Numerical simulations of industrial-scale combustion chamber - LES versus RANS

Kamil Kwiatkowski\textsuperscript{1\hspace{1em}2}, Daniel Jasiński\textsuperscript{3}, Konrad Bajer\textsuperscript{1\hspace{1em}2}

\textsuperscript{1} Institute of Geophysics, Faculty of Physics, University of Warsaw, Pasteura 7, 02-093, Warsaw, Poland
\textsuperscript{2} Interdisciplinary Centre for Mathematical and Computational Modelling, Pawiński 5a, 02-106, Warsaw, Poland
\textsuperscript{3} Faculty of Power and Aeronautical Engineering, Warsaw University of Technology, Nowowiejska 24 00-665 Warsaw, Poland

E-mail: kamil@igf.fuw.edu.pl, daniel.jasinski@gmail.com

Abstract. In this work we focus on the simulation of the process of biomass syngas combustion in the industrial combustion chamber directly linked with gasification chamber, where this gas is continuously producing from the biomass.

Conflicting demands from the engineers to have rapid results and hints how to ensure the best conditions for combustion of this particular fuel and to lower the emission of pollutants, with simultaneously deep view inside the process and its stability motivates us to use both the RANS and LES techniques of turbulence modelling, compare it and take their advantages. We designed and performed series of 3D numerical simulations of both cold flow and combustion in complex geometry of industrial burner. It seems to us that the proper approach for modelling of biomass syngas combustion is steady flamelets model.

Simulations performed with RANS closure are used as the initialisation of LES models, but their main goal is to predict the long-time oscillation of pressure and temperature observed in the working combustion chamber. On the other hand the main goal of the simulations with LES closure is to predict the proper level of short-time behaviour of the flame and local phenomena.

1. Introduction

Searching for renewable energy sources encourages to use completely new fuels produced from biomass but poses new challenges for both researchers and engineers. One of this new fuels, which popularity grows up, is syngas, the direct product of biomass gasification and pyrolysis processes. The biomass syngas contains hydrogen, carbon monoxide and carbon dioxide and when the gasification agent is air - nitrogen, but has relatively low mean calorific value, strongly fluctuating composition and possibly admixture of solid components ((Dudyński \textit{et al.}, 2011), which suggest that default application is direct burning in combustion chamber. The biomass syngas, which we focused on in this research, comes from wood chips gasification has the following composition (in mass fraction): $N_2$ 0.567, $CO$ 0.222, $H_2$ 0.0006, $CO_2$ 0.121, $H_2O$ 0.016, $CH_4$ 0.012 (Dudyński \textit{et al.}, 2011).

Design the way of proceedings the turbulent combustion, which ensure accepted level of stability independently of the strongly fluctuating compositions, is a demanding task. Stringent norm of pollutants emission and requirement of process completeness makes this task even more
difficult. The emissions from the standard, commercially available burners used in industry critically depend on the small differences of chemical composition of the gas and often exceed the norms even by an order of magnitude. There is a great need for custom burners designed for specific types of syngas in different gasifying installations. It is, in fact, critical in the case of syngas coming from waste disposal which considerably varies with the type of disposed waste (very different in a furniture factory and, for example, in a meat processing factory).

Increasing power of computational resources, accessible for researchers, makes Computational Fluid Dynamics common tool used to understand the process of flow and combustion in industrial devices. Flow in this type of devices is clearly turbulent, with Reynolds number more than $10^5$ and usually very complex.

Dealing with turbulence requires an averaging technique, which leads to two different approaches, first Reynolds-Averaged Navier-Stokes (RANS) based on time-averaging, and second LES based on spatial-averaging. RANS approach had been thoroughly studied and use, its deficiencies are known. Thanks to easier access to computational power the latter closure (LES) is becoming more and more popular.

Work, which we present in this paper, summaries our results with both of the turbulence closures applied to simulations of turbulent non-premixed combustion. It lead us to the conclusion that application of LES for simulation industrial-scale flows and processes is still very limited, however it can provide realistic results.

2. Turbulence and combustion modelling

2.1. RANS closure

Reynolds Averaged Navier-Stokes is based on the concept of time-averaging. In this concept all instantaneous variables, for example velocity components $u(x, t)$, are split into the mean value $\bar{u}(x, t)$ and the fluctuating component $u'(x, t)$, where the mean value is defined:

$$\bar{u}(x, t) = \frac{1}{T} \int_{-T}^{T} u(x, \tau) d\tau$$

The averaging operation applied to the Navier-Stokes equation leads to an equation for averaged variables, which is analogical to original equation except for one additional term $(-\bar{u}_i u_j')$, which has to be modelled. The most common approach to deal with this additional term is the turbulent viscosity hypothesis, which states that the additional term in the averaged N-S equation can be expressed as:

$$\nu_t \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)$$

where turbulent viscosity $\nu_t$ is usually calculated as:

$$\nu_t = C_\mu \frac{k^2}{\varepsilon}$$

where $k$ is the turbulent kinetic energy and $\varepsilon$ is its dissipation rate. This requires additional models and solving two new equation for this two variables. There are many variations of so called “$k - \varepsilon$” model, for our purpose we use “Realisable $k - \varepsilon$” model, which should perform best in modelling free-shear flows (Shih et al., 1995).

2.2. LES closure

Large Eddy Simulation is based on spatial filtering of equations, which may be treated as some sort of spatial averaging. This approach also introduces separation of field variables into filtered
(spatially averaged) variables $\langle u \rangle$ and subscale fluctuations $u''$. In this case the spatially averaged variable is expressed as:

$$\langle u \rangle(x, t) = \int_{\mathbb{R}^3} u(r, t) G(x - r) dr$$

where $G(x, t)$ is the filter convolution kernel.

Filtering operation applied to the N-S equation, similarly to time-averaging operation, introduces additional terms in the equation for filtered variables, which also have to be modelled, with so-called Subgrid Scale Models. This additional terms are also in the form of divergence of some tensor and are similarly modelled using subgrid scale viscosity assumption. The most popular model for the subgrid scale stress tensor is the Smagorinski-Lilly model (Smagorinsky, 1963). In this model the subgrid scale viscosity $\nu_T$ is expressed as:

$$\nu_T = (C_S \Delta)^2 |\langle S \rangle|$$

where $C_S$ is a constant, $\Delta$ is the filter size an $\langle S \rangle$ is the resolved strain rate tensor.

### 2.3. Turbulent Non-premixed Combustion Modelling

One of the most popular and successful approach for modelling turbulent diffusive flames is the laminar flamelet concept in industrial applications. In this model a concept of conserved scalar mixture fraction is used to simplify thermo-chemistry in turbulent flows. This allows to describe all possible states in reacting system using only the value of mean mixture fraction, mixture fraction variance and scalar dissipation rate. This approach allows to compute all chemistry before actual calculation and store it in so-called PDF tables (Peters, 1984, 2000).

In this type of combustion modelling LES shows an advantage because it requires only one transport equation for mixture fraction and the remaining two variables required for model closure are calculated based on subgrid scale model values (Peters, 2000).

Biomass syngas, which is the fuel in our case, contains methane and other hydrocarbons, so have to use mechanism of chemical reactions that allow us to consider the combustion of not only hydrogen and CO but also combustion of lower hydrocarbons (less than three atoms of carbon). We decide to use the GRI3 (Smith et al., 2000) detail mechanism of chemical reactions and thermodynamic data for combustion processes to produce the steady flamelets. GRI based on 6 elements and 53 species suitable for combustion of syngas and includes more than 300 reactions. Chemistry tables were calculated for the whole set of 53 species and stored for a simplified set of 20 species.

### 3. Case settings

#### 3.1. Computational domain

The first challenge in LES simulations is the density of the mesh which should be able to resolve all large scale vortices and at least 80% of kinetic energy contained in the system (Pope, 2000). To ensure this we created mesh containing 4.5M cells and adapted it dividing all cell into eight pieces, which gave us around 36M cells. The characteristic cell length scale is around 1cm. This mesh is presented in figure 1. Both RANS and LES calculations were performed on the same computational mesh, however RANS based simulations mainly use the “coarse” mesh, and LES based simulations use mainly the “fine” mesh. It allows us also to check the mesh independence. Time step for simulations for finer mesh should be around $5 \times 10^7(-4)$s, times around 20 iterations per one time step, times two seconds as a characteristics residence time in the combustion chamber gives us $10^5$ iterations. For these simulations we currently use around 32 processors (cores), one iteration takes usually one minute.
3.2. Boundary and initial conditions for LES calculations

The second issue concerns initial and boundary conditions of the flow. We perturbate the inlet velocities using two approaches: Vortex Method and Spectral Synthesiser (Kraichnan, 1970). Brief comparison presented at pictures 2 shows that after few inlet diameters the results are in good agreement, but Vortex Method of adding the fluctuations working slightly better close to the inlet.

Our initialisations based on the results of unsteady RANS simulations, with perturbated velocity fields (see fig. 3).

3.3. Solver settings

Based on the observations from the installation and on the previous calculations (Kwiatkowski et al., 2011) we assume that unsteady calculations are essential. RANS or Unsteady-RANS calculation was performed using Realisable $k - \epsilon$ model, which is best suited for cases with free-shear flows. For all equations we used second order upwind discretisation scheme.
Figure 4. The isosurface of stoichiometric value of mixture fraction coloured by the temperature, time change is equal 0.6s. Sequential picture of the simulations shows that the flame precessing during combustion. This behaviour has been confirmed by high-speed camera recording.

For LES calculations second-order temporal discretisation (Crank-Nicolson scheme) was used. For spatial discretisation Bounded Central Differencing scheme (second-order) was applied. Time step was chosen so that the Courant number based on the smallest cells was about $C_0 = 2$. As a subgrid-scale model standard Smagorinski-Lilly model was applied. To provide not only the instantaneous values of flow but also the statistics, sampling of the solution variables was performed.

4. Results

Unsteady RANS Simulations were performed for the time of about 30s, sample of results is presented in figure 4. This simulations have shown that flow pattern in the combustion chamber is nearly periodic with characteristic time scale of about 5 seconds, which has been confirmed both by observation of the flame and by formal Fourier analysis of the parameters measured from the working installation. The oscillatory behaviour of the flow field was not yet confirmed with LES simulations since it requires significantly more computational time.

Comparison of LES and RANS results show that both models give similar exhaust temperature which is agreement with measurements. This is due to large size of the combustion chamber, where gases near outlet are able to reach equilibrium conditions (see picture 6).

Temperature field predicted in RANS simulation is very smooth and the highest temperature is much lower then the temperature in LES simulation. This is because in LES simulation large fluctuation of mixture fraction field are resolved explicitly, while RANS requires use of presumed shape PDF to account for turbulent fluctuation. The difference in temperature field has significant impact on prediction of NOx emission since it has very strong dependence on temperature, and is mainly caused by local high temperature fluctuation. In RANS simulations the temperature fluctuations are introduced through another PDF, which effectiveness in a refined task such NOx prediction should be verified on a case by case basis.
Figure 5. Sample of result comes from LES simulations. The general quantities like the length of the flame is in very good agreement with RANS simulations and with observations.

Figure 6. Qualitative comparison of LES and RANS results. Despite the fact that temperature of the flame are significantly different, the exhaust temperature are similar and consistent with measurements.

5. Discussion and Summary

Resulting flows were complex and definitely nonsymmetrical, with clearly recognisable large vertical structures. Qualitatively, these results were confronted with (still very limited) experimental observations and measurements. Temperature range and asymmetry agree with measurements in working burners. Comparison of RANS and LES predicted temperature field show significant differences in prediction of local phenomena which can be crucial for proper determination of the \( NO_x \) emission. Detailed validation of the flow field is not yet completed as the first trials of precise flow visualisation were unsuccessful. However there is qualitative agreement with observations. More efforts in flow visualisation are planned in the near future.
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