Influences of Obstacles to Burning-out Rate of Mixture in a Closed Vessel

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1 Introduction

A fictitious domain method (FDM) allows to compute in a regular domains using a regular meshes independently of the geometry of the actual domains. The main reason for popularity of FDM is that they allow using of fairly structured meshes on a simple shape of fictitious domain containing the actual one, therefore allows using of fast solvers. The stability condition of the resulting scheme is the same as the one of the finite difference scheme. Up to now FDM was used for problems of physics with Dirichlet boundary conditions. But many problems of science are Neumann problems and applications of FDM to them have peculiarities.

In this work FDM extended and implemented for reactive flow problems in a non-regular domains. The most prominent example of those problems is the propagation of flame in a tube with obstacles. A computer code has been developed to describe the propagation of laminar flames in closed vessel with obstacles of different shapes and various locations. Evolution of the average pressure, buning-out rate, velocity, vorticity, and temperature in the vessel are calculated. The obtained results are compared with numerical data of authors obtained without FDM and experimental data available in the literature. The efficiency of FDM for combustion problems in non-regular domain is demonstrated.

2 Computations

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It is considered the cases when 2D flame propagates in a closed rectangular tube with length L and a cross section of 2hx2h and we focus our attention to study the hydrodynamic structure of the flame and influence of obstacles to the burning rate. The combustible gas is a stoichiometric methane-air mixture. The study is based on the assumption of a low Mach number flow and uses a one-step global chemistry model of the methane-air laminar flame. The problem is simulated using unsteady conservation equations of energy, species, mass, momentum and equation of state. The transport coefficients, thermodynamic data, kinetic coefficients and numerical algorithm are given elsewhere [1]. The fictitious transport coefficients are

$$\lambda^{\mathcal{E}}(\vec{x}) = \begin{cases} \lambda, & \text{if } \vec{x} \in \Omega \\ \varepsilon, & \text{if } \vec{x} \in \Omega_f \end{cases}, \quad D^{\mathcal{E}}(\vec{x}) = \begin{cases} D, & \text{if } \vec{x} \in \Omega \\ \varepsilon, & \text{if } \vec{x} \in \Omega_f \end{cases}, \quad \xi^{\varepsilon}(\vec{x}) = \begin{cases} 0, & x \in \Omega \\ 1/\varepsilon, & \vec{x} \in \Omega_f \end{cases},$$

where λ is the heat conductivity, D is the diffusion coefficient, Ω is the actual flow domain, Ω_f is the fictitious domain (obstacle domain), ε is the small positive parameter. The term $-\xi^{\varepsilon} \overline{v}$ added to the right hand side of momentum equation and provides vanishing of flow velocity into the fictitious domain. Boundary conditions are non-slip and heat- and mass isolated at the solid boundaries and symmetric at the symmetry line. At initial time

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the gas mixture is at rest at a temperature of 300 K and pressure of $P_t(0)=P_0=10^5 Pa$, $p_d=0$, $\varepsilon = 10^{-6}$. A line igniter placed near the left side wall and perpendicular to the x-y plane.

The numerical technique consist two steps. In the first step the transport equations for enthalpy and mass fraction of methane are solved by a Crank-Nicolson scheme, then temperature is calculated from the caloric equation and density – from the equation of state. In the closing step, the velocity and the dynamic pressure fields are obtained from Navier-Stokes equations in the low Mach number limit using a projection method for a known value of the density. At that for each numerical time step the intermediate value of velosity \vec{V}^* is calculated in the usual way and the final value of velosity is calculated from the next term $\vec{V}^{n+1} = \psi^{\varepsilon} (\vec{V}^* - \nabla \Pi^{n+1})$, where $\psi^{\varepsilon} (x) = (1 + \tau \xi^{\varepsilon} (\vec{x}))^{-1}$, $\Pi = p + \frac{2}{3} \mu \operatorname{div} \vec{V}$, τ is numerical time $(1, if \ \vec{x} \in \Omega)$

step. Thus $\psi^{\varepsilon}(x) = (1 + \tau \xi^{\varepsilon}(\vec{x}))^{-1} = \begin{cases} 1, & \text{if } \vec{x} \in \Omega \\ \varepsilon/(\varepsilon + \tau), & \text{if } \vec{x} \in \Omega_f \end{cases}$, and if $\varepsilon \to 0$ then

 $\psi^{\mathcal{E}}(\vec{x}) \to H(\vec{x}) = \begin{cases} 1, & \text{if } \vec{x} \in \Omega \\ 0, & \text{if } \vec{x} \in \Omega_f \end{cases}$ which is coincident with ordinary projection method for actual domain.

3 Results

The calculations are performed on a uniform mesh $\Delta x = \Delta y = 0.05mm$ which provides a fine resolution of the flame front including preheat and reaction zones. The efficiency (in terms of computer cost) and accuracy of the fictitious domain method is demonstrated by comparing FDM results with ones which obtained without FDM. A good agreement between results of two ways is found (Fig. 1) at the same stability condition of the resulting finite difference scheme. Snapshots demonstrate the influence of the three flat plates mounted at various distances from the bottom side wall (from the ignition point) on the propagation of the enclosed flame. Similar to experiments of [2] the flame flattening as it approaches the first obstacle, jetting past the obstacles, turning behind the obstacles, and the flame reconnection. Despite the fact that in the experiment flow was turbulent the flame shape around and behind of the obstacles is predicted very well. In particular the three flat flames approach each other in a certain order behind the obstacles as in the experiment.



Fig. 1 Comparison of flame positions and flow velocity obtained with (left snapshots) and without FDM (right snapshots)

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Simulations are performed for different types of obstacles:

a) a flat plate with a height of h/2 placed at the walls of the vessel at various distances from the ignition point, the blockage ratio (*BR*) of obstacles is 0.5;

b) a flat plate with a height of h placed at the center of the vessel at various distances from the ignition point, BR=0.5;

c) a new moon like obstacles mounted at the center of vessel at various

distances;

d) a circular wire grid 2*h* in height with a mesh width of h/3.3 and wire diameter of h/10 placed across the vessel, BR=0.3.

In cases a) and b) in agreement with experiments [3] it is found that (Fig. 2a, b):

the mixture burning out is distinctly differing in depend of the position of obstacles;

the fastest mixture burning out occurs when a plate obstacle placed at the distance 0.6L from the ignition point, then 0.4L;

the real tulip formation occurs only when the obstacle is placed close to end-flanges;

the flame front refraction takes place when a plate obstacle placed at the midway between end-flanges;

the strongest pressure jump takes place when a plate obstacle placed at the distance 0.6L from the ignition point. In addition the arising an isolated burning zone around the obstacle is established and the baroclinic vorticity generating and increasing at the refracting flame is observed.



Fig. 2 The average pressure records (P/Po) and unburned fuel fraction (M/Mo) in cases of the flat plates placed: a) at the walls of the vessel and b) at the center of the vessel at four distances from the ignition point. I – $X_{obs}/L=0.154$; II – $X_{obs}/L=0.4$; III – $X_{obs}/L=0.6$; IV – $X_{obs}/L=0.85$.

Simulations are performed for circular, co-flow and contra-flow new moon like obstacles mounted at the axis of vessel too. In Fig. 3 shown the average pressure records P/Po and unburned fuel fraction M/Mo in cases a new moon like obstacles mounted at various distances from the ignition point. It is found that the mixture burning out is distinctly differing in depend of the number of obstacles



Fig. 3 The average pressure records P/Po and unburned fuel fraction M/Mo in cases a new moon like obstacles mounted at the center of vessel at various distances from the ignition point. I – one obstacle mounted at the distance L/3.5 from the ignition point; II – two obstacles mounted at the distances L/3.5 and 2L/3.5; III – three obstacles mounted at the distances L/3.5, and 3L/3.5, BR=0.5.

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Fig.5 The flame propagates through a circular wire grid mounted at 88mm from the point of ignition.

The propagation of flames through a circular wire grid mounted at 88*mm* from the point of ignition is illustrated in Fig.5. The developing of flame front depends completely from the vorticity field generated by grids. After the passing through grid the flame was split into three flamelets as number of circular wires. The burning rate is increasing noticeably at this time.

4 Conclusions

The fictitious domain method to simulate reactive flow problems in non-regular domains is elaborated. The efficiency of the fictitious domain method is demonstrated.

The obtained results on flame propagation in a closed vessel with obstacles are compared with experimental data available in the literature and showing well agreement with them.

A generalization to 3D space, to multicomponent flows and detailed chemistry is straightforward within the framework of our method and will be studied in the near future.

References

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