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Combustion modeling in large scale volumes using EUROPLEXUS code

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ABSTRACT

Most of the numerical benchmarks on combustion in large scale volumes for hydrogen safety, which were performed up until today have demonstrated, that current numerical codes and physical models experience poor predictive capabilities at the industrial scale, both due to under-resolution and deficiencies in combustion modeling. This paper describes a validation of the EUROPLEXUS code against several large scale experimental data sets in order to improve its hydrogen combustion modeling capabilities in industrial settings (e.g. reactor buildings). The code is based on the Euler equations and employs an algorithm for the propagation of reactive interfaces, RDEM, which includes a combustion wave, as an integrable part of the Reactive Riemann problem, propagating with a fundamental flame speed (being a function of initial mixture properties as well as gas dynamics parameters). Validation of the first combustion model implemented in the code is based on obstacle-laden channels, interconnected reactor-type compartments, vented enclosures and covers all major premixed flame combustion regimes (slow, fast and detonation) with an aim to obtain conservative results. An improvement of this model is found in a direction of transient interaction of flame fronts with regions of elevated integral length scales presented in the velocity gradient field due to e.g. interactions with geometrical non-uniformities and pressure waves.

1. Introduction

During certain severe accidental scenarios in a nuclear power plant (NPP), hydrogen gas is released into the reactor building. In the case of ignition various combustion regimes are possible depending on the local concentrations of hydrogen and steam, as well as temperature and pressure distributions. These regimes may include jet fires, slow or fast deflagrations and detonations. Therefore, in order to improve hydrogen risk management strategies one has to find means to estimate the severity of combustion processes involved into various regimes of flame propagation under given initial conditions.

The use of CFD methods for industrial applications implies a capability to deal with geometries very large with respect to characteristic scales involved in flame acceleration processes. Although, many types of approximations might be employed (e.g. for thermal and species diffusion, viscosity, turbulence, etc.), in general, main pressure loads/transients can be correctly predicted if the flame propagation speed is properly resolved. One of the first approaches to combustion modeling on a large scale was proposed in Efimenko and Dorofeev (2001) and resulted in the CREBCOM model. This algorithm is simple to implement as it resolves non-reactive Euler equations with a reactive contribution added by introducing a source term. This model was successfully employed in several industrial CFD codes, including TONUS, Kudriakov et al. (2008) and COM3D, Bielert et al. (2001).

Recently, numerical benchmarks which have been performed, in particular, within a framework of OECD/NEA (ISP49 (2012)), demonstrated that current numerical models experience poor predictive capabilities due to deficiencies in combustion modeling, especially during the so-called “Blind Phase” exercises. Moreover, the fast combustion regime, which is of major importance for the safety analysis of an accident at NPP, was validated only by the experiments performed at a relatively medium-scale (ENACCEF). Therefore, these combustion models were not examined in a case of significant mesh under-resolution associated with large industrial scale (i.e. NPP).

This paper describes two combustion models, which were recently implemented in the EUROPLEXUS code EUROPLEXUS (2012). At this point, their validation is based on the

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experimental data obtained in several large and middle scale experimental facilities for homogeneous hydrogen-air and hydrogen-air-steam mixtures, covering all major flame regimes (slow, fast and detonations). An emphasis is placed on the achievement of moderately accurate or conservative results for these models to be further employed in an NPP under severe accidental scenarios.

2. Numerical modeling

2.1. RDEM model

A combustion model was developed in CEA (Tang et al. (2014a, 2014b)) and employed in the EUROPLEXUS code to deal with hydrogen hazards in large scale facilities. On the large scale it is out of question to be able to resolve either small scale turbulent structures or the flame front itself. Therefore, the thermal conduction and species diffusion (includes the case of non-uniform premixed mixture), which are important phenomenons in a deflagration propagation, are not directly modelled; their action is taken in part into account by introducing a correlation for the velocity of the reactive wave into the Euler equations. The numerical scheme (see below) allows consideration of all major combustion regimes (in terms of a Mach number) relevant for nuclear safety. In addition, since numerical viscosity is always present in the numerical algorithms due to a discretization error, certain similarity with viscous flows does exist. In particular, the turbulent r.m.s. velocity can be calculated in accelerating flows (flames) from a viscous stress tensor, which is supposed to implicitly exist due to presence of a numerical viscosity. The studies in the case of typical shear flows confirming that the effective numerical viscosity can easily achieve the values of the molecular one, depending on the grid, have been reported by Grinstein since 1990s, Grinstein and Guirguis (1992).

Thus, the equations to be solved are the reactive Euler equations:

$$\begin{cases} \frac{\partial}{\partial t}\rho + \vec{\nabla}\cdot(\rho\vec{U}) = 0 \\ \frac{\partial}{\partial t}(\rho\vec{U}) + \vec{\nabla}\cdot(\rho\vec{U}\otimes\vec{U} + P) = 0 \\ \frac{\partial}{\partial t}(\rho\tilde{e}_t) + \vec{\nabla}\cdot\left(\rho\vec{U}\tilde{h}_t\right) = 0 \\ \frac{\partial}{\partial t}(\xi) + \vec{D}\cdot\vec{\nabla}\xi = 0 \end{cases} \quad (1)$$

The first three equations are the classical conservation equations for mass, momentum and energy. The fourth equation is the transport equation for the progress variable ξ. This equation is in non-conservative form. The apparent flame speed $\vec{D}$ has to be defined only on the interface (with the same value ahead and behind it) and represents its velocity. In this work we compute $\vec{D}$ as a function of the fundamental flame speed K_0 via

$$\vec{D} = \vec{U} + K_0\vec{n} \quad (2)$$

where $\vec{n}$ is a normal to the flame surface going from a burnt to an unburnt region, $\vec{U}$ is the velocity of the unburnt gas. It is assumed that we know the fundamental flame speed K_0 as a function of space and time.

In literature there exist several approaches to model a flame as an interface. Some of these approaches require a solution of the reactive Riemann problem between a burnt and an unburnt region. In order to propagate the flame front we use the reactive discrete equation method (RDEM) Le Metayer et al. (2005), which was initially developed to deal with evaporation fronts and detonation waves. The extention of this method for the propagation of flame interfaces is described in Tang et al. (2014a, 2014b), while the Reactive Riemann solver used for this approach is given in Beccantini and Studer (2009). This method is conservative, since in a close and isolated system the total mass and energy are conserved. It does not suffer from the problem of pressure and velocity oscillations at the combustion interface when the specific heat ratios are different. Finally, an implementation of the RDEM in an existing Finite Volume code is rather straightforward and does not require an interface reconstruction.

2.2. Fundamental flame velocity modeling

The only parameter of the combustion model developed in EUROPLEXUS is K_0 which represents a fundamental flame velocity, i.e. the flame velocity relative to the fresh mixture just ahead of it. Transition from one combustion regime to another occurs continuously with respect to the initial conditions and the fundamental flame speed. We consider thermally perfect gases, because the temperature dependence of the specific heats is important in the case of deflagration and detonation waves, Beccantini and Studer (2009).

The first model (Model I) for this parameter was expressed as a product of several factors following Bauwens et al. (2010):

$$K_0 = S_L^0\Theta_{TH}\Theta_{TURB}\Theta_{WRIN} \quad (3)$$

where S_L^0 is the laminar flame speed of a gas mixture under consideration determined at reference temperature and pressure (P_0,T_0), Θ_{TH} is the thermodynamic factor which takes into account an influence of elevated pressure and temperature, Θ_{TURB} is the turbulence factor, and Θ_{WRIN} is the flame wrinkling factor. A typical form of the model, which takes into account an influence of elevated temperature and pressure on the laminar flame speed determined according to their reference values (T_0,P_0) is

$$\Theta_{TH} = \left(\frac{P}{P_0}\right)^{\alpha}\left(\frac{T}{T_0}\right)^{\beta} \quad (4)$$

For mixtures containing hydrogen gas experimental results give $\alpha = -0.5$ and $\beta = 2.2$ Malet (2004).

The wrinkling factor (exists only for Model I) accounts for a flame surface area increase in the fully-turbulent velocity region. In the case of flame propagation in an unbounded free space, it has been shown by Gostintsev and co-authors Gostintsev et al. (1987) that the ratio between the surface of a spherically propagating flame and the surface of the equivalent sphere increases according to $(R/R_0)^{1/3}$, where R is a distance from the ignition point, and R_0 is a distance at which the fully-turbulent regime is reached. R_0 has been shown to be of the order of 1 m for a stoichiometric hydrogen-air mixture, Gostintsev et al. (1987). However, at present there exist no model or an experimental correlation for this parameter for various mixtures and/or in the presence of other factors, such as pressure waves. In this work a constant value of $R_0 = 1$ m was chosen.

The influence of turbulence on flame velocity can be taken into account using different methods. Bauwens et al. Bauwens et al. (2010), among others, propose to add a transport equation for the value of Θ_{TURB} having source terms responsible for increase and decrease of this value, which is similar to surface flame density modeling. For the turbulence factor we prefer to use an algebraic model in the form of correlation for turbulent flame velocity, as given in Bradley et al. (1992):