

MARCHI


Real Gas Effects for Compressible Nozzle Flows

D. Drikakis¹

S. Tsangaris

Department of Mechanical Engineering,
 National Technical University of Athens,
 Athens, Greece

Numerical simulation of compressible nozzle flows of real gas with or without the addition of heat is presented. A generalized real gas method, using an upwind scheme and curvilinear coordinates, is applied to solve the unsteady compressible Euler equations in axisymmetric form. The present method is an extension of a previous 2D method, which was developed to solve the problem for a gas having the general equation of state in the form $p = p(\rho, i)$. In the present work the method is generalized for an arbitrary P-V-T equation of state introducing an iterative procedure for the determination of the temperature from the specific internal energy and the flow variables. The solution procedure is applied for the study of real gas effects in an axisymmetric nozzle flow.

1 Introduction

The numerical solution of the compressible Euler equations has been reported by several authors, but all of these methods were developed mainly for perfect air. The incorporation of the real gas effects requires the introduction of a general equation of state. In the present paper a generalized method is presented for the simulation of real gas flows and test cases are presented for nozzle flows.

In recent years efforts have been made by many authors for the construction of algorithms for the solution of the equations of gas dynamics with real gas effects (Collela and Glaz, 1985; Liou et al., 1990; Grossman and Walters, 1989; Glaister, 1988; Drikakis and Tsangaris, 1991). These efforts mainly originated in the numerical investigation of hypersonic flow fields using an equation of state in the form $p = p(\rho, i)$, where p , ρ , i are the pressure, density, and specific internal energy of the gas. In the aforementioned papers modern numerical methods, as Flux Vector Splitting methods and Riemann solvers, have been modified for hypersonic flow simulation. All the above methodologies concern a $p = p(\rho, i)$ E.O.S. and they can not directly be used for a P-V-T equation of state.

Drikakis and Tsangaris (1991) developed a real gas method, in combination with a Riemann solver, for the discretization of the inviscid fluxes, introducing thermodynamic parameters, such as the pressure derivatives with respect to density and specific internal energy. This method can not directly be used for an arbitrary P-V-T E.O.S., because it needs the definition of the pressure as a function of the density and the specific internal energy. In the present paper, this method is extended to apply to any P-V-T equation of state by an iterative procedure for the determination of the temperature from the specific internal energy. On the other hand, the extension of the 2-D method in axisymmetric form, with source terms, is presented. The solution of the inviscid axisymmetric gas dynamic

equations with source terms is obtained by a Godunov type, finite volume scheme. The variation of the pressure along a characteristic line is calculated in terms of the thermodynamic parameters. The present method is general because it does not make any assumption in the real gas manipulation, formulating the real gas problem along the characteristic lines in conservative form. The method has the advantage that it can also be used for P-V-T equations of state, while the methods mentioned in the literature have been developed on the basis that pressure is a function of the density and the specific internal energy or on the basis of an "equivalent" ratio of specific heats.

The solution procedure is used for the numerical simulation of real gas effects in an axisymmetric convergent-divergent nozzle. Results and differences from the perfect gas assumption are presented for nitrogen and superheated steam flow. The study of real gas effects is also presented for the gas flow with the addition of heat. The introduction of the heat source terms causes large variations in the gas flow, especially in the temperature field.

2 Governing Equations

The Euler equations for axisymmetric gas flow with real gas effects and source terms, such as a volumetric heat addition, are solved. The equations can be written in an extended conservation law form for a generalized coordinate system as:

$$U_t + E_\xi + G_\zeta + r\dot{H} = Q \quad (1a)$$

where

$$U = J(\rho, \rho u, \rho w, e)^T$$

$$E = J(\rho \bar{U}, \rho \bar{U} u + p \xi_x, \rho w \bar{U} + p \xi_z, (e + p) \bar{U})^T$$

$$G = J(\rho \bar{W}, \rho u \bar{W} + p \zeta_x, \rho w \bar{W} + p \zeta_z, (e + p) \bar{W})^T$$

¹Present address: Lehrstuhl für Strömungsmechanik, Universität Erlangen-Nürnberg, D-8520, Erlangen, Germany.

Contributed by the Fluids Engineering Division for publication in the JOURNAL OF FLUIDS ENGINEERING. Manuscript received by the Fluids Engineering Division March 30, 1991. Associate Technical Editor: C. J. Freitas.

$$\bar{H} = \frac{J}{z} (\rho w, \rho u w, \rho w^2, (e+p)w)^T$$

$$\bar{U} = u\xi_x + w\xi_z$$

$$\bar{W} = u\zeta_x + w\zeta_z$$

$$e = \rho i + .5\rho(u^2 + w^2) \quad (1b)$$

If $r=1$ the equation is in axisymmetric form. If $r=0$ it is in 2-D form. The source term Q contains a volumetric heat addition.

$$Q = J(0, 0, 0, q)^T$$

Body fitted arbitrary coordinates ξ, ζ are used and the Jacobian of the transformation $\xi = \xi(x, z), \zeta = \zeta(x, z)$ from Cartesian coordinates x, z to generalized coordinates ξ, ζ is written as:

$$J = x_\xi z_\zeta - z_\xi x_\zeta$$

The quantities ρ, p, u, w represent the density, the pressure and the Cartesian velocity components respectively and e, i represent the total energy and the specific internal energy. The indices $(\cdot)_\xi, (\cdot)_\zeta$ denote partial derivatives with respect to ξ, ζ . The formulation of the governing equations is completed by a general equation of state in the form:

$$p = p(\rho, i) \quad \text{or} \quad p = p(\rho, T)$$

where T is the temperature of the gas.

The solution is obtained by an implicit procedure. The first order in time discretized implicit form of Eq. (1) is written as:

$$\frac{U^{n+1} - U^n}{\Delta t} + E_\xi^{n+1} + G_\zeta^{n+1} + r\bar{H}^n = Q \quad (2)$$

A Newton method can be constructed for U^{n+1} by linearizing the fluxes in Eq. (2) about the known time level n . Then Eq. (2) is written as follows:

$$\frac{\Delta U}{\Delta t} + (A^n \Delta U)_\xi + (C^n \Delta U)_\zeta = RHS \quad (3a)$$

where

$$RHS = - (E_\xi^n + G_\zeta^n + r\bar{H}^n) + Q \quad (3b)$$

A, C are the Jacobians of the flux vectors E, G , respectively, and ΔU is the time variation of the solution.

The fluxes on the right-hand side are calculated at the cell faces of the finite volume by a linear, locally one dimensional Riemann solver (Godunov type differencing) (Eberle, 1985). The characteristic flux averaging scheme is of third accuracy

in space and locally monotonic. The Jacobians of the fluxes of the left-hand side are formulated for a general equation of state.

3 Real Gas Formulation

The Euler equations are splitted into two one-dimensional equations.

$$U_i + E_\xi = 0$$

$$U_i + G_\zeta = 0$$

The Riemann invariants are a transformation of nonconservative Euler equations on the characteristic directions. These invariants are given by the following expressions:

$$p - p_0 - s^2(\rho - \rho_0) = 0 \quad (4a)$$

$$(w - w_0)\bar{x} - (u - u_0)\bar{z} = 0 \quad (4b)$$

$$p - p_1 + \rho s[\bar{x}(u - u_1) + \bar{z}(w - w_1)] = 0 \quad (4c)$$

$$p - p_2 + \rho s[-\bar{x}(u - u_2) - \bar{z}(w - w_2)] = 0 \quad (4d)$$

The subscripts indicate the point locations (points on the characteristic lines) at which $p_j, \rho_j, u_j, w_j, j=0, 1, 2$, should be interpolated.

Since we make use of the homogeneous property, the invariants have to be inverted into conservative variables. Considering that the pressure can be written as a function of the density and specific internal energy, $p = p(\rho, i)$, we obtain:

$$\Delta p = p_\rho \Delta \rho + p_i \Delta i \quad (5)$$

Our goal is to formulate the equations by means of the pressure derivatives p_ρ and p_i . The development of the method for a general equation of state is analytically presented in the literature (Drikakis and Tsangaris, 1991).

Finally, we find the conservative cell face flow values $\rho, l = \rho u, n = \rho w, e$ from which the Euler fluxes on the right-hand side of Eq. (3), can be calculated. All the conservative values are given by the following equations:

$$\rho = \rho_0 + \bar{\rho} + r_1 + r_2 \quad (6a)$$

$$l = l_0 + r_1(u + s\bar{x}) + r_2(u - s\bar{x}) + \bar{x}d + u\bar{\rho} \quad (6b)$$

$$n = n_0 + r_1(w + s\bar{z}) + r_2(w - s\bar{z}) + \bar{z}d + w\bar{\rho} \quad (6c)$$

$$e = d\lambda_0 + (H + s\lambda_0)\rho_1 + (H - s\lambda_0)\rho_2 + \bar{e} + \bar{\rho} \left(q^2 + \rho \frac{Q}{p_i} \right) - \rho_0 \frac{p}{p_i} Q \quad (6d)$$

with

Nomenclature

A, C = Jacobians of the flux vectors
 e = total energy per unit volume
 E, G = flux vectors
 i = specific internal energy
 J = Jacobian matrix
 H = total enthalpy
 p = pressure
 p_i = pressure derivative with respect to internal energy

p_ρ = pressure derivative with respect to density
 ρ = density
 s = sound velocity
 T = gas temperature
 u, w = Cartesian velocity components
 U = conservative solution vector

ΔU = time variation of the conservative solution vector
 ξ, ζ = Body fitted coordinates
 x, z = Cartesian coordinates
 λ_k = eigenvalues

Indices

n = iteration level

$$\bar{\rho} = \frac{p_i}{\rho s^2} \left(\bar{e} - e_0 - \rho_0 Q \frac{\rho}{p_i} \right) \quad (7a)$$

$$\bar{e} = ul_0 + wn_0 \quad (7b)$$

$$d = \rho_0 \lambda_0 - l_0 \bar{x} - n_0 \bar{z} \quad (7c)$$

and

$$\lambda_0 = u\bar{x} + w\bar{z}$$

$$r_1 = \frac{0.5}{s^2} \left\{ \rho_1 (-s\lambda_0 + Q) + l_1 \left(-u \frac{p_i}{\rho} + s\bar{x} \right) + n_1 \left(-w \frac{p_i}{\rho} + s\bar{z} \right) + e_1 \frac{p_i}{\rho} \right\} \quad (7d)$$

$$r_2 = \frac{0.5}{s^2} \left\{ \rho_2 (s\lambda_0 + Q) - l_2 \left(-u \frac{p_i}{\rho} + s\bar{x} \right) + n_2 \left(-w \frac{p_i}{\rho} + s\bar{z} \right) + e_2 \frac{p_i}{\rho} \right\} \quad (7e)$$

H is the total enthalpy while the sound velocity s and the term Q are given as:

$$s^2 = p \frac{p_i}{\rho^2} + p_\rho \quad (8a)$$

and

$$Q = p_\rho + p_i \frac{q^2}{2\rho} - i \frac{p_i}{\rho} \quad (8b)$$

The \bar{x} , \bar{z} terms contain metric derivatives:

$$\bar{x} = \frac{\xi_x}{\sqrt{\xi_x^2 + \xi_z^2}}, \quad \bar{z} = \frac{\xi_z}{\sqrt{\xi_x^2 + \xi_z^2}}$$

The implementation of the method in the right-hand side of the equation, in order to include real gas effects, is obtained by the derivation of the Jacobian matrices and the eigenvectors for a general equation of state. For this reason, as with the expressions on the right-hand side, the matrices on the left-hand side are defined by introducing the pressure derivatives. The Jacobian matrix A is defined as follows:

$$A = \frac{\partial E}{\partial U} = \left(\frac{\partial E}{\partial \rho}, \frac{\partial E}{\partial l}, \frac{\partial E}{\partial n}, \frac{\partial E}{\partial e} \right)$$

In accordance with the assumption that the pressure is a function of the density and the internal energy, the partial derivatives for the pressure are given by the following relations:

$$\frac{\partial p}{\partial \rho}(\rho, i)|_{l, n, e} = \frac{\partial p}{\partial \rho}(\rho, i)|_i + \frac{\partial i}{\partial \rho}(\rho, l, n, e)|_{l, n, e} \frac{\partial p}{\partial i}(\rho, i)|_\rho$$

$$\frac{\partial p}{\partial l}(\rho, i)|_{\rho, n, e} = \frac{\partial p}{\partial l}(\rho, i)|_\rho \frac{\partial i}{\partial l}(\rho, l, n, e)|_{\rho, n, e}$$

$$\frac{\partial p}{\partial n}(\rho, i)|_{\rho, l, e} = \frac{\partial p}{\partial n}(\rho, i)|_\rho \frac{\partial i}{\partial n}(\rho, l, n, e)|_{\rho, l, e}$$

$$\frac{\partial p}{\partial e}(\rho, i)|_{\rho, l, n} = \frac{\partial p}{\partial e}(\rho, i)|_\rho \frac{\partial i}{\partial e}(\rho, l, n, e)|_{\rho, l, n}$$

and the internal energy is defined by:

$$i(\rho, l, n, e) = \frac{e}{\rho} - 0.5 \frac{(l^2 + n^2)}{\rho^2}$$

The analytical expressions of Jacobian matrices and the eigenvectors for a real gas can be found in reference (Drikakis and Tsangaris, 1991).

The above formulation of the method imposes the calculation of the thermodynamic derivatives of the pressure. These derivatives are approximated by the values of the pressure, density and the specific internal energy on the left and right states of the volume cell face. These approximations are defined as follows:

$$p_i = \frac{1}{\Delta i} \left\{ \frac{1}{2} (p(\rho_R, i_R) + p(\rho_L, i_R)) - \frac{1}{2} (p(\rho_R, i_L) + p(\rho_L, i_L)) \right\} \quad (9a)$$

$$p_\rho = \frac{1}{\Delta \rho} \left\{ \frac{1}{2} (p(\rho_R, i_R) + p(\rho_R, i_L)) - \frac{1}{2} (p(\rho_L, i_R) + p(\rho_L, i_L)) \right\} \quad (9b)$$

for $\Delta i \neq 0$, $\Delta \rho \neq 0$ and

$$p_i = \frac{1}{2} \{ p_\rho(\rho_L, i) + p_\rho(\rho_R, i) \} \quad (9c)$$

$$p_\rho = \frac{1}{2} \{ p_\rho(\rho, i_L) + p_\rho(\rho, i_R) \} \quad (9d)$$

for $\Delta i = 0$, $\Delta \rho = 0$, respectively.

Where

$$\Delta(\cdot) = (\cdot)_R - (\cdot)_L$$

The indices R , L represent, for a cell face $i + 1/2$, the volumes $i + 1$, i , respectively (Fig. 1(a)).

4 Coupling of the Temperature With the Specific Internal Energy

The equations of state for real gases are defined either by the density and the specific internal energy or by the density (or specific volume) and the temperature (P-V-T equation of state). To the second category belong the best known equations of state. In this case the calculation of the temperature of the gas is needed because from the conservative variables only the internal energy can be defined. For a real gas the specific internal energy is defined by the following relation:

$$i(\rho, T) = \int \left(\frac{\partial i}{\partial v} \right)_T dv + \int \left(\frac{\partial i}{\partial T} \right)_v dT \quad (10a)$$

The derivative in the second term of the above relation is the specific heat for constant volume v .

The derivative of the internal energy in the first term can be calculated by the pressure and the pressure derivative with respect to temperature as follows:

$$\left(\frac{\partial i}{\partial v} \right)_T = T \left(\frac{\partial p}{\partial T} \right)_v - p \quad (10b)$$

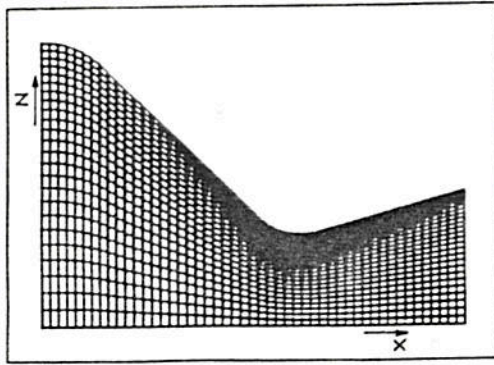


Fig. 1 Typical control volume and labeling scheme-Computational mesh 50 x 25 for the JPL nozzle

The specific heat for constant volume c_v for a real gas depends on the specific volume and the temperature, while for a perfect gas depends on the temperature alone. On the other hand, if the temperature of the gas is greater than the critical temperature (T_c) the variations of the c_v are not large (Hittmair and Adam, 1971). Thus a first approximation can be considered with constant c_v .

For the Van der Waals equation of state:

$$p = \frac{RT}{v-b} - \frac{a}{v^2}$$

and using Eqs. (10a, b), the specific internal energy can be defined as follows:

$$i(T, v) - i(T_0, v_0) = \int c_v dT - a \left(\frac{1}{v} - \frac{1}{v_0} \right) \quad (11a)$$

Thus a value for the temperature can be defined by the known specific internal energy. If we consider that c_v is a function of the pressure and the density, an iterative procedure is needed in order to satisfy Eq. (11a). An iterative procedure, such as the Newton-Raphson technique, is also necessary if the internal energy from the Eq. (10a) is a complex function of the temperature. For instance if we consider the Benedict-Webb-Rubin equation of state and assuming, for the sake of simplicity, that $T > T_c$, the Eq. (10a) is written as follows:

$$i = T - T^{-2} f_1(v) + f_2(v) \quad (11b)$$

where $f_1(v)$, $f_2(v)$ are functions of the specific volume. From Eqs. (11a) or (11b) by an iterative procedure we can find the temperature and consequently the pressure from the P-V-T equation of state.

5 Heat Addition

In the computational method, source terms have also been introduced in order to simulate real gas flows with the addition

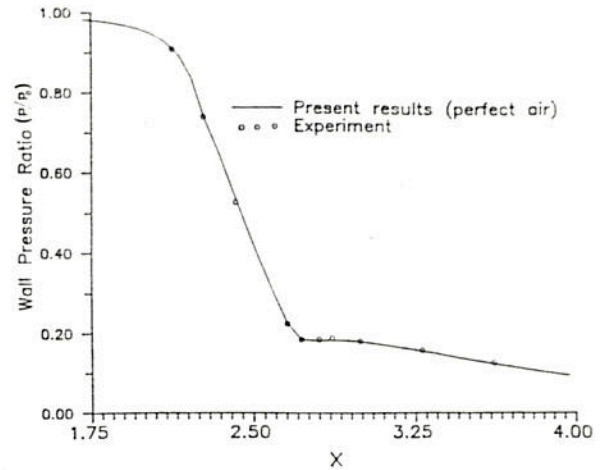


Fig. 2 Wall pressure distribution. Perfect air

of heat. As it seems from the results in the following section of the real gas effects are stronger when heat is added in the gas flow. The source term is defined in terms of an algebraic function $F(x, y)$ as (Merkle and Choi, 1987):

$$q = P \min\{2F^{3/2} - 3F + 1, 1\}$$

where

$$F(x, y) = \frac{(x-x_1)^2 + (z-z_1)^2}{(x_2-x_1)^2 + (z_2-z_1)^2}$$

(x_1, z_1) is the position of the maximum heat addition. The source term is normalized by the coordinate (x_2, z_2) . In the nozzle calculations we consider the position of the maximum heat addition at the axis of the nozzle in the throat region. The parameter P is defined as input parameter. For the present test cases $P = 1 \times 10^7 \text{ W/m}^3$.

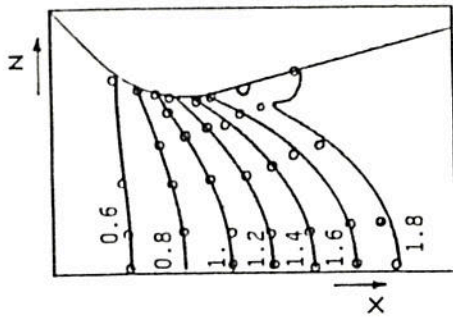
6 Results and Discussion

The computational code in axisymmetric form is used for the simulation of the gas flow into JPL nozzle (Fig. 1(b)). For the present conical nozzle with angles of convergence 45 deg and divergence 15 deg, experiments for the perfect air have been performed by Cuffel et al. (1969). The computational mesh is 50 x 25 grid points. Grid dependence studies (Drikakis, 1991) have shown that finer meshes do not influence the accuracy of the solution in the case of the axisymmetric nozzle flow. The present flow is a steady flow problem. In order to accelerate the convergence to steady state solution, the local time stepping technique is used. The time step is varied in the computational domain by the following relation:

$$\Delta t = \frac{\text{CFL}}{\max(|\lambda_j|)}$$

where λ_j , $j=0, 1, 2$ are the eigenvalues of the equations while CFL is the Courant-Friedrichs-Lewy number. The unfactored implicit procedure allows the use of CFL numbers up to 150. The CPU time on a workstation computer system (main processor consists of the R3000 and R3010 floating point coprocessor with 20-MHz clock frequency) is 30 min for the perfect gas case.

Comparison, in Fig. 2, of the ratio of static pressure to stagnation pressure along the wall with the corresponding experimental results shows the reliability of the numerical method. In Fig. 3 comparison is also presented with the experimental results for the Mach number distributions.



— Present Results
o Experiment

Fig. 3 Iso-Mach lines. Perfect air

Table 1 Summary table of the equations for the test problems

Euler equations written in curvilinear coordinates system and axisymmetric form.

$$U_t + E_\xi + G_\zeta + r\bar{H} = Q$$

Van der Waals EOS

$$p = \frac{RT}{v-b} - \frac{a}{v^2}$$

Benedict-Webb-Rubin EOS ($A_0, B_0, C_0, a, b, c, \gamma, \alpha$ constants)

$$p = \frac{RT}{v} + \left(B_0 RT - A_0 - \frac{C_0}{T^2} \right) \frac{1}{v^2} + (bRT - a) \frac{1}{v^3} + \frac{aa}{v^6} + \frac{c \left(1 + \frac{\gamma}{v^2} \right)}{T^2} \frac{1}{v^3} \exp \left(-\frac{\gamma}{v^2} \right)$$

Coupling of the specific internal energy with the temperature

$$i(T, v) - i(T_0, v_0) = \int_{T_0}^T c_v dT - a \left(\frac{1}{v} - \frac{1}{v_0} \right)$$

As a first test case for the real gas flow in the JPL nozzle, the nitrogen flow has been studied. For the present cases the Van der Waals E.O.S., the Benedict-Webb-Rubin E.O.S. and the constant compressibility factor have been used. The set of equations which are solved for the test problems is summarized in Table 1.

In Figs. 4(a) and 4(b), comparisons of the pressure and the temperature distributions at the wall are presented. In those figures comparisons between "perfect" nitrogen with Van der Waals E.O.S., Benedict-Webb-Rubin (BWR) E.O.S. and nitrogen with a constant compressibility factor $z = pv/RT = 0.3$ are presented. From these figures we observe small differences in the temperature distributions, between the two equations of state (Van der Waals, BWR) and the perfect gas assumption. Greater differences are presented for the constant compressibility factor $z = 0.3$ especially in the temperature distribution. A significant result is that the ideal gas assumption underpredicts the temperature distribution in the supersonic region of nozzle. The influence of real gas on the supersonic region is stronger because of the compressibility effect.

The pressure rise in the throat region just downstream of the tangency is larger for $z = 0.3$. This result is important because the pressure rise influences significantly the boundary layer and the heat transfer in high temperature gas flows. For the above test cases the calculation of the temperature is obtained for each computational volume by an iterative process (Newton-Raphson) and for each time step. This increase the computational cost by a factor of two.

Another test case is the flow of superheated steam through

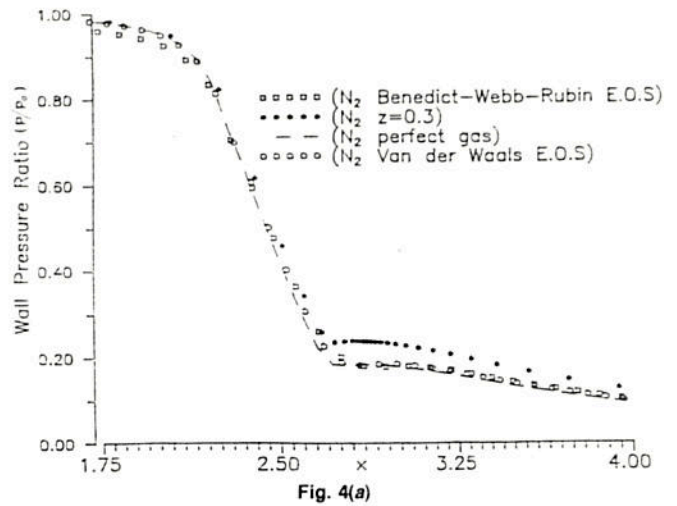


Fig. 4(a)

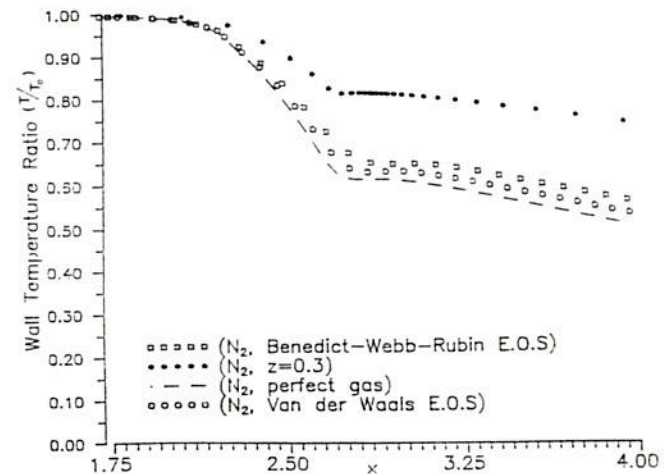


Fig. 4(b)

Fig. 4(a,b) Wall pressure and temperature distributions for nitrogen (N_2)

the JPL nozzle. The real gas behavior of the steam is described by thermodynamic relations (Galitskiy, 1990) which have been incorporated as thermodynamic subroutines in the computational code in order to obtain real gas flow simulation. These subroutines also define the specific heats for constant volume and pressure as function of the p, T :

$$c_v = c_v(p, T), \quad c_p = c_p(p, T)$$

The flow of superheated steam has also been studied with the addition of heat using the source term. In Fig. 5 the pressure distributions for perfect and real steam are shown and the differences are small. In the case of heat addition, not shown here, the pressure rise is larger than the corresponding rise in the case with no heat addition. On the other hand, large differences between steam as perfect gas and steam as real gas are presented in the temperature field (Fig. 6). The influence of real gas effect is stronger in the case of heat addition (Fig. 6). Finally in Fig. 7 differences for perfect and real steam (without heat addition) in the location of the isotherm lines are shown. The real gas effects are significant especially in the divergent region (supersonic) of the nozzle where the compressibility is stronger.

7 Conclusions

[A previous real gas method (Drikakis and Tsangaris, 1991)

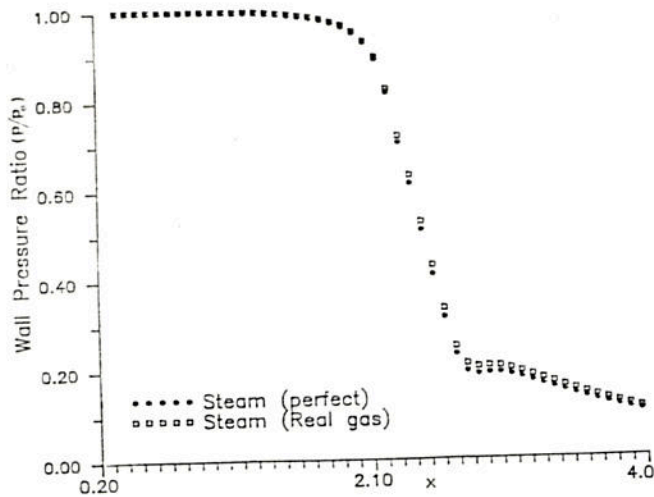


Fig. 5 Wall pressure distributions for superheated steam

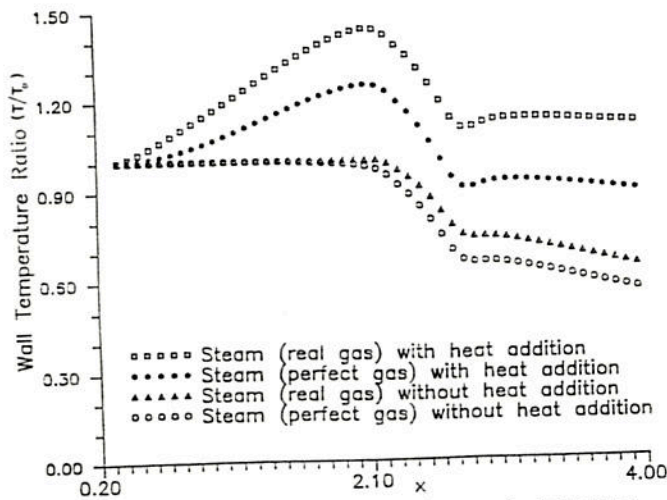


Fig. 6 Wall temperature distributions for superheated steam

is generalized for any P-V-T equation of state. Using the present method it is not necessary to consider the pressure as a function of the density and the specific internal energy. The pressure can be a complex function of the density or the specific volume and the temperature. In this case thermodynamic equations are used in order to correlate the thermodynamic and the flow variables. Numerical simulation of the nitrogen and

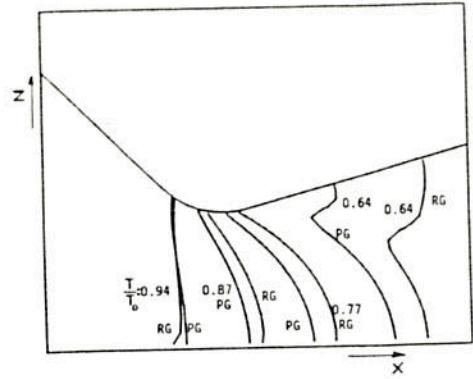


Fig. 7 Iso-temperature lines for superheated steam (PG = perfect gas, RG = real gas)

steam flow in an axisymmetric nozzle shows that the ideal gas assumption underpredicts the temperature distribution along the wall of the nozzle, while there are significant differences between perfect and real gas in the temperature profiles. Differences between perfect and real gas in the pressure distribution are small. On the other hand, in the case of heat addition the influence of the real gas on the temperature distribution is more intense; that means that the reformulation of the computational methods for real gases is necessary for the understanding of the complex gas flows.

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