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A DESCRIPTION OF THE "ENGULF" COMPUTER CODES - CODES TO MODEL THE THERMAL RESPONSE OF AN LPG TANK EITHER FULLY OR PARTIALLY ENGULFED BY FIRE

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ABSTRACT

Simple computer codes have been developed at the Safety and Reliability Directorate to model the thermal and pressure response of LPG tanks involved in fire engulfment accidents. The present code, ENGULF II, can model either total or partial fire engulfment of an LPG tank, including jet flame impingement. Other features available within the code are safety relief vent valves, bulk boiling of the liquid contents, external tank wall thermal insulation, water spray cooling, tank failure prediction and the modeling of a gas or petrol filled tank. Code predictions have been in good agreement with available experimental data.

INTRODUCTION

The assessment of the safety of liquid filled tanks when engulfed in fire usually forms part of most risk studies carried out on chemical plants today. This requires a comprehensive study of the heat and mass transfer processes involved within the tank in order to be able to accurately predict how the tank's temperatures and pressure will vary with time during the fire. From this data, it is then possible to predict under what conditions failure of such tanks, sometimes resulting in Boiling Liquid Expanding Vapour Explosions (BLEVEs) can occur.

As tools for such safety assessments, the Safety and Reliability Directorate (SRD) of the United Kingdom Atomic Energy Authority, has been involved in the development of simple computer codes to model the response of an LPG tank in a fire engulfment accident. This work has been carried out under contract for the Health and Safety Executive (HSE) in the United Kingdom.

Two codes have been developed to date, ENGULF and ENGULF II.

ENGULF was the first code to be written (refs. 1,2) and this models only the total fire engulfment of a tank partially filled with a hydrocarbon liquid. When this basic code had been developed, it was decided to extend the model to be able to simulate partial fire engulfment of a tank, as in practice partial engulfment is usually more likely than full engulfment, especially for larger sized tanks. This development led to the writing of a new code - ENGULF II.

The fire engulfment geometries modeled by ENGULF II are full tank engulfment, less than 100% tank engulfment in a pool fire, jet flame impingement and radiation from a distant fire source. ENGULF II has now, therefore, totally superceeded ENGULF. Both codes are completely general for any tank material and any liquid inside the tank. To date the liquid properties which have been coded up and used in the ENGULF codes include propane, butane, toluene, pentane and petrol.

The ENGULF codes are written in standard Fortran 77 and are, at present, being run on an ICL 2982 mainframe and the Apricot XI and XENi microcomputers.

DESCRIPTION OF THE MODELS

A brief outline of the major aspects of the two models, ENGULF and ENGULF II follow. When developing ENGULF II applicable parts from the original ENGULF code were used wherever possible.

Tank geometry

In ENGULF the tank was represented as a cuboid or box shape. When a cylindrical tank was being simulated an equivalent cuboid tank was made by matching volumes and surface areas. However, this could lead to discrepancies in the relative sizes of the internal tank areas in contact with the vapour and liquid masses at extremes of fill. This would effect the relative amounts of heat transferred into the bulk fluids thus leading to slight errors in predicted temperatures.

To overcome this, the tank geometry used in ENGULF II is that of a plane cylinder. Note that the model does not allow for a cylinder with domed ends.

The parameters which are important in the geometry calculations for the tank are, therefore, its length (L), radius (r), and the angle that the liquid level to tank centre line makes with the vertical (Θ) (Fig. 1). These parameters are used to calculate the tank wall temperature node dimensions.

Tank temperature nodes

Figures 2a and 2b show typical temperature node schemes which are used in ENGULF II. Fig. 2a represents a completely fire-engulfed tank and Fig. 2b, a partially engulfed tank. In the latter case, there are four wall temperatures which are calculated (i.e., the heated liquid and vapour walls and the unheated liquid and vapour walls). Also calculated are the mean bulk liquid and vapour temperatures (i.e., a single temperature for each of the fluid masses). ENGULF II does not model any stratification of temperature within the fluid masses.

The liquid level angle Q, shown in Fig. 2, is used to calculate the heated and unheated liquid and vapour wall temperature node heat transfer areas and hence the node heat capacities used in the code. It is calculated by equating the geometrical expression for the liquid volume at any time to the actual liquid volume calculated from its mass and density and solving for Q, as

$$V_L = L.r^2 \, (\pi - (\theta - \sin\theta . \cos\theta)) \qquad (1)$$

FIG. 1 CYLINDRICAL TANK GEOMETRY

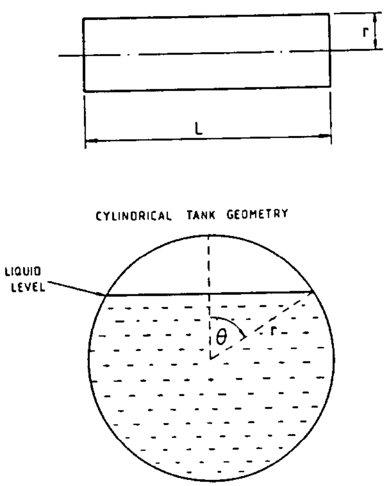


FIG. 2a TANK TEMPERATURE NODES - FULL ENGULFMENT

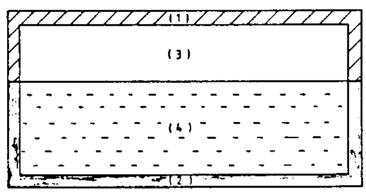
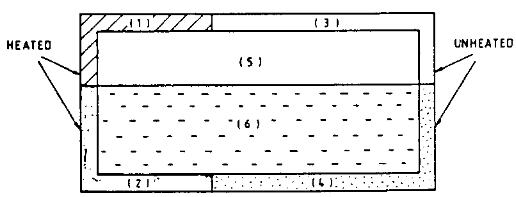


FIG. 2b PARTIAL ENGULFMENT



Once θ has been calculated then the heat transfer areas can be evaluated. As an example of the sort of analysis in ENGULF II, consider a mid-tank partial engulfment. IF L_1 and L_2 are the extremities of the engulfed region and L and r are the tank's length and radius, then the four wall temperature node heat transfer areas can be shown to be

Heated vapour wall	$= 2r\theta\ (L_2-L_1)$	(2)
Heated liquid area	$= 2r\ (\pi-\theta)(L_2-L_1)$	(3)
Unheated vapour area	$= 2r^2(\theta-\mathrm{Sin}\theta.\cos\theta) + 2\theta r(L-L_2+L_1)$	(4)
Unheated liquid area	$= 2r\ (\pi-\theta)(L_2-L_1) + r^2\ (\pi-(\theta-\mathrm{Sin}\theta.\cos\theta))$	(5)

Equations similar to (2-5) have been derived for all the fire scenarios in the code.

Heat transfer modeling

This section describes how the heat transfer terms between the six temperature nodes, fire and outer atmosphere are calculated in ENGULF II. The heat transfer analysis of a partially-engulfed tank is much more complex than that of the full tank engulfment considered in ENGULF. This is because there are now unheated liquid and vapour wall areas in addition to the heated walls. Heat can, therefore, be low through these unheated areas to the outside atmosphere.

To model the partial engulfment fire cases requires many extra heat transfer terms to those needed for simple full fire engulfment. The heat transfer model used in ENGULF has, therefore, had to be extensively revised and extended for ENGULF II.

Heat transfer for the fire into the tank

Mid, end and full tank engulfment. With these cases, the heat input into the tank is calculated in the same way as for total tank engulfment in ENGULF (i.e., it is assumed that there is uniform radiative heat input into the tank from the fire over the heated regions).

The radiative heat transfer rate (in Watts) into the vapour wall, for example, is (ref. 3):

$$\frac{\sigma \cdot (T_F^4 - \mathrm{YOUTV}(1)^4)}{(1/\varepsilon_f + 1/\varepsilon_{out} - 1)} \cdot \mathrm{HTA}(1) \qquad (6)$$

The flame emissivity (ε_f) can be altered to account for any enhanced convective heat transfer from the fire, if necessary, as in ENGULF

<u>Jet flame torching</u>. The model used to represent heat transfer into the tank from an impinging jet flame is different to that used for mid, end or full tank engulfment. From a jet torch most of the heat is transferred to the tank surface by convection and not radiation as with an engulfing pool fire. A simplified convective heat transfer mechanism has been used in ENGULF II to model heat input from an impinging jet torch.

The user inputs the heat flux from the torch and also the flame temperature. These are then used to calculate the convective heat transfer coefficient from the torch by

$$H_{TORCH} = \frac{\mathrm{TORFLX}}{(T_F - \mathrm{YOUT})} \qquad (7)$$

This heat transfer coefficient is then fixed and used throughout the fire run to calculate the rate of heat input into the tank. Again, the heat input is assumed to be uniform over the torched area.

<u>Distant fire sources</u>. The remote fire source cases in ENGULF II are modeled as pure radiation sources. A similar

analysis to the mid, end and full tank engulfments is sued. The user must have some knowledge of the situation of the fire so that he can calculate the radiant heat flux onto the tank surface. The user must, therefore, know the distance of the fire form the tank, the geometrical position of the fire in relation to the tank and atmospheric attenuation factors, etc. Once the incident flux is known then an equivalent flame temperature is calculated so that the distant source is treated just as if it were an engulfing pool fire with a reduced heat flux.

Heat transfer out of the tank

In the partial engulfment cases there are areas of the tank which are open to the atmosphere (i.e., unheated liquid and vapour walls). These, therefore, provide pathways for heat to escape from the tank and so limit the build-up of a pressure and temperature within the tank compared to the full tank engulfment. In ENGULF II, heat can escape from the tank by convective and radiative mechanisms. The heat transfer by convection from the unheated walls to the atmosphere is calculated using natural convection empirical heat transfer coefficients (ref. 3). For the unheated liquid wall to the atmosphere

$$h_{lvair} = 0.105\left(\frac{K^2_{air}\cdot\rho^2_{air}\cdot\alpha_{air}\cdot Cp_{air}\cdot g\cdot\Delta T}{\mu_{air}}\right)^{1/3} \tag{8}$$

The thermodynamic properties of air are used in the above heat transfer coefficient correlation. These care calculated at the average of the unheated wall and atmosphere temperatures.

There is a subroutine, AIRPRO, in ENGULF II which contains the temperature dependencies of all the air properties used in these correlations. The radiant heat loss from the tank is modeled using a similar analysis to equation 6. For the special case of a distant fire source, there is also convective and radiative heat transfer from the heated areas of the tank to the atmosphere, as these surfaces are also in contact with the outside air. These heat transfer terms are modeled in ENGULF II.

Heat transfer into the tank contents

The modeling of the heat transfer into the tank contents is treated in a similar way to that in ENGULF.

Heat transfer into the liquid. The heat transfer from the inner heated liquid wall is modeled, as in ENGULF, using standard pool boiling theory (ref. 4). This is one of the areas which has been transferred directly from ENGULF to ENGULF II.

Heat transfer in the vapour spaces. The modeling of the radiative heat transfer within the vapour space of the tank is one of the main areas which has been developed extensively for the partial engulfment cases.

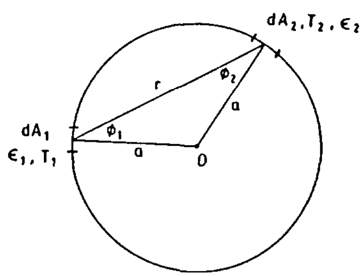
In the fire engulfment of a tank the heated vapour wall rises to a very high temperature (500-600^{o}C) due to the poor heat transfer into the bulk vapour. This means that in the vapour space enclosure, there is a hot wall area which is radiating into the vapour space and to the cooler unheated vapour wall within the enclosed vapour volume.

In ENGULF there was simply radiation from the inner heated vapour wall to the vapour with no unheated vapour wall. Because of this radiation from heated to unheated areas, and the relative orientation of the two areas to each other, a more rigorous approach is required when calculating the radiative heat transfer terms within the vapour space in ENGULF II.

Consider the simple case (ref. 5) of radiation within a sphere where area dA_1 at temperature T_1, emissivity ε_1 , is radiating inside the sphere shown in Fig. 3. To calculate the incident flux on an area dA_2, temperature T_2, emissivity ε_2, from dA_1 it can be shown that

$$\Delta\emptyset = \sigma\ (\varepsilon_1 T_1^4 - \varepsilon_2 T_2^4)\ \frac{dA_1 . dA_2}{4\pi a^2} \tag{9}$$

FIG. 3 RADIATION HEAT TRANSFER WITHIN A SPHERE



As the radiation passes from the heated vapour wall to the unheated vapour wall, some of it will be absorbed by the vapour itself. Equation 9 does not take this into account and only applies to the ideal situation where there is no absorbing medium inside the enclosed volume which is not the case within the vapour space.

Consider an enclosed volume which has three separate, distinct areas A_1, A_2 and A_3 with temperatures T_1, T_2 and T_3, emissivities $\varepsilon_1, \varepsilon_2$, & ε_3 and where ε_3 equals unity. The enclosed volume holds a vapour with an absorption coefficient for radiant energy of α.

The radiant heat transfer between areas 1 and 2 is made up of many separate components. The direct component is

$$Q = \sigma \cdot \varepsilon_1 \varepsilon_2 \, T_1^4 \cdot A_1 \cdot (1-\alpha) \, A_2/A \tag{10}$$

but in addition to this there are many reflected radiation terms due to radiation which is not initially absorbed by A_2 and reflects back to A_1. It can be shown that the expression for the total radiated heat transfer term is

$$\begin{aligned} Q_2 = {} & \sigma \, \varepsilon_1 \varepsilon_2 T_1^4 A_1 \, (1-\alpha) \, A_2/A \\ & + \sigma \, \varepsilon_1 \cdot T_1^4 \cdot A_1 (1-\alpha)(1-\varepsilon_2)\left(\frac{A_1+A_2}{A}\right)(1-\alpha) \, \frac{\varepsilon_2 A_2}{A} \\ & + \sigma \, \varepsilon_1 \cdot T_1^4 \cdot A_1 (1-\alpha)(1-\varepsilon_2)\left(\frac{A_1+A_2}{A}\right)(1-\alpha)(1-\varepsilon_2) \cdot \left(\frac{A_1+A_2}{A}\right)(1-\alpha)\frac{\varepsilon_2 A_2}{A} \end{aligned} \tag{11}$$

+ further reflection terms, diminishing in magnitude to higher order.

Using an identical analysis for the radiant heat from areas 2 to 1, it can be shown that the net radiant heat flux between areas 1 and 2 is therefore:

$$Q_{12} = \frac{\alpha \; \varepsilon_1 \varepsilon_2 (1-\alpha) A_1 A_2}{(1-(1-\alpha)(1-\bar{\varepsilon})) \cdot A} \, (T_1^4 - T_2^4) \tag{12}$$

This technique is used in ENGULF II to calculate the internal vapour space heat transfer terms between the heated and unheated vapour walls and the liquid surface and vapour bulk.

Heat conduction within the tank walls

There are some important heat conduction terms which must be modeled for the partial engulfment cases. These are the conduction terms across the boundaries between the heated and unheated wall nodes.

As explained earlier, the tank wall is not split into many small temperature nodes along its length and circumference. Lumped wall nodes are used instead. The technique used in the modeling of conductive heat transfer across the heated boundaries is to calculate a "typical conduction length" across each boundary and this is then used to calculate the conduction heat transfer terms between the lumped wall nodes; for example:

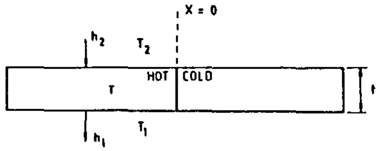
$$QCnn = k \cdot (\text{conduction length scale})^{-1} \cdot \text{area} \cdot \Delta T \tag{13}$$

To calculate the conduction length scales, consider the tank wall situation shown in Fig. 4. The wall thickness is "t", the hot wall temperature "T", the external heat transfer coefficient into the tank "h_2", the external temperature "T_2", the internal wall heat transfer coefficient into the contents "h_1", and the internal bulk temperature "T_1".

From consideration of the heat fluxes across the wall boundaries and the conduction across the hot/cold boundary, it can be shown that the effective conduction length scale is given by

$$\Delta X = (Kt)^{\frac{1}{2}} \left(\frac{1}{(h_1+h_2)^{\frac{1}{2}}} + \frac{1}{(h_3+h_4)^{\frac{1}{2}}}\right) \tag{14}$$

FIG. 4



The heat conduction length scales calculated above can now be used in the calculation of the wall conduction heat fluxes using equation (13). The area in equation (13) is the cross sectional area of the boundary between the wall nodes under consideration across which the heat conduction is taking place. This will obviously be different, from each of the conduction terms, for each of the separate engulfment cases modeled in ENGULF II.

An example of a typical expression for a cross conduction area is now given for the mid-tank engulfment fire geometry for the unheated vapour to unheated liquid wall boundary. Similar expressions are used within ENGULF II for the other fire geometries.

$$(4 \cdot r \cdot \sin\theta + 2L_1 + 2(L - L_2))t \qquad (15)$$

Tank thermal protection systems

Thermal insulation. ENGULF II has the option of having a simple thermal insulation layer on the outside of the tank. This can be used to model non-ablative types insulation. The code simply puts a thermal resistance, with the properties of the particular insulating material, in series with the outer wall temperature nodes when calculating the tank wall temperatures. The code does not model any temperature profile within the insulating layer itself. The thermal resistance slows down the flow of heat into the tank.

Water spray cooling. Water spray cooling of an LPG tank can be modeled by both ENGULF and ENGULF II. If water sprays are selected by the user, an extra heat transfer term is included in the equations to calculate the outer wall temperatures. This is a convective cooling term out from the tank wall to the water film on the tank's surface. The empirical heat transfer coefficient used for this cooling term is taken from (ref. 3) and is

$$h = 8500\ (Sr)^{1/3} \qquad (19)$$

Thermodynamic properties of the liquid and vapour phases

In ENGULF II, many empirical heat transfer coefficient correlations are used to calculate rates of heat transfer.

These correlations are functions of the thermodynamic properties of the liquid and vapour inside the tank. They are used throughout the fire, as the nodes heat up, so a range of values for each thermodynamic property is required covering a wide temperature range. Without such property data for the liquid and vapour phases, the accurate calculations of the heat transfer rates into and out of the tank could not be made.

The thermodynamic properties required for the liquid phase are: i) special latent heat of vapourization, ii) dynamic viscosity, iii) specific heat capacity at constant volume, iv) thermal conductivity, v) saturated vapour pressure curve, vi) density, vii) surface tension, and viii) volumetric expansion coefficient. For the vapour phase, the thermodynamic properties required are: i) dynamic viscosity, ii) specific heat capacity at constant pressure, iii) thermal conductivity, iv) saturated conductivity, v) volumetric expansion coefficient, and vi) ratio of specific heat capacity, γ (single value).

All these properties are coded up into two separate property data files, one for the liquid and one for the vapour. These property files are then called at various times throughout the fire run when needed. ENGULF II is completely general for any fluid and so a user only has to code up the properties of the fluid required to run for any new one.

Liquid mixture modeling

ENGULF II has been developed to model a multi-component liquid mixture (i.e., one whose physical properties can be synthesized as a combination of its individual component and vapour properties). This was done in particular to model the properties of petrol in a fire engulfed tank, as it was not possible to simulate petrol by a single hydrocarbon (e.g., octane or heptane). The method used is described in detail (ref. 6) for readers who may be interested in this option of the code.

Vapour venting and bulk liquid boiling

ENGULF II uses the same venting and bulk boiling models as ENGULF. These models have been directly transferred from the original code.

Tank failure prediction

The tank failure prediction method used is that proposed by Moodie (ref. 7) which assumes that the tank fails in a longitudinal (hoop stress) tensile model. The maximum pressure which can be sustained by the tank is

$$P_{burst} = \frac{2}{\sqrt{3}} \cdot \sigma_y . A . \ln\left[\frac{(r+t)}{r}\right] \quad (20)$$

where $A = (2-\sigma_u/\sigma_y)$ for $T < 700°C$
$A = 1$ for $T > 700°C$

Coded into ENGULF II are the ultimate tensile and yield stress values for various steels over a wide range of temperatures. At every timestep during a fire run the code, therefore, calculates the burst pressure of the tank and compares this with the actual tank pressure. The user selects the tank material properties required via the input file.

Numerical model for calculating transient temperatures

The numerical model used to calculate the wall and bulk fluid temperatures throughout the fire in ENGULF II is the same as the one used in the original code ENGULF (i.e., a fourth order Runge-kutta algorithm).

CODE PREDICTIONS AND COMPARISONS WITH EXPERIMENTAL DATA

Running parallel with SRDs development of the ENGULF computer codes has been a series of fire engulfment experiments being carried out by the Health and Safety Executive in the United Kingdom, which have provided data to compare our codes against. The tests were originally with 0.25 and 1 tonne tanks (ref. 7) and more recently with 5 tonne tanks of propane (ref. 8). All these tests have been with full tank fire engulfment and no data has been available thus far for any of the partial engulfment or torching cases modeled in ENGULF II. It has not been possible to do any code comparisons for these options of the new code but ENGULF II has been extensively tested theoretically and from our experience it appears to predict the results one would expect for such partial engulfment situations.

This section will, therefore, compare only experimental and code results for fully engulfed, uninsulated propane tanks. Only comparisons with the 5 tonne results will be shown as comparisons with the 0.25 and 1 tonne results are covered in refs. 1 and 2. Figs. 5-10 show a selection of

FIG. 5 OUTER VAPOUR WALL TEMPERATURE

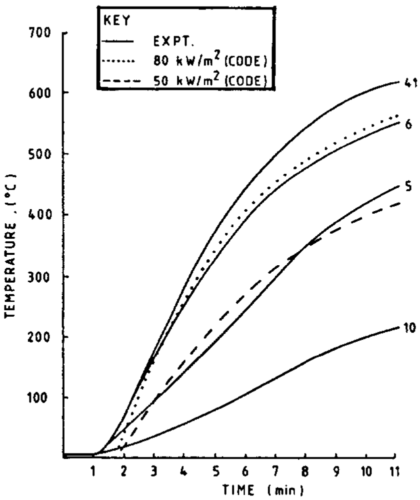


FIG. 6 OUTER LIQUID WALL TEMPERATURE

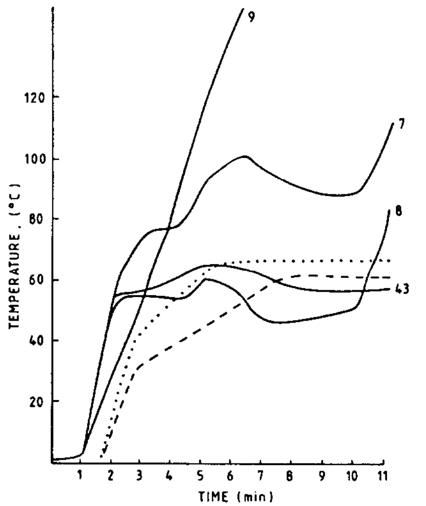


FIG. 7 LIQUID TEMPERATURE

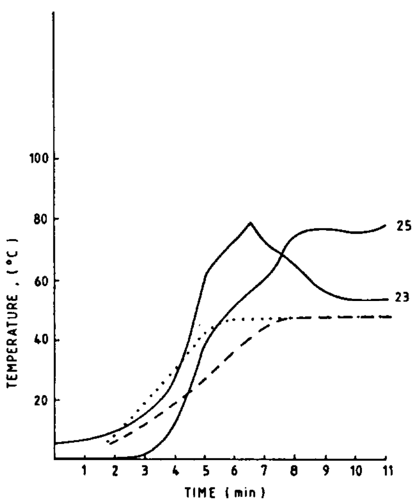


FIG. 8 TANK PRESSURE

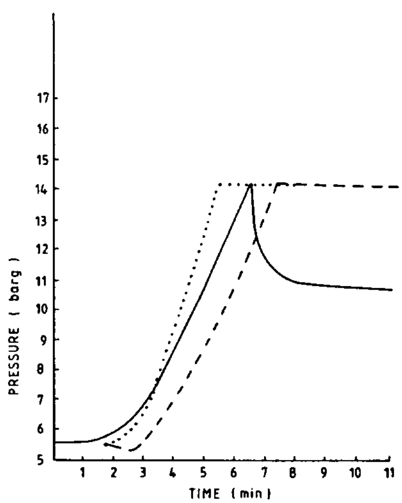


FIG. 9 VAPOUR TEMPERATURE

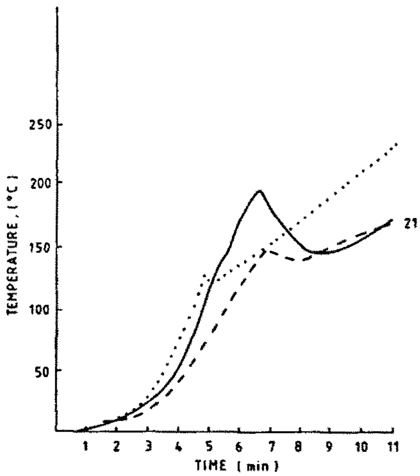
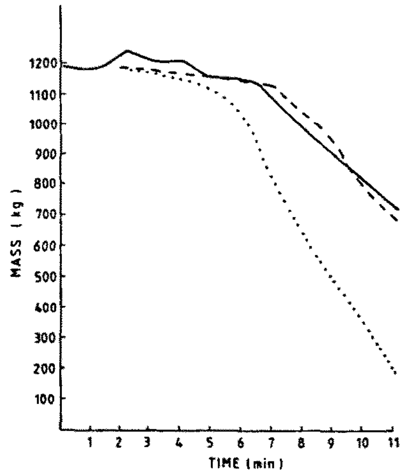


FIG. 10 LIQUID MASS



comparisons for the main tank parameters in a fire-engulfed vessel. These results are for 20% full propane trials. The experimental thermocouple numbers on the graphs refer to the thermocouple identifiers as given in ref. 8.

For the code predictions, a range of heat fluxes were run and on the comparison graphs the 80 KW/m^2 and 50 KW/m^2 results are shown. It was assessed that in the fire trial it took about 2 minutes for the tank to become fully engulfed and so this time delay is taken into account on the comparison graphs.

As can be seen from the figures, both the 50 and 80 KW/m^2 code predictions show reasonable agreement with the test data. One feature which is obvious from Fig. 5 is the non-homogeneity of the engulfing fire as there is such a wide variation in the vapour wall temperature profiles. The thermocouple results in Fig. 8 are all from one side of the tank. This should be taken into account when comparing ENGULF

II with experiments as the heat input is assumed to be of uniform flux over all the tank's surface in the code.

Figure 10, the liquid propane mass graph, shows excellent agreement between code and experiment for an average flux of 50 KW/m^2. This suggests that in the actual fire test the mean overall heat flux into the tank is about 50 $KW/^2$ which would agree with the wall temperature profiles which suggest areas of the tank receiving 80-90 KW/m^2 but other areas only receiving 20-30 KW/m^2.

ENGULF II could be extended in the future to model a varying heat flux over the tank's surface by simple extension of the ideas involved in the present partial engulfment cases.

CONCLUSIONS

A computer code ENGULF II has been written to model full and partial fire engulfment of partially-filled liquid tanks. Reasonable agreement has been achieved with the available experimental data for full tank engulfments. To date, no experimental data is available to compare the partial and torching scenarios of ENGULF II against but the results for these cases appear satisfactory.

SYMBOLS

a	radius
A	total internal surface area (m^2)
dA	infinitesimal area (m^2)
C_p	vapour specific heat capacity at constant pressure (J/kg/K)
g	acceleration due to gravity (m/s^2)

HTA(i)	heat transfer area of "i"th node (m^2)
H_{TORCH}	torching heat transfer coefficient ($W/m^2/K$)
h	convective heat transfer coefficient ($W/m^2/K$)
h_{1vair}	heat transfer coefficient from unheated liquid wall to ambient ($W/m^2/K$)
K	thermal conductivity (W/m/K)
L	tank length (m)
Q	heat flux (W)
QCnm	conduction heat flux from node n to m (W)
r	tank radius (m)
S	water spray rate ($kg/s/m^2$)
t	wall thickness (m)
T_F	flame temperature (^oK)
Δ T	temperature difference (K^o)
T	temperature (^oK)
TORFLX	torching heat flux (W/m^2)
TOUTV(i)	outer vapour wall skin temperature (^oK)
YOUT	outer wall temperature (^oK)
Y(1)	}
Y(2)	}
Y(3)	} temperature nodes (^oK)
Y(4)	}
Y(5)	}
Y(6)	}
α	gas absorption coefficient
α_{air}	volumetric expansion coefficient of air (/K)
γ	ratio of specific heat capacities for the vapour
ε_{out}	outer wall emissivity
ε_{in}	inner wall emissivity

ε_f	flame emissivity
$\bar{\varepsilon}$	mean emissivity
ϕ	liquid angle (rads)
μ	dynamic viscosity (Ns/M^2)
ρ	density (kg/m^3)
σ	Stephan-Boltzmann constant ($W/m^2/K4$)
σ_u	ultimate tensile stress (Pa)
σ_y	yield stress (Pa)

Subscripts

air	refers to air properties
L	liquid
V	vapour
W	wall
1,2	distinguishing flags

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