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The influence of a source term, an example:
chemically reacting hypersonic flow

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Abstract

We show, by way of an example, that the solution of a system of hyperbolic conservation laws exhibits an unexpected behavior if a source term is present. The example is the system of Euler equations for N species in two space dimensions. If the source term is not present and in the initial and inflow conditions a fixed mixture of species is prescribed then the solution basically behaves like the flow of an ideal gas, except that there are additional equations for the different species. However, introducing the chemical reaction terms produces a thin boundary layer, which makes numerical computations of the two-dimensional problem extremely difficult, if not impossible for todays computers. In addition this boundary layer is unphysical. We shall analyse the boundary layer in a one-dimensional calculation along the stagnation point stream line. In M. Fey and R. Jeltsch, in *Proceedings of the 9th GAMM Conference on Numerical Methods in Fluid Dynamics*, a modification of the Van Leer flux vector splitting is presented which is able to indicate the presence of the boundary layer in a two-dimensional calculation.

Key words: chemical boundary layer, geometrical singularities

Subject Classification: 35L65, 65M99, 76K05, 76N15

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1 Introduction

When developing numerical schemes for hyperbolic conservation laws, most authors consider a scalar one-dimensional conservation laws without a source term. New phenomena have to be taken into account when one wants to generalize such methods to systems in several space dimensions. Here we consider an effect which arises from an interaction of the source term with a geometric singularity. We consider hypersonic Euler flow of N chemically reacting species around a blunt body in two space dimensions. We shall indicate that an extreme chemical boundary layer will develop at the stagnation point. However, if the chemical reactions are turned off then no boundary layer develops. In Section 2 we formulate the mathematical problem and report on the fact that todays 'general purpose' numerical schemes with todays computers do not give the correct stagnation point temperature. In Section 3 we consider analytically the steady state flow along the stagnation point stream line if one assumes that the flow is symmetric with respect to this line. This leads to a free boundary value problem for a system of $N + 2$ ordinary differential equations. If one uses N equations for the mass fractions and one for the pressure and velocity along the stagnation point stream line, one can observe nicely the effect of the source term. A heuristic argument is given to show why the boundary layer depends on the geometry of the body and the reaction rates. In Section 4 we give a brief outline of a scheme which is able to at least indicate the existence of a boundary layer in two-dimensional computations.

2 Mathematical Problem

We consider the unsteady Euler equations with N chemical species in two dimensions. The equations have the form

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + \frac{\partial G(U)}{\partial y} = S(U) \tag{2.1}$$

where $U = (\rho_1, ..., \rho_N, \rho u, \rho v, \rho E)^T$. ρ_i is the partial density of the i-th species,

$$\rho = \sum_{i=1}^{N} \rho_i \tag{2.2}$$

is the density of the gas, u and v are the velocities in x- and y-direction. ρE is the total energy per unit volume. The fluxes F(U), G(U) and the source terms are given by

$$F(U) = \begin{pmatrix} \rho_1 u \\ \vdots \\ \rho_N u \\ \rho u^2 + p \\ \rho v u \\ (\rho E + p)u \end{pmatrix}, \quad G(U) = \begin{pmatrix} \rho_1 v \\ \vdots \\ \rho_N v \\ \rho u v \\ \rho v^2 + p \\ (\rho E + p)v \end{pmatrix}, \quad S(U) = \begin{pmatrix} s_1 \\ \vdots \\ s_N \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{2.3}$$

p is the pressure and the s_i are the source terms due to chemical reactions. The chemical source terms have to satisfy

$$\sum_{i=1}^{N} s_i = 0 \qquad (2.4)$$

and depend on the partial densities and the temperature, i. e. $s_i = s_i(\rho_1, ..., \rho_N, T)$, $i = 1, 2, ..., N$. The functions s_i are known functions given by the law of mass action. Since we have the unknowns $\rho_1, ..., \rho_N, u, v, E, p$ and T we need two further equations. One is the equation of state for a mixture of N species

$$p = RT \sum_{i=1}^{N} \frac{\rho_i}{W_i} \qquad (2.5)$$

where R is the universal constant of gas and W_i is the molecular weight of the i-th species. The temperature is related to the energy by the equations

$$a) \;\; E = e(T) + \frac{1}{2}(u^2 + v^2) + \sum_{i=1}^{N} \frac{\rho_i}{\rho} h_i^0 \quad \text{where} \quad b) \;\; e(T) = \frac{1}{\rho} \sum_{i=1}^{N} \rho_i e_i(T) \qquad (2.6)$$

Here $e_i(T)$ is the internal energy of the i-th species, which is a known highly nonlinear function describing, in addition to the usual translational and rotational motion, vibrational excitation and electronic energies. h_i^0 is the known formation enthalpy of the i-th species. (2.1), (2.5) and (2.6) form a system of $N + 5$ equations for the unknowns $\rho_1, ..., \rho_N, u, v, p, E, T$. Once the quantities are known, ρ can be computed from (2.2) and T from (2.6).

Note that we have included the formation enthalpy in our total energy E. This implies that the last component of the source term $S(U)$ in (2.3) is zero, i. e. the energy conservation equation becomes homogeneous.

When computing flow problems with these equations we shall adopt a five species model for the species N, N_2, O, O_2 and NO described by Park [16] and [10]. Geometrically we consider the unsteady flow around a blunt object such as a double ellipse, see test problem 6.2-3 in [8], or a simple circular cylinder. The free-stream values at the inflow are $p_\infty = 2.53 \, Pa$, $\rho_\infty = 4.15 \times 10^{-5} \, kg/m^3$, $T_\infty = 211 \, K$, $M_\infty = 25$, $Y_{N_2,\infty} = 0.79$, $Y_{O_2,\infty} = 0.21$ and $Y_{O,\infty} = Y_{N,\infty} = Y_{NO,\infty} = 0$. Here Y_i always denotes the mass fraction $Y_i = \rho_i/\rho$, $i = 1, 2, ..., N$ of the i-th species and $M := \sqrt{u^2 + v^2}/c_f$ is the Mach number where c_f is the frozen speed of sound given by $c_f^2 := \gamma(T)p/\rho$ with $\gamma(T) := 1 + R/(\rho c_v) \sum_{i=1}^{N} \rho_i/W_i$. $c_v = c_v(T) := \partial e(T)/\partial T$ is the specific heat of the gas mixture. At the body surface one assumes that the velocity is tangential to the body, i. e. $(u, v) \cdot n = 0$ where n is the normal to the body.

Let us consider 'general purpose' numerical schemes to solve this initial boundary value problem. By 'general purpose' we mean a scheme which is more or less easily extendable to a three-dimensional problem, does not use special information of this particular problem and can be used for time accurate calculations. For example in the Antibes workshop in 1990, see [8], out of the six contributions [3], [12], [2], [17], [19] all except for [17] can be considered to be 'general purpose'. There are the following two major problems to be overcome by such a scheme. The first one is due

to the very strong bow shock which may give rise to unphysical values, e. g. negative pressures. If a scheme is explicit, such unphysical values have to be avoided. This can be done for example with a Van Leer flux vector splitting. The second problem is much more serious. If one integrates in time to steady state, the stagnation point temperatures in the contributions in [8] vary between $8455\,K$ and $9653\,K$ for 'general purpose' schemes compared to $5783\,K$ for the specialized method proposed in [17]. Note that the contribution by [12] had an even higher stagnation point temperature. However, using a new low diffusion Van Leer flux vector splitting, LDVL, introduced in [11], this temperature is reduced to approximately $8575\,K$. In the Antibes workshop of 1991 for 'general purpose' schemes, again the stagnation point temperatures vary between $8500\,K$ and $9200\,K$, see [1]. Long time ago one has already observed that the solution of (2.1) – (2.6) has a chemical boundary layer, see [5], [6], [7], [18] and [9]. In the next section we shall demonstrate this phenomena.

3   Analysis along the stagnation point stream line

In order to demonstrate mathematically why 'general purpose' methods have difficulties when computing the stagnation point temperatures we shall consider here the steady state solution in a simple geometric setting. We shall consider the flow around a two-dimensional blunt object which is symmetric with respect to the x-axis. We assume that there exists a steady state solution which is also symmetric with respect to the x-axis. Hence the stagnation point stream line is the x-axis and one has $v(x,0) \equiv 0$ and all unknown variables are even functions in y except v. For $y \equiv 0$ the solutions have to satisfy the conservation of species equations, the momentum equations in x- and y-direction and the conservation of energy equation:

$$(\rho_i u)_x + (\rho_i v)_y = s_i, \quad i = 1, ..., N \tag{3.1}$$
$$(\rho u^2 + p)_x + (\rho u v)_y = 0 \tag{3.2}$$
$$(\rho u v)_x + (\rho v^2 + p)_y = 0 \tag{3.3}$$
$$[(\rho E + p)u]_x + [(\rho E + p)v]_y = 0 \tag{3.4}$$

Due to (2.2) and (2.4) the sum of the N equations in (3.1) gives the conservation of mass

$$(\rho u)_x + (\rho v)_y = 0. \tag{3.5}$$

Introducing the enthalpy $H = E + p/\rho$ in (3.4) and using (3.5) and $v \equiv 0$ yields

$$\rho u H_x = 0. \tag{3.6}$$

If we assume that there is no vacuum, i. e. $\rho > 0$, and that the flow is in positive x-direction except at the stagnation point x_s, i. e. $u(x,0) > 0$ if $x \neq x_s$, we have by (3.6) that $H(x,0) =: H_0 = const$. Even across the bow shock the enthalpy is constant and therefore H_0 can be computed using the free-stream condition:

$$H_0 = \sum_{i=1}^{N} Y_{i,\infty} e_i(T_\infty) + \frac{1}{2}u_\infty^2 + \sum_{i=1}^{N} Y_{i,\infty} h_i^0 + \frac{p_\infty}{\rho_\infty}$$

Hence one can replace the conservation of energy equation (3.4) by the algebraic equation

$$H_0 = \frac{u^2}{2} + \sum_{i=1}^{N} Y_i \left(e_i(T) + h_i^0 + \frac{RT}{W_i} \right) \tag{3.7}$$

which relates the temperature T to u and Y_i, $i = 1, ..., N$ but not to density or pressure. Clearly, since we consider the solution along the stagnation point stream line $y \equiv 0$, the momentum equation in y-direction cannot give us any information. Moreover, to simplify the notation we drop the independent variable y and denote the differentiation with respect to x by a prime. Hence the solution satisfies the conservation of species equations

$$\rho_i' u + \rho_i u' = s_i(\rho_1, ..., \rho_N, T) - \rho_i v_y, \quad i = 1, ..., N \tag{3.8}$$

and the momentum equation in x-direction (3.2) which takes after some manipulation the form

$$\sum_{i=1}^{N} \alpha_i \rho_i' + \rho u u' = 0 \quad \text{where} \quad \alpha_i = (\gamma - 1) \left(H_0 - \frac{u^2}{2} - e_i(T) - h_i^0 \right) + \frac{RT}{W_i}. \tag{3.9}$$

Note that (3.8) and (3.9) represent a system of $N + 1$ ordinary differential equations for the $N + 4$ unknowns $\rho_1, ..., \rho_N, T, \rho, u$ and v_y. Since we have only two additional algebraic equations, namely (2.2) and (3.7), we are missing one equation. It is clear that the system has to be underdetermined since somehow the flow should depend on the geometry of the object around which it has to flow, e. g. the standoff distance of the bow shock will definitely depend on the size of the body. To a certain extend this reflects the fact that in subsonic flow, and that is what we have in front of the stagnation point, information is flowing upstream. Note that in our derivation we have up to now not made any approximation.

Before making this approximation we consider the condition at the bow shock and at the stagnation point. By definition of the coordinate system the bow shock occurs at $x = x_0 = 0$. Using the Rankine-Hugeniot condition, one can compute the conditions behind the shock with subscript zero using the free-stream values with subscript ∞. One finds the following equations:

$$a) \quad Y_{i,0} = Y_{i,\infty}, \quad i = 1, 2, ..., N$$

$$b) \quad u_0 = u_\infty \frac{\rho_\infty}{\rho_0}$$

$$c) \quad p_0 = p_\infty + \rho_\infty u_\infty^2 \left(1 - \frac{\rho_\infty}{\rho_0} \right) \tag{3.10}$$

$$d) \quad e_0 = e_\infty + \left(\frac{p_\infty}{\rho_\infty} - \frac{\rho_\infty}{\rho_0} u_\infty^2 \right) \left(1 - \frac{\rho_\infty}{\rho_0} \right) + \frac{u_\infty^2}{2} \left(1 - \left(\frac{\rho_\infty}{\rho_0} \right)^2 \right)$$

The $Y_{i,0}$ are uniquely determined from (3.10a). (3.10b–d) form a system of three equations for the unknowns u_0, ρ_0, p_0 and e_0. The equation of state (2.5) and (2.6b) provide two additional equations:

$$e) \quad \rho_0 = p_0 \left/ \left(RT_0 \sum_{i=1}^{N} \frac{Y_{0,i}}{W_i} \right) \right. \qquad f) \quad e_0 = \sum_{i=0}^{N} Y_{i,0} e_i(T_0) \tag{3.10}$$

This set of equations can be solved giving initial conditions at $x = 0$ for all unknowns in (3.8), (3.9) except for v_y.

We want to investigate the behavior of the solution of the stagnation point. If there exists a solution to the original problem then at the stagnation point x_s the velocity u is equal to zero, i. e.

$$\lim_{x \to x_s^-} u(x, 0) = 0.$$

We assume that the physical quantities are continuous functions up to the stagnation point, in particular we assume that they remain bounded. However, infinite gradients at the stagnation point are allowed. We assume that the following limits exist and are zero:

$$a) \quad \lim_{x \to x_s^-} \rho_i' u = 0, \quad i = 1, 2, ..., N \qquad\qquad b) \quad \lim_{x \to x_s^-} \rho' u = 0 \qquad\qquad (3.11)$$

Substituting this into the conservation of mass equation (3.5) using $v \equiv 0$ gives

$$\lim_{x \to x_s^-} (\rho u' + \rho v_y) = 0. \qquad\qquad (3.12)$$

Using (3.11b), (3.12) and the symmetry in the momentum equation (3.2) gives $\lim_{x \to x_s^-} p' = 0$. We see that u and p have rather smooth behavior near the stagnation point. If there is no vacuum at the stagnation point, i. e. $\rho(x_s, 0) > 0$, then using (3.12) and (3.11a) in (3.8) implies

$$\lim_{x \to x_s^-} s_i(\rho_1, ..., \rho_N, T) = 0, \quad i = 1, 2, ..., N. \qquad\qquad (3.13)$$

Hence we have chemical equilibrium at the stagnation point.

Observe that if we assume that $v_y(x)$ is known, one can solve the system of ordinary differential equations (3.8), (3.9) using the initial conditions at $x = 0$ until u becomes 0. This gives the stagnation point x_s which is also the standoff distance. To do this we have made experiments with $v_y = const$. The results are given in Fig. $1 - 4$. One observes that for large values of v_y one obtains a boundary layer in the density, temperature and mass fraction of nitrogen atoms. The boundary layer becomes more pronounced as v_y increases, i. e. the smaller the body becomes. If the body is large, i. e. $v_y = 100$, no boundary layer can be observed. Note that the code DASSL [4] which we have used stops short of the point x where u becomes zero due to the steep gradient.

To analyse this boundary layer analytically let us rewrite the system (3.8), (3.9) as

$$A(y(x))\dot{y}(x) = b(y(x)), \quad x \in [0, x_s) \qquad\qquad (3.14)$$

with

$$A = \begin{pmatrix} u & & & \rho_1 \\ & \ddots & & \vdots \\ & & u & \rho_N \\ \alpha_1 & \cdots & \alpha_N & \rho u \end{pmatrix}, \quad b = \begin{pmatrix} s_1(\rho_1, ..., \rho_N, T) - \rho_1 v_y \\ \vdots \\ s_N(\rho_1, ..., \rho_N, T) - \rho_N v_y \\ 0 \end{pmatrix}, \quad y = \begin{pmatrix} \rho_1 \\ \vdots \\ \rho_N \\ u \end{pmatrix}.$$

The quantities ρ and T are given by (2.2) and (3.7). One easily finds, see [15], [14], that

$$\det A = -u^{N-1}\rho c_f^2 \left(1 - M^2\right).$$

Hence if $N > 1$ then A becomes singular in a vacuum, which is not of interest, or if $u = 0$. Thus, at the stagnation point A becomes singular, in fact the rank drops from $N + 1$ to 2. To find the solution at the stagnation point we use two smooth functions, the pressure $p_s = \lim\limits_{x \to x_s^-} p$ and the velocity $u_s = \lim\limits_{x \to x_s^-} u = 0$.

One can now obtain the other variables $Y_1, ..., Y_N, \rho$ and T using the fact of equilibrium chemistry (3.13), constant enthalpy (3.7) and the equation of state (2.5). To do this observe that some of the equations in (3.13) are linearly dependent since one has $m \leq N$ kind of atoms which are conserved. Using the equations of conservation of these atoms, one can eliminate m of the unknowns Y_i, w. l. o. g. one could eliminate $Y_1, ..., Y_m$. Hence (3.13) reduces to

$$s_i(Y_{m+1}, ..., Y_N, \rho, T) = 0, \quad i = m+1, ..., N$$

After eliminating $Y_1, ..., Y_m$ from the equation of state and (3.7) we obtain the two additional equations. Observe that this system of equations does depend on the geometry of the body only through the pressure p. The pressure p is obtained from the integration of (3.14) and thus depends on v_y. Hence all thermodynamic variables at the stagnation point depend on the geometry of the body. To illustrate this dependence we have solved this initial value problem (3.14) for the five species model and the initial conditions given above under the assumption that $v_y = const.$, see Table 1.

In order to show that the chemical boundary layer is due to the chemistry source term we rewrite the equations (3.14) in the variables Y_i. The equivalent system has the form

$$
\begin{aligned}
a) \quad & Y_i' = \frac{1}{u\rho} s_i(Y_1, ..., Y_N, \rho, u), \quad i = 1, 2, ..., N \\
b) \quad & u\rho' + \rho u' = -\rho v_y \\
c) \quad & c_f^2 \rho' + \rho u u' = -\frac{1}{u} \sum_{i=1}^{N} \alpha_i s_i(Y_1, ..., Y_N, \rho, u)
\end{aligned}
\tag{3.15}
$$

for the unknowns $Y_1, ..., Y_N, \rho, u$. From this one sees easily that if the source terms are identically zero then by (3.15a) the mass fractions are constant, i. e. one has a flow of a nonreactive mixture of gases. Then (3.15b) and (3.15c) are the usual equations one obtains along the stagnation point line of an ideal gas flow. Hence there is no boundary layer.

Since p and u are the variables which have a smooth limit as x tends to the stagnation point one should see the singular behavior of the equations better if we replace the dependent variable ρ by p. After simple manipulations one obtains

$$
\begin{aligned}
a) \quad & Y_i' = \frac{1}{u\rho} s_i(Y_1, ..., Y_N, p, u), \quad i = 1, 2, ..., N \\
b) \quad & p' + \rho u u' = 0 \\
c) \quad & (1 - M^2)u' = -v_y + \frac{1}{\rho c_f^2} \sum_{i=1}^{N} \alpha_i s_i(Y_1, ..., Y_N, p, u)
\end{aligned}
$$

where $M = u/c_f$ along the stagnation point line. Here one needs the algebraic equation (3.7) and the equation of the state (2.5). Again one sees easily that there is no boundary layer if there is no source term present.

Let us briefly get a rough idea of the boundary layer. Assume that in (3.15) the conservation of atoms has been used to eliminate m of these mass fractions. Moreover we use the dependence on the smooth functions u and p. Hence (3.15a) reduces to $Y' = S(Y, u, p)/(u\rho)$ where $Y = (Y_{m+1}, ..., Y_N)^T$. At the stagnation point we have equilibrium chemistry. Hence we can assume an expansion of the form

$$S(Y, u, p) = J(Y, u, p)(Y - Y^*) + O(||Y - Y^*||^2). \qquad (3.16)$$

Let us further assume that there exists a regular matrix T independent of Y, u, p such that $TJT^{-1} = \Lambda$ is a real diagonal matrix. If we omit the higher order terms in (3.16), we obtain for the new variable $Z = T(Y - Y^*)$ a system of $N - m$ independent ordinary differential equations

$$Z' = \frac{1}{u\rho}\Lambda(u, p)Z, \quad Z(x_s) = 0.$$

Expanding the solution around x_s and using $u = -v_y(x_s - x)$ gives for each component z_i

$$z_i(x) = c_s(x_s - x)^{-\frac{\lambda_i}{v_{ys}\rho_s}} \qquad (3.17)$$

where λ_i is the i-th eigenvalue of J, ρ_s is the density at the stagnation point and v_{ys} is $v_y(x_s)$. Observe that the eigenvalues λ_i are negative. One sees that there is a boundary layer if there is one eigenvalue λ_i with $-\lambda_i < v_{ys}\rho_s$. Moreover, it becomes more extreme if v_{ys} is increasing.

If the reactions become infinitely fast, i. e. $-\lambda_i$ tends to infinity, then one does not have a boundary layer and in fact one has a flow with equilibrium chemistry. One knows from the results in the two Antibes workshops that todays schemes have no problem computing equilibrium Euler flow, i. e. one obtains the correct stagnation point temperature. In order to set this last derivation in the proper perspective let us briefly discuss a particular example. In Fig. 5 we plot λ_i/ρ along the stagnation point stream line in the case of a circular body with the five species chemistry model described above. Since one has conservation of the total number of the N and O atoms two eigenvalues are identically zero. Directly behind the shock two eigenvalues are complex and we have indicated only $|\lambda_i|/\rho$. Further downstream this pair of conjugate complex eigenvalues becomes two real eigenvalues and λ_i/ρ is approximately $-1.03\,\mu sec^{-1}$ and $-0.33\,\mu sec^{-1}$ at the stagnation point. Since $v_y \sim 0.0327\,\mu sec^{-1}$, these two eigenvalues do not give rise to a boundary layer. However, the third eigenvalue λ_3 does. If we use the value of $\lambda_3/\rho \sim 0.01\,\mu sec^{-1}$ which occurs just before the stagnation point, we obtain an exponent of 0.3 in (3.17). Note that in 2D calculations we get estimates of approximately 0.4 for this exponent. However from Fig. 5 we see that the eigenvalue becomes zero at the stagnation point, a fact which contradicts our assumption. Hence one has to improve the above analysis. There are indications that the singularity is stronger than of the type $(x_s - x)^\alpha$. Perhaps it is of the form $c/\ln[d(x_s - x)]$, see [15], [14]. Without going into more details it is clear that the slow reactions are causing the

chemical boundary layer and that this fact will be even more pronounced if the corresponding eigenvalue goes to zero.

Let us briefly relate the present analysis to earlier investigations. Conti [6] and Vinokur [18] give good surveys on earlier work on analysing chemical boundary layers. Conti uses in [5] and in more detail in [6] the method of successive truncations. The idea is that one expands unknown functions with respect to powers of $sin\theta$ and $cos\theta$, where θ is the angle in polar coordinates. This leads to a sequence of systems of ordinary differential equations. However, each system requires knowledge of at least one unknown which originates from the next system. This is similar to our v_y function. While in our analysis v_y is taken from a 2D computation and incorporates the geometry of the body as the needed additional function, Conti [6] uses the bow shock radius r_s as a geometrical parameter and truncates the expansion of the pressure after one term. To get more accurate results one solves successively several of these systems of ordinary differential equations. In Vinokur [18] the chemical boundary layers are shown to exist using a local analysis at the stagnation point similar to the derivation we proposed to obtain the necessary condition $-\lambda_i < v_{ys}\rho_s$ for existence of a boundary layer. The basic behavior of the boundary layer given by Vinokur is $(x_s - x)^\alpha$. We have mentioned above that this cannot be correct if an eigenvalue goes to zero. Moreover it seems that our method to compute the standoff distance x_s using v_y is new. Finally we want to mention that in [9] the existence of a possible chemical boundary is pointed out but the assumption of incompressibility at the stagnation point seems to be contrary to our results, see Fig. 1.

4   2D - computations and the low diffusion Van Leer flux vector splitting

We briefly explain the overall scheme for the two-dimensional numerical solution of (2.1). We use an operator splitting, i. e. alternatively one solves the system of ordinary differential equations

$$\frac{\partial U}{\partial t} = S(U) \tag{4.1}$$

and the system of $N + 3$ partial differential equations

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + \frac{\partial G(U)}{\partial y} = 0. \tag{4.2}$$

From (2.3) we see that the last three equations of (4.1) are homogeneous. Moreover, using (2.2) and (2.4) the sum of the first N equations in (4.1) gives $\partial\rho/\partial t = 0$. Hence, when solving (4.1) we can assume that ρ, u, v and E are constant. Thus, in this chemistry step one has to solve only a subsystem of (4.1) consisting of the first N equations. Of course, for the s_i one has to know the temperature T but this can be computed from (2.6). Since in our examples the eigenvalues of the Jacobian of the right hand side are moderate only compared to the integration stepsize there is no difficulty in integrating this system. In fact one could use an explicit Euler scheme.

In the flow step one can solve (4.2) using a dimensional splitting and the Van Leer flux vector splitting in the modification for real gas given by Yee [20]. This

standard Van Leer, SVL, has too much numerical viscosity and does therefore not resolve the boundary layer. This can clearly be seen from Fig. 6. Instead we use a modification called low diffusion Van Leer, LDVL. The basic idea is to reduce the number of contact discontinuities by summing up the first N equations. If the formation enthalpy is removed from the energy equation, this results in the usual Euler equations. These are solved by the standard Van Leer. To update the mass fractions we model the contact discontinuities exactly by complete upwinding according to the total density flux. However, to add the changes of the energy due to formation enthalpy we use these fluxes for the partial densities constructed according to the standard Van Leer scheme. In [11] it is shown that this new low diffusion Van Leer scheme is consistent and has less numerical viscosity in areas of subsonic flow, hence the chemical boundary layer is better resolved, see Fig. 6. For comparison we show in Fig. 6 also the numerical solution, BVP, of the boundary value problem (3.8), (3.9) along the stagnation point line with (3.10), condition $u(x_s) = 0$ and $v_y = const. = 32\,437\,sec^{-1}$.

5 Conclusions

In our analysis we have found a boundary layer at the stagnation point due to the chemical source term. It turns out that the boundary layer is so thin that it is not physical. This means that the Euler equations with chemistry are not modeling physics correctly. However, numerical 'general purpose' schemes should be able to give the correct mathematical solution in order to show the incorrectness of the model. We observe that all 'general purpose' schemes for solving the unsteady Euler flow with chemical reactions give a stagnation point temperature which is wrong by more than $2700\,K$, i. e. more than 45 %. If one shows the solution along the stagnation point stream line, which is rarely done, one does, for example with standard Van Leer, not observe the boundary layer at all. To compare the quality of numerical discretizations one should relate the results to the cell size at the stagnation point. To get better numerical results one should perhaps formulate different boundary condition. In [13] we used the boundary layer behavior discussed here to get better boundary conditions. This leads to a decrease of the stagnation point temperature by approximately $300\,K$ but does still not solve this problem satisfactory.

We observed that if the source terms are turned off then the boundary layer vanishes. This indicates that it is not enough to analyse schemes only for homogeneous conservation laws. Instead one also has to consider source terms. In this conference this has been done for singular perturbed problems by Engquist and LeVeque, see this book. However, in the present example the situation is worse in the sense that the perturbation parameter depends on the solution and becomes zero at least in one point of the domain.

References

[1] *Book of Abstracts of the Workshop on Hyperbolic Flows for Reenry Problems, Part II, April 15 − 19, 1991*, volume 4, 1991.

[2] S. Borelli and M. Pandolfi. A contribution to the prediction of hypersonic non-equilibrium flows. In [8], 1992.

[3] N. Botta, M.-C. Ciccoli, J.-A. Désidéri, L. Fezoui, N. Glinsky, E. Hettena, and C. Olivier. Reactive flow computation by upwind finite elements. In [8], 1992.

[4] K. E. Brenan, S. L. Campbell, and L. R. Petzold. *Numerical Solution of Initial Value Problems in Differential Algebraic Equations*. North Holland, 1989.

[5] Raul J. Conti. Stagnation equilibrium layer in nonequilibrium blunt body flow. *AIAA J.*, 2:2044–2046, 1964.

[6] Raul J. Conti. A theoretical study of non-equilibrium blunt body flow. *J. Fluid Mech.*, 24(1):65–88, 1966.

[7] Raul J. Conti and Milton Van Dyke. Reacting flow as an example of a boundary layer under singular external conditions. *J. Fluid. Mech.*, 38(3):513–535, 1969.

[8] J.-A. Désidéri, R. Glowinski, and J. Périaux, editors. *Hypersonic Flows for Reentry Problems, Proceedings of the Workshop held in Antibes, France, 22-25 January, 1990*, volume 2. Springer Verlag, 1992.

[9] Jean-Antoine Désidéri. Some comments on the numerical computations of reacting flows over the double-ellipse (double ellipsoid). In [8], volume 2, 1992.

[10] Michael Fey, Helmut Jarausch, Rolf Jeltsch, and Peter Karmann. On the Interaction of Euler and ODE Solver when Computing Reactive Gas Flow. In J. E. Flaherty, P. J. Paslow, M. S. Shephard, and J. D. Vasilakis, editors, *Proceedings of the Workshop on Adaptive Computational Methods for Partial Differential Equations*. SIAM, 1988.

[11] Michael Fey and Rolf Jeltsch. Influence of numerical diffusion in high temperature flow. In I. L. Rhyming, editor, *Proceedings of the 9th GAMM Conference on Numerical Methods in Fluid Dynamics, Notes on Numerical Fluid Mechanics*. Vieweg Verlag, 1992.

[12] Michael Fey, Rolf Jeltsch, and Peter Karmann. Numerical analysis of chemically reacting inviscid flow in 2-d. In [8], 1992.

[13] Michael Fey, Rolf Jeltsch, and Peter Karmann. Special aspects of reacting inviscid blunt body flow. In J.-A. Désidéri, R. Glowinski, and J. Périaux, editors, *Hypersonic Flows for Reentry Problems, Proceedings of the Workshop held in Antibes, France, April, 1991*, volume 3. Springer Verlag, to appear.

[14] Michael Fey, Rolf Jeltsch, and Siegfried Müller. Stagnation point computations of non-equilibrium inviscid blunt body flow. *Computers & Fluids*. to appear.

[15] Michael Fey, Rolf Jeltsch, and Siegfried Müller. *Stagnation Point Analysis*. Research Report No. 92-03, Seminar für Angewandte Mathematik, ETH Zürich, 1992.

[16] Chul Park. On convergence of computation of chemically reacting flows. Technical Report 085-0247, AIAA, 1985.

[17] F. Sabetta, B. Favini, G. Moretti, M. Onofri, and M. Valorani. Reactive and inert inviscid flow solutions by quasi-linear formulations and shock fitting. In [8], 1992.

[18] Marcel Vinokur. On stagnation point conditions in non-equilibrium inviscid blunt body flows. *J. Fluid. Mech.*, 30:49–75, 1970.

[19] J. B. Vos and C. M. Bergmann. Inviscid hypersonic flow simulations using an explicit scheme. In [8], 1992.

[20] Helen Yee. Upwind and symmetric shock-capturing schemes. Technical Report TM 89464, NASA, 1987.

| Table 1: Solution at the stagnation point with chemical equilibrium					
$v_y =$	100	1000	10000	32437	100000
Y_N	4.62112E–01	4.62173E–01	4.62272E–01	4.62344E–01	4.62414E–01
Y_{N_2}	3.27454E–01	3.27394E–01	3.27296E–01	3.27225E–01	3.27156E–01
Y_O	2.09498E–01	2.09499E–01	2.09501E–01	2.09502E–01	2.09503E–01
Y_{O_2}	5.67648E–06	5.66061E–06	5.63479E–06	5.61623E–06	5.59804E–06
Y_{NO}	9.30253E–04	9.28473E–04	9.25572E–04	9.23485E–04	9.21436E–04
ρ	7.58529E–04	7.54662E–04	7.48387E–04	7.43892E–04	7.39496E–04
p	2.10363E+03	2.09248E+03	2.07439E+03	2.06144E+03	2.04877E+03
T	5.76834E+03	5.76695E+03	5.76468E+03	5.76305E+03	5.76144E+03
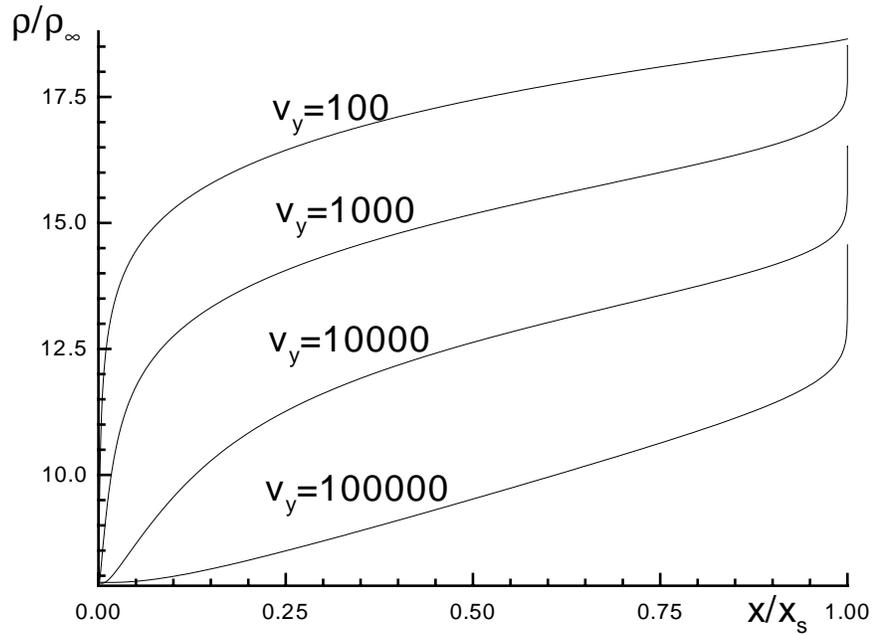
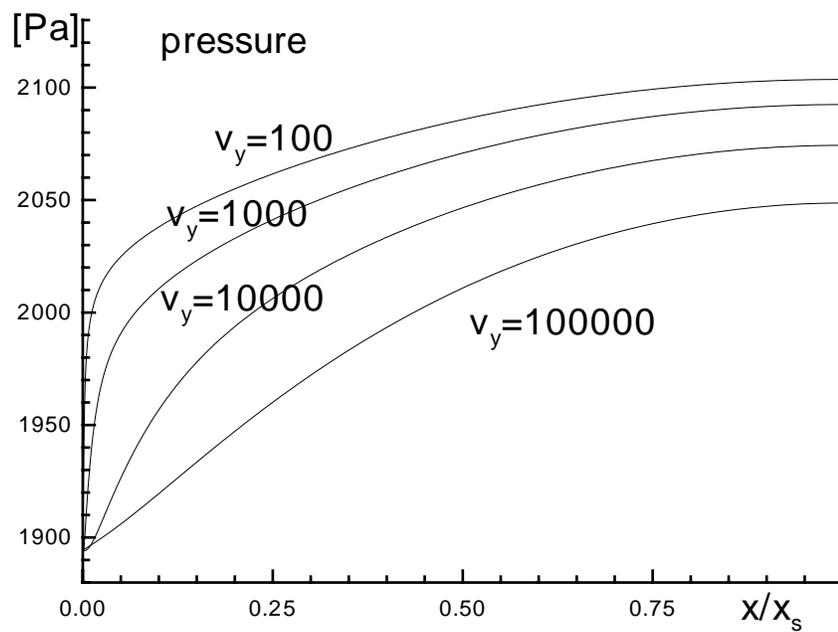Figure 1: Density along the stagnation point streamline.

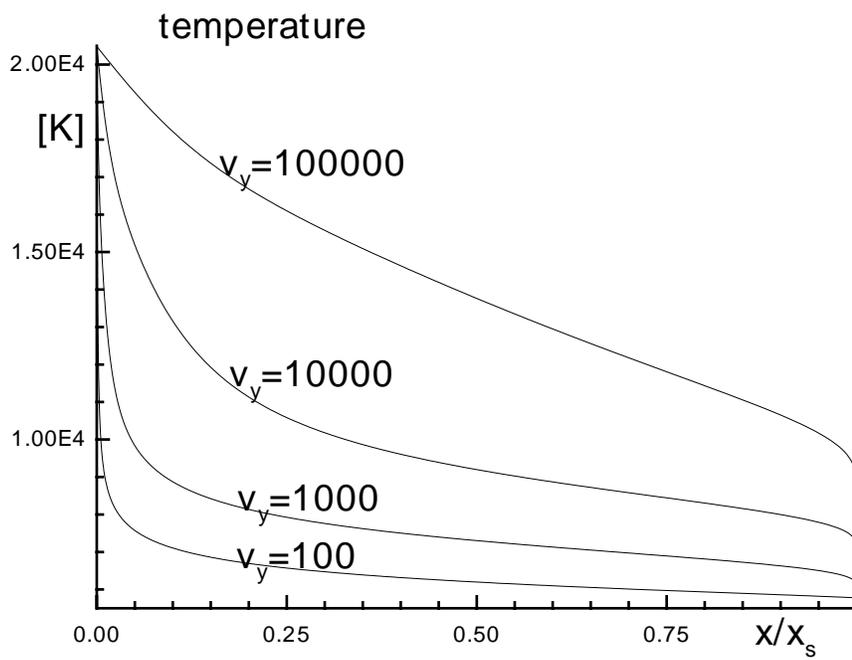Figure 2: Pressure along the stagnation point streamline.

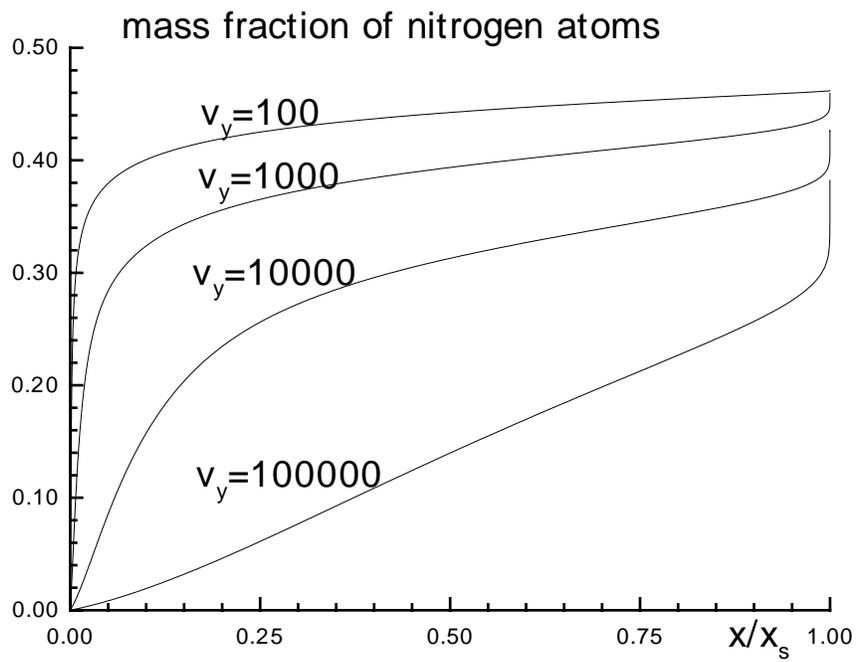Figure 3: Temperature along the stagnation point streamline.

Figure 4: Mass fraction of nitrogen atoms along the stagnation point streamline.
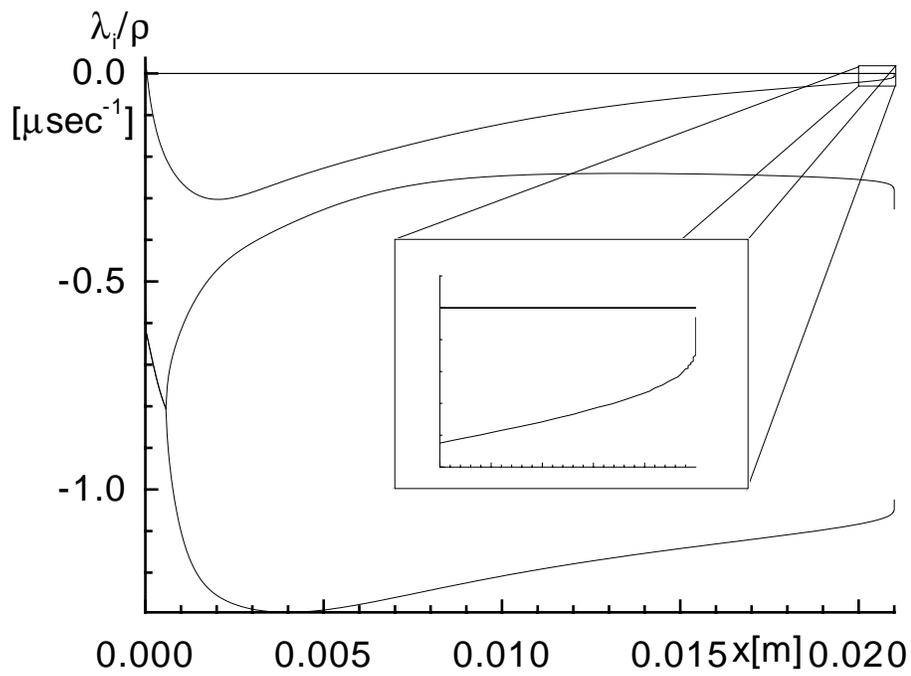
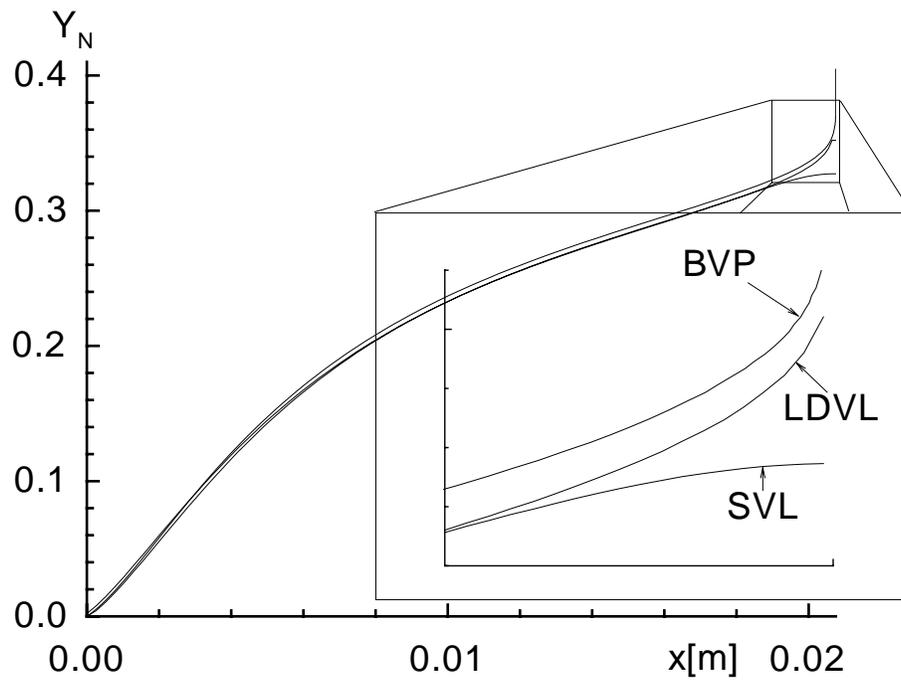Figure 5: λ_i/ρ along the stagnation point streamline.

Figure 6: Comparrison between the solution of the boundary value problem (BVP) and 2-D calculations (SVL), (LDVL).

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