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Computation of an ideal gas nozzle flow with basically different codes

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Abstract

A finite difference code and a code based on the method of characteristics applied to the calculation of a stationary flow of an ideal gas through a convergent-divergent nozzle are compared. The stationary profiles of the flow variables are obtained as asymptotic solutions of the transient calculation. An analytical solution serves as a basis to criticize the two different codes: while the code based on characteristics agrees fairly well with the analytical solution, the finite difference code supplies strongly smoothed, unrealistic profiles due to numerical damping.

Berechnung einer idealen Gas-Strömung durch eine Düse mit grundsätzlich unterschiedlichen Rechenprogrammen

Zusammenfassung

Ein Finite-Differenzen Code und ein Charakteristiken-Code werden anhand der Berechnung einer stationären Strömung eines idealen Gases durch eine konvergent-divergente Düse verglichen. Die stationären Profile der Strömungsvariablen werden als asymptotische Lösungen der transienten Rechnung erhalten. Eine analytische Lösung ist die Grundlage zur Beurteilung der beiden unterschiedlichen Programme: während der Charakteristiken-Code recht gut mit der analytischen Lösung übereinstimmt, liefert der Finite-Differenzen Code stark geglättete, unrealistische Profile, verursacht durch numerische Dämpfung.

1. Introduction

The fluid dynamic computer codes used for the current light water reactor safety analysis are mainly finite difference codes of first order in space /¯1_7, /¯2_7. As they fortunately allow for a rather flexible adaption to the geometry of the problem (one- or multidimensional, obstacles, free surfaces etc.) in contrary to a code based e.g. on the method of characteristics and as physical modelling seems to be of primary importance one is easily tempted to ignore the numerical background of finite difference codes. The main problem of a transient calculation is its stability, which is often solved using the donor-cell technique (upwind differencing) /¯3, pp. 64_7. This again leads to a so called first order code of which the numerical damping is a well-known effect. Second order codes enlarge the expense but due to first order errors resulting from geometry modelling, coarse resolution possibilities, non-linear equation of state etc. they are not that much superior to first order codes. Moreover first order methods can be more accurate when only coarse grids are treatable due to computing time /¯4_7 or when the solutions contain discontinuities /¯5_7.

The following investigation, which clearly shows some weak points of both a finite difference code and a code based on the method of characteristics, was initiated by an experiment with the "HENRY-nozzle" (Semiscale Mod-1, Idaho) and its check with several codes by Travis & Hirt /¯6_7. There, as well as in some of our calculations /¯7_7 emphasis was laid on the effect of dimensionality, i.e. whether a one dimensional (1D-)calculation of such an axisymmetric nozzle flow is satisfying or whether a 2D-calculation is required. Here the main interest was focused on a comparison between

- a quasi analytical solution of the stationary critical nozzle flow of an ideal gas
- a calculation with a code based on the method of characteristics (1D, transient)
- a calculation with a finite difference code (1D/2D, transient)

The test example was insofar modified with regard to the above mentioned experiment with the HENRY-nozzle, as the two-phase steam-water mixture flow was modelled by an ideal gas flow with $\kappa = cp/cv = 1.07$. This simulation matches the real two-phase flow quite well due to the uncommon value of κ and permits a quasi analytical solution. So the comparison between the codes due to the simple equation of state is possible. Therefore in this investigation only calculations are compared with each other and not with the experimental results. The stationary nozzle flow is calculated by both the codes as an asymptotic solution of a transient calculation starting from constant initial values.

1.1 Geometry

The HENRY-nozzle (see fig. 1, original and model in different scales) consists of a convergent conical part followed by a cylindrical part representing the nozzle throat and a divergent concical part for the acceleration in the supersonic range. It should be noted that the straight contour lines cause discontinuities of the derivatives of the radius and the cross-section area with respect to the axial coordinate. The cylindrical part before the nozzle entry was added for the calculations in order to make the radial profiles of the flow entering the converging part more realistic. The nozzle was axially divided into 45 and 49 cells for the calculations by the finite difference code and the method of characteristics code, respectively.

1.2 Basic equations

The basic system of equations to be solved for the one dimensional transient flow in a nozzle neglecting viscosity and heat- und mass transfer consists of:

the Euler equation ,
the continuity equation,
the energy equation.

If a shock occurs in the flowfield, the well-known shock equations (see /‾8, pp. 42_7, for example) for calculating the gas properties across a shock have to be used in addition to the equations mentioned above.

1.3 Equation of state

The fluid is considered to be an ideal gas, the flow to be inviscid and adiabatic. Thus the equation of state is

$$\frac{p}{p_o} = \left(\frac{\rho}{\rho_o}\right)^{\kappa} \qquad (1)$$

p is the pressure and ρ is the denisty, $\kappa = 1.07$ the adiabatic exponent. Thus the experimental two-phase mixture is approximated. This unusual value of κ only quantitatively influences the results but it does not change the generality of the conclusions.

1.4 Boundary and initial conditions

At the nozzle entry the following values were fixed for all times t:

$$p_{entry} = 4.8 \text{ MPa}, \quad \rho_{entry} = 56 \text{ kg/m}^3, \quad T_{entry} = 534 \text{ K}.$$

At the exit for different calculations the pressure was reduced beginning from p_{exit} = 4.5 MPa to p_{exit} = 1.5 MPa in 0.5 MPa-steps.

Initially (t=0) the state in the whole nozzle except the exit plane equals the state at the entry, the velocity u is zero everywhere. At the exit the downstream pressure is given.

2. The codes

2.1 STRUYA

The finite difference code STRUYA /¯9_7 is an enhancement of the transient code YAQUI from LASL /¯10_7. It is an arbitrary Eulerian-Lagrangian computer program for fluid flow at all speeds. 1D- as well as 2D-calculation is possible, the option for structure coupling is not used here.

The mesh does not necessarily have to be rectangular, which allows an exact modelling of the HENRY-nozzle geometry (see fig. 1). In STRUYA the conservation equations are included in a more general form than required by this application. Therefore the viscosity terms of the Navier-Stokes equations are incorporated. At the walls free slip is assumed. The donor cell technique is applied. Because neither the shock equations are included nor a shock detection occurs in STRUYA, a "smeared" appearance of a possible shock is to be expected. Each calculation cycle consists of three principal steps (ICE-technique /¯11_7):

1. Explicit calculation of guess velocities, densities and pressures for the entire mesh using the equation of state, momentum and the flowfield variables of the previous time step.

2. Implicit solution of the continuity equation by means of pressure iteration with appropriate adjustment of velocities.

3. Explicit calculation of the energy, using the energy equation and the iterated flow field variables from the second step.

2.2 Method of characteristics for the one-dimensional transient problem

The Euler equations reduce to

$$u_t + uu_x = -\frac{1}{\rho}p_x . \tag{2}$$

x and t are the independent variables in space and time, the indices denote derivatives with respect to space and time, u is the velocity in x-direction, ρ the density and p the pressure. With regard to the variation of the cross-section of the nozzle, the continuity equation is given by

$$\rho_t + u\rho_x + \rho u_x = -u\rho\frac{d}{dx}(\ln(A(x)). \tag{3}$$

A(x) is the cross-section of the nozzle. For the HENRY-nozzle the function $\frac{d}{dx}(\ln(A(x))$ is piecewise defined corresponding to the piecewise linear radius.

The energy equation can be written in the form [12, p. 307]

$$p_t + up_x - a^2(\rho_t + u\rho_x) = 0, \tag{4}$$

where a is the speed of sound.

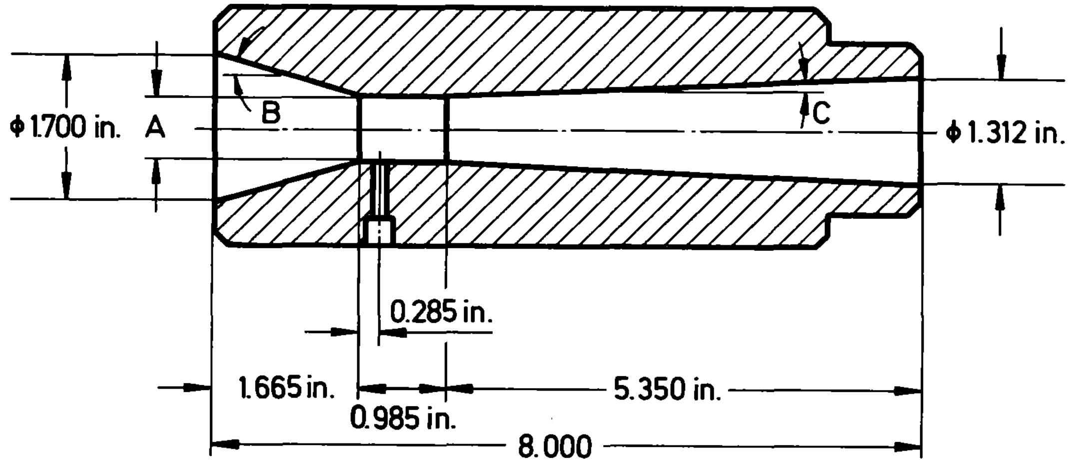
According to the method of characteristics [12, p. 307] the system of conservation equations is transformed into:

$$\left(\frac{dt}{dx}\right)_o = \frac{1}{u} , \tag{5a}$$

$$dp_o - a^2 d\rho_o = 0 , \tag{5b}$$

$$\left(\frac{dt}{dx}\right)_\pm = \frac{1}{u \pm a}, \tag{6a}$$

$$dp_\pm \pm \rho a du_\pm = -\frac{\rho u}{A}\frac{dA}{dx} . \tag{6b}$$



A	0.593
B	16° 50'
C	3° 19'

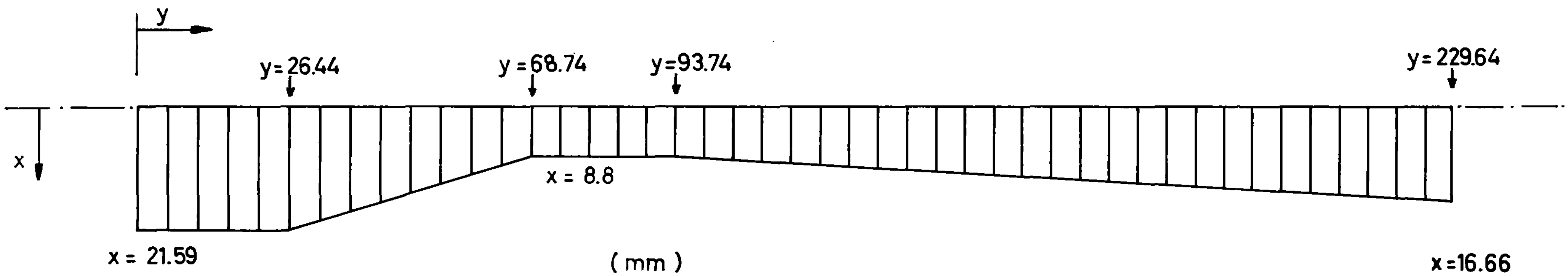


Fig. 1: HENRY- Nozzle and STRUYA Computing- mesh

Equations (5a) and (6a) define the slope of three characteristic curves, which are denoted by the indices o,+,-, while equation (5b) and (6b) are differential relations, which represent the flow equations. Each of the three equations (5b) and (6b) is valid only along the appropriate characteristic curve given by (5a) and (6a), respectively. At an intersection point of all three characteristic curves all equations (5b) and (6b) are valid and so provide three equations for the three unknown quantities u, p and ρ. But this intersection point where values for u, p and ρ could be calculated can only be found, if the solutions for u, p and ρ are already known, because u and a are used in (5a) and (6a). Hence an iterative solution scheme is necessary.

Replacing the differentials in (5) and (6) by finite differences leads to a set of difference equations, which can be used to solve the initial value problem in two different ways.

The first method is called the "direct" one. Initial values are given at three points of the flowfield on time level t, and at the intersection point of the three characteristic curves the gas properties u, p and ρ for the time level $t + \Delta t$ are calculated. Both the time step Δt and the location in x of the "solution point" are given by the computation. In order to achieve equal time steps in the whole flow field and the same spacing of the computational grid for all time steps, the "inverse" method according to /¯12, p. 333_/ was used for the calculations in the HENRY-nozzle.

For the inverse method (fig. 2) the characteristics, which are approximated by straight lines, are traced back from the new solution point P4 on time level $t + \Delta t$ to their intersections with time level t. At the intersection points P1, P2, P3 the initial values of u, p and ρ are linearly interpolated between the grid points P5, P6, P7 for which all variables are known. The iterative process of localisation of P1, P2, P3 and then evaluating u, p and ρ at the solution point P4 is done by a predictor-corrector algorithm, the localisation of P1, P2, P3 being the predictor - and the evaluations in P4 the corrector-step. In order to avoid extrapolations, the time step Δt was chosen such that the characteristics calculated using

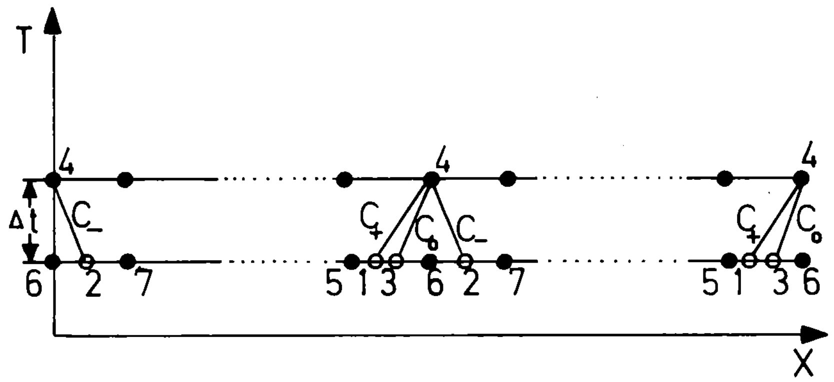


Fig. 2: "inverse" solution method of characteristics (nozzle inlet, inside and exit)

the stagnation-speed-of-sound would intersect at a distance of 1/3 of the grid spacing from point P6. This prevents from extrapolation for a Mach number below 2.

3. "Exact" solution for the steady flow

The onedimensional transient calculation of the flow in the HENRY-nozzle approaches the onedimensional, steady flow asymptotically for long times. So the steady solution can be used as check for the unsteady calculation. All equations necessary for the onedimensional steady solution can be found in /‾8, pp. 42, 49_7.

The following equation gives a connection between two cross-sections, A_1 and A_2, of a nozzle and the Mach numbers M_1 and M_2 of the flow at these cross-sections:

$$\frac{A_1}{A_2} = \frac{M_2}{M_1} \left(\frac{1 + \frac{\kappa-1}{2} M_1{}^2}{1 + \frac{\kappa-1}{2} M_2{}^2}\right)^{\frac{\kappa+1}{2(\kappa-1)}} . \qquad (7)$$

A special form of (7) is used, if one of the cross-sections is the nozzle throat because the Mach number corresponding to the throat is equal to 1, according to the theory of the Laval nozzle. If two of the cross-sections A_1 and A_2 and one of the corresponding Mach numbers are given, the other Mach number can be calculated iteratively.

The energy equation for onedimensional steady flows reads:

$$i + \frac{u^2}{2} = \frac{\kappa}{\kappa-1}\frac{p}{\rho} + \frac{u^2}{2} = \frac{\kappa}{\kappa-1}\ \frac{p_o}{\rho} = \text{const.} \tag{8}$$

An almost analytical solution for the one-dimensional steady flow in a nozzle including a shock can be found in the following way:

1. Using the inlet cross-section and the throat cross-section, the inlet Mach number can be found by (7).

2. Taking the inlet Mach number and the given boundary conditions p_1 and ρ_1 at the inlet plane, the stagnation pressure and density p_o and ρ_o are calculated with the energy equation (8).

3. Assuming a position of the shock, the Mach number at the supersonic side of the shock is calculated by (7) and with this Mach number and the stagnation quantities the flow quantities at the supersonic side of the shock can be found.

4. With the help of the well-known shock equations /‾8, p. 42_/ the flow quantities at the subsonic side of the shock are calculated and from them the stagnation quantities behind the shock.

5. The Mach number at the subsonic side of the shock and the nozzle cross-sections at the location of the shock and in the exit plane make it possible to calculate the Mach number in the exit plane via (7).

6. The Mach number in the exit plane and the stagnation quantities behind the shock allow to find the pressure in the exit plane, which can be compared to the pressure given as a boundary condition in the exit plane.

The whole process from 3. to 6. has to be iterated using the Regula Falsi, till the computed pressure in the exit plane meets the given one. This makes the solution "quasi analytical". Then the location of the shock is known and the flow quantities in the flow field can be calculated at any points desired, using (7) and (8).

4. Calculation and special problems in connection with the method of characteristics

The treatment of the combined initial and boundary value problems, which exist in the inlet and outlet plane of the nozzle made necessary a modification of the scheme for the initial value problem in the flowfield. In the inlet plane only the characteristic C_- (fig. 2) was used and the pressure and density were prescribed as boundary conditions. So only the velocity had to be calculated.

In the exit plane of a subsonic flow the pressure was prescribed and the C_+- and C_o-characteristics were used to determine u and ρ (fig. 2). The exit plane of a supersonic flow can be treated as a field point, because all three characteristics reach the exit plane from inside the nozzle and so make it impossible and unnecessary to give boundary conditions. A shock occuring in the flowfield was treated as a special boundary dividing the flowfield into two regions, which were connected only by the shock equations (fig. 3).

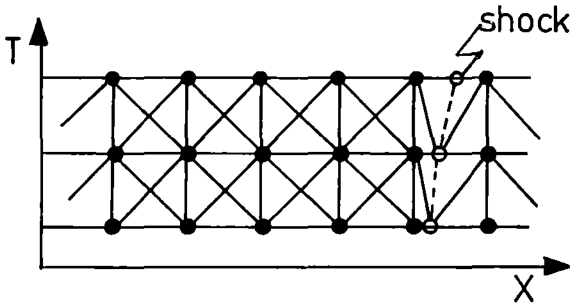


Fig. 3: Treatment of a shock in the flowfield

Computation was carried on until the steady state was reached, which took between 1200 and 1800 time steps depending on the outlet pressure ($\Delta t \approx 5 \cdot 10^{-6}$ sec). The computing time always remained below 15 min on a UNIVAC-1108.

Detection of a shock:
For most of the outlet pressures a slowly moving and finally resting shock was expected during the computation. Up to the time when the beginning of a shock was ascertained no shock calculations were performed in the field, but after its detection the shock was traced trough the flowfield and treated as a special boundary in it. The following criteria were used to detect the beginning of a shock:

1. The flowfield upstream from the point where the beginning of a shock was supposed had to be supersonic and the flowfield downstream subsonic.

2. Two neighbouring characteristics of the same family of Mach lines had to intersect within a time interval $(\Delta t)_{sh} = 45\ \Delta t/4$. This empirical value of $(\Delta t)_{sh}$ allowed to find the shock at the earliest time, when its fitting into the flowfield was numerically stable.

Once the shock was detected, its position was taken to be in the middle of the grid interval in which it was found and the starting flow quantities on both sides of the shock were taken from the neighboring grid points (fig. 4). The initial shock velocity was taken to be zero.

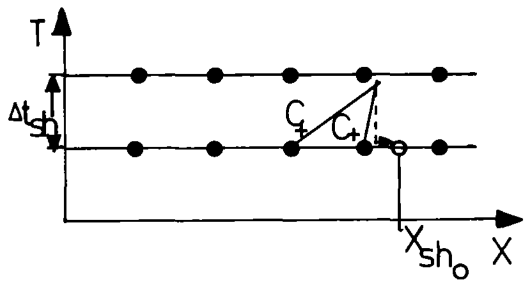


Fig. 4: detection of a shock in the flowfield

5. Calculation by STRUYA

STRUYA calculates the stationary nozzle flow as the asymptotic solution of a transient calculation starting with the above mentioned initial conditions. "Stationarity" of the calculation was obtained per definition when the maximum change in locally corresponding velocities in 0.5 ms was less than 0.1 %. This is - arbitrarily chosen - 1/12 of the time for the flow to reach stationarity. The convergence criterion for the iteration in each cycle was

$$(\text{mass source term}) \cdot \Delta t < \varepsilon \cdot \rho, \qquad \varepsilon = 10^{-4}$$

Full donor cell technique was applied (α=1); in some examples α was set equal to 0.75 with negligible effect on the stationary results. Each test was run over 8 ms corresponding to 8000 cycles, stationarity was reached after 6 to 6.5 ms in all cases. This is about 2.5 times as large as the characteristic run-through time of the nozzle in steady state. The computation time was 20.5 min on an IBM 370/168.

Due to the - in some cases - initially rather large pressure difference at the exit problems of stability arose. Stability was obtained by making the viscosity terms in the Navier-Stokes equation non-zero. As will be discussed later, this had the effect of not only damping instabilities but also the flow velocity. In addition to the work presented here, calculations were performed with four mesh cells in radial direction ("2D"). They generally showed the same results as the 1D-calculations and therefore will not be discussed further.

6. Results

In figs. 7 and 8 (figures with numbers > 7 see appendix) the transient development of some typical profiles is documented. Figs. 11 through 18 show the quasi-analytical solution (solid line) together with the corresponding stationary results of STRUYA (dashed line) and the calculation by characteristics (dotted line), respectively.

The "correct" - according to gas dynamics - solution clearly distinguishes the acceleration phase in the converging part of the nozzle, a section of indifference in the cylindrical part followed by further acceleration in all examples (the exit pressure, below which critical flow occurs, is 4.72 MPa!). For downstream pressures between 4.72 MPa and 1.89 MPa deceleration is introduced by a shock. Its location is determined by the exit pressure. In the 1.5 MPa case (< 1.89 MPa) no shock occurs due to a totally supersonic solution downstream of the throat. The denisty profiles resemble the pressure profiles. The local sonic velocity is nearly constant.

6.1 Method of characteristics

The solution obtained by the method of characteristics shows the following discrepancies as compared to the analytical solution:

- influence of the time-step
- the location of the shock is not detected correctly
- even at large times t there remains a small but negligible pressure gradient in the nozzle throat

These discrepancies are results of the combination of constant cross-section parts and corners in the contour of the nozzle which is rather unfavourable for using a method of characteristics. The first mentioned influence of the time-step size on the results can be seen in fig. 5. A small pressure peak appears at the connection between the cylindrical inlet part and the convergent part of the nozzle if the time step is taken to be half of the one used for the other calculations. The effect of the unfavourable nozzle shape on the numerical process can be shown easily in the case of this pressure peak and works similarly in the cases of the other discrepancies. Information on the nozzle cross-section is used by this method of characteristics only along the C_+- and C_--characteristics and only in the term $\frac{1}{A}\frac{dA}{dx}$ in eq. (6b). For points in regions with constant cross-section, the whole term becomes zero and therefore along characteristics coming out of constant cross-section regions no information about the area of the duct is used. If two grid points are located as shown in fig. 6 and a time-step like Δt_1 in fig. 6 is used, all characteristics used for calculations in the left point on time level $t+\Delta t_1$ originate in a

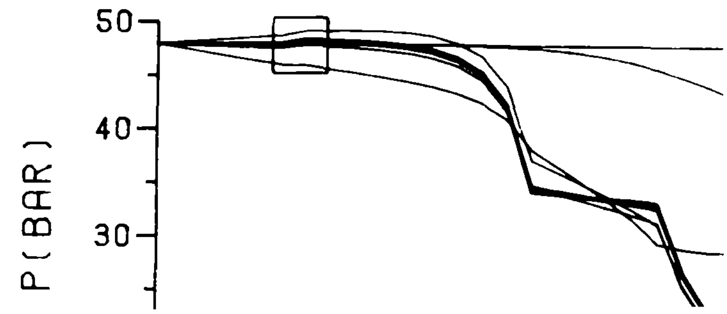


Fig. 5: pressure peak due to time-step size

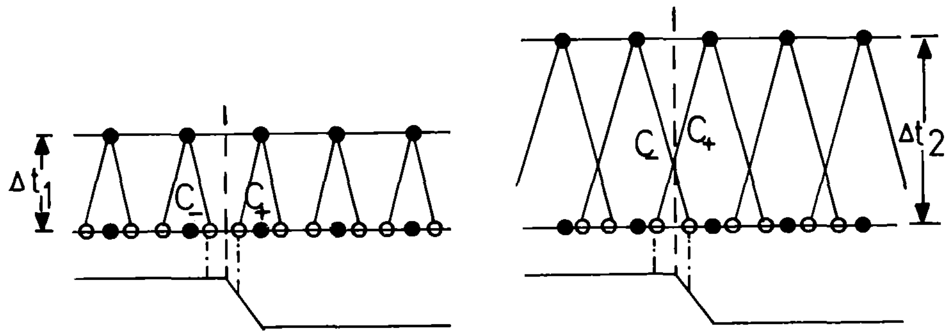


Fig. 6: influence of time-step size; here $\Delta t_1 = 3.87 \cdot 10^{-6}$ sec, $\Delta t_2 = 5.16 \cdot 10^{-6}$ sec

constant cross-section region while all characteristics used in the right point on time level $t+\Delta t_1$ come out of a region with varying cross-section. Concerning the information on the cross-section the two parts of the nozzle are disconnected, and therefore the peak in the pressure distribution appears. If the time-step is increased to Δt_2 in fig. 6, the nozzle parts are connected again and the peak disappears. Calculations in nozzles without contour corners or parts with constant cross-section did not show any connection between time-step size and results. They can be taken as proof for the statement that the problems with the HENRY-nozzle calculations are caused by its special, unfavourable form.

6.2 STRUYA

The calculations with the finite difference code STRUYA show deviations from the correct solution, which principally change the shape of the profiles.

The shock is smoothed out over a length of about three diameters. In the 1.5 MPa - case, where there should be no shock, still one exists close to the exit due to the - now senseless - pressure boundary condition. The "edges" of the curves which are caused by the cylindrical section of the nozzle are totally smoothed, not the slightest change in the inclination can be detected. This effect is not influenced by the physical viscosity.

Fig. 10 demonstrates the effect of the physical viscosity in STRUYA. While the viscous flow calculation supplies a totally subsonic solution ($M_{max} = 0.96$), where due to the pressure ratio a supersonic flow should result, the inviscid flow solution reaches at least M = 1.12. In the 4.5 MPa-case even the inviscid calculation amounts to a subsonic solution ($M_{max} = 0.62$!, see fig. 12). Surprisingly the local speed of sound is reached first - if it is ever reached - at the same location (z = 0.085 m) in all test examples. At this site the critical pressure

$$p_{exit} = p_{entry} \left(\frac{2}{\kappa+1}\right)^{\frac{\kappa}{\kappa+1}}$$

is calculated correct with a maximum error of 1.5 %. Out-of-throat and out-of-shock profiles for "non-extreme" cases (3.5 - 2.0 MPa exit pressure) are computed correctly. The mass flux at the throat is slightly rising with falling exit pressure though sonic speed is attained. Only at exit pressures below ~ 3.0 MPa it remains constant as it should do.

It is worth mentioning that the 2D-calculations of the two-phase nozzle flow with STRUYA agreed very well with the experimental data /‾6_7 concerning the mass flux. The calculated pressure at z = 0.075 m (pressure tap in the nozzle wall) was always ~ 9 % above the experimental value, indicating the same tendency as in this work. It should be added, that after all the 2D-effect for the HENRY-nozzle with a relatively small angle of convergence is negligible compared with the discrepancies deducted here. Finally we should note that STRUYA and its predecessor YAQUI were mainly developed for analysis of highly transient flow situations and are not particularly tuned for steady flows.

7. Conclusions

In the application on a critical nozzle flow of an ideal gas it was demonstrated that a first order finite difference code compared to a code based on the method of characteristics may produce results which are extremely damped. The resulting errors are of an intolerable magnitude though the physics of the code are derived from first principles.

The calculations with the code based on the method of characteristics match the exact solution fairly well, especially if the derivatives of the contour are steady. The quantitative deviations show that with geometries like the HENRY-nozzle the method of characteristics reaches limits as well.

Due to the numerical damping and the enormous computation time the first order finite difference code seems not to be the adequate tool for this kind of problem though easy handling suggests its application. A code of second order in space should supply better results though geometry and the nonlinear equation of state for example imply errors of first order anyway. On the other hand, while the method of characteristics is far superior in this comparison, certain problems (e.g. 2D-calculations of a steam-water flow through the same nozzle) exclude its practical application. Moreover the damping effects are sometimes desired for transient processes where they are expected to be of minor influence on the results (like filters are used for experimental evaluation). It is therefore recommended to test these codes before application on a similar but analytically resolvable example to make sure that the numerical effects such as difference formulation, stepsize, mesh discretisation, stability parameters etc. do not dominate (in an unnoticed way!) over the physical effects which are to be simulated.

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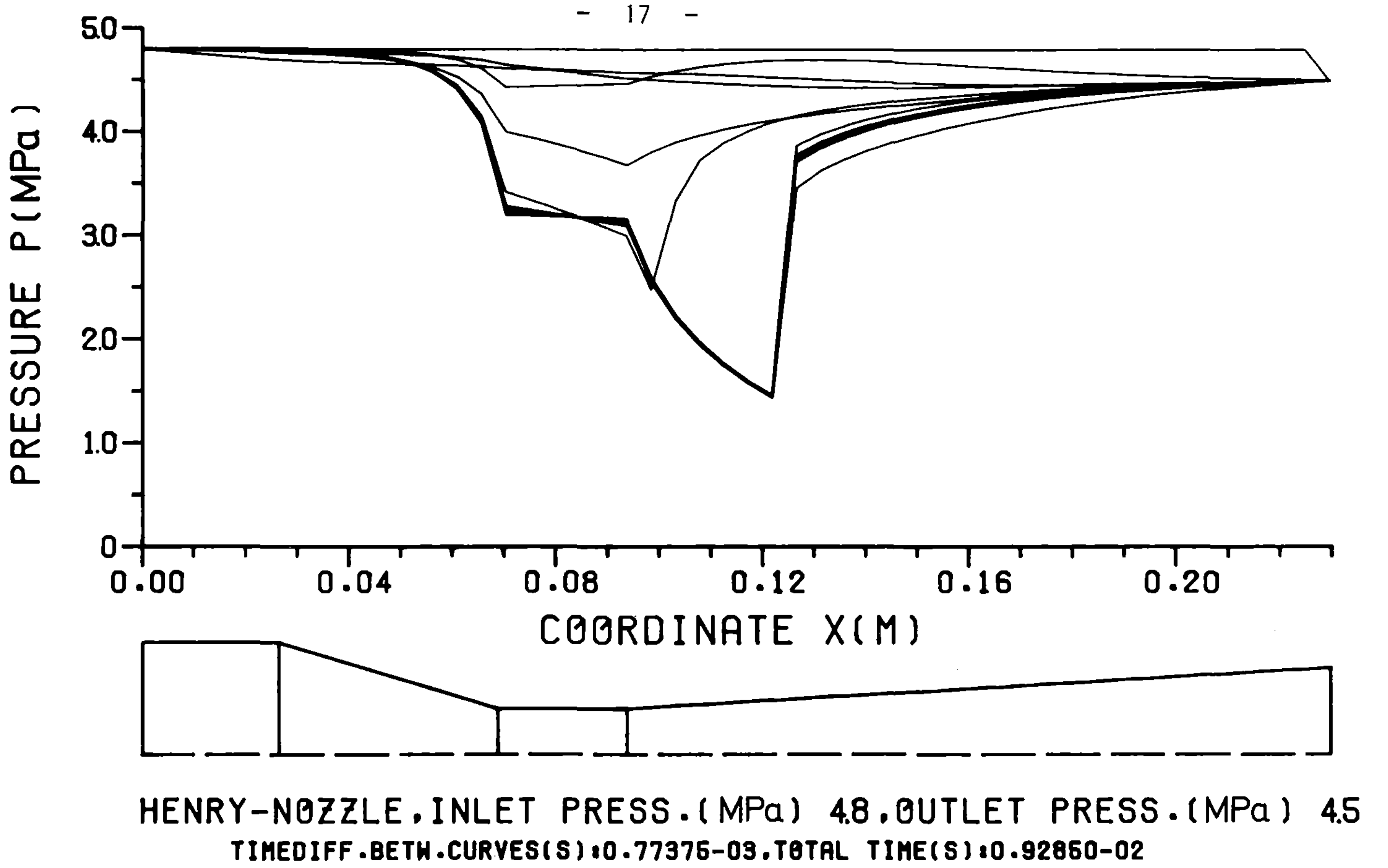
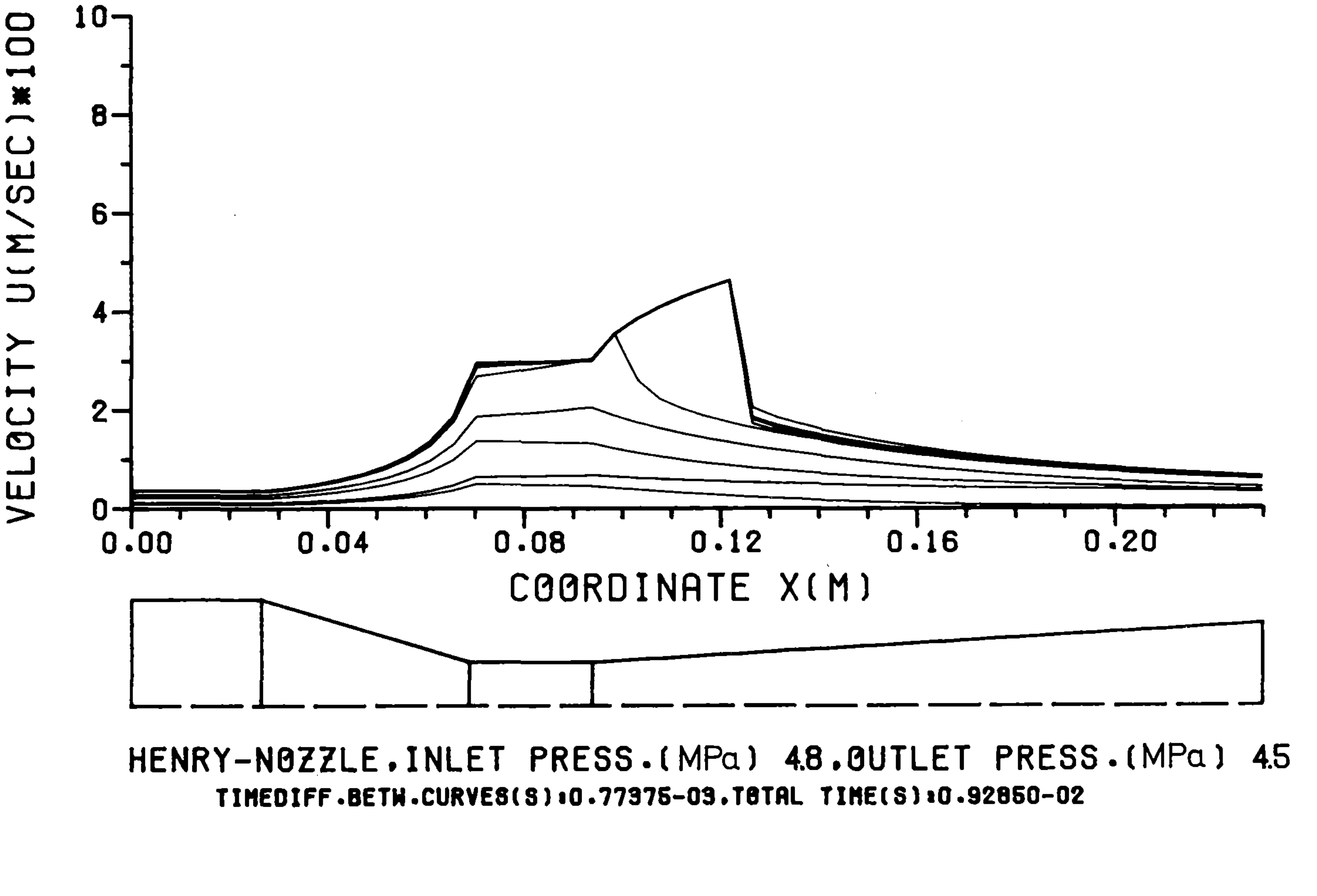


Fig. 7 & 8: transient development of pressure- and velocity profile



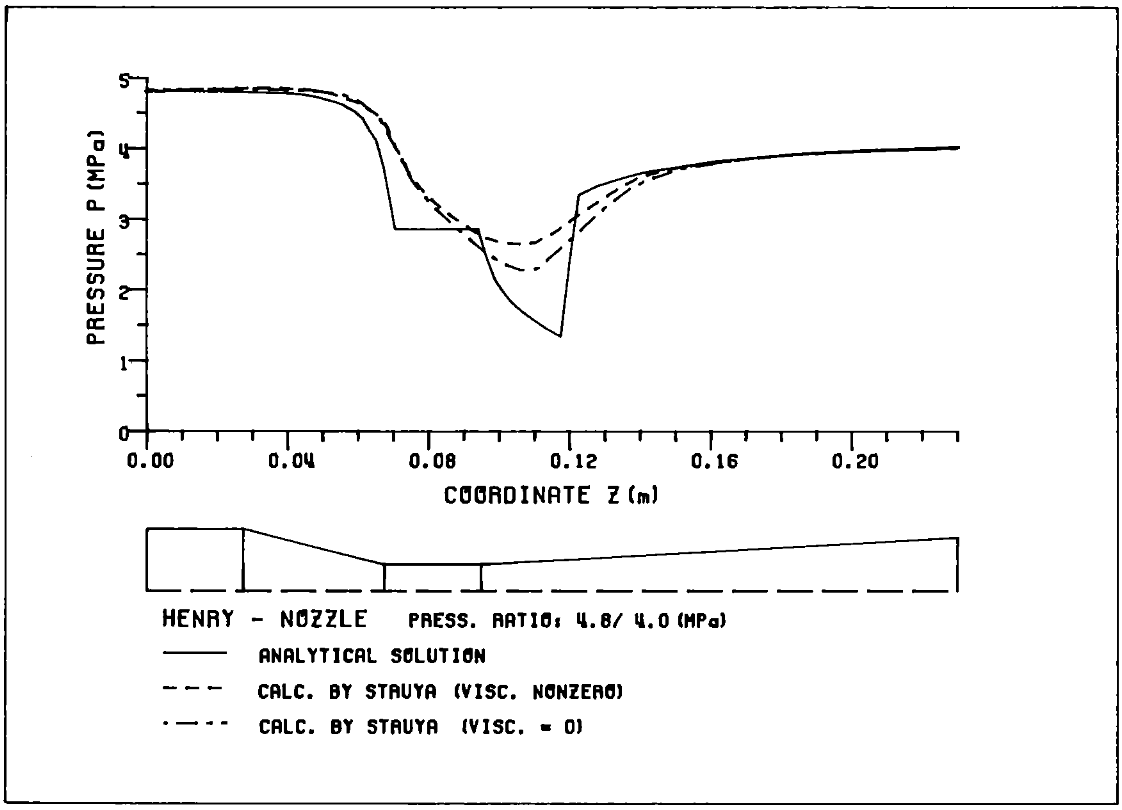
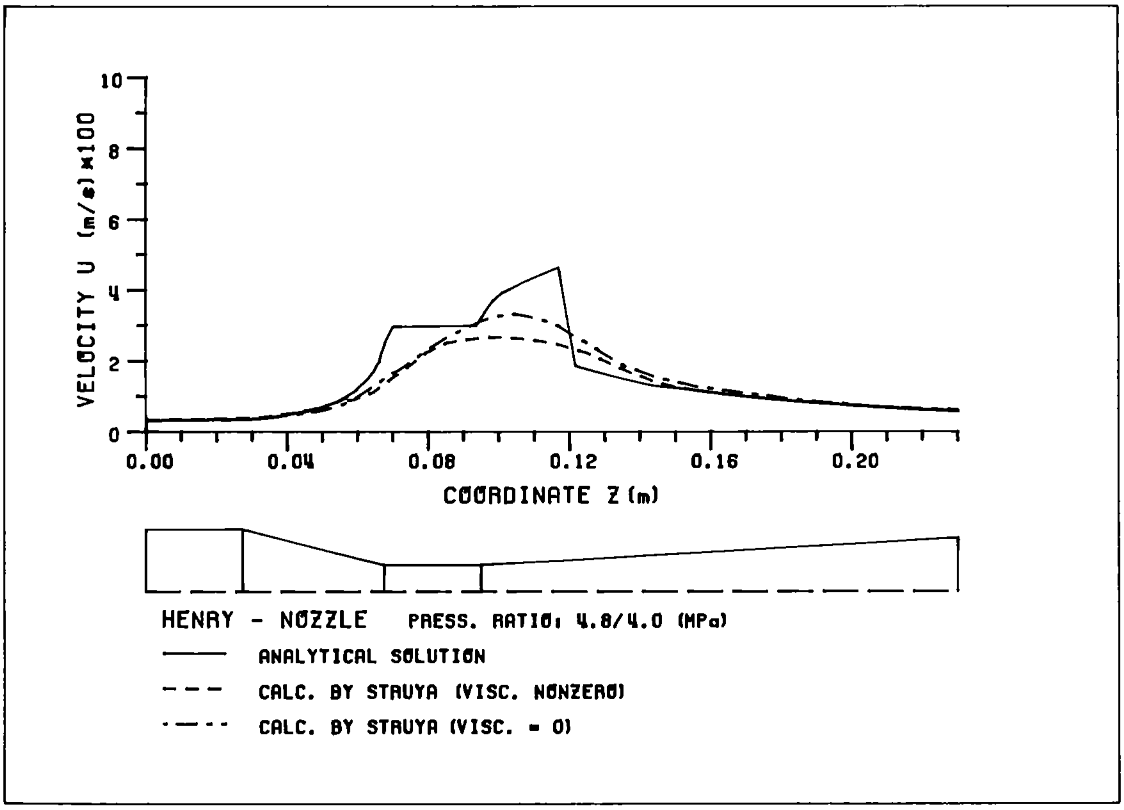


Fig. 9 & 10: influence of the viscosity in STRUYA



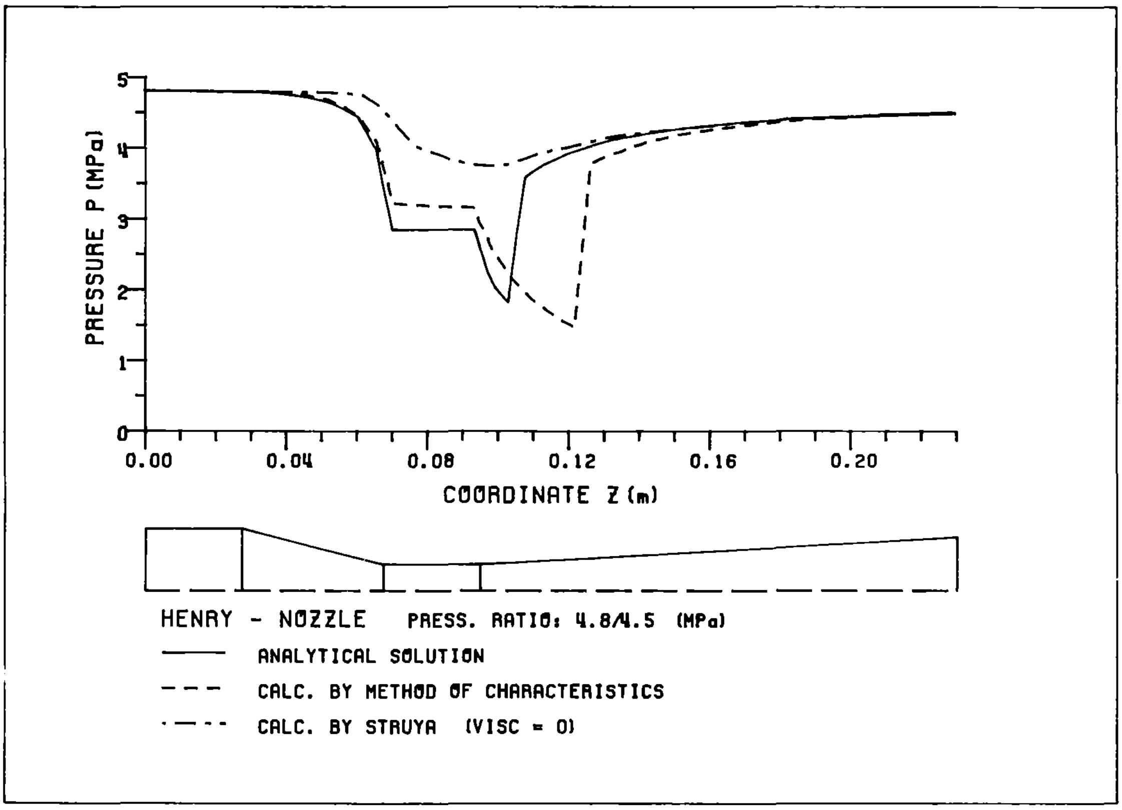
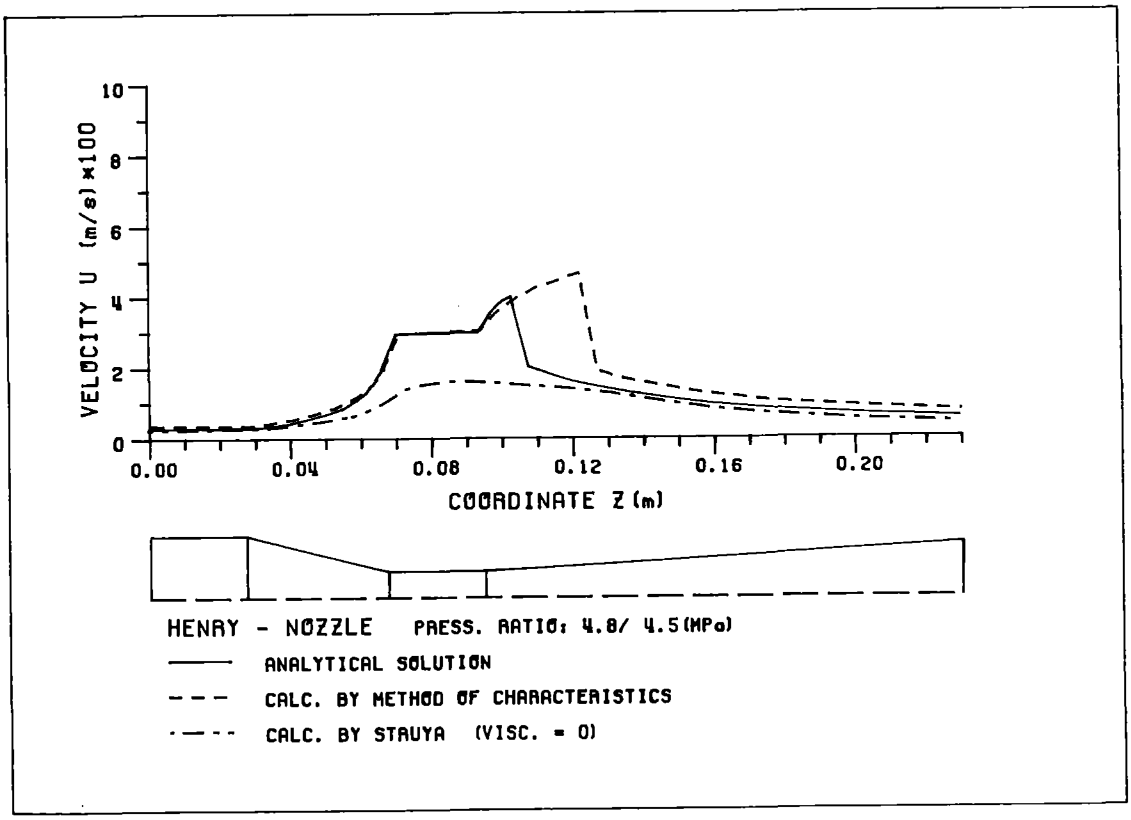


Fig. 11 & 12: downstream pressure 4,5 MPa



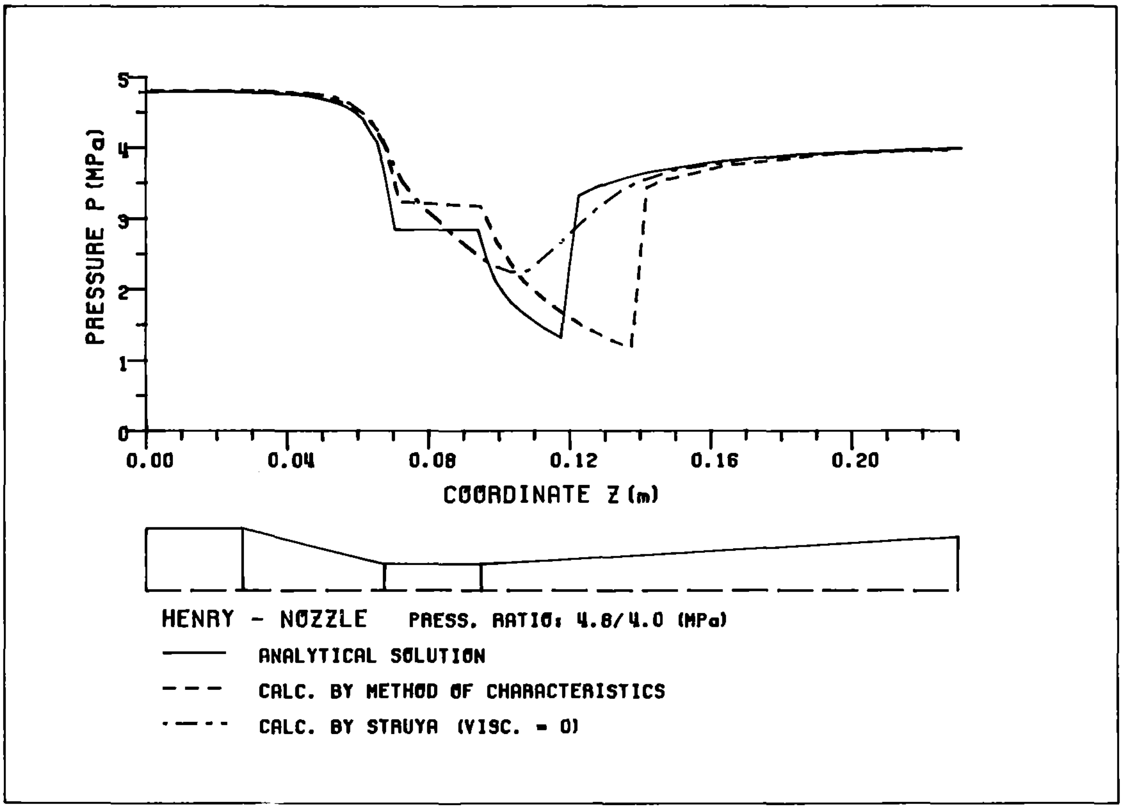
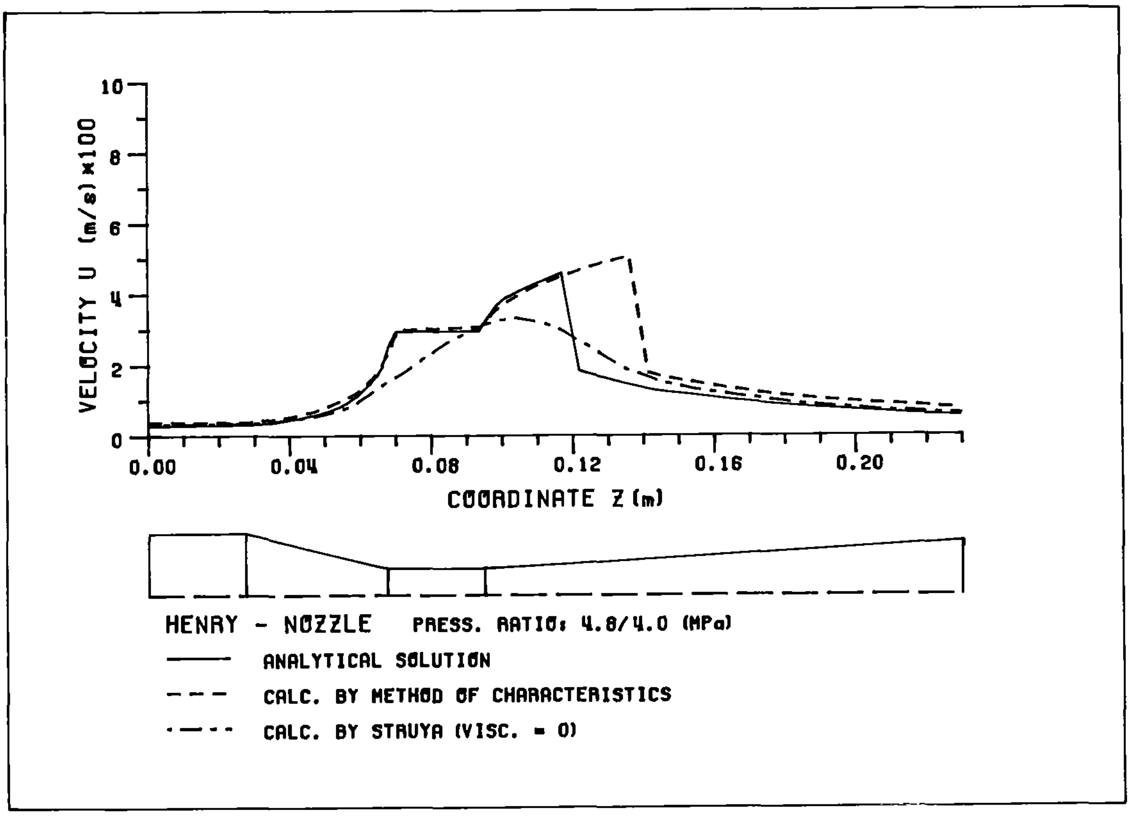


Fig. 13 & 14: downstream pressure 4.0 MPa



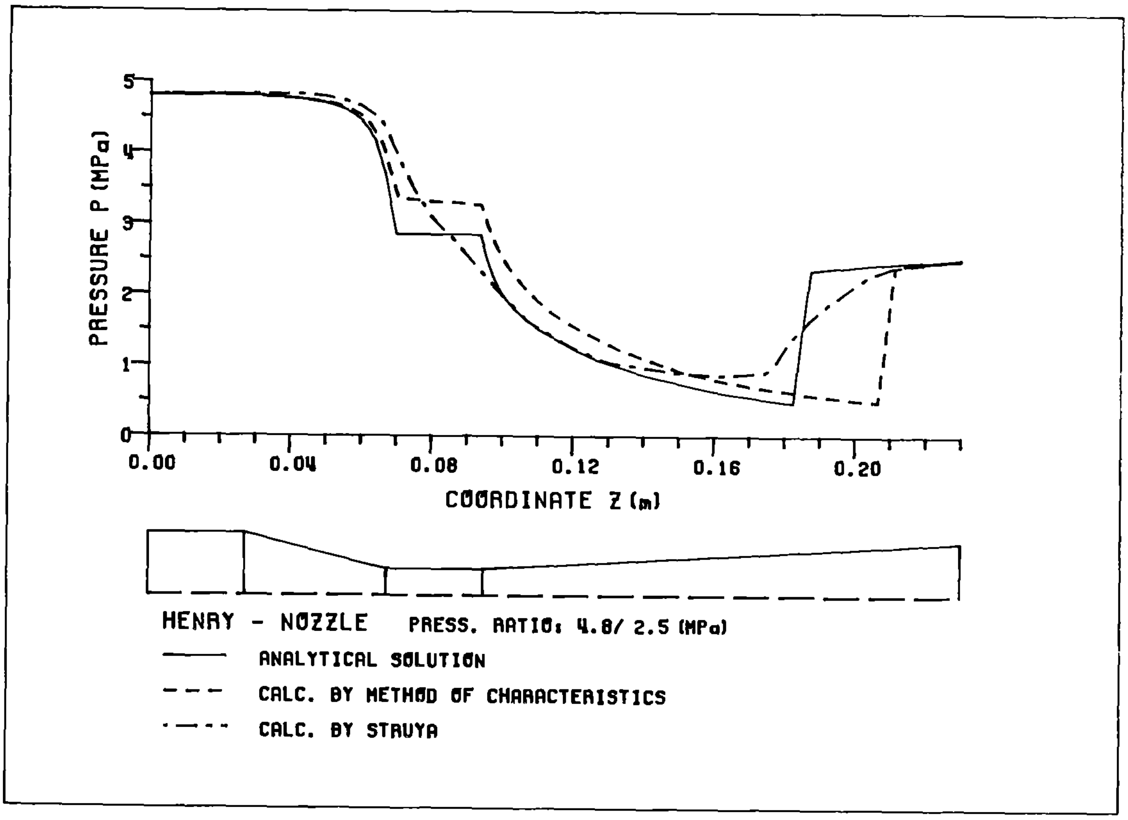
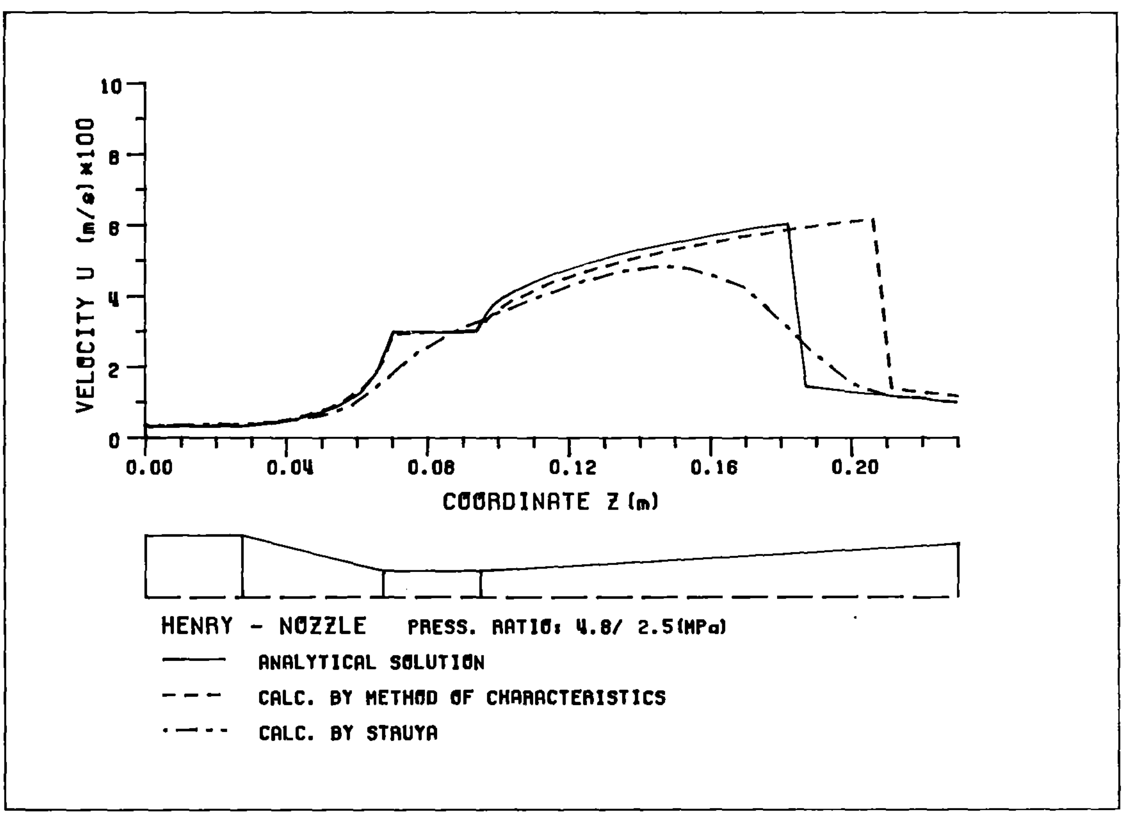


Fig. 15 & 16: downstream pressure 2.5 MPa



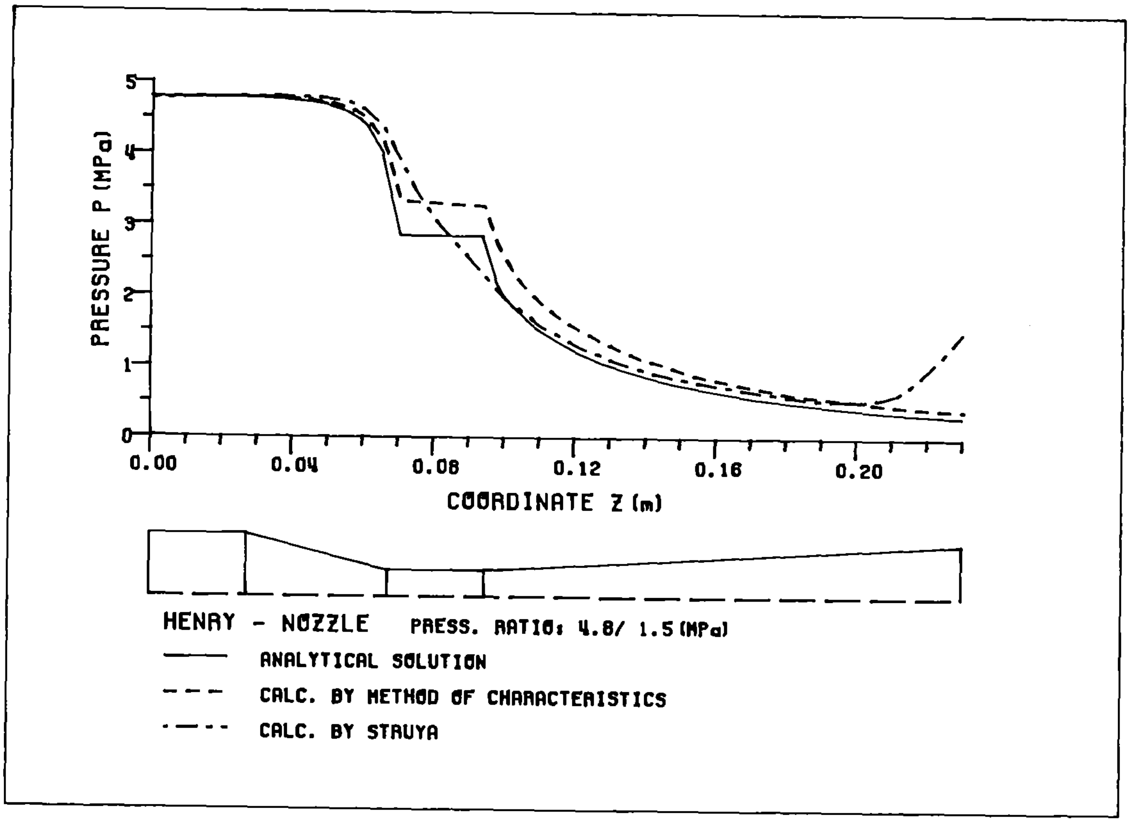


Fig. 17 & 18: downstream pressure 1.5 MPa