# Birth and evolution of the gas dynamic disturbance and shock wave formation in spatially inhomogeneous self-igniting media

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## 1 Introduction

In the detonation science the problem of detonation initiation is important for safety (where the detonation must be prevented) and for development of the prospective aircraft engines (where reliable and repeatable detonation initiation is required). There are two approaches to detonation initiation. First is strong initiation, which is governed by the strength of the power source in the combustible mixture. There are no general problems to initiate detonation in this way (except of the choice of the source power due to economical reasons).

The second way is mild detonation initiation. Zel'dovich pointed out, that small disturbances in the explosive medium can generate detonation, and the energy deposited is much less than in the case of the strong initiation.

The problem of mild detonation initiation was addressed in the numerous researches (Zel'dovich et al., Gelfand et al., Makhviladze, Kapilla, Dold, Short). It was shown that mild detonation initiation includes several important stages, such as propagation of the supersonic shockless combustion wave, shock wave formation, its amplification and transition to ZND detonation. Most of the works dealt with the numerical analysis of the problem for a simple Arrhenius kinetics (Zel'dovich, Gelfand, Makhviladze), on the combination of the asymptotic techniques and numerical methods with the same kinetics (Dold, Kapilla, Short), restricting the possible range of the systems and conditions.

The present work concentrates on the description of the birth of the gas dynamic disturbances and shock wave formation in the mild initiation of detonation. The difference from the other works and main result is that the ordinary differential equation is proposed that much simpler to solve than partial differential equations, used in other researches (Gelfand, Kapilla, Short). In addition, no restrictions are imposed on the type of the chemical kinetics and activation energy value.

In the work of J.F. Clarke [1] the influence of the exothermic chemical reaction on the amplitude of the initially given gasdynamic disturbance and the shock wave formation was investigated for the spatially uniform medium.

In the present work the approach of [1] is extended on the spatially inhomogeneous medium. Using the asymptotic approach and Zel'dovich spontaneous flame [2] as a zero-order approximation to solution, the equation, describing the evolution of the gas-dynamic disturbances is derived. The procedure of its solution, accounting for the absence of the initial gasdynamic disturbance, is developed (this is the difference with [1]).

Application of the derived equation is illustrated on the problem of the shock wave formation in the initially undisturbed spatially inhomogeneous media, when the heat release is described by simple first-order chemical reaction with Arrhenius-like kinetics. Comparison with the CFD solution of the same initial problem is made.

## 2 Transport equation for disturbances and its solution

The evolution of the system is described by a full system of equations of the reactive fluid dynamics

$$\begin{gathered}\rho_t + (\rho u)_x = 0, \quad \frac{dp}{dt} = -c^2 \rho \frac{\partial u}{\partial x} + HR(p, \rho, \vec{y}) \\ p_t + (c+u) p_x + \rho c (u_t + (c+u) u_x) = HR(p, \rho, \vec{y}), \\ \vec{y}_t + u \vec{y}_x = \vec{\omega}(p, \rho, \vec{y})\end{gathered} \qquad (1)$$

where *HR* is a heat release rate during the chemical reaction, $\omega$ is reaction rates vector, *c* is frozen sound speed. The kinetics is assumed to be arbitrary. The gas is assumed to be ideal.

***Zel'dovich spontaneous flame*. *Small parameter***. If the temperature in the medium is distributed non-uniformly, than intensive chemical reaction starts at different times for a different points. According to Zel'dovich [2], this process is viewed as spontaneous flame propagation, ignoring any compressible particle communication occurring during the reaction. The speed of this flame depends on initial conditions only and is defined according to Eq. (2):

$$\vec{w}_{sp} = grad\, t_i \Big/ \left| grad\, t_i \right|^2 , \qquad (2)$$

where $t_i$ is a suitably chosen induction time. Spontaneous flame is the wave of self-ignition process of a constant volume.

The amplitude of the disturbance, appearing in the medium after the passage of the Zel'dovich spontaneous flame is $\Delta u/c_0 \approx c_0/w_{sp} = \varepsilon$ ($\varepsilon$ is small parameter notation), and small if

$$\varepsilon << 1. \qquad (3)$$

***Governing equations of the Zel'dovich spontaneous flame***. If the inequality (3) is satisfied, than the amplitude of the disturbances, appearing after self-ignition of every volume of the medium, will be small. Therefore, Zel'dovich spontaneous flame can be chosen as a zero-order approximation to solution of the system (1). Its equations are

$$u_0 = 0, \frac{\partial \rho_0}{\partial t} = 0, \frac{\partial p_0}{\partial t} = HR(p_0, \rho_0, \vec{y}_0), \frac{\partial \vec{y}_0}{\partial t} = \vec{\omega}(p_0, \rho_0, \vec{y}_0), , \qquad (4)$$

where subscript «0» refers to zero-order solution.

***Transport equation, its interpretation***. Substituting of (4) into system (1), collecting the terms of the first order, and differentiating resultant equation with respect to $\xi$, one obtains the following equation

$$\left(\frac{\partial \varphi}{\partial \tau}\right)_\beta = \frac{\gamma+1}{2} \cdot \varphi^2 + \frac{1}{2} \varphi \cdot \left( \frac{\partial HR}{\partial p} + \frac{1}{c_0^2} \frac{\partial HR}{\partial \rho} - \frac{1}{\rho_0 c_0} \left( \frac{\partial (\rho_0 c_0)}{\partial \tau} \right)_\beta \right) + \frac{1}{2 \rho_0 c_0} \left( c_0 p_{0\xi} \right)_\xi , \qquad (5)$$

where $\tau$ is time, $\xi$ is acoustic line parameter, $\beta$ is characteristic line parameter. They are defined by relations

$$d\tau = dt, \, d\xi = c_0(t, x) dt - dx, \, \left(\frac{\partial \xi}{\partial \tau}\right)_\beta = -\left(u^{(1)} + c^{(1)}\right), \varphi = u_\xi^{(1)} . \qquad (6)$$

The first term in Eq. (5) is a Riemann non-linear term, which is responsible for shock wave formation. The second term is similar (but not the same) to that, presented in the work [1] and is responsible for amplification/attenuation of the disturbances by chemical heat release and changing background. The third one is responsible for birth of the gasdynamic disturbances inside the spatially inhomogeneous region of the intensive chemical reaction of the Zel'dovich spontaneous flame.

***Solution of the transport equation***. The transport equation (5) is solved along characteristic line, and it is necessary to calculate zero-order solution along these lines. The main problem is to find the equation of the characteristic line, because its definition includes unknown flow speed.

To resolve this problem, the following is proposed: to calculate zero-order solution along acoustic lines, which are close to characteristic lines, i.e. to use relation $(dx/d\tau)_\beta = c_0(x, \tau)$ instead of $(dx/d\tau)_\beta = c_0(x, \tau) + c^{(1)} + u^{(1)}$. Than, the steps in solution of the equation, and particularly in determination of the point, where shock wave forms will be as follows:

1. For a given heat release model to find the values of $c_0(x, \tau)$.
2. For a given $c_0$ to solve the equation of the acoustic line with appropriate initial condition $x_0$, $\tau_0$.
3. To solve the equation (5) along the found characteristic line and determine the time moment $\tau^b$ and spatial position $x^b$ of the shock wave formation.
4. To find the minimum of $\tau^b$ (denote as $\tau_{cr}$) and corresponding $x^b$ (denote as $x_{cr}$) for changing values of $x_0$ and $\tau_0$ (so, exists $x_{0cr}$ and $\tau_{0cr}$).

## 3 Example: Arrhenius kinetics of the heat release

In the present section the analysis will be concentrated on the basic features of the shock wave formation in the medium with initial temperature gradient in the absence of gas dynamic disturbances. Initial condition for Eq. (5) is $\varphi(x_{0cr}, \tau_{0cr})=0$. The set of the parameters, used in calculations, is representative of hydrogen-air system.

***Chemical model***. The exothermic reaction of the first order with the Arrhenius-like rate is considered

$$\frac{dy}{dt}=-k(T)\cdot y,\ \frac{dT}{dt}=\frac{Q}{c_v}\cdot k(T)\cdot y,\ k(T)=k_0\exp\left(-\frac{E_a}{RT}\right),$$

where $y$ is a fuel mass fraction, $T$ is temperature. This system has an analytical solution, found by Todes [3]. Non-dimensional representation of the solution is ($Ei(x)$ is integral exponent function)

$$\tau(\theta)=Ei\left(\frac{\varepsilon_a}{\theta}\right)-Ei\left(\frac{\varepsilon_a}{\theta_{ini}}\right)-\exp\left(\frac{\varepsilon_a}{\theta_{ini}+1}\right)\cdot\left\{Ei\left(\frac{\varepsilon_a(1+\theta_{ini}-\theta)}{\theta(1+\theta_{ini})}\right)-Ei\left(\frac{\varepsilon_a}{\theta_{ini}(1+\theta_{ini})}\right)\right\}, \quad (7)$$

where $\varepsilon_a = E_a/RT_b$, $\theta_{ini} = T_{ini}/T_b$ are dimensionless activation energy and initial temperature, $T_b = Q/c_v$ is temperature scale, $\tau = t\cdot k_0$ is dimensionless time.

***Parametric analysis.*** In the non-dimensional units there are four parameters: activation energy $\varepsilon_a$, initial temperature gradient $g$, temperature in the center of the hot spot $\theta_m$ and ambient temperature $\theta_a$. The scales are: pressure scale is initial pressure $p_{ini}$, time scale is $1/k_0$, temperature scale is $T_b = Q/c_v$, speed scale is $c_b = \sqrt{\gamma RT_b/M}$. Below the ambient temperature is not considered.

For a small initial gradients the characteristics on which shock wave forms begins at $x_{0cr} > 0$ and $\tau_{0cr} = 0$, and

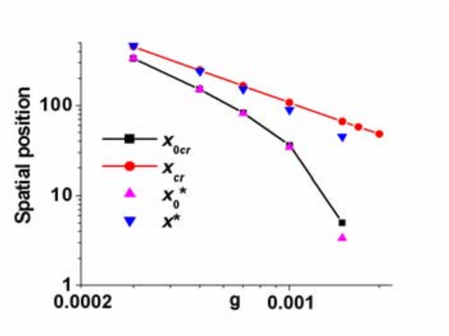


Figure 1a. Initial and final point of the characteristics vs. temperature gradient. Points, connected by straight lines – obtained from solution of the Eq. (5). Separate points (*) – predictions from estimates (9) and (10).
$\varepsilon_a = 2{,}27$, $\theta_m = 0.42$, $\theta_a = 0.2$, $\gamma = 1.4$

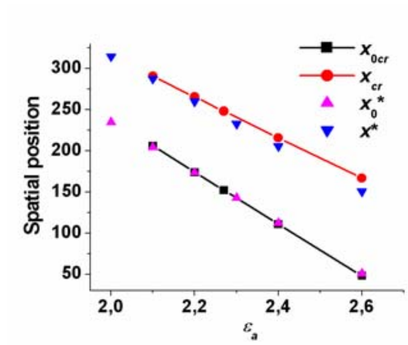


Figure 1b. Initial and final point of the characteristics vs. activation energy. Points, connected by straight lines – obtained from solution of the Eq. (5). Separate points (*) – predictions from estimates (9) and (10).
$g = 0.0005$, $\theta_b = 0.42$, $\theta_a = 0.2$, $\gamma = 1.4$

moves until the point $x_{cr}$. The dependences of $x_{0cr}(g)$ and $x_{cr}(g)$ are presented on the Fig. 1a (points, connected by the lines). Beginning from the specific value of the temperature gradient $x_{0cr} = 0$ and $\tau_{0cr} \geq 0$.

For the $\tau_{0cr} > 0$ the zero initial condition for the Eq. (5) needs to be modified because of the flow speed must be zero at this point. This modification was not applied and results of the calculations, where $x_{0cr} = 0$ must be considered as approximate.

The dependences $x_{0cr}(\varepsilon_a)$, $x_{cr}(\varepsilon_a)$ are linear with the good accuracy (Fig. 1b, points, connected by the lines).

Solution of the Eq. (6) shows that the variation of the temperature $\theta_m$ does not influence the process of the shock wave formation, i.e. though the $x_{0cr}$ changes, the temperature $\theta_{0cr}(\varepsilon_a,g)=\theta_{ini}(x_{0cr})$ and the distance $x_{cr} - x_{0cr}$ remain constant. Hence, only two parameters, $g$ and $\varepsilon_a$, determine the characteristic line, on which the shock wave will form and only the part of the medium between the points $x_{0cr}$ and $x_{cr}$ directly influences the process of the shock wave formation.

***Interpretation***. The trajectory of the spontaneous flame is a line of maximum heat release rate $\tau_{indhr} = \tau(\theta_{hr\max})$, where $\theta_{hr\max}(x)=\left(\sqrt{\varepsilon_a^2+4\varepsilon_a\theta_{ini}(x)+4\varepsilon_a}-\varepsilon_a\right)/2$.

Introduce the speed of the spontaneous flame

$$w_{sphr}(x)=(dt_{indhr}(x)/dx)^{-1}. \tag{8}$$

Analysis of the results of the solution of the Eq. (6), shows that for the whole set of the parameters at the initial point of the characteristic line, speed

$$w_{sphr}(x_{0cr}) \approx 2.5, \tag{9}$$

deviation from this value is less than 5%. Eq. (9) can be used to estimate initial position of the characteristics. Its solution $x_0$* is shown on the Figs. 1a and 1b by a separate points.

As calculations show, for shallow initial temperature gradients $g$, the specified characteristic begins on the $x$ axis at the point $x_{0cr}$ ($\tau_{0cr} = 0$), is tangent with the line of maximum heat release rate and the point of shock wave formation $x_{cr}$ ,$\tau_{cr}$ is near the same line, i.e. the point $x_{cr}$ is near the point, where the characteristics and maximum heat release line are tangent at the point $x$*

$$w_{sphr}(x^*) = \sqrt{\theta_{hr\max}(x^*)}\,. \tag{10}$$

The value of $x$* is used as estimation for $x_{cr}$ and shown on the Figs. 1a and 1b by a separate points.

***Comparison with the solution of the full system of equations (1)***. To validate the prediction of the approach, proposed in the present work, the comparison with the full solution of the reactive fluid dynamics equations (1) with first order Arrhenius kinetics was made.

In the table the comparison of the model predictions (solution of the Eq. (5)) and CFD solution results is presented. The following quantities are compared: the point of shock wave formation $x_{cr}$ and corresponding time $\tau_{cr}$. The presented results cover all the range of parameters, reported in the previous sections. The difference between predicted and CFD-obtained results is less than 8% and is supposed to be an excellent accuracy for assumptions, which are the basis for the present theory.

| | | Eq. (5) | | Full solution | |
|---|---|---|---|---|---|
| $\varepsilon$ | $g$ | $x_{cr}$ | $\tau_{cr}$ | $x_{cr}$ | $\tau_{cr}$ |
| 2.27 | 0.001 | 107.84 | 94.09 | 108.93 | 101.22 |
| 2.27 | 0.0005 | 248 | 130.1 | 243.75 | 139.65 |
| 2.2 | 0.0005 | 265.5 | 125.47 | 266.96 | 135.77 |
| 2.4 | 0.0005 | 215.85 | 138.89 | 204.46 | 149.57 |

## 4 Conclusions

In the present work the problem of birth of the gas dynamic disturbances and shock wave formation inside the spatially inhomogeneous self-igniting medium is addressed.

Using the asymptotic approach and Zel'dovich spontaneous flame [2] as a zero-order approximation to solution, the ordinary differential equation, describing the evolution of the gas-dynamic disturbances is derived and procedure of its solution is developed. Derived equation can be applied to all types of the kinetics and does not impose any restrictions on the kinetic parameters of the model, e.g. the value of the activation energy.

Application of the derived equation is illustrated on the problem of the shock wave formation in the spatially inhomogeneous media without gasdynamic disturbances at initial time moment, when the heat release is governed by simple first-order chemical reaction. It is shown that only activation energy and initial temperature gradient determine the point, where shock wave will form. In addition, an invariant quantity exists, which does not depend on any parameter. It is a speed of the Zel'dovich spontaneous flame at the initial point of the characteristics, on which the shock wave will form. Its value is 2.5 (dimensionless, see above) for a $\gamma = 1.4$.

## References

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