Effect Of Radiation Preheating On Dynamics of Wrinkled Flames

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1 Introduction

Actualisation of the deflagration to detonation transition (DDT) in a combustible gaseous mixture depends on a variety of circumstances and may develop in a number of physical scenarios. Among all of these scenarios, the mechanisms not involving interference from effects, substances and objects external to the released fuel, i.e. incident shock waves, jets, particular geometry of nearby walls and objects, pose special interest.

Probably the first successful attempt to explain possible mechanism of self-initiated DDT was the idea of the promoting temperature gradient. According to [1], temperature gradient in the reacting media results in a gradient of induction times of chemical reactions. If the gradient of the latter matches the speed of propagation of the reaction front, then the synergy of the two processes may transform the flame into a detonation wave.

Consideration of time scales specific to heat transfer via conduction and radiation, shows that the most likely heat transfer mode which is able to modify the temperature gradient is radiation [2]. Normally, gaseous fuels do not absorb radiative heat significantly, however even minor quantities of water vapour can change this behaviour dramatically. Moreover, fine aerosol and dust fuels often are good radiation heat absorbents.

The depth of the wrinkles of spherical flames reaches up to 1/10-th of the averaged flame radius, see e.g. [3]. This suggests that unburnt fluid particles may spend significant time inside the wrinkle before reaching the flame front itself. Thus, preheating of the unburnt mixture, traveling inside the wrinkles, with the heat radiation from surrounding flame surfaces might be significant.

In what follows we investigate if the effect of radiation preheating is able to trigger the DDT. A Navier-Stokes based numerical model and results of a set of computer simulations of the phenomena in question are presented. They indicate that the DDT in combustible mixtures with essential heat emissivity and absorption is possible. Physical mechanism of such heat radiation triggered self-initiated DDT 's is explained too.

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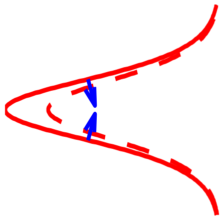

Figure 1: Formation of an optimal temperature gradient by radiation preheating.

2 Mathematical model and its numerical implementation

Numerical simulations of dynamics of deflagration fronts in presence of intensive radiation preheating was studied in the case of planar flames propagating in tubes open from one end. The approach used Navier-Stokes description of compressible fluid and employed drastically simplified chemistry and radiation models. The governing equations can be written as follows

$$\frac{\partial V}{\partial t} + \frac{\partial \mathcal{F}(V)}{\partial x_1} + \frac{\partial \mathcal{G}(V)}{\partial x_2} = \frac{\partial \mathcal{F}^{(d)}(V)}{\partial x_1} + \frac{\partial \mathcal{G}^{(d)}(V)}{\partial x_2} + \mathcal{Q}(V),$$

where $V = \left[\rho, \rho u_1, \rho u_2, \frac{\rho T}{\gamma - 1} + \frac{\gamma M^2}{2}\rho\left(u_1^2 + u_2^2\right), \rho Y\right]$. Formulas for convective $\mathcal{F}(V)$, $\mathcal{G}(V)$, and dissipative $\mathcal{F}^{(d)}(V)$, $\mathcal{G}^{(d)}(V)$ fluxes can be found elsewhere. The source term $\mathcal{Q}(V)$ is combined of contributions from chemistry and radiation. Tube diameter d and laminar burning speed relevant to the burnt gases u_b were used as scales, so that the Mach number $M = \dfrac{u_b}{a_0}$, where a_0 is the speed of sound in the fuel at initial temperature T_0. Other nondimensional governing parameters used were the Reynolds number $Re = \dfrac{\rho_0 u_b d}{\mu}$, $T_a = \dfrac{E_a}{RT_0}$, and $Q = \dfrac{\bar{Q}}{c_v T_0}$. Prandtl $Pr = \dfrac{c_p \mu}{\kappa}$ and Lewis $Le = \dfrac{\kappa}{c_p D \rho_0}$ numbers were set to one.

Chemistry was modelled with a single irreversible $\mathcal{A} \to \mathcal{B}$ reaction of Arrhenius type. The radiation model was reduced to the heat flux driven by temperature according to the Stefan-Boltzmann law. In addition, emission by cold gas and gas too far away from the flame as well as absorption by hot gas and gas too far away from the flame were not taken into account, because gases in those areas are in nearly thermodynamical equilibrium from the view point of radiation. In spite of its roughness, the model governs interaction of all relevant energy fluxes reasonably well.

The governing equations of the model were solved with a high order upwind shock capturing finite difference scheme without any fractional steps. Numerical approximation is implicit in the stream-wise coordinate, and is explicit in the other one, similar to [4], providing satisfactory compromise between limitations of numerical stability and efficient parallelization. Computational domain was moving together with the flame front and absorbing boundary conditions were implemented on its up- and downstream boundaries. The resulting code is reasonably efficient for Mach numbers greater than 0.01, Reynolds numbers less than 1000, and for the nondimensional activation energy T_a less than 50.

3 Computer simulations

In our numerical simulations self-initiation of DDT never took place in smooth open pipes without obstacles and absorption of radiation heat. On the other hand, significant absorption of radiation heat was able to alter behavior of the flame front dramatically. It was found that self-initiation of DDT in radiation heat absorbing media progresses via formation of an optimal temperature gradient on the sides of wrinkles on the flame surface. Successful DDT was resulting from interaction ("collision") of two flame segments accelerating through such promoting temperature gradients as illustrated in Fig 1. Zone of intensive chemical reaction is indicated with a solid line in there, while the boundary of the layer of unburnt gas at essentially elevated temperature is shown with a dashed line. Normals to the flame surface indicate presence of parts of the preheated layer in which structure of the temperature gradient is the most advantageous for the deflagration front to transform into a detonation wave. Appearance of such a thick preheated layer of the unburnt gas can be seen in the second row in Fig. 3 as well.

Sufficient amount of fuel available between two opposing flame segments of the wrinkle is critical for success of the DDT. In addition, the effect is sensitive to the shape of the flame front, which in turn depends on a set of governing parameters of the problem. For example, chemical reactions of orders higher than one widen range of flames able to experience the DDT significantly, confirming observations [5].

In contrast to expectations based on common sense, success of the self-initiated DDT depends on the depth of the flame wrinkle in a lesser degree. The self-initiated DDT based on the mechanism just described might work for much smaller flames. An asymptotic estimation of the critical radius of outward propagating unconfined flames for this new self-initiated DDT mechanism is possible, but would deserve a separate investigation.

As absorption rate grows, flame dynamics evolves through a sequence of distinctive regimes. First, the flame is not affected by the radiation at all. Rise of the absorption rate leads to formation of promoting temperature gradients able to generate powerful compression waves. However, these temperature gradients are insufficient to allow for proper acceleration of deflagration fronts yet and generated compression waves are not strong enough to maintain supersonic combustion behind them. As a result, the steady flame propagation is altered by a sequence of failed detonations as illustrated in Fig. 2. The last row of the figure shows a weak compression wave rushing away from the flame front, which remains subsonic.

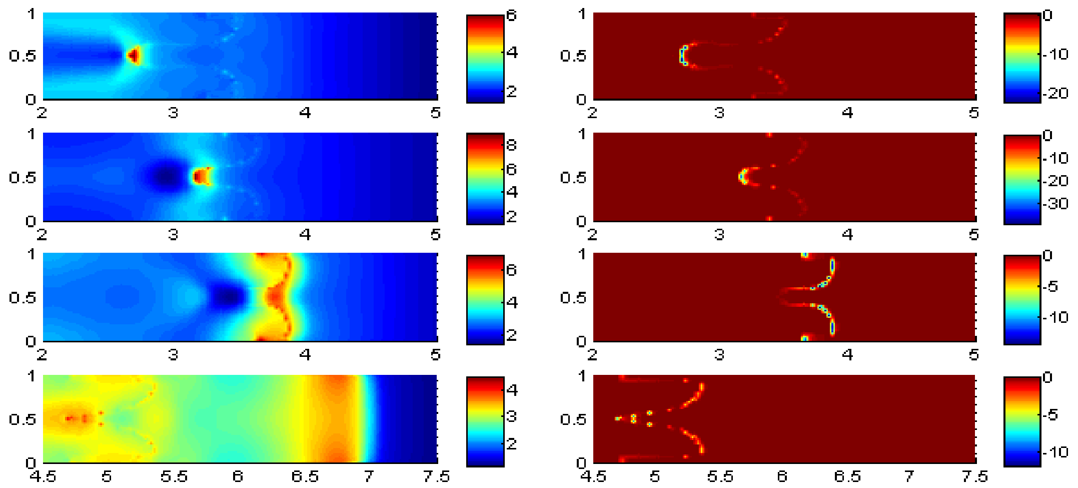

Figure 2: Example of evolution of pressure (left) and reaction rate (right) fields in the failed self-initiation of DDT.

Eventually, when absorption rate is high enough, stable self-initiated DDT takes place [2] as this is illustrated in Fig 3. The first row depicts the flame just before the DDT. The next row illustrates formation of the preheated layer of the unburnt gas in front of the flame. Soon after events begin to unfold really fast. The third row shows the moment when a "micro-explosion" inside the wrinkle just took place. Generated powerful compression wave kick starts the detonation front shown in the following rows. Reminiscences of the shock waves brought forth by the opposing flame segments continue to interfere with the downstream propagating detonation front for some time as can be seen in the forth row of Fig. 3. However, they decay eventually and the detonation wave settles gradually to a perfect ZND detonation structure exemplified in the fifth row.

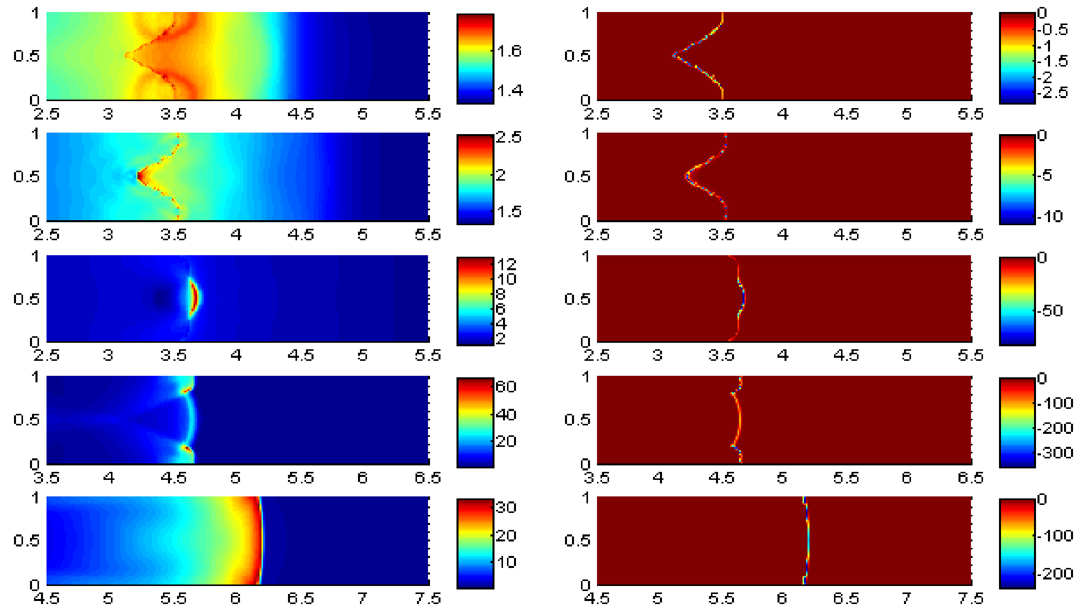

Figure 3: Example of evolution of pressure (left) and reaction rate (right) fields in the self-initiation of DDT.

Relatively low Reynolds numbers and activation energies were used in our numerical simulations. Character of changes as the Reynolds number grows does not suggest any problems up to transition to turbulence. The latter looks just a technical challenge rather than the undoer of the proposed DDT scenario. Changes in the character of flame dynamics when activation energy grows suggest just further shrinking of the range of absorption rate for which detonation repeatedly fails. The tendency explains lack of experimental observations of the regime of successively failing detonations.

4 Conclusions

A simple mathematical model of propagation of laminar flames in heat radiating and absorbing combustible gas was suggested and investigated numerically. As absorption rate grows, flame dynamics evolves through a sequence of regimes. Initially flame is not affected by the radiation. At certain rate of radiation heat absorption flame propagation is altered by a sequence of failed detonations. Eventually, stable self-initiated DDT takes place demonstrate plausibility of the idea of the radiation preheating as the principal effect in the self-initiated DDT .

Practical realization of the self-initiated DDT mechanism in question is expected for mixtures containing water vapour, fine liquid sprays and dusts because variation of concentration of the admixtures affects values of the dissipation factor in a very wide range. Many experimentalists report that moist atmospheres increase chances of DDT significantly, see e.g. [6]. However, in practice, choice of mixtures with required properties might be limited and further experimental validation of the proposed mechanism of DDT is required.

References

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