Radiation preheating can trigger transition from deflagration to detonation

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Abstract

In this article effect of radiation preheating of unburnt mixture by propagating deflagration front is studied from the viewpoint of its ability to form a promoting temperature gradient and trigger transition to detonation. First, we investigate the effect of radiation preheating of the unburnt mixtures, when they are traveling through the wrinkles on the flame surface, in order to estimate a possibility of significant temperature rise. Subsequently, numerical simulations of a simplified mathematical model are carried out. They demonstrate plausibility of the proposed mechanism of the deflagration to detonation transition.

Keywords: Premixed combustion, transition to detonation, DDT, radiation heat transfer.

1 Introduction

If a large amount of accidentally released gaseous fuel is within the limits of flammability and ignition takes place, a chance for transition of the deflagration front into the detonation wave (DDT) appears. Actualisation of the DDT 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. This is virtually the only possible mechanism of DDT in open atmosphere, and thus is especially important for safety in large storage and processing petrochemical plants and pipelines, see e.g. [1].

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Research in explosion safety usually assumes that principles of safety by design rule out powerful sources of ignition in explosion prone industrial environment leaving chances to more delicate mechanisms of the DDT. For example obstacles placed in the way of the deflagration front or incident shock waves, see e.g. [2][3]. Alternatively, they can be self-initiated.

Probably the first successful attempt to explain possible mechanism of self-initiated DDT was the idea of the promoting temperature gradient. According to [4], 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. This scenario was carefully investigated in a number of later studies, see e.g. [5], where an idealized medium with simple, rate-sensitive kinetics and an initially prescribed linear gradient of temperature was studied exhaustively.

Once it was understood that temperature nonuniformities may induce transition to detonation, an investigation of possible physical mechanisms leading to such uniformities was undertaken. Amongst theoretical achievements in the area we would mention the concept of the equivalent drag force, which works to create temperature nonuniformities ahead of the flame front [6]. Numerical simulations demonstrating importance of the effect of viscous friction in the boundary layer [7] were carried out in relatively narrow channels. Although, further work [8] indicates that the effect remains relevant in quite realistic cases too.

Another approach is based on the collective thermal effect of shock waves generated in front of a very fast flame by the flame itself [9]. The theory looks feasible for flames, which are naturally very fast and, in addition, experience immense exponential acceleration. Both computational and experimental examples given in [9] demonstrate possibility of such exponential acceleration of flames in tubes up to supersonic propagation speeds with Mach numbers well in excess of one. At such speeds supersonic deflagration fronts are able to generate downstream shocks strong enough to change thermal and reactive properties of the fuel cardinaly. It is not clear how to extend these ideas to unconfined outward propagating flames.

1.1 Acceleration of expanding flames

It was discovered in [10], that expanding flames do accelerate. This acceleration was linked to appearance of wrinkles, as wrinkles increase flame surface area allowing to burn larger quantities of fuel and thus expand faster. Theoretical and numerical analysis, see e.g. [11][13], revealed physical mechanism and basic characteristics of the acceleration. It was established that flame fronts become extremely sensitive to the upstream velocity perturbations as their size grows. From
the physical point of view, the sensitivity of cellular flames to perturbations of the upstream flow velocity is explained by the possibility of a pseudoresonant interaction between them [14]. The pseudoresonant interaction amplifies certain upstream velocity perturbations and transforms them into pairs of coupled vortices of size proportional to the thermal flame thickness, which are located just behind the flame front. These pairs of vortices suck the unburnt gas into the areas occupied by the products of combustion and form wrinkles which significantly increase the bulk burning rate and hence the averaged flame propagation speed.

The power law of growth of the averaged flame radius \( \bar{r}(t) \propto (t - t_*)^\beta \) for large enough times \( t > t_* \), in accordance with the fractal analysis [15], was confirmed. Values of the power \( \beta \) depend on the dimension of the problem and equal 3/2 for three dimensional flames and 5/4 for two-dimensional ones. In expanding flames, the pseudoresonant interaction between the flame and the upstream flow velocity perturbations is weakened by stretch. As a result set up of the acceleration at \( t_* \) can be delayed significantly. On the other hand, permanent growth of the size of the flame results in its permanent acceleration unlike the non-stretched planar flames, which have a finite limit on their propagation speed [13]. Using a realistic set of dimensional parameters, e.g. planar flame speed relative to the burnt gases \( u_b = 0.5 \) m/s and thermal diffusivity \( D_{th} = 2.5 \times 10^{-5} \) m\(^2\)/s, our findings for \( t_* \) in dimensional terms can be put as \( \bar{r}(t_*) \approx 20 \) m.

Theoretically, continuous acceleration of the flame should lead to supersonic speeds and further to DDT. However, the rate of expansion of spherical flames \( \bar{r}(t) \propto (t - t_*)^{3/2} \), is so slow that even an optimistic estimation, e.g. assuming initial flame expansion rate of about \( v_0 \approx 66 \) m/s for flame of averaged radius \( r_0 \approx 20 \) m, gives flame radius \( \bar{r} \) of order of \( r_0(v/v_0)^{3} \approx 2.5 \) km for which supersonic speeds \( v \approx 330 \) m/s can be reached. This means that if self-initiated DDT of expanding flames takes place at all, it should be assisted, and even more likely dominated, by an effect other than flame acceleration.

### 1.2 Radiation preheating

Upon realizing that flame acceleration due to flame cellularization alone cannot lead to self-initiated DDT, appearance of a promoting temperature gradient in front of expanding flames looks the only factor which can. The question is how such temperature gradient can be generated in front of the expanding flame? 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. Normally, gaseous fuels do not absorb radiative heat significantly, however even minute quantities of water vapour can change this behaviour dramatically. Moreover, fine aerosol and dust fuels often are good
radiation heat absorbents. Initiation of detonation by ultraviolet radiation was demonstrated in [16], where the radiation was an external factor and its direct action was photochemical rather than the thermal one.

Calculations show that the depth of the wrinkles on two-dimensional circular flame surface reaches up to 1/10-th of the averaged flame radius. Comparison with the three-dimensional spherical flames shows that the latter expand and grow cellular structures even faster, see Fig. 1 from [12]. Their cellular structures are better developed and wrinkles are even deeper. This suggests that some 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 important.

![Figure 1](image.png)

Figure 1: Development of a fractal structure on surface of circular flame (left). Comparison of the circular flame and the equatorial cross-section of the three-dimensional spherical flame at nearly the same time instances (right).

In this work we carry out tentative estimations of a possibility of the effect of radiation preheating to trigger the DDT. In Section 2 we consider a simple analytical model of the phenomena confirming a possibility of significant growth of temperature due to radiation in deep enough wrinkles. Further, in Section 3 a Navier-Stokes based numerical model is presented. Results of a set of computer simulations of the phenomena in question are discussed in Section 4, indicating 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.
2 Preliminary estimations

2.1 Heat balance equation

Let us assume that a combustible fluid particle $P$ is moving inside a flame wrinkle and estimate its temperature growth because of heat radiated from hot flame. The estimation will be by order of amplitude, similar to that one outlined in [17]. For the sake of simplicity the products of combustion are assumed at the same uniform temperature $T_W$ and particle $P$ is not very close to the flame yet. Under this conditions, the only heat which matters is the heat from the flame absorbed by the particle. All other elements of the radiating system are in nearly thermodynamical equilibrium and radiation heat exchange between them can be neglected. Furthermore, the wrinkle will be modelled as a conical cavern of depth $L$ and of the apex semi-angle $\alpha$, see Fig. 2. Under assumptions in question, variations of the geometry of the wrinkle result just in a coefficient of order one and are not essential.

![Figure 2: Model of a wrinkle on the surface of an expanding flame.](image)

Every element $W$ of area $dA_W$ of the cone surface radiates heat according to the Stefan-Boltzmann law with the coefficient of emissivity $\varepsilon_W$. So that heat radiated per unit time is $\left. \frac{dE}{dt} \right|_W = \varepsilon_W \sigma T_W^4 dA_W$. The heat is transferred from $W$ to $P$, which is at a distance $l$, dissipating according to the exponential law with
the dissipation factor $\chi$. It means that heat radiated from point $W$ per unit time will be weakened by $e^{-\rho_a x l}$ times upon travelling through distance $l$. Here $\rho_a$ is the density of the absorbing species, which might be quite different from the averaged density $\rho$ of the combustible mixture.

The heat flux incident on the fluid particle $P$ of cross-section area $dA_P$ is the areal fraction $dA_P/(2\pi l^2)$ of the radiation energy which reaches $P$ after being radiated from $W$ is
$$\frac{dE}{dt}\bigg|_{W \to P} = \frac{dA_P}{2\pi l^2} e^{-\rho_a x l}\varepsilon_W T_W^4 dA_W.$$ Hence, the fraction of this radiation heat which will dissipate within the small fluid particle $P$ of thickness $dl$ is
$$\frac{dE}{dt}\bigg|_{P \to W} = \frac{dA_P}{2\pi l^2} (\rho_a x dl) e^{-\rho_a x l} (\varepsilon_W T_W^4) dA_W.$$ Denoting volume of the fluid particle $P$ as $dV = dA_P dl$, the total rate of heat gain of the fluid particle $P$ is
$$\frac{dE_P}{dV dt} = \frac{\varepsilon_W \rho a x T_W^4}{2\pi} \int A_W l^{-2} e^{-\rho_a x l} dA_W.$$

Noticing that the $x, \xi$-averaged $l^2 = (\xi - x)^2 + (\xi - L)^2 (\tan \alpha)^2$ is proportional to $L^2$, $dA_W = \frac{L - \xi}{\cos \alpha} d\xi d\phi$, and that the integrand of the above integral is positive, the integral itself can be approximated as follows
$$\frac{dE_P}{dV dt} \approx \frac{\varepsilon_W \rho a x T_W^4}{2\pi c_g} e^{-\rho_a x l \sqrt{c_g \cos \alpha}}.$$

As temperature of the fluid particle grows due to radiation heating, intensity of chemical reaction starts to grow too. We estimate the rate of this heat release assuming an overall exothermic uni-molecular irreversible chemical reaction $A \rightarrow B$. For example, $A$ is a mixture of $CH_4$ and air and $B$ is a mixture of air, $CO_2$, and gaseous $H_2O$. If the reaction produces energy $Q$ per mole of reacted species $A$, then the heat release because of chemical reactions in the fluid particle per unit volume per unit time is $\rho \frac{dc_P T}{dT} = Q \rho' k_a e^{-\frac{E_a}{RT}}$, where $c_P$ is the specific heat capacity at constant pressure, $\nu$ is the order of the reaction, $k_a$ is the pre-exponential factor, and $E_a$ is the activation energy. Assuming that the fluid particle is moving toward the flame front with velocity $u_n$, we can replace time $t$ with $x = u_n t$:
$$c_P \rho u_n \frac{dT}{dx} = Q \rho' k_a e^{-\frac{E_a}{RT}}.$$

Combining heats produced by radiative heat flux from the flame surface (1) and chemical reactions (2):
$$\frac{d\Theta}{d\zeta} \approx q_e e^{\frac{\tau_a \Theta}{1+\tau_a}} + q_r,$$
where \( q_c = \frac{Q\rho^{-1}k_aLe^{-T_a}}{c_p u_n T_0} \), \( q_r = \frac{\varepsilon W \sigma T_W^4 \rho_a \chi L e^{-\rho_a \chi L \sqrt{T_a}}}{c_g \rho e c_p u_n T_0 \cos \alpha} \), \( T_a = \frac{E_a}{R T_0} \), \( \Theta = \frac{T - T_0}{T_0} \), and \( \zeta = \frac{x}{L} \).

2.2 Approximate solution

In the early stages of heating, fluid particle temperature does not differ from \( T_0 \) significantly and the Arrhenius exponent can be approximated as \( \exp \left( \frac{T_a \Theta}{1 + \Theta} \right) \approx e^{T_a \Theta} \). Then, the correspondingly approximated heat balance equation (3) is integrated exactly \( \Theta(\zeta) \approx -\frac{1}{T_a} \ln \left[ \left( 1 + \frac{q_c}{q_r} \right) e^{-q_r T_a \zeta} - \frac{q_c}{q_r} \right] \), yielding the solution blowup distance for \( \zeta = x/L \) equal

\[
\zeta^* \approx \frac{1}{q_r T_a} \ln \left( 1 + \frac{q_c}{q_r} \right). \tag{4}
\]

It is interesting to compare the latter to the blowup distance \( \zeta^*_0 \approx \frac{1}{q_c T_a} \) for \( q_r \equiv 0 \).

Considering parameters typical to combustion of hydrocarbons in air \( T_a = 80 \), \( Q/(c_p T_0) = 8 \), \( u_n = 0.5 \text{ m/s} \), \( k_a = 5 \times 10^{12} \text{ s}^{-1} \), \( \nu = 1 \), one obtains \( q_c \approx 2 \times 10^{-22} \text{ L}^{-1} \). Taking into account that function \( f(x) = xe^{-x} \) reaches its maximum equal \( e^{-1} \) for \( x = 1 \), we conclude that \( q_r \) is maximal for \( \rho_a \chi L = c_g^{-1/2} \) and this maximum is

\[
q_{r,\text{max}} \approx \frac{\varepsilon W}{e c_g^{3/2} \cos \alpha} \times \frac{\sigma T_W^4}{\rho e c_p u_n T_0}. \tag{5}
\]

Assuming that the first factor in (5) is about \( 1/2 \), \( \rho = 1 \text{ kg/m}^3 \) and \( T_W = 1500 \text{ K} \), one obtains from (4) that \( \zeta^* \approx 0.9 \) for \( L \gtrsim 1 \text{ m} \). Numerical integration of (3) shows that significant growth of temperatures can be reached for even smaller flames. According to our earlier analysis, wrinkles of depth \( 1 \text{ m} \) can appear on flames of radius \( r_c \gtrsim 10 \text{ m} \).

Our choice of \( \rho_a \chi L = c_g^{-1/2} \) may look artificial. However, it is not, because the value of the product is effectively controlled by the density \( \rho_a \) of the heat absorbing admixture and by the wrinkle depth \( L \). The former, is at the disposal of the experimentalist. For some particular species values of \( \rho_a \) suitable for efficient combustion might be limited and the limit may lie below the requirements of the efficient radiation heat absorption for given \( \chi \) and \( L \). Even so, required values of \( \rho_a \) can be always lowered below this limit for deeper wrinkles, i.e. for larger \( L \).

These simplified estimations were carried out for some “typical” values of combustion and heat transfer parameters and for an optimal radiation heat absorption. Thus, they just show that radiation preheating of fuel in front of the
deflagration flame might be significant in principle. Such temperature rise alone not necessarily leads to the DDT yet and more detailed numerical simulations are still required in order to validate the hypothesis. Furthermore, mixtures with such a combination of the parameters in question might be difficult to find in practice even if theoretical numerical simulations confirm that radiation preheating can cause the DDT.

As we have mentioned in Section 1.2, two heat transfer mechanisms potentially able to produce promoting temperature gradient are heat conduction and radiation. According to (5), the time scale of the radiation preheating over distances of order \( l_a = (\rho_a \chi)^{-1} \) is of order \( \tau_r = \frac{\rho c_p l_a}{\varepsilon_W \sigma T_W^3} \). In contrast, the time scale of heat transfer by conduction over the same distance is \( \tau_c = l_a^2 / \kappa \), where \( \kappa \) is the thermal diffusivity. By representing \( \kappa \propto \delta_{th} u_n \) in terms of the thermal flame thickness \( \delta_{th} \) and laminar burning velocity \( u_n \), the ratio of the time scales takes the form

\[
\frac{\tau_r}{\tau_c} = \frac{\rho c_p u_n}{\sigma T_W^3} \times \frac{\delta_{th}}{l_a} \varepsilon_W^{-1}.
\]

For gases value of \( \rho c_p \) is typically about \( 10^3 \) J/(m\(^3\)×K) and \( u_n \) is of order 1 m/s. Then, value of the Stefan-Boltzmann constant \( \sigma \approx 5.67 \times 10^{-8} \) kg/(s\(^3\)×K\(^4\)) and reasonable flame temperatures of at least \( T_W = 1800 \) K ensure that the first factor in (6) does not exceed 3. Hence, for typical gaseous fuels

\[
\frac{\tau_r}{\tau_c} = \frac{3}{\varepsilon_W} \times \frac{\delta_{th}}{l_a}.
\]  

(6)

Thickness of the preheated layer \( l_T \), which renders optimal temperature gradient, exceeds \( \delta_{th} \) by a few orders of magnitude [5]. Thus, for reasonably radiating flames, i.e. \( \varepsilon_W > 0.03 \), and if we manage to adjust \( \rho_a \) to make the dissipation length \( l_a \) match \( l_T \), radiation heat transfer will dominate conductivity.

Relationship between the leading time scales is getting more complicated for multi-component and especially for multiphase fuels. For example, if radiation absorbing and reacting species are different, then the speed of heat transfer between them should be taken into account too. Further complications are linked to the time scales of evaporation and pyrolysis processes, which are relevant to burning of mist and dust mixtures.

3 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 rather than for expanding spherical flames in the open. This geometrical simplification made it possible to carry out investigations with relatively limited resources.

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

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

where $V = [\rho, \rho u_1, \rho u_2, \rho \frac{T}{\gamma - 1} + \gamma \frac{M^2}{2} \rho (u_1^2 + u_2^2), \rho Y]$. Formulas for convective $F(V)$, $G(V)$, and dissipative $F^{(d)}(V)$, $G^{(d)}(V)$ fluxes can be found elsewhere. The source term $Q(V)$ 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 $M = \frac{u_b}{a_0}$, 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 $Re = \frac{\rho_0 u_b d}{\mu}$, $Ta = \frac{E_a}{RT_0}$, and $Q = \frac{\bar{Q}}{c_v T_0}$. Prandtl $Pr = \frac{c_p \mu}{\kappa}$ and Lewis $Le = \frac{\kappa}{c_v D \rho_0}$ numbers were set to one.

Chemistry was modelled with a single irreversible $A \rightarrow B$ reaction of Arrhenius type similar to the assumptions in Section 2.1. 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 [18], 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 $Ta$ less than 50.
4 Computer simulations and discussion

4.1 Numerical experiments

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 3. 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. 5 as well.

Figure 3: Formation of an optimal temperature gradient by radiation preheating.

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 suitable flames able to experience the DDT significantly, confirming earlier observations of other researchers, see e.g. [19]. Note, heat radiation from the flame not only heats up the unburnt fuel in front, but cools down the flame itself too, which levels out the gradient even faster.

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, which makes our estimation of critical flame radius of order $r_c \approx 10$ m in Section 2.2 less relevant. The self-initiated DDT based on the mechanism just described might work for much smaller flames. An asymptotic estimation of the critical radius of out-
ward 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. 4.

![Figure 4: Example of evolution of pressure (left) and reaction rate (right) fields in the failed self-initiation of DDT.](image)

Eventually, when absorption rate is high enough, stable self-initiated DDT takes place [20] as this is illustrated in Fig 5. 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. 5. However, they decay eventually and the detonation wave settles gradually to a perfect ZND detonation structure exemplified in the fifth row.

Effect of radiation heat transfer at very high radiation absorption rate was not
studied yet, but is believed to be similar to the case of high thermal conductivity. Hence, dynamics of the self-initiated DDT at very high radiation absorption rate is expected to be similar to the case when optimal temperature gradient is formed by means of heat conductivity rather than by the radiation heat transfer \( (6) \). It is interesting to note that the detonation initiations presented in \( [19] \) were obtained for rather high thermal conductivity and that the range of flame wrinkles, able to generate a detonation, widens as heat conductivity grows. All this can be explained in terms of formation of an optimal temperature gradient by means of conduction. It is also known that at high thermal conductivity flames lose ability to form properly shaped wrinkles and an artificial corrugated wall was needed in \( [19] \) to create them. Introduction of strong fuel diffusion, i.e. consideration of small Lewis numbers, see e.g. \( [21] \), might fix the problem too.

### 4.2 Critical analysis

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 \( \rho_a \chi \) in a very wide range. Many experimentalists report that moist atmospheres
increase chances of DDT significantly, see e.g. [22]. However, in practice, choice of mixtures with required properties might be limited. Moreover, mixtures with specific characteristics, which can be easily considered theoretically, may simply not exist in real at all. Hence, validation of practical usefulness of the proposed mechanism of DDT requires development of realistic chemical and heat radiation/absorption models. These models should be coupled, i.e. changes in the concentration of water vapours should affect not only rates of heat radiation and absorption in the mixture, but rates of chemical reactions as well. High enough concentration of water vapours will result in almost as high heat radiation/absorption rate as required, but at certain stage their excess will begin to slow down or even completely extinguish the flame.

On the other hand, once quite detailed chemistry is going to be considered, the heat radiation/absorption model has to be refined too. As concentration of water vapour changes, new intermediate species with special radiation properties may appear. Therefore, the heat radiation/absorption model should take into account the spectral structure of the radiation fluxes rather than their total energy alone. Furthermore, if heat absorbing and reacting species are not the same, then heat exchange between them should be taken into account too.

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.

Eventually, this investigation is based on a simplified geometrical model of the phenomena. The original problem of self-initiated DDT is a three-dimensional one and is in the open atmosphere, whereas only a planar two-dimensional combustion in a pipe was considered in this paper.

5 Conclusions

Possible temperature rise of gas fuel in front of propagating flame as a result of radiation heat transfer was estimated. The estimation demonstrated that temperature rise of fuel approaching flame inside a wrinkle can match the adiabatic burning temperature for relatively small flames of radii just 10 m as soon as the gas mixtures involved are able to emit and absorb radiation heat at high enough rate.

A variety of numerical experiments on flame dynamics in pipes open from one end was carried out as well. 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.
Undertaken simulations demonstrate plausibility of the idea of the radiation
preheating as the principal effect in the self-initiated DDT. However, the self-
initiated DDT is a very delicate phenomena. More accurate and detailed numerical
simulations are needed in order to clarify issues highlighted in this work.

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