

DELAYED THERMAL EXPLOSION IN INERT POROUS MATRIX FILLED WITH EVAPORATING LIQUID FUEL

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Introduction

The present paper is concerned with the mathematical modeling of unusual and hazardous phenomenon, which is known as self-ignition within porous media filled in with evaporating fuel (the phenomenon is also known in industry as spontaneous insulation fires). A fluid leaks from the pipe into porous heat insulation and disperses over an extremely large internal surface. Due to highly insulated environment, heat losses are remarkably low, and self-ignition may occur as a result of an exothermic oxidation reaction. The problem of spontaneous insulation fires in insulation materials has been discussed both theoretically and experimentally (see for example, Bowes, 1974; Britton, 1990; McIntosh and Griffiths, 1995; Goldfarb *et al*, 1997, Gol'dshtein *et al*, 1999). Despite an intensive study of this subject, it is still a partly understood phenomenon.

The present paper proposes an original simplified model describing the influence of evaporating fuel film on thermal explosion in porous solid matrix. The main purpose is to investigate *analytically* delay effects before the final self-ignition.

Problem Statement

This paper concerns the problem of thermal explosion in a *three-phase medium (combustible gas mixture - combustible liquid - solid inert skeleton of the porous medium)*. An original physical model is suggested, using the spatially uniform approach and adiabatic approximation. The constructed model is based on the conventional cell approach to the analysis of dynamical processes in multiphase media (Nigmatulin, 1990). Specifically, the porous medium is modeled as a set of equal parallel capillaries of the same inner radius. In order to make the problem tractable analytically, the internal porous structure of the medium is assumed to be ideal. The natural assumption is that within all capillaries the same processes take place simultaneously. We assume that the combustible gas mixture is placed in the center of the capillary, and the combustible liquid is spread in a form of uniform thin layer on the inner surface of the capillary. Hydrodynamic effects (gas filtration through the porous media, combustible liquid flow, etc) are supposed to be negligible. The influence of pressure disturbances on the thermal explosion dynamics is ignored. Essentially, the gas temperature inside the fixed pore is controlled by the two main processes: heat release associated with an oxidation reaction and heat sink due to cooling caused by an evaporation process. The chemical reaction is modeled as a first order highly exothermic reaction taking place in the gas phase. Heat flux from the gas phase to the liquid film is considered to be proportional to the temperature difference between gas and film. The initial temperatures of the liquid and gas phases are assumed to be equal. Finally, the governing equations read

$$\pi R_{g0}^2 c_{pg} \rho_g \frac{dT_g}{dt} = \pi R_{g0}^2 Q_r \mu_r C_r A \exp\left(-\frac{E}{BT_g}\right) - \alpha_{gl}(T_g - T_l)H(R_{ci} - R_g)2\pi R_g \quad (1)$$

$$\pi R_{g0}^2 \frac{dC_f}{dt} = -\pi R_{g0}^2 C_f A \exp\left(\frac{-E}{BT_g}\right) + \frac{2\pi R_g}{L\mu_f} \alpha_{gl} (T_g - T_l) H(R_{ci} - R_g) (1 - \psi(T_l)) \quad (2)$$

$$\pi (R_{ci}^2 - R_{g0}^2) c_l \rho_l \frac{dT_l}{dt} = \alpha_{gl} (T_g - T_l) H(R_{ci} - R_g) 2\pi R_{g0} \psi(T_l) \quad (3)$$

$$\frac{d}{dt} [\pi (R_{ci}^2 - R_g^2(t)) \rho_l] = \frac{1}{L} \alpha_{gl} (T_g - T_l) H(R_{ci} - R_g) (2\pi R_g) (1 - \psi(T_l)) \quad (4)$$

$$\psi(T_l) = \frac{T_{ls} - T_l}{T_{ls} - T_{l0}} \quad \left\{ \psi(T_l)|_{T_l=T_{l0}} = 1; \quad \psi(T_l)|_{T_l=T_{ls}} = 0 \right\} \quad (5)$$

The initial conditions of the system (1)-(5) are given by

$$T_g = T_{g0}; \quad T_l = T_{g0}; \quad C_f = C_{f0}; \quad R_g = R_{g0} \quad (6)$$

The following notations were used here: **T**- temperature (K); **R** - radius (m); **C** - concentration of combustible component in gaseous mixture (kmol/m³); **c** – thermal capacity (J/kg/K); **q**- heat flux (J/m²/s); **ρ**- density (kg/m³); **φ** - volumetric phase (dimensionless); **Q** - heat combustion (J/kg); **L** - latent heat of evaporations (J/kg); **E** - activation energy (J/kmol); **B** - universal gas constant; **R_{ci}**- internal radius of the model cylindrical cell (capillary without fuel) (m); **R_{ce}** - external radius of the model cell (capillary with its walls) (m); **R_g** - radius of the gas phase inside a capillary (when a sample is loaded by fuel) (m); **H**- Heaviside function, describe effects existing in a presence of fuel film (dimensionless); **ψ(T_l)** - describes the heat flux from the burning gas to the fuel film, and it takes the following approximation: Subscripts: **c** – capillary; **f** - combustible component of gaseous mixture; **g** - gas phase; **l** - liquid fuel film; **m**-solid matrix; **s** - at saturation conditions; **0** - undisturbed state of the system.

Results and Discussion

The conventional Semenov approach is used for non-dimensionalisation, based on the initial values of the key variables (Semenov, 1928). The dimensionless model can be treated as a multi-scale system with a small parameter, due to a great difference in characteristic times of the processes involved (highly exothermic chemical reaction, evaporation). The system is analyzed by the method of integral manifolds (MIM, Gol'dshtein and Sobolev, 1992; Gol'dshtein *et al* 1999; Goldfarb *et al* 2000, McIntosh *et al*, 1998).

It was shown that under the typical parameter values (which were extracted from the available experimental data - Britton, 1990; Pegg and Pan, 2000), the system demonstrates explosive behavior with *long-time delays* before the final ignition. It was also shown, that the final

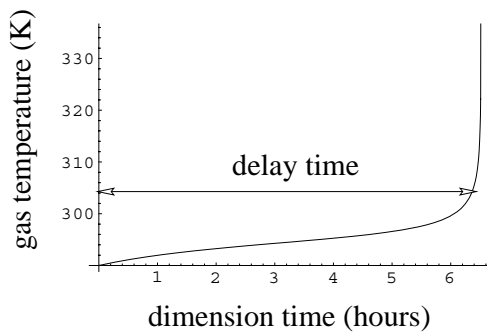


Figure 1. Typical time history and the delay time definition.

thermal explosion normally occurs in the temperature interval below the boiling point of the liquid fuel. The latter conclusion means that accepted safety regulations (chemical industry, heavy processing plants, etc) might be a subject of additional thorough verification versus the obtained results.

This work focused on the delay effects, especially the delay time as one of the mostly important practical characteristics. Physically, the delay time is related to the temporary balance between the chemical heat release and the *internal* heat losses due to intensive

liquid fuel evaporation. The analytical approximate formula for the delay time was derived:

$$t_{\text{delay}} \approx t_{\text{react}} \frac{\int_0^{\ln(\varepsilon_1)} \frac{\exp(-v) dv}{(1 - v/\theta_s) \left(\frac{\varepsilon_2}{\varepsilon_1} - \psi_f v + \theta_s (1 - \psi_f) \ln(1 - v/\theta_s) \right)} \quad (7)$$

$$\beta = \frac{BT_{g0}}{E}, \quad t_{\text{react}} = \frac{\exp(1/\beta)}{A}, \quad \psi_f = \frac{Q_f}{L}, \quad \theta_s = \frac{T_s - T_{g0}}{\beta T_{g0}},$$

$$\varepsilon_1 = \frac{2\alpha_{gl} T_{g0} \beta \exp(1/\beta)}{AC_{f0} \mu_f Q_f R_{g0}}, \quad \varepsilon_2 = \frac{2\alpha_{gr} R_{g0} \exp(1/\beta)}{AR_{ce}^2 (C_i \phi_i \rho_i + C_m \phi_m \rho_m)}$$

The delay time depends on the six key system parameters. The reaction time t_{react} is the time required for the reactant concentration to fall by a factor e from its initial value under the isothermal conditions. The parameter θ_s is the saturation liquid temperature.

The obtained approximate formula (7) allows us to investigate the important dimensional characteristics of the delay time and its dependence on the key system parameters. From the practical point of view, the dependence of the delay time on the reciprocal of the initial gas temperature is very informative (see for example McIntosh, *et al*, 1998; Pegg and Pan, 2000). The Figures 2a, 2b depict comparison between the approximate delay time formula (7) and the numerical simulations of the original system (1)-(6), versus the reciprocal of the initial gas temperature. It can be seen that the theoretical predictions of the delay time are in a good agreement with the numerical simulations.

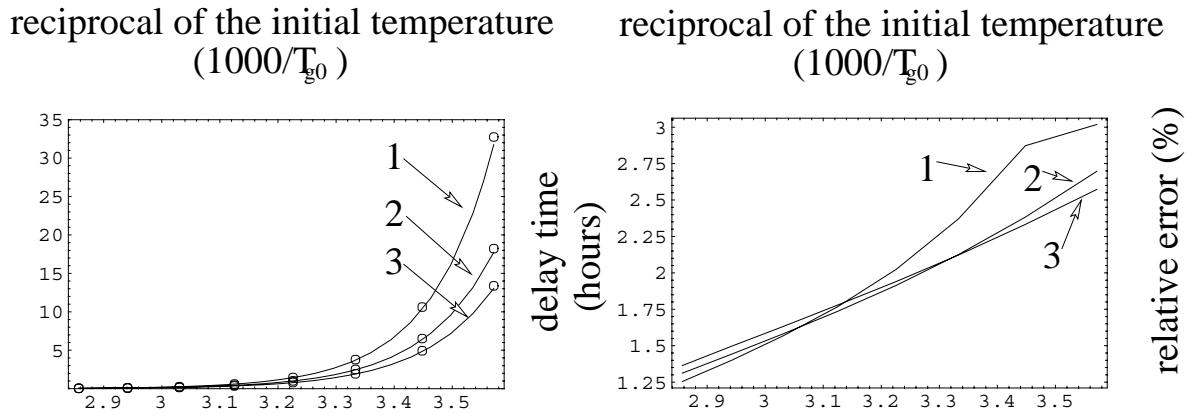


Figure 2. a (left). The delay time versus the reciprocal of the initial gas temperature ($1000/T_{g0}$), for the various thickness of the fuel film $\delta=(R_{ci} - R_{g0})$. Comparison between the derived estimation (7) (plotted as a smooth curve) and the direct numerical simulations of the original system (1)-(6) (plotted as circles). Numbers designate: 1 - $\delta=0.16$ (μm); 2 - $\delta=0.08$ (μm); 3 - $\delta=0.008$ (μm); **b (right).** Relative error between the two distinct data sets (the derived estimation (7) and the direct numerical simulations of the original system (1)-(6)), illustrated on the left. The following parameter values were used: $\rho_l=1.003$ (kg/m^3); $C_{f0}=0.6$ (mol/kg); $L=0.529$ (MJ/kg); $c_p=1.26$ ($\text{kJ}/\text{kg}/\text{K}$); $T_s=518$ (K); $\mu_f=119.2$ (kg/kmol); $Q_f=25.7$ (MJ/kg); $E=65$ (MJ/kmol); $A=1.15 \cdot 10^6$ ($1/\text{sec}$); $R_{ci}=1.2$ (μm); $R_{ce}=1.25$ (μm); $\alpha=50$.

There is another important use of the approximate delay time formula (7). More specifically, an original approach to determine experimentally the fuel activation energy is suggested. The suggested approach is based on the delay time measurements under controlled initial

conditions (see for example Britton, 1990; Pegg and Pan, 2000). Suppose that the dimensional experimental results of the delay time measurements are depicted versus reciprocal of the initial gas temperature (the idea is illustrated by the Figure 3). The scattered experimental results (small circles; measured with some accuracy) can be approximated by the linear least-squares fit:

$$\ln(t_{\text{delay}}) \approx a\left(\frac{1000}{T_{g0}}\right) + b \quad (8)$$

Detailed numerical simulations showed that the value of the dimensionless integral in the formula (7) depends weakly on reciprocal of the initial temperature (the dashed line on the Figure 3). It means that the upper bound of the activation energy can be obtained from the equations (7-8) as:

$$E^{up} = 1000 B a$$

The correction due to the value of dimensionless integral can be easily calculated numerically (for the typical parameters mentioned in the Caption of the Figure 2, the relative error lies within interval 5-8 percents).

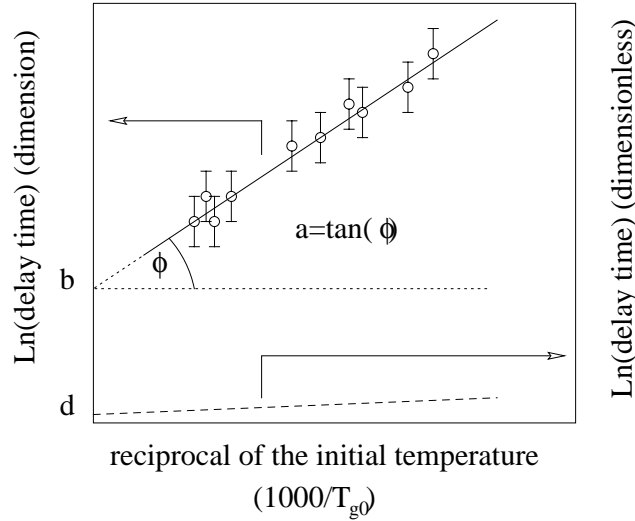


Figure 3 . Illustration of suggested method of activation energy determination on the basis of delay time measurements.

Conclusions

The purpose of this paper was to study theoretically the phenomenon of gaseous thermal explosion in porous media filled with a combustible evaporating fuel. An original physical model was suggested. The relevant mathematical model was studied analytically using the method of integral manifolds (MIM). It was shown that under the realistic parameter values the system behavior is explosive with long-time delays. The analytical estimation of the delay time was gained and compared with the results of the direct numerical simulations. The comparison witnesses that the accuracy of the derived estimation is quite high. A novel approach to determination of the activation energy on the basis of delay time measurements was suggested.

Acknowledgment

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