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Simulation of Combustion in Cylinder of Internal Combustion Engine Using Chemical Kinetics and Computational Fluid Dynamics

Simulace spalování ve válci spalovacího motoru s využitím chemické kinetiky a výpočetní dynamiky plynů

Summary

The lecture deals with a simulation of in-cylinder phenomena at internal combustion engines. It is mainly focused on combustion. Combustion has strong impact on properties of internal combustion engines in terms of an engine efficiency and emission formation. The complex model can be based on RANS equations, turbulence models and full chemistry description. The CFD model for simulation of internal combustion engines is described in the lecture. The involvement of chemical kinetics to the model is shown. The chemical kinetics equations are stiff which causes problems with a numerical solution. A method of split integration of the fluid governing equations and chemical kinetics terms is described. The algorithm is applied to an unconventional engine using porous media combustion. A discussion of results is involved. It is focused on an analysis of the extended model possibilities arisen from the chemical kinetics involvement.

Souhrn

Přednáška se zabývá problematikou simulace dějů ve válci spalovacího motoru, především spalování. Spalování významným způsobem ovlivňuje vlastnosti spalovacího motoru s ohledem na účinnost motoru a tvorbu škodlivin. Komplexní model spalovacího motoru může být založen na Navier-Stokesových rovnicích s Reynoldsovým průměrováním, modelu turbulence a chemické kinetice. V přednášce je popsán CFD model použitelný pro simulaci spalovacích motorů. Jsou konkretizovány zdrojové členy chemických reakcí. Rovnice chemické kinetiky mají nepříjemné vlastnosti z hlediska jejich numerického řešení. V práci je popsán algoritmus rozdělené integrace rovnic popisujících proudění a rovnic chemické kinetiky. Metoda je aplikována na nekonvenční spalovací motor využívající spalování v porézním médiu. Je provedena stručná diskuse výsledků s ohledem na možnosti, které nabízí zahrnutí chemické kinetiky do simulačních modelů.

Klíčová slova: počítačová dynamika plynů, spalovací motor, spalování, chemická kinetika, numerické řešení, spalování v porézním médiu

Keywords: Computational Fluid Dynamics (CFD), internal combustion engine, combustion, chemical kinetics, numerical solution, porous media combustion

Contents

1 Introduction

An internal combustion (IC) engine is the most widely used source of energy for mobile applications. It is very likely that the IC engine will remain the prime mover for automobiles at least during several next decades – [1]. Due to this fact, the progress of IC engines plays a very important role in the sustainable development of all countries over the world. However it is foreseeable that future engines will be driven by current alternative and new fuels such as hydrogen, biofuels, synthetic fuels, etc.

There still exists a space for the development of current IC engines. The new fuels and permanent pressure on improving engine fuel economy and reducing emission formation will call for an optimization of existing combustion systems and development of new ones. The task is very complex and it is convenient to use advanced simulation tools to reduce time-to-market during research and development. It further enables the manufacture significant cut down on costs.

Ever increasing computer power enables formulation of very comprehensive but computationally demanding algorithms which can be applied to practical problems. The methods are helpful in understanding complicated phenomena at the initial development phase. An experimental calibration is necessary to make the methods reliable (and general enough) to be further used in design and optimization work. Complex CFD models combined with detailed combustion models based on chemical kinetics are the typical representative of the methods. In fact, they represent a virtual reality tool providing extremely comprehensive information on explored phenomenon. Typical problem is that current experimental techniques lag the numerical simulations. The level of models is so high that it is even possible to regard simulation results as results of numerical experiments.

The presented lecture deals with premixed (or immediately mixed) mixture flames. Spray models have to be employed for diffusion flames of liquid fuels.

2 Combustion Systems and Models of Internal Combustion Engines

The lecture deals with combustion in IC engines. It is strongly affected by turbulence and it makes sense to further consider turbulent flames only. Currently used combustion systems and flame types can be adequately categorized according to type of used mixture and ignition system.

The premixed mixture combustion is typical for spark ignition (SI) engines. The combustion is characterized by a propagating flame front while the burning is initiated by an external energy source – electric discharge, auxiliary fuel, etc. The flame front (flame brush) is usually very thin compared to dimensions of a combustion chamber. The turbulence intensity has very strong influence on combustion as laminar burning occurs in individual turbulent eddies. The turbulence significantly promotes in-cylinder transport phenomena. It leads to significant increase in flame front propagation velocity.

The diffusion flame is another combustion system widely used. It is typical for compression ignition (CI) engines. The fuel is injected into air and combustion is initiated by a spontaneous auto-ignition. The ignition energy is supplied through mixture compression, which increases its temperature. The ignition occurs after an ignition delay. A droplet break-up, fuel evaporation, fuel/air mixing (physical phase) and chemical processes are simultaneously running during the ignition delay and consecutive combustion. The fuel/air mixing is strongly affected by a diffusion of fuel, burnt gas and air to or out of the reaction zone. It is clear that turbulence strongly impacts the combustion as well.

It is possible to combine both combustion systems to integrate their advantages. The diffusion flame enables using low overall air excess but formation of soot is inevitable – [2] – if a carbon based fuel is used. On contrary, the premixed combustion does not allow for using as lean mixture as diffusion flame does. However the emission formation (nitrogen oxide mainly) can be more easily aftertreated and the soot is not formed at all. The engine integrating the premixed mixture combustion with the compression ignition is called a homogeneous charge compression ignition (HCCI) engine. Such combustion is mainly controlled by chemical kinetics. The turbulence effect depends on a mixture formation system used.

A simulation model to be used to in-cylinder phenomena modeling has to include suitable turbulence model and combustion model. It has to correctly treat an interaction between the turbulence and combustion. A hierarchy of turbulent combustion models, in terms of chemistry and mixing treatment, is summarized in [3]. There are models considering an infinitely fast chemistry. They apply an equilibrium assumption to combustion. They are not suitable for the systems in which either slow reactions might play an important role or their products are of interest. It is typical for low temperature combustion systems and nitrogen oxide formation. A finite rate chemistry models, such as PDF, flamelet or complex chemistry ones, has to be employed in this case. The combination of the CFD algorithm with chemical kinetics represents the most general formulation of the combustion model.

3 Reaction mechanisms

Reaction mechanisms represent a very important model input when the complex chemistry is considered. In simpler models it is usually adequate to use net (overall) reactions only. It is possible to apply the chemical kinetics to the single overall reaction in cases when knowledge of chemical transformation of main species only is important. On the contrary, a set of elementary reactions including intermediate products and defining a chemical transformation pathway is necessary in problems in which detailed combustion or emission simulation is required. The set of elementary reactions describing the chemical process is called a reaction mechanism – [4]. A reaction mechanism should consider all possible chains of the chemical transformation to describe correctly auto-ignition, emission formation, etc. Therefore, it has to include both fast (fuel oxidation) and slow (emission formation) reactions. To describe combustion and auto-ignition of hydrocarbons and hydrogen, the reaction mechanism has to consider following chains – [4]: initiation, propagation, branching and termination. In fact it is impossible to find reaction mechanism describing all possible details of combustion.

It is utmost important to find correct (and minimized) reaction mechanism for the considered problem to model the process successfully. From the practical application point of view, problems with obtaining the appropriate reaction mechanism represent an important limitation of the current state-of-the-art. It typically restricts the applications to fuels such as hydrogen, methane, n-heptane, etc. Number of species and elementary reactions in the full reaction mechanism of hydrogen, methane and n-heptane are summarized in Table 1.

Reaction mechanism	**Number of species *K***	**Number of reactions *L***
$H_2 - O_2$	≈ 10	> 20
$CH_4 - O_2 - N_2$	≈ 50	> 300
nC_7H_{16} - air	≈ 800	> 3000

Table 1: *Number of species and reactions in typical reaction mechanisms.*

It is possible to reduce number of species and reactions in a reaction mechanism. The reduction techniques can be found in [11]. The mechanisms are then usually tailored to a particular task and they must be used with care.

4 The Simulation Model Background

The simulation model is based on the AMEM algorithm – [5]. The AMEM represents typical CFD algorithm for simulation of turbulent flow in cylinder of IC engines. It employs the finite volume (FV) method. Governing equations of flow, source terms due to chemical transformation and numerical solution are described further. See [6] for the turbulence model involvement.

4.1 Basic System of Governing Equations

The governing equations describing flow and combustion in a cylinder of IC engines can be based on a budgeting equation in integral form. In the case of IC engine simulations, it is necessary to take into account movable boundaries of a computational domain.

$$\frac{d}{dt}\int_{V_{lib}}\phi dV = -\int_{\partial V_{lib}}\phi\left(w_j - w_{Gj}\right)n_j dS + \int_{V_{lib}}P_\phi dV + \int_{\partial V_{lib}}S_{\phi j}n_j dS$$
$$\Phi = \int_{V_{lib}}\phi dV \tag{1}$$

The equation (1) is written for a volume specific quantity ϕ. Index j defines a direction of a reference coordinate system. Tensor form and Einstein summation rule is used further. The term on the left hand side represents an accumulation of the quantity ϕ in a control volume chosen independently of a fluid flow. The first term on the right left side describes a convective flux of the quantity ϕ through the control volume surface S. In this term, a relative velocity on the control volume surface appears - w stands for a fluid (material) velocity on a FV interface and w_G is a grid velocity respectively. Next two terms represents bulk and surface sources. n_j denotes outer normal to the surface S.

The continuity equation has to take into account changes of a mixture composition due to combustion. Therefore, the continuity equation has to be written for all individual species:

$$\frac{d}{dt}\int_{V_{lib}}\sigma_k\rho dV = -\int_{\partial V_{lib}}\sigma_k\rho\left(w_j - w_{G,j}\right)n_j dS - \int_{\partial V_{lib}}j_{mass,k,j}n_j dS + \frac{dm_{k,chem}}{dt}, \tag{2}$$

where index $k=1,...,K$ indicates overall number of species, σ_k is mass fraction of the k-th specie and ρ is the mixture density. The diffusion and source term due to chemical reactions appear on the right hand side of the continuity equation together with the convective flux. The diffusion can be modeled in the standard way using the Fick law – [7]. The chemical term will be discussed further.

The momentum equation has a standard form as no chemical source has to be explicitly involved in. However, flow pattern of a chemically reactive mixture can be very different comparing it to a non-reactive flow. The influence of chemical reactions is considered through significant changes in density, temperature and pressure in the reaction zone.

$$\frac{d}{dt}\int_{V_{lib}}\rho w_i dV = -\int_{\partial V_{lib}}\rho w_i\left(w_j - w_{Gj}\right)n_j dS + \int_{V_{lib}}\rho g_i dV + \int_{\partial V_{lib}}\left(-p\delta_{ij} + \tau_{ij}\right)n_j dS \tag{3}$$

In this equation p is pressure, τ_{ij} is the tensor of viscous stresses.

$$\frac{d}{dt}\int_{V_{lib}}\rho e dV = -\int_{\partial V_{lib}}\rho e\left(w_j - w_{Gj}\right)n_j dS + \int_{V_{lib}}\rho g_j w_j dV + \int_{\partial V_{lib}}\left(-p\delta_{i,j} + \tau_{i,j}\right)\left(w_j - w_{Gj}\right)n_j dS +$$
$$-\int_{\partial V_{lib}}q_j n_j dS - \int_{V_{lib}}P_V dV - \int_{V_{lib}}\dot{Q}_V dV \tag{4}$$

$$e = u + \frac{1}{2}w_j w_j$$

Energy equation (4) is derived for total internal energy e. Since the movable control volume is considered, the energy equation has to include a term describing the work due to the volume changes.

$$-\int_{V_{lib}} P_v dV = \int_{V_{lib}} \left(-p\delta_{ij} + \tau_{ij}\right) w_{G,i} n_j dS \tag{5}$$

In general, it is necessary to include turbulent heat conduction when the turbulent reactive flow is considered. The heat conduction strongly affects the flame propagation in some combustion systems. The reason for that is the mixture pre-heating ahead of the reaction zone – [4]. In case of the ICE simulations, the heat transfer to the cooled walls is very important as well. It can cause flame quenching and it influences knock onset, etc.

$$\dot{q}_i = -\lambda_{eff}(T)\frac{\partial T}{\partial x_i} - \rho\sum_{k=1}^{K} h_k D_{k,eff}^{M} \frac{\partial \sigma_k}{\partial x_i} + \dot{q}_{wall} \tag{6}$$

The heat conduction is incorporated in the model through the Fourier law – [7]. The effective heat conduction coefficient (sum of molecular and turbulent one) is used. The second term in (6) describes energy diffusion flux caused by the diffusion of species – [7]. Dufour and Soret effects are neglected what is justifiable in the presented problem – [4]. h_k is sensible enthalpy – see (13) – and $D_{k,eff}^{M}$ is the effective diffusion coefficient. The application of the effective transport parameters is very important as it forms the coupling between the turbulent flow and the chemical transformation. The last term in (6) describes heat transfer to the cooled wall if the FV is closed to it. The thermal boundary layer is very thin ($\delta \approx 0.1$ mm). The mesh size of used computational grid does not enable solving the heat transfer coefficient correctly. Time when computational mesh resolution will be sufficient for direct numerical simulation of the heat transfer coefficients seems to be far off. The same comment could be made on turbulence simulation. For that reason, the heat transfer to the cooled walls is included in a simplified manner. The heat transfer coefficient is determined according to known correlations – Eichelberg, Woschni – [8]. These correlations are not valid locally and they use mean in-cylinder thermodynamic parameters to define the heat transfer coefficient. However, they are well verified. It is quite reliable and easy-to-adopt approach to include the heat transfer to the engine simulations. Finally, heat flux density is given by

$$\dot{q}_{wall} = -\alpha\left(T_{wall} - \bar{T}\right), \tag{7}$$

where α is the heat transfer coefficient, $\boldsymbol{T}$ is the mean in-cylinder temperature and T_{wall} is the wall temperature.

The released heat due to chemical transformation is included in a bulk source term – the last term on the right hand side of (4). In general, the term can include different bulk sources of energy/heat in the FV. For that reason, it is convenient to divide it into two parts:

$$\dot{Q}_v = \dot{Q}_{chem} + \dot{Q}, \tag{8}$$

where Q_{chem} is the heat released/consumed by the chemical transformation and Q is a general term respecting other bulk energy and heat sources such as radiation, spark discharge energy, etc. The chemical source term is discussed further.

The system of governing equations is not sufficient for the solution. It has to be amended for closures and constitutive relations (equation of state, turbulence models, etc.) – [5].

4.2 Combustion Description – Chemical Kinetics

In the detailed combustion model, a suitable reaction mechanism describing the combustion, i.e. fuel oxidation and emission formation, has to be incorporated and chemical kinetics has to be applied to. The reaction mechanism is a set of elementary reactions describing significant branches of the combustion process. *l-th* reaction of the reaction mechanism can be written in a general form (9).

$$\sum_{k=1}^{K} \upsilon'_{k,i}\chi_{k,i} \leftrightarrow \sum_{k=1}^{K} \upsilon''_{k,i}\chi_{k,i} \tag{9}$$

In equation (9), χ_k is the chemical symbol and ν_k is the stoichiometric coefficient of the *k-th* specie. The superscripts ′ and ′′ indicate forward and reverse reaction respectively. Overall production rate ω_k of the *k-th* specie can be written as a summation of contributions to its transformation of all reactions of the reaction mechanisms involving the *k-th* specie.

$$\dot{\omega}_k = \frac{dC_k}{dt} = \sum_{l=1}^{L} \Delta\upsilon_{k,l} q_l,\ k = 1,\dots,K,\ \Delta\nu_{k,l} = \upsilon''_{k,l} - \upsilon'_{k,l} \tag{10}$$

Index *l=1,...,L* indicates number of all individual elementary reactions of the reaction mechanisms. C_k is molar concentration of the *k-th* specie and q is the rate of progress variable for the *l-th* reaction. Using definition of the molar concentration, equation (10) can be rewritten in the form defining the source term due to chemical reactions in the continuity equation:

$$\frac{dm_{chem,k}}{dt} = V_{lib} M_k \dot{\omega}_k = \int_{V_{lib}} M_k \left(\sum_{l=1}^{L} \Delta\upsilon_{k,l} \dot{q}_l \right) dV\ , \tag{11}$$

where M_k is the molecular weight of the *k-th* specie, V is the volume of the control volume.

Heat released by the combustion is necessary source term to the energy equation. Assuming the reaction mechanisms, it can be written in the Hess law form. Therefore, overall released/consumed heat can be expressed as a sum of heat effects of individual reactions. The source term for constant temperature yields

$$\int_{V_{lib}} \dot{Q}_{chem} dV = -\sum_{k=1}^{K} h_k^{chem} \frac{dm_{k,chem}}{dt} = -V_{lib} \sum_{k=1}^{K} M_k h_k^{chem} \dot{\omega}_k = -\int_{V_{lib}} \left[\sum_{k=1}^{K} M_k h_k^{chem} \left(\sum_{l=1}^{L} \nu_{k,l} \dot{q}_l \right) \right] dV\,. \tag{12}$$

Enthalpy of the *k-th* specie h_k involves sensible enthalpy and heat of formation of the specie. In equation (13), $c_{p,k}$ is the specific isobaric heat capacity and $h_{f,k}$ is the heat of formation of the *k-th* specie.

$$h_k^{chem} = h_k(T_k) + h_{f,k}(T_{ref}) = \int_{T_{ref}}^{T_k} c_{p,k} dT + h_{f,k}(T_{ref}) \tag{13}$$

The rate of progress variable *q* remains the last unknown to be defined. In general, a chemical reaction runs in both forward and reverse directions. Resulting rate of progress variable for *l-th* reaction is given by the difference of forward and reverse rates:

$$\dot{q}_l = k_{f,l} \prod_{k=1}^{K} C_{k,l}^{\upsilon'_{k,l}} - k_{r,l} \prod_{k=1}^{K} C_{k,l}^{\upsilon''_{k,l}} , \tag{14}$$

where $k_{f,l}$ and $k_{r,l}$ are the forward and reverse rate constants. The forward/reverse rate constant can be evaluated using well known Arrhenius law – [9]. Usually the Arrhenius temperature dependence is used to evaluate the forward rate constant and the reverse one is determined from the equilibrium constant – [9].

$$k_{f,l} = A_l \cdot T^{b_l} \cdot e^{-\frac{E_{a,l}{}^{f}}{RT}} , \; k_{r,l} = \frac{k_{f,l}}{K_{C,l}} \tag{15}$$

The pre-exponential factor A_l, the temperature exponent b_l and the activation energy $E_{a,l}$ are specified empiric parameters (known from the numerical solution point of view) of the reaction mechanism. The equilibrium constant $K_{C,l}$ is easily obtained from thermodynamic properties of species – [9].

4.3 Numerical Solution

In general, the numerical solution of the governing equation set is quite demanding in case of solely non-reactive flow simulation. The chemical kinetics involvement further significantly increases the demands on the numerical solution. The reaction mechanism consists of both fast and slow reactions. It leads to the existence of a wide range of time scales which strongly affects the system dynamics. The system is characterized by the Jacobian matrix which eigenvalues range in several orders of magnitude. The stiffness of the system does not usually enable using standard numerical procedures with reduced time step only. It is necessary to use special methods for solution of the stiff problems. However, they are usually demanding as for computational time. Therefore, it is very convenient and favorable to split solution into two threads and to integrate the flow equations and chemical kinetics ones separately with tailored methods.

Mathematical model is formed by governing equations in the integral form (2), (3) and (4). The vector of unknown variables *W* can be defined as

$$W = \left\| \rho\sigma_1, \ldots, \rho\sigma_k, \rho w_1, \rho w_1, \rho w_3, \rho e \right\|^T . \tag{16}$$

Note that it is not the vector of conservative properties in the case of the movable FV boundaries considered. The system of equations can be rewritten in a general form using the *W* vector:

$$\frac{d}{dt} \int_V W_{u,v} \, dV + R(W)_{u,v} = 0 . \tag{17}$$

It is suitable to split the operator *R* into two parts in the case of the turbulent reactive flow solution.

$$\frac{d}{dt}\int_V W_{u,v}dV + R_{flow}\left(W\right)_{u,v} + R_{chem}\left(W\right)_{u,v} = 0 \tag{18}$$

Subscripts *u* and *v* indicate the finite volume in *i* and *j* directions of the coordinate system. The operator *R* is split into two parts – part describing only flow and that describing the chemical transformation. The R_{chem} can be written in the vector form as

$$R_{chem}\left(W\right) = -\int_V \dot{Q}_{chem}\, dV \tag{19}$$

$$\dot{Q}_{chem} = \left\| M_1\left(\sum_{l=1}^{L}\upsilon_{1,l}\dot{q}_l\right),\dots,M_k\left(\sum_{l=1}^{L}\upsilon_{k,l}\dot{q}_l\right),0,\sum_{k=1}^{K}M_k h_{chem,k}\left(\sum_{l=1}^{L}\upsilon_{k,l}\dot{q}_l\right)\right\|^T \tag{20}$$

The integration of the equation set can be performed in two steps using (18). In the presented case, the part describing flow phenomena has been integrated using explicit Runge-Kutta method – [10].

$$\begin{aligned} W_{u,v}^{(0)} &= W_{u,v}^{n} \\ W_{u,v}^{(k)} &= W_{u,v}^{(0)} - \alpha^{(k)}\Delta t\, R_{proud}(W^{(k-1)})_{u,v},\ k = 1,\dots,K \\ W_{u,v}^{n+1} &= W_{u,v}^{(k)} \end{aligned} \tag{21}$$

The time step Δt is chosen according to the CFL criterion in dependence on the order of the method. The standard coefficients $\alpha^{(k)}$ for three and four stage method has been used – [11].

The chemical source term represents an ordinary differential equation. It can by rewritten in a general form as

$$\frac{dy\left(x_1,\dots,x_n\right)}{dt} = f\left(x_1,\dots,x_n,y\right). \tag{22}$$

Backward differentiation formulas (BDF) are very often used to the integration of stiff problems. The BDF method represents a linear multi-step method and it can be formulated in form suitable for the stiff problems as

$$y^{n+k} = \Delta t \beta^k f^{n+k} - \sum_{j=0}^{k-1}\alpha^j y^{n+j}\,, \tag{23}$$

where *n* indicates the time level. An order of the method is given by number of steps *k*. Coefficients α_0 and β_0 may not equal *0*. Therefore the formula (23) describes an implicit method. The method coefficients are summarized in Table 2. The solution leads to a set of algebraic equations which is usually solved using Newton methods – [11].

K	β_k	α_0	α_1	α_2	α_3	α_4
1	1	-1	1			
2	2/3	1/3	-4/3	1		
3	6/11	-2/11	9/11	-18/11	1	
4	12/25	3/25	-16/25	36/25	-48/25	1

Table 2: *Table of coefficients for the BDF method.*

The integration splitting allows for almost arbitrary combination of numerical methods. Moreover, each integration thread may use different time step chosen according to its specific criterion. It is very important feature as the chemical kinetics usually requires much shorter time steps compared to the flow solution. The integration splitting considerably reduces computational time. Both integration paths have to be synchronized. It is the only requirement on the used time step. The solution decomposition leads to the fact that resulting solution is of the 1st order of accuracy in time. Taking into account used time steps and uncertainties in inputs (reaction mechanisms, etc.) this is not an issue restricting the applicability of the method.

In practical applications, it is possible to use generally available routines for solving the stiff problems. In chemistry problems, DVODE and LVODE – [12] - procedures are widely used. Those procedures incorporate the BDF method.

5 Application of the Methodology to an Unconventional Cycle Simulation – Porous Media Engine

The methods presented are very suitable for exploring a potential of unconventional cycles such as those using porous media. The CFD simulation of in-cylinder flow coupled with the complex chemistry represents the most efficient way to understand the combustion system behavior at the research stage. Moreover, the detailed simulation is necessary as the system does not allow for an optical access, etc.

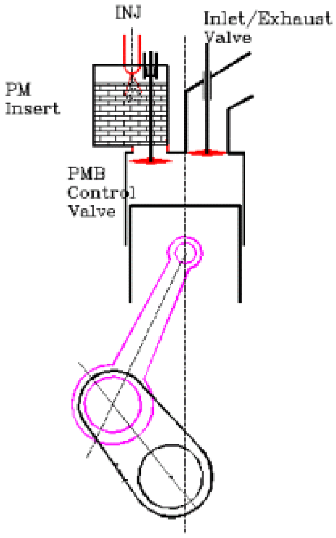

Fig 1: *Scheme of the PM engine with a possibility of gas access control to a PM insert.*

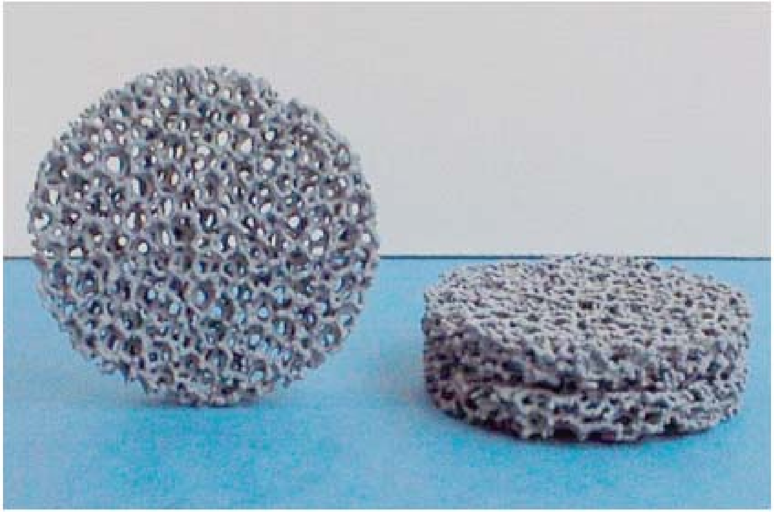

Fig 2: *Porous media.*

Basic layout of the porous media (PM) engine is shown in Fig 1. A ceramic insert – porous media - with high porosity is placed in the engine head. The PM is made of SiC. It has structure like a “sponge”. The purpose of the PM should be to homogenize combustion, to accumulate and regenerate heat between consecutive engine cycles and to restrict in-cylinder temperature. The basic idea of the system is to burn mixture without soot and NO formation.

From the mathematical model point of view, it is necessary to describe fluid – solid phase interaction. The interaction of fluid and PM has to be included in the momentum equation and energy equation. The model has to be extended for the energy equation of the solid phase to solve the accumulation and regeneration capability. A detailed model description is beyond the scope of the text. The source terms to the momentum equation and energy equation of solid phase are presented only. The detailed description can be found in [13].

The PM filaments have been considered to have circular section of known diameter d_{PM}. Assuming that the filaments distribution to the coordinate system direction is isotropic, the drag force caused by filaments can be defined as

$$F_{PM,j} = \int_{V_{lib}} \rho g_j dV = -\frac{4}{3\pi} \cdot c_x \cdot \frac{(1-P)}{P} \cdot m \cdot \frac{w_j \cdot |w_j|}{d_{PM}}, \tag{24}$$

where P is the ceramic matrix porosity, c_x is drag coefficient and m is mass of fluid in the FV. The force is included in the momentum equation (3) as an additional bulk source term.

The energy equation of porous media can be derived in a very simple form. Temperature profile across the filament has been neglected.

$$c_{PM} m_{PM} \frac{\partial T_{PM}}{\partial t} = \alpha_{PM} A_{PM} (T - T_{PM}) - \lambda_{PM} A_{PM,j} \frac{\partial T_{PM}}{\partial x_j} - \frac{dQ_{PM,chlaz}}{dt} \tag{25}$$

The accumulation is given by balance among heat transfer from/to the PM, heat conduction and heat transfer to the cylinder walls on the PM/cylinder contact surface.

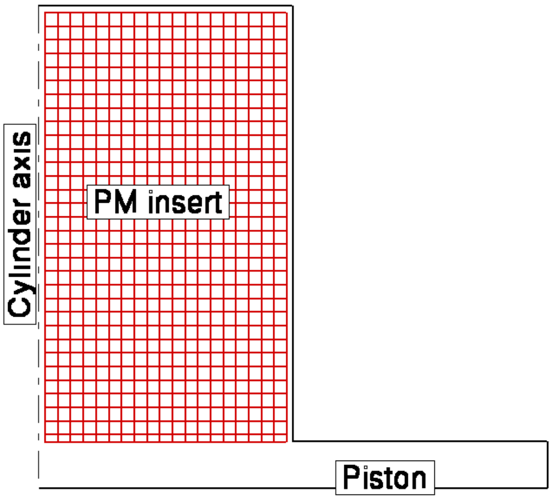

Fig 3: *Lay-out of the combustion chamber used to the simulation of the PM engine.*

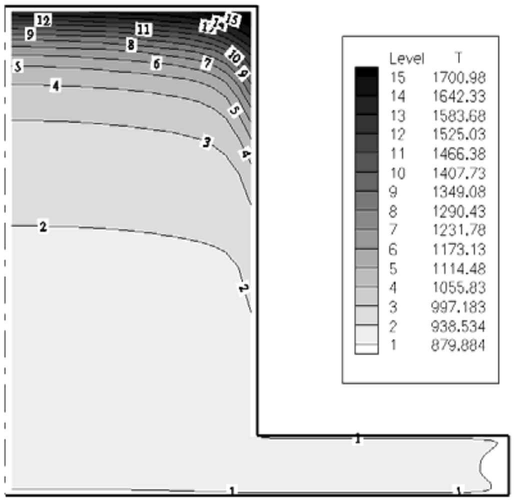

Fig 4: *In-cylinder gas temperature at the start of injection (10 degCA BTDC).*

The drag coefficient and heat transfer coefficient can be estimated from correlations for flow past a cylinder at low Reynolds numbers – [14], [15].

The procedure has been applied to simulation of a PM engine with very simple geometry - Fig 3. The combustion is simulated using two models which are combined to make the simulation faster. As it will be demonstrated later, very high temperature occurs in the PM burner during combustion. It promotes rate of the chemical reactions and it is possible to use the infinitely fast chemistry model using a fictitious fuel. The chemical kinetics model is connected to it to solve chemical transformation of real fuel including intermediate products. Moreover, the used reaction mechanisms includes detailed scheme of NO formation.

Temperature fields in the cylinder at various stages of the engine cycle are shown in Fig 4 and Fig 5. The temperature contours are presented since temperature strongly affects all chemical processes and it has very strong influence on NO formation. The rate of NO formation is one of the limiting factors for an applicability of the combustion system. The local in-cylinder temperature is very high which is very unfavorable to the reduction of NO formation. It is caused by several factors. An initial temperature of PM insert has been 1000K. It has been estimated using simple thermodynamic analysis of the cycle. During the compression stroke, the mixture is pushed to the PM insert and it is preheated. The Fig 4 clearly indicates that as it depicts the in-cylinder temperature field before combustion. Mixture which was compressed in the PM at early stage of the compression stroke has the highest temperature. The fuel is injected into the PM insert only which is other important factor causing mixture stratification. It has several consequences and the high local temperature is one of them.

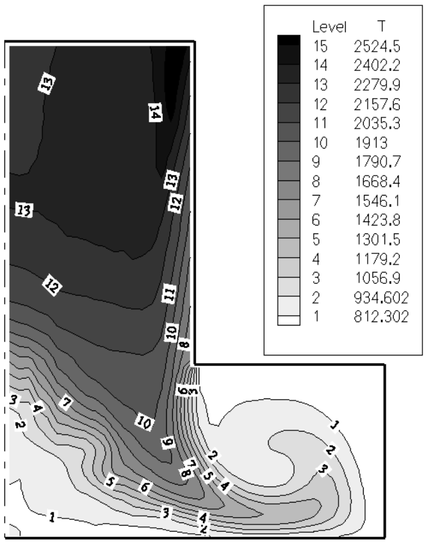

Fig 5: *In-cylinder gas temperature after end of combustion (40 degCA ATDC).*

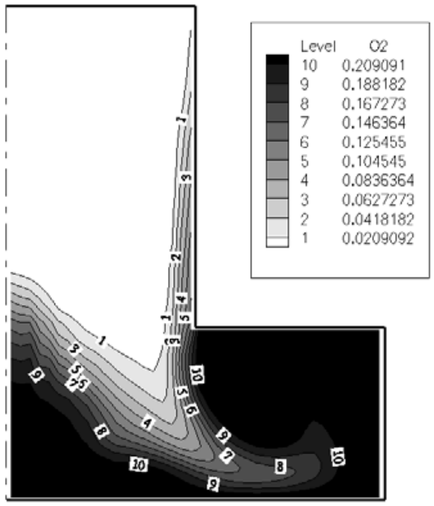

Fig 6: *Oxygen mass fraction at 40 degCA ATDC.*

The chemical kinetics provides very detailed information on combustion and emission formation. In the presented case, methane combustion has been considered. The reaction mechanism according to [16] has been used. In Fig 6, oxygen mass fraction at the end of combustion is shown. It indicates drawbacks of the unoptimized combustion system design. The mixture stratification leads to the lack of oxygen for methane oxidation although overall air excess is 4. It causes a formation of CO - Fig 7. Carbon monoxide is formed due to the incomplete oxidation and partially due to carbon dioxide dissociation at high temperature.

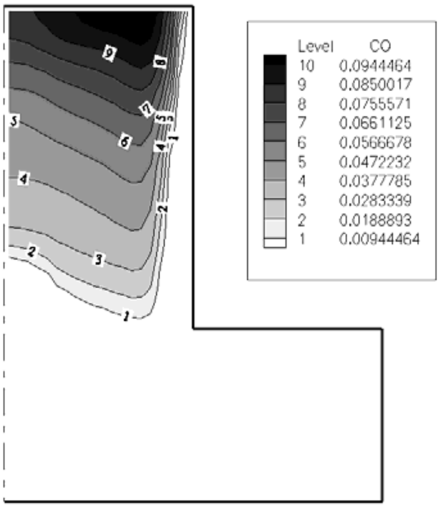

Fig 7: *Carbon monoxide mass fraction at 40 degCA ATDC.*

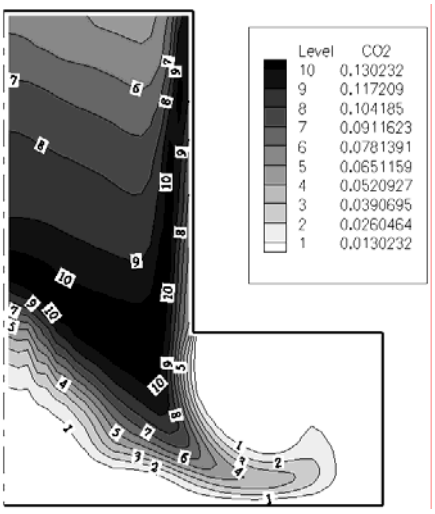

Fig 8: *Carbon dioxide mass fraction at 40 degCA ATDC.*

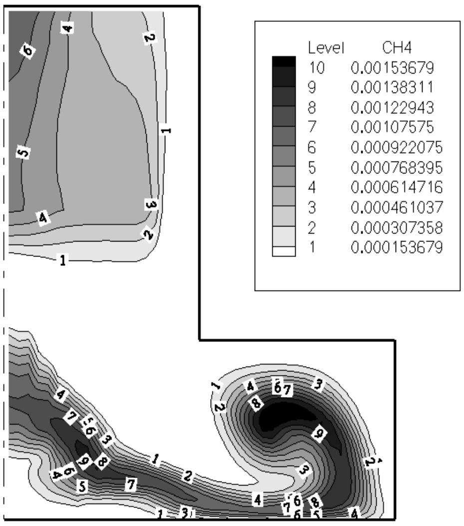

Fig 9: *Methane mass fraction at 40 degCA ATDC.*

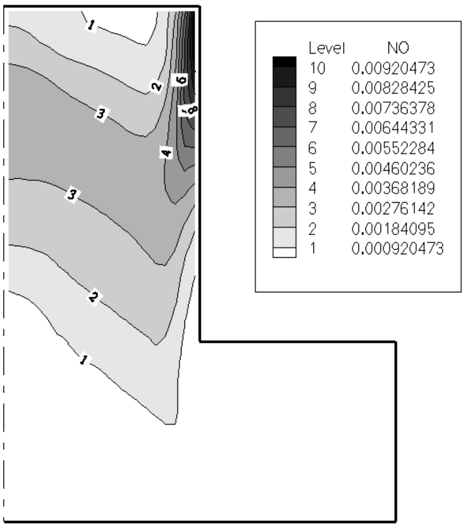

Fig 10: *Nitrogen oxide mass fraction at 40 degCA ATDC.*

The products of incomplete burning are expelled from the PM burner during combustion and expansion strokes. It is necessary to make it burned in the cylinder to compensate for the strong mixture stratification. The phenomena depend on the temperature of expanding gas and on mixing. Fig 9 shows methane mass fraction after the end of combustion. Quite high amount of the fuel remains unburned in the upper part of the PM insert because of the local lack of oxygen. The mixing and in-cylinder temperature is not sufficient for diffusion afterburning and significant amount of fuel remains unburned in the main combustion chamber as well. It is a drawback of the combustion system when it is operated under unsteady conditions.

Nitrogen oxide mass fraction is shown in Fig 10. It clearly demonstrates the inconvenience of the locally high temperature to the NO formation rate. It is compensated by the lack of oxygen to some extent.

6 Conclusion

The model for the simulation of in-cylinder phenomena at IC engines has been presented. The algorithm is based on a general CFD method and it incorporates the complex combustion model based on chemical kinetics. The proposed procedure represents the comprehensive tool which can be used to explore new combustion system. The chemical kinetics involvement significantly extends the IC engine model capabilities.

Application of the chemical kinetics equation to a reaction mechanism and definition of the source terms to the flow governing equation is not very complicated. It is necessary to find correct reaction mechanism to describe a fuel oxidation correctly. It is possible to do it quite easily in the case of simple gaseous fuels like hydrogen or methane. However, it is quite complicated to find a reaction mechanism for multi-component hydrocarbons fuels including gasoline and diesel fuel. In some particular tasks, it is possible to use a reduced reaction mechanism to decrease number of considered species and reactions.

The model of flow has to treat turbulent flow in cylinder of an engine at least qualitatively correctly. The chemical kinetics is usually tuned to describe well the nature of the chemical transformation itself. Unlike the standard turbulent combustion models, it is not possible to simply use some tuning parameters to match the reaction mechanism to the turbulence model. There is no explicit dependence between turbulence and reaction mechanism but turbulence has significant influence on energy, momentum and mass transports. The reaction mechanism is usually formulated in a general manner or it matches a particular problem, i.e., a particular combustion system, temperature and pressure range, air excess, etc. For that reason, the reaction mechanism has to be chosen and employed with care.

The integration of the chemistry source terms is a drawback of the method. The chemical kinetics equations are stiff. It requires the application of suitable numerical methods. It is very convenient to split integration of flow governing equations and chemistry. The simulation is very time consuming and it typically takes in orders of days/month if fine enough computational mesh is used. This restricts an application of the models for multi-parametric optimizations.

The model is capable of very detailed simulation. It is very well suited for exploring new combustion systems, especially in cases lacking experimental data. The simulations of the porous media burner demonstrate it. The problems of model calibrations are still open for the future amendment.

From the practical application of the PM burner point of view, it does not represent the low emission system in the considered setup. Hot spots inside the PM insert are formed due to low material heat conductivity despite the SiC matrix use. It is not convenient to have most mixture burn in the high volume PM chamber since it leads to the significant mixture stratification. In-cylinder air/fuel mixing is not sufficient to ensure efficient afterburning at the late combustion stage.

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