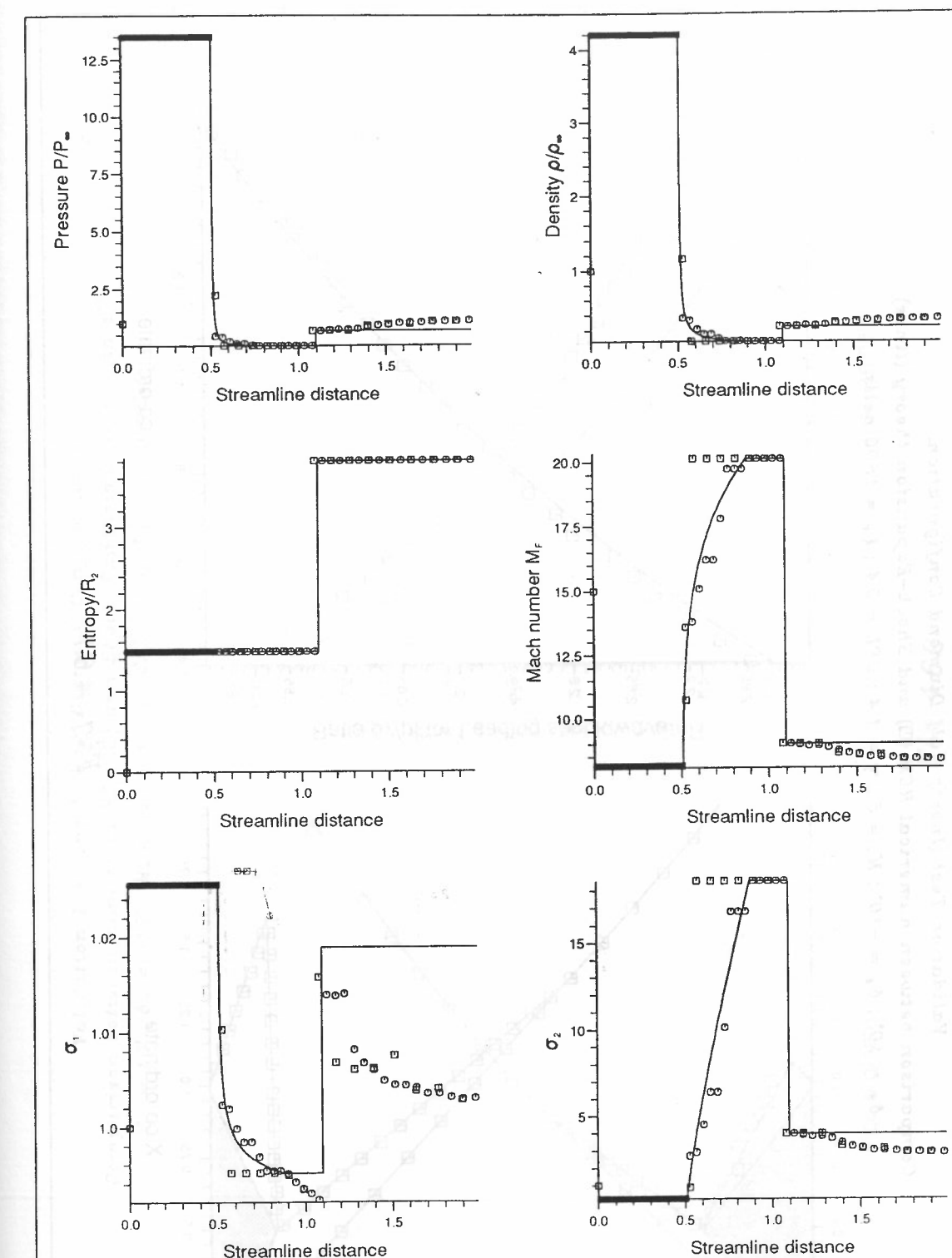






Validation (Inert): Half Diamond Configuration.
Comparison between two numerical RCM solutions ($\square$ coarse,
 $\circ$ fine mesh) with Shock Expansion Theory (line) for $\xi_2 = 0.025$
 $\delta_1 = 10^\circ$; $\delta_2 = -10^\circ$; $M_\infty = 5$; $\gamma = 1.4$; CFL = 0.4

Fig. 4.59



Validation (Inert): Half Diamond Configuration.
Comparison between two numerical RCM solutions ($\square$ coarse,
 $\circ$ fine mesh) with Shock Expansion Theory (line) for $\xi_2 = 0.001$
 $\delta_1 = 10^\circ$; $\delta_2 = -10^\circ$; $M_\infty = 15$; $\gamma = 1.4$; CFL = 0.4

Fig. 4.60

Validation Test (Inert): Half Diamond Configuration.
Comparison between numerical RCM (□) and Shock-Expansion theory (lines)

$\delta_1 = 10^\circ$; $\delta_2 = -10^\circ$; $M_\infty = 5$; $\gamma = 1.4$; $CFL = 0.4$; $\xi_z = 1500$ cells.

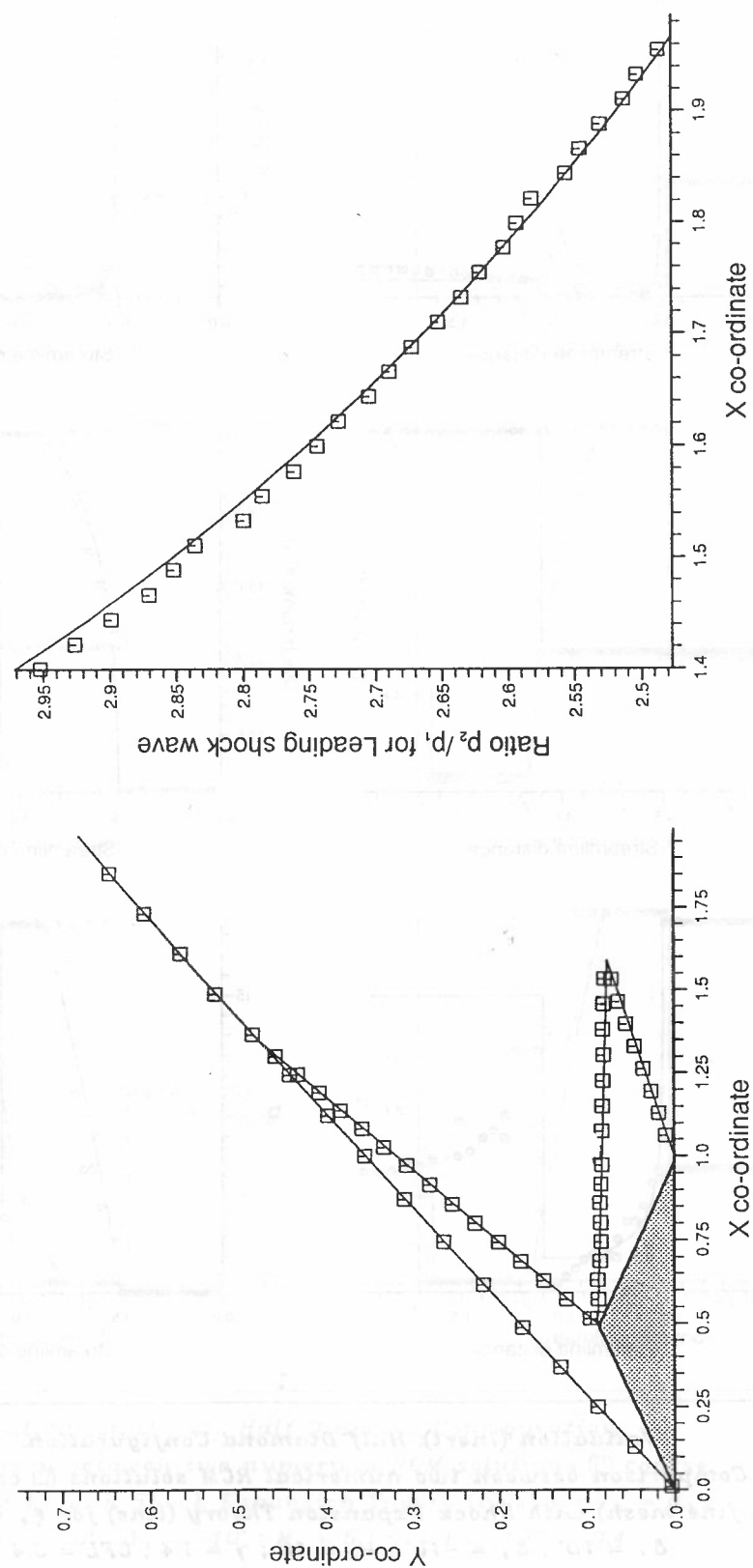


Fig. 4.61

Validation Test (Inert): Half Diamond Configuration.
Comparison between numerical RCM (□) and Shock-Expansion theory (lines)

$\delta_1 = 10^\circ$; $\delta_2 = -10^\circ$; $M_\infty = 15$; $\gamma = 1.4$; $CFL = 0.4$; $\xi_z = 1500$ cells.

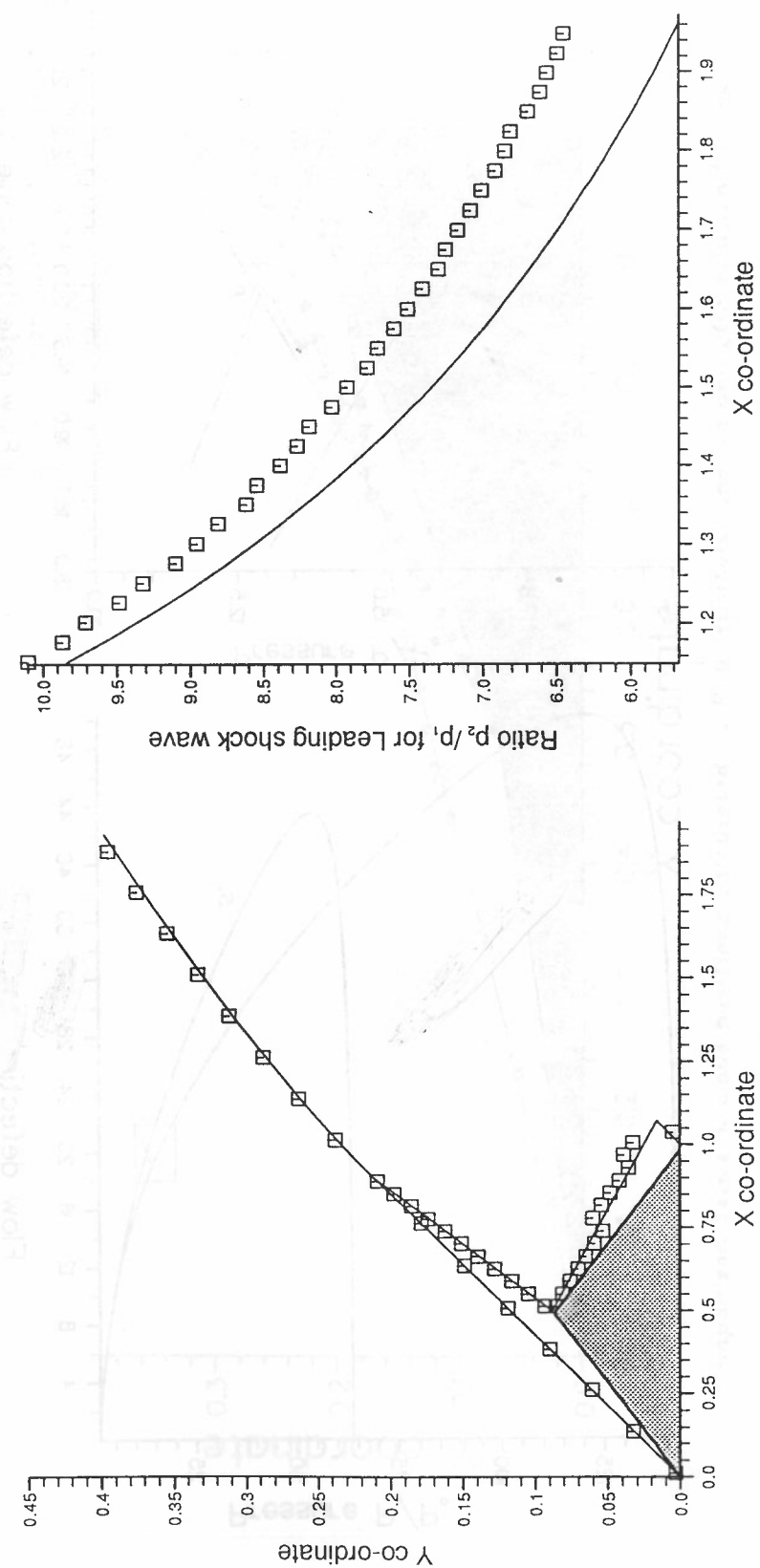
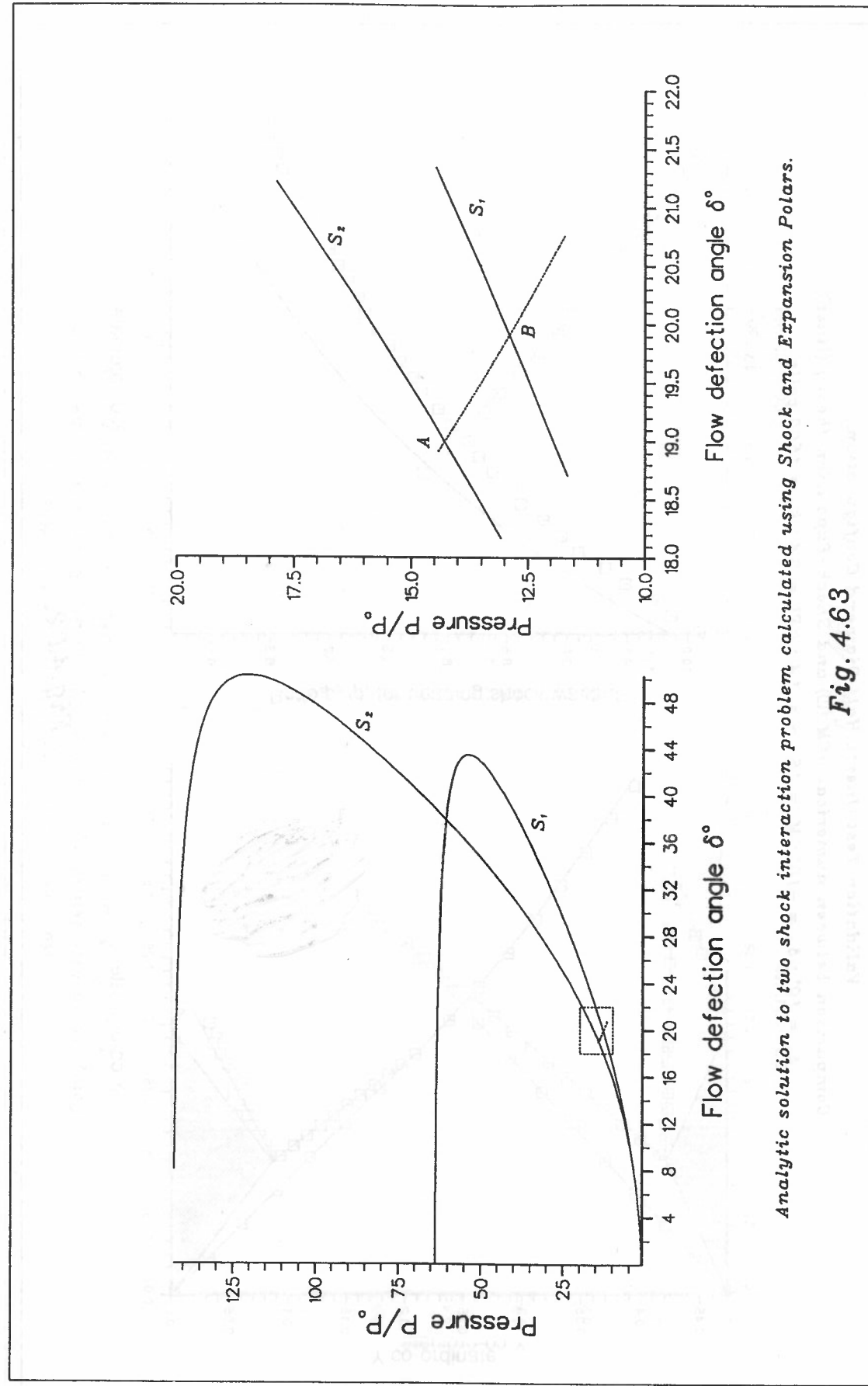
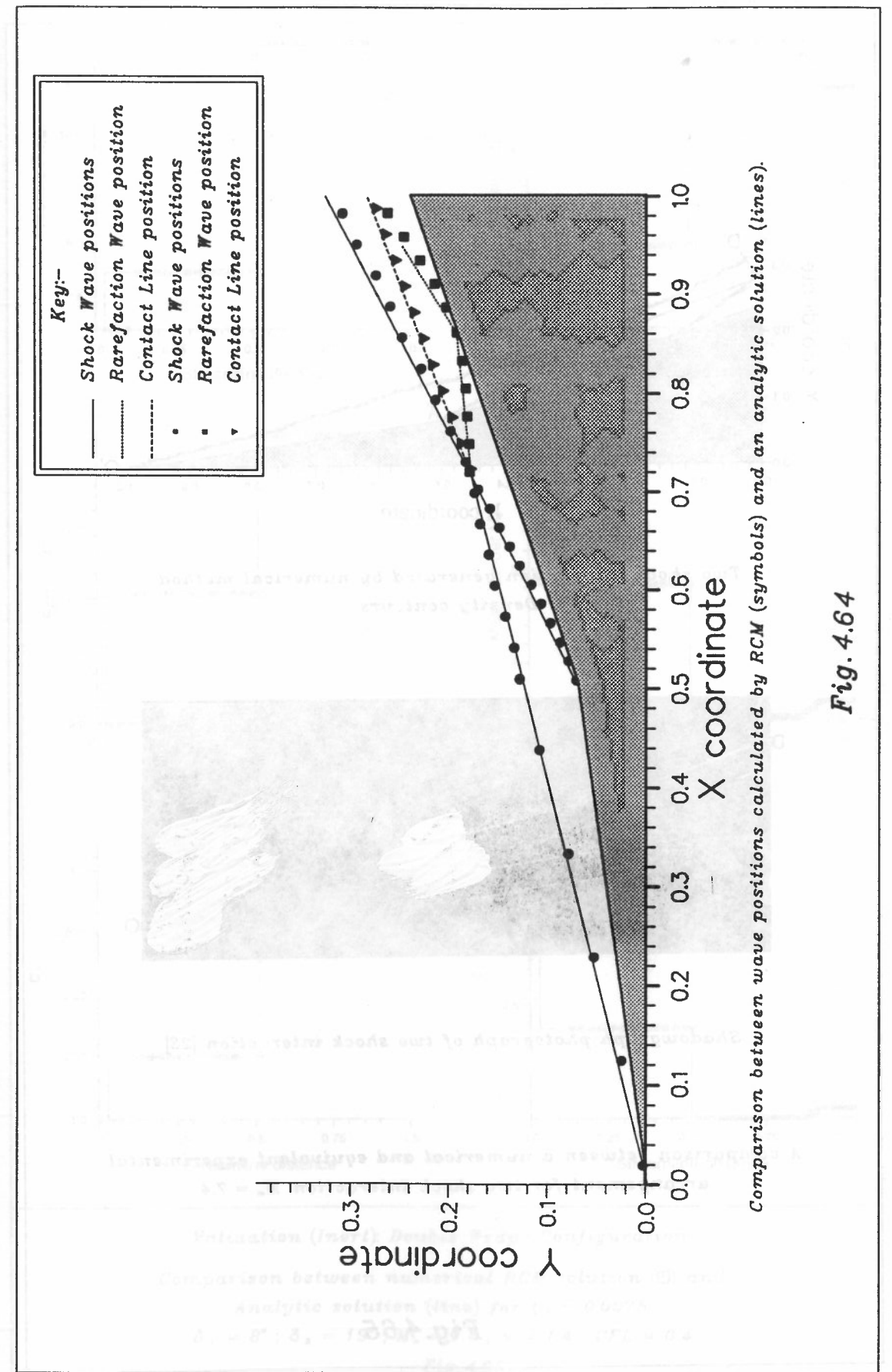


Fig. 4.62



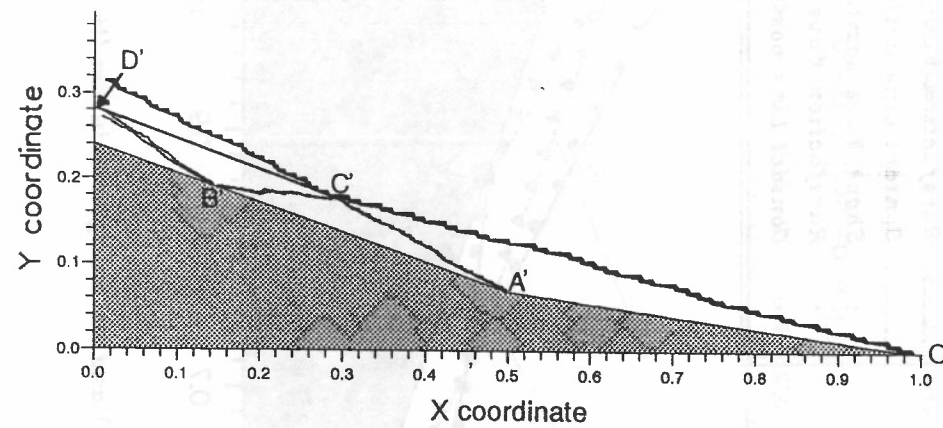
Analytic solution to two shock interaction problem calculated using Shock and Expansion Polars.

Fig. 4.63

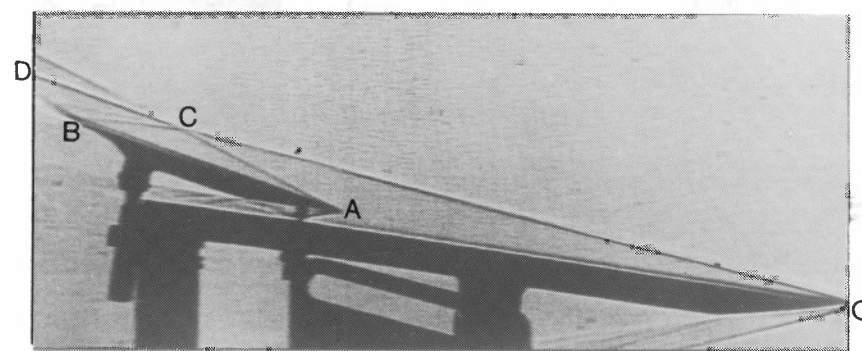


Comparison between wave positions calculated by RCM (symbols) and an analytic solution (lines).

Fig. 4.64



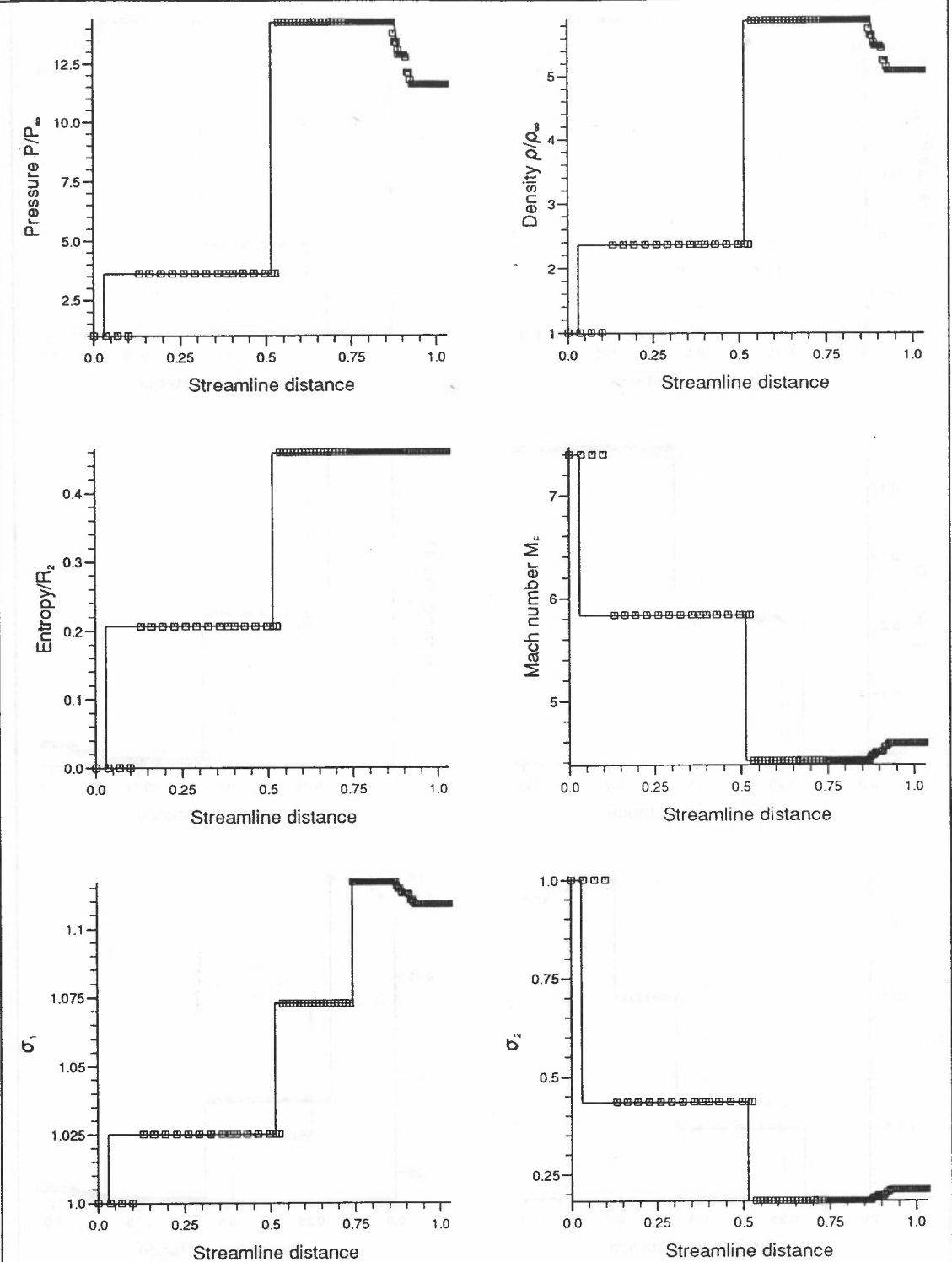
Two shock interaction generated by numerical method
Density contours



Shadowgraph photograph of two shock interaction [23]

A comparison between a numerical and equivalent experimental
arrangement for two shock interaction. $M_\infty = 7.4$

Fig. 4.65



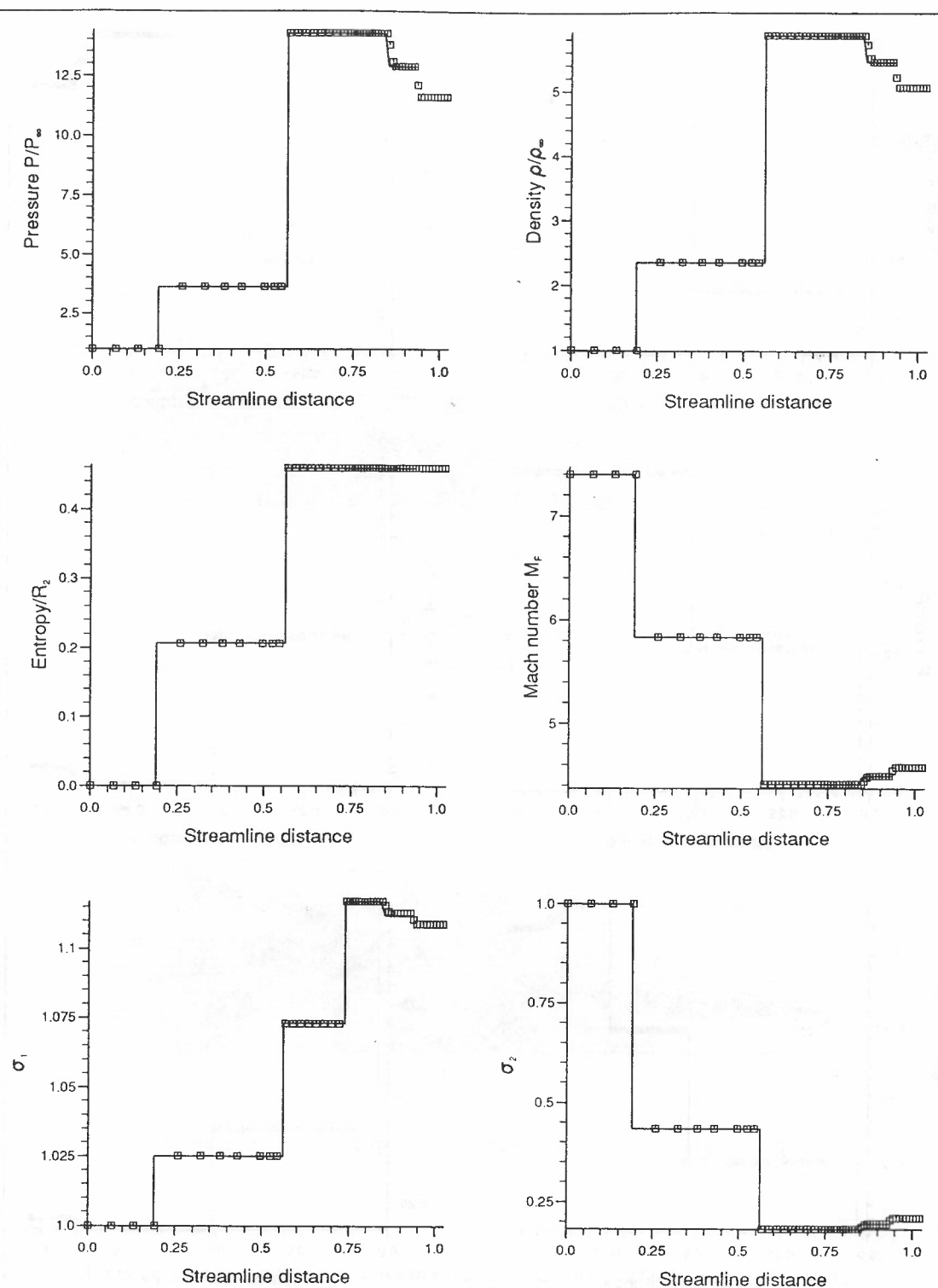
Validation (Inert): Double Wedge Configuration.

Comparison between numerical RCM solution ($\square$) and

Analytic solution (line) for $\xi_2 = 0.0075$

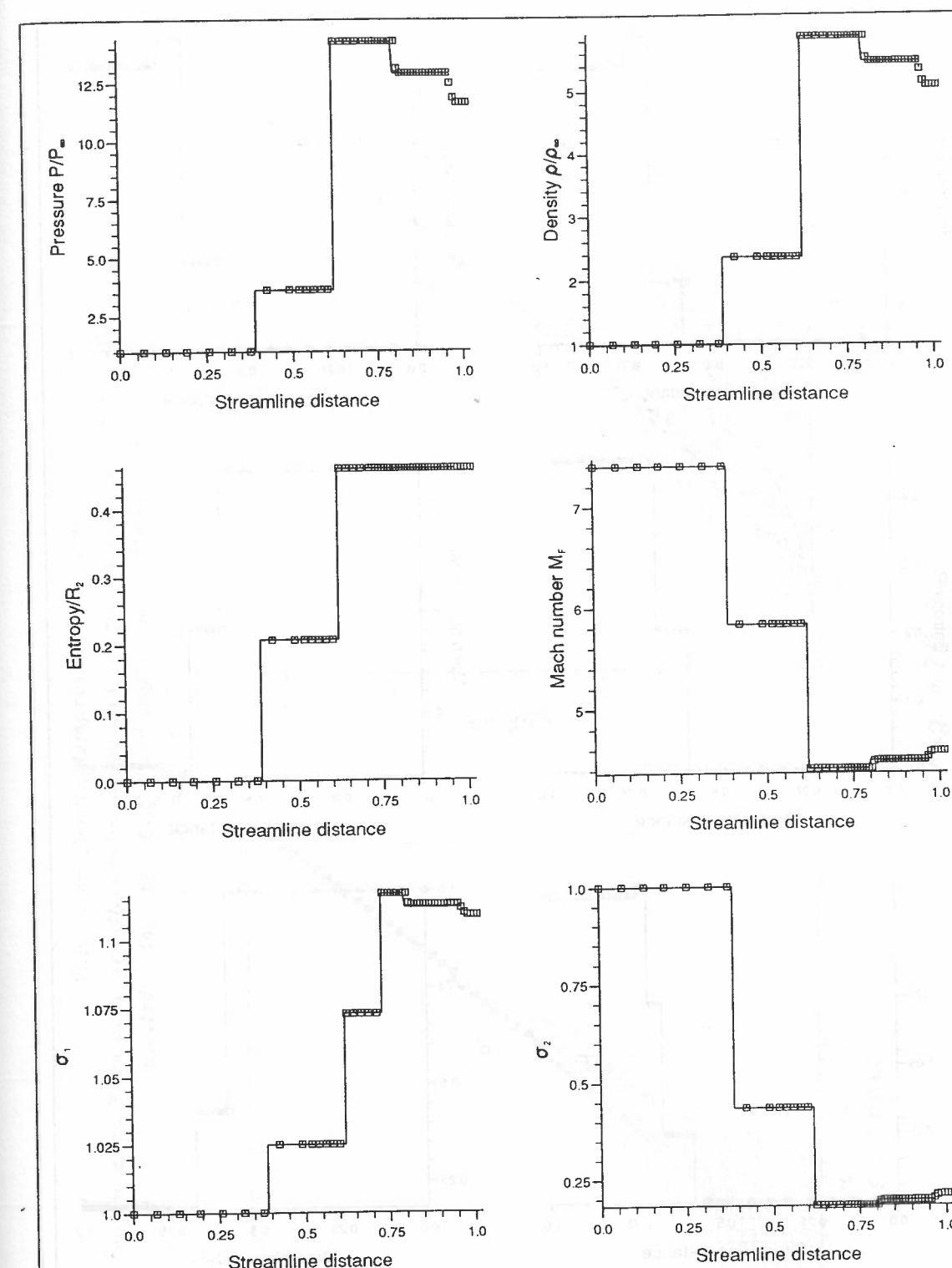
$\delta_1 = 8^\circ$; $\delta_2 = 19^\circ$; $M_\infty = 7.4$; $\gamma = 1.4$; $CFL = 0.4$

Fig. 4.66



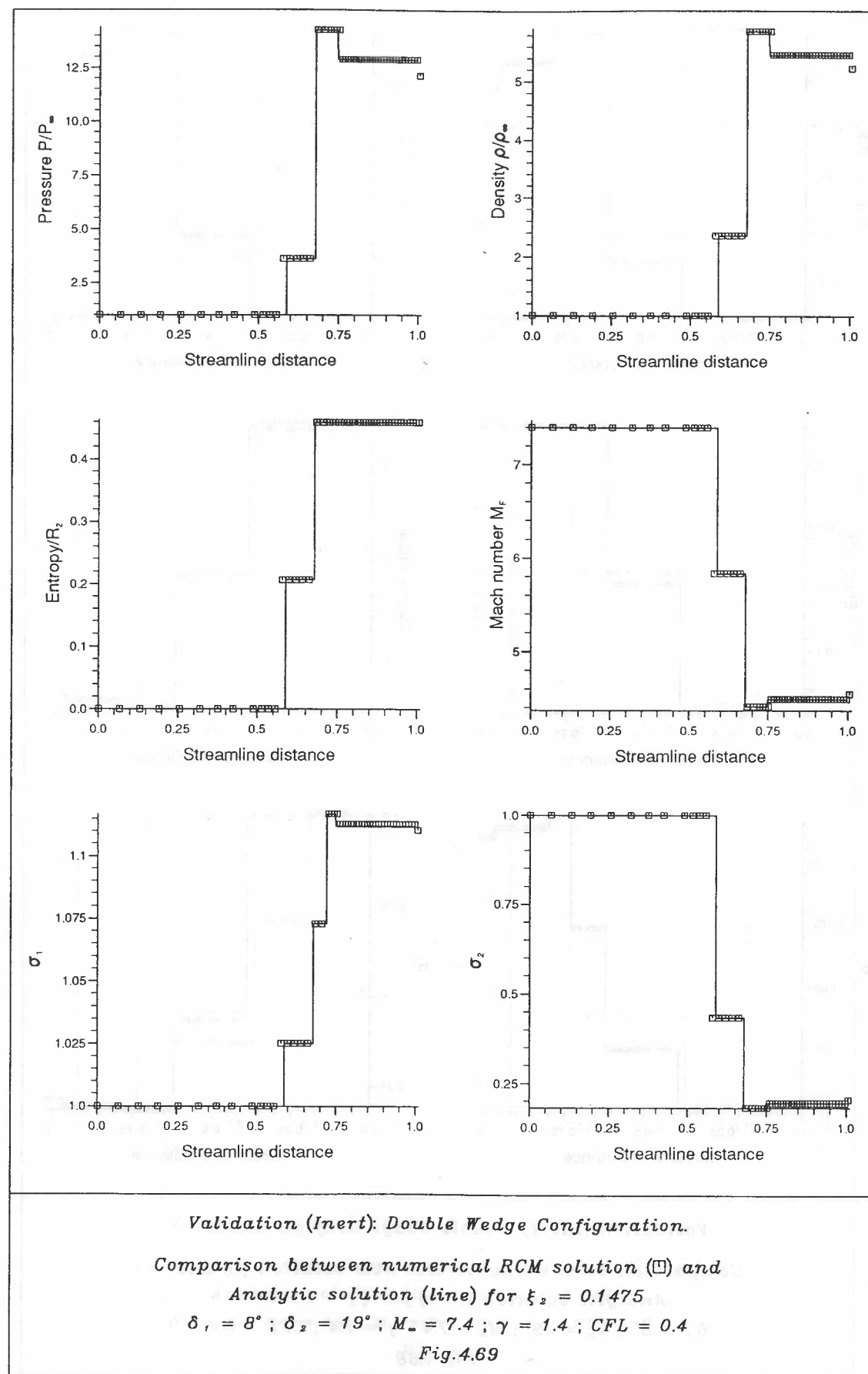
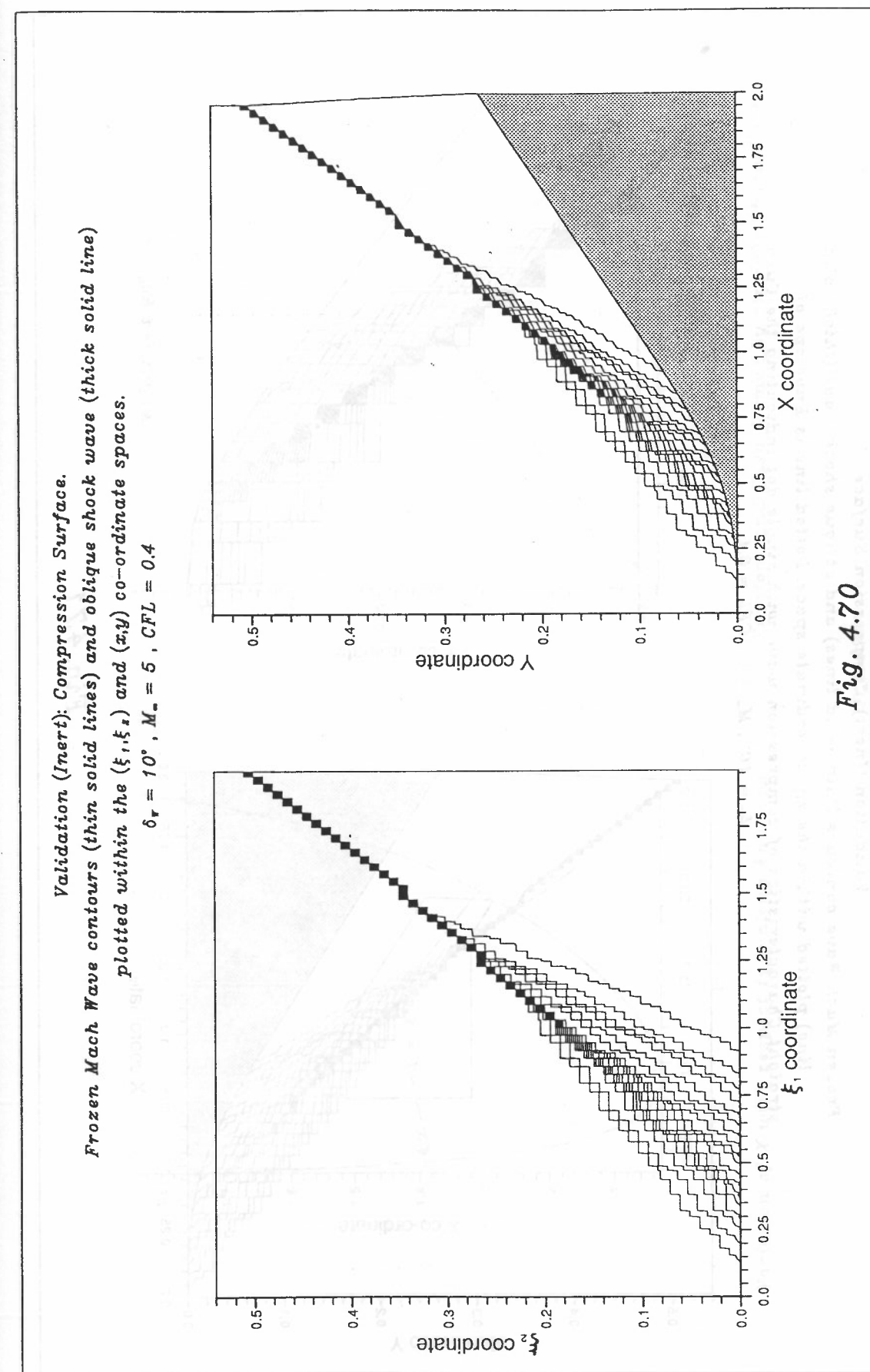
Validation (Inert): Double Wedge Configuration.
Comparison between numerical RCM solution ($\square$) and
Analytic solution (line) for $\xi_2 = 0.0475$
 $\delta_1 = 8^\circ$; $\delta_2 = 19^\circ$; $M_\infty = 7.4$; $\gamma = 1.4$; CFL = 0.4

Fig. 4.67



Validation (Inert): Double Wedge Configuration.
Comparison between numerical RCM solution ($\square$) and
Analytic solution (line) for $\xi_2 = 0.0975$
 $\delta_1 = 8^\circ$; $\delta_2 = 19^\circ$; $M_\infty = 7.4$; $\gamma = 1.4$; CFL = 0.4

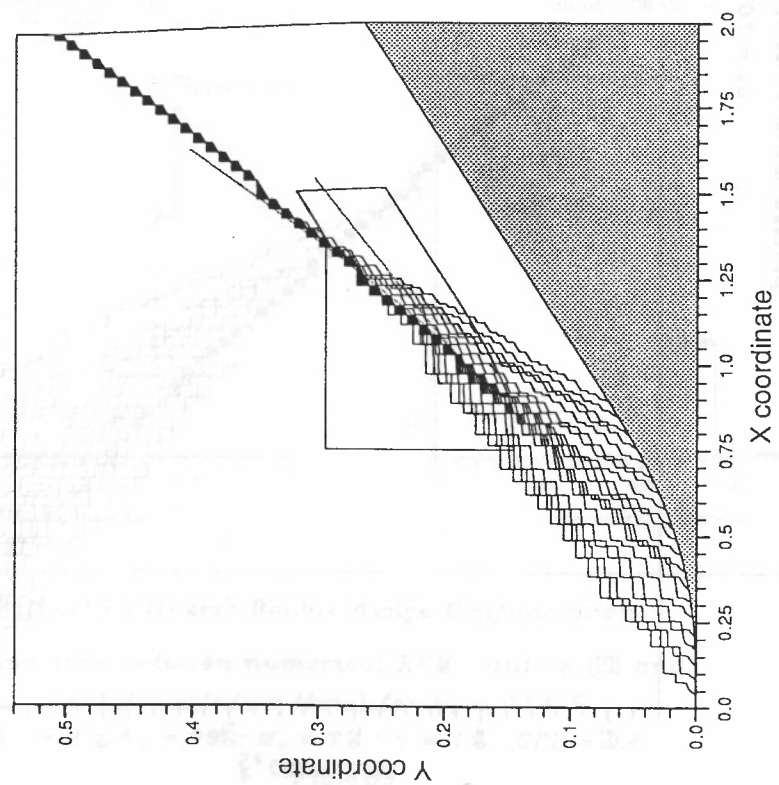
Fig. 4.68



Validation (Inert): Compression Surface.

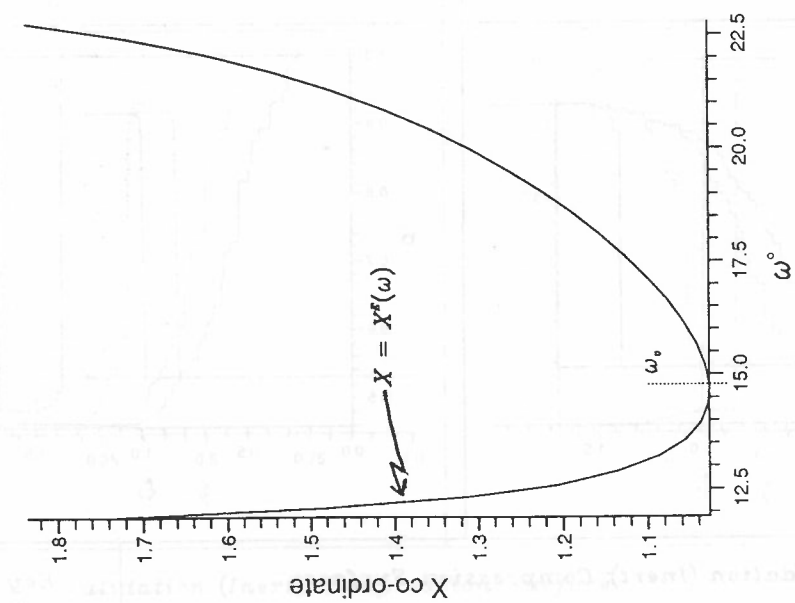
Frozen Mach Wave contours (thin solid lines) and oblique shock wave (thick solid line) plotted within the xy co-ordinate space. Dotted line is Envelope of straight Characteristics of compression wave with single dot indicating the Cusp.

$$\delta_r = 10^\circ, M_\infty = 5, CFL = 0.4$$

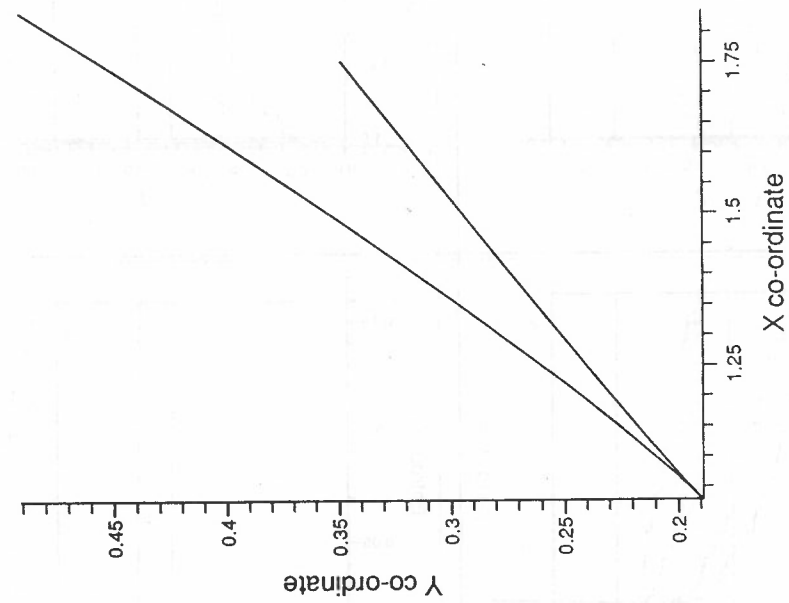


Magnified Region.

Fig. 4.71

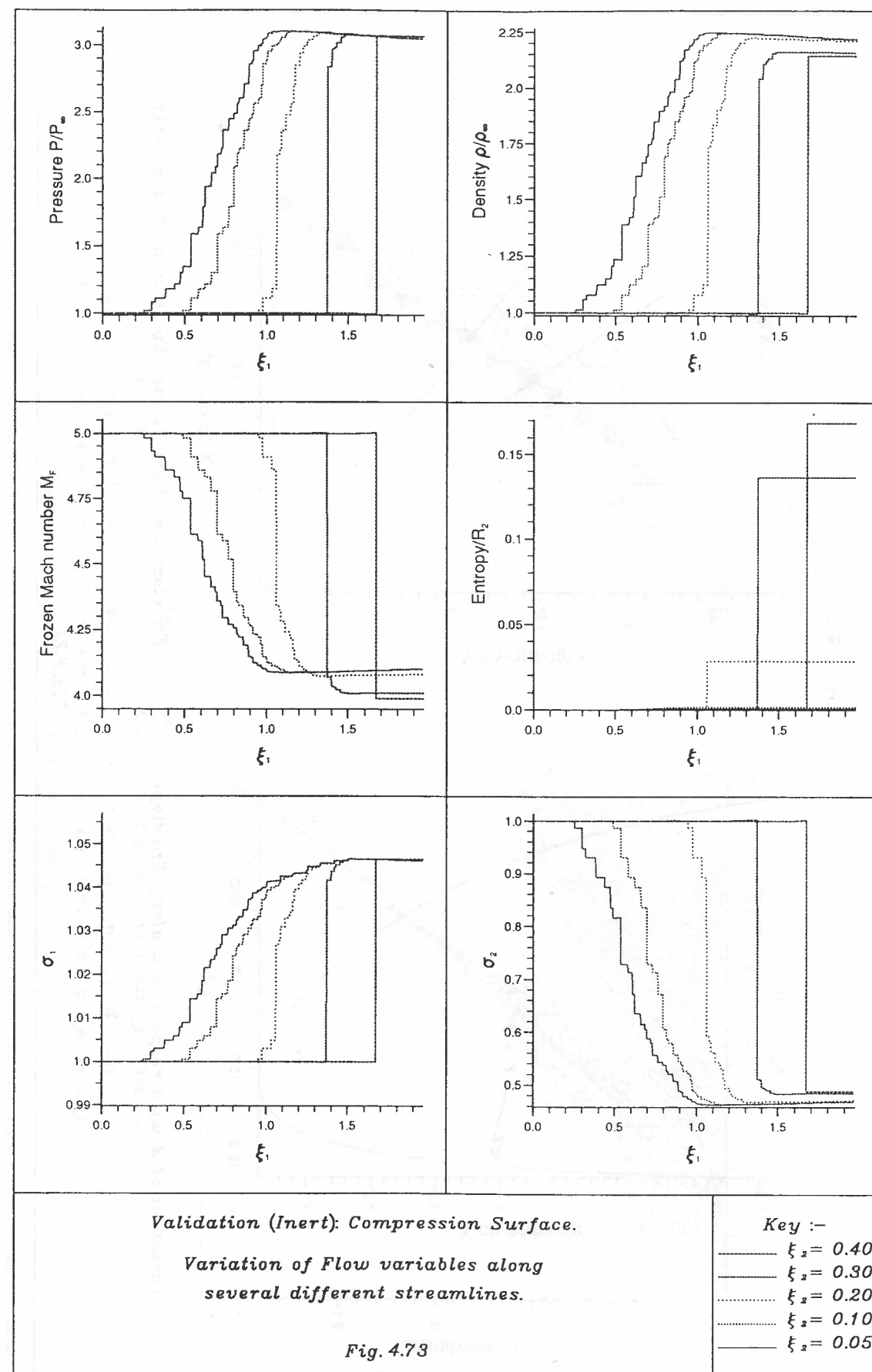
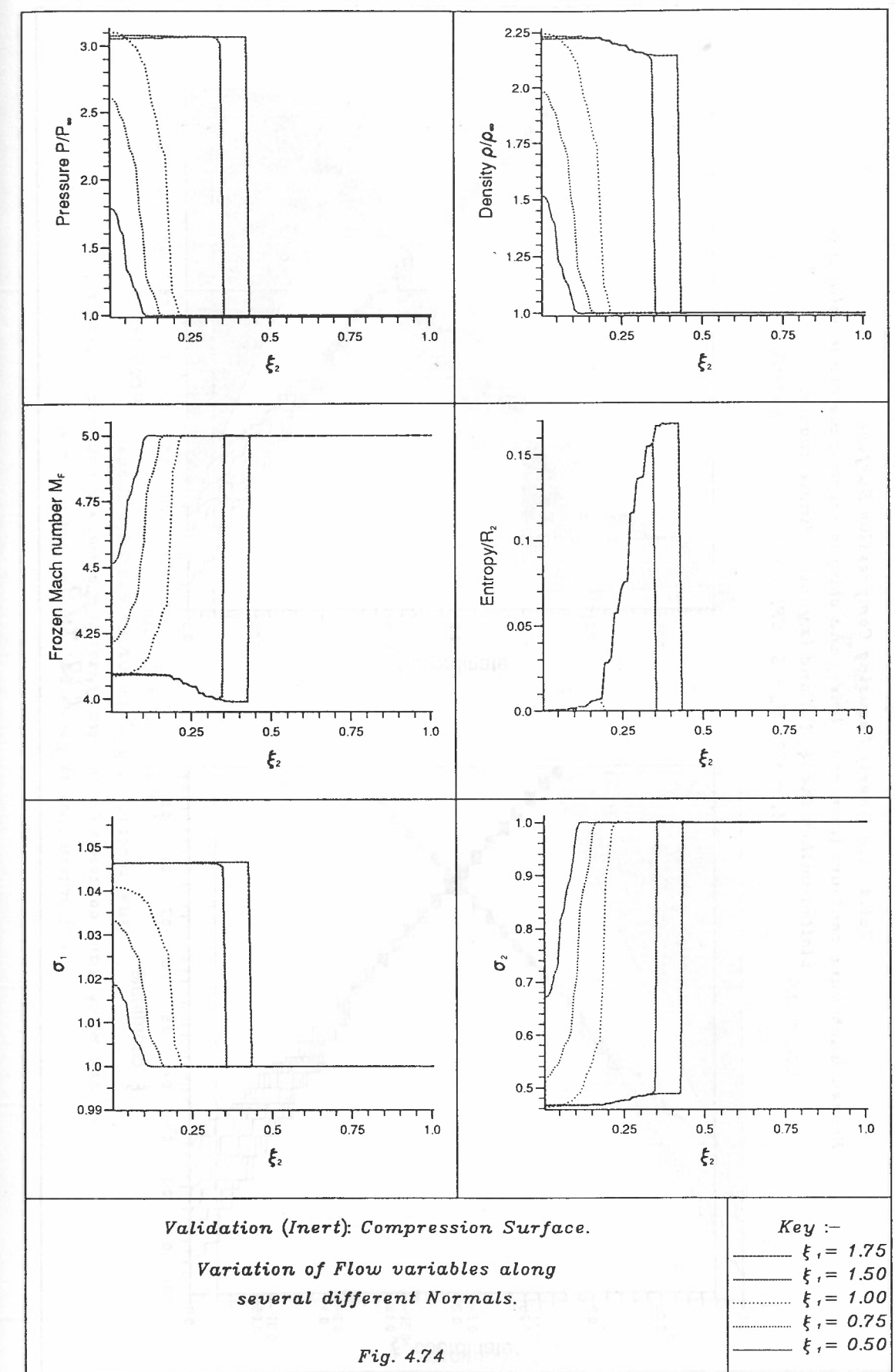


Variation of X with respect to ω along Envelope.



Envelope and Cusp formed by straight Characteristics.

Fig. 4.72



Validation (Inert): Focusing Compressive Surface.
Frozen Mach Wave contours (thin solid lines) and oblique shock wave (thick solid line)
plotted within the (ξ, ξ_*) and (x, y) co-ordinate spaces.
 $\delta_r = 10^\circ$, $M_\infty = 5$, $CFL = 0.4$

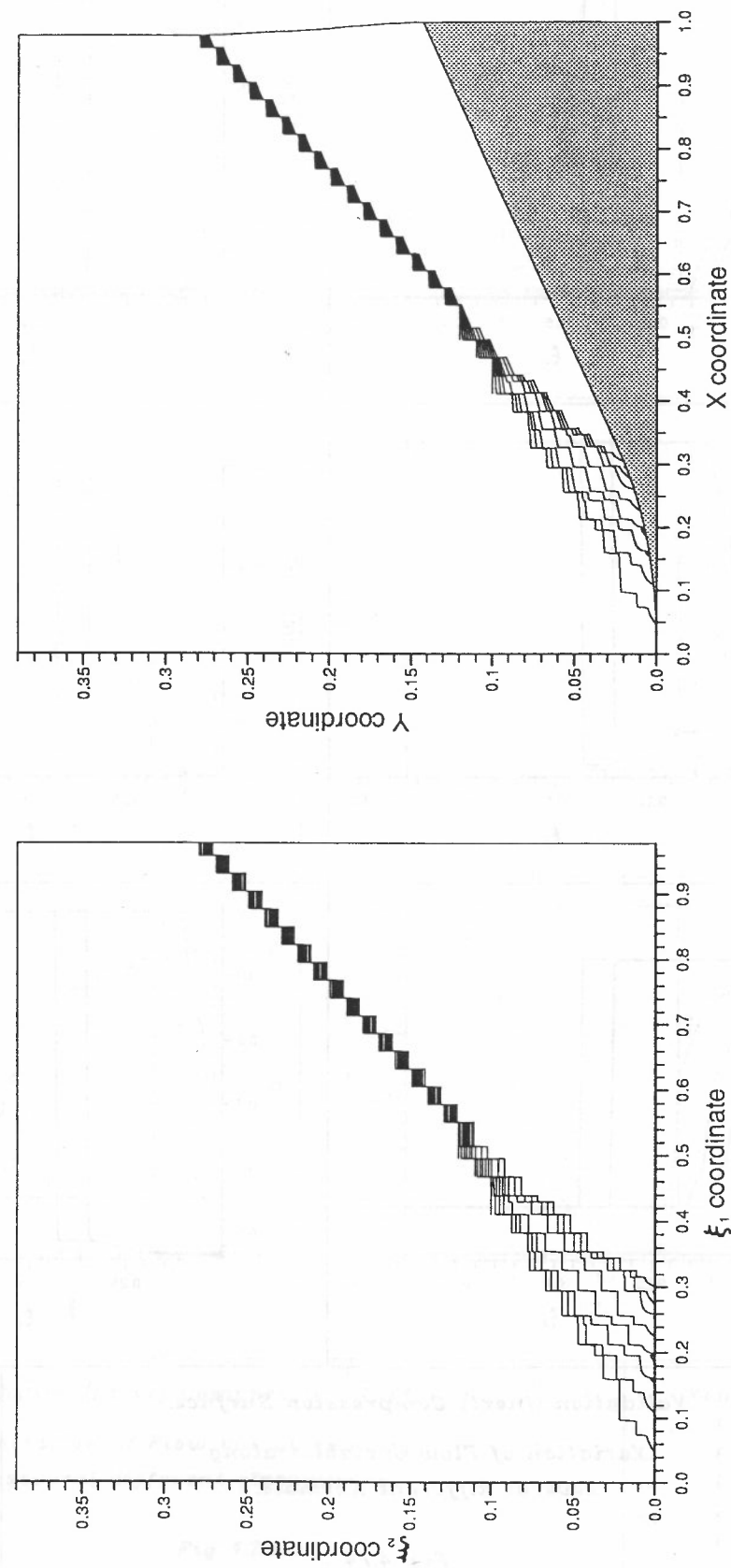


Fig. 4.75

Validation (Inert): Focusing Compressive Surface.
Frozen Mach Wave contours (thin solid lines) and oblique shock wave (thick solid
line) plotted within the x, y co-ordinate space.
 $\delta_r = 10^\circ$, $M_\infty = 5$, $CFL = 0.4$

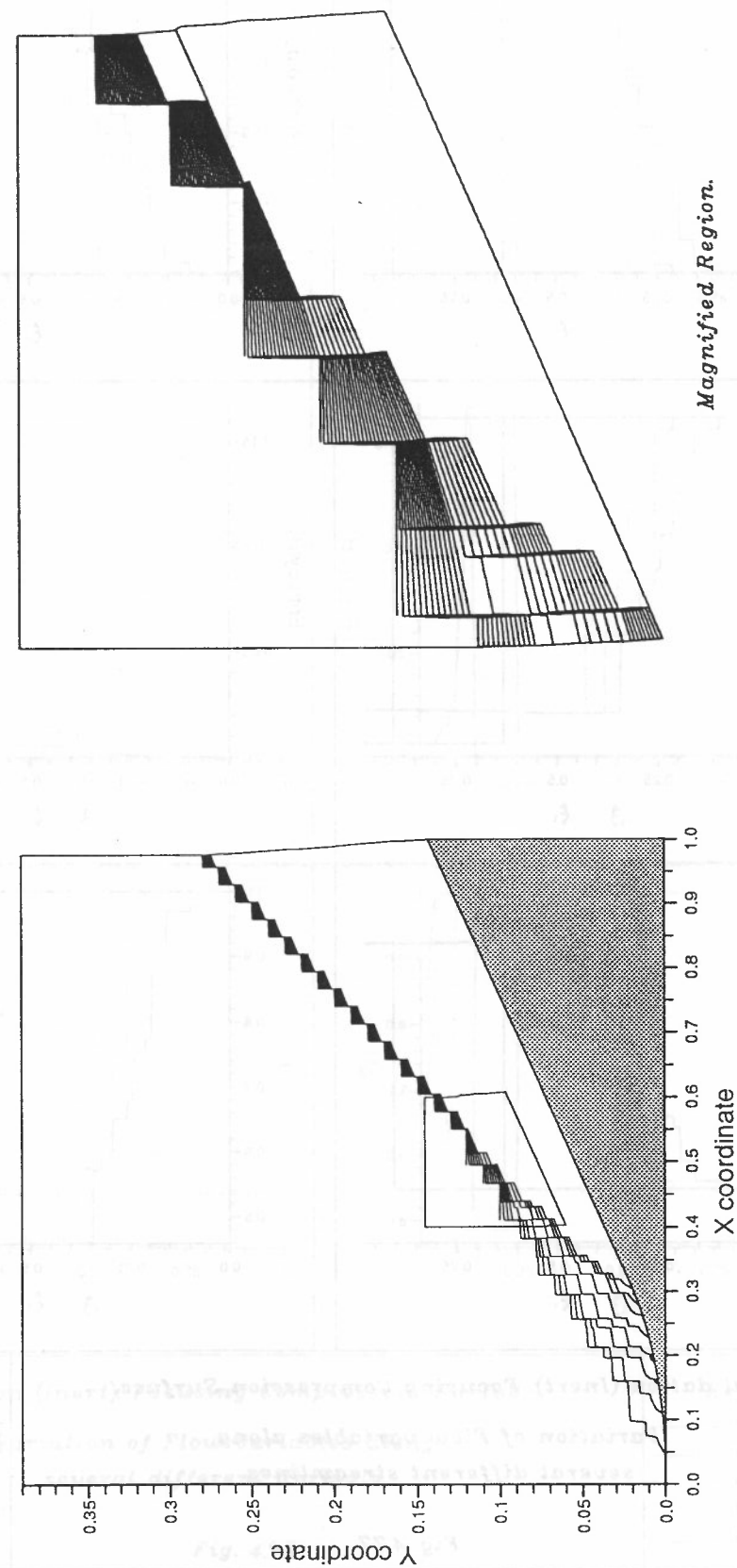
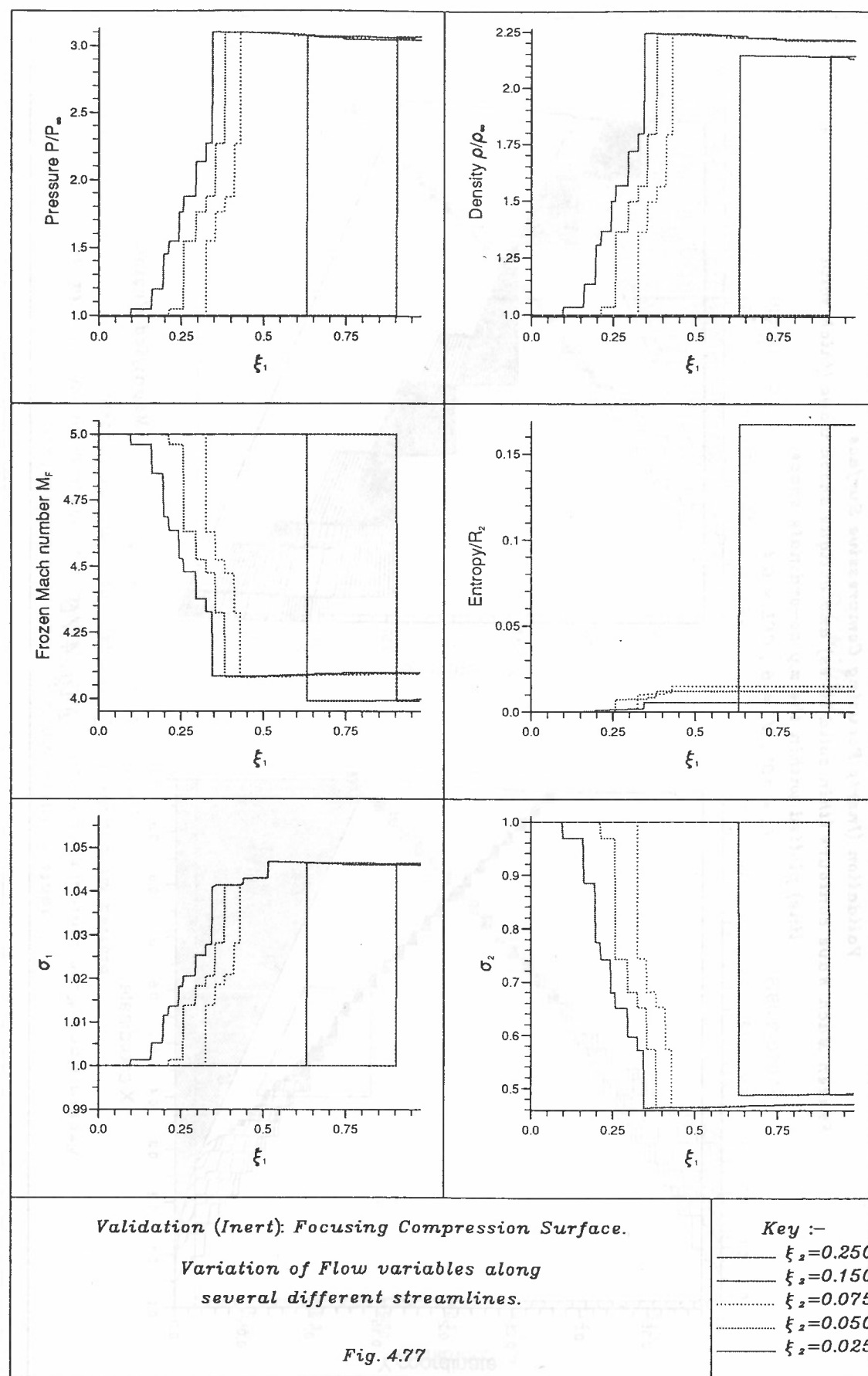
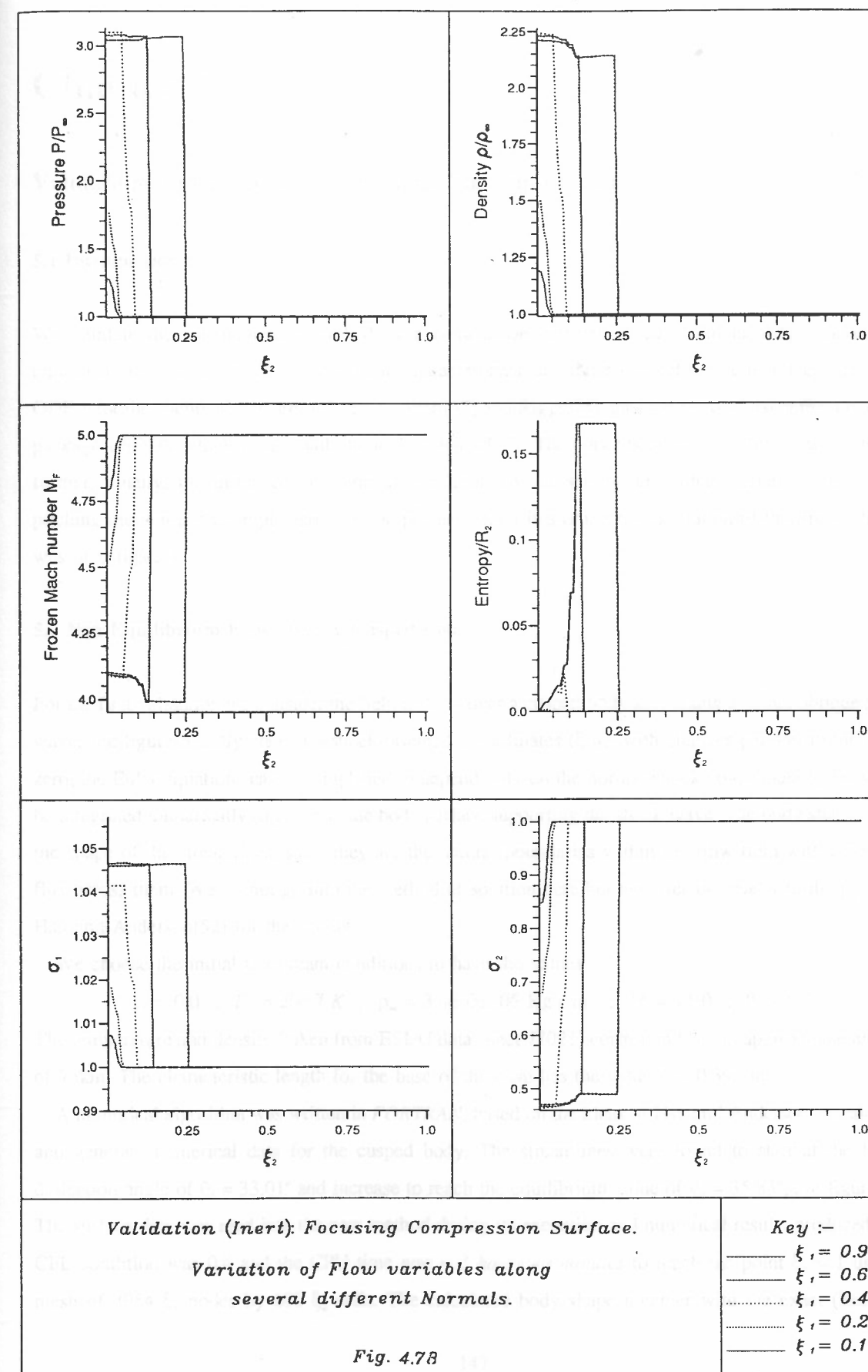
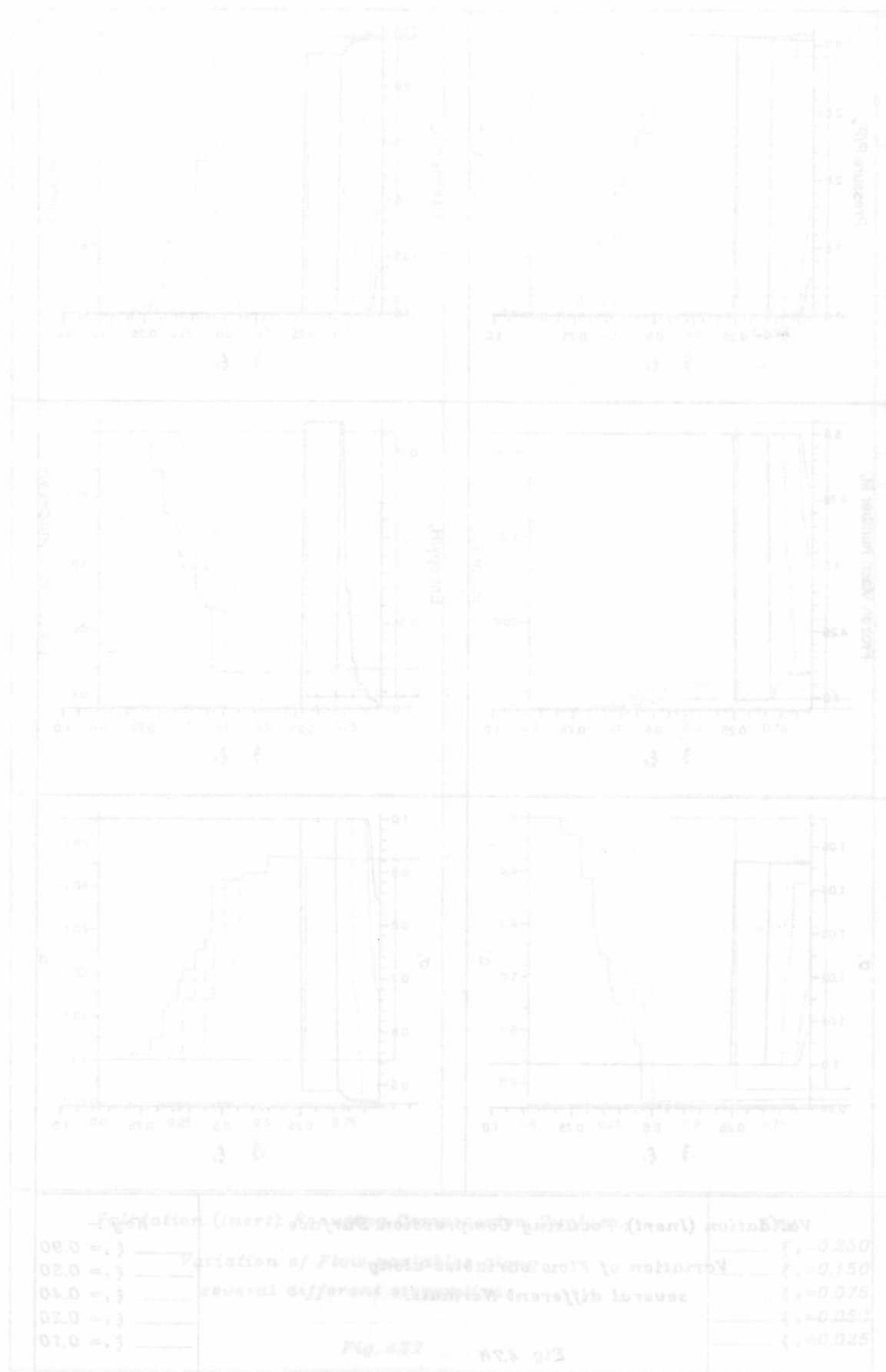


Fig. 4.76





Chapter 5

Validation And Results For Chemical Non-Equilibrium

5.1 Introduction

We validate the full numerical method by a comparison between results from existing analytic and numerical methods, such as the Method of Characteristics, and those created by the new technique. The ODE's for the chemical step are *stiff*, see Lambert[57] and Riggs[75], and were solved using the numerical package LSODE which comes with the text by Riggs[75]. The upper boundary conditions were studied further. Finally, the influence of chemical relaxation on the aerodynamic characteristics, such as the pitching moment, of a simple aerodynamic profile, which is a crude representation of the Space shuttle, was investigated.

5.2 Non-Equilibrium Flow Over A Cusped Body

For the first validation we consider the field of flow over a cusped body supporting a plane, oblique shock wave, see figure 5.1. By choosing shock-oriented co-ordinates (ξ, η) , with changes parallel to the shock zero, the Euler equations can be simplified to depend only on the normal shock co-ordinate ξ . These can be integrated numerically to generate the body surface supporting the shock wave. The body shape is also the shape of the streamlines, since they are the natural boundaries within the flow field with zero mass flux across them. We do not go into the method of solution here but we refer the reader to the paper by Hsu and Anderson[52] for the details.

We choose the initial freestream conditions to have the values

$$c_1 = 0.0 ; T_\infty = 206.7 K ; \rho_\infty = 3.4863E-05 \text{ Kg / m}^3 ; M_\infty = 25.0 ; \beta = 40^\circ$$

The temperature and density (taken from ESDU data sheet 77021) corresponds to an approximate altitude of 75km. The characteristic length for the base of the cusp has the value $L = 0.395 \text{ m}$.

A numerical algorithm was written in *FORTRAN*, based on the ideas of Hsu and Anderson, to calculate and generate numerical data for the cusped body. The streamlines were found to start at the frozen deflection angle of $\theta_f = 33.01^\circ$ and increase to reach the equilibrium value of $\theta_e = 35.83^\circ$, see figure 5.7. The surface data was read into the new method during its execution and numerical results produced. The CFL condition was 0.4 and the CPU time was $\approx 3 \text{ hours } 40 \text{ minutes}$ to reach the point $\xi_1 = 1$ using a mesh of 7054 ξ_1 nodes by 600 ξ_2 cells. The calculated body shape together with the exact (line) and

numerical (symbol) shock position can be viewed in figure 5.7. There is excellent agreement between the shock positions. A comparison between the exact (solid line) and calculated (circles) flow variation along a streamline are to be found in figure 5.8. On the whole there is excellent agreement between the two results. However, the density and particularly the pressure show signs of non-monotonicity behaviour about the analytic solution. The temperature appears to oscillate very weakly. These are due to the size of the mesh. Because the method does not contain any natural dissipation, numerical oscillations that are created will not be dissipated by the method.

Because the rate equation is dominated by the dissociation reaction it can be written without loss of accuracy as

$$\frac{\partial c_1}{\partial \xi_1} = \rho L \frac{4k_b \rho_d}{q W_2^2} (1 - c_1^2) \exp(-\theta_d/T) \quad (5.1)$$

For different flow fields with the same freestream velocity and temperature but different density and characteristic length, we note that the rate equation will be unchanged if $\rho L = \text{constant}$. This is the *binary scaling law* [6, pages 580-583]. As a second test we adopted this scaling procedure. We choose to take a third of the original density and triple the characteristic length. Whence

$$\rho_\infty = 1.621\text{E-}05 \text{ Kg / m}^3 ; L = 1.185 \text{ m}$$

The numerical results for this run can be observed in figure 5.8. The flow field variation is the same as the original data and we have therefore not plotted them. However, there is a discrepancy in the entropy variations and this is plotted (triangle's). The lower density has produced a larger degree of chemical non-equilibrium with the difference in the chemical potentials bigger. One may note that work undertaken in Hypersonic windtunnels, where the binary scaling law is used (see Stalker[88]), are performed at higher densities to that encountered during re-entry into the Earth's atmosphere. In this case the entropy due to the chemical non-equilibrium will be less than that found in practice. This will imply that the vorticity will ultimately be lower in the experimental arrangement due to these reactions.

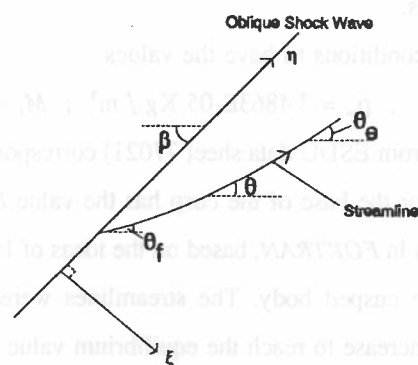


Figure 5.1 Streamline in shock-oriented co-ordinates.

5.3 Non-Equilibrium Flow Past a Wedge

The chemical non-equilibrium flow field past a wedge has been investigated by a considerable number of people many years ago. The details of these results have been compiled within the excellent texts by Clarke and McChesney[21,22] and Vincenti and Kruger[98]. A much more recent study of the wedge has been performed by Pandolfi et al[70] using Moretti's *Lambda scheme* with multiple reactions.

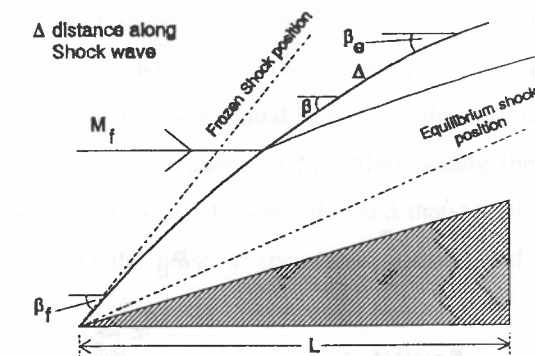


Figure 5.2 Flow over wedge with non-equilibrium.

One such investigation was performed by Capioux and Washington[15] using the method of characteristics. They performed four runs using different initial data. We use the initial data for their first case as the starting point for our second validation. The initial data has the form

$$M_\infty = 32 ; q_\infty = 9988.6114 \text{ M / s} ; \rho_d/\rho_\infty = 8.11\text{E}07 ; c_1 = 1\text{E-}10 ; \beta = 30^\circ$$

The rate equation was of the form (2.97) with constant C (which was derived from Matthews[63] dissociative rate equation) having the numerical value

$$C = 3.5488061 \times 10^{20} (1 + c_1) \quad (5.2)$$

from which the reverse reaction rate has the form

$$k_b = 6.0566291 \times 10^{11} T^{-n} \quad (5.3)$$

The characteristic length used for non-dimensionalization was defined as

$$L = \frac{q_\infty^{1+2n}}{\rho_\infty R_2^n C} \quad (5.4)$$

where $n = 2.5$ and $L \approx 1.397 \text{ m}$.

For 2000 ξ_2 cells and CFL = 0.4 there where 9250 ξ_1 nodes used reach the point $X/L = 0.1$. The program took roughly 41 hours 46 minutes to complete. This is to be compared with a similar frozen calculation which took roughly 3 hours 24 minutes. There is an order of magnitude increase in the CPU

time. The numerical oscillations, particularly those that increase, will be due to the creation of oblique shock waves in the RCM method. These waves will reduce the computational step size and will increase significantly the number of steps needed to reach a given point in the flow. Because there are no oscillations in the frozen case the step size will be larger.

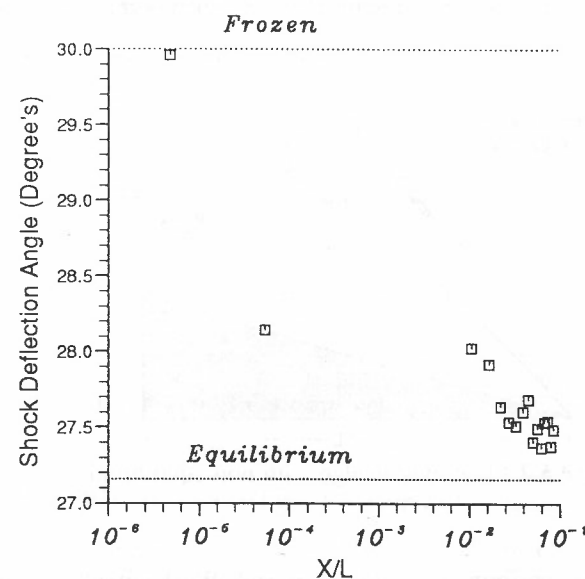


Figure 5.3 Variation of shock deflection angle.

Numerical results for the variation of the flow field variables along several different streamlines can be found in figure 5.9. These are compared with the equilibrium values (solid lines) which were calculated using the numerical technique described within appendix B. For the streamline along the body surface the agreement between Capioux and Washington's results and ours is good. However, the pressure and density again oscillates widely. These oscillations are now apparent, but of lower magnitude, in the temperature profiles. These effects are attributed to the very large freestream Mach number and large jump in the temperature across the shock. Because of this the chemical source will have a large influence on the behaviour of the flow field. The pressure will approach the equilibrium value asymptotically downstream because the flow field must be parallel to the wedge surface. The profiles show clearly that there is an entropy and vorticity layer close to the body surface, see also figure 5.2. These layers will be due to the non-equilibrium as well as that generated by the weakening of the shock wave. For inert flows a decrease in deflection angle will cause the shock to weaken and ultimately produce an entropy/vorticity layer. For non-equilibrium the shock is weakened by the presence of the reactions causing an entropy/vorticity layer to be formed. This will be in addition to the entropy created by the reactions themselves. At the leading edge of the wedge, the shock wave starts at its frozen wave angle β_f . However, along the shock this decreases until its equilibrium value β_e is reached (since there must be a zero pressure gradient along a

normal away from the wedge infinitely far downstream). For the calculation performed, the shock angle is seen to decrease and then to oscillate close to the equilibrium value, see figure 5.3. The amount of vorticity created downstream by the shock wave curvature can be derived from [23,48]:

$$\zeta = q_\infty \frac{(1-r)^2}{r} \cos \beta \frac{\partial \beta}{\partial \Delta} ; \quad r = \frac{\rho_2}{\rho_1} \quad (5.5)$$

where Δ is the distance along the shock wave and β is the wave angle. A comparison between the vorticity just downstream of the shock wave and that calculated from the shock can be done. The shock wave is approximated by using a Least Squares polynomial fit through the calculated numerical shock angle vs position. The curvature of the wave is calculated by differentiating the polynomial and the vorticity derived from equation (5.5). A comparison between this and that calculated downstream revealed poor accuracy. This was attributed to the noise in the shock position and subsequent inaccuracy of the polynomial fit.

5.4 Non-Equilibrium Flow Over a Downward Sloping Wedge

We make two further validations of the numerical method by a comparison with the results from Cleaver [24] and Appleton [8] for a wedge with negative deflection angle. Both of these authors using the Method of Characteristics. Also of notable importance in this area is the work by Glass and Takano [41].

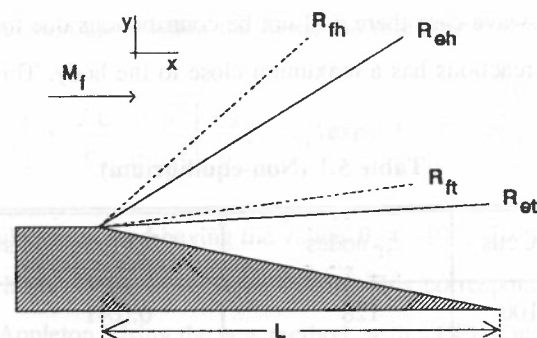


Figure 5.4 Frozen and Equilibrium Mach waves.

5.4.1 Validation using Cleaver's Initial Data

We use the freestream equilibrium conditions suggested by Cleaver [24]:

$$M_f = 1.83 ; \quad \rho_\infty = 0.0516604 \text{ Kg/m}^3 ; \quad T_\infty = 4250 \text{ K} ; \quad q_\infty = 3235.3388 \text{ m/s}$$

$$\theta_w = -5^\circ ; \quad c_{1e} = 0.777445$$

These are slightly more accurate than those given within his paper. For instance Cleaver uses an

equilibrium mass fraction of $c_{1e} = 0.78$. With the initial conditions this value is not accurate enough for our purposes.

The reaction rate was constant and fixed at

$$k_b = 1000 \text{ m}^6 \text{ mol}^{-2} \text{ s}^{-1} \quad (5.6)$$

The characteristic length was defined to be $L = q_\infty \tau_{1\infty}$ and has the approximate value 0.175.

Two runs were performed using different degrees of grid fineness with 100 and 500 cells respectively. The CFL number was 0.4 and the program was terminated when X/L reached a non-dimensional length of 0.15. The CPU times and number of ξ_1 nodes are given in table 5.1. These are to be compared with similar calculations for frozen conditions table 5.2. There is a slight increase in CPU time due to the addition of chemical non-equilibrium.

A comparison between the results calculated using the new method and that by Cleaver reveals a remarkable agreement. This is surprising since Cleaver's calculations were performed by hand. The results from the new method for the 500 cell case are plotted, with the calculated equilibrium values (see appendix B), in figure 5.10. At the singular point there is a sudden discontinuous decrease in the flow variables. The distance over which this occurs as compared with that for the reactions is extremely small. Thus frozen conditions exist at the singular point. The sudden drop causes recombination of the Oxygen atoms and drop in the mass fraction c_1 . The energy released causes the gas temperature to rise slowing the recombination. The pressure close to the wall is observed to reach its equilibrium value quickly downstream of the singular point. It is clear that there is an entropy layer generated by the non-equilibrium. However, unlike for shock wave case there will not be contributions due to the curvature of the waves. The dissipation due to the reactions has a maximum close to the body. This is observed in the entropy variation for $\xi_2 = 0.0$.

Table 5.1 (Non-equilibrium)

ξ_2 Cells	ξ_1 nodes	CPU time h:m:s
100	128	0:0:41
500	634	0:17:12

Table 5.2 (Frozen)

ξ_2 Cells	ξ_1 nodes	CPU time h:m:s
100	130	0:0:35
500	649	0:15:14

5.4.2 Validation Using Appleton's Initial Data

Appleton[8] assumed that the atmosphere was composed entirely of ideal Oxygen. That the conditions corresponded roughly to the state behind an attached bow shock wave at the nose cone travelling at an altitude of 39.624Km and speed of 6705.6 m/s. The initial conditions thus have the values:

$$\rho_\infty = 0.015 \text{ Kg/m}^3; p_\infty = 21029.71 \text{ N/m}^2; T_\infty = 3540 \text{ K}; q_\infty = 2908.1273 \text{ m/s}; c_{1e} = 0.52427$$

These were non-dimensionalized, by Appleton, with respect to Lighthill characteristic constants for Oxygen p_d , ρ_d , θ_d , and u_d (see table 5.5 for values). Where $p_d = \rho_d u_d^2$ and $u_d = (R_2 \theta_d)^{1/2}$.

The reaction rate equation used was of the form

$$q \frac{\partial c_1}{\partial s} = \left(\frac{k_b (1 + c_1) \rho_d^2}{W_1^2} \right) \frac{\rho}{\rho_d} \left((1 - c_1) \exp(-\theta_d / T) - \frac{\rho}{\rho_d} c_1^2 \right) \quad (5.7)$$

where the reverse reaction rate k_b had the form of equation (5.3). It was assumed for simplicity that the squared bracketed term of equation (5.7) was constant, having the numerical value C , taken within the freestream, as

$$C = 11.25 \times 10^{16} \text{ s}^{-1} \quad (5.8)$$

The characteristic length was thus defined by u_d / C having the numerical value $\approx 3.48 \text{E-12}$ Metres. In terms of the non-dimensionalization used within the thesis the rate equation becomes

$$\frac{\partial c_1}{\partial \xi_1} = \frac{LC}{q_\infty} \frac{\bar{\sigma}_1}{q} \frac{\bar{\rho}^2}{\bar{\rho}_d^2} \left(\frac{\bar{\rho}_d}{\bar{\rho}} (1 - c_1) \exp(-\bar{\theta}_d / \bar{T}) - c_1^2 \right) \quad (5.9)$$

Three wedge deflection angles were used having the values $\theta_w = -10^\circ$, -20° , and -30° respectively. The characteristic length L was chosen to have the value 9.57m. This corresponds to the furthest distance downstream calculated to by Appleton. Using the new method, with a CFL condition of 0.4, a comparison was made between the new and old results. The grids used and CPU times required to reach the non-dimensional distance $x/L = 1.0$ can be found in table 5.3. The results are plotted in figures 5.11 to 5.12 where the variables are related to the frozen conditions at the wedge singular point and are non-dimensionalized with respect to Lighthill's characteristic constants. The distance x_w has been non-dimensionalized with respect to the length u_d / C . The dotted lines are the equilibrium values. There is good agreement between the two results. The behaviour of the flow field close to the wall is expected to be similar to Cleaver's test case. Thus the discussion above is applicable here.

As a measure of the increase in CPU time due to the chemical non-equilibrium numerical runs were

performed under frozen conditions. The CPU times and grids used are found in table 5.4. We observe that there is a increase in CPU time due to the reactions. This is particular evident for the smallest deflection angle $\theta_w = -10^\circ$ where the system reaches equilibrium quickly. The stiffness of the chemical equations will be the highest here. Therefore the greatest amount of work by the ODE solver will occur causing the difference in CPU times (non-equilibrium and frozen) to be the most. To confirm this we can calculate the stiffness of each of the reactive systems directly. To do this we assume locally at each nodal point that the mass fraction has the exponential behaviour

$$c_1 = A \exp(-\lambda \xi_1) \quad (5.10)$$

where λ is the stiffness parameter and A a constant determined for the nodal position. Thus by differentiating this equation twice with respect to c_1 we have the condition

$$-\lambda = \frac{1}{Da_w} \frac{\partial}{\partial c_1} \left(\frac{\bar{\sigma}_1 K_1}{\bar{\rho} q} \right) \quad (5.11)$$

where K_1 is given by equation (2.113). During execution of each test case λ was calculated. Its absolute variation with position can be viewed in figure 5.13. It is clear that the stiffness of the system has the highest values for $\theta_w = -10^\circ$; which confirms our original assumption. It is apparent that λ is a measure of the inverse of the local Damkhöler number. Thus for $\theta_w = -20^\circ$ we observe clearly the smooth transition from frozen to equilibrium conditions.

Table 5.3 (non-equilibrium)

θ_w	Grid used ($\xi_1 \times \xi_2$)	CPU time h:m:s
-10°	4,242 X 600	3:34:53
-20°	3,125 X 600	2:48:15
-30°	2,388 X 600	2:22:18

Table 5.4 (frozen)

θ_w	Grid used ($\xi_1 \times \xi_2$)	CPU time h:m:s
-10°	4,488 X 600	2:09:39
-20°	3,256 X 600	1:44:48
-30°	2,157 X 600	1:10:44

Table 5.5

p_d	2.2994E12 N / M ²
ρ_d	150,000 Kg / M ³
u_d	3,915.2988 M / s
θ_d	59,000 K

5.5 Upper Boundary Conditions Re-Visited

The effectiveness of the upper boundary (along $\xi_2 = 1$) was investigated further for chemical non-equilibrium. An expansion wave, generated using Cleaver's initial data, was allowed to impinge onto the boundary. Two length scales were chosen: $L = 0.0068$ Metres and $L = 0.0272$ Metres respectively; where the latter is four times that of the former. It was found that the waves were reflected at the upper boundary, downwards, towards the solid boundary. These causing a secondary wave system to be created. By assuming, approximately, that specular reflection occurs at the upper boundary the distance downstream where the wave first interacts with the solid boundary can be shown to be $\approx 3.5 L$ (see figure 5.5). Pressure and density profiles have been plotted for the two different length scales within figure 5.14. We observe that at $\approx 3.5 L$ the profiles increase; this suggests that the incident expansion was reflected as a compression causing the profiles to rise. By quadrupling the length scale the non-dimensional position at which the profiles increase should remain the same; this is indeed observed. An indication of the path of the reflected waves through the field of flow can be observed by plotting density contours, see figure 5.15. The contours are clearly distorted by the passage of the reflected waves. A line (dotted) can be drawn through the contours where they start to curve downwards. The point at which this line hits the solid boundary is in excellent agreement with our approximate distance for interaction.

We observe that secondary waves are generated at the upper boundary. These are non-physical, should not occur in practice, and will affect the accuracy of the flow field downstream. Therefore waves should not be allowed to interact with the boundary if the accuracy of the flow field is to be maintained.

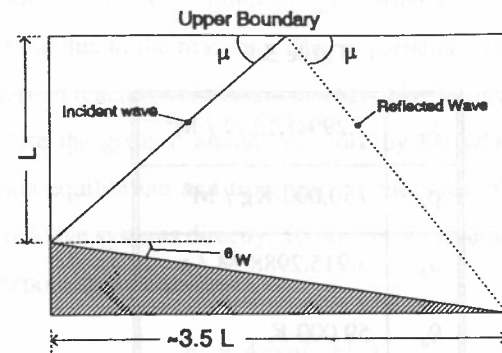


Figure 5.5 Specular Reflection of Mach Wave.

5.6 Aerodynamic Characteristics of Simple Re-Entry Configuration

The affect of the relaxation processes on the aerodynamic characteristics of the Space Shuttle vehicle has been examined earlier by Woods et al[102]. For the continuum flow regime (altitudes below 85Km) the lift and drag were smaller during the shuttle flight then that predicted based on windtunnel tests using perfect gas flow. The centre of pressure (CP) was shown to move forward due to the non-equilibrium, causing an upwards pitching moment, which can be as much as 0.7% of the length of the vehicle. This is to be compared with the built in shift, due to the control surfaces, which is a maximum of 1%. Numerical studies of this phenomena by Park[71], Park and Yoon[73] in the U.S.A. and by Kosorukov et al[56] in Russia have confirmed these effects qualitatively.

We purpose a crude model for the Space Shuttle OB, figure 5.6, and investigate the affect of the chemical non-equilibrium on its aerodynamic characteristics as compared to those for a perfect, constant γ , gas. The flap AB was added to represent a form of controlling surface. We only consider the changes on the underside of the profile. The shuttle experienced its greatest aerodynamic difficulties at the altitude of 74Km. Using this as the starting conditions the density and temperature (from ESDU data sheet 77021) have the values:

$$T_{\infty} = 210 \text{ K} ; \rho_{\infty} = 4.070675\text{E-}05 \text{ Kg / m}^3$$

We assume that the shuttle has an approximate characteristic length $L = OA = 33$ Metres, the flap AB = 2.5 Metres, angle of attack of $\theta_a = 40^\circ$, and speed¹⁴ of $q_{\infty} = 5000$ m/s.

Calculations were performed for constant $\gamma = 7/5, 4/3$, and $9/7$. The flap deflection angle δ , with respect to θ_a , was varied in steps of 10° within the range -20° and 20° . Calculations were performed for chemical non-equilibrium with a fixed reverse reaction rate given by equation (5.6) and a variable temperature rate

¹⁴ For $c_1 = 0.0$ ($\gamma = 4/3$) these initial conditions give a temperature downstream of the leading shock which is in the range of approximation for the Lighthill model.

given by equation (5.3). Execution was terminated when the end of the profile was reached determined by

$$x/L = \frac{1}{OB} (OA \cos \theta_a + AB \cos \delta) \quad (5.12)$$

Using a CFL number of 0.4 the CPU for 400 ξ_2 cells (minimum thought necessary to resolve the flow field) and 29,114 ξ_1 nodes was over 31 hours for the zero flap configuration. This is to be compared with a frozen calculation which took roughly 1 hour 40 minutes and used 2,421 nodes.

Aerodynamic coefficients were calculated for each of the cases (see Anderson[4] for definitions). We have defined the abbreviations *frr* and *vrr* to represent fixed and variable reverse reaction rates respectively. These are plotted in figure 5.16. It is clear that the real gas effects have the overall effect of reducing the lift, drag, and normal forces. The force parallel to the body appears to be unaffected. The variable rate does not reduce them as much since it is initially an order of magnitude less than for the fixed rate. It will be obvious that as the strength of the source term goes to zero the aerodynamic characteristic for the real gas case will increase/decrease to match up with does for $\gamma = 4/3$. By considering $\gamma = 9/7$ and zero flap deflection angle, a flap deflection of $\approx 14^\circ$ is necessary for the real gas case to yield the same lift and normal force coefficients. Therefore it will be necessary to have a larger flap angle for real gases as compared a perfect gas law model. The CP shift is observed to move forwards for negative flap deflection angles but backwards for positive deflections. It is clear from the data for the pitching moment¹⁵ that the real gas effects cause the nose to pitch upwards. To compensate for this it is necessary to have a larger flap deflection angle. It is observed that the real gas effects can be modelled approximately by reducing γ . However, this will not correctly model the compressibility effects due to the reactions and thus will be of limited use. A comparison was made, for zero flap angle in figure 5.17, between the oblique shock positions produced within an inert flow field $\gamma = 4/3$ and produced when real gas effects prevail. It is clearly observed that the shock weakens due to the reactions. These findings are in good qualitative agreement with the those from Park[71], Park and Yoon[73], Kosorukov[56], and Woods[102].

We now investigate the effect of the two different reverse reaction rates on the flow field profiles. These are done in figures 5.18 - 5.21. For the first two it is clear from them that the variable rate produces less noise. This rate is lower in the initial stages of development downstream of the shock wave. Considering the temperature variation along the streamline $\xi_2 = 0.1$, it is clear that both rates are approximately the same downstream. This suggests that the pressure and density profiles should behave in a similar way. However, this is not the case. An explanation could be that the initial strength of the

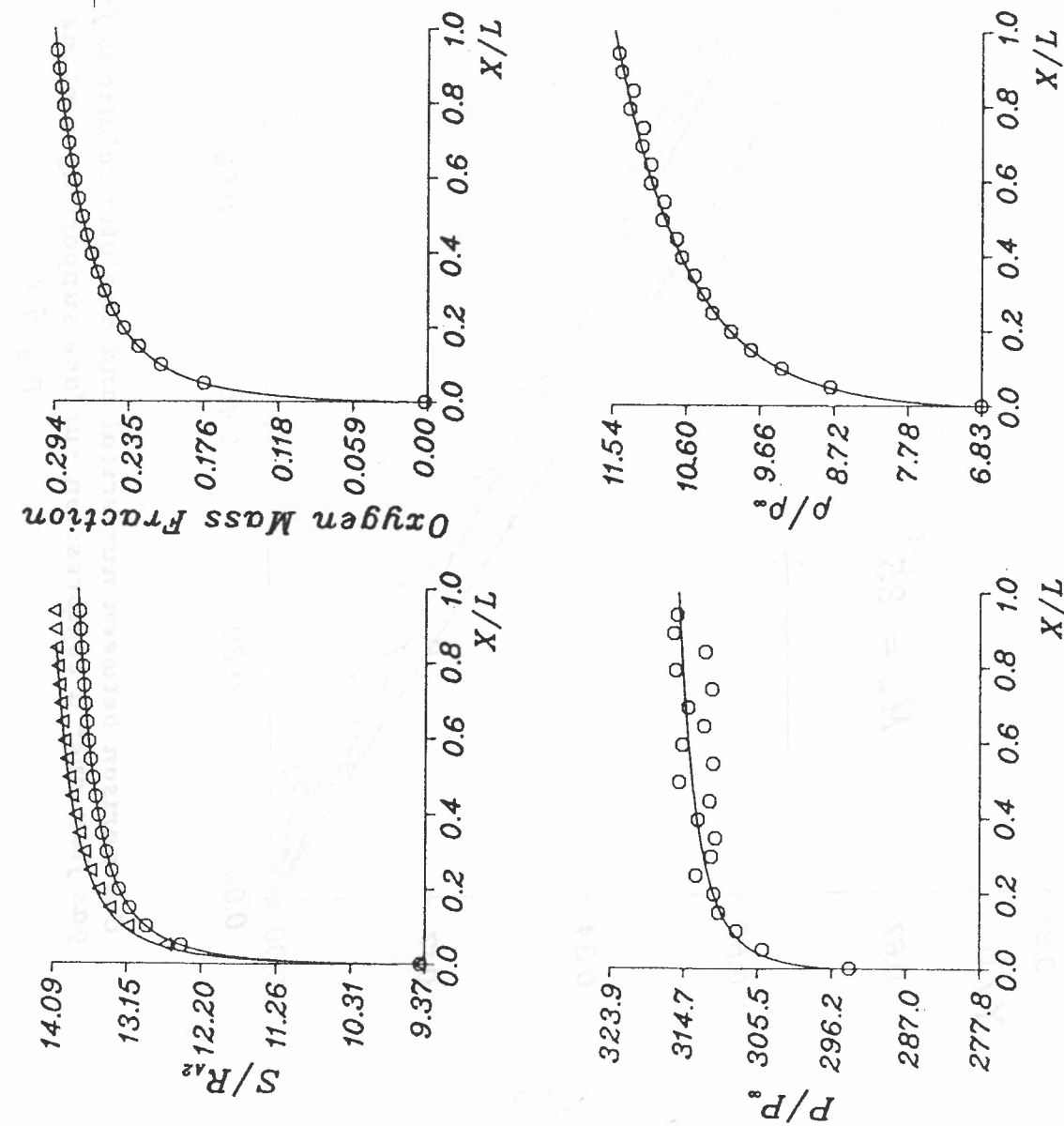
¹⁵ Convention dictates that a +ve pitching moment is nose upwards. Here moments are taken about the leading edge.

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Comparison between numerical and analytic solutions for nonequilibrium gas flow over a compression surface supporting a plane, oblique shock wave.

Δ RCM for $L=1.185m$, $\rho_\infty=1.1621 \times 10^{-6} \text{ Kg/M}^3$
 $\circ$ RCM for $L=0.395m$, $\rho_\infty=3.4863 \times 10^{-6} \text{ Kg/M}^3$
 — Analytic Solution



Comparison between numerical and analytic flow variable profiles.
Fig. 5.8

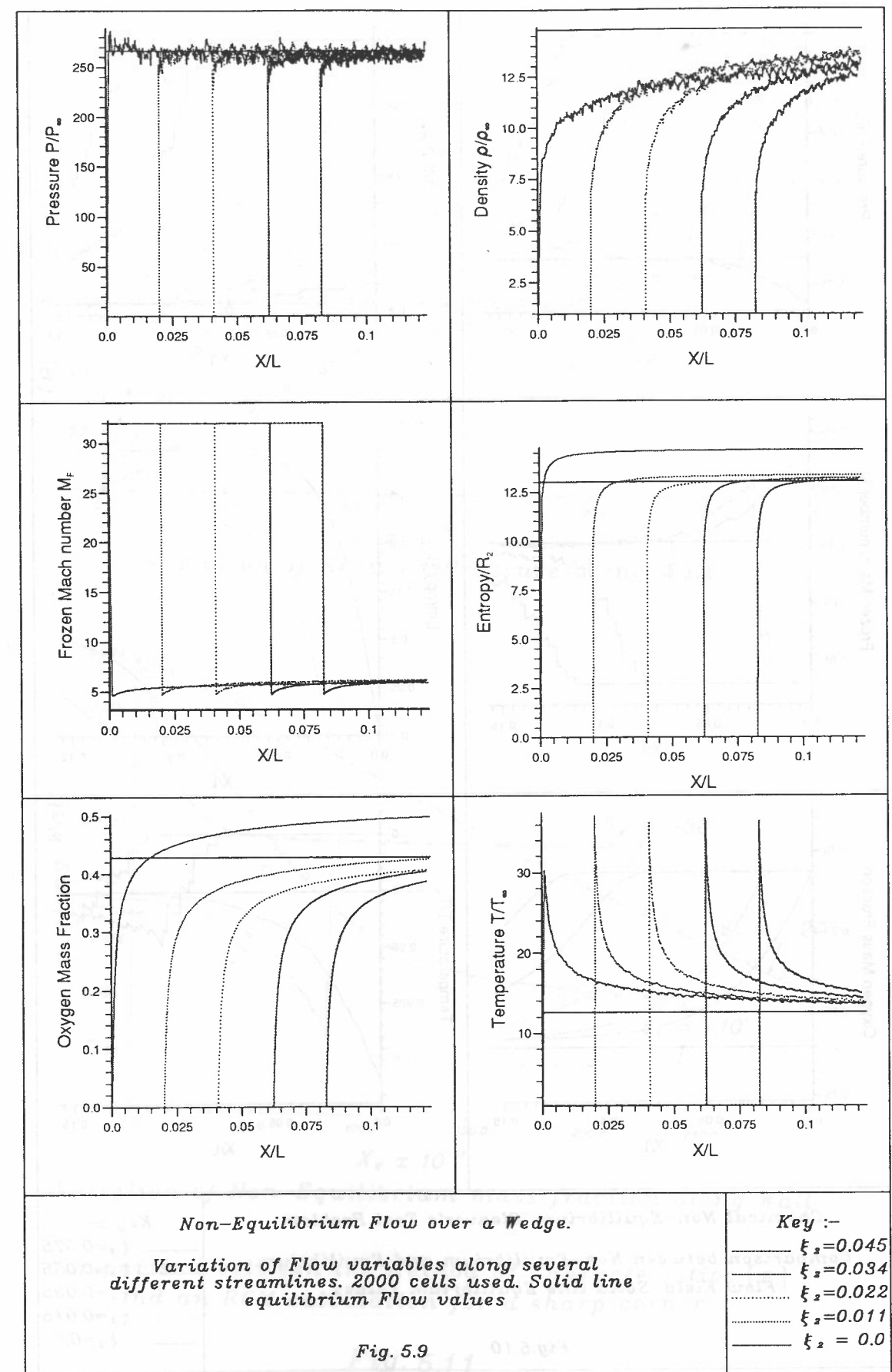


Fig. 5.9

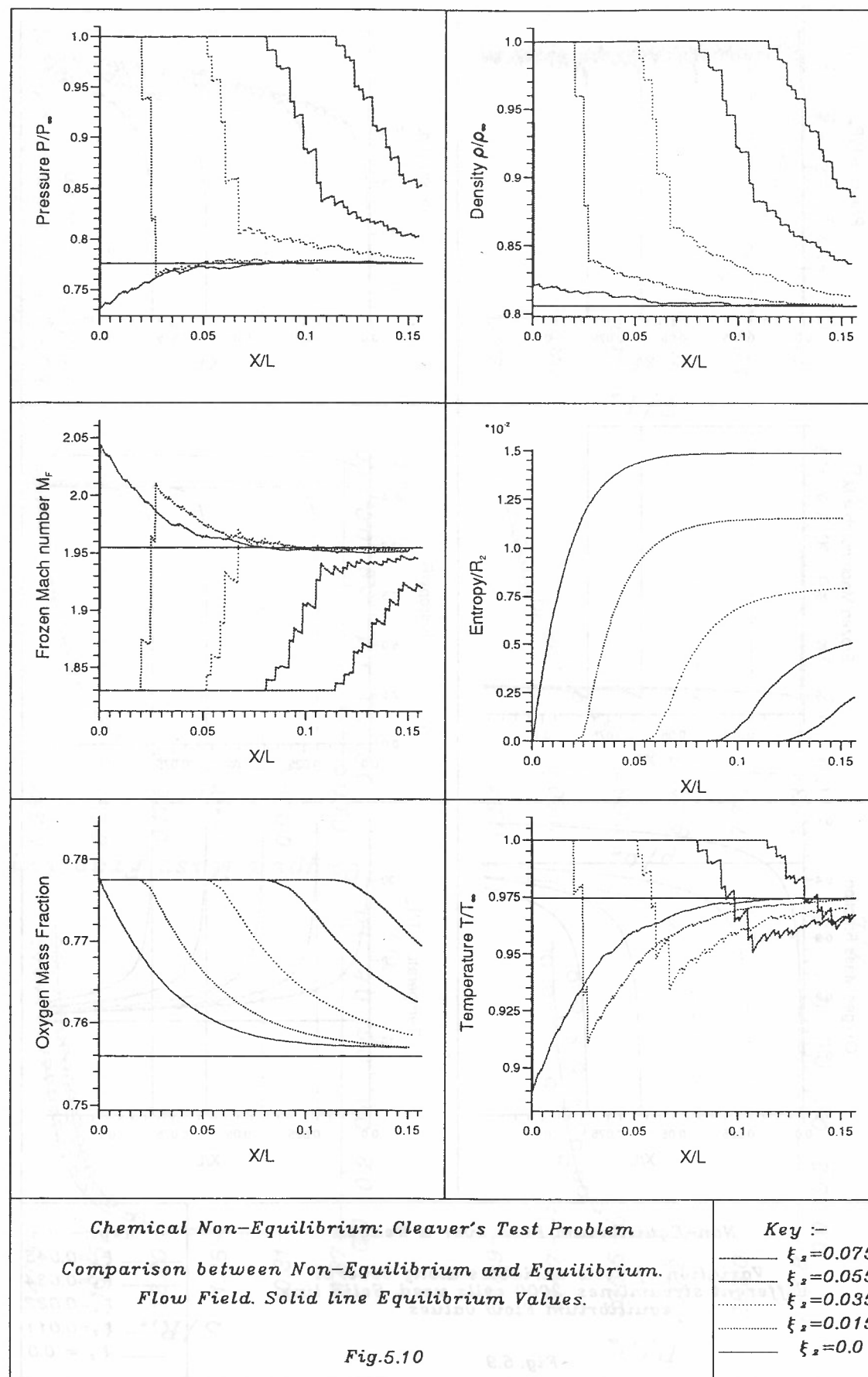
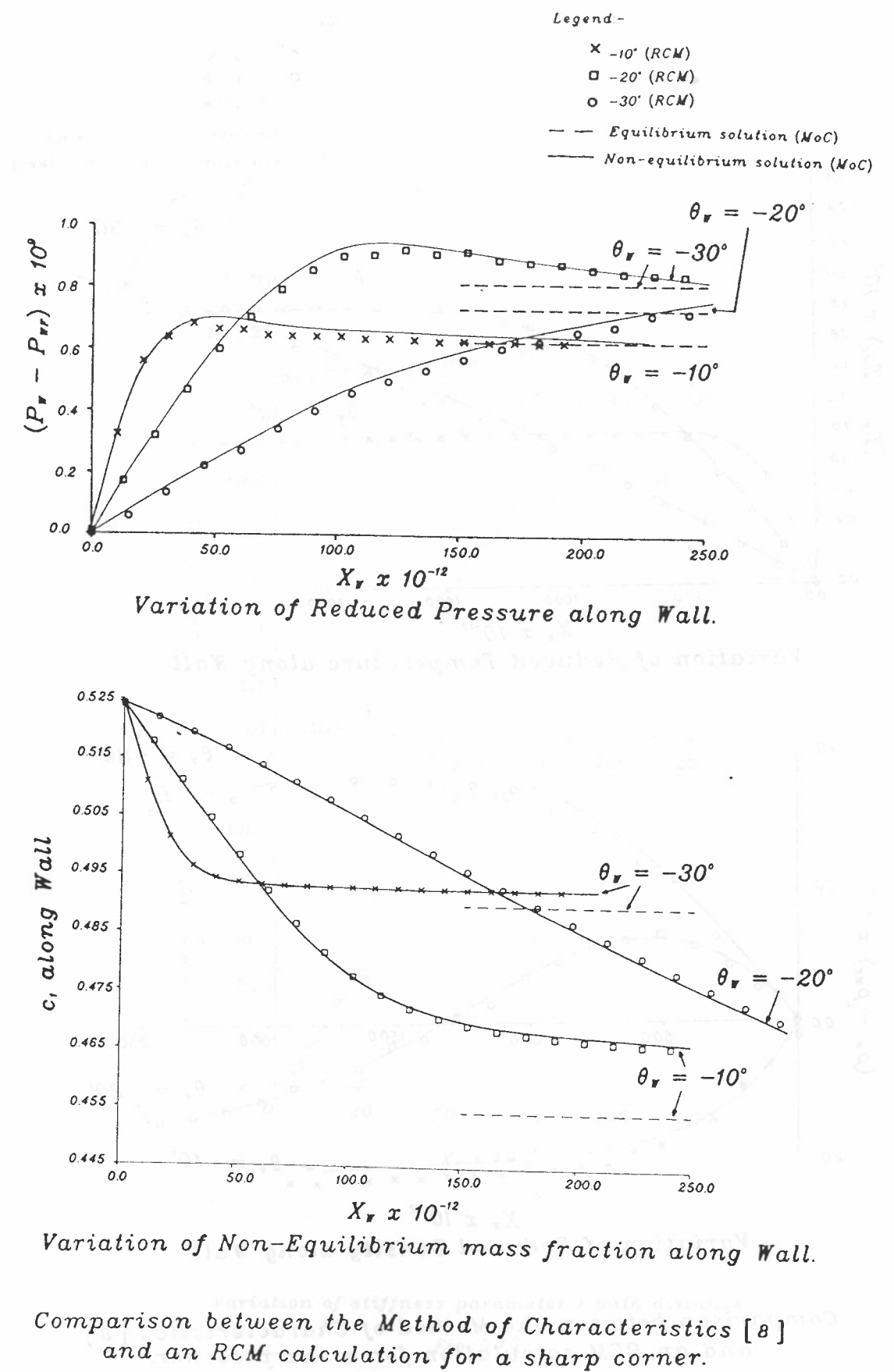
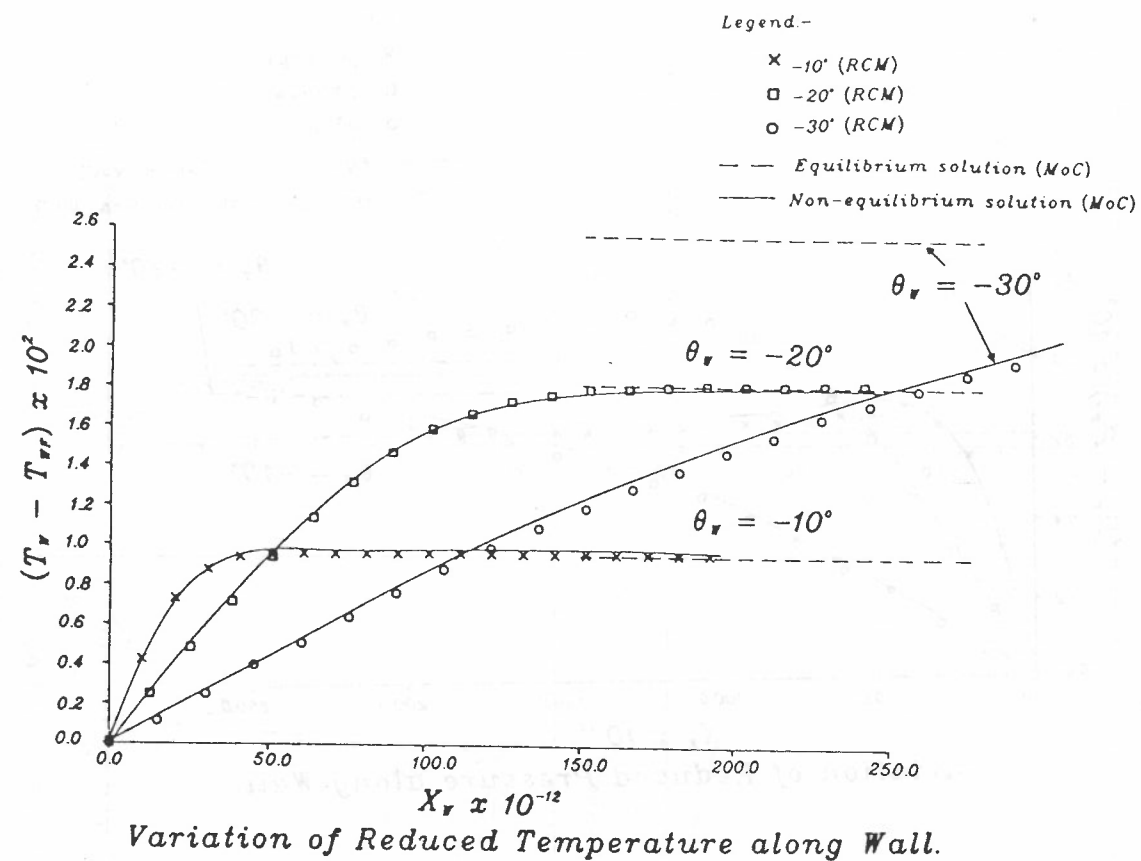
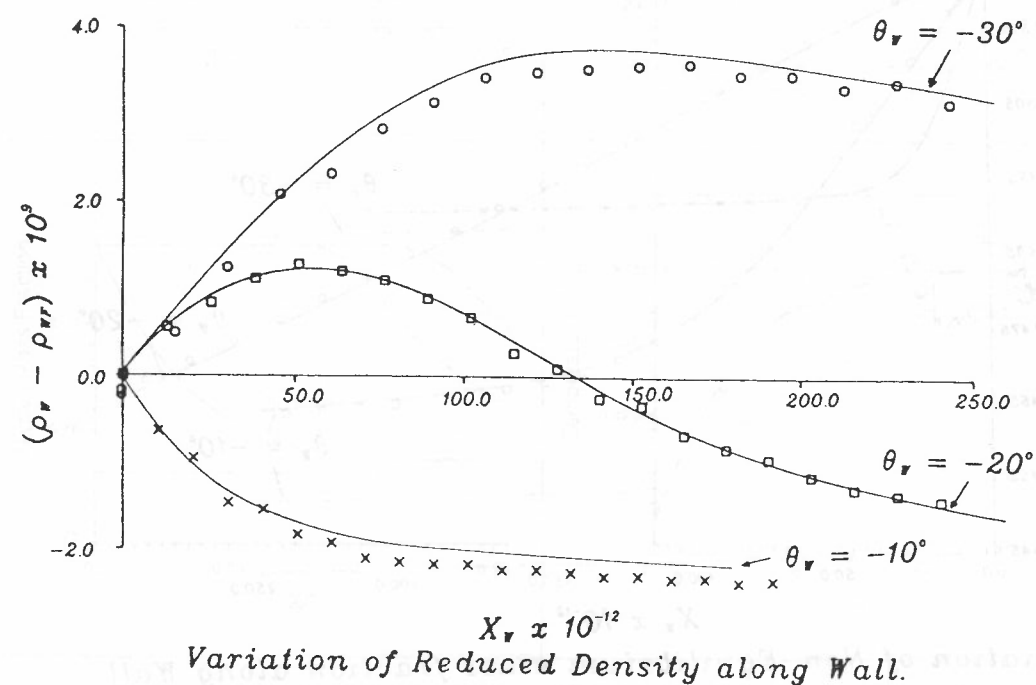
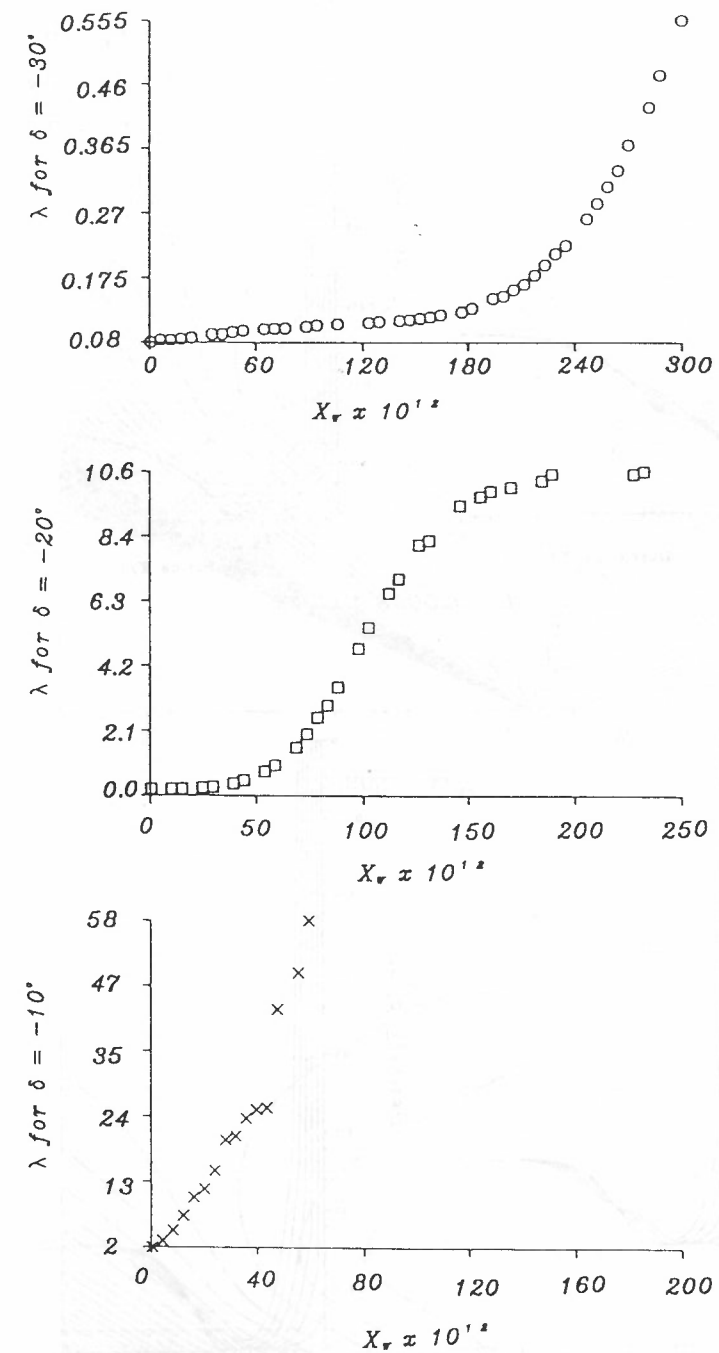


Fig. 5.11



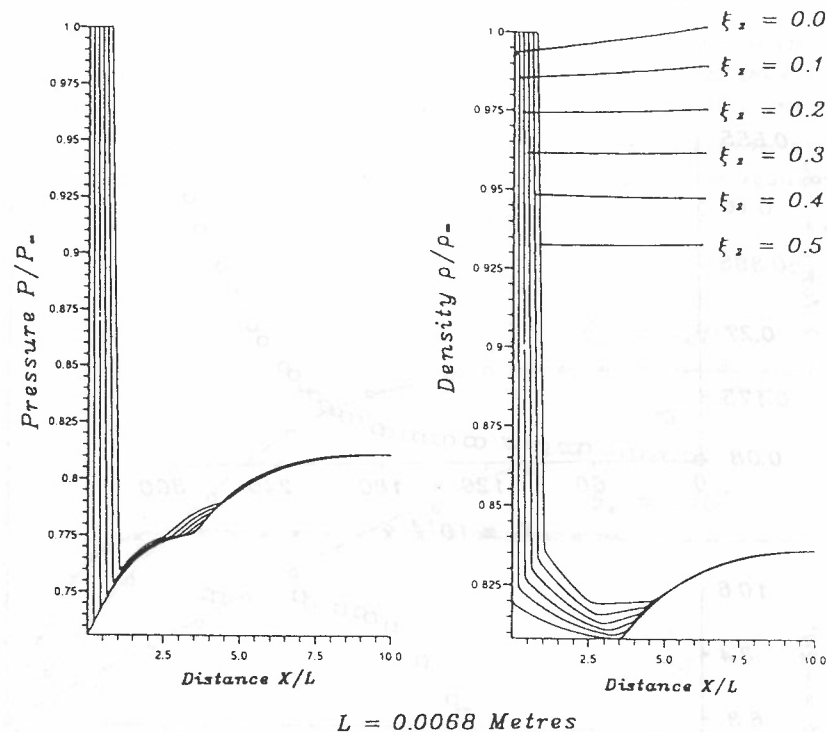
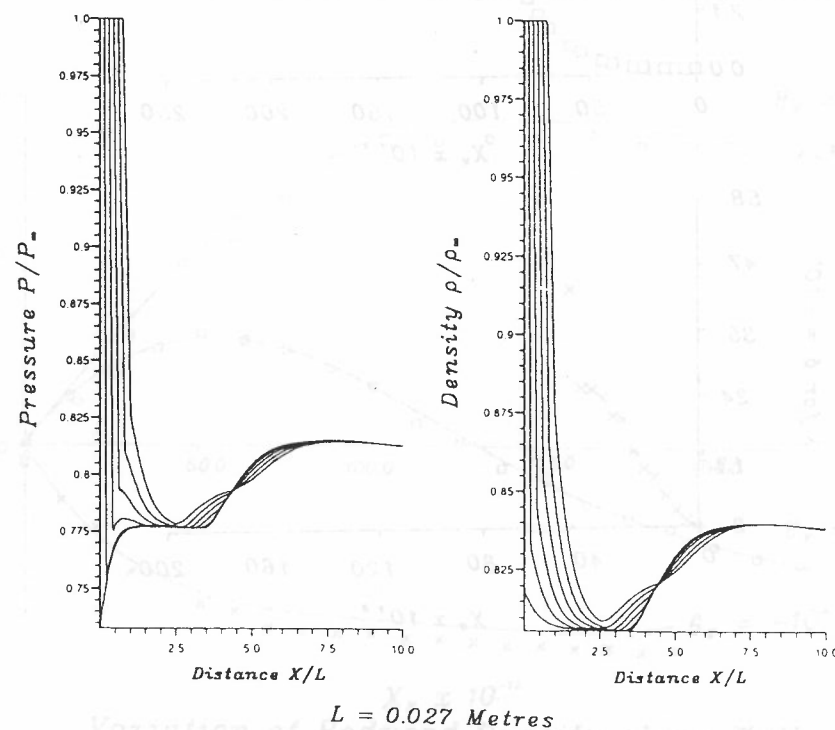
Comparison between the Method of Characteristics [8]
and an RCM calculation for a sharp corner.

Fig. 5.12



Variation of stiffness parameter λ with distance

Fig. 5.13



Upper Boundary Test Problem

Fig. 5.14

Upper Boundary Test Problem

Comparison between Density contours generated in ξ_1 , ξ_2 and x , y co-ordinate spaces
 $M_\infty = 1.83$ $CFL = 0.45$

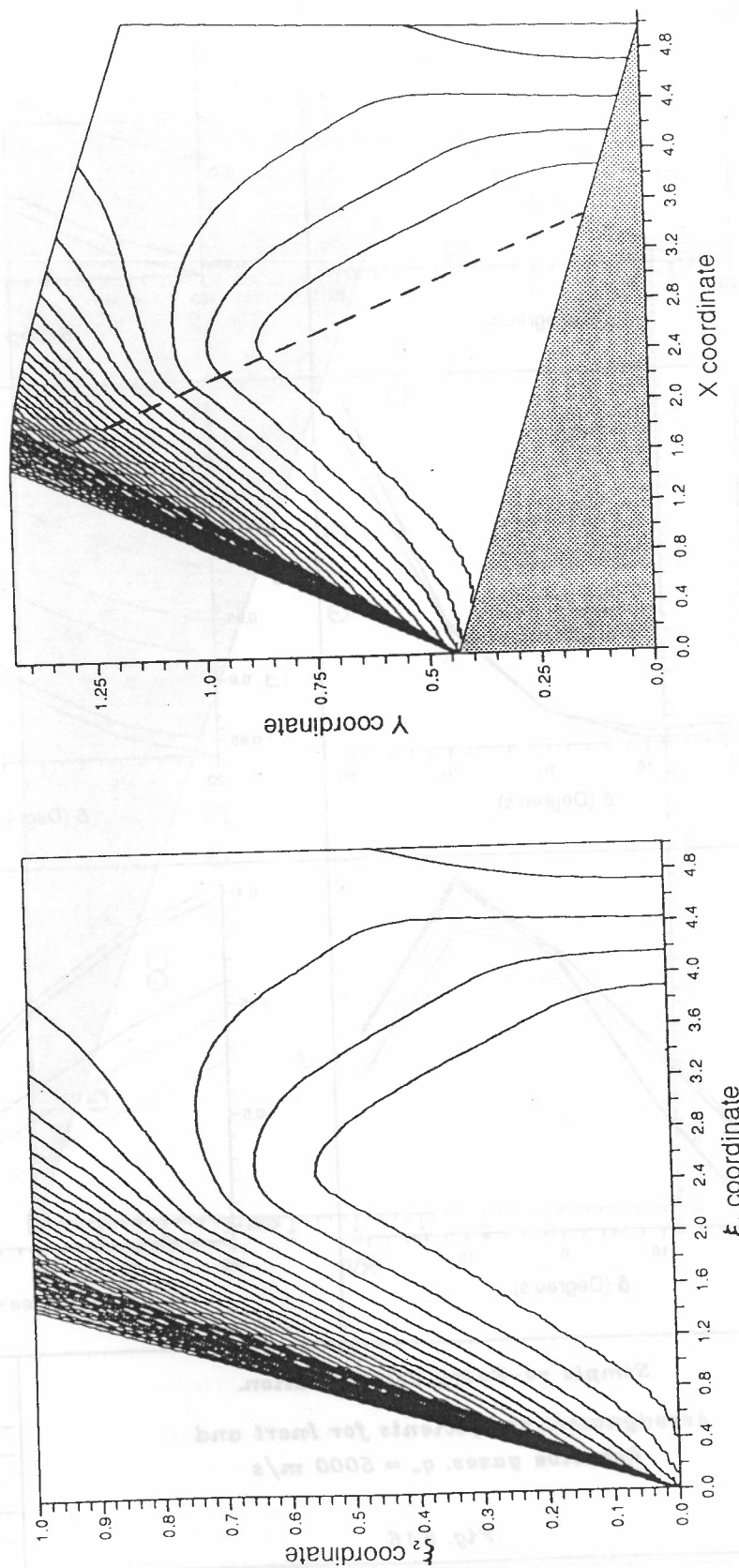
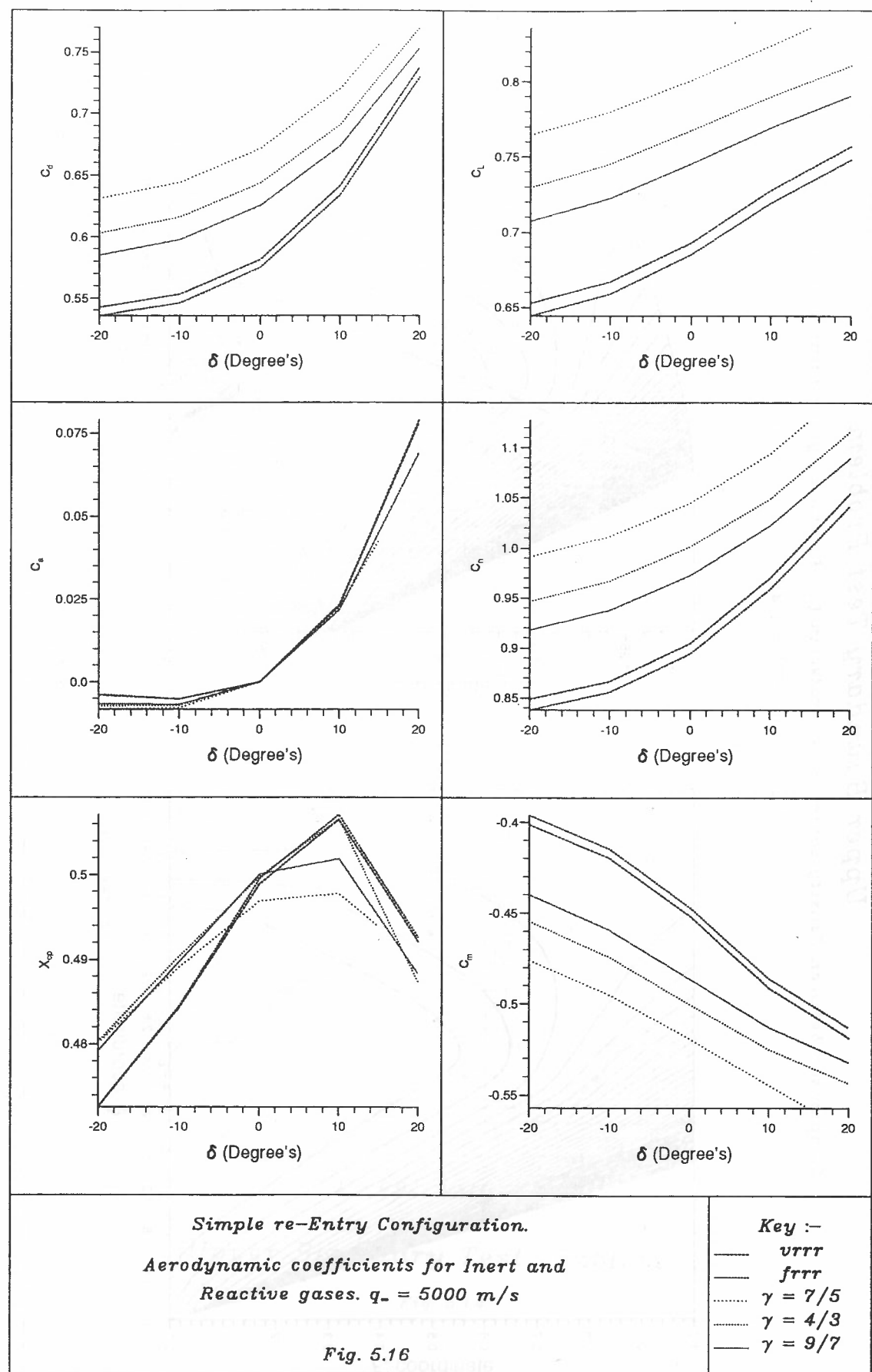
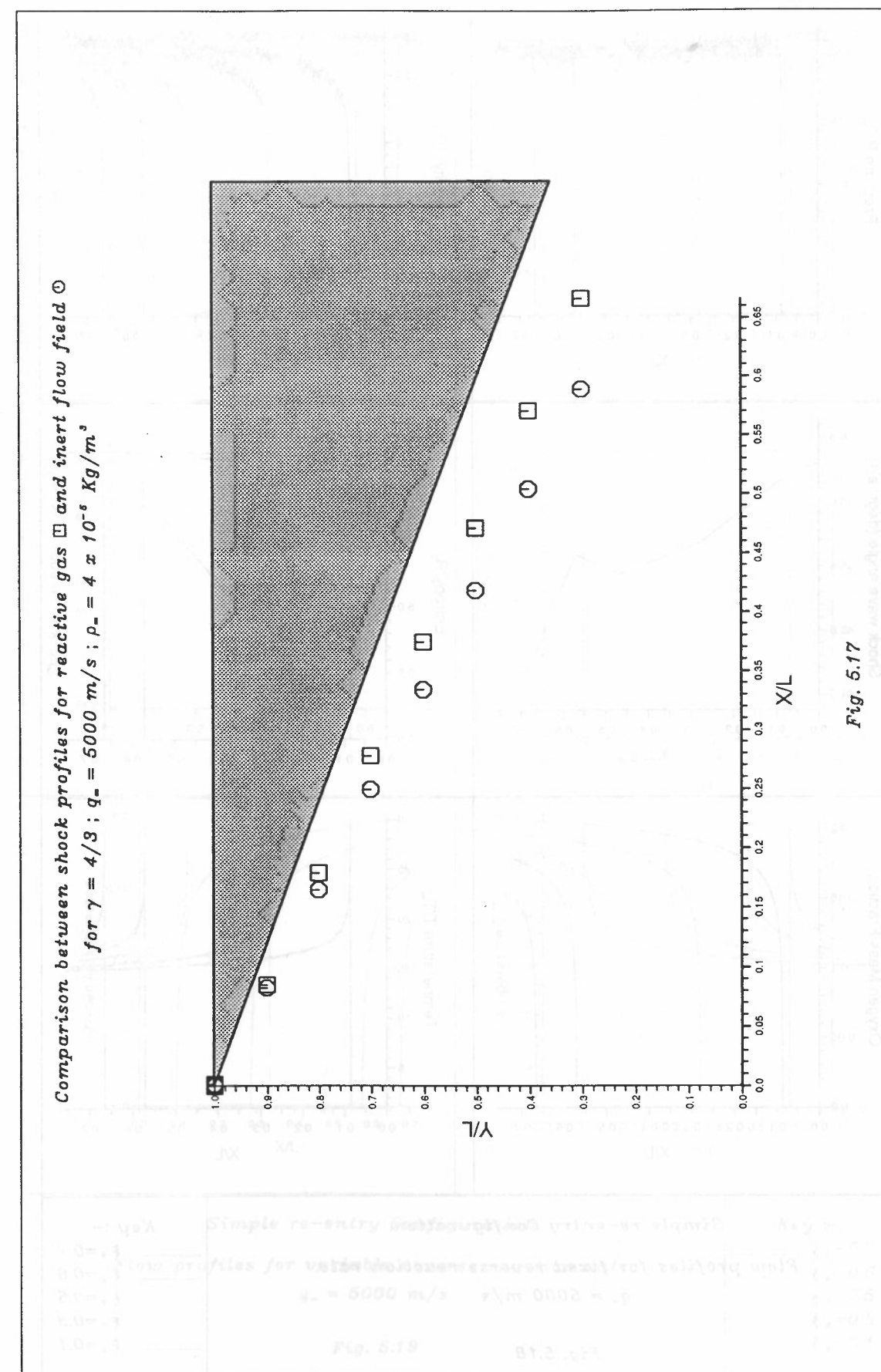
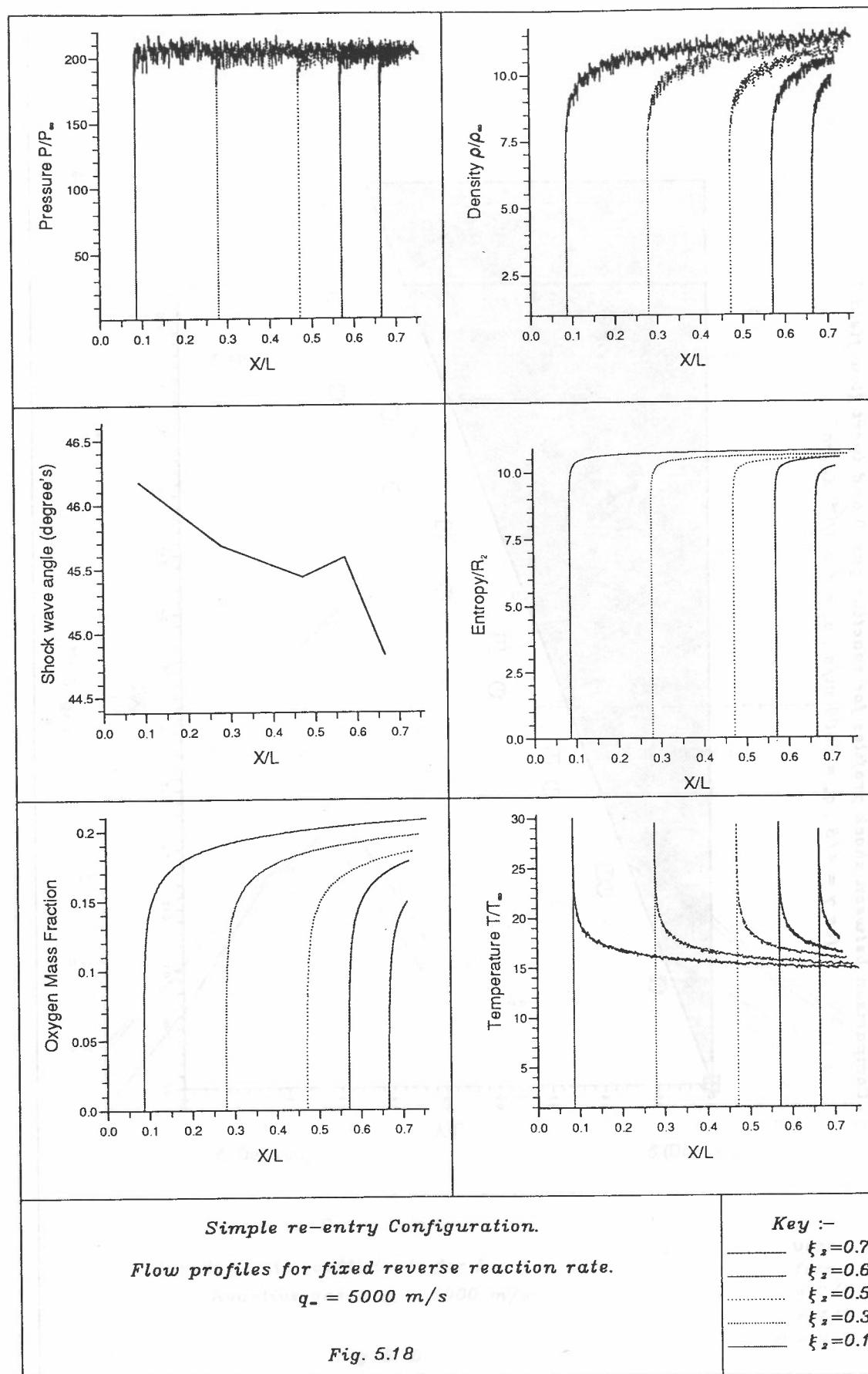
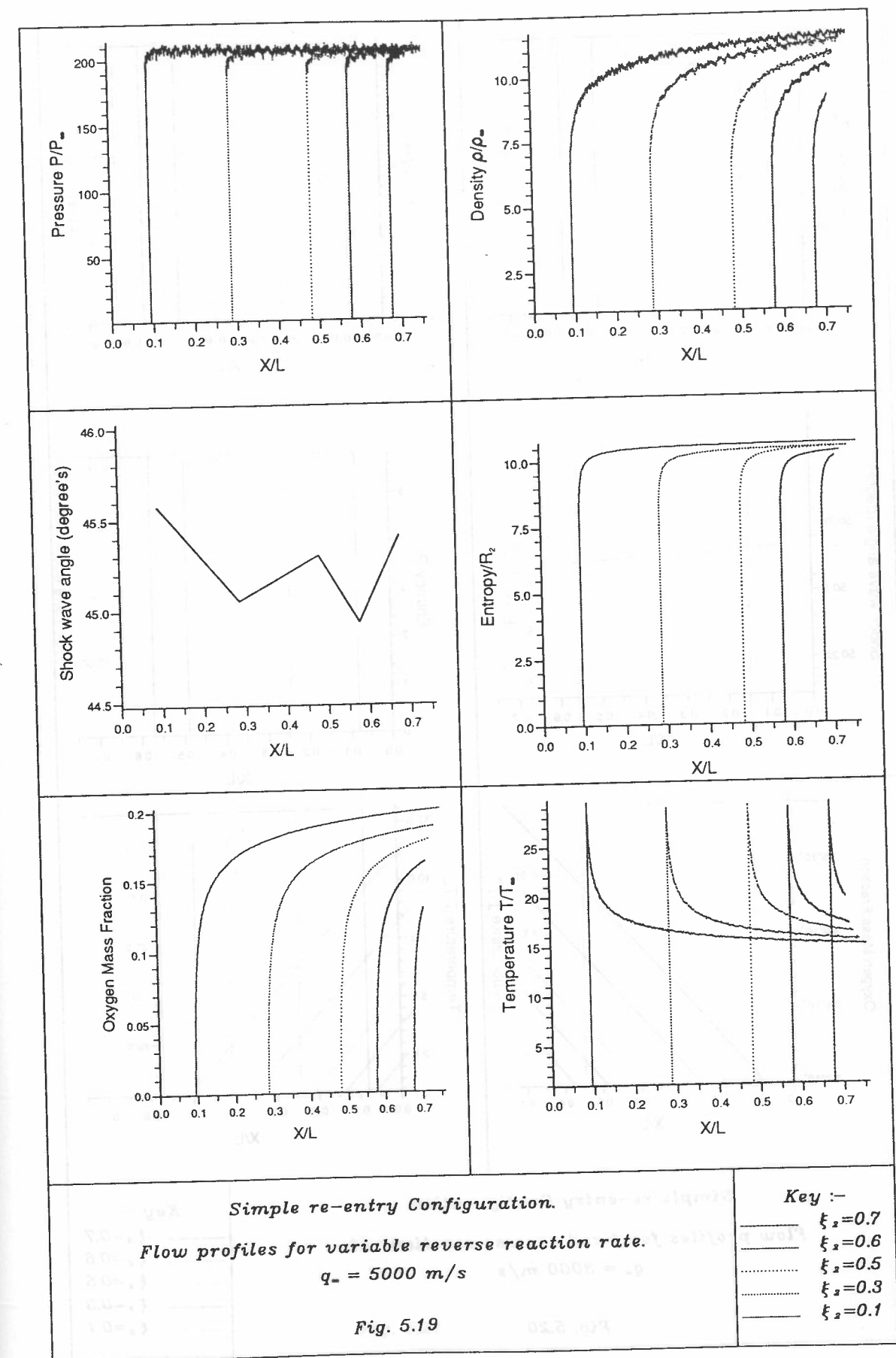
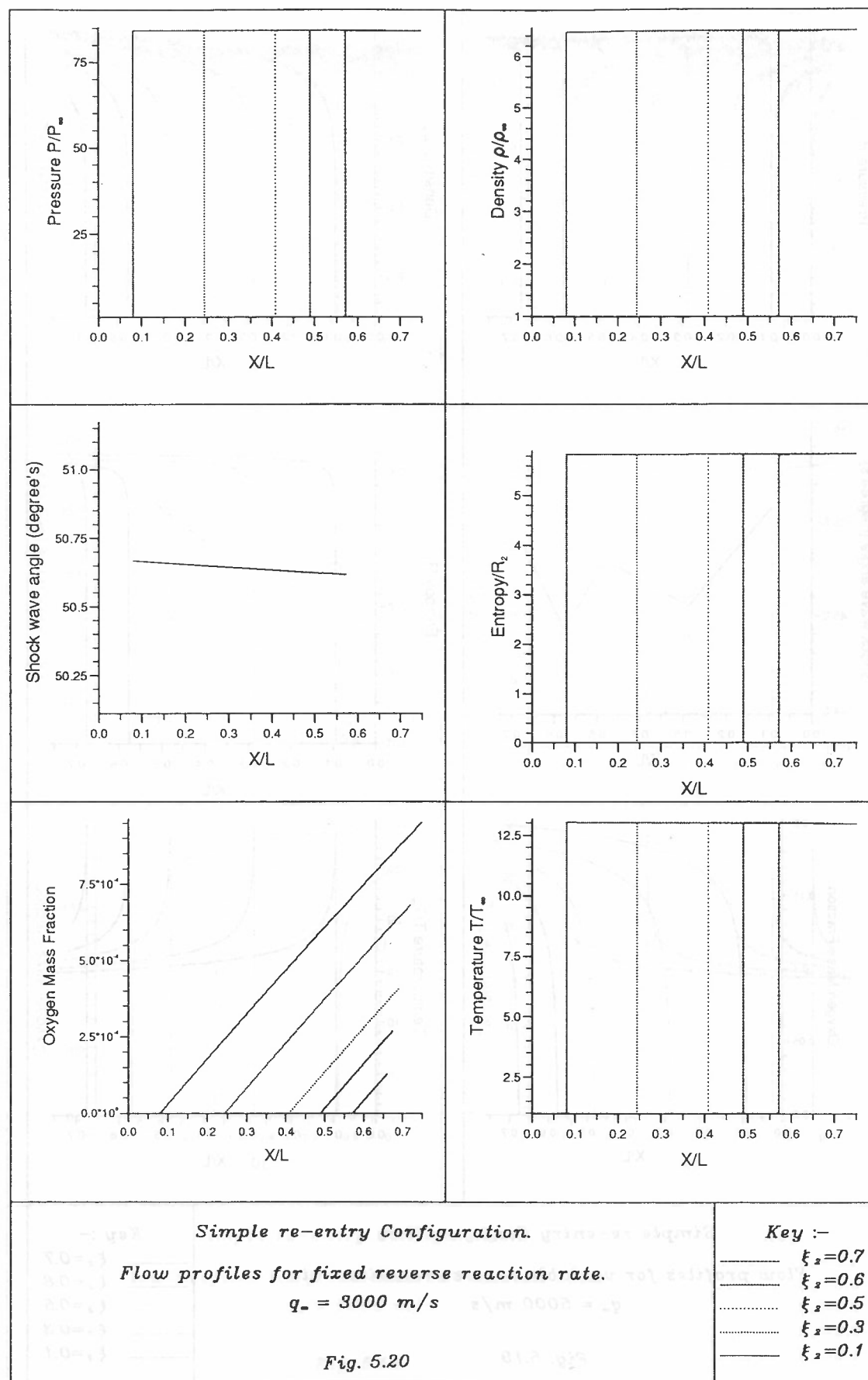
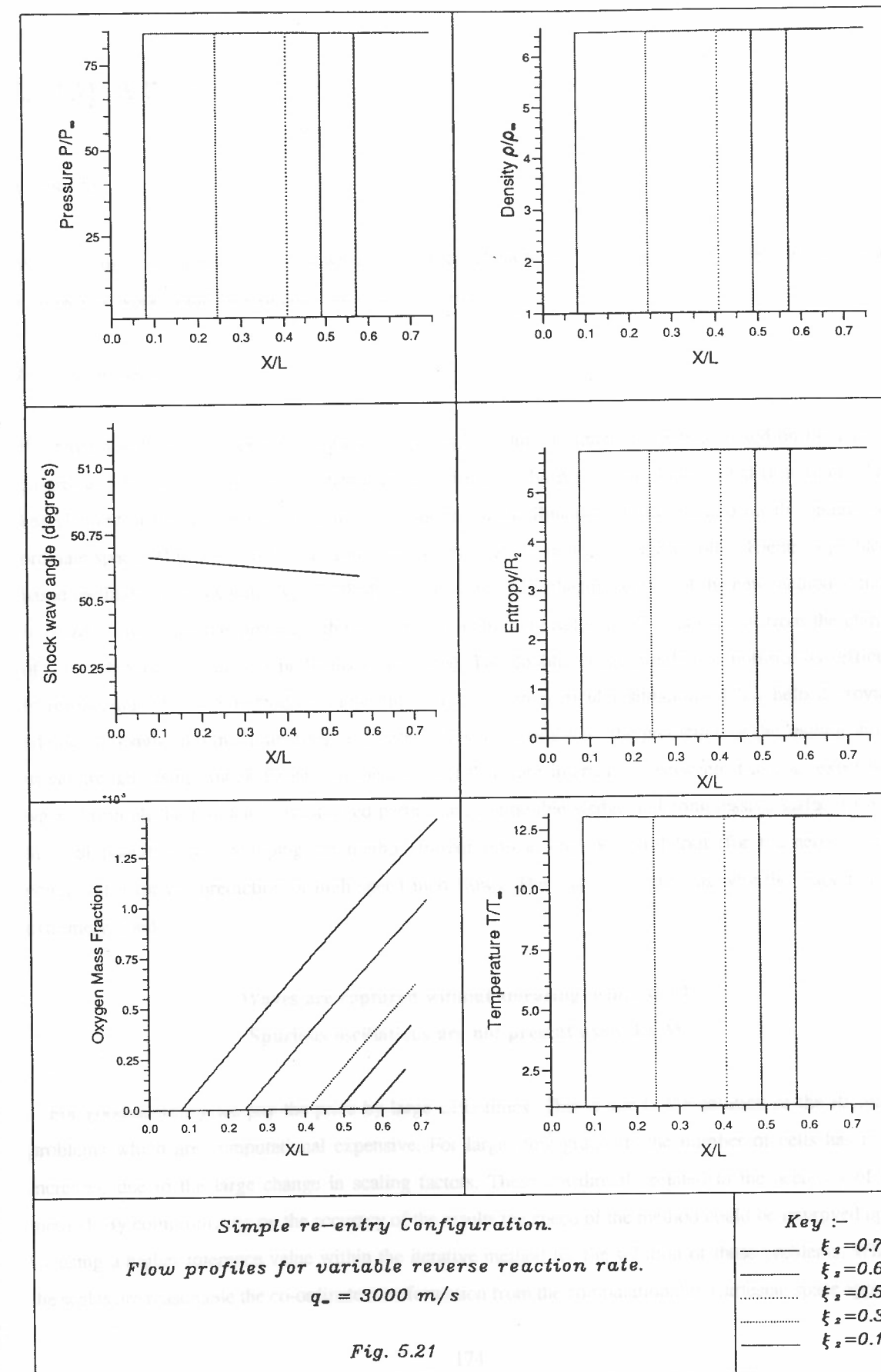
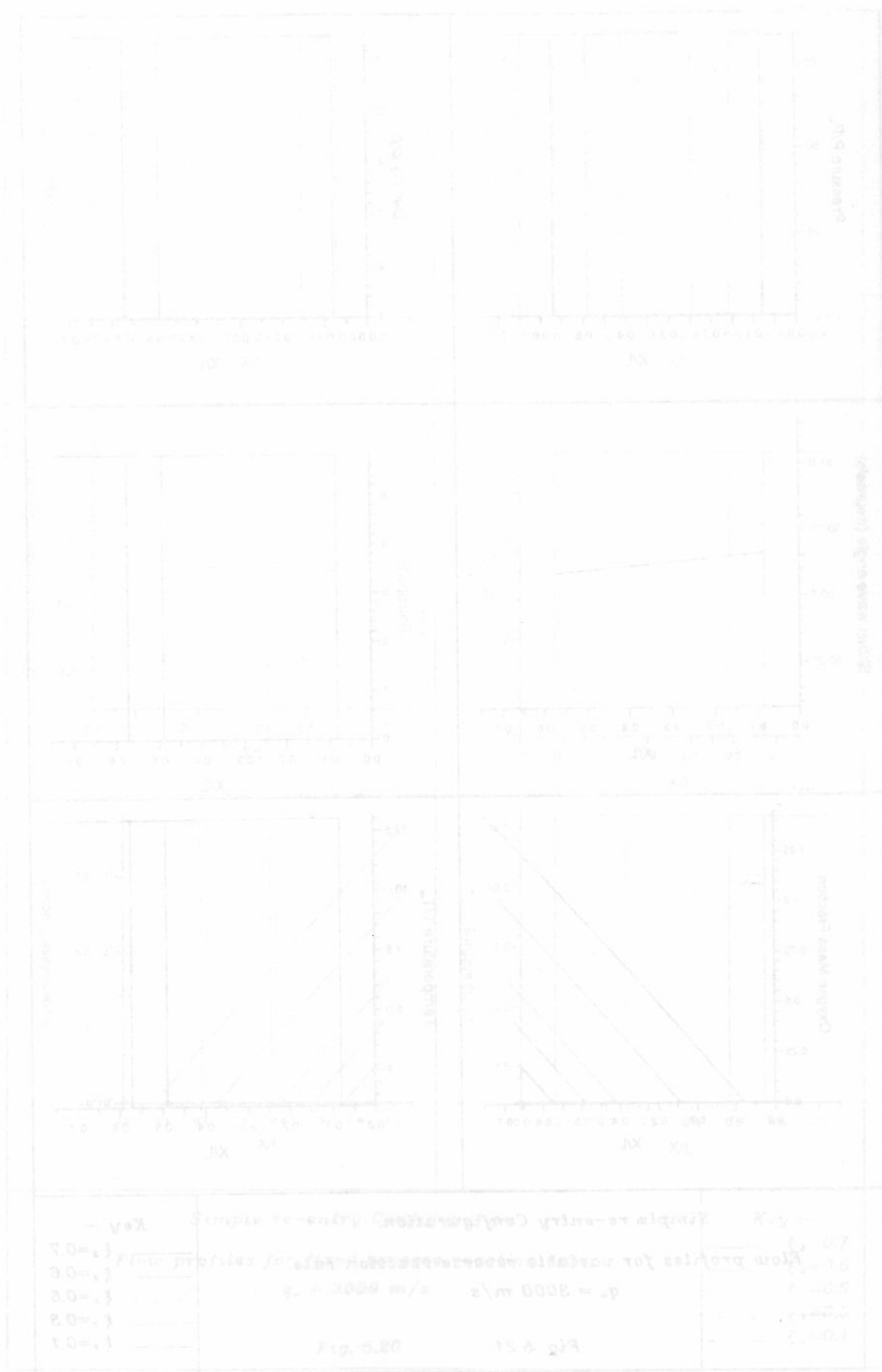


Fig. 5.15









Chapter 6

Closure

We bring the thesis to a close by drawing up some conclusions based on our work. A few suggestions as to how our work could be extended are also presented.

6.1 Conclusions

We have developed a successful fractional step, high resolution numerical method based on the natural co-ordinate system for high speed, chemically reacting, steady, planar two dimensional flow fields. The key element of the new algorithm is the development of the Random Choice method for the natural co-ordinate space. This has clearly not been done before and has great potential for other Riemann problem based methods such as Godunov[44], PPM[26], and WAF[92]. The application of the new method to inert or frozen flow fields has proved both excellent and extremely accurate. This is evident from the clarity of results from numerous test problems investigated. The double wedge problem is notoriously difficult to resolve but the new method has done this with ease. In particular situations it has helped provide additional insight into the limitations of a theory. This was evident for the prediction of the leading shock wave strength using Shock Expansion theory when there are interactions between it and an expansion wave. From all the problems investigated particularly the double wedge and compressive surfaces stems the real potential of developing the method further into a very powerful tool (for the aerodynamic community) for the prediction of high speed inert flows. There are clear reasons why the resolution is extremely good

Waves are captured without smearing using RCM

Spurious oscillations are not present using RCM

For good accuracy we pay the price by large CPU times. This is due to the solution of the Riemann problems which are computational expensive. For large flow gradients the number of cells has to be increased due to the large change in scaling factors. These are directly related to the accuracy of the method. By compromising on the accuracy of the results the speed of the method could be improved upon by using a higher tolerance value within the iterative method for the solution of these problems. Where the scales are reasonable the co-ordinate transformation from the computational to Cartesian space appears

to have the minimal effect on the numerical results. For severe flow changes where σ_2 changes significantly these numerical transformations will become less accurate.

For chemical non-equilibrium the scheme appears to be affected, in the form of oscillations in the flow variables, initially by the strength of the chemical source term. This is due to its exponential dependence on the absolute temperature and the form of reverse reaction rate equation used. By using a variable rate the oscillations are reduced but not removed. The ODE solver has been shown to have a minimal effect on the CPU time where the *stiffness* of the system of equations is low with reactions slow. Where the *stiffness* increases the CPU time is observed to increase accordingly due to the extra work performed by the ODE package. On the whole the numerical results agree well with other methods. The results from the simple re-entry profile have produced the right qualitative behaviour. Therefore the power of the full algorithm is very good.

For visualization purposes in-house routines for graph and contour plotting were written as the off-the-shelf packages such as *GINO-F* and *UNIRAS* were felt to be inadequate.

6.2 Future Work

The high resolution method for inert flow fields has proved in some instances to be very expensive in terms of CPU time. This is because at each spatial level the wave interactions are modelled by solving the local Riemann problems. It was implied earlier that the type of seeding conditions for an iterative method and the convergence rate of the method itself will have an influence on the convergence time or number of steps. It would not be a trivial task to determine the optimum seeding conditions and iterative method for a general problem, but would be worth pursuing.

Another way to reduce the CPU time is to use an approximate Riemann problem. Harten & Lax[47] have shown that under appropriate circumstances this approximate can be applied to the Random Choice Method and still preserve its power.

The power of the natural co-ordinate space lies in the flexibility in the initial choice of the scaling factor σ_2 . Currently it was fixed within each cell. In physical space the nodes start with the same distance apart along a normal. However, some regions may be less important than others. For example, the region downstream of an oblique shock wave will be more important than the freestream where nothing happens. Thus σ_2 could be scaled so that some regions are finely resolved while others are coarsely resolved. Scaling should be done where the flow changes are sudden and large, particularly for expansions with high Mach numbers and deflection angles. In this way the nodes do not have to be moved in the computational

grid to get these desired features; one has only to initially scale σ_2 appropriately. This scaling procedure is similar to the variable node spacing used by Gottlieb[45] for the one dimensional unsteady RCM.

The inclusion of additional reactions goes without saying. We have attempted to lay the ground work for this in appendix F. However, the strength of chemical source term and its influence on the flow field must be looked at further. We have only touched upon this problem within this thesis. It is clear that the choice of rate equation will influence the behaviour. By including a vibrational relaxation model one could use the rate equations suggested by Park[72] which employs the geometric temperature

$$T = \sqrt{T_t T_v} \quad (6.1)$$

where T_t and T_v are the translational and vibrational temperatures. Therefore the vibrational relaxation has a direct influence on the strength of the chemical reactions by reducing the effective temperature.

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Appendices

APPENDIX A

Vector Relations and Identities

For generalized orthogonal curvilinear coordinates (ξ_1, ξ_2, ξ_3) with basis vectors $(\underline{e}_1, \underline{e}_2, \underline{e}_3)$ the gradient of the scalar function ϕ can be expressed as

$$\nabla\phi = \sum_{i=1}^3 \frac{1}{h_i} \frac{\partial\phi}{\partial\xi_i} \underline{e}_i \quad (\text{A.1})$$

and similarly the Divergence and Curl of the general vector $\underline{A} = A_1\underline{e}_1 + A_2\underline{e}_2 + A_3\underline{e}_3$

$$\nabla \cdot \underline{A} = \frac{1}{h_1 h_2 h_3} \left\{ \frac{\partial(h_2 h_3 A_1)}{\partial\xi_1} + \frac{\partial(h_1 h_3 A_2)}{\partial\xi_2} + \frac{\partial(h_1 h_2 A_3)}{\partial\xi_3} \right\} \quad (\text{A.2})$$

$$\nabla \wedge \underline{A} = \frac{1}{h_1 h_2 h_3} \begin{vmatrix} h_1 \underline{e}_1 & h_2 \underline{e}_2 & h_3 \underline{e}_3 \\ \frac{\partial}{\partial\xi_1} & \frac{\partial}{\partial\xi_2} & \frac{\partial}{\partial\xi_3} \\ h_1 A_1 & h_2 A_2 & h_3 A_3 \end{vmatrix} \quad (\text{A.3})$$

where h_1, h_2, h_3 are the scaling factors given by

$$h_i = \left| \frac{\partial \underline{r}}{\partial \xi_i} \right| ; i = 1, 2, 3 \quad (\text{A.4})$$

with the basis vectors

$$\underline{e}_i = \frac{1}{h_i} \frac{\partial \underline{r}}{\partial \xi_i} ; i = 1, 2, 3 \quad (\text{A.5})$$

$\underline{r}$ is the positional vector $\underline{r} = x\underline{i} + y\underline{j} + z\underline{k}$ of a point P in the Cartesian coordinate space (x, y, z) .

Gauss' Divergence theorem states that if the vector $\underline{A}$ and its derivatives are continuous functions of position within the volume v enclosed by the surface S then

$$\int_S \underline{A} \cdot \underline{n} dS = \int_v \nabla \cdot \underline{A} dv \quad (\text{A.6})$$

The gradient theorem is a corollary of the above for the scalar ϕ :

$$\int_S \phi \underline{n} dS = \int_v \nabla \phi dv \quad (\text{A.7})$$

$\underline{n}$ is a positive (outward pointing) normal from S .

Useful vector identities are

$$\nabla \cdot (\phi \underline{A}) = \phi (\nabla \cdot \underline{A}) + (\underline{A} \cdot \nabla) \phi \quad (\text{A.8})$$

$$\nabla \cdot (\underline{A} \underline{B}) = (\underline{A} \cdot \nabla) \underline{B} + \underline{B} (\nabla \cdot \underline{A}) \quad (\text{A.9})$$

$$(\underline{A} \cdot \nabla) \underline{A} = \nabla(A^2/2) - \underline{A} \wedge (\nabla \wedge \underline{A}) \quad (\text{A.10})$$

APPENDIX B

Numerical Computation of Equilibrium Flows

The equilibrium flow field conditions for a Lighthill symmetric diatomic gas downstream of an oblique shock wave and a rarefaction wave are calculated via two numerical algorithms. The results are then used as a comparison with the non-equilibrium results presented in chapters four and five found in the main text. Note all the variables used have been non-dimensionalized.

B.1 Equilibrium Oblique Shock Wave

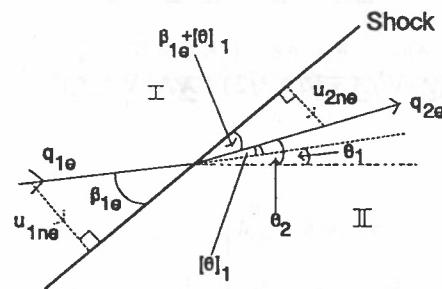


Figure B.1 Parameters for Equilibrium Oblique shock.

The Rankine-Hugoniot jump relations across an equilibrium shock wave are written

$$\begin{aligned} [\rho_e u_{ne}] &= 0 \\ [\rho_e u_{ne}^2 + p_e] &= 0 \\ [u_{te}] &= 0 \\ [h_{te}] &= 0 \end{aligned} \quad (\text{B.1a,b,c,d})$$

The subscripts n and t are the normal and tangential velocity components to the shock wave respectively and the subscript e referring to equilibrium conditions. Equations (B.1b) and (B.1d) can be re-written as

$$\begin{aligned} [p_e] &= -Q_e^2 [v_e] \\ 2[h_e] &= [p_e]([v_e] + 2v_{1e}) \end{aligned} \quad (\text{B.2a,b})$$

where Q_e is the mass flux through the wave given by $\rho_{1e} u_{1ne} = \rho_{1e} q_{1e} \sin(\beta_{1e})$. The change in specific volume ($v_e = 1/\rho_e$) across the wave $[v_e]$ in terms of the equilibrium shock angle β_{1e} and the flow deflection angle $[\theta]_1$ ($=\theta_2 - \theta_1$) is given by

$$[v_e] = \frac{-v_{1e} \csc^2(\beta_{1e}) \tan[\theta]_1}{\tan[\theta]_1 + \cot \beta_{1e}} \quad (\text{B.3})$$

The specific intrinsic enthalpy for the fluid will be a function of the pressure and specific volume (say) and the equilibrium mass fractions. For a Lighthill[60] two component gas it has the form

$$h_e = h_e(p_e, v_e, c_{1e}) \equiv \frac{4+c_{1e}}{1+c_{1e}} p_e v_e + \theta_d c_{1e} \quad (\text{B.4})$$

By equation (B.2b) the enthalpy downstream of the shock can be written in terms of the initial upstream conditions and the jump conditions across the wave

$$2h_e(p_{1e} + [p_e], v_{1e} + [v_e], (c_{1e})_1 + [c_{1e}]) = 2h_e(p_{1e}, v_{1e}, (c_{1e})_1) + [p_e]([v_e] + 2v_{1e}) \quad (\text{B.5})$$

where $(c_{1e})_1$ is the initial equilibrium mass fraction. The equilibrium mass fraction downstream of the shock can be calculated from the 'law of mass action' given by

$$\frac{(c_{1e})_2}{1-(c_{1e})_2} = \frac{v_{2e}}{v_d} \exp(-\theta_d/T_{2e}) \quad (\text{B.6})$$

where v_{2e} , $(c_{1e})_2$ and T_{2e} are the upstream specific volume, equilibrium mass fraction and equilibrium absolute temperature respectively. v_d and θ_d are Lighthill's characteristic specific volume and characteristic temperature for dissociation respectively. The equation can best be written in terms of the jump conditions as

$$\frac{\{(c_{1e})_1 + [c_{1e}]\}^2}{1-(c_{1e})_1 - [c_{1e}]} = \frac{v_{1e} + [v_e]}{v_d} \exp(-\theta_d/T_{2e}) \quad (\text{B.7})$$

The temperature of the gas is related through the equation of state and can be written in terms of the jumps in pressure, specific volume and mass fraction across the shock as

$$T_{2e} = \frac{(v_{1e} + [v_e])(p_{1e} + [p_e])}{(1 + (c_{1e})_1 + [c_{1e}])} \quad (B.8)$$

By substituting equations (B.2a), (B.3) and (B.8) into the equations (B.5) and (B.7) we now have two equations for the unknowns β_{1e} and $[c_{1e}]$. These are written in concise form as

$$\begin{aligned} F_1(\beta_{1e}, [c_{1e}]) &= 0 \\ F_2(\beta_{1e}, [c_{1e}]) &= 0 \end{aligned} \quad (B.9)$$

where the unknowns are the now the roots of the equations. Because they are nonlinear no analytic solution exists. However, they can be solved using a numerical iteration technique such as Newton Raphson's method for two unknowns which is written as

$$w^{m+1} = w^m - \frac{F^m}{dF^m} \quad (B.10)$$

where m is the iteration number with $m=0$ the initial or starting values to begin the iteration. w is the column vector of unknowns, F the column vector for the functions to be solved and dF the Jacobian matrix for F . A program was written based on the NAG routine C05NBF and this was used to solve these equations. For all circumstances encountered the freestream was assumed frozen with the initial atomic mass fraction zero.

C.1.1 Calculation of Entropy

Once the downstream conditions have been calculated the jump of entropy across the wave can be determined from the First of Thermodynamics. For continuous flow field regions (such as regions one and two in figure B.1 above) the first law has the form

$$dS = \frac{de}{T} - \frac{p}{\rho^2 T} d\rho \quad (B.11)$$

By substituting equations for the equation of state, specific total energy, and 'law of mass action' the first law can then be written

$$dS = \frac{3dT}{T} + \ln \left\{ \frac{\rho_d(1-c_{1e})}{c_{1e}^2} \right\} dc_{1e} - \frac{(1+c_{1e})d\rho}{\rho} \quad (B.12)$$

and can be integrated to give

$$S = 3 \ln T + c_{1e} \ln \rho_d - (1+c_{1e}) \ln(1-c_{1e}) + c_{1e}(1-2 \ln c_{1e}) + S_0 \quad (B.13)$$

Where S_0 is some constant reference entropy. The equation is valid for all continuous regions. However, across the shock there is a jump of entropy given by the difference in entropy between the two regions written mathematically as

$$[S] = 3[\ln T] + [c_{1e}] \ln \rho_d - [(1+c_{1e}) \ln(1-c_{1e})] + [c_{1e}(1-2 \ln c_{1e})] \quad (B.14)$$

we make the assumption that the reference entropy for both regions is the same. For frozen flow fields with $(c_{1e})_1 = (c_{2e})_2 \Rightarrow \gamma = \gamma_1 = \gamma_2$ the entropy equation reduces to a more familiar result

$$[S] = 3 \ln \left\{ \frac{p_1 + [p]}{p_1} \left(\frac{\rho_1 + [\rho]}{\rho_1} \right)^\gamma \right\} \quad (B.15)$$

with

$$\gamma = \frac{4+c_1}{3} \quad (B.16)$$

B.2 Equilibrium Rarefaction Wave

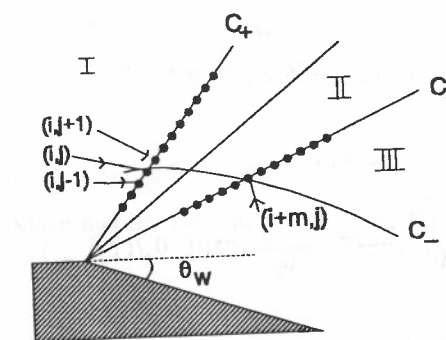


Figure B.2 Computational Grid and Characteristics for Expansion Wave.

The characteristic equations governing equilibrium flow fields are written as

$$\begin{aligned}
\frac{\sqrt{M_e^2-1}}{\rho_e q_e^2} \frac{\partial p_e}{\partial \chi_{\pm}} \pm \frac{\partial \theta_e}{\partial \chi_{\pm}} &= 0 \\
\rho_e q_e \frac{\partial q_e}{\partial s} + \frac{\partial p_e}{\partial s} &= 0 \\
\rho_e \frac{\partial h_e}{\partial s} - \frac{\partial p_e}{\partial s} &= 0
\end{aligned} \quad (B.17a,b,c)$$

where s and $\chi_{\pm}$ are the distances measured along a streamline and the $C_{\pm}$ characteristics respectively. The specific enthalpy and equation of state are given by

$$\begin{aligned}
h_e &= \{(4+c_{1e})T_e + c_{1e}\theta_d\} \\
p_e &= \{\rho_e(1+c_{1e})T_e\}
\end{aligned} \quad (B.18a,b)$$

these are both dependent on the equilibrium mass fraction through the 'law of mass action' written

$$\frac{c_{1e}^2}{1-c_{1e}} = \frac{v_e}{v_d} \exp(-\theta_d/T_e) \quad (B.19)$$

Unlike the characteristic equations for inert flow fields those for equilibrium cannot in general be integrated to give a closed form analytic solution. However, a numerical step-by-step method based on the familiar finite difference technique can be used to obtain an approximate solution. It is convenient for numerical purposes to choose the coordinate system based on the characteristic directions.

The equations are written in finite difference form as

$$\frac{\sqrt{(M_e^2)_{i,j\pm 1}-1}}{(\rho_e)_{i,j\pm 1} (q_e^2)_{i,j\pm 1}} \Delta_{\pm} (p_e)_{i,j} \pm \Delta_{\pm} (\theta_e)_{i,j} = 0 \quad (B.20)$$

$$(\rho_e)_{i,j} (q_e)_{i,j} \Delta (q_e)_{i,j} + \Delta (p_e)_{i,j} = 0 \quad (B.21)$$

$$(\rho_e)_{i,j} \Delta (h_e)_{i,j} - \Delta (p_e)_{i,j} = 0 \quad (B.22)$$

and

$$\frac{(c_{1e}^2)_{i,j\pm 1}}{1-(c_{1e})_{i,j\pm 1}} = \frac{(v_e)_{i,j\pm 1}}{v_d} \exp(-\theta_d/(T_e)_{i,j\pm 1}) \quad (B.23)$$

where the subscripts i and j represent the values of the variables at the discrete mesh point i,j (see figure B.2). The differences, for an arbitrary function f , are defined by

$$\begin{aligned}
\Delta_{\pm} f_{i,j} &= f_{i\pm 1,j} - f_{i,j\pm 1} \\
\Delta f_{i,j} &= f_{i+1,j} - f_{i,j}
\end{aligned} \quad (B.24)$$

Given the initial freestream conditions and the wedge flow deflection angle θ_w we wish to calculate the equilibrium conditions downstream of the rarefaction fan defined by the C_{+} characteristics. To solve the equations we use a predictor corrector type method based on the Method of Characteristics which is presented in the texts by Zucrow and Hoffman[107,108]. The coordinate lines are defined along the characteristic directions with the C_{+} and C_{-} directions represented by $i=\text{constant}$ and $j=\text{constant}$ respectively. Thus for the initial freestream Mach wave we have $i=0$. We wish to calculate those conditions at the next spatial level $i+1$ with the deflection angle $\Delta\theta=\theta_w/(nstep-1)$. Where $nstep$ is the number of computational steps needed we to get the desired accuracy for the downstream flow conditions.

Predictor step

The predicted flow conditions at the next level $(i+1, j)$ are given by the equations above as

$$\begin{aligned}
p'_e &= \frac{(\rho_e)_{i,j+1} (q_e^2)_{i,j+1} \Delta_{-} \theta}{\sqrt{(M_e^2)_{i,j+1}-1}} + (p_e)_{i,j+1} \\
q'_e &= -\frac{p'_e - (p_e)_{i,j}}{(\rho_e)_{i,j} (q_e)_{i,j}} + (q_e)_{i,j} \\
h'_e &= \frac{p'_e - (p_e)_{i,j}}{(\rho_e)_{i,j}} + (h_e)_{i,j}
\end{aligned} \quad (B.25)$$

where the prime represents the predicted values and we have used the property that along the C_{+} characteristic the flow variables remain constant. To calculate the predicted mass fractions we must solve iteratively the equation for the 'law of mass action'

$$\frac{(c'_{1e})^2}{1-(c'_{1e})^2} = \frac{\rho_d}{p'_e} \left[\frac{h'_e - c'_{1e} \theta_d}{4+c'_{1e}} \right] \exp \left(-\frac{\theta_d(4+c'_{1e})}{h'_e - c'_{1e} \theta_d} \right) \quad (B.26)$$

from which the temperature and density can be calculated from equations (B.18a) and (B.18b) respectively. To evaluate the equilibrium Mach number the equilibrium speed of sound a_e must be obtained from the ratio found in Cleaver[24]

$$\left(\frac{a_f'}{a_e'}\right)^2 = 1 + \frac{c_{1e}'(1-c_{1e}')}{3} \frac{\{(1+\theta_d/T_e')(1+c_{1e}')-(4+c_{1e}')\}^2}{(1+\theta_d/T_e')^2 c_{1e}'(1-(c_{1e}')^2)+8+2c_{1e}'} \quad (\text{B.27})$$

with the predicted frozen speed of sound a_f' is given by

$$a_f' = \sqrt{\frac{4+c_{1e}'}{3} T_e'} \quad (\text{B.28})$$

thus the equilibrium Mach number can be calculated from the equation

$$M_e' = \frac{q_e'}{a_e'} \equiv \frac{q_e'}{a_f'} \left(\frac{a_f'}{a_e'}\right) \quad (\text{B.29})$$

Corrector step

The corrector step is given by

$$\begin{aligned} p_e'' &= \frac{\rho_e'(q_e')^2 \Delta \theta}{\sqrt{(M_e')^2 - 1}} + (p_e)_{i,j} \\ q_e'' &= -\frac{p_e'' - (p_e)_{i,j}}{\rho_e' q_e'} + (q_e)_{i,j} \\ h_e'' &= \frac{p_e'' - (p_e)_{i,j}}{\rho_e'} + (h_e)_{i,j} \end{aligned} \quad (\text{B.30})$$

$$\frac{(c_{1e}'')^2}{1-(c_{1e}'')^2} = \frac{\rho_d}{p_e''} \left\{ \frac{h_e'' - c_{1e}'' \theta_d}{4+c_{1e}''} \right\} \exp \left(-\frac{\theta_d(4+c_{1e}'')}{h_e'' - c_{1e}'' \theta_d} \right) \quad (\text{B.31})$$

$$\left(\frac{a_f''}{a_e''}\right)^2 = 1 + \frac{c_{1e}''(1-c_{1e}'')}{3} \frac{\{(1+\theta_d/T_e'')(1+c_{1e}'')-(4+c_{1e}'')\}^2}{(1+\theta_d/T_e'')^2 c_{1e}''(1-(c_{1e}'')^2)+8+2c_{1e}''} \quad (\text{B.32})$$

$$a_f'' = \sqrt{\frac{4+c_{1e}''}{3} T_e''} \quad (\text{B.33})$$

$$M_e'' = \frac{q_e''}{a_e''} \equiv \frac{q_e''}{a_f''} \left(\frac{a_f''}{a_e''}\right) \quad (\text{B.34})$$

where the double primes represents the corrected values.

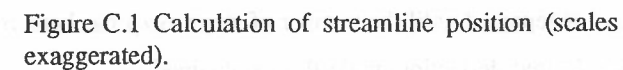
The solution

To obtain the values at the new updated point we take the average of the predicted and corrected values thus

$$(U_e)_{i+1,j} = \frac{1}{2} (U_e' + U_e'') \quad (\text{B.35})$$

Here U represents all the variables stated earlier; for example the pressure p_e . With all the new updated values the procedure above is repeated until the number of steps $nstep$ has been reached. At this stage the equilibrium values for the desired deflection angle θ_w are obtained.

Calculation of Streamline Distance Through Expansion Wave


$$\frac{r dv}{dr} = -\tan(\mu_f) \quad (\text{C.1})$$
$$dV = -\frac{\gamma+1}{2} \frac{M_f dM_f}{\sqrt{M_f^2-1} \left(1 + \frac{\gamma-1}{2} M_f^2\right)} \quad (C.2)$$
$$r = r_1 \left\{ \frac{1 + \frac{\gamma-1}{2} M_f^2}{1 + \frac{\gamma-1}{2} M_{f1}^2} \right\}^{\frac{\gamma+1}{2(\gamma-1)}} \quad (\text{C.3})$$

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Figure C.2 Calculation of the local Radius of Curvature R for the streamline (Not to Scale).

$$\frac{r dv}{R d\theta} = \sin(\mu_f); \quad dv = d\theta + d\mu \equiv d\theta - \frac{dM_f}{M_f \sqrt{M_f^2 - 1}} \quad (C.5)$$
$$\frac{d\theta}{dv} = \frac{2}{\gamma+1} \left(1 - \frac{1}{M_f^2} \right) \Rightarrow R = \left\{ \frac{\gamma+1}{2} \frac{M_f^3}{M_f^2-1} \right\} r \quad (\text{C.6})$$
$$R = \frac{(\gamma+1)r_1}{2} \frac{M_f^3}{M_f^2-1} \left\{ \frac{1+\frac{\gamma-1}{2}M_f^2}{1+\frac{\gamma-1}{2}M_f^2} \right\}^{\frac{\gamma+1}{2(\gamma-1)}} \quad (C.7)$$

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$$ds = R|d\theta| ; d\theta = \frac{-\sqrt{M_f^2-1} dM_f}{M_f \left(1 + \frac{\gamma-1}{2} M_f^2\right)} \quad (C.8)$$

or $ds = F(M_f, \gamma) dM_f$ where

$$F(M_f, \gamma) = \frac{(\gamma+1) M_f^2 r_1 \left(1 + \frac{\gamma-1}{2} M_f^2\right)^{\frac{3-\gamma}{2(\gamma-1)}}}{2\sqrt{M_f^2-1} \left(1 + \frac{\gamma-1}{2} M_f^2\right)^{\frac{\gamma+1}{2(\gamma-1)}}} \quad (C.9)$$

The total distance through the rarefaction can be calculated from the integral:

$$\Delta s = \int_{M_{f,r}}^{M_f} F(M_f, \gamma) dM_f \quad (C.10)$$

This can be integrated numerically using Simpson's rule. However, for $\gamma = 1.4$, $F(M_f, \gamma)$ has the particular simple form

$$F(M_f, \gamma=1.4) = \frac{\alpha M_f^2 \left(1 + \frac{1}{5} M_f^2\right)^2}{\sqrt{M_f^2-1}} ; \alpha = \frac{1.2 r_1}{\left(1 + \frac{1}{5} M_{f,r}^2\right)^3} \quad (C.11)$$

from which equation (C.10) can be shown to integrate as:

$$\Delta s = \left\{ \alpha \left[\frac{53 \ln \left\{ \sqrt{M_f^2-1} + M_f \right\}}{80} + \frac{M_f \sqrt{M_f^2-1} \{8M_f^4 + 130M_f^2 + 795\}}{1200} \right] \right\}_{M_{f,r}}^{M_f} \quad (C.12)$$

APPENDIX D

Contour Plotting

In order to acquire full information from the numerical results it was necessary to view them as contours. However, at an early stage it was found that the *off the shelf packages* (otsp) such as Gino-F and Unimap (Uniras Product) were inadequate for the job and a customized, in house, package would have to be developed. Three clear faults with the otsp were identified which were found by experience:

1. Data generated from the RCM algorithm was stored at discrete, spatially irregular, points. This irregularity will be extremely evident for the (transformed from computational space) Cartesian plane. The otsp will first try to regularize the irregular data by an internal interpolation procedure such as a Bilinear or Polynomial interpolation. This procedure is effectively producing an approximate surface to the data. From the new regular data set the contours are generated. However, to regularize irregular data can cause serious problems when physical boundaries are present.
2. The interpolation operation will smooth the data. If shock waves are present then these will be smeared. Also the type of interpolation used will cause the generation of different types of spurious contours. These must therefore be kept to an absolute minimum. Results from an RCM calculation for $M_{\infty}=3$, $\theta_w=30^\circ$, $\gamma=1.4$, using 20 ξ_2 nodes are displayed for Bilinear and Polynomial interpolation procedures, using Unimap, in Figures D.1 and D.2 respectively. The interval between the contours remains the same for both plots. These plots demonstrate that different interpolations produces different spurious contours.
3. Because the otsp are designed for the general user they can be rather inflexible for a specific application.

The in house developed basic contouring package was based on the idea by Quirk[74]. We refer the reader to the reference for the details. The new contour package was applied to the test case above and the results are to be found in Figure D.3. It is clear that there are no spurious contours. The stepping of the shock wave is due to the coarseness of the grid and will become less noticeable as the mesh is refined.

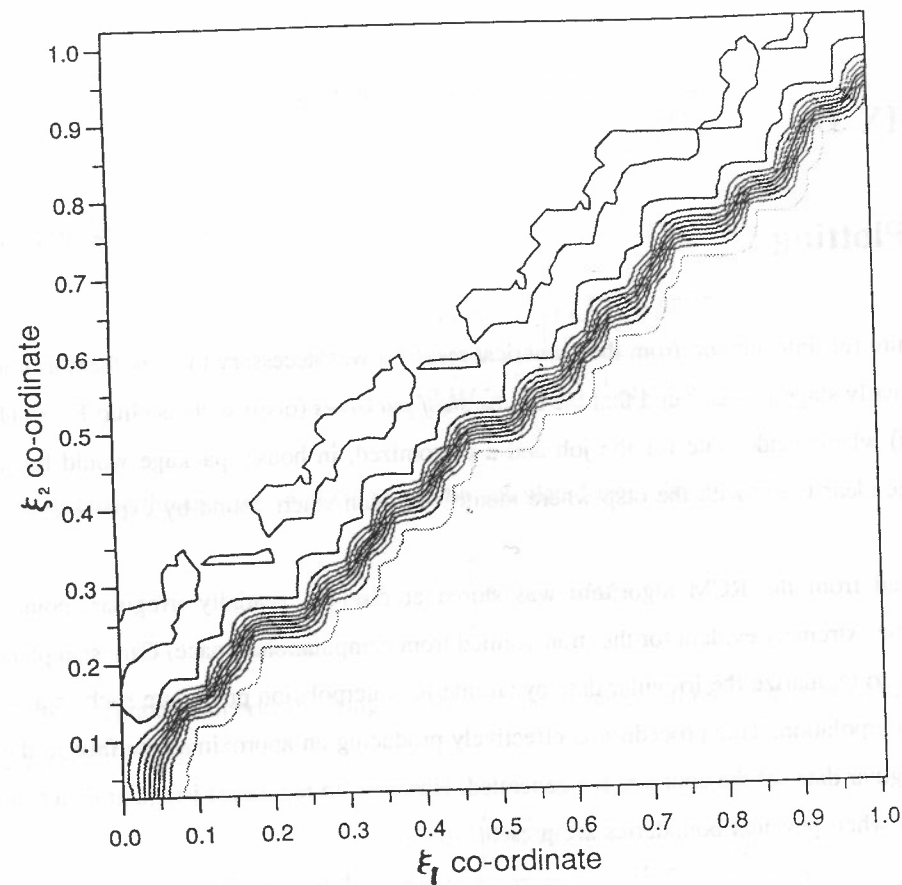


Figure D.1 Bilinear Interpolation of Data using Unimap.

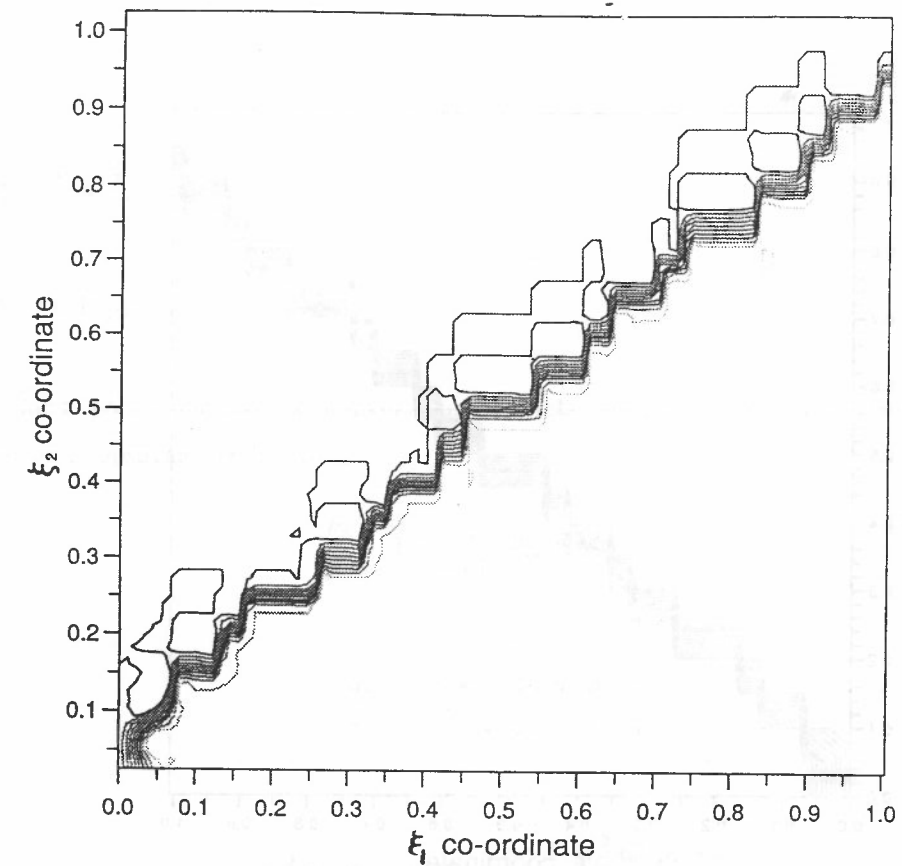


Figure D.2 Polynomial Interpolation of data using Unimap.

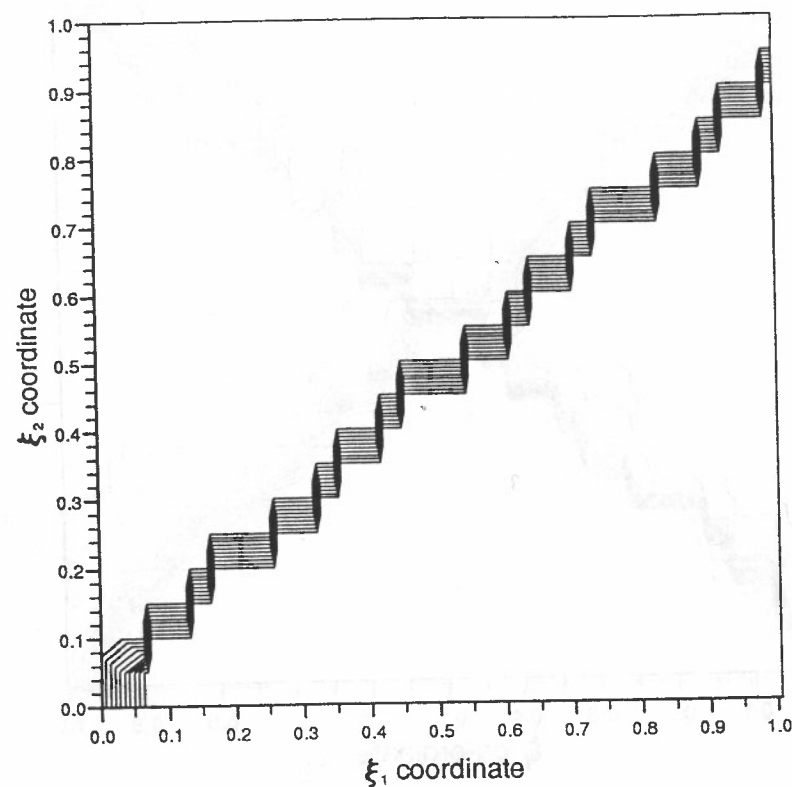


Figure D.3 Contours generated by new in house package.

Appendix E

Frozen Oblique Shock relations

For an inert, polyatomic gas the Rankine-Hugoniot relations can be written in terms of the ratio downstream to upstream conditions as

$$\frac{p_2}{p_1} = 1 + \frac{2\gamma}{\gamma+1} (M_{f1}^2 \sin^2 \beta_{f1} - 1) \quad (\text{E.1})$$

$$\frac{\rho_2}{\rho_1} = \frac{2\gamma + (\gamma+1)(p_2/p_1 - 1)}{2\gamma + (\gamma-1)(p_2/p_1 - 1)} \quad (\text{E.2})$$

$$M_{f2}^2 \sin^2(\beta_{f1} - [\theta]) = \frac{(\gamma-1)M_{f1}^2 \sin^2 \beta_{f1} + 2}{2\gamma M_{f1}^2 \sin^2 \beta_{f1} - (\gamma-1)} \quad (\text{E.3})$$

where $[\theta]$ is jump of θ across the wave or the flow deflection angle. The shock wave angle can be calculated by solving the equation

$$\tan([\theta]) = 2 \cot \beta_{f1} \left(\frac{M_{f1}^2 \sin^2 \beta_{f1} - 1}{M_{f1}^2 (\gamma + \cos(2\beta_{f1}) + 2)} \right) \quad (\text{E.4})$$

There are no closed form solutions to this and a root finding technique such as the Secant Method or Newton-Raphson Method can be used.

Appendix F

A general description of a mixture of chemically reacting perfecting gases will be given. These ideas are used within the main text for a two component gas.

Thermodynamic Equations

The field of flow is composed of a mixture of n perfect gases with chemical formula represented by A_α ($\alpha = 1, 2, \dots, n$). The subscript α is used to distinguish between the different chemical properties associated with each chemical species. Initially the mixture is in thermodynamic equilibrium and either it is in chemical equilibrium or is chemically frozen. Any perturbations, such as a change in flow deflection angle, will cause non-equilibrium behaviour to develop. To analyze the system¹⁶ we define that locally there is thermodynamic equilibrium but chemical non-equilibrium (unless frozen conditions are specified throughout). The rotational, vibrational, and electronic energy modes are defined to be in equilibrium with the translational degrees of freedom. Thus we do not need to specify rate equations for these modes of vibration. At a local level the concepts of Chemical Equilibrium Thermodynamics, Classical Boltzmann Statistics, and Quantum Mechanics can be applied¹⁷.

Chemical non-equilibrium will cause the system to relax back to a new chemical equilibrium state. During this process finite rate chemical reactions will occur. If there are m independent chemical reactions then the chemical equation for the r -th reaction ($r = 1, 2, \dots, m$) can be written



where $\nu_{\alpha}^{(r')}$, $\nu_{\alpha}^{(r'')}$ are the stoichiometric coefficients for reactants and products respectively, and $k_f^{(r)}$, $k_b^{(r)}$ are the forward and backward reaction rate constants respectively and are functions of the absolute temperature only.

The reaction rate constants are dependent on the type of non-equilibrium. For chemical non-equilibrium,

¹⁶The properties of a mixture of perfect gases are known and are well documented. For them, we shall refer to the texts by Clarke and McChesney[21,22] and Vincenti and Kruger[98], using the abbreviations C&M and V&K respectively, throughout the appendix.

¹⁷The details of which can be found in V&K chapter three and four.

where the internal energy modes are in equilibrium with the translational temperature (i.e. only one temperature specified), the forward reaction rate constant has been found experimentally to have the Arrhenius form:

$$k_f^{(r)} = c_f^{(r)} T^{-\eta_f^{(r)}} \exp(-\theta_f^{(r)}/T) \quad (F.2)$$

where $c_f^{(r)}$, $\eta_f^{(r)}$, and $\theta_f^{(r)}$ are all constants and $\theta_f^{(r)}$ is the forward activation temperature for the r -th reaction.

For non-equilibrium with multiple temperatures (such as vibrational and electronic non-equilibrium) work by Park[72] has shown the need to modify the Arrhenius equation to include these effects. We will only deal with a single temperature model and do not discuss this aspect further. The reverse reaction rate constant has the general form

$$k_b^{(r)} = c_b^{(r)} T^{-\eta_b^{(r)}} \exp(-\theta_b^{(r)}/T) \quad (F.3)$$

where $\theta_b^{(r)}$ is not the usually activation temperature but combined with the exponent it is a measure of the probability of the recombination reaction taking place at a given temperature. Usually $\theta_b^{(r)}$ is taken as zero.

Mixture of Perfect Gases

The equation of state for a single component gas has been found empirically to have the form

$$p_{\alpha} = \rho_{\alpha} R_{\alpha} T ; R_{\alpha} = \frac{R}{W_{\alpha}} \quad (F.4)$$

where p_{α} , ρ_{α} , R_{α} , R , W_{α} and T are the partial pressure, partial density, specific gas constant, Universal gas constant, molar weight of the α -th species, and absolute temperature respectively. From Dalton's Law of partial pressures the equation of state for the mixture becomes

$$p = \rho \frac{R}{W} T \quad (F.5)$$

$$W^{-1} = \sum_{\alpha=1}^n \frac{c_{\alpha}}{W_{\alpha}}$$

The specific intrinsic energy for each species e_{α} will be dependent on the molecular structure. For atoms the energy contributions are due to the translational and electronic degrees of freedom

$$e_{\alpha} = e_{\alpha}^{tr} + e_{\alpha}^{el} + e_{\alpha}^{ref} \quad (F.6)$$

while for molecules there are additional contributions from the rotational and vibrational modes

$$e_{\alpha} = e_{\alpha}^{tr} + e_{\alpha}^{rot} + e_{\alpha}^{vb} + e_{\alpha}^{el} + e_{\alpha}^{ref} \quad (F.7)$$

where the different energy modes are measured with respect to their zero point energies at absolute zero and e_{α}^{ref} is a reference energy from which measurements are made. The specific intrinsic energy and enthalpy for each species can be determined from the Partition functions defined for each energy mode by

$$\begin{aligned} e_{\alpha} &= R_{\alpha} T^2 \left(\frac{\partial \ln Q_{\alpha}}{\partial T} \right) \\ h_{\alpha} &= e_{\alpha} + p_{\alpha} v_{\alpha} \end{aligned} \quad (F.8)$$

where Q_{α} is the Partition function for all the degrees of freedom. For atoms it has the form

$$Q_{\alpha} = Q_{\alpha}^{tr} Q_{\alpha}^{el} Q_{\alpha}^{ref} \quad (F.9)$$

and for molecules

$$Q_{\alpha} = Q_{\alpha}^{tr} Q_{\alpha}^{rot} Q_{\alpha}^{vb} Q_{\alpha}^{el} Q_{\alpha}^{ref} \quad (F.10)$$

The exact form of the Partition functions are given by

$$Q_{\alpha}^{tr} = v \left(\frac{2\pi m_{\alpha} k T}{h^2} \right)^{3/2}; \quad Q_{\alpha}^{rot} = \frac{1}{\sigma} \left(\frac{T}{\theta_{r\alpha}} \right); \quad Q_{\alpha}^{el} = \sum_{l=0}^{\infty} g_l \exp(-\theta_{l\alpha}^{el}/T) \quad (F.11)$$

and

$$Q_{\alpha}^{vb} = \frac{1}{1 - \exp(-\theta_{v\alpha}/T)}; \quad Q_{\alpha}^{ref} = \exp\left(-\frac{e_{\alpha}^{ref}}{R_{\alpha} T}\right) \quad (F.12)$$

where k , m_{α} , N_A , h , g_l , $\theta_{r\alpha}$, $\theta_{v\alpha}$, and $\theta_{l\alpha}^{el}$ are the Boltzmann constant, mass of single entity per kilogram $= (W_{\alpha} / N_A)$, Avogadro Number, Plank's constant, degeneracy of l -th electronic state, characteristic rotational excitation temperature, characteristic vibrational excitation temperature, and characteristic electronic excitation temperature respectively. σ is the symmetry factor which has the value two for homonuclear molecules and unity for heteronuclear molecules.

The specific intrinsic energy and enthalpy have the form for atoms and molecules

$$\begin{aligned} e_{\alpha} &= \left(\frac{3}{2} + \phi_{\alpha} (1 + \chi_{\alpha}^{vb}) + \chi_{\alpha}^{el} \right) R_{\alpha} T + e_{\alpha}^{ref} \\ h_{\alpha} &= \left(\frac{5}{2} + \phi_{\alpha} (1 + \chi_{\alpha}^{vb}) + \chi_{\alpha}^{el} \right) R_{\alpha} T + h_{\alpha}^{ref} \end{aligned} \quad (F.13)$$

where the functions

$$\begin{aligned} \chi_{\alpha}^{vb} &= \frac{\theta_{v\alpha}/T}{\exp(\theta_{v\alpha}/T) - 1} \\ \chi_{\alpha}^{el} &= \frac{\sum_{l=0}^{\infty} g_l (\theta_{l\alpha}/T) \exp(-\theta_{l\alpha}/T)}{Q_{\alpha}^{el}} \\ \phi_{\alpha} &= \begin{cases} 0 & \text{; atoms} \\ 1 & \text{; molecules} \end{cases} \end{aligned} \quad (F.14)$$

are non-dimensional.

The specific heat capacities for each species at constant volume $c_{v\alpha}$ and pressure $c_{p\alpha}$ are determined by

$$\begin{aligned} c_{v\alpha} &= \left(\frac{\partial e_{\alpha}}{\partial T} \right)_v = \left(\frac{3}{2} + \phi_{\alpha} (1 + \psi_{\alpha}^{vb}) + \psi_{\alpha}^{el} \right) R_{\alpha} \\ c_{p\alpha} &= \left(\frac{\partial h_{\alpha}}{\partial T} \right)_p = \left(\frac{5}{2} + \phi_{\alpha} (1 + \psi_{\alpha}^{vb}) + \psi_{\alpha}^{el} \right) R_{\alpha} \end{aligned} \quad (F.15)$$

where

$$\begin{aligned} \psi_{\alpha}^{vb} &= \left(\frac{\theta_{v\alpha}/(2T)}{\sinh(\theta_{v\alpha}/(2T))} \right)^2 \\ \psi_{\alpha}^{el} &= \frac{\sum_{l=0}^{\infty} g_l (\theta_{l\alpha}/T)^2 \exp(-\theta_{l\alpha}/T)}{Q_{\alpha}^{el}} - \{\chi_{\alpha}^{el}\}^2 \end{aligned} \quad (F.16)$$

The ratio of specific heat capacities for the α -th species γ_{α} is defined by

$$\gamma_{\alpha} = \frac{c_{p\alpha}}{c_{v\alpha}} = \frac{\frac{5}{2} + \phi_{\alpha} (1 + \psi_{\alpha}^{vb}) + \psi_{\alpha}^{el}}{\frac{3}{2} + \phi_{\alpha} (1 + \psi_{\alpha}^{vb}) + \psi_{\alpha}^{el}} \quad (F.17)$$

It is clear from this equation that any changes in the mass fractions or vibrational/electronic energies will cause the ratio to vary. Note that for Inert gases where the mass fractions are fixed and the internal

degrees frozen or un-excited the ratio γ_α remains fixed. The specific energies and enthalpies for the α -th species can be written concisely as

$$\begin{aligned} e_\alpha &= \frac{P_\alpha}{\rho_\alpha(\gamma_\alpha - 1)} + e_\alpha^{ref} \\ h_\alpha &= \frac{\gamma_\alpha P_\alpha}{\rho_\alpha(\gamma_\alpha - 1)} + h_\alpha^{ref} \end{aligned} \quad (F.18)$$

The total specific energy, enthalpy, and specific heat capacities are the mass averages of all the individual components. i.e.

$$e = \sum_{\alpha=1}^n c_\alpha e_\alpha; \quad h = \sum_{\alpha=1}^n c_\alpha h_\alpha \quad (F.19)$$

etc. Whence

$$\begin{aligned} e &= \frac{P}{\rho(\gamma - 1)} + \sum_{\alpha=1}^n c_\alpha e_\alpha^{ref} \\ h &= \frac{\gamma P}{\rho(\gamma - 1)} + \sum_{\alpha=1}^n c_\alpha h_\alpha^{ref} \end{aligned} \quad (F.20)$$

where the ratio of specific heat capacities γ is given by

$$\gamma = \frac{c_p}{c_v} = \frac{\sum_{\alpha=1}^n \frac{c_\alpha}{W_\alpha} \left(\frac{5}{2} + \phi_\alpha (1 + \psi_\alpha^{wb}) + \psi_\alpha^{el} \right)}{\sum_{\alpha=1}^n \frac{c_\alpha}{W_\alpha} \left(\frac{3}{2} + \phi_\alpha (1 + \psi_\alpha^{wb}) + \psi_\alpha^{el} \right)} \quad (F.21)$$

The changes in specific intrinsic enthalpy h_α , specific entropy S_α , and the specific volume $v_\alpha (= 1/\rho_\alpha)$ for each species are related by the *First law of Thermodynamics* as

$$T dS_\alpha = dh_\alpha - v_\alpha dp_\alpha \quad (F.22)$$

For a mixture of gases the First law becomes

$$T dS = dh - v dp - \sum_{\alpha=1}^n \mu_\alpha dc_\alpha \quad (F.23)$$

where the total specific entropy is the mass average of the individual entropy components. Also μ_α is the chemical potential per unit mass for α th species. It is equivalent to the specific Gibbs free energy

$$\mu_\alpha = g_\alpha = h_\alpha - TS_\alpha \quad (F.24)$$

and has the general form (see C&M page 51):

$$\mu_\alpha(p_\alpha, T) = \mu_\alpha(p_*, T) + R_\alpha T \ln(p_\alpha/p_*) \quad (F.25)$$

where p_* is an arbitrary reference pressure.

The *Second law of Thermodynamics* states that the total entropy for the system must remain fixed or increase. It can be divided up into contributions from the fluid motion due to transport phenomena and the chemical reactions. Written mathematically as

$$dS = dS_T + dS_R \geq 0 \quad (F.26)$$

The neglect of the transport processes, such as viscosity, reveals through equations (2.14) and the First law of Thermodynamics for inert gases that there can be no entropy production along streamlines¹⁸ for regions where the flow variables and derivatives remain continuous. By substituting equations (2.13) and (2.14) into equation (F.23) the entropy is shown to be due exclusively to the chemical reactions

$$dS_R = - \frac{1}{T} \sum_{\alpha=1}^n \mu_\alpha dc_\alpha \geq 0 \quad (F.27)$$

However, where the flow variables and derivatives become discontinuous, such as across an oblique shock wave or contact surface, entropy will be generated in addition to the reactions within the fluid.

The change in mass fraction for the r -th reaction $dc_\alpha^{(r)}$ will be proportional to the difference $(v_\alpha^{(r)'} - v_\alpha^{(r)'})W_\alpha$. Therefore from equation (F.27) we have the condition for the r -th reaction

$$\sum_{\alpha=1}^n v_\alpha^{(r)'} \hat{\mu}_\alpha^{(r)} \geq \sum_{\alpha=1}^n v_\alpha^{(r)''} \hat{\mu}_\alpha^{(r)} \quad (F.28)$$

where $\hat{\mu}_\alpha^{(r)} = \mu_\alpha^{(r)} W_\alpha$ is the molar chemical potential.

¹⁸ Since by definition the substantial derivative of entropy dS is equivalent to $\underline{V} \cdot \nabla S$

The Law of Mass Action

For equilibrium there must be no entropy production. Whence

$$\sum_{\alpha=1}^n (v_{\alpha}^{(r')} - v_{\alpha}^{(r'')}) \hat{\mu}_{\alpha e}^{(r)} = 0 \quad (\text{F.29})$$

where the subscript e refers to the equilibrium state.

Upon substituting equation (F.25) for equilibrium into equation (F.29) an expression for the *Law of Mass Action* can be obtained in terms of the equilibrium mass fractions (see C&M, page 54), which are evaluated at the local temperature and pressure, as

$$K_e^{(r)} = \prod_{\alpha=1}^n c_{\alpha e}^{(r)} (v_{\alpha}^{(r'')} - v_{\alpha}^{(r')}) \quad (\text{F.30})$$

$$K_e^{(r)} = \exp(-\Delta \hat{\mu}/RT) \prod_{\alpha=1}^n \left(\frac{p_{\alpha}}{\rho R_{\alpha} T} \right)^{(v_{\alpha}^{(r'')} - v_{\alpha}^{(r')})} \quad (\text{F.31})$$

$$\Delta \hat{\mu} = \sum_{\alpha=1}^n (v_{\alpha}^{(r'')} - v_{\alpha}^{(r')}) \hat{\mu}_{\alpha e}^{(r)}$$

where $\hat{\mu}_{\alpha e}^{(r)}$ stands for $\hat{\mu}_{\alpha}^{(r)}(p_e, T)$ and $K_e^{(r)}$ is the equilibrium constant for the mixture which is dependent only on T and reference value p_e . The equilibrium constant is normally determined experimentally but an explicit analytic form can be derived from the Partition functions as

$$K_e^{(r)} = \exp\left(-\frac{\Delta e}{RT}\right) (\rho v)^{-\sum v_{\alpha}^{(r)}} \prod_{\alpha=1}^n \left\{ (m_{\alpha} Q_{\alpha})^{(v_{\alpha}^{(r'')} - v_{\alpha}^{(r')})} \right\} \quad (\text{F.32})$$

where

$$\sum v_{\alpha}^{(r)} = \sum_{\alpha=1}^n \{ v_{\alpha}^{(r'')} - v_{\alpha}^{(r')} \} \quad (\text{F.33})$$

$$\Delta e = \sum_{\alpha=1}^n \{ v_{\alpha}^{(r'')} - v_{\alpha}^{(r')} \} W_{\alpha} e_{\alpha}^{ref}$$

Clarke's Rate Equation For Chemical Non-Equilibrium

The mass rate of production per unit volume for the r -th reaction has been shown (see C&M chapter

three) to have the general form

$$K_{\alpha}^{(r)} = \frac{\rho W_{\alpha} (v_{\alpha}^{(r'')} - v_{\alpha}^{(r')})}{\tau_{\alpha}^{(r)}} \left(K^{(r)} \prod_{\alpha=1}^n (c_{\alpha})^{v_{\alpha}^{(r')}} - \prod_{\alpha=1}^n (c_{\alpha})^{v_{\alpha}^{(r'')}} \right) \quad (\text{F.34})$$

where

$$\tau_{\alpha}^{(r)} = \frac{\rho}{k_b^{(r)}} \prod_{\alpha=1}^n \left(\frac{\rho}{W_{\alpha}} \right)^{-v_{\alpha}^{(r'')}} \quad (\text{F.35})$$

and

$$K^{(r)} = \prod_{\alpha=1}^n (\rho_e c_{\alpha e} / \rho)^{(v_{\alpha}^{(r'')} - v_{\alpha}^{(r')})} \quad (\text{F.36})$$

provided that

$$\frac{k_{fe}^{(r)}}{k_{be}^{(r)}} = \frac{k_f^{(r)}}{k_b^{(r)}} \quad (\text{F.37})$$

where ρ_e and $c_{\alpha e}$ are the local equilibrium values for density and mass fractions respectively. The mass fractions are evaluated at the local temperature, i.e. $T_e = T$. Also $\tau_{\alpha}^{(r)}$ has the units of time and is proportional to the time taken for a small deviation from equilibrium to fall to e^{-1} of its original value as a result of the r -th reaction alone. Since there are m independent chemical reactions the total mass production for each species is the sum over all the reactions

$$K_{\alpha} = \sum_{r=1}^m K_{\alpha}^{(r)} \quad (\text{F.38})$$

For equilibrium the net rate of mass production for the forward reaction is balanced by the net rate of removal for the reverse reaction. Therefore $K_{\alpha}^{(r)} = 0$ for all the chemical reactions with the equilibrium constant defined by equation (F.31).

Entropy Production

The specific entropy generated due to the chemical reactions can be directly calculated from equation (F.27) which is re-written as

$$dS = -\frac{1}{\rho T} \sum_{r=1}^m \sum_{\alpha=1}^n \mu_{\alpha}^{(r)} K_{\alpha}^{(r)} \quad (\text{F.39})$$

upon substituting equations (F.25), (F.29) and (F.34) we obtain the result

$$dS = -\frac{R}{\rho} \sum_{r=1}^m R^{(r)} \ln \left\{ \prod_{\alpha=1}^n \left(\frac{p_{\alpha}}{p_{\alpha e}} \right)^{(v_{\alpha}^{(r)''} - v_{\alpha}^{(r)'})} \right\} \quad (\text{F.40})$$

where $R^{(r)}$ is the rate of progress of the r -th reaction measured in moles per unit volume per unit time and has the form

$$R^{(r)} = k_b^{(r)} \prod_{\alpha=1}^n (\rho / W_{\alpha})^{v_{\alpha}^{(r)'}} \left(K^{(r)} \prod_{\alpha=1}^n c_{\alpha}^{v_{\alpha}^{(r)'}} - \prod_{\alpha=1}^n c_{\alpha}^{v_{\alpha}^{(r)''}} \right) \quad (\text{F.41})$$