Effect of Inert Particle Evaporation on the Chemical Reaction in a Combustible Medium

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Abstract

Dispersions of various solid or liquid materials are often used as a fire safety measure in chemical processing plants or mine galleries. In this paper the effect of inert particles evaporation on the preself-ignition chemical reaction in a gaseous combustible medium is investigated. It is shown that under certain conditions the evaporation process may promote the chemical activity and may become a reason for strong secondary shock or detonation wave onset. Monodisperse particles uniformly distributed in a combustible mixture were considered first. A quenching criterion was derived indicating the amount of particles required for the suppression of the mixture self-ignition. A comparison was made between the quenching ability of H_2O, \text{P}(\text{C}_2\text{H}_6)_4 and KBr particles. It was shown that self-ignition can be promoted, if particle inertia effects in the fluid flow were taken into account. The latter is due to momentum losses during vapor acceleration and drag forces. Nonuniformly distributed evaporating particles produce temperature and dilution ratio nonuniformities in the reactive mixture. Under conditions close to self-ignition this may become a reason for strong shock or detonation wave generation in accordance with the Zeldovich mechanism. Detailed calculations were carried out indicating characteristic regions of spontaneous detonation onset. A comparison was made between the calculated results and predictions obtained on the basis of an analytical criterion.
Introduction

Dispersions of various liquid or solid materials are often used as a safety expedient in chemical processing plants or mine galleries\(^1\) for preventing high dynamic or thermal loading of construction elements. The quenching of a flame can be achieved, for example, by the formation of fog in front of it. The influence of these aerosol particles on the flame consists in chemical inhibition by loss of free radicals or in physical inhibition by gas cooling due to heat transfer during particle evaporation. Drag forces between particles and gas can also play an important role, see, for example, Ref.\(^2\). According to Ref.\(^3\), powders can be used for detonation suppression. Additionally, a whole class of detonable media exists, where chemically inert dust particles play a significant role, for example, dusty detonations. It is shown in Ref.\(^4\) that inert particles dispersed in a gaseous reactive mixture cause a widening of the detonation limits as compared to the pure gas. The influence of inert particles on the propagation of detonation waves was theoretically studied in Ref.\(^5\), in regard to heat transfer and friction between particles and gas.

In the present paper the effect of mass addition by inert particle evaporation on the chemical reaction in a combustible gas mixture was studied. It is shown that in some cases the particle evaporation process can promote the onset of strong secondary shock and detonation waves. Of particular interest is the coupling between gas phase reaction and fast evaporation of the dispersed particles. This can take place either in a flame front or in a high-temperature gas mixture, which is close to self-ignition conditions. In the present case, we restrict ourselves by considering only the problem, concerning self-igniting mixture behavior.

One-Dimensional Two-Phase Flow Conservation Equations

The flow behavior of a gas/particle mixture\(^4\) including inter- and intra-phase rate processes can be described by the conservation equations of two interactive continua. In a simplified strategy the volume fraction of the particle phase is introduced by

\[ \varepsilon = \frac{V_p}{V} = \frac{\rho_p}{\rho} \]

where \( V \) and \( V_p \) are the volume of the suspension and the respective volume of all particles in the suspension. The quantities \( \rho_p \) and \( \rho \) are the material density of the particles and the "smeared" density of the particle phase (mass of the particles per volume of suspension). In the later equations, we only consider the limiting case of very low volume fraction of the suspended particles. This assumption facilitates the description of the two-phase-flow problem and allows the consideration of only the gas-phase properties with the respective source terms.
The conservation equations of mass, momentum and energy for the gas phase of two interactive gas/particle continua can be formulated under the assumptions of Ref.6 in the following one-dimensional way:

\[
\frac{dp}{dt} + \rho \frac{du}{dt} = 0
\]  \hspace{1cm} (1)

\[
\frac{d\rho u}{dt} = -\frac{\partial p}{\partial x} + F_d + J(u_p - u)
\]  \hspace{1cm} (2)

\[
\frac{d\rho e}{dt} = -\rho \frac{\partial u}{\partial x} + J \left[ (h_D - e) + \frac{(u_p - u)^2}{2} \right]
\]  \hspace{1cm} + F_d(u_p - u) + Q + Q_R \hspace{1cm} (3)

In these equations \(d/dt\) is the substantial derivative and \(\rho, u, p,\) and \(e\) are the density, flow velocity, pressure, and internal energy of the gas phase, respectively. The quantities \(J, F_d,\) and \(Q\) are the source terms or interphase flux terms for mass, momentum, and heat, \(u_p\) is the mean velocity of the particle phase, and \(Q_R\) is the chemical energy source term. The quantity \(J \left[ (h_D - e) + \frac{(u_p - u)^2}{2} \right]\) is the energy transferred from the particle phase to the gas phase due to mass transfer, where \(h_D\) is the specific enthalpy of the vapor when leaving the particle surface. It was introduced instead of \(e_D\) because of the possible expansion work of the vapor. Similar equations for the particle phase can also be formulated, see Ref.6.

The different source terms in Eqs. (1)-(3) are, in general, complicated functions of the gas- and particle-phase properties. In the present case we assume the particles to be spherical and monodisperse. In this case the particle phase can be described by the two properties \(n_p\) and \(d_p\), the number concentration and the mean particle diameter. According to Ref.6, the interphase flux terms are

\[
J = -n_p \cdot \frac{d\rho \Delta p}{dt} = -n_p \rho 0 \pi \frac{d d_p^2}{dt}
\]

\[
J = n_p \cdot \rho 0 \pi \Delta p \cdot K
\]

\[
F_d = n_p \cdot \frac{\pi}{2} \rho C_D(u_p - u) \mid u_p - u \mid
\]

\[
Q = n_p \cdot \pi d_p \lambda N u(T_p - T)
\]

In these equations, \(K = -dd_p^2/dt\) is the evaporation coefficient, \(C_D\) and \(\lambda\) are the drag coefficient and the heat conductivity of the gas phase, respectively, \(T_p\) and \(n_p\) are the particle surface temperature and the particle mass, and \(N u\) the particle Nusselt number.

The chemical reaction in the gas phase is introduced in the simplest possible way by a one-step kinetics, characterized by a global rate parameter
a. The source term $Q_R$ then results in

$$Q_R = -\varrho h_R \frac{da}{dt}$$

where $h_R$ is the heat of reaction. The rate parameter $a$ ranged between $a = 1$ (unreacted mixture) and $a = 0$ (combustion products).

The rate laws for $d_p$ and $a$ can be introduced in the following simplified way:

$$\frac{dd}{dt} = -K$$

$$\frac{da}{dt} = -a^n Z \exp(-E/RT) \quad (4)$$

In Eq. (5), $Z$ is the pre-exponential frequency factor, $n$ the reaction order, $R$ the gas constant, $E$ the activation energy, and $T$ the gas-phase temperature. Equation (4) can be integrated if $K$ is independent of $d_p$ and $t$. The result is\textsuperscript{8,9}

$$d_p^2 = d_{p0}^2 - K t \quad (6)$$

where $d_{p0}$ is the particle diameter at time $t = t_0$, $K = 2D_{eq} p_v M_v / \varrho_p^0 RT_p$. Here $D_{eq}$ is the diffusion coefficient, $p_v$ the vapor pressure, $M_v$ the vapor molecular weight, $T_p$ the particle temperature. Note that the $d^2$-law given by Eq. (6) is a reasonable realistic model because we consider processes during the long induction period with insignificant temperature and pressure rise\textsuperscript{9}.

**Uniformly Distributed Particles in a Closed Volume**

In this section we consider a volume of the linear dimension $L$, which contains a premixed reactive gas mixture loaded with uniformly distributed suspended inert particles of initial size $d_{p0}$. The initial conditions $(p, T)_0$ of the gas/particle mixture are such that self explosion is possible. The effect of particle evaporation on the chemical reaction was studied under the following assumptions:

1. All thermophysical parameters of gas and vapor are identical.
2. The particle velocity is equal to the gas velocity, $u = u_p$.
3. The enthalpy of the vapor (added energy) is equal to the interphase heat flux, $J \cdot h_D = -Q$.

Under these conditions, the conservation equations of mass and energy for a quiescent mixture result in the simple form

$$\frac{dg}{dt} = J \quad (7)$$
EFFECT OF PARTICLE EVAPORATION

\[ \frac{de}{dt} = Q_R - J_e \]  

(8)

The energy equation (8) expresses the fact that the energy \( e \) (or the temperature \( T \)) of a gas/particle mixture can be increased or decreased depending on the relative effects of gas cooling due to mass addition (\( J_e \cdot e \)) or gas heating due to chemical reaction (\( Q_R \)). It is clear from the above differential equation that the quenching criterion for the chemical reaction is

\[ Q_R < J_e \]  

(9)

This criterion is fulfilled if the cooling effect exceeds the gas heating by the exothermic reaction.

The quenching criterion will now be applied to a high-temperature gas/particle mixture, in which at time \( t = 0 \) the reaction and evaporation processes were simultaneously started.

\[ t = 0: \quad T = T_0, \quad e = e_0, \quad a = a_0 = 1 \]
\[ J_0 = J(t = 0), \quad Q_{R0} = Q_R(t = 0) \]

The source terms \( J_0 \) and \( Q_{R0} \) can be expressed by the respective evaporation time \( \tau_{ev} \) or chemical induction time \( \tau_{ind} \), which are

\[ \tau_{ev} = \frac{e}{J_0} \]
\[ \tau_{ind} = \frac{c_p T_0}{Q_{R0}} \frac{R T_0}{E} \]

(10)

The quenching criterion (9) can be then rewritten in the following form:

\[ \frac{\tau_{ev}}{\tau_{ind}} < \frac{E}{R T_0} \]

(11)

If this condition is satisfied, then the chemical reaction is quenched by the particle evaporation process.

The source term \( J_0 \) or the evaporation time \( \tau_{ev} \) are mainly determined by the evaporation coefficient \( K \), which is a complicated function of the particle as well as the gas phase properties. It includes, for example, the Sherwood number, which expresses the convective mass transfer due to the relative motion between a suspended single particle and the surrounding gas. In the present case we only assume diffusive processes of a spherical particle, that means \( Sh = 2 \). From the energy balance applied to a single suspended particle under stationary conditions, the difference between gas temperature \( T \) and particle temperature \( T_p \) can be determined. For the particle materials KBr, H₂O, and Pb(C₂H₅)₄, the calculated evaporation coefficients are summarized in Table I. The Stefan flow conditions are
Table I. Calculated evaporation coefficient $K$ obtained from stationary, diffusive energy exchange between a single particle and the surrounding gas; $T$ = gas temperature and $T_p$ = particle surface temperature.

<table>
<thead>
<tr>
<th></th>
<th>KBr</th>
<th></th>
<th>Water</th>
<th></th>
<th>Pb(C$_2$H$_5$)$_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$</td>
<td>$T_p$</td>
<td>$K$</td>
<td>$T_p$</td>
<td>$K$</td>
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</tr>
<tr>
<td>K</td>
<td>K</td>
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<td>K</td>
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<td>300</td>
<td>300</td>
<td>-</td>
<td>299</td>
<td>18</td>
<td>299.7</td>
</tr>
<tr>
<td>400</td>
<td>400</td>
<td>-</td>
<td>359</td>
<td>314</td>
<td>377</td>
</tr>
<tr>
<td>500</td>
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<td>-</td>
<td>320</td>
<td>677</td>
<td>406</td>
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<td>700</td>
<td>-</td>
<td>371.9</td>
<td>1345</td>
<td>425</td>
</tr>
<tr>
<td>800</td>
<td>800</td>
<td>-</td>
<td>372.1</td>
<td>1724</td>
<td>427</td>
</tr>
<tr>
<td>900</td>
<td>900</td>
<td>-</td>
<td>372.2</td>
<td>2140</td>
<td>432</td>
</tr>
<tr>
<td>1000</td>
<td>1000</td>
<td>2.07</td>
<td>372.3</td>
<td>2594</td>
<td>434</td>
</tr>
<tr>
<td>1100</td>
<td>1100</td>
<td>8.65</td>
<td>372.3</td>
<td>3082</td>
<td>436</td>
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<tr>
<td>1200</td>
<td>1200</td>
<td>24.6</td>
<td>372.3</td>
<td>3605</td>
<td>437</td>
</tr>
<tr>
<td>1300</td>
<td>1300</td>
<td>48.9</td>
<td>372.4</td>
<td>4167</td>
<td>438</td>
</tr>
<tr>
<td>1400</td>
<td>1400</td>
<td>79.7</td>
<td>372.4</td>
<td>4763</td>
<td>438.7</td>
</tr>
<tr>
<td>1500</td>
<td>1500</td>
<td>115.4</td>
<td>372.4</td>
<td>5395</td>
<td>439.4</td>
</tr>
</tbody>
</table>

Table II. Reaction quenching criterion of Eq. (11) applied to the reaction conditions behind the leading shock of methane-air detonation waves; particles of KBr with $n_p = 10^{15}$ m$^{-3}$ and $d_{p0} = 1$ mm.

<table>
<thead>
<tr>
<th>$\Phi$</th>
<th>$D$</th>
<th>$p_f p_0^{-1}$</th>
<th>$T_f$</th>
<th>$\tau_{nd}$</th>
<th>$\tau_{ev}$</th>
<th>$\tau_{ev/\tau_{nd}}$</th>
<th>$E/RT_f$</th>
<th>$\tau_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>m/s</td>
<td>K</td>
<td></td>
<td>ms</td>
<td>ms</td>
<td>ms</td>
<td></td>
<td></td>
<td>ms</td>
</tr>
<tr>
<td>0.5</td>
<td>1430</td>
<td>19.70</td>
<td>1150</td>
<td>4.180</td>
<td>16.00</td>
<td>3.8</td>
<td>20.1</td>
<td>6.20</td>
</tr>
<tr>
<td>0.8</td>
<td>1660</td>
<td>26.40</td>
<td>1370</td>
<td>0.200</td>
<td>1.40</td>
<td>7.0</td>
<td>15.9</td>
<td>0.50</td>
</tr>
<tr>
<td>0.9</td>
<td>1710</td>
<td>28.03</td>
<td>1430</td>
<td>0.120</td>
<td>1.00</td>
<td>8.3</td>
<td>16.2</td>
<td>0.33</td>
</tr>
<tr>
<td>1.0</td>
<td>1750</td>
<td>29.30</td>
<td>1465</td>
<td>0.086</td>
<td>0.75</td>
<td>8.7</td>
<td>15.8</td>
<td>0.25</td>
</tr>
<tr>
<td>1.5</td>
<td>1760</td>
<td>29.22</td>
<td>1430</td>
<td>0.140</td>
<td>1.00</td>
<td>8.3</td>
<td>16.2</td>
<td>0.33</td>
</tr>
<tr>
<td>2.0</td>
<td>1680</td>
<td>26.24</td>
<td>1290</td>
<td>0.880</td>
<td>3.00</td>
<td>3.4</td>
<td>17.9</td>
<td>1.00</td>
</tr>
<tr>
<td>2.5</td>
<td>1590</td>
<td>23.25</td>
<td>1170</td>
<td>6.320</td>
<td>15.00</td>
<td>2.4</td>
<td>19.7</td>
<td>5.00</td>
</tr>
</tbody>
</table>

Included in the given set of data. It is clear from Table I that at a gas-phase temperature of $T = 1000 K$ the evaporation coefficient of H$_2$O and Pb(C$_2$H$_5$)$_4$ is two to three orders of magnitude larger than that of KBr.

The quenching condition of Eq. (11) is now applied to the properties behind the leading shock (index f) of a stationary methane-air detonation. The induction time of the gas-phase reactions $^{11}$ was compared to the evaporation time of KBr particles with $n_p = 10^{15}$ m$^{-3}$ and $d_{p0} = 1$ mm. The suspension density was assumed to be $\varphi_p = 1$ kg/m$^3$. The result of the calculations are shown in Table II. The gas-phase detonation is characterized by the equivalence ratio $\Phi$, the detonation velocity $D$, the pressure $p_f$, and the temperature $T_f$. The equivalence ratio $\Phi$ is defined as the ratio of the fuel mass to the oxidizer mass in the stoichiometric mixture.
ratio $p_f/p_0$ of the leading shock, and the temperature $T_f$ in the induction zone. The reaction induction time $\tau_{ind}$ and the calculated evaporation time $\tau_{ev}$ are given. The comparison of $\tau_{ev}/\tau_{ind}$ with the dimensionless activation energy $E/RT_f$ indicates that according to Eq. (11) the detonation is always suppressed. The property in the last column of Table II is the particle life time, $\tau_p$, according to Eq. (6). The condition $\tau_{ind} < \tau_p$ is always fulfilled (except for $\Phi = 2.5$). Note that in this simplified theory, heat consumption by the particles and the influence of mixture dilution was not considered. It is also clear from Table I that the reaction quenching by $\text{H}_2\text{O}$ or $\text{Pb}(\text{C}_3\text{H}_5)_4$ particles is much more effective than that of KBr, because of the considerably higher evaporation coefficients.

**Relative Motion Between Particles and Gas**

We now consider the case of relative motion between the particles and the combustible gas mixture. To simplify Eq. (4) we assume the following:

1. The particle velocity is zero, $u_p = 0$.
2. The drag force $F_d$ is of minimum importance, $F_d = 0$.

For flow conditions the energy equation results in

$$\frac{d\varepsilon}{dt} = Q_R - J \left( \varepsilon - \frac{u^2}{2} \right)$$

(12)

It can be seen from the right hand side of Eq. (12) that because of the explosion suppression criterion

$$Q_R < J \left( \varepsilon - \frac{u^2}{2} \right)$$

the gas cooling effect due to particle evaporation is qualitatively less efficient than in the case considered before. This is a result of momentum loss due to

Fig. 1 Dependence of the kinetic to thermal energy ratio behind a shock wave on the shock Mach number.
vapor acceleration. When making quantitative analysis one should take into account the dependence of the evaporation coefficient on the flow Reynolds number. At $u^2/2 > e$ the evaporation process promotes self-explosion. Figure 1 shows the dependence of the quantity $u^2/2e$ behind the shock wave on the shock Mach number for fuel-air mixtures. It appears that particle evaporation behind the shock wave always leads to temperature decrease ($u^2/2e < 1$). The effect of reaction promotion may come into play in nozzle flows. If the process of kinetic energy dissipation due to drag force is also considered, the full energy equation (3) must be discussed. Remember, the term $F_d(u_p - u)$ is always positive and contributes to the effect of ignition promotion.

Nonuniformly Distributed Particles

In the case of nonuniformly distributed particles $n_p = n_p(x)$, the source term $J$ of the gas/particle mixture no longer depends only on $t$ but also on $x$, $J = J(x, t)$. This means that the gas cooling effect by the particles is nonuniform resulting in pressure, temperature, and velocity gradients, as can be seen from the conservation equations (1)-(3) with the simplified assumptions $F_d = 0$ and $Jh_D = -Q$:

\[
\begin{align*}
\frac{d\rho}{dt} + \rho \frac{\partial u}{\partial x} &= J(x, t) \\
\frac{\partial u}{dt} &= -\frac{\partial p}{\partial x} + J(u_p - u) \\
\frac{\partial e}{dt} &= -\rho \frac{\partial u}{\partial x} + Q_R + J(x, t)[-e + \frac{(u_p - u)^2}{2}]
\end{align*}
\]

Stationary conditions are no longer possible, and waves will be generated by the particle nonuniformity. Spatially nonuniform chemical energy release can be expected in this case. According to the Zel’dovich mechanism 12,13 under conditions close to self-ignition this may become a reason of strong shock or detonation wave generation.

The physical meaning of the Zel’dovich coupling criterion 13 consists in a requirement for the reaction wave to propagate at the local sound velocity. Now we consider conditions when particle evaporation promotes spontaneous detonation onset in the preheated combustible mixture. Evaporation of particles produces the temperature gradient of the order

\[
\omega(t) \approx \frac{\Delta T(t)}{L}
\]

where $\Delta T$ is the temperature increment at the length $L$. According to Eqs. (6)-(8) and using Taylor series

\[
\Delta T = T_0 \delta(1 + \delta)
\]
with $\delta = (\pi/6)(d_p^3 - d_p^3(t))n_p(L)d_p^6/\rho_0$ for particles distributed initially as $n_p = n_p^0\pi/L$. The parameter $\delta$ is approximately equal to $\tau_{ind}/\tau_{ev}$ to first order for $k\tau_{ind}d_p^2 \ll 1$. A further simplification gives $\Delta T = T_0\delta$ because $\tau_{ind}/\tau_{ev} \ll 1$ due to the occurrence of self-ignition.

Here $n_p^0$ is the reference value of particle number concentration. The temperature gradient given by Eq. (14) should be compared with the characteristic temperature gradient for the Zel’dovich mechanism to come into effect:\footnote{\textsuperscript{13}}

$$\omega_c \approx \frac{RT_0^3a/c_0}{L\tau_{ind}(e - 1)} \quad (15)$$

where $c_0$ is the sound velocity in the initial mixture. Eq. (15) can be derived from Eq. (10) using high activation energy asymptotics. Equating Eq. (14) to Eq. (15) and taking into account Eqs. (10) gives

$$\frac{\tau_{ev}}{\tau_{ind}} \approx \frac{E}{RT_0} \frac{c_0\tau_{ind}(e - 1)}{L} \quad (16)$$

A comparison between criteria (11) and (16) shows that at

$$\frac{c_0\tau_{ind}(e - 1)}{L} < 1$$

reaction quenching by evaporating particles may produce conditions for spontaneous onset of strong shock waves. This may become a case if particles are nonuniformly distributed in the volume.

To verify the criterion (16) we integrated numerically Eqs. (13) for initially quiescent methane-air mixture. The following set of parameters was used for the computational example, which corresponds closely to Eq. (16): $\rho = 0.3$ kg/m$^3$, $T_0 = 1200$ K, $p_0 = 0.1$ MPa, $C_p = 8.67$ kcal/kmol K, $\mu = 30$ kg/kmol, $E = 44.5$ kcal/mole, $n = 1$, $Q = 15$ kcal/mole s, $Z = 10^{10}$ s$^{-1}$, $L = 0.1$ m, $n_p^0 = 10^{11}$ m$^{-1}$, $\phi_p^0 = 2225$ kg/m$^3$, $d_{p0} = 20$ $\mu$m (KBr particles).

The evaporation coefficient for KBr particles was calculated by the use of the dependence\footnote{\textsuperscript{8}}

$$k = 2.126 \cdot 10^{(-1.7618 - 8665/T)(T/T_e)^{0.75}(p_e/p)}$$

where $T_e = 300$ K, $p_e = 1$ bar.

The kinetic parameters $Z$, $n$, and $E$ of the mixture have been chosen by comparison of an adiabatic induction period with an empirical correlation for ignition delay\footnote{\textsuperscript{14}}. The ratio of specific heats is assumed to be constant and equal to the average value between the corresponding quantities for the initial mixture and combustion products, the composition of the latter being calculated through the use of a stoichiometric formula neglecting dissociation. The heat release $Q$ is then determined from the experimental value of the ideal detonation velocity.
Initial conditions for Eqs. (13) are as follows:

\[ t = 0, \quad 0 \leq x \leq L : \quad p = p_0, \quad \varepsilon = \varepsilon_0, \quad u = 0, \quad a = 1 \]

Boundary conditions:

\[ u(t > 0, x = 0) = u(t > 0, x = L) = 0 \]

Two limiting cases were considered:

1. Particles were assumed taken in motion immediately, i.e., \( u - u_p = 0 \)

2. The particle velocity was assumed zero, i.e., \( u - u_p = u \)

The integration procedure of Eqs. (13) was the same as proposed in Ref. 15.

Shown in Fig. 2 is the calculated temporal evolution of various quantities. Results of the calculations are similar whether or not the relative motion of the phases is taken into account. This is due to the fact that the most important stage of the process is the pre-ignition stage. Figure 2a shows the evolution of the parameter \( n_p d_p (n_p^0 d_{p0})^{-1} \) representing a modified particle diameter. At time \( t \approx 400\mu s \) self-ignition occurs near the boundary \( x = 0 \) where the particle number concentration is minimum. In the further evolution, particles disappear behind the reaction wave.

Figure 2b shows the dimensionless temperature history. At time \( t = 300 - 400\mu s \) one can see the formation of nonuniform temperature distribution induced by nonuniform cooling effect of the particle ensemble. After the self-ignition event at \( t \approx 400\mu s \) spontaneous detonation onset is evident. The fully developed detonation wave originates at \( t \approx 420\mu s \). The detonation wave forms as a result of spatially nonuniform chemical energy release^{12,13}. Also evident is the reaction proceeding at the far end of the vessel.

Figure 2c shows the dimensionless pressure history. Relatively low-pressure values in the detonation wave are due to the high initial temperature \( T_0 \). Unstable character of the detonation wave propagation is due to one-dimensional instability of the detonation front at given \( E \) and \( Q \) values.

Figure 2d shows dimensionless gas-phase velocity history. The detonation velocity is of about 1750 m/s which is somewhat less than the CJ value (\( \approx 1810 \) m/s). The difference should be attributed to momentum losses on vapor acceleration^{16}.

Thus the computational example confirms the criterion given by Eq. (16). It should be mentioned that experiments on detonation suppression by water-based foams reveal a possibility of strong secondary shock formation behind a decaying precursor blast wave^{16}. The secondary explosions may be attributed to reaction onset in nonuniformly preheated zones in a two-phase combustible mixture.

To verify the criterion in general, we made calculations for the whole variety of fuel-air and fuel-oxygen mixtures with different quenching agents.
Fig. 2 Calculated temporal evolution of reaction in an initially quiescent methane-air mixture loaded with nonuniformly distributed inert evaporating particles: a) modified particle diameter, b) gas-phase temperature, c) pressure, and d) gas-phase velocity.
Fig. 2 (continued) Calculated temporal evolution of reaction in an initially quiescent methane-air mixture loaded with nonuniformly distributed inert evaporating particles: a) modified particle diameter, b) gas-phase temperature, c) pressure, and d) gas-phase velocity.
Fig. 3 Resultant dimensionless diagram indicating parametric domains with and without spontaneous shock/detonation formation: solid line corresponds with the approximate coupling criterion of Eq. (16). Dashed line is the numerically calculated boundary between reaction regimes with (upper region) and without (lower region) shock/detonation formation.

Presented in Fig. 3 is the resultant dimensionless diagram. It shows parametric domains with and without spontaneous shock or detonation formation. The dashed line is the numerically calculated boundary separating the two characteristic regions. In the upper region the maximum pressure during system evolution is more than 10% larger than the pressure of constant volume explosion at $T = T_0$. In the lower region the maximum pressure differs less than by 10% from it. The 10% criterion is somewhat conditional here. It is used to indicate only a possibility of considerable local pressure jumps (shocks) during system evolution. The solid line in Fig. 3 represents the approximate criterion given by Eq. (16). If one takes into account strong dependence of $\tau_{ex}$ and $\tau_{ind}$ on temperature, the agreement of results is satisfactory.

Conclusion

A simplified theory developed in this paper shows that evaporating inert particles may quench or promote chemical activity in the combustible mixture. Physically clear criteria are proposed to predict critical conditions for gaseous detonation quenching. It is shown that suppression of chemical activity in the combustible gas may be accompanied by strong secondary shock formation and even detonation onset. It is a matter of great concern now to study a combined effect of particle evaporation and drag due to relative motion of phases.
Acknowledgments

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