CFD-modeling of the pulsed combustion in vortex chamber

A R Khalilov, V M Larionov, A O Malahov, S A Nazarychev
Kazan Federal University, 18 Kremlyovskaya str., Kazan 420008, Russian Federation

E-mail: nartline@inbox.ru

Abstract. The article is a review of existing mathematical methods used in modeling the combustion process of gaseous fuels in order to determine the most suitable model for pulsed combustion.

1. Introduction
At present, the study of pulsating combustion of hydrocarbon fuels is becoming increasingly important. Computer simulation of pulsating combustion is a complex non-stationary task, the solution of which requires taking into account many factors and conducting preliminary calculations. A review of the literature showed that the focus is on modeling swirl combustion. However, few take into account the oscillatory, pulsating components, which have a significant effect on the nature of combustion.

The purpose of the work is to create a computer model of the pulsation combustion process in a vortex combustion chamber.

Modeling of combustion processes covers the following stages characterizing the objectives of the study:
• selection of the optimal mathematical model (viscosity, combustion, convective heat transfer);
• selection and simplification of the geometric model and meshing, mesh convergence;
• setting boundary conditions;
• choice of time step for non-stationary solution.

Grid convergence is the process of finding the optimal computational grid to obtain a high-quality calculation in the task. When modeling the processes of hydro-gas dynamics, it is worth paying attention to the type of grid, since depending on the task, it is essential to choose a tetra- or hexagonal grid. The size of the cells in the grid also plays an important role, i.e., the smaller the size of the calculated cells relative to the dimensions of the region under consideration, the higher the resolution of the calculated volume and, accordingly, the accuracy of the calculations increases. However, the use of a grid with a very high resolution is not rational, since this leads to an increase in the consumption of computing resources. When solving the problems of hydro-gas dynamics by
numerical methods, one inevitably encounters the unsatisfactory accuracy of the results obtained. A common problem is the insufficient resolution of the computational grid. When modeling physical processes, it is always necessary to imagine which feature of the process is decisive, key to the task and has the greatest influence on the result. It is this feature that must be resolved by the computational grid in the first place.

The study of convergence on the grid is divided into the following stages:

- selection of a mathematical model: at this stage, it is necessary to correctly select a set of solvable equations that fully describe the key physical processes occurring in the simulated device;
- selection of control (characteristic) parameters: here it is necessary to determine which device or current parameters are key, reflect the correctness of the solution obtained;
- simplification of the calculation task: very often, the convergence study on the grid can be carried out on an incomplete statement of the task, taking only part of the simulated device with the most important physical process. The use of simplified task statements makes it possible to reduce the time and computational resources by orders of magnitude at the stage of convergence study on the grid;
- analysis of the results.

2. Models overview

There are many models that describe turbulent flows, among them:

2.1 Spalart-Allmaras model

This model is relatively simple, it solves the simulated transport equation for the kinematic eddy (turbulent) viscosity. The Spalart-Allmaras model was developed specifically for problems associated with flow restrictions along the wall, and it was shown that it gives good results for boundary layers.

2.2 $k - \omega$ model

This model is one of the most commonly used turbulence models. This is a two-equation model, that is, it includes two additional transport equations to represent the turbulent properties of the flow. This allows a model with two equations to take into account effects such as convection and diffusion of turbulent energy. The first variable is the turbulent kinetic energy $k$. The second variable in this case is the specific dissipation of $\omega$. Namely, it determines the scale of turbulence, while the first variable $k$ determines the energy of turbulence.

2.3 $kk - l - \omega$ model

This model is used to predict the development of the boundary layer and calculate the beginning of the transition. This model can be used to effectively solve the problem of the transition of the boundary layer from laminar to turbulent mode.

2.4 $v^2 - f$ model

The model is similar to the standard $k - \varepsilon$ model, but includes near-wall turbulence of anisotropy and nonlocal deformation effects. The limitation of the $v^2 - f$ model is that it cannot be used to solve the Euler problem of a multiphase medium, while the $k - \varepsilon$ model is usually used in such problems. A distinctive feature of the $v^2 - f$ model is the use of a velocity scale, instead of turbulent kinetic energy, to estimate turbulent viscosity.
2.5 Large eddy simulation model (LES)

In LES, large eddies are resolved directly, and small eddies are modeled. The rationale for LES can be summarized as follows:

- Momentum, mass, energy and other passive scalars are carried mainly by large eddies;
- Large eddies are more problem-dependent. They are dictated by the geometry and boundary conditions of the flow involved;
- Small eddies are less dependent on geometry, tend to be more isotropic and, therefore, more universal;
- The probability of finding a universal turbulence model is much higher for small eddies. [1]

2.6 SST (Menter’s Shear Stress Transport) turbulence model

The SST transition model is based on the use of $k - \omega$ transport equations, with two other transport equations, one for discontinuity and one for transition start criteria. [2]

2.7 Reynolds stress model (RSM)

It is the most complex turbulence model. Having abandoned the isotropic eddy viscosity hypothesis, RSM closes the Reynolds-averaged Navier-Stokes equations by solving the transport equations for the Reynolds stresses together with the equation for the dissipation rate. This means that in 2D streams, five additional transport equations and seven additional transport equations, solved in 3D, are required. Since RSM takes into account the effects of streamlined curvature, swirl, rotation, and rapid changes in the strain rate in a more rigorous way than models with one or two equations, it has great potential for accurate prediction of complex flows. However, the accuracy of the RSM forecasts is still limited by the closure assumptions used to model the various terms in the exact transport equations for Reynolds stresses. [3]

3. $k - \varepsilon$ turbulence models

When choosing a turbulence model, the choice fell on the $k - \varepsilon$ model family. As the most of suitable candidates have been considered the standard model and the RNG $k - \varepsilon$ turbulence.

The standard model introduces two important concepts — generation and dissipation. The physical meaning of turbulence generation is the generation of new eddies and pulsations, which form turbulence. Dissipation, on the contrary, is the scattering of large eddies into smaller ones, which leads to averaging of the flow and a decrease in turbulence. Two transport equations allow us to consider turbulence in space and time. This model is semi-empirical and relies on a phenomenological approach and experimental results.

The model includes two additional transport equations (1) to represent the turbulent properties of the flow, which allows you to take into account various fundamental phenomena, such as convection and diffusion of turbulent energy:

$$
\begin{align*}
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k u_i) & = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k \\
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_i} (\rho \varepsilon u_i) & = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_3 \varepsilon G_b) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} + S_\varepsilon
\end{align*}
$$

The first equation of the system describes the kinetic energy of turbulence $k$, the second equation of the system describes the eddy dissipation $\varepsilon$. The values of the constants $\sigma_k$, $\sigma_\varepsilon$, $C_{1\varepsilon}$, $C_{2\varepsilon}$ were...
obtained as a result of numerous iterations of data selection for a wide range of turbulent flows. They have the following meanings: $C_\mu = 0.09$, $\sigma_k = 1.00$, $\sigma_\varepsilon = 1.30$, $C_{1\varepsilon} = 1.44$, $C_{2\varepsilon} = 1.92$ [4]

The RNG model has a similar shape to the standard $k-\varepsilon$ model, but includes the following improvements:

- has an additional term in the equation for $S$, which improves the accuracy of calculations for flows with high strain rates;
- the model takes into account the effect of vorticity on turbulence, which increases accuracy for high-vortex flows;
- this theory offers analytical formulas for turbulent Prandtl numbers, while the standard model uses user-defined constant values;
- the RNG model offers analytically obtained formulas for effective viscosity, which is designed for flows with low Reynolds numbers.

However, the effective use of this option depends on the proper consideration of the parietal region.

These improvements make the RNG model more accurate and reliable, allowing it to be effectively applied to a wider class of currents compared to the standard $k-\varepsilon$ model.

The equations of the RNG model are as follows:

$$
\begin{align*}
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k u_i) &= \frac{\partial}{\partial x_j} \left( a_{k \mu} \frac{\partial k}{\partial x_j} \right) + G_k + G_b - \rho \varepsilon - Y_M + S_k, \\
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_i} (\rho \varepsilon u_i) &= \frac{\partial}{\partial x_j} \left( a_{\varepsilon \mu} \frac{\partial \varepsilon}{\partial x_j} \right) + C_{1\varepsilon} \frac{\varepsilon}{k} \left( G_k + G_b \varepsilon - G_3 \varepsilon \right) - C_{2\varepsilon} \frac{\varepsilon^2}{k} - R_\varepsilon + S_\varepsilon,
\end{align*}
$$

(2)

The main difference between the RNG model and the standard one is an additional term in the equation (2) for $\varepsilon$. $R_\varepsilon$ is calculated by:

$$
R_\varepsilon = \frac{C_\mu \rho \eta^3 (1 - \eta_0) \varepsilon^2}{1 + \beta \eta^3} \frac{\varepsilon^2}{k},
$$

where $\eta = 5k/\varepsilon$, $\eta_0 = 4.38$, $\beta = 0.012$. Constants $C_{1\varepsilon}$ and $C_{2\varepsilon}$ have the following meanings: $C_{1\varepsilon} = 1.42$, $C_{2\varepsilon} = 1.68$.

Turbulent heat transfer is modeled using the concept of Reynolds analogy with turbulent momentum transfer. So, the energy equation is defined as follows:

$$
\frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x_i} \left[ u_i (\rho E + \rho) \right] = \frac{\partial}{\partial x_j} \left[ k_{eff} \frac{\partial T}{\partial x_j} + u_i (\tau_{ij})_{eff} \right] + S_h,
$$

where $E$ is the total energy, $k_{eff}$ is the effective thermal conductivity, and $(\tau_{ij})_{eff}$ is the deviator voltage tensor, which is defined as:

$$
(\tau_{ij})_{eff} = \mu_{eff} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - 2 \frac{\mu_{eff}}{\partial x_k} \delta_{ij}.
$$

For standard and realizable $k-\varepsilon$ model effective thermal conductivity is defined as:

$$
k_{eff} = k + \frac{C_{\rho e \mu}}{Pr},
$$

where $k$ is the thermal conductivity. The default turbulent Prandtl number is 0.85.
For the $k-\varepsilon$ RNG model, the effective thermal conductivity is defined as:

$$k_{\text{eff}} = \alpha c_p \mu_{\text{eff}},$$

where $\alpha$ is calculated according to the equation

$$\left| \frac{\alpha - 1.3929}{\alpha_0 - 1.3929} \right|^{0.3679} \left| \frac{\alpha - 2.3929}{\alpha_0 - 2.3929} \right|^{0.6321} = \frac{\mu_{\text{mol}}}{\mu_{\text{eff}}} - 1,$$

where $\alpha_0 = 1/\Pr = k/c_p \cdot \mu_{\text{mol}}/\mu_{\text{eff}} \ll 1, \alpha_k = \alpha_{\varepsilon} \approx 1.393$. [5]

4. Conclusion
As a result, based on the review, the $k-\varepsilon$ RNG model was selected. This mathematical model has the necessary parameters that take into account secondary flows and the influence of acoustic oscillations on the flow as a result of swirling motion.

Acknowledgements
The work is performed according to the Russian Government Program of Competitive Growth of Kazan Federal University.

References
[1] URL: https://www.afs.enea.it/project/neptunius/docs/fluent/html/th/node42.html
[2] URL: https://www.cfd-online.com/Wiki/SST_k-omega_model
[3] Kozelkov A S, Kurulin V V, Puchkova O L, Lashkin S V 2014 Vychislitel'naya mekhanika splavnikh sred 7 (1) 40–51
[4] Korkodinov Ya. A. 2013 Obzor semeystva k-ε modeley dlya modelirovaniya turbulentnosti pp 8–11.
[5] Korkodinov Ya. A. 2013 Obzor semeystva k-ε modeley dlya modelirovaniya turbulentnosti pp 12–13.