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DISCUSSION ON NUMERICAL MODELLING OF PHYSICAL PROCESSES IN A COMBUSTION ENGINE*

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Abstract. The contribution presents our approach to numerical modelling of processes in a combustion engine and its present situation. The modelling was motivated by the aim of computation of production of nitrogen oxides during the work cycle of such engine. There are the models of flow of compressible gas, heat and mass transport, and chemical reactions and their connection presented here. The model of flow is made by solution of Navier-Stokes and compressible continuity equations by the finite element method. Transport problem is described by the advection equation and the energy equation; both are solved applying the finite volume method. Chemical reactions are modelled locally in each finite volume. All three models use the same mesh in each time step; the mesh is changing in time.

Key words. modelling, finite element method, finite volume method.

AMS subject classifications. 76N15, 76V05, 93A30.

1. Introduction. The main motivation of working on the model is a task of modelling of production of nitrogen oxides in a gas combustion engine. We decided to develop a complete model of relevant physical and chemical processes and compute the nitrogen oxide production as an outcome from it.

The task was divided into three main problems: flow, mass and heat transport, and chemical reactions. Each of them was modelled separately. The models are solved in a cycle and outputs from one model form inputs to another one.

In the paper, a brief description of the three models is set, the algorithm of the computation is shown and a short summary of the first calibration computations is presented.

The model is not able to compute the nitrogen oxide production, yet. The present program assumes gas fuel, it does not model diffusion and turbulent processes and it has many other limitations. The calibration shows that the global behaviour of the model is good and we are optimistic in our prognoses of its future capabilities.

2. Physical model.

2.1. Governing equations. The model is governed by the equation of convection, the mass balance equation, the energy equation, the mass transport equation, and the equations of chemical reactions, which are solved in a time-dependent bounded region with boundary conditions and initial conditions.

As the equation of convection, the Navier-Stokes equation is used. We neglect the gravity term, since it has no considerable effect:

$$\frac{\partial}{\partial t}\mathbf{u} + (\mathbf{u}\cdot\mathbf{grad})\mathbf{u} = -\frac{1}{\rho}\,\mathbf{grad}\,p + \frac{\eta}{\rho}\Delta\mathbf{u}. \tag{2.1}$$

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Here $\mathbf{u}$ denotes the flow velocity vector, p is pressure, ρ means mass density of the gas, and $\eta(T)$ is the dynamic viscosity.

The continuity (mass balance) equation has to be used in the general compressible form:

$$\frac{\partial}{\partial \mathrm{t}}\rho + \operatorname{div}(\rho\mathbf{u}) = 0. \tag{2.2}$$

The simplified energy equation models heat advection and production by combustion and mechanical forces:

$$\frac{\partial}{\partial \mathrm{t}}(\rho E) + \operatorname{div}(\rho E\mathbf{u}) = -\operatorname{div}(p\mathbf{u}) + \rho\mathbf{u}\cdot\mathbf{F} + \rho q, \tag{2.3}$$

where E denotes the density of total energy of gas $E = u + \frac{1}{2}\mathbf{u}^2$, T is temperature, q denotes the energy produced by chemical reactions, and $\mathbf{F}$ denotes the density of external mechanical forces.

The mass transport is modelled by the advection equation:

$$\frac{\partial}{\partial \mathrm{t}}(\rho c_i) + \operatorname{div}(\rho c_i\mathbf{u}) = 0, \tag{2.4}$$

where c_i means the concentration of i-th gas in the gas mixture.

The chemical reactions can be described by very general chemical equations of the following structure:

$$k_{l1}\mathrm{A}_{l1} + k_{l2}\mathrm{A}_{l2} + k_{l3}\mathrm{A}_{l3} + \ldots \overset{\text{time } t}{\longrightarrow} k_{r1}\mathrm{A}_{r1} + k_{r2}\mathrm{A}_{r2} + \ldots + q. \tag{2.5}$$

The time t consumed by the chemical reaction depends on temperature T, pressure p, and concentrations of reacting species. The produced energy q depends only on the amount of chemicals having been reacted.

The relation connecting temperature, pressure, and mass density is the equation of state:

$$\frac{p}{\rho} = RT, \tag{2.6}$$

where R is a constant dependent only on type of gas.

The relations of the other thermodynamical coefficients of particular gases in the mixture to temperature are:

$$\begin{array}{rcl} c_{Vi}(T) & = & c_{Vi0} + a_iT + b_iT^2 + c_iT^3, \\ c_{pi}(T) & = & R_i + c_{Vi}(T), \end{array} \qquad \begin{array}{rcl} R_i(T) & = & R_i, \\ \kappa_i(T) & = & \frac{c_{pi}(T)}{c_{Vi}(T)}, \end{array} \tag{2.7}$$

where c_{Vi}, c_{pi}, R_i, and κ_i are isochoric thermal capacity, isobaric thermal capacity, gas constant, and adiabatic exponent of i-th gas respectively.

All equations hold in a time-dependent region $\Omega(t)$ with boundary $\Gamma(t)$.

2.2. Boundary conditions. The flow problem consists of Navier-Stokes equation (2.1), continuity equation (2.2), and Dirichlet and/or Newton boundary conditions prescribed on $\Gamma_D(t)$ and $\Gamma_N(t)$ respectively, where $\Gamma_D(t)$ and $\Gamma_N(t)$ are disjoint parts of the boundary $\Gamma(t)$:

$$p = p_D \quad \text{on } \Gamma_D, \tag{2.8}$$

$$\mathbf{u}\cdot\mathbf{n} - \sigma(p - p_D) = u_N \quad \text{on } \Gamma_N. \tag{2.9}$$

On the major part of the boundary, the homogeneous Neumann boundary condition (i.e. Newton boundary condition with $\sigma = u_N \equiv 0$) is prescribed, which expresses the impermeability of the walls. The Dirichlet and Newton boundary condition may appear when the vents are open, or exceptionally there, where the pressure is known, e. g. from an experiment.

The other equations are completed with the Dirichlet boundary conditions of concentrations of chemical species and temperature:

$$\left.\begin{array}{rcl} c_i & = & c_{j,i} \\ T & = & T_j \end{array}\right\} \text{ at } \Gamma_j(t), j = 1, \ldots, J, \tag{2.10}$$

where the boundary $\Gamma(t)$ is decomposed into J disjoint parts with various boundary conditions. It allows to model more different vents in the engine.

2.3. Initial conditions.

$$\begin{array}{rclrcl} \rho\mathbf{u}(t=0) & = & \mathbf{f}_0, & \rho(t=0) & = & \rho_0, \\ c_i(t=0) & = & c_{0,i}, & T(t=0) & = & T_0 \end{array} \tag{2.11}$$

The initial conditions are chosen such that the initial mass density ρ_0, temperature T_0, and concentrations $c_{0,i}$ are constant in the whole volume $\Omega(0)$ and the initial flux $\mathbf{f}_0$ could be fixed either directly experimentally, or indirectly by identification.

3. Numerical model.

Decomposition of the problem. The time-dependence of the domain complicates the mathematical formulation of the problem. The problem (2.1)–(2.11) is then decomposed to time steps, which are solved in several substeps the following way:

- Isochoric processes:
  - Production of mass and energy (chemical processes)
  - Flow
  - Transport of mass and energy
- Adiabatic expansion/compression

Numerical solution of flow. For numerical simulations the Navier-Stokes equation (2.1) and mass balance equation (2.2) was discretised by finite difference method in time and the mixed-hybrid weak solution of the discretised system was derived. The approximation of the weak solution is searched in the space discretised by finite element method using trilateral prismatic elements.

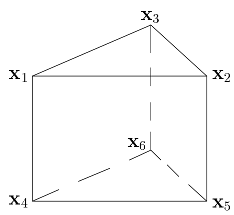

FIG. 3.1. *A typical shape of a finite element/finite volume*

The application of the method results into solution of the nonlinear algebraic system

$$\begin{pmatrix} \mathbf{A}(\mathbf{p},\mathbf{f}) & \mathbf{B} & \mathbf{C} \\ \mathbf{B}^T & \mathbf{D} & \mathbf{0} \\ \mathbf{C}^T & \mathbf{0} & \mathbf{E} \end{pmatrix} \begin{pmatrix} \mathbf{f} \\ \mathbf{p} \\ \lambda \end{pmatrix} = \begin{pmatrix} \mathbf{r_1}(\mathbf{p},\mathbf{f}) \\ \mathbf{r_2} \\ \mathbf{r_3} \end{pmatrix} \begin{array}{l} \Leftarrow \text{Navier-Stokes equation} \\ \Leftarrow \text{Mass balance equation} \\ \Leftarrow \text{Local balance} \end{array},$$

which is linearised either by explicit method, or solved iteratively ($\mathbf{p}$ and $\mathbf{f}$ are estimated and iterated – see Fig.3.2). The system matrix of such a way linearised problem is large sparse symmetrical indefinite.

The vector $\mathbf{p}$ describes elementwise constant approximation of pressure function, the vector λ includes values of facewise constant approximation of traces of pressure function on element boundaries, and the vector $\mathbf{f}$ describes elementwise linear Raviart-Thomas approximation of flux function $\mathbf{f} = \rho\mathbf{u}$.

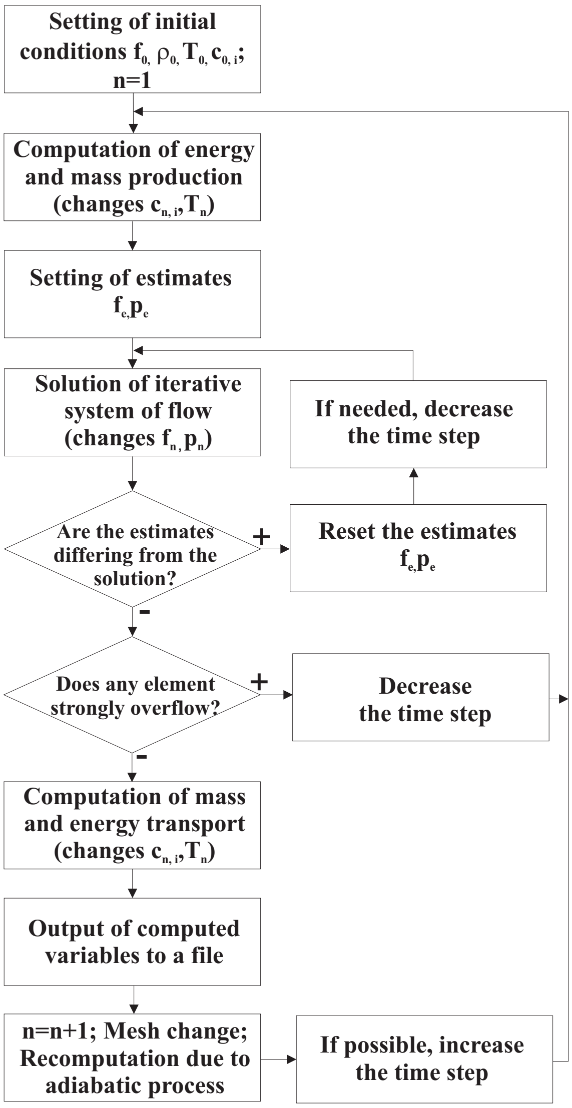

FIG. 3.2. *Rough diagram of the computational algorithm*

Numerical solution of transport. The equations of transport of energy (2.3) and the equation of transport of mass (2.4) are solved by finite volume method. The shape of finite volumes is identical to the shape of finite elements of the flow model.

The right-hand side terms in (2.3) are modelled separately – the term of energy sources in the step of chemical processes computation and the term of transformation of mechanical energy in the step of adiabatic volume change.

The method then results in solution of a large number of simple equations

$$(3.1)\quad \frac{V^e}{\Delta t}\rho^e c_i^e + \sum_{l=0}^{4} c_i^{e_l} f_l^e = \frac{V^e}{\Delta t}\rho^{e0} c_i^{e0}, \qquad \frac{V^e}{\Delta t}\rho^e E^e + \sum_{l=0}^{4} E^{e_l} f_l^e = \frac{V^e}{\Delta t}\rho^{e0} E^{e0},$$

where ρ^e, c_i^e, and E^e denote average mass density, average concentration of the i-th part of gas mixture, and density of total energy in the finite volume e respectively, V^e means the volume of the finite volume e, Δt is the time step, the exponent ^{0} means the initial condition for the computed time step, f_l^e is the outer flux through the l-th face of the volume e, and

$$c_i^{e_l} = \begin{cases} c_i^e & \text{for } f_l^e > 0 \\ c_i^{e_l^*} & \text{else} \end{cases}, \qquad E^{e_l} = \begin{cases} E^e & \text{for } f_l^e > 0 \\ E^{e_l^*} & \text{else} \end{cases},$$

where e_l^* denotes the finite volume neighbouring e through its l-th face.

There is a complication in the solution of (3.1). When the fluxes, computed by flow model, are large in the sense that during one time step inflows and outflows more mass than it is present inside the finite volume at the start of the time step, but the final mass density inside the element stays positive (we say that the element "weekly overflows"), it is needed to shorten the time step for transport computations. In such a case the computation of transport is made in several time substeps. The worst situation is, when the flow model gives such a solution that there is a "strongly overflowing" element, i. e. that after the whole time step computed with the given flow array, the element would include non-positive mass. It has to be solved by shortening the global time step and re-starting the computation.

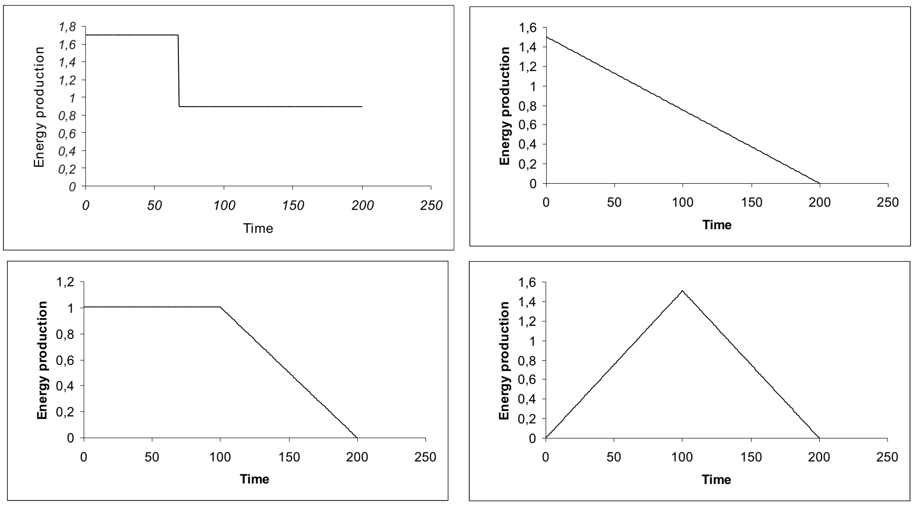

FIG. 3.3. *Various local models of energy production*

Model of chemical reactions. Each reaction is started when temperature reaches a defined critical temperature. The kinetics of chemical reactions can be computed by one of several simplified local kinetic models (see Fig. 3.3). The simplified model is applied locally (on each element separately), i. e. it is supposed that elements are isolated from each other during the chemical reactions take place. In fact, the speed of the reaction does not depend on time from start (like it is drawn on Fig. 3.3), but it depends on concentration of "burning gas" (a pre-defined part of gas mixture) inside the finite volume – see Fig. 3.4.

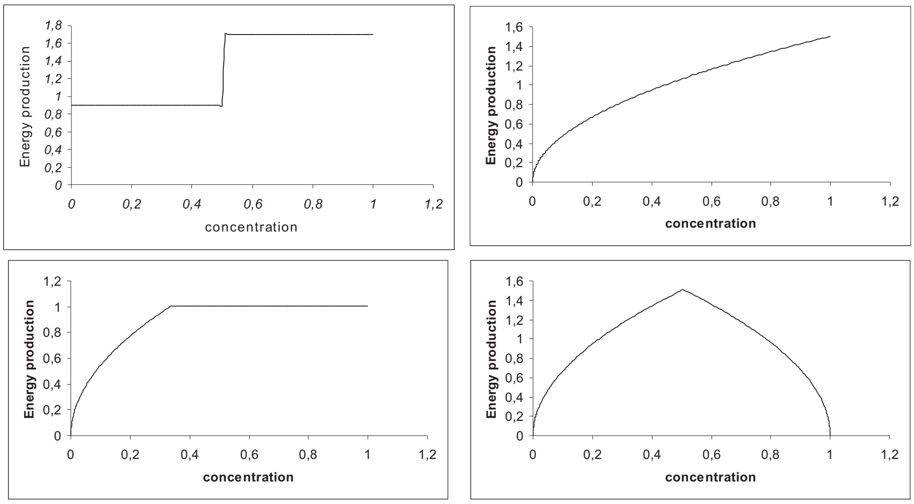

FIG. 3.4. *The dependency of reaction speed on concentration of the "burning gas" due to the local models*

The process of chemical reaction is modelled by change of concentration of reacting gases and by production of heat (increase of temperature).

Moving mesh. The changing part of the region has cylindrical form and only the height of it changes. The moving mesh is built using these properties. In top view, the circle is discretised by triangles, and in side view, the cylinder is split to layers. The resulting form of all finite elements/finite volumes is trilateral prism. The top view discretisation does not change in time; height and number of layers may differ.

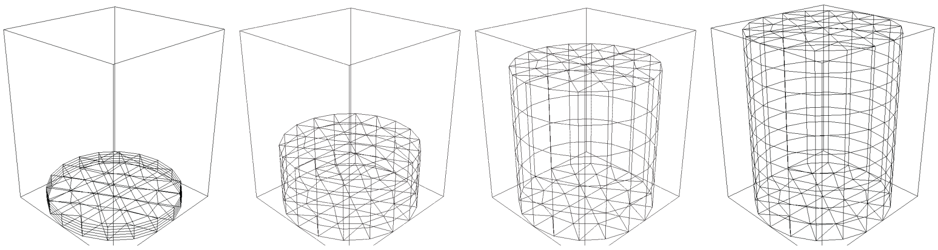

FIG. 3.5. *An example of a moving mesh*

The mesh is changing always between computations of two time steps. Concurrently the recomputation due to adiabatic process takes place. The meshes are built so that each "new element" (or a few of them) corresponds to an "old element" (or a few of them) so that it is uniquely defined, which mass is placed in which element of the new mesh. To ensure such a correspondence, each two sequential meshes have either the same number of layers, or the ratio between their numbers of layers is integer.

4. First calibration tests. There were some tests of the flow, transport, and mesh changing modules performed and the following conclusions may be done:

- In the cylinder changing its volume with homogeneous initial and homogeneous Neumann boundary conditions, temperature and density are changing due to the adiabatic process, vortices are preserved, linear flows are vanishing in time, and mass balance is preserved.
- Applying Dirichlet or Newton boundary condition, mass is inflowing, or outflowing, local mass balance is preserved.

These tests show that the global behaviour of the flow, transport and adiabatic parts of the model is good.

- When large fluxes appear, the stability of computation is damaged.

It shows the weakness of the algorithm of iterations of nonlinear system of the flow problem.

Calibration of the module of chemical reactions was made independently on the other computing modules of the simulation software (flow and transport were not computed at all). After calibrating non-physical parameters of the model, we observed rather good behaviour of the energy production.

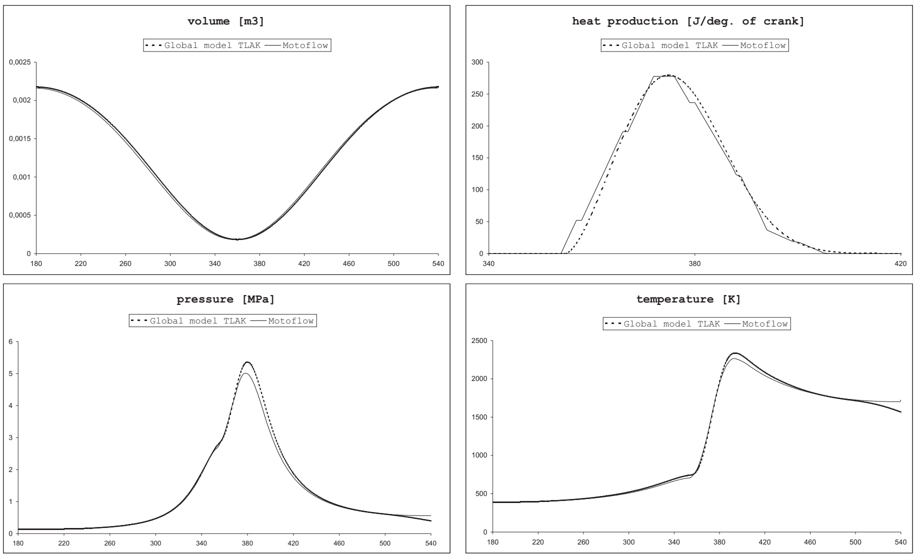

FIG. 4.1. *Global characteristics of the work-cycle of a gas combustion engine computed by the described model* `MOTOFLOW` *compared with data obtained from the calibrated global model* `TLAK` *(in all graphs dashed) – computation with no open vents, i. e. no gas inflow or outflow (using the upper left model of energy production from Figs 3.3 and 3.4)*

Further calibration of complete model was made on such a problem: a cylindrical engine with all vents closed. The initial conditions are homogeneous, chemically corresponding to well mixed methane-air mixture. The results of our model `MOTOFLOW` were compared with results of another model `TLAK` developed at the Department of Transport Machines of TU in Liberec. `TLAK` is a model computing global physical parameters of the gas inside the engine (mean pressure and mean temperature) and it was well calibrated using measurements on real engine of simple cylindrical geometry. Our parameters and initial conditions correspond to the real engine. The only difference from reality was closing all vents.

Figure 4.1 shows the result of one of performed computations in comparison with data obtained from the global model `TLAK`.

Calibration of the behaviour with open vents is complicated by appearing very large fluxes around the open vents and it would be done after improvement of the iterative process of the flow module, which becomes unstable now.

5. Conclusion. There was a model of physical processes in a combustion engine formulated and implemented. Many calibration tests were made and the results show that the model is able to produce globally relevant data. We did not calibrate the local outputs, since we had not good data for comparison.

The tests showed also the need of some changes in the model, especially in the iteration cycle of the flow model. The model does not include diffusion transport and it does not include turbulence, it does not consider fluid fuel. There is a lot of work to do, yet.

REFERENCES

[1] Šembera J., Čížková L., Maryška J. (2000) First Steps to Modelling of Processes in Combustion Engine, Proceedings of Colloquium Fluid Dynamics, Prague, pp.123–126.
[2] Čížková L., Maryška J., Šembera J. (2001) Modelling of Processes in a Combustion Engine–Model of Transport Phenomena. Proceedings of 4rd Seminar Euler and Navier-Stokes Equations, Prague, May 23–25, 21–24
[3] Šembera J., Maryška J. (2002) On the Local Model of Energy Production Inside a Combustion Engine. Proceedings of Seminar on Topical Problems of Fluid Mechanics 2002, Prague, February 2002, pp. 71–74.
[4] Brezzi F., Fortin M. (1991) Mixed and Hybrid Finite Elements Methods. Springer series in Computational Mathematics, Vol. **15**
[5] Landau L. D., Lifshitz E. M. (1982) Fluid Mechanics. Pergamon Press, Oxford