# Numerical Modeling of Combustion of Fuel-Droplet-Vapour Releases in the Atmosphere 

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#### Abstract

The paper is concerned with a numerical simulation of fuel cloud behaviour which follows releases of a liquid fuel. The main aim of the work is to develop further a mathematical model to simulate such releases into the atmosphere. The model is validated by a comparison with experimental results. The influence of boundary conditions for turbulent kinetic energy $k$ and its dissipation rate $\varepsilon$ on the solution is investigated. It is concluded that the solution depends mainly on the combination of $k$ and $\varepsilon$ in the form $k^{3 / 2} / \varepsilon$ rather than each of these values separately. A way to define the boundary conditions for $k$ and $\varepsilon$ is suggested. The KIVA-II code has been used as the base of the code used. The original code has been modified to simulate low Mach number atmospheric flows, radiation, soot formation and turbulent combustion.


Key words: boundary conditions, combustion, fuel-droplet, turbulence.

## 1. Introduction

Many chemical industry accidents are accompanied by fuel releases. Usually, a large quantity of fuel is stored at high pressure in a liquid state. Even a small rupture can cause a quick release of fuel from a tank. For example, 100 tons of fuel are released in about 10 s . A failure of a tank with pressurised fuel is followed by abrupt decrease of pressure, explosive boiling and evaporation two-phase outflows of a liquid-vapour-air mixture. An ignition of such a fuel-droplet-vapour-air cloud can cause shock-free combustion with the formation of a fireball. The powerful radiation flux emitted by the fireball is dangerous for people and the environment.

There are a number of papers devoted to numerical investigations of the combustion of vapour fuel clouds in the atmosphere. However, combustion of twophase releases of liquid fuel has not been studied well up to now. The present paper is a further development of the model presented in [1]. In a comparison with [1], a more comprehensive model for a droplet motion is used, a nonvertical fuel release is allowed. Special attention is paid to the boundary and initial values for turbulent variables.

The flow of a fuel-droplet-air mixture from a ruptured tank is considered. A Euler-Lagrange approach is used to solve the Navier-Stokes equations. The combustion process (the eddy break-up model), turbulence (the $k-\varepsilon$ model) and radiation (the weighted-sum-of-gray-gases model) are taken into consideration. The Lagrangian approach is used to simulate the behaviour of dispersed droplets and describe the mass, momentum and energy exchange between the gas and liquid phase via the source terms. A one-phase gas model, where instantaneous evaporation of fuel liquid is assumed, is used along with the two-phase model. Numerical results obtained on the basis of the one-phase and two-phase models are compared with each other and with the experimental results.

The present investigations may be directly used in numerical simulation of the tank failure. The process of a tank failure is complicated since it is accompanied by the destruction of the tank, fuel release under high pressure, the intermixing of fuel and air, and combustion. Furthermore, these processes can take place simultaneously. It is very difficult or even impossible to describe all these processes in detail. Therefore, a simple model of the initial stage of the process is desirable. The main aim of this investigation is to develop such a model. A comparison with experimental data enables one to validate the model.

## 2. Problem Statement

### 2.1. Governing EQUATIONS

The gas phase is described by the system of Favre averaged Navier-Stokes equations completed by the $k-\varepsilon$ model of turbulence and the eddy break-up model for turbulent combustion [2]. The gas is considered as a mixture of fuel vapour, oxygen, nitrogen, carbon dioxide and water vapour.

The liquid phase consists of liquid propane droplets. The influence of droplets on the gas is taken into account by the source terms in the conservation equations.

The governing equation system can be rewritten as follows:

$$
\begin{align*}
& \frac{\partial \rho}{\partial t}+\nabla(\rho \mathbf{U})=S_{m}  \tag{1}\\
& \frac{\partial \rho U}{\partial t}+\nabla(\rho \mathbf{U} \mathbf{U})=-\nabla p+\nabla \hat{\mathbf{R}}+\left(\rho-\rho_{a}\right) \mathbf{g}+\mathbf{f}_{d}  \tag{2}\\
& \frac{\partial h}{\partial t}+\nabla(\rho \mathbf{U} h)=\nabla\left(\frac{\mu}{\operatorname{Pr}} \nabla h\right)+H_{c} w-S_{R}+S_{h}  \tag{3}\\
& \frac{\partial \rho Y_{i}}{\partial t}+\nabla\left(\rho \mathbf{U} Y_{i}\right)=\nabla\left(\frac{\mu}{\mathrm{Sc}} \nabla Y_{i}\right)+w_{i}+\delta_{i 1} S_{m}, \quad i=1, \ldots, N,  \tag{4}\\
& \frac{\partial \rho k}{\partial t}+\nabla(\rho \mathbf{U} k)=\nabla\left(\frac{\mu}{\sigma_{k}} \nabla k\right)+G-\rho \varepsilon+S_{t} \tag{5}
\end{align*}
$$

$$
\begin{align*}
& \frac{\partial \rho \varepsilon}{\partial t}+\nabla(\rho \mathbf{U} \varepsilon)=\nabla\left(\frac{\mu}{\operatorname{Pr}} \nabla \varepsilon\right)+\frac{\varepsilon}{k}\left(C_{1} G-C_{2} \rho \varepsilon+C_{S} S_{t}\right),  \tag{6}\\
& \hat{\mathbf{R}}=\mu\left((\nabla \mathbf{U}+\nabla \mathbf{U})^{T}-\frac{2}{3}(\nabla \mathbf{U}) \hat{\mathbf{I}}\right)-\frac{2}{3} \rho k \hat{\mathbf{I}},  \tag{7}\\
& G=\mu_{t}\left(\left(\nabla \mathbf{U}+\nabla \mathbf{U}^{T}\right)^{i j} \nabla_{i} \mathbf{U}_{j}-\frac{2}{3}(\nabla \mathbf{U})^{2}\right)-\frac{2}{3} \rho k(\nabla \mathbf{U})-\frac{\mu_{t} \mathbf{g}}{\rho} \nabla \rho,  \tag{8}\\
& \mu=\mu_{1}+\mu_{t}, \quad \mu_{t}=C_{\mu} \rho \frac{k^{2}}{\varepsilon}, \quad P=\rho R T \sum_{i=1}^{N} \frac{Y_{i}}{m_{i}}, \quad \sum_{i=1}^{N} Y_{i}=1,  \tag{9}\\
& w=\rho A \frac{\varepsilon}{k} \min \left(Y_{F}, \frac{Y_{O}}{v_{O}}, \frac{B Y_{P}}{v_{P}}\right) . \tag{10}
\end{align*}
$$

Here $t$ is time, $\rho$ is the density, $\rho_{a}$ is the undisturbed atmosphere density, $p$ is the deviation of pressure $P$ from the atmospheric one, $\mathbf{U}$ is the velocity, $\hat{\mathbf{R}}$ is the stress tensor, $\mathbf{g}$ is the gravity acceleration, $h$ is enthalpy, $H_{c}$ is the heat of combustion, the source terms $S_{R}, S_{t}, S_{m}, S_{h}$ are determined below, $k$ is the kinetic energy of turbulence, $\varepsilon$ is turbulent dissipation rate, $\hat{\mathbf{I}}$ is the unit tensor, $\mu_{l}$ and $\mu_{t}$ are the laminar and turbulent viscosities, $R$ is the universal gas constant, $T$ is temperature, index 1 corresponds to the fuel vapour, $N$ is the total number of gas species. The gas phase consists of five components (fuel, $\mathrm{O}_{2}, \mathrm{~N}_{2}, \mathrm{CO}_{2}, \mathrm{H}_{2} \mathrm{O}$ ) with mass fractions $Y_{i}$ and the molecular mass $m_{i}$. The reaction rates for individual components are $w_{i}= \pm v_{i} w, v_{F}=1, v_{P}=v_{\mathrm{CO}_{2}}+v_{\mathrm{H}_{2} \mathrm{O}}=1+v_{\mathrm{O}}, Y_{P}=Y_{\mathrm{CO}_{2}}+Y_{\mathrm{H}_{2} \mathrm{O}}$, where the indexes $O$ and $P$ correspond to the oxidiser and combustion products, respectively. Propane $\mathrm{C}_{3} \mathrm{H}_{8}$ is considered as the fuel. The constants in (1) are as follows $C_{\mu}=$ $0.09, C_{1}=1.44, C_{2}=1.92, C_{s}=1.5, \sigma_{k}=1.0, \sigma_{\varepsilon}=1.3, \operatorname{Pr}=0.7, \mathrm{Sc}=0.7$, $A=4, B=0.5$.

To take into account radiative heat transfer, the weighted-sum-of-gray-gases model is used [3]. This model is based upon an approximation of the optical properties of a real gas by a number of gray gases with different absorption coefficients $\kappa$. The total radiation is represented by the sum of the contributions from each spectral group. The contribution of the molecular band radiation of carbon dioxide and water vapour mixture is approximated by three spectral groups, which correspond to optically thin, thick and intermediate spectrum bands. One additional gray gas, characterised by zero absorption coefficient, is added for a continuous spectral representation of the total gas-soot mixture. The radiative heat transfer associated with the soot is approximated by two groups. Thus, the gas-soot mixture is represented by eight gray gases as in [1] and the total radiative source term $S_{R}$ is

$$
\begin{equation*}
S_{R}=\sum_{k=1}^{8} \nabla \mathbf{q}_{R, k} \tag{11}
\end{equation*}
$$

For optically thick gray gases, the radiative heat fluxes $\mathbf{q}_{R, k}$ are determined by the diffusion approximation method, which is reduced to the solution of an elliptic equation

$$
\begin{equation*}
\mathbf{q}_{R, k}=-\frac{1}{3 \kappa_{k}} \nabla U_{k}, \quad \nabla \mathbf{q}_{R, k}=-\kappa_{k}\left(a_{k} U_{b}-U_{k}\right) \tag{12}
\end{equation*}
$$

where $a_{k}$ is a weight coefficient, $U_{k}$ is the radiative energy density of $k$-th gray gas, $U_{b}=4 \sigma T^{4}$ is the black body radiative energy density, $\sigma$ is the Stefan-Boltzman constant.

For optically thin gray gases, a simpler model of the "volume emission" is used. In this case

$$
\begin{equation*}
\nabla \mathbf{q}_{R, k}=4 \kappa_{k} a_{k} \sigma\left(T^{4}-T_{a}^{4}\right) \tag{13}
\end{equation*}
$$

where $T_{a}=293 \mathrm{~K}$ is the atmospheric temperature.
The optical thickness $\iota_{k}$, corresponding to $k$-th gray gas, is determined as the maximal value among the integrals of the absorption coefficient $\kappa_{k}$ along vertical and horizontal lines. The value $\iota_{*}=1$ is considered as the critical point. If $\iota_{k}$ is less than $\iota_{*}$ the gray gas is treated as a thin one; otherwise, the gas is thick.

The soot formation is described by the following equations [4, 5]:

$$
\begin{align*}
\frac{\mathrm{d} N_{s}}{\mathrm{~d} t}= & \nabla\left(\frac{\mu}{\mathrm{Sc}} \nabla \frac{N_{s}}{\rho}\right) \\
& +g_{0} N_{r}\left(N_{s}+N_{r}\right) / K-A \frac{\varepsilon}{k} N_{s} \min \left(1, \frac{v_{s} \rho_{O_{2}}}{v_{S} m_{s} N_{s}+v_{O} \rho_{F}}\right)  \tag{14}\\
\frac{\mathrm{d} N_{r}}{\mathrm{~d} t}= & \nabla\left(\frac{\mu}{\mathrm{Sc}} \nabla \frac{N_{r}}{\rho}\right)+A_{s} Y_{F} \exp \left(-\frac{E}{R T}\right) \\
& +(f-g) N_{r} \frac{Y_{F}}{Y_{F_{0}}}-g_{0} N_{r}\left(N_{S}+N_{R}\right) \\
& -A \frac{\varepsilon}{k} N_{r} \min \left(1, \frac{v_{s} \rho_{\mathrm{O}_{2}}}{v_{S} m_{s} N_{s}+v_{O} \rho_{F}}\right) \tag{15}
\end{align*}
$$

where $\mathrm{d} / \mathrm{d} t$ is the convection derivation operator, $m_{S}=\rho_{S} \pi D_{S}^{3} / 6, \rho_{S}=2$. $10^{3} \mathrm{~kg} / \mathrm{m}^{3}, D_{S}=200 \mathrm{~A}, A_{S}=6.2 \cdot 10^{40} \mathrm{sm}^{-3} \mathrm{~s}^{-1}, E=7.54 \cdot 10^{5} \mathrm{~J} / \mathrm{mole}$, $f-g=100 \mathrm{~s}^{-1}, Y_{F_{0}}=0.2, g_{0}=10^{-15} \mathrm{~m}^{3} / \mathrm{s}, K=5$.

Soot particles are considered as passive ones without influence on gas except through radiation. The soot volume fraction is determined as $f_{v}=m_{S} N_{s} / \rho_{S}$. In the calculations the mass fraction of soot was not more than $10^{-2}$.

Droplets are described by using the Lagrange approach as in [6]. This dispersion phase is presented by sample parcels, each containing a large number of physically
identical droplets. In the $i$-th parcel, all droplets have the same diameter $d_{i}$, coordinate $\mathbf{r}_{i}$, velocity $\mathbf{U}_{i}$ and temperature $T_{i}$. Drop collisions can be taken into account, but for simplicity they are not considered in this research.

The motion equation of a droplet is as follows:

$$
\begin{align*}
& m_{i} \frac{\mathrm{~d}^{2} \mathbf{r}_{i}}{\mathrm{~d} t^{2}}=\mathbf{f}_{d_{i}}+m_{i} \mathbf{g} \\
& \mathbf{f}_{d_{i}}=C_{d} \frac{\pi d_{i}^{2}}{8} \pi\left|\mathbf{U}_{g}-\mathbf{U}_{i}\right|\left(\mathbf{U}_{g}-\mathbf{U}_{i}\right) \tag{16}
\end{align*}
$$

where $\mathbf{U}_{g}=\mathbf{U}+\mathbf{U}^{\prime}$ is local velocity, $\mathbf{U}^{\prime}$ is turbulent fluctuating velocity, and $\mathbf{U}_{i}$ is droplet velocity.

$$
C_{d}= \begin{cases}\frac{24}{\operatorname{Re}_{i}}\left(1+\frac{\mathrm{Re}_{i}^{2 / 3}}{6}\right), & \text { if } \mathrm{Re}_{i}<10^{3}  \tag{17}\\ 0.44, & \text { else }\end{cases}
$$

$\left.\operatorname{Re}_{i}=\rho d_{i}\left|\mathbf{U}_{g}-\mathbf{U}_{i}\right| \mu / \hat{/ T}\right), \hat{T}=\left(T+2 T_{d_{i}} / 3, T_{d_{i}}\right.$ is the temperature of $i$-th droplets.
It is assumed that $\mathbf{U}^{\prime}$ corresponds to the Gaussian probability distribution with the mean $2 / 3 k$. The correlation time $t_{\text {cor }}$ for $\mathbf{U}^{\prime}$ is estimated as the minimum of an eddy breakup time and the time needed for a droplet to traverse an eddy. Thus

$$
\begin{equation*}
t_{\mathrm{cor}}=\Lambda_{e} \min \left(\frac{1}{(2 k / 3)^{1 / 2}}, \frac{1}{\left|\mathbf{U}_{i}-\mathbf{U}_{g}\right|}\right) \tag{18}
\end{equation*}
$$

where $\Lambda_{e}=C_{\mu}^{3 / 4} k^{3 / 2} / \varepsilon$ is the characteristic size.
Evaporation of a droplet is simulated by using the Frossling formula [7]

$$
\begin{equation*}
\frac{\mathrm{d} d_{i}}{\mathrm{~d} t}=-\frac{2 D_{d}(\hat{T})}{\rho_{l} d_{i}} \frac{Y_{1}^{*}-Y_{1}}{1-Y_{1}^{*}} \mathrm{Sh}_{d} \tag{19}
\end{equation*}
$$

where $Y_{1}^{*}$ is fuel vapour mass fraction at the droplet surface, $D_{d}$ is fuel vapour diffusivity in air, $\mathrm{Sh}_{d}$ is the Sherwood number, $\rho_{l}$ is fuel density,

$$
\begin{align*}
\mathrm{Sh}_{d} & =\left(2+0.6 \mathrm{Re}_{d}^{1 / 2} \mathrm{Sc}_{d}^{1 / 3}\right) \frac{\ln \left(1+b_{d}\right)}{b_{d}} \\
\mathrm{Sc}_{d} & =\frac{\mu(\hat{T})}{D_{d}(\hat{T})}, \quad b_{d}=\frac{Y_{1}^{*}-Y_{1}}{1-Y_{1}^{*}} \tag{20}
\end{align*}
$$

Droplet temperature $T_{d}$ is determined by the energy balance equation

$$
\begin{equation*}
\frac{1}{6} \rho_{l} d c_{l} \dot{T}_{d}-\rho_{l} R L\left(T_{d}\right)=Q_{d} \tag{21}
\end{equation*}
$$

$Q_{d}$ is determined by Ranz-Marshall correlation

$$
\begin{equation*}
Q_{d}=\lambda \frac{T-T_{d}}{d} \mathrm{Nu}_{d} \tag{22}
\end{equation*}
$$

where $\mathrm{Nu}_{d}$ is the Nusselt number

$$
\begin{equation*}
\mathrm{Nu}_{d}=\left(2+0.6 \mathrm{Re}_{d}^{1 / 2} \operatorname{Pr}_{d}^{1 / 3}\right) \frac{\ln \left(1+b_{d}\right)}{b_{d}} \tag{23}
\end{equation*}
$$

$\operatorname{Pr}_{d}=\operatorname{Pr}_{d}(\hat{T})$ is the Prandtl number, $\lambda$ is the molecular heat conductivity.
The following equation [7] is solved to simulate break-up of droplets:

$$
\begin{equation*}
\rho_{l} d_{i}^{2} \frac{\mathrm{~d}^{2} s}{\mathrm{~d} t^{2}}+20 \mu_{l} \frac{\mathrm{~d} s}{\mathrm{~d} t}+64 \alpha s / d_{i}=2.7 \rho\left(\mathbf{U}_{g}-\mathbf{U}_{i}\right)^{2} \tag{24}
\end{equation*}
$$

where $\alpha$ is the surface tension coefficient, $s$ is the formal distortion parameter. The criteria of breaking up is $s>1$. After break up the new droplet radii satisfy to a distribution with the following distribution function:

$$
\begin{equation*}
g(d)=2 / d_{c} \exp \left(-d / d_{c}\right), \quad d_{c}=\bar{d} /\left(7+0.05 \rho_{l} \bar{d}^{3} \bar{s}_{t}^{2} / \alpha\right) \tag{25}
\end{equation*}
$$

The magnitudes $\bar{d}$ and $\bar{s}_{t}\left(s_{t}=\mathrm{d} s / \mathrm{d} t\right)$ correspond to $s=1$.
The source terms in Equations (1-10) are determined by summing contributions of all individual droplets in parcels as follows:

$$
\begin{align*}
\mathbf{f}_{d} & =-\frac{1}{\nabla V} \sum_{\nabla V} N_{i} \mathbf{f}_{d, i} \delta\left(\mathbf{r}-\mathbf{r}_{i}\right), \quad S_{m}=-\frac{1}{\nabla V} \sum_{\nabla V} N_{i} \dot{m}_{i} \delta\left(\mathbf{r}-\mathbf{r}_{i}\right), \\
S_{t} & =-\frac{1}{\nabla V} \sum_{\nabla V} N_{i} m_{i} \frac{\mathrm{~d}^{2} \mathbf{r}}{\mathrm{~d} t^{2}} \cdot \mathbf{U}^{\prime} \delta\left(\mathbf{r}-\mathbf{r}_{i}\right), \\
S_{h} & =-\frac{1}{\nabla V} \sum_{\nabla V} N_{i} \dot{m}_{i}\left(h-H_{v}\right) \delta\left(\mathbf{r}-\mathbf{r}_{i}\right), \tag{26}
\end{align*}
$$

Here $m_{i}=\rho_{l} \pi d_{i}^{3} / 6, h=h\left(T_{d}\right)$ is the fuel vapour enthalpy, $H_{v}$ is the heat of evaporation, $N_{i}$ is the number of droplets in $i$-th parcel, $\Delta V$ is the computational cell volume. The summation is performed over all droplets within the computational volume $\Delta V$ surrounding the end of the vector $\mathbf{r}$.

The effect of the liquid volume fraction has been neglected because the evaporation time is essentially less than the total time of the problem and the flow is mainly considered much further from the source, where the liquid phase can be essential.

### 2.2. INITIAL AND BOUNDARY CONDITIONS

The problem is considered as an axysimmetrical one in the cylindrical coordinate system $(r, z)$. It is assumed that fuel vapour and droplets are injected into an undisturbed atmosphere with constant temperature $T_{a}$ and pressure $P_{a}$.

The principal question is how to define initial data for liquid-vapour fuel. We assumed that the fuel is injected from a circular source. The other way of defining
the initial data is to consider a given initial fuel distribution, which is established instantaneously. As our study shows, the latter approach failed to give sufficiently satisfactory results.

The source is considered to be a plane disk of diameter $D$. The source height is negligibly small in comparison with the characteristic size of the region. Initially, the source injects a fuel vapour-liquid mixture into the atmosphere. The injection velocity is represented by a piecewise function of time. It is assumed that spatial distribution of the velocity follows the Gaussian distribution with the maximum value of $U_{\text {in }}(0)$ on the axis $z$ and decrease of the velocity at the source boundary by a factor of $\sqrt{2}$.

The incompressible Bernoulli equation is used to estimate the maximum outflow velocity $U_{\text {in }}(0)$, so that

$$
\begin{equation*}
U_{\text {in }}(0)=\left(2\left(P_{0}-P_{a}\right) / \rho_{l}\right)^{1 / 2}, \tag{27}
\end{equation*}
$$

where $P_{0}$ is the pressure in the tank at the moment of failure, $\rho_{l}$ is the liquid propane density at pressure $P_{0}$.

The injection is realised at an angle $\theta=\theta(r)$ to the axis of symmetry, so that $\theta(0)=0, \theta(D / 2)=\theta^{*}$. In calculations $\theta^{*}=70^{\circ}$ was assumed. Fuel consists of fuel vapour characterised by the mass fraction $x_{v}$ while the liquid part is represented by droplets with the same initial diameter $d_{0}$ for simplicity. We assumed $d_{0}=50 \mu \mathrm{~m}$. The initial droplet diameter has been taken as a constant and is equal to $50 \mu \mathrm{~m}$ because, according to [1], the initial diameter slightly influences the solution if the fuel mass is above 1 kg .

It is difficult to estimate the fraction $x_{v}$ of the fuel mass discharged as vapour. We considered two approaches. In the first simplistic approach we assumed that the fuel is evaporated instantaneously, so that $x_{v}=1$. The second approach for the estimation $x_{v}$ was used in [1], where $x_{v}$ was calculated by an average balance assuming that the liquid heat capacity $C_{l}$ and heat of evaporation $H_{v}$ are constant. Then $x_{v}=\operatorname{Cl}\left(T_{0}-T_{\mathrm{bp}}\right) / H_{\nu}$, where $T_{0}$ is the lading temperature at the point of failure $\left(58^{\circ} \mathrm{C}\right), T_{\mathrm{bp}}$ is the temperature at the boiling point $\left(-42^{\circ} \mathrm{C}\right)$.

After the depressurisation, the density of the two-phase mixture is

$$
\begin{equation*}
\rho_{\mathrm{in}}=\frac{1}{\frac{x_{v}}{\rho_{v}}+\frac{1-x_{v}}{\rho_{l}}}, \tag{28}
\end{equation*}
$$

where $\rho_{v}=\rho_{v}\left(P_{a}\right)$ is the vapour density on the saturation line at ambient pressure, $\rho_{l}=\rho_{l}\left(P_{a}\right)$ is the liquid fuel density at ambient pressure.

We assumed that the vapour-liquid mixture is injected from the source with the total density $\rho_{\text {in }}$ and mass vapour fraction $x_{v}$.

Since $\rho_{\text {in }} \neq \rho_{l}$, it is necessary to consider the equivalent source with the diameter $D_{\text {eff }}$

$$
\begin{equation*}
\rho_{l} D_{b}^{2}=\rho_{\mathrm{in}} D_{\mathrm{eff}}^{2}, \tag{29}
\end{equation*}
$$

where $D_{b}$ corresponds to the breach area $S_{b}$.

The right and upper boundaries are located far enough so that droplets do not reach these boundaries. After termination of the release, the inlet flow boundary conditions in the source were changed to the solid wall boundary conditions.

On the solid wall the following boundary conditions for $k$ and $\varepsilon$ were used

$$
\begin{equation*}
k=0, \quad \nabla \varepsilon \cdot \mathbf{n}=0 . \tag{30}
\end{equation*}
$$

Here $\mathbf{n}$ is the internal unit normal vector.
The following boundary conditions for radiative fluxes were used for optically thick gray gases

$$
\begin{equation*}
2 \mathbf{q}_{R, k} \cdot \mathbf{n}=\left.\left(a_{k} U_{b}-U_{k}\right)\right|_{w} . \tag{31}
\end{equation*}
$$

We assumed that an ignition is sparklike and takes place near the source surface in a small volume.

## 3. Numerical Procedure

The small Mach number approximation [8] was used to solve the system of governing equations. In this approach, a pressure deviation from the atmospheric value $P_{a}$ (proportional to the square of the Mach number) is neglected everywhere except in the pressure gradient in the momentum equation. The Poisson equation for the pressure correction has to be solved. This simplification allows one to remove the stiffness associated with propagation of sound waves.

A staggered rectangular nonuniform mesh was used. The approximation was of the second order for the spatial derivatives and the first order for the time derivatives. Usually, a computational mesh included $100 \times 200$ mesh points. The elliptic equations were solved by a preconditioned conjugate gradient method.

The elliptic equations were solved by the preconditioned conjugate gradient method [9] as follows. Let us assume that a finite-difference analog of the elliptic equation is the following system of linear equations

$$
\begin{equation*}
A \mathbf{X}=\mathbf{b} . \tag{32}
\end{equation*}
$$

Then, an approximate solution of the system is defined by the following procedure:

$$
\begin{align*}
& \mathbf{x}_{j+1}=\mathbf{x}_{j}+\alpha_{j} \mathbf{p}_{j}, \quad \alpha=\left\|\mathbf{r}_{j}\right\|^{2} /\left(A \mathbf{p}_{j}, M \mathbf{p}_{j}\right),  \tag{33}\\
& \mathbf{r}_{j+1}=\mathbf{r}_{j}-\alpha_{j} A \mathbf{p}_{j}, \quad \beta_{j+1}=\left\|\mathbf{r}_{j+1}\right\|^{2} /\left\|\mathbf{r}_{j}\right\|^{2},  \tag{34}\\
& \mathbf{p}_{j+1}=M^{-1} \mathbf{r}_{j+1}+\beta_{j} \mathbf{p}_{j} . \tag{35}
\end{align*}
$$

Here $M$ is a preconditioning symmetric positive definite matrix, the vectors are considered in the Euclidean space with the following inner product

$$
\begin{equation*}
(\mathbf{a}, \mathbf{b})=M_{i j}^{-1} \mathbf{a}_{j} \mathbf{b}_{i} . \tag{36}
\end{equation*}
$$

The radiation problem is the most difficult to solve due to a stiffness caused by a wide range of the absorption coefficients. A successful choice of the preconditioning matrix $M$ is very important here. The Jacobi matrix is a simple suitable way to choose $M$. The other way, used in this work, is to choose $M$ as the matrix corresponding to matrix $A$ when there is an uniform mesh and constant "effective" absorption coefficient. In this case, the inverse matrix $M^{-1}$ may be obtained very quickly by the method of quick Fourier transformation in one direction along with the Thomas algorithm in the other one. Usually, the second way has proved more effective. As a result, calculation of the radiation part of the problem was not time consuming and added only about $20 \%$ to the total computing time.

The system of Equations $(14-15)$ for the soot formation was integrated at each time step after all the other governing equations had been integrated by using the method of splitting into physical processes. The most difficult subsystem for the solution is the chemical kinetic one

$$
\begin{align*}
\frac{\mathrm{d} N_{s}}{\mathrm{~d} t} & =g_{0} N_{r}\left(N_{s}+N_{r}\right) / K  \tag{37}\\
\frac{\mathrm{~d} N_{r}}{\mathrm{~d} t} & =A_{s} Y_{F} \exp \left(-\frac{E}{R T}\right)+(f-g) N_{r} \frac{Y_{F}}{Y_{F_{0}}}-g_{0} N_{r}\left(N_{s}+N_{R}\right), \tag{38}
\end{align*}
$$

because of its stiffness. To integrate this system, we use the method of total approximation splitting the system into the differential equations, which include the free term, linear term with $N_{r}$ and nonlinear part into the right side accordingly. The final approximate solution at the next time step $t=t_{n+1}$ can be received analytically in quadratures as follows:

$$
\begin{align*}
& N_{r}\left(t_{n+1}\right)=N_{r}^{\prime \prime} D_{r s}(\Delta t) D_{e}(\Delta t)  \tag{39}\\
& N_{s}\left(t_{n+1}\right)=\left(N_{s}\left(t_{n}\right)+N_{r}^{\prime \prime}\right) D_{r s}(\Delta t)-N_{r}\left(t_{n+1}\right)  \tag{40}\\
& N_{r}^{\prime}=A_{S} Y_{f} \int_{t_{n}}^{t_{n+1}} \exp (-E /(R T))  \tag{41}\\
& N_{r}^{\prime \prime}=N_{r}^{\prime} \exp \left((f-g) / Y_{F_{0}} \int_{t_{n}}^{t_{n+1}} Y_{F}\right) \tag{42}
\end{align*}
$$

where

$$
\begin{aligned}
& D_{r s}(\Delta t)=N_{s}\left(t_{n}\right)+N_{r}^{\prime \prime}-(1-\beta) N_{r}^{\prime \prime} D_{e}(\Delta t) \\
& D_{e}(\Delta t)=\exp \left(-g_{0}\left(N_{s}\left(t_{n}\right)+\beta N_{r}^{\prime \prime}\right) \Delta t\right), \quad \beta=1 / K, \quad \Delta t=t_{n+1}-t_{n}
\end{aligned}
$$

It is easy to show that scheme (39-42) is positively defined. It means the scheme guarantees positivity of $N_{r}$ and $N_{s}$ in calculations.

## 4. Comparison with Experimental Data

We considered test 93-12 from the report [10] since this experiment is presented with the most comprehensive set of measurements. The tank failure was accompanied by the BLEVE phenomena in this experiment. The main parameters of the experiment were $M_{0}=110 \mathrm{~kg}, P_{0}=2.1 \mathrm{MPa}, T_{0}=331 \mathrm{~K}, S_{b} \approx 0.01 \mathrm{~m}^{2}$. In this case we have $x_{v} \approx 0.6, \rho_{\text {in }} \approx 4 \mathrm{~kg} / \mathrm{m}^{3}, \rho_{v} \approx 2.4 \mathrm{~kg} / \mathrm{m}^{3}, U_{\mathrm{in}}(0)=94.7 \mathrm{~m} / \mathrm{s}$.

The influence of the initial and boundary conditions for $k$ and $\varepsilon$ on the solution was investigated. Our calculations showed that the solution depends mainly on the combination of $k$ and $\varepsilon$ in the form $k^{3 / 2} / \varepsilon$ rather than each of these values separately. Even a variation of $k$ and $\varepsilon$ within several orders of magnitude had a weak effect on the solution if the combination $k^{3 / 2} / \varepsilon$ was held constant. This prompts the following way of defining the initial and boundary conditions for $k$ and $\varepsilon$. According to Prandtl's mixing-length hypothesis, the mixing length $\Lambda=k^{3 / 2} / \varepsilon$ may be obtained by using the local equilibrium assumption $(G=\varepsilon)$ and eddy viscosity model. Originally, values of $\Lambda$ at the source $\left(\Lambda_{\text {in }}\right)$ and in the atmosphere $\left(\Lambda_{a}\right)$ have to be estimated. Thereafter values of $k$ and $\varepsilon$ may be estimated roughly.

We assumed that the inlet value of $\Lambda$ at the boundary is

$$
\begin{equation*}
\Lambda_{\mathrm{in}}=0.05 D \tag{43}
\end{equation*}
$$

which is the natural correlation between a typical path scale and $\Lambda$, e.g. in case of a round jet $\Lambda=0.04 D$ [11].

It is difficult to estimate $\Lambda_{a}$ for the initial boundary conditions in advance. It depends on atmospheric conditions near the experimental equipment. In the experiment, just one quantitative characteristic is available that is the span $t_{\mathrm{FB}}$ of the fireball ( $t_{\mathrm{FB}}$ as the time taken for the fireball to be visible). Calculations show that increasing $\Lambda_{a}$ causes a decrease in $t_{\mathrm{FB}}$. The value of $t_{\mathrm{FB}}$ has been used as a characteristic value to determine $\Lambda_{a}$.

In the experiment, $t_{\mathrm{FB}}$ was about 4 s . In calculations, $\Lambda_{a}$ was taken as 0.7 m that corresponds to $D / 2$ approximately. The relation between $\Lambda_{a}$ and $D$ is just formal (of course, they are physically independent parameters) and it is used here to find reference point for the estimation of $\Lambda_{a}$.

The certain dependence of the fireball span on the turbulence length scale $\Lambda_{a}$ seems unexpected. Possibly, it takes place due to the use of the equilibrium $k$ $\varepsilon$ turbulence model in nonequilibrium conditions. The use of such a model, with the value $\Lambda_{a}$ as a free parameter, is justified by its simplicity in comparison with nonequilibrium turbulence models.

To estimate the inlet and initial turbulent kinetic energy at a given $\Lambda$, it is sufficient to satisfy such clear demands as

$$
\begin{equation*}
k_{\mathrm{in}} \ll U_{\mathrm{in}}^{2}, \quad k_{a} \ll k_{\mathrm{in}} \tag{44}
\end{equation*}
$$



Figure 1. Fireball. Temperature. Two-phase model. $M_{0}=110 \mathrm{~kg}, t_{\mathrm{in}}=0.2 \mathrm{~s}$. Simulation of experiment [10]. Dashed line corresponds to the visible fireball in the experiment. Dotted line indicates the visible fireball in the calculations.
where $k_{\text {in }}$ is the inlet kinetic turbulence energy, $k_{a}$ is the initial value for $k$.
In the calculations we assumed that

$$
\begin{equation*}
k_{\mathrm{in}}=10^{-2} U_{\mathrm{in}}^{2}, \quad k_{a}=10^{-7} U_{\mathrm{in}}^{2} . \tag{45}
\end{equation*}
$$

Calculation results are presented in Figure 1 for the two-phase model. The injection period tin was 0.2 s . The fireball dynamic is presented at the time instants $t=0.5,1.5,2.5$ and 3.5 s . The predictions are shown as a contour plot of temperature. The dashed line is the visible fireball boundary in the experiment. The
boundary is indicated approximately since the fireball was essentially asymmetric. The dotted line indicates the fireball boundary, obtained in the calculations, from the outside point of view.

A reasonable agreement can be claimed between the experimental and computational positions of the upper fireball edge, except the first instant $(t=0.5 \mathrm{~s})$. The latter can be explained by simplifications of our model, which were accepted for the initial stage of the process. In the experiment, the fireball is essentially asymmetric. Possibly, this is the main reason for the difference between the experimental and computational fireball location at the last instant $(t=3.5 \mathrm{~s})$.

The lower edge location depends strongly on the injection time. Afterburning fuel affects the location of the lower boundary in the experiment. To show the role of this effect, we considered a case where the liquid fuel was injected for 1.4 s but the injection time for the vapour fuel remained as in the previous example. The computational results are presented in Figure 2. Due to the delay in the fuel injection, the computational fireball lower edge is essentially closer to the experimental edge.

It is useful to compare these results with the ones obtained for the simpler gas model with $x_{v}=1$, which means instantaneous evaporation of fuel. In this case $\rho_{\text {in }}=\rho_{v}$ and $D_{\text {eff }}=1.5 \mathrm{~m}$. The fuel is ignited faster in the case of the gas model since the stage of droplet evaporation is absent. It takes time for droplet evaporation. The last droplets disappeared in about 0.5 s . Since the fuel evaporates much faster than the fireball span, the fireball structure is similar to that of the two-phase model (Figure 1).

It is interesting to verify the proposed approach to the definition of boundary conditions for the turbulent variables $k$ and $\varepsilon$ at another experiment. A comparison with Hasegawa-Sato's experiment [12] on the vertical combustion of fuel-vapour clouds created by an impulse source was done. Test $P_{r}-5$ has been considered as in [1]. The experiment is characterised by the following data: $M_{0}=5.85 \mathrm{~kg}$, $T_{0}=301 \mathrm{~K}, P_{0}=10 \mathrm{~atm}$. No precise data on the size $S_{b}$ is given in [12]. The equivalent diameter was taken to be $D_{\text {eff }}=0.5 \mathrm{~m}$, which corresponds to an actual breach diameter of Dreal, release time of $t_{\text {in }}=0.13 \mathrm{~s}$ and the vapour fraction $x_{v}=0.386$. These parameters coincide with the data chosen in [1]. The calculation results, presented in [1], showed that the breach diameter influences the fireball characteristics weakly as long as the release time is relatively short.

The ignition source corresponds to the pilot flame in the experiment. It has coordinates $(r, z)=(0.5 \mathrm{~m}, 4 \mathrm{~m})$ and the typical size $d_{\mathrm{ig}}=0.2 \mathrm{~m}$. In the calculations the reactions were artificially completed in this region up to the end in each time step.

To compare with the calculation results [1], as well, we only considered a vertical release with a constant injection velocity $U_{\text {in }}=60.6 \mathrm{~m} / \mathrm{s}$. According to Makhviladze et al. [1], the initial droplet diameter is not essential for fuel masses exceeding about 1 kg , so that we used the same diameter $d_{0}$ as for the previous test case.


Figure 2. Fireball. Temperature. Two-phase model. $M_{0}=110 \mathrm{~kg}, t_{\mathrm{in}}=1.45 \mathrm{~s}$. Simulation of experiment [10]. Dashed line corresponds to the visible fireball in the experiment. Dotted line indicates the visible fireball in the calculations.

A fireball dynamic is presented at the time instants $t=1.17,1.45$ and 2 s in Figure 3. The dashed line corresponds to the visible cloud shape in the HasegawaSato experiment $P_{r}-5$. A good correspondence between our results and both the experimental and computational results [1] has been obtained, but in [1] the initial and boundary conditions were chosen specially to coincide with the experiment [12].


Figure 3. Fireball. Temperature. Two-phase model. $M_{0}=5.85 \mathrm{~kg}, t_{\mathrm{in}}=0.13 \mathrm{~s}$. Simulation of the Hasegawa-Sato experiment [12]. Dashed line corresponds to the visible fireball in the experiment.

In Figure 4, the comparison of the maximum temperature as the function of time is given for different radiation models. The continuous line corresponds to the model (20-24). The dashed line represents the case where the radiation has not been taken into account. The comparison shows that due to the radiation the temperature decreases by up to 400 K . The soot contribution has not been so essential: the change of temperature was within 50 K . The dotted line represents a


Figure 4. Maximum temperature in fireball as function of time for different radiation models.
simplified radiation model which uses just one "average" absorption coefficient $k=\sum_{1}^{8} a_{j} k_{j}$. This model is much less time-consuming, because we only need to solve one radiation equation, and the model gives quite reasonable results.

## 5. Conclusions

A mathematical model was developed to simulate the behaviour of releases, following tank failures with hydrocarbon fuels at high pressures.

The $k-\varepsilon$ model is used to simulate the turbulent processes. Inlet and initial boundary conditions for $k$ and $\varepsilon$ have to be specified. In this work, an approach was suggested to estimate the initial and inlet boundary conditions for $k$ and $\varepsilon$. This approach is based on the results of our calculations which show that the mixing length $\Lambda$ is a governing parameter to choose initial and boundary values for $k$ and $\varepsilon$. It means that the solution depends more strongly on the inlet and boundary conditions for $\Lambda$ than on the inlet and initial values of $k$ and $\varepsilon$ separately. The choice of inlet value of $\Lambda$ is suggested.

It was shown that it is acceptable to use a pure gas model to simulate fuel cloud behaviour in the case of nondelayed ignition.

The mathematical model developed was verified by a comparison with different experimental data.

Three-dimensional effects can be essential in the simulation of real phenomenon and will be considered in future research.

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