NUMERICAL MODEL OF DIFFUSION OF SPECIES IN AN INTERNAL COMBUSTION ENGINE

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ABSTRACT

This thesis is a contribution to solution of the problem of numerical modelling of physical processes in an internal combustion engine. The model of mass transport was precised with the mechanism of molecular diffusion. There are some numerical problems like the estimation of the stability condition for the time step or the reduction of numerical diffusion arising from the upwind method used to approximate the advective term. These problems were successfully tested for one-dimensional mass transport with uniform fluid flow.

1 INTRODUCTION

The main objective of the model of processes in an internal combustion engine is to predict the production of nitrogen oxides during the work of an engine by a complete simulation of relevant physical and chemical processes. Whole model is divided into three main problems: flow, mass and energy transport, and chemical reactions. They are solved as isochoric processes and then adiabatic expansion (or compression) is applied to all of the resulting quantities because the studied volume is changing in time.

This thesis precised the original advective mass transport model with the mechanism of molecular diffusion. There are some problems which should be solved for successful use of the derived numerical model of diffusion based on the finite volume method. The explicit method for time discretization was used, therefore the stability condition for the time step is necessary to be evaluated. It was successfully solved for incompressible fluid flow in the meantime. The next problem is the phenomenon of numerical diffusion arising from the upwind method used to approximate the advective term of the transport equation. It can be reduced by a convenient reduction of diffusion coefficients.

The precised model was successfully tested on 1D problems with uniform fluid flow. Two 2D tests were made, too. They show quantitatively good results.

2 PHYSICAL MODEL

2.1 GOVERNING EQUATION

The model is governed by the equation of mass conservation which can be written for a control volume $V \subset \Omega$ (here Ω respresents the inner volume of a cylinder) and the gas component ℓ ($1 \leq \ell \leq n_\ell$) as

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho c_\ell \mathrm{d}\mathbf{x} + \int_{\partial V} (\rho c_\ell \mathbf{v} + \mathbf{j}_\ell)\cdot \mathbf{n}\mathrm{d}S = \int_V q_\ell \mathrm{d}\mathbf{x}, \tag{1}$$

where ρ is the density of a gas mixture, c_ℓ is the mass fraction of the ℓ-th component, $\mathbf{v}$ is the velocity vector, $\mathbf{j}_\ell$ is the diffusion flux, q_ℓ is the density of sources and sinks of the component and $\mathbf{n}$ denotes the outer normal vector to the boundary ∂V of the control volume V.

The diffusion flux is approximated by the equation similar to the Fick's law of diffusion

$$\mathbf{j}_\ell = -\rho \mathcal{D}_\ell \nabla c_\ell, \tag{2}$$

where $\mathcal{D}_\ell$ is the effective diffusion coefficient of the ℓ-th component.

2.2 BOUNDARY AND INITIAL CONDITIONS

The open valve of an engine is described by the Dirichlet boundary condition

$$\begin{aligned} \rho &= \rho_D \\ c_\ell &= c_{\ell,D} \end{aligned} \qquad \text{on } \Gamma_D, \tag{3}$$

where Γ_D is the part of the boundary $\partial\Omega$. On the remaining part $\Gamma_N = \partial\Omega \setminus \Gamma_D$, the homogeneous Neumann boundary condition $v_n = 0$, $(\nabla c_\ell)_n = 0$ is assigned (index n denotes the projection to the outer normal of the boundary). That represents the impermeability of the walls.

The initial conditions are chosen such that the density and mass fractions at the beginning are constant in whole volume of Ω, i. e.

$$\begin{aligned} \rho &= \rho^0 \\ c_\ell &= c_\ell^0 \end{aligned} \qquad \text{at } t = 0. \tag{4}$$

3 NUMERICAL MODEL

At first, the discretization of the volume Ω must be done. It is approximated by the mesh of control volumes $\mathcal{T}$, the set of their sides $\mathcal{E}$ and the set of points $\mathcal{P}$, where every point $x_K \in \mathcal{P}$ has assigned exactly one control volume $K \in \mathcal{T}$. This mesh must fulfil the properties of admissible meshes (see definition in [2]). Let's denote: $m(K)$ and $m(\sigma)$ the 3D and 2D Lebesgue measure of $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}$, respectively; h the maximum of diameters of all control volumes. Furthermore for each control volume $K \in \mathcal{T}$ we denote: $\mathcal{N}(K)$ the set of adjacent control volumes of K, $\mathcal{E}_K$ the set of sides common to the volume

K and volumes $L \in \mathcal{N}(K)$ (for adjacent control volumes K and L let $\sigma = K|L$ means that σ is the common side of K and L); $d_{K,\sigma}$ is the distance between the point x_K and the side σ; $d_{K|L}$ is the distance between points x_K and x_L for all (adjacent) pairs $(K,L) \in \mathcal{T}^2$. At last we denote $\tau_{K|L} = m(K|L)/d_{K|L}$ and $\tau_{K,\sigma} = m(\sigma)/d_{K,\sigma}$.

The time discretization is realized by the ascending sequence of time values t_n, $n \in \mathbb{N}_0$, $t_0 = 0$ with the difference (time step) $\Delta t_n = t_{n+1} - t_n$.

In whole model, the same mesh is used by all submodels (for the model of fluid flow solved by the finite element method, for the model of mass and energy transport, and the model of chemical reactions). This mesh is constructed from trilateral prismatic elements (control volumes) and suits conditions of admissible meshes.

3.1 NUMERICAL SCHEME

The numerical scheme is based on the finite volume method which is derived from the equation (1). With the explicit method used for time, the resulting discrete equation may be written for each control volume K from $\mathcal{T}$ as

$$m(K)\frac{\rho_{\ell,K}^{n+1} - \rho_{\ell,K}^{n}}{\Delta t_n} + \sum_{\sigma \in \mathcal{E}_K} F_{\ell,K,\sigma}^{n} + \sum_{\sigma \in \mathcal{E}_K} f_{K,\sigma}^{n} c_{\ell,\sigma,+}^{n} = m(K) q_K^n c_{\ell,K,+}^{n}, \tag{5}$$

where $\rho_{\ell,K}^{n} = \rho_K^n c_{\ell,K}^{n}$. The lower index K denotes the quantity in the point x_K of the control volume K and the upper index n means its value in the time t_n.

The other symbols have the following meaning. The mass fraction $c_{\ell,\sigma,+}^{n}$ is chosen by the upwind method (analogical approximation is applied to the fraction $c_{\ell,K,+}^{n}$), i. e.

$$c_{\ell,\sigma,+}^{n} = \begin{cases} c_{\ell,K}^{n} & \text{for } f_{K,\sigma}^{n} \geq 0, \\ c_{\ell,L}^{n} & \text{for } f_{K,\sigma}^{n} < 0, \text{ where } \sigma = K|L, \end{cases} \qquad c_{\ell,K,+}^{n} = \begin{cases} c_{\ell,K,q}^{n} & \text{for } q_K^n \geq 0, \\ c_{\ell,K}^{n} & \text{for } q_K^n < 0. \end{cases} \tag{6}$$

The mass fraction $c_{\ell,K,q}^{n}$ is given by the composition of a mixture at the source of mass. The resulting variables of the model are expressed as

$$\rho_K^{n+1} = \sum_{\ell=1}^{n_\ell} \rho_{\ell,K}^{n+1}, \qquad\qquad c_{\ell,K}^{n+1} = \frac{\rho_{\ell,K}^{n+1}}{\rho_K^{n+1}}. \tag{7}$$

The diffusion flux $F_{\ell,K,\sigma}^{n}$ is computed by the four point difference method. All of these approximations are conservative which implies a conservative character of the numerical scheme.

3.2 STABILITY

Because of the use of the explicit method for time, the stability analysis must be performed. The stability condition was derived only for incompressible flow with the constant density ρ. It may be written in the form

$$\Delta t_n \leq \frac{\rho m(K)}{\sum\limits_{\sigma \in \mathcal{E}_{K,+}^{n}} f_{K,\sigma}^{n} + \rho \sum\limits_{L \in \mathcal{N}(K)} \tau_{K|L} \mathcal{D}_{\ell,K|L}^{n} + \rho \sum\limits_{\sigma \in \mathcal{E}_{K,\Gamma_D}} \tau_{K,\sigma} \mathcal{D}_{\ell,\sigma}^{n}}, \quad \forall K \in \mathcal{T}. \tag{8}$$

Here $\mathcal{E}^n_{K,+}$ represents the set of sides with nonnegative sing of the advective flux $f^n_{K,\sigma}$, $\mathcal{E}_{K,\Gamma_D}$ is the set of sides from $\mathcal{E}_K$ which hold $\sigma \subset \Gamma_D$, The symbol $\mathcal{D}^n_{\ell,\sigma}$ represents the diffusion coefficient on the side σ. It can be seen that this condition sets the upper bound for the time step proportionally to the second order of the spatial discretization parameter h; in case of pure advection transport the stability condition is the first order of h.

4 TESTS

The implemented model was tested on simple meshes. The 1D test problem is described by the equation

$$\frac{\partial c}{\partial t}(x,t) + v\frac{\partial c}{\partial x}(x,t) - \mathcal{D}\frac{\partial^2 c}{\partial x^2}(x,t) = 0,\ c(0,t) = 1,\ c(x,0) = 0,\ (x,t) \in (0,\infty) \times (0,T), \quad (9)$$

where $\mathcal{D}$ and v are positive numbers. The numerical solution can be compared with the analytic solution

$$c(x,t) = \frac{1}{2}\left[\exp\left(\frac{vx}{\mathcal{D}}\right)\texttt{erfc}\left(\frac{x+vt}{2\sqrt{\mathcal{D}t}}\right) + \texttt{erfc}\left(\frac{x-vt}{2\sqrt{\mathcal{D}t}}\right)\right]. \quad (10)$$

For high values of $vx/\mathcal{D}$ the first term may be neglected (especially for numerical evaluation).

If the control volumes are numbered by the sequence of indices $0 \leq i \leq N$ then the numerical scheme can be rewritten as

$$c_i^{n+1} = c_i^n - v\frac{\Delta t}{h}(c_i^n - c_{i-1}^n) + \mathcal{D}\frac{\Delta t}{h^2}(c_{i-1}^n - 2c_i^n + c_{i+1}^n) \quad (11)$$

It can be shown that the estimate of the numerical diffusion coefficient has the form

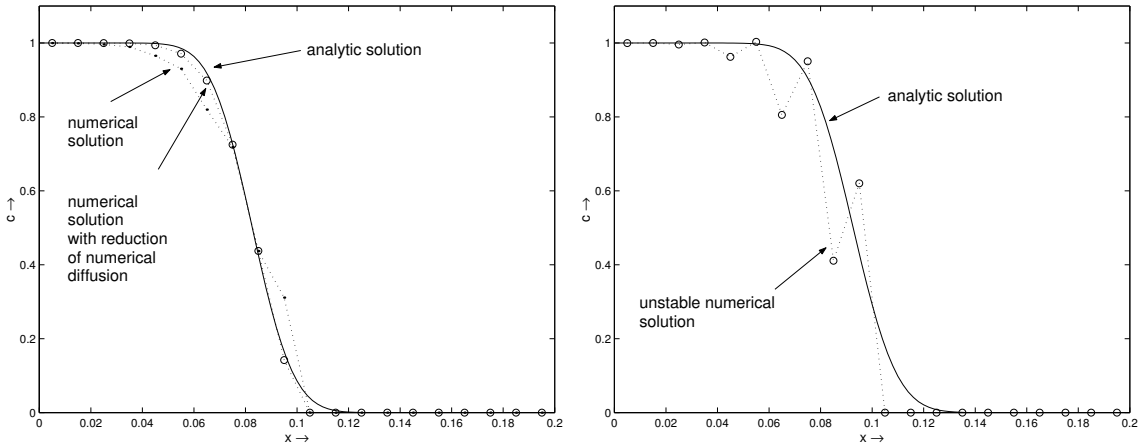
$$\mathcal{D}_{num} = \frac{1}{2}vh\left(1 - v\frac{\Delta t}{h}\right). \quad (12)$$

The simplest way to reduce the magnitude of numerical diffusion is to subtract this artificial coefficient from the "physical" diffusion coefficient $\mathcal{D}$. Naturally, the condition for the time step Δt must be achieved in order to ensure non-negativity of the reduced coefficient together with the stability condition. It can be rewritten in the form

$$\tilde{\mathcal{D}} = \mathcal{D} - \mathcal{D}_{num} \geq 0, \qquad \Delta t \leq \frac{h^2}{hv + 2\mathcal{D}}. \quad (13)$$

Analysis of both of these conditions shows that for rougher meshes the time step must be set close to the stability boundary to keep the reduced coefficient nonnegative but for fine meshes this problem does not occur.

Numerical tests of the problem (9) were made for various input parameters (including tests of pure diffusion and advection). All of their results was accorded to our theoretical prepositions (see fig. 1 for representative examples).



(a) (b)

Figure 1: Numerical solutions of two tests with the analytic solution of advection-diffusion equation): (a) stable solutions with and without correction of numerical diffusion, (b) unstable solution

5 CONCLUSIONS

There was the diffusive-advective model of mass transport formulated and implemented. The stability analysis was performed for incompressible fluid flow and successfully tested for one and two-dimensional problems. On these problems, the reduction of numerical diffusion was analyzed and tested (quantitatively for 1D, qualitatively for 2D tests). The calibration cannot be done at present because valid data for comparison are not currently available.

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REFERENCES

[1] R. B. Bird, W. E. Stewart, E. N. Lightfoot: Transport phenomena. John Wiley & Sons, Inc., New York, 2002.

[2] R. Eymard, T. Gallouët, R. Herbin: The finite volume method. In preparation for 'Handbook of Numerical Analysis', Ph. Ciarlet et J. L. Lions eds., 1994.

[3] J. H. Ferziger and M. Perić, Computational methods for fluid dynamics. Springer-Verlag, Berlin, 1996.

[4] J. Šembera, J. Maryška: Discussion on Numerical Modelling of Physical Processes in a Combustion Engine. Proceedings of Algoritmy 2002, pp. 179-186.