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

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Abstract

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 scales 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].

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 was successful in circumventing 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 (*GP–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 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 as shown in figure 1.

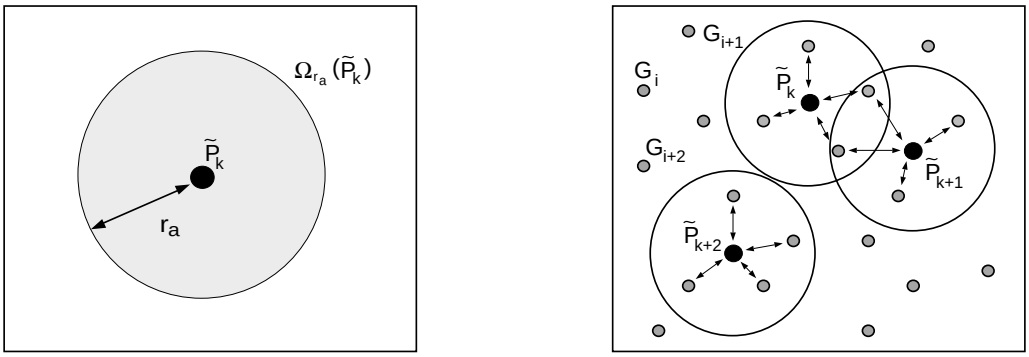

Figure 1: Left: Action sphere, $\Omega_{r_a}(\tilde{P}_k)$, attached to a pseudo condensed phase (CP) particle, $\tilde{P}_k$
Right: Interaction of three pseudo CP–particles with GP–particles, G_i, located inside their action spheres.

This means that only those gas and pseudo CP–particles interact with each other, which are inside the same action-sphere.

Results of test implementation

First test implementations for two-phase combustion in non-flowing systems of isotropic and homogeneous turbulence are described in a previous work [7]. This paper shows results for flowing systems, with initial and boundary conditions similar to those used for experimental studies [2]. The evolution of a hot spot is investigated which is transported in a turbulent flow field. Calculations are performed for a turbulent air flow and a premixed methane/air mixture with and without reactive particles.

Initial and boundary conditions

A schematic diagram of the computational set-up under consideration is sketched in figure 2.

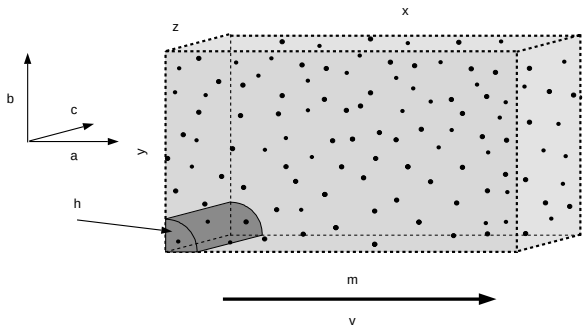

Figure 2: Sketch of boundary conditions: open volume of a methane/air mixture enriched with CO–devolatilizing reactive particles. The darker region in the lower left corner represents a hot spot, which is initially of higher temperature than the bulk volume.

The figure shows on open volume of length 5 cm, heigth 2.5 cm, and depth 1 mm. The gas/particle mixture flows with an uniform mean velocity of 2.5 m/s in the x-direction under conditions of isotropic constant turbulence. Calculation were made for four different mixture compositions:

(1) turbulent air flow,

(2) turbulent air/particle flow,

(3) turbulent lean methane/air flow,

(4) turbulent lean methane/air/particle flow.

Initially the temperature in the bulk volume is 300 K and the temperature in the lower left corner of the volume is set to a higher value to represent the hot spot. The temperature value of this hot spot is 2200 K for calculations (1) and (2) and 1700 K for calculations (3) and (4), respectivly. The composition in the hot spot is assumed to be in thermochemical equilibrium.

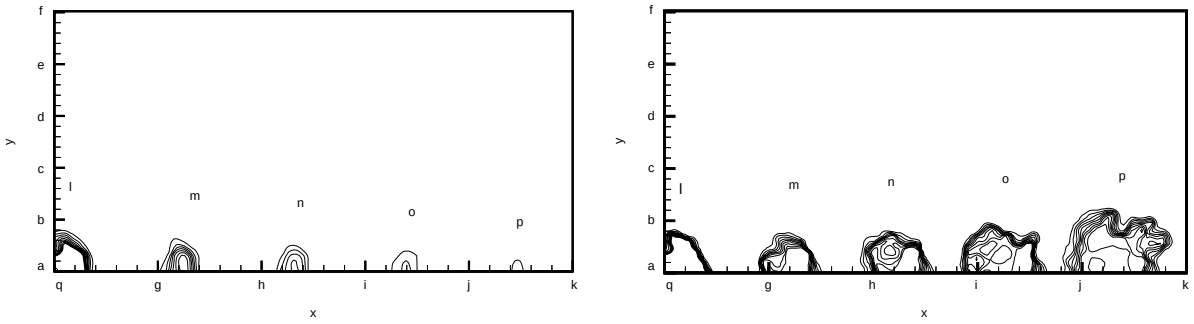

Figure 3: Turbulent air flow ($k = 0.01\,\mathrm{J/kg}$, $\epsilon = 9.8\,\mathrm{J/kg\,s}$) without particles (left part) and with particles (right part) with an initial hot spot of $T = 2200\,\mathrm{K}$. Lines of constant temperature for five time steps. The outer isoline corresponds to $T = 420\,\mathrm{K}$.

Evolution of the Hot Spot

The evolution of the hot spot in the turbulent flow field is illustrated in Figs. 3 and 4 for the four different mixtures. Each figure shows lines of constant temperature in the x/y–plane for five points in time. Common to all four mixtures is the convective transport of the flame with a mean velocity of 2.5 m/s. But the evolution of the shape of the hot spot is completely different in all four cases.

In turbulent air (left part of Fig. 3) the hot temperature region diffuses isotropically due to turbulent mixing processes. After 16 ms the maximum local temperature in the volume is less than 540 K. Without any fuel supply, the hot spot is dispersed in the non–reactive gas flow.

If particles are added to the turbulent air flow (right part of Fig. 3), the mixture is ignited by the hot spot and the maximum temperature in the flame rises up to about 2260 K due to intensive heat release by homogeneous burning of the devolatilized CO and heterogeneous reactions at the surface of the particles. The isotherms of the reaction zone of this flame are convoluted, which indicates an irregular structure of the flame front due to a local, non-uniform influence of particles. Very similar flame structures have been observed experimentally [2].

Turbulence on its own would not directly result in the convolution of the flame front, because turbulence is assumed to be isotropic. This is consistent with calculations made for a methane/air mixture of equivalence ratio 0.58 as shown in the left part of Fig. 4. In this case the structure of the reaction zone is much more smooth and non-wrinkled. The computed turbulent burning velocity is 0.61 m/s, which is slightly less than the experimentally obtained value of 0.625 m/s for similar conditions [2]. The computation shows the total consumption of methane in a thin flame front and leads to a temperature of burned products of 1623 K, which is 3 K less than the adiabatic burning temperature obtained from the Chemkin code [3].

In a forth calculation, particles are added to the methane/air mixture (Fig. 4, right side). The simulation shows a more rapid growth of the flame, a regular, non-convoluted shape of the reaction front, and a non-uniform temperature distribution in the region of burned methane. The temperature evolution in the flame front is dominated by the spatially homogeneous burning of methane. Particles do significantly disturb the shape of the flame front because of the timed elay needed to heat the particles until they significantly start to devolatilize CO. This fuel is spatially inhomogeneously burned in a secondary step with the oxygen remaining from the methane combustion.

Conclusions

A new method for two-phase turbulent reactive flow modelling has been developed and 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 incorporates the intrinsic feature of the exchange processes between the fluid– and the particle–phase, that is *the finite dynamic depth of interphase fluxes*.

Numerical calculations were performed to investigate the evolution of a hot spot in a turbulent air and methane/air flow with and without particles. The calculations show the strong local influence of individual particle clouds on the evolution of the hot spot. In the case of turbulent air flow, the addition of particles leads to the ignition of the mixture and a flame ball develops, which consists of a convoluted

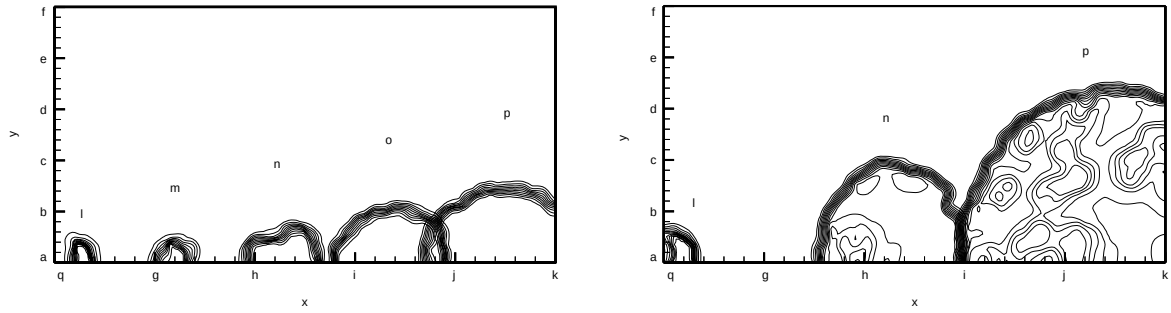

Figure 4: Turbulent methane/air flow ($k = 0.01\,\mathrm{J/kg}$, $\epsilon = 9.8\,\mathrm{J/kg\,s}$) without particles (left part) and with particles (right part) with an initial hot spot of $T = 1700\,\mathrm{K}$. Lines of constant temperature for five time steps. The outer isoline corresponds to $T = 420\,\mathrm{K}$.

flame front and a non-homogeneous temperature distribution behind this front. The addition of particles to the premixed methane/air flow also has a strong influence on the reaction activity in the system. First, the burning velocity of the flame is enhanced by the addition of CO–devolatilizing, reactive particles, and second, the local addition of this fuel leads to a secondary type of combustion, which is diffusion controlled and mainly concentrated to the vicinity of individual particle clouds or enveloping groups of particle clouds.

These numerical tests indicate that the method is capable of providing information on the local structure of combustion zones with species formation and transport. The method provides extensive statistics of various correlations of properties and 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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