Modelling and Scaling of Fireballs from Single -and Two-Phase Hydrocarbon Releases

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ABSTRACT

Numerical modelling of evolution, behaviour and radiation of fireballs occurring in the atmosphere as a result of hydrocarbon fuel releases is reported. Transient reacting flows developing upon vertical outflows are considered for the cases of single-phase releases (relevant to discharge of hydrocarbons in the case of low storage overpressure) and two-phase releases (relevant to discharge of pressure-liquefied hydrocarbons). The calculations performed are for methane and propane fireballs in a wide range of fuel masses from 1 g up to 1000 kg. The scaling of fireball size and lifetime as functions of fuel mass and release velocity is studied. Unified description of single- and two-phase cloud burning times in terms of Froude number is given. The internal structure of fireballs of different linear scales is obtained. The radiation characteristics of small (optically thin) and large (optically thick) fireballs are compared. Good agreement between the calculated results and experimental data available is demonstrated.

KEYWORDS : External fires, fire safety, hydrocarbon releases, fireballs, modelling, scaling

INTRODUCTION

Fireballs occurring upon ignition of hydrocarbon fuel accidentally released into the atmosphere emit powerful heat radiation which is considered one of the major hazards of modern chemical industry [1]. The outflows of flammable substances in a typical accident may be either single-phase or two-phase. In the latter case a mixture of fuel vapour and droplets formed as a result of flash evaporation of pressure-liquefied gas escapes into the atmosphere. Studying the conditions for fireball formation, properties and behaviour of the burning cloud and its impact on the environment (including hazards to people and materials) is an important part of risk analysis.

Experimental studies of fireballs performed over the past two decades were focused primarily on measuring the maximum diameter, elevation, lifetime, surface temperature and emissive power [2–4]. This led to the development of engineering methods for the prediction of integral parameters of burning clouds which proved very useful in quantitative risk assessment practice (e. g., [5, 6]), providing a fast screening tool for analysis of possible accident scenarios and a number of relevant computer codes are available commercially. Very little information, however, was obtained about the internal structure of fireballs, which may be attributed to the experimental difficulties in studying such short-duration and intrinsically transient combustion.

A "big issue" in studies of fireballs is the role of scale effects on the structure, size and duration of burning clouds as well as on their environmental impact mostly attributed to the heat radiation. The asymptotic scaling laws may be derived from dimensional analysis. However, to obtain a meaningful relationship between multiple non-dimensional parameters, a significant degree of simplifications has to be introduced. For example, the dependence of the fireball lifetime on the fuel mass and release conditions can be obtained in the limiting cases of momentum-dominated and buoyancy-controlled fireballs. For a wide range of practically important parameters, however, both momentum and gravity forces are of importance and the scaling laws need special study (see e. g., [7]). Even more complicated is the problem of scale effects on two-phase releases when additional time and length scales related to motion and evaporation of the dispersed phase arise in the problem.

Many questions related to the internal structure of a burning cloud are not yet studied adequately at the moment. In particular, it has not been clarified to what extent the temperature, concentration and radiation fields in the fireball depend on the cloud size and how the heat fluxes received by the ground surface change with fireball scale. The data available from large-scale experiments tend to be specific to a particular test and in any case remain quite scarce. However, an insight into these problems may be achieved by using the CFD methods. In this paper single- and two-phase fireballs are studied numerically. Methane and propane fireballs are modelled and the scale effects are considered. This work extends the numerical analysis of fireballs presented earlier [8, 9].

MODEL

The mathematical model used for studying the fireballs is based on a system of Favre-averaged mass, momentum, energy and species conservation equations closed by the $k-\varepsilon$ model of turbulence [10] and eddy break-up model of turbulent combustion [11]. The gaseous phase consists of O_2, N_2, fuel vapour, CO_2 and H_2O. Temperature dependencies of enthalpies and heat capacities of all components are taken into account. In general, the model for the gas phase is similar to the one used in [8, 9] for gaseous fireball calculations, the main difference being the additional source terms accounting for two-phase effects and radiative heat transfer.

The Lagrangian approach is adopted for the description of the dispersed phase. Each of the liquid fuel droplets is characterised by its own diameter and velocity which may differ from the local gas velocity. The net drag force between the gas and dispersed phase is allowed for by introducing an appropriate source term into the momentum equation. Evaporation rate for each droplet is described by the quasi-steady model with correction for the relative motion of droplet with respect to the gas. Mass and energy exchange between the dispersed and gaseous phases are taken into account by source terms in the continuity and energy equations. It is assumed that droplets do not burn individually, rather they serve as a volumetric fuel vapour source while the reaction proceeds in the surrounding gas phase. No allowance for influence of droplets on turbulent characteristics is made.

Formation and oxidation of soot particles are allowed for using the two-step global kinetics model [12] with the modifications and constant adjustments for large-scale flames offered in [13]. The first stage consists in pyrolysis of fuel molecules and formation of radical nuclei, while at the second stage solid soot particles are being formed. The soot oxidation is considered to be mixing-controlled and described according to the eddy break-up model [11].

The radiative properties of hot combustion products are described by the Weighted-Sum-of-Gray-Gases (WSGG) model [14]. Total of $N_g = 8$ gray gases are used for the mixture of CO_2, H_2O and soot, the model absorption coefficients κ_i and polynomial approximations for the weighting coefficients a_i are taken according to [16, 17]. For each gray gas the radiative transfer equation

$$\nabla \mathbf{q}_{R,i} = \kappa_i (a_i E_b - E_i), \quad i = 1 \ldots N_g \tag{1}$$

is solved, where $\mathbf{q}_{R,i}$ is the radiative flux, E_i is the radiative energy density corresponding to the i-th gray gas, $E_b = 4\sigma T^4$ is the blackbody energy density, σ is the Stefan-Boltzmann constant. The radiative transfer equation (1) for individual gray gases is solved using either the volumetric emission approximation or the P_1-approximation of spherical harmonics method depending on the optical thickness of fireball in the corresponding spectral group [15]. Namely, for optically thin gray gases radiation reabsorption is neglected and Eq. (1) reduces to

$$\nabla \mathbf{q}_{R,i} = 4\kappa_i a_i \sigma (T^4 - T_a^4).$$

For optically thick gray gases the radiative flux is proportional to the gradient of radiative energy density, so that an elliptic equation has to be solved for E_i:

$$\mathbf{q}_{R,i} = -\frac{1}{3\kappa_i} \nabla E_i, \qquad \nabla \frac{1}{3\kappa_i} \nabla E_i + \kappa_i (a_i E_b - E_i) = 0$$

The total radiative source term in the energy equation is assessed as the sum of source terms relevant to all individual gray gases: $\nabla \mathbf{q}_R = \sum_{i=1}^{N_g} \nabla \mathbf{q}_{R,i}$. To calculate the radiative fluxes from the burning cloud incident onto the ground surface, the Monte Carlo method was used.

The scenario for fireball formation considered below is that used in the previous work [8, 9]: some finite mass of fuel M_0 is released into the initially quiescent atmosphere from a circular source located on the ground surface. The fuel velocity U_0 is directed vertically upward, the ignition occurs near the axis at some elevation above the source. The calculations are performed until total fuel burnout and cooling of combustion products.

PARAMETERS AND SCALES

To determine the role of scale effects, calculations were performed in a wide range of fuel masses spanning six orders of magnitude M_0 = 1 g – 1000 kg. Isothermal subsonic outflow conditions were used for gaseous releases, which corresponds to low-to-medium storage overpressures. On the other hand, two-phase outflow parameters were chosen to represent depressurisation of a vessel filled with a volatile pressure-liquefied gas (propane). The storage pressure was taken equal to the saturated vapour pressure at the storage temperature. The fuel was assumed to escape from the vessel in an all-liquid state undergoing flash evaporation in the near zone. As a result of flash evaporation, the remaining liquid disintegrates into fine droplets of the diameter 10–100 μm while the temperature of the resulting aerosol-vapour mixture drops to the boiling temperature at the ambient pressure. Further downstream the flow is virtually isobaric. The near zone was excluded from calculations by substituting the "equivalent orifice" parameters calculated from thermodynamics. The velocities of droplets and vapour at the source were assumed the same. The range of source diameters was chosen such that the release time was shorter than the fireball burning time. Also, the ignition height was of the order of several source diameters which resulted in rapid ignition of escaping fuel. In this way the influence of source diameter and ignition source was quite insignificant, and these values are not considered below as governing parameters.

To tackle the scaling issue it is necessary to introduce meaningful characteristic values which could be used to reduce the problem to a non-dimensional form. In particular, the length scale should be chosen taking into account gas heating and expansion in the burning cloud. An appropriate length scale was defined in [9] as

$$L_* = \left(\frac{QM_0}{\rho_a C_{p,a} T_a} \right)^{1/3}, \tag{2}$$

where Q is the heat of combustion, index a denotes parameters taken at the ambient conditions. The maximum diameter of fireball observed experimentally scales with the mass of fuel as $D_{FB} = AM_0^{1/3}$ where, according to different authors, the average proportionality constant A ranges from 5.8 to 6.28 [5, 6]. In terms of the length scale (2), this range is expressed as $D_{FB} = (1.15 - 1.25)L_*$, where the proportionality constants are calculated using $Q \approx 50$ MJ/kg typical of hydrocarbon fuels. Thus, the length L_* practically coincides with the experimental maximum diameter of fireball and may be considered as a "natural" length scale for the burning cloud. The velocity and time scales are introduced as

$$U_* = (L_* g)^{1/2}, \qquad t_* = (L_*/g)^{1/2}. \tag{3}$$

The relationship between the momentum and buoyancy forces acting on the burning cloud is given by the Froude number

$$\mathrm{Fr} = \left(\frac{U_0}{U_*} \right)^2 = \frac{U_0^2}{g \left(\dfrac{QM_0}{\rho_a C_{p,a} T_a} \right)^{1/3}}. \tag{4}$$

Note that the above parameters are applicable both to single- and two-phase releases because they are based only on the integral characteristics — total fuel mass and release velocity.

SIZES AND BURNING TIMES OF SINGLE- AND TWO-PHASE FIREBALLS

The calculations performed for single-phase (methane, propane) as well as two-phase (propane) fireballs have shown that the experimental relationship between the maximum fireball diameter and the cubic root of fuel mass $D_{FB} = (5.8 - 6.28)M_0^{1/3}$ (or its equivalent form $D_{FB} = (1.15 - 1.25)L_*$) is reproduced quite well [8,9]. The maximum fireball size is primarily determined by the expansion of air entrained and heated in the burning cloud. Since hydrocarbon fuels have a relatively narrow range of heats of combustion, the influence of fuel type remains insignificant.

The burning time of a fireball t_{FB} may be estimated from dimensional analysis: in the case of momentum-dominated release $t_{FB} \propto L_*/U_0$, while for buoyancy-controlled clouds $t_{FB} \propto L_*/U_* = t_*$. The dependence of fireball lifetime on the fuel mass and release velocity in the intermediate cases was determined experimentally in [7] where gaseous methane and propane releases were studied and approximating formulae were offered for vertical and horizontal releases. In particular, the burning time of a fireball resulting from a vertical outflow of hydrocarbon gas was found to be described by the correlation

$$\frac{t_{FB}}{\hat{t}_*} = \frac{10.6}{1 + \dfrac{1}{50}\dfrac{U_0}{\hat{U}_*}}, \quad \text{where} \quad \hat{t}_* = \left(\frac{M_0}{\rho_a}\right)^{1/6} g^{-1/2}, \quad \hat{U}_* = \left(\frac{M_0}{\rho_a}\right)^{1/6} g^{1/2}. \tag{5}$$

This formula gives correct functional dependencies in the cases of large and small release velocities, it can be rewritten (see [9]) in terms of the non-dimensional variables (2)–(4) as

$$\left(\frac{t_{FB}}{t_*}\right)^{-1} = 0.22 + 0.01\,(U_0/U_*) = 0.22 + 0.01\mathrm{Fr}^{1/2}. \tag{6}$$

Thus, in the experiments the inverse non-dimensional burning time was found to be a linear function of the square root of Froude number. The same representation of the calculated results is used below.

In Fig. 1 burning times calculated in this work for gaseous methane and propane releases are shown by the open points, while the filled points correspond to the two-phase propane releases. The variation of Froude number was achieved in two ways — either by changing the total fuel mass released M_0, or by changing the outflow conditions, source size and ignition height. Also, in the case of two-phase outflow the droplet size was varied in the range 10–100 μm. In the calculations performed without radiative processes taken into account (see [9]) the fireball duration was defined as the time it takes for the maximum temperature to fall to 1000 K after all fuel was consumed, while in the calculations with radiative submodel included, the fireball lifetime was defined as the moment by which the total radiative power of the cloud fell to 5 % of its maximum value. The solid line corresponds to the experimental dependence (5) obtained by Roper *et al* [7] and presented in its equivalent form (6). It may be seen that the calculated points concentrate around the experimental dependence, the scatter of points being comparable with the experimental scatter caused by the intrinsic irregularity of turbulent flow.

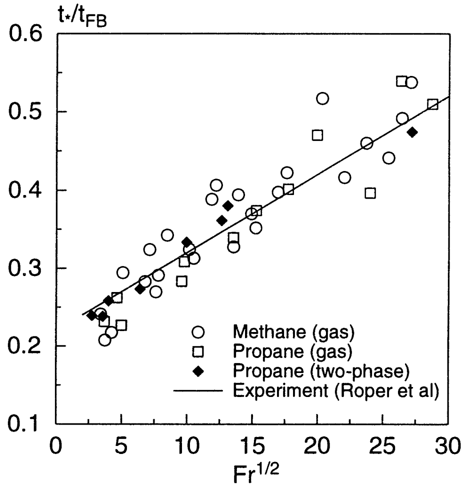

FIGURE 1. Dependence of the inverse non-dimensional burning time on the square root of Froude number for single- and two-phase releases. The experimental dependence obtained by Roper *et al* [7] is presented by the solid line

It is important to note that both single-phase and two-phase fireballs are described by the same dependence. The reason for this similarity is that propane has a quite low boiling temperature (-42°C) and is highly volatile when released into the ambient atmosphere. The calculations have shown that total evaporation of all liquid droplets occurs shortly after release, the evaporation rate becomes especially high as soon as ignition occurs. Hence, evaporation is a faster process than diffusion combustion, and at the later stages even for the two-phase release the fireball behaves as though from a single-phase release. The main influence of two-phase effects is thus reflected in changing the release velocity with changes in the storage conditions. We note that two-phase effects may have a more pronounced impact in the case of delayed ignition affecting the evolution of two-phase clouds prior to ignition. Also, such effects may be more important for liquids with higher boiling points discharged as aerosol clouds into the atmosphere.

RADIATION FROM BURNING CLOUD

An important parameter directly related to the hazards of fireballs is the fraction of total combustion energy being emitted as heat radiation. This value is often used in the empirical models to estimate the effects of the burning cloud on the environment (e. g., [6]). In the calculations the total power of radiation emission $Q_R(t)$ was determined first by integrating the radiative source term (equal to the divergence of radiative heat flux $\nabla \mathbf{q}_R$ and giving the difference between local emission and absorption of radiative energy per unit time per unit volume) over the volume of the fireball. After that the radiative energy fraction χ_R was obtained by integrating the total power of radiation $Q_R(t)$ with respect to time and dividing it by the total heat of combustion of all fuel:

$$Q_R(t) = \int_{V_{FB}} \nabla \mathbf{q}_R \, dV, \qquad \chi_R = \frac{\int_0^\infty Q_R(t)\,dt}{QM_0}.$$

The calculated values of radiative fraction χ_R are presented in Fig. 2 for three values of Froude number Fr = 5, 50 and 250. It may be seen that in all the parameter ranges considered the calculated values of χ_R are in the region 0.18–0.27, which correlates well with the experimental range 0.20–0.24 given for turbulent propane flames in [18] and 0.20–0.32 according to [19,20]. Direct comparison of the calculated values with the experimental data obtained for different (however, similar in their nature) flames is complicated because the radiative fraction depends somewhat on the flame scale: for example, for large-scale optically thick clouds this value is expected to decrease with increase in the total fuel mass as $M_0^{-1/6}$ (see [21]). On the other hand, for small-size fireballs measurements give the radiative fraction around 0.15 [22]. With these reservations, reasonable agreement between the calculated and experimental ranges of radiative fraction may be considered to substantiate the validity of the radiation submodel used.

To study the dependence of radiative properties of fireball on its scale, the total emissivities were estimated as

$$\varepsilon_{FB} = \sum_{i=1}^{N_g} a_i [1 - \exp(-\tau_i)], \quad \text{where} \quad \tau_i = 2\int_0^{R_{FB}} \kappa_i \, dr$$

The optical thickness τ_i for the i-th gray gas in the WSGG model was calculated by integrating the absorption coefficient κ_i along a radial line passing through the point of maximum temperature. The integration was performed over the interval $0 \le r \le R_{FB}$ corresponding to the fireball interiour where the gas temperature exceeded 500 K, which excluded the emission/absorption in the ambient atmosphere. In Fig 2 the emissivities obtained for Fr = 50 are presented by the dashed line (for each fuel mass the maximum value of emissivity over the fireball lifetime is shown). It can be seen that emissivities close to unity (corresponding to optically thick clouds) are achieved for fuel masses higher than 1 kg, or for fireballs which are larger than several meters in diameter. This agrees well with other estimates available [4,7,19,21].

Although the integral parameters of burning clouds scale with respect to the total fuel mass and release velocity as discussed above, such scaling does not mean full similarity in the internal structures of fireballs. The reason for this is that the radiative heat transfer processes possess their own length scale related to the mean beam path length of radiation which, in turn, depends on the absorbing properties of the combustion products. Hence, the radiation field is quite different in small-scale (optically thin) and large-scale (optically thick) clouds.

To elucidate the differences in the internal structures of fireballs of different scales, it is convenient to compare the spatial distributions of the non-dimensional radiative source term

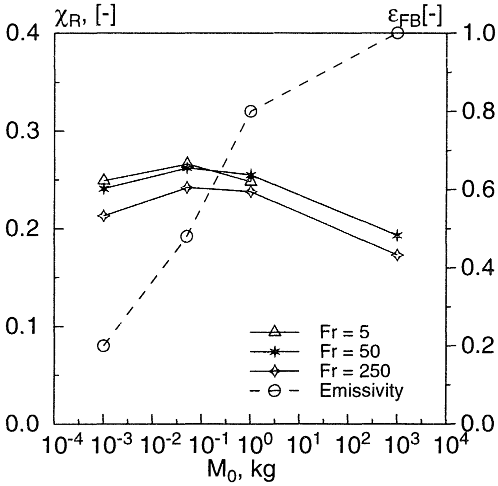

FIGURE 2. Radiative fraction of combustion energy χ_R for propane fireballs, M_0 = 1 g–1000 kg

$S_R = \nabla \mathbf{q}_R/(QM_0/L_*^3 t_*)$ calculated for the same Froude number and corresponding to the same moments of non-dimensional time, but obtained for different initial masses of fuel M_0. In the absence of radiative processes the resulting temperature distributions in non-dimensional coordinates r/L_*, z/L_* would coincide, so that any differences observed may be attributed to the scale effects. In Fig. 3 the temperature and radiative source term fields are presented for M_0 = 1 g and 1000 kg gaseous propane fireballs at the same moment of non-dimensional time t/t_* = 1.4 (the corresponding dimensional parameters are $L_* = 0.51$ m, $t = 0.32$ s for the smaller fireball and $L_* = 51$ m, $t = 3.2$ s for the bigger one). The Froude number in these calculations was Fr = 50, so that the release velocity was $U_0 = 15.8$ m/s for the smaller cloud and 158 m/s for the bigger one.

It can be seen that the distributions of the radiative source term in the small and large fireballs are qualitatively different. The small fireball is optically thin in almost all spectral subregions (typically, only for one or two of the eight gray gases in the WSGG model the fireball turned out to be optically thick, i. e., in the corresponding spectral subregions its optical thickness exceeded unity), the radiation emitted by hot combustion products leaves the cloud almost without being reabsorbed. As a result, the fireball emits radiation all over its volume and the radiative power has a maximum inside the cloud. The large fireball, however, is optically thick for all gray gases, radiation reabsorption plays an important role blocking the radiation inside the cloud. The cloud emits primarily from its surface where the radiative source term has its maximum in a narrow near-surface layer. In this case the radiative field inside the cloud is essentially non-uniform, there even exist regions where absorption prevails over emission.

Despite such big differences in the radiation fields, the temperature fields inside small-scale and large-scale clouds do not differ substantially. High temperature inside the cloud is maintained

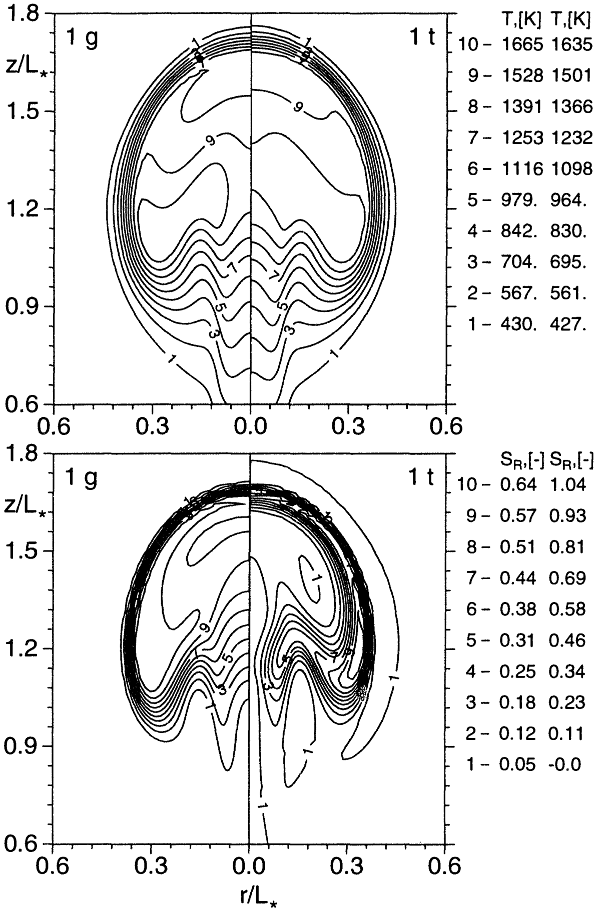

FIGURE 3. Temperature fields (top) and radiative source term distributions (bottom) for 1 g (left) and 1000 kg (right) gaseous propane fireballs calculated at $t/t_* = 1.4$, $\mathrm{Fr} = 50$.

due to combustion energy release in chemical reactions, also, the vortex flowfield rolls up the fireball into an almost spherical cloud. These two factors prove to be the most significant in determining the internal temperature-concentration structure of a fireball. The radiation heat losses decrease the maximum temperature of fireball from about 2500 K (in the case when the radiative heat transfer is not taken into account, see [8]) to about 1700 K, but the dynamics of fireball motion is not affected noticeably by this temperature drop.

The estimation of hazards of fireballs requires the fluxes from the burning cloud onto the ground surface to be calculated. An important feature of fireballs is short duration of the radiative impulse compared to steady-state jet fires, flares etc. For such transient events the heat flux q_S itself is not sufficient to characterise the effects of radiation. A value which better describes the heat impact of fireball is the received radiation dose [5,23] obtained by integrating the flux q_S with respect to time over the entire duration of the fireball:

$$\psi_S = \int_0^{\infty} q_S(t)\, dt.$$

The heat fluxes on the ground surface were calculated at different moments of time by the Monte Carlo method. For each gray gas 10^7 energy bundles were emitted and traced until absorption either in the volume or on the bounding surfaces. The ground surface was treated as a black body, so that no reflection was allowed there. This gives the worst-case estimates for the fluxes received by the ground. Further integration with respect to time gave the dose ψ_S, the radial distributions of which are presented in Fig. 4 for the smallest (1 g) and largest (1000 kg) fireballs. The radial coordinate is non-dimensionalised using the length scale L_*, the dose of received radiation is related to the characteristic value QM_0/L_*^2. The curves clearly show that differences in the radiative fields described above are also reflected in the radiation dose distributions: while for the optically thin cloud the radiation dose reaches its maximum on the axis under the cloud centre, in the case of optically thick cloud the dose has its maximum at some distance (approximately equal the fireball radius) from the axis. This may be attributed to radiation blockage inside the cloud.

CONCLUSIONS

The results of CFD modelling of fireballs from single- and two-phase releases of hydrocarbon fuels presented in this paper show that while the integral parameters of burning clouds (size, lifetime) can be described by unified dependencies on the fuel mass and outflow velocity (in terms of Froude number), the radiative field inside the cloud and heat fluxes generated by the burning cloud turn out to be scale-dependent. In this work only fireballs resulting from vertically directed releases of hydrocarbon fuels are studied, which is relevant to fuel releases in the case of partial loss of storage vessel containment. In the further work the study will be extended to vapour-droplet clouds following the instantaneous release of pressure-liquefied gas into the atmosphere upon total loss of containment. Also, flame propagation through the two-phase mixture after ignition of such clouds will be studied in detail. *This work has been carried out under the grants GR/K 13486 and GR/M18263 from the UK Engineering and Physical Sciences Research Council (EPSRC).*

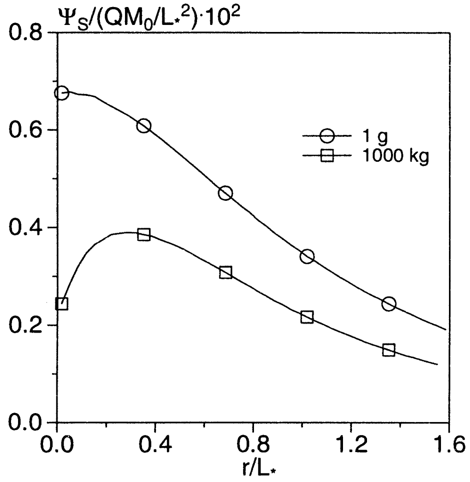

FIGURE 4. Radial distributions of radiation dose ψ_S received on the ground surface from 1 g and 1000 kg propane fireballs

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