Modelling of Turbulent Flame Propagation in a Gas/Particle Mixture by a Lagrangian PDF Method

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Introduction

A turbulent flow field is characterized by a local distribution of eddies causing variations in the flow field properties. In a reactive mixture, turbulence leads to additional local heat release and dilatation, which in turn reinforces turbulence and chemical reactions. The very short lenght scale of chemical processes are hardly resolved in a numerical simulation, especially if the properties of the flow field are smeared over cells in the computational domain. In addition to the problems being known in gas phase turbulent combustion, a dispersed condensed phase and its interaction with the local flow structure increases the combustion complexity. This leads to the task of modelling additional features such as particle evaporation/devolatilization, heterogeneous reactions, and absorption/emission of radiation. In contrast to pure gas mixtures, combustion in two–phase flows involves all modes of flames, ranging from premixed over partially–premixed to diffusion flames [1].

Keywords: Two–Phase Combustion, Turbulence, Proberbility Density Function, Particle Method

Modelling

Our approach to model turbulent gas/particle combustion is based on a joint velocity–composition probability density function (PDF) according to Pope [6]. This method had successfully shown to circumvent the closure problem of chemical source terms in turbulent combustion without any special requirements concerning the combustion mode. The evolution of the PDF is calculated by a Lagrangian approach modelling the dynamics of so called "gas–phase particles" G_i, $i = 1, \ldots, N_G$ in a turbulent flow [5, 7]. While moving through physical space, gas–phase particles are influenced by the condensed phase due to exchange fluxes of mass, momentum, and energy. The differential equations for total mass, partial masses, momentum and enthalpie of gas particle

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G_i read in Lagrangian form:

$$\frac{D^{G_i}\left(\rho_{G_i} V_{G_i}\right)}{Dt} = \mathcal{Q}_{G_i \leftrightarrow P}\,, \qquad \frac{D^{G_i}\left(\rho^l_{G_i} V_{G_i}\right)}{Dt} = \nabla \cdot \mathbf{j}^l_{G_i} + \dot{\omega}^l_{G_i} + \mathcal{Q}^l_{G_i \leftrightarrow P}\,, \qquad l = 1, \ldots, N_S\,, \tag{1}$$

$$\rho_{G_i} \frac{D^{G_i}\mathbf{v}_{G_i}}{Dt} = \nabla(p\,\mathbf{E} - \tau) + \mathcal{R}_{G_i \leftrightarrow P}\,, \qquad \rho_{G_i}\,\frac{D^{G_i} h_{G_i}}{Dt} = -\nabla \cdot \mathbf{q}^{diff}_{G_i} + h^{hom}_{G_i} + \mathcal{S}_{G_i \leftrightarrow P} \quad . \tag{2}$$

In these equations, exchange terms between gas–particle G_i and condensed phase particles P in its surrounding are denoted with an index $G_i \leftrightarrow P$. The second type of source term influencing gas–particle G_i on its trajectory are due to molecular fluxes, which are modelled by means of stochastic Langevin and Dopazo equations [4].

Using the same methodology, the deterministic equations for individual solid particles read:

$$\frac{D^{P_k} m_{P_k}}{Dt} = -\mathcal{Q}_{G \leftrightarrow P_k}\,, \qquad m_{P_k}\frac{D^{P_k}\mathbf{v}_{P_k}}{Dt} \;=\; -\mathcal{R}_{G \leftrightarrow P_k}\,, \qquad m_{P_k}\,\frac{D^{P_k} h_{P_k}}{Dt} = -\mathcal{S}_{G \leftrightarrow P_k}\,. \tag{3}$$

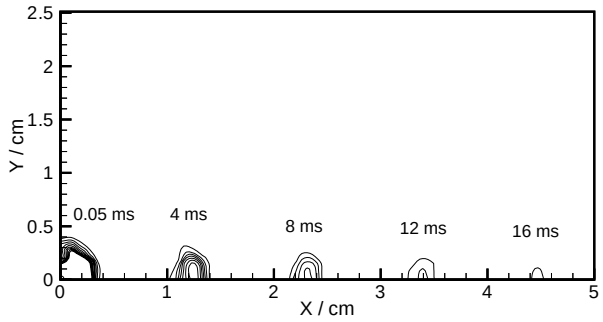
Due to computational limitations one cannot calculate the dynamics of every condensed phase particle. Thefore we define "pseudo condensed phase (cp–) particles" $\tilde{P}_k, k = 1, \ldots, N_{\tilde{P}}$, which represent clouds of real condensed phase particles. Pseudo cp–particles move in space and interact with the gas phase like individual real particles, but their effect on the gas phase is amplified by the number of real particles they represent. The interaction between both phases is restricted to the vicinity of pseudo cp–particles by the definition of an "action–sphere" which is attached to every pseudo cp–particle. This means that only those gas and pseudo cp–particles interact with each other, which are inside the same action-sphere.

Results

The details of this approach and first test implementations for non-flowing systems of isotropic and homogeneous turbulence are described in [7].

This paper shows results for flowing systems. The evolution of an ignition kernel is investigated which is transported in a turbulent flow field. Calculations are performed for a premixed methane/air mixture, a turbulent air flow, and an air/dust mixture. Dust particles are assumed to be spherical with a diameter of 50 μm and a loading ratio of 90 g/m^3. Devolatilization of particles is modelled by assuming release of CO. Homogeneous and heterogeneous reactions are included in the model by one–step reactions. The reaction rates determining devolatilisation, homogeneous, and heterogeneous reactions are described by Arrhenius laws.

Figure 1 shows the strong influence of particles on the evolution of the flame. In the case without dust particles (left), the hot temperature region diffuses rapidly, whereas with dispersed particles (right), the air/particle mixture is ignited and a flame is convected downstream. This flame grows due to intensive heat



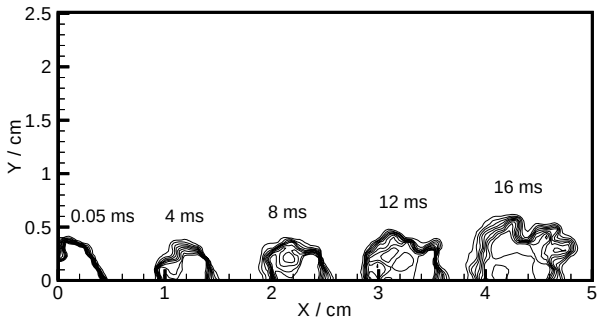


Figure 1: Lines of constant temperature in X/Y–plane for five points in time for air (left) and an air/particle mixture (right). Turbulence is characterized by constant values of k = 0.01 J/kg and $\epsilon = 9.8\ J/kg\ s$. Isolines range from 300 K to a maximum of about 2000 K in steps of 120 K.

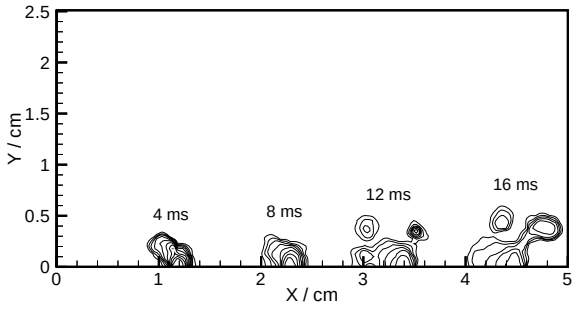


Figure 2: Lines of constant CO mass fraction in the X/Y–plane for five time steps for an air/dust mixture. Turbulence is charakterized by constant values of k = 0.01 J/kg and $\epsilon = 9.8\ J/kg\ s$.

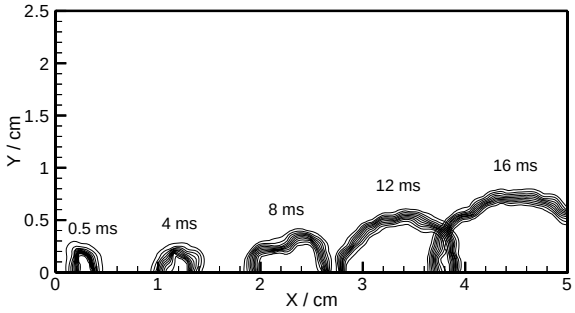


Figure 3: Lines of constant temperature in X/Y–plane for five time steps for a methane/air mixture of equivalence ratio 0.58. Turbulence is charakterized by constant values of k = 0.01 J/kg and $\epsilon = 9.8\ J/kg\ s$.

release by homogeneous burning of devolatilized CO and heterogeneous reactions on the surface of condensed particles. The local influence of particles is clearly indicated by the highly convoluted flame front and by the distribution of devolatilized, unburned CO shown in Fig. 2. Very similar flame structures have been observed experimentally [2].

The evolution of a flame kernel in a premixed methane/air mixture of equivalence ratio $\Phi = 0.58$ is shown in Fig. 3. The computed turbulent burning velocity is about 0.61 ms^{-1}, which is slightly less than the experimentally obtained value of 0.625 ms^{-1} for similar conditions [2]. The computed temperature of burned products is 1623 K, which is 3 K less than the adiabatic burning temperature obtained from the Chemkin code [3].

Conclusions

A new method for modelling two-phase turbulent reactive flows is applied to isotropic, homogeneous turbulence. Contrary to existing approaches, the method is based on considering both interacting continua in Lagrangian manner. In this formulation, gas and condensed phase properties are calculated along the trajectories of "particles" representing the system. The method is applied to turbulent premixed and non-premixed reactive systems with and without dispersed particles. The computed results show very good agreement with experimental data. The calculations indicate that the method is capable of providing information on the local structure of combustion zones with species formation and transport. Furthermore it is applicable independent of the combustion mode in the gas phase, *i.e.* no assumption regarding the degree of premixedness is required.

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