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PTNSS-2011-SC-071

Combustion of Ethanol-air Mixtures in Closed Vessel – Comparison of Simulations with the use of RANS and LES method

Large Eddies Simulations (LES) has become recently a powerful computational tool with application to turbulent flows. It links classical Reynolds Averaged Navier–Stokes (RANS) approach and Direct Numerical Simulation (DNS). This modeling approach computes the large eddies explicitly in a time-dependent simulation using the filtered Navier-Stokes equations. Filtering is essentially a mathematical manipulation of the exact Navier-Stokes equations to remove the eddies that are smaller than the size of the filter. LES resolves the large flow scales that depend directly on the geometry where small scales are modeled by the sub-grid-scale models. LES is expected to improve the description of the aerodynamic and combustion processes in Internal Combustion Engines. With LES it is possible to resolve the essential part of the flow energy, yielding reliable results. Proper predictions depend on the quality of sub-grid-scale (SGS) models.

In this paper the results of computational analysis are compared with experimental results for combustion in constant volume chamber. In that way there is a possibility to see the difference in results of initial flame kernel and laminar flame development. Simulations were made with two CFD codes: Fire and Fluent, which allowed to compare the experimental and simulation results for RANS and LES method and make further improvement in LES combustion model for application in full engine simulation.

Key words: *LES, RANS, Internal Combustion Engines, Sub-Grid-Scale models, Combustion, Constant volume chamber.*

Spalanie mieszaniny etanolu z powietrzem w komorze o stałej objętości - Porównanie wyników symulacji przy uzyciu metody LES i RANS

LES jest znakomitym narzędziem obliczeniowym przepływów turbulentnych łączącym powszechnie używaną metodę RANS (Reynolds Average Navier Stokes Eqution) z DNS (Direct Numerical Simulation). W skrócie metoda LES opiera się na zastosowaniu filtru do równań Naviera-Stokesa i wprowadzeniu rozdziału na zjawiska wielko-skalowe (duże wiry) oraz drobno-skalowe. Zjawiska wielko-skalowe są obliczane przez bezpośrednie rozwiązanie przefiltrowanych równań N-S, natomiast drobno-skalowe są modelowane w skali podsiatkowej. Możliwe jest dzięki temu bezpośrednie obliczenie dużych wirów i wirów biorących udział w procesie kaskadowym. Wiry małe, zależne głównie od lepkości są modelowane, ale wymaga to zastosowanie odpowiednio gęstej siatki od której zależy proces filtrowania. Filtrowanie jest matematyczną manipulacją równań N-S polegającą na wyodrębnieniu wirów z turbulentnego pola przepływu, które są większe niż wielkość zastosowanego filtru. Mimo to właściwe wyniki symulacji uzależnione są również od jakości modelowania w skali podsiatkowej.

W pracy przedstawiono porównanie wyników badań eksperymentalnych i symulacyjnych procesu spalania mieszanki ethanolu z powietrzem w komorze o stałej objętości. Celem tej pracy jest przedstawienie pierwszych wyników dla tworzonego modelu spalania w LES.

Słowa kluczowe: *LES, DNS, RANS, Silniki tłokowe, Model SGS (Podsiatkowy), Spalanie*

1. Introduction

Modern combustion research regarding the operating efficiency demands and the environmental sustainability needs to face two major objectives, reduction of the pollutants and efficient optimization of combustion. An accurate prediction of the essential chemical and physical properties of the reactive flows is required to achieve these purposes. These tasks cannot be solved by the experiments and empirical equations. Nowadays all industrial companies which develop new technologies use CFD to predict and to optimize flow processes. Turbulent combustion systems involve many processes and phenomena like heat and mass transfer mixing, turbulence, and multiphase flows. They are configuration dependent and flows typically exhibit strong large coherent structures and evolve in an unsteady manner making steady state computations an approximation. Numerical methods must be capable to provide the necessary information on the flow and highly unsteady behavior must be predicted by the scalars like chemistry turbulence interactions.

The aim of the models must be a prediction of combustion systems of technical and practical importance [1].

Extreme conditions inside the Internal Combustion Engines (ICE), like high combustion temperatures and pressures, precipitation of soot and other combustion products cause that experimental techniques are limited or too expensive in approaching investigation of complicated phenomena. Alternatively, computer simulations (Computational Fluid Dynamics, CFD) offer the opportunity to carry out repetitive parameter studies with clearly defined boundary conditions in order to investigate various configurations.

These days standard in engine simulations are Reynolds Averaged Navier-Stokes (RANS) methods [2][3]. In RANS, the local instantaneous value of a computed dependent variable represents an ensemble- or phase-average over many engine cycles at a specified spatial location and crank phasing. Two-equation (k-ε) closures have been used to model turbulent transport, with standard equilibrium wall functions. Shortcomings of RANS models have been documented by several generations of turbulence researchers [4][5]. This method allows to accurately predict the mean characteristics of stabilized engine operation, and are therefore widely used to choose the most promising engine configuration, before going to actually test it. These techniques are inherently not adapted to predict unsteady phenomena [6]. A better candidate for a tool allowing for such predictions is Large Eddy Simulation (LES) technique [7]. The governing equations are spatially filtered. Explicit account is taken of flow structures larger than the filter width, which is on the order of the mesh spacing, while the influence of unresolved scales is modeled using a subgrid-scale (SGS) model (Figure 1).

Because statistics of small-scale turbulence are expected to be more universal than those of the large scales, LES offers the promise of wider generality and reduced modeling uncertainty. Turbulence model formulation and calibration traditionally have been carried out in statistically stationary and/or homogeneous flows for simple geometric configurations [8].

RANS and LES differ in the way they resolve the scales present in engine flows related to turbulence, combustion and liquid jets. The RANS simulations are based on a statistical averaging to solve only the mean flow. This approach causes that the whole spectrum of scales is being modeled and the predictivity of RANS depends on the models used. Also the statistical averaging extremely complicates addressing unsteady phenomena. In LES, modeling concerns a much smaller part of the spectrum, which leads to the improvement of predictivity. LES allows to address large scale unsteady phenomena, and it has a good potential to predict engine unsteadiness.

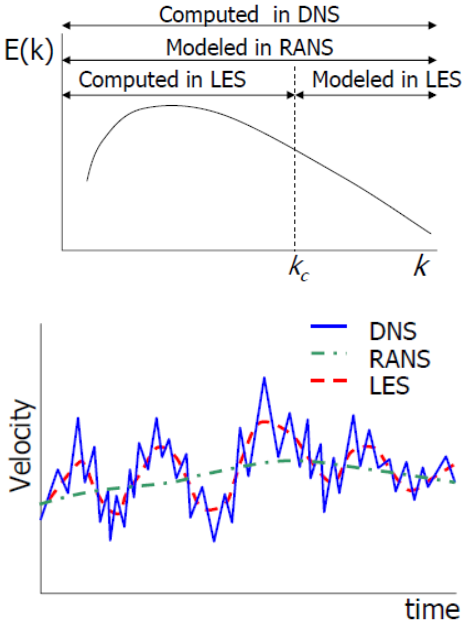

Figure 1. Comparison of Direct Numerical Simulations (DNS), LES and RANS methods [9].

The effect of the modeled part of the turbulence in LES and RANS on the resolved part is diffusive and is taken into account by introducing a turbulent viscosity. The level of turbulent viscosity directly depends on the amount of modeled energy leading to high levels for RANS and far less important levels for LES. This explains the different requirements of LES and RANS in terms of numerical schemes. In RANS, the main requirement is to be robust and stable on distorted meshes. Upwind schemes are known to be very stable but dissipative which is only a second order. In LES method vortices must be accurately resolved with as little numerical dissipation as possible [10]. The best schemes which can handle this problem are the precise and energy-conserving numerical schemes, as Finite-Volume Center-Differencing (FVCD) [11]. It has been estimated that grid-independent (to a 10±20% level) profiles of in-cylinder flow and combustion of dependent mean variables in RANS computations require at least 100^3 mesh points using second-order or higher numerical methods [5]. This corresponds to sub-millimeter mesh spacings in a typical automotive IC engine, and is not far beyond current practice of 250,000 to 500,000 nodes. This mesh density should suffice to capture large- and intermediate-scale flow structures. LES mesh requirements for ICE are expected to be comparable to those of RANS [8].

2. Turbulence models

The most important part is to use proper SGS turbulence model that will not take much computational time and give the most reasonable results. Many SGS models were developed and verified with experimental data.

2.1 Smagorinsky Model

This is the one of the simplest SGS models based on the equilibrium hypothesis [12]. In this model eddy viscosity is proportional to the local strain-rate tensor.

$$\upsilon_t = l^2 \sqrt{2\overline{S}_{ij}\overline{S}_{ij}} \tag{1}$$

Quantity l is the length scale that characterizes small eddies. Its value depends on so called Smagorinsky constant (C_S = 0.18 - 0.23) that has to be tuned for simulated application. Δ is the grid filter width and $\overline{S}_{ij}$ is a strain rate tensor of the filtered flow.

$$l = C^{\frac{1}{2}}\Delta \quad C_S = C^{\frac{1}{2}} \tag{2}$$

2.2 Modified Smagorinsky Model

For the modified Smagorinsky model another equation is used for length scale determination:

$$l = \min\left(C_S * \Delta, \kappa d, \alpha d'\right) \tag{3}$$

where κ is von Karman constant, α is a constant which depends on the application, d is distance to the wall and d' is the characteristic length of the combustion chamber. Eddy viscosity equation stays the same (1).

2.3 Van Driest wall damping SGS Model

For this model also equation (1) is used and the length scale is equal to:

$$l = C_S f_u \overline{\Delta} \tag{4}$$

The Smagorinsky constant and grid filter are the same. The new parameter is f_u the van Driest wall damping function [13] which takes to account the near wall effect.

2.4 Dynamic SGS model

All models described above are based on the constant C_S value, but the difference in sub grid scale turbulence should be taken to the account. For dynamic SGS model the Smagorinsky number is not constant, and is defined by equation proposed by Germano et al. [14].

$$l^2 = C_S \overline{\Delta}^2 \tag{5}$$

$$C_S = \frac{1}{2}\frac{\left\langle A_{ij}B_{ij}\right\rangle}{\left\langle B_{ij}B_{ij}\right\rangle} \tag{6}$$

$$A_{ij} = \left(\overline{\overline{\rho}\,\tilde{u}_i\,\tilde{u}_j}\right) - \frac{1}{\overline{\overline{\rho}}}\left(\overline{\overline{\rho}\,\tilde{u}_i}\right)\left(\overline{\overline{\rho}\,\tilde{u}_j}\right) \tag{7}$$

$$B_{ij} = \overline{\Delta}^2\left(\overline{\overline{\rho}\left|\tilde{\overline{S}}\right|\tilde{\overline{S}}_{ij}}\right) - \overline{\overline{\rho}\left|\tilde{\overline{S}}\right|}\,\hat{\Delta}^2\,\tilde{\overline{S}}_{ij} \tag{8}$$

Where $\hat{}$ is taken to indicate a test filter process, $\langle\rangle$ indicates volume averaged, and the width of test filter $\hat{\Delta}$ is twice the width of grid filter $\overline{\Delta}$.

2.5 Lagrangian Dynamic Model

Meneveau at al. [16] proposed to accumulate the averages required in the dynamic model over flow pathlines rather than over direction of statistical homogeneity. This again leads to a closed-form expression for $C_S\Delta^2$ that involves the two second-order tensors of equations (7) and (8). The Lagrangian form of the dynamic models requires the two additional transport equations for quantities that represent weighted averages of $A_{ij}B_{ij}$ and $B_{ij}B_{ij}$ over fluid particle trajectories. In addition it requires the specification of the relaxation time scale that corresponds to the Lagrangian memory time for fluid elements. The model is applicable to arbitrary statically non-homogenous turbulent flows.

2.6 WALE Wall Adapting Local Eddie Viscosity

This model was described in work of Devesa et al. [31]. Local viscosity is described by equation:

$$\nu_t = (C_w\Delta)^2 \frac{\left(s_{ij}^d s_{ij}^d\right)^{3/2}}{\left(\overline{S}_{ij}\overline{S}_{ij}\right)^{5/2} + \left(s_{ij}^d s_{ij}^d\right)^{5/4}} \tag{9}$$

where Δ is the size of filter used, C_w is a modeling constant, S_{ij}^d is a square product from gradient of the velocity for tensor of $\overline{g_{ij}}$.

$$s_{ij}^d = \frac{1}{2}\left(\overline{g_{ij}}^2 + \overline{g_{ij}}^2\right) - \frac{1}{3}\overline{g_{kk}}^2\delta_{ij} \tag{10}$$

2.7 Model SGS Yakhot-Orszag

This model is presented in work of Naitoh et al. [32]. Turbulent viscosity is calculated from the equation:

$$\nu_t = \nu_0\left[1 + H\left\{\frac{a\Delta^4}{2(2\pi)^4\nu_0^3}\nu_T\left(\overline{u}_{i,j} + \overline{u}_{j,i}\right)^2 - C\right\}\right]^{1/3} \tag{11}$$

where Δ is the size of used filter and C is a modeling constant.

3. Combustion models in Sub-Grid Scale (SGS)

In previous chapter the turbulent SGS models were presented. Nevertheless in case of piston engine there is a need to describe also the combustion process. This models needs to describe in SGS scale the relation between chemical reactions and turbulent flow. Models presented in this chapter are taken from literature review.

3.1 Flame Tracking Model

The flame surfaces are analyzed by G variable (or progress variable) in G-equation. Models of flame surfaces are assumed to be infinitely thin. Flame surfaces are represented by constant contour surface of G in the G-equations models [16]. Turbulent burning velocities in SGS are represented by a monotonically increasing function with respect to the SGS turbulence intensity [17]. In several studies such as Im et al. [17], the SGS turbulent burning velocities are estimated dynamically by applying a test filter similar to the dynamic procedure (Dynamic Smagorinsky model). Since G variable changes its value from 0 to 1 discontinuously at the flame front, numerical viscosity should be introduced to stabilize the numerical solution. To improve this problem, a level-set approach is applied for the numerical simulation of the G-equation as reported by Wang and Bai [18] and Pitsch and Duchamp De Lageneste [19]:

$$\frac{\partial\breve{G}}{\partial t} + \tilde{v}\nabla\breve{G} = -\frac{\rho_u}{\overline{\rho}}\overline{(s_L + s_\kappa)n} * \nabla\breve{G} \tag{12}$$

where t is time, $\tilde{v}$ is filtered velocity (Favre-filtered), s_L is burning velocity of laminar fronts, s_K is describing the flame front propagation, D describe temperature molecular diffusion, n is a normal vector to the flame front.

3.2 The PDF Model

The PDF methods are based on probability density functions for RANS modeling. In LES based on PDF models, conservation equations are exchanged with transport equations of joint probability density function concerning the mass fraction of chemical species. In these models, joint probability density functions are defined based on mass-weighted average (or Favre average) as described by Jeberi et al. [20]. For PDF models, no model for chemical source is required. Whereas SGS scalar flux models such as those in LES of non-reactive scalar transport and mixing model similar to PDF models for RANS should be developed. The probability density function can be solved by Monte Carlo simulation as shown by Sheikhi et al. [21].

3.3 Thickened Flame Method

For turbulent combustion, the flame thickness is significantly thinner, than computational grid size and LES grid filter. To avoid a problem of "losing the flame" the special variable has to be applied which thickens the flame. This method was proposed by Colin et al. [22]. In this method, selection of parameters for the variable transformation is very important to obtain stable and correct solution. The basic assumption for TFLES model is to thickened the area for the species transport equation. The flame thickness δ_L^0 is multiplied by variable F like it is presented in eq. 13. Used variable does not influence the flame speed. It is because when the thermal diffusion coefficient D_{th} will be multiplied by F then the pre-exponential coefficient A will be divided by F.

$$S_L^0 \propto \sqrt{D_{th}A} \quad \delta_L^0 \propto \frac{D_{th}}{S_L^0} = \sqrt{\frac{D_{th}}{A}} \tag{13}$$

4. Gradient method combustion model

For proper basic representation of the combustion process there is a need to control energy and species source term of the continuity equation. Energy source term is represented by heat of combustion product multiplied by the reaction rate:

$$\overline{S}_e = S_c \cdot H_c \tag{14}$$

where S_c [kg/m^3/s] is source term for species transport equation (reaction rate), H_c is lower heating value for used fuel [J/kg].

The source term of species transport eq. is presented by:

$$\overline{S}_c = \rho_u \cdot S_t \cdot \left|\nabla \tilde{c}\right| \tag{15}$$

where ρ_u is a density of unburnt mixture, S_t is a turbulent burning velocity solved for the SGS scale, $\left|\nabla \overline{c}\right|$ is a gradient of the fuel or products mass fraction [26,27].

The equation describing the turbulent burning velocity:

$$S_t = S_u\left(Y_{H_2}, T, p\right) \cdot \left(\psi \cdot \chi_{Karl_{MAX}}\right) \cdot \exp\left(\frac{u'}{S_t}\right)^2 \tag{16}$$

where S_u is laminar burning velocity calculated as a function of temperature and pressure, χ_{Karl} is a Karlovitz coefficient and u_{sgs} is a local SGS velocity of the flow. Knowing that the sub-grid scale unresolved root mean square velocity is defined by:

$$u'_{SGS} = \sqrt{2/3\, k_{SGS}} \tag{17}$$

with k_{SGS} as the subgrid scale unresolved kinetic energy defined by

$$k_{SGS} = \frac{v_t^2}{L_{SGS}^2} = \frac{\mu_t^2}{\rho^2 \cdot L_{SGS}^2} \tag{18}$$

it follows that:

$$u'_{SGS} = \sqrt{\frac{2}{3}} \cdot \frac{\mu_t}{\rho \cdot L_{SGS}} \tag{19}$$

Using the SGS Smagorinsky-Lilly mixing length with C_s=0.157:

$$L_s = 0.157 \cdot V^{1/3} \tag{20}$$

the sub-grid-scale residual velocity can be modelled for highly turbulent flows by

$$u'_{sgs} = \sqrt{\frac{2}{3}} \frac{\mu_t}{\rho\left(0.157 V_{CV}^{1/3}\right)} \tag{21}$$

Presented combustion model is easy to adopt for the other SGS turbulence models. There is no direct connection to the chemical reaction, the process is described by mean of one chemical reaction equation.

5. Results comparison

Experimental results were taken from Liao et al. [23,24]. Simulations were made for the same conditions. Constant-Volume chamber size was 108x108x135 mm. The mixture of ethanol and air was made in the chamber for different ER (equivalence ratio), 358 K temperature and 1 bar pressure. For all calculated cases the maximum pressures were compared (Figure 2.). The results shows that in all simulation cases pressure is higher than experimental. The difference is about 0,2 MPa. Also LES combustion model results of maximum pressure have linear characteristic with ER, because of no connection with chemistry. At this stage reaction is assumed to be ideal (Fire LES 1). There is a possibility to control increase of the pressure with energy equation source term by introducing an empirical correlation (Fire LES 2). But that kind of approach probably will need tuning for different cases. In authors opinion there is a need to introduce a chemistry connection for better results in next step. Result from ECFM Fire combustion model is presented only for three points of calculation because of the much slower combustion process. Approximately for ECFM combustion model time needed for combustion is two times higher than experimental one. For this model laminar burning data is prepared for combustion in IC engines and doesn't cover the whole range of pressures. Comparison should be done again for higher initial pressure to see if the ECFM model will represent the flame front correctly.

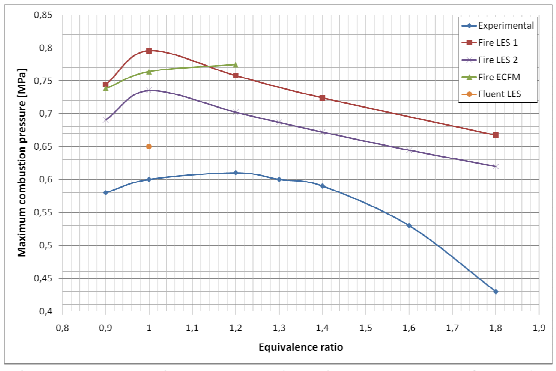

Figure 2. Maximum combustion pressure for ethanol-air mixture as a function of equivalence ratio. Initial temperature 358 K, pressure 0,1 MPa.

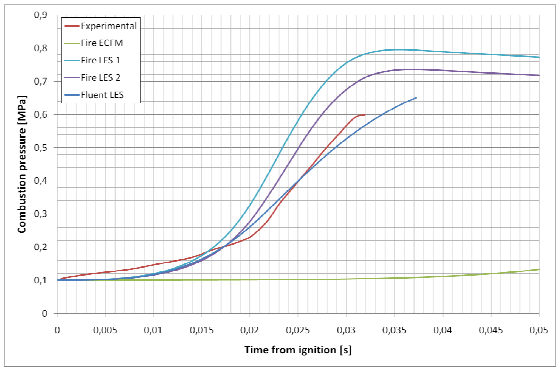

Figure 3. The variations of combustion pressure with time for ER = 1. Initial temperature 358 K, pressure 0,1 MPa.

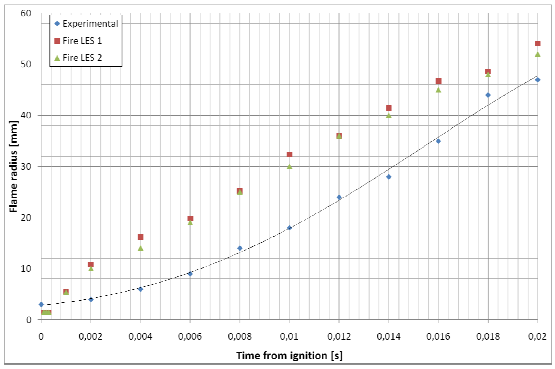

Figure 4. Flame front growths for stoichiometric ethanol-air mixture. Initial temperature 358 K, pressure 0,1 MPa.

In Figure 3 the increase of combustion pressure in time is presented. The time needed for flame growth is in good correlation with experimental results. Still the increase of the pressure is slower for first stage of combustion process. According to the flame growth (Figure 4.) results the increase of the pressure should be faster in the first stage of combustion for simulation. At that point of work it is hard to answer this problem. In Figure 3. the results from ECFM combustion model are presented too. Only slight increase of pressure can be seen for time 0,05 s. The flame growth for this model is much slower what was described earlier.

6. Conclusion

Results obtained from the simulations are satisfactory at that point for presented combustion model. Presented combustion model is based on the gradient method. Chemistry in this approach is represented by one step reaction model and this is the reasons for higher pressure results and linear characteristic of the maximum pressure profile (Figures 2-3). Presented combustion model was previously used for VLES (Very Large scale Eddy Simulation) simulation with good results [25]. In case of ICE Engine chemistry becomes more important and it needs to be introduced to the model. Also for better development of the model other experimental results should be used like for iso-octane and n-heptane air mixtures.

7. Acknowledgement

This research was supported by Polish Ministry of Science and Higher Education under the grant No NW509082437.

Nomenclature/*Skróty i oznaczenia*

LES Large Eddy Simualtion/*symulacje dla wirów wielkoskalowych*
SGS Sub-grid Scale/*Skala podsiatkowa*
RANS Raynolds Average Navier-Stokes Equation/*równania N-S*
ICE Internal Combustion Engine/*silniki spalania wewnętrznego*
CFD Computational Fluid Dynamics/*komputerowa mechanika płynów*
PDF Probability Density Function/*probabilistyczna funkcja gęstości*
FVCD Finite-Volume Center-Differencing/*różnice centralne dla skończonej objętości*
ER Equivalence ratio/*współczynnik stechiometrii*

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