Journal of Hazardous Materials, 20 (1988) 227-238
Elsevier Science Publishers B.V., Amsterdam - Printed in The Netherlands

FIRE ENGULFMENT OF LPG TANKS: HEATUP, A PREDICTIVE MODEL

G.V. Beynon, L.T. Cowley, L.M. Small and I. Williams

Shell Research Ltd., Thornton Research Centre, P.O. Box 1, Chester CH1 3SH, U.K.

SUMMARY

A predictive model of the behaviour of horizontal pressurised LPG vessels engulfed by fire is described. Complete fire engulfment is treated with a heat flux distribution that is both variable in the vertical direction and time dependent. Heat flow through the tank walls, convective and radiative exchange to the fluid and heat and mass transfer between the liquid and vapour are incorporated. The liquid and vapour zones are each assumed to be separately well mixed. The operation of different designs of pressure relief valves is simulated.

Model validation was against extensive measurements on 0.25, 1 and 5 tonne LPG tanks filled to a range of levels and engulfed in kerosine pool fires. HEATUP successfully predicted pressure relief valve opening times, discharge rates, pressure histories and average liquid and vapour temperatures for the different tank sizes and fill levels. Predicted mean wall temperatures in both liquid and vapour zones also agreed with measurements.

INTRODUCTION

The ability to understand and accurately predict the behaviour of pressurised LPG vessels engulfed by fire is necessary to assist the definition of design and operating procedures for LPG storage and transport.

A model that is to be a reliable predictive tool must take adequate account of a number of complicated and strongly interacting processes. A fire might partially or wholly engulf an LPG vessel, even in the latter case the incident convective and radiative heat flux may be non uniform because of wind and other effects. Part of the incident flux will be conducted through the tank walls. At the tank inner surface heat is convected and radiated to the liquid and vapour. Radiation from the dry inner walls is partially absorbed by vapour before reaching the liquid surface where reflection and absorption occur. Convective heat transfer from the wet inner surface to the liquid may be by free convection, nucleate boiling or film boiling, depending on the heat flux. The vapour is convectively heated (or cooled) at the dry inner walls. As the fire burns, the liquid temperature increases with consequent vapourisation and pressure rise. The vapour will usually be superheated. At a given pressure the pressure relief valve (PRV) opens and discharges fluid. The resulting pressure history depends on the PRV size, the incident heat flux and the complex interaction of the above processes. Vapour is a less effective heat sink than liquid and dry wall temperatures usually exceed those of wetted walls. A combination of the dry wall temperatures, vessel structural characteristics and the internal pressure determine the ultimate integrity of the tank.

The HEATUP model described here has been developed in conjunction with and validated against measurements on the behaviour of 0.25, 1 and 5 tonne LPG tanks filled to a range of levels and engulfed in kerosine pool fires.[1,2] Models of Ramskill and Hunt[3] and Sousa and Venart[4] also make use of some of these data.

The plan of subsequent sections is to outline the assumptions that form the model basis, predictions are then compared with experiments and finally details of the model are described.

MODEL BASIS AND ASSUMPTIONS

Our approach was to start with a set of well defined assumptions, test their validity during development and modify as necessary. The major assumptions are now described, starting with the geometry, then the fire and working inwards to the tank contents.

The tanks considered are horizontal cylinders of length to diameter ratio sufficient to permit heat flow calculations in a vertical cross section only neglecting end effects. The fire totally engulfs the tank with a flux that is constant along the tank length but height dependent. There is a vertical plane of symmetry in which lies the tank axis.

Fire to tank heat transfer is radiative. There is, of course, a convective component but provided the radiative component chosen to represent the fire transmits the appropriate total flux (including the convective component) our treatment is adequate. Any PRV flare radiation is ignored, but could to some extent be incorporated by modificaion of the vertical heat flux distribution.

Wall heat transfer is via radial and azimuthal conduction. The wall may be multilayered in order to describe insulated vessels.

At the inner tank surface heat is transmitted to the contents by convection and radiation. Between the wall and the liquid, different convective regimes are considered depending on the temperature difference. There is free convection to the vapour space. The vapour is considered as a partially absorbing medium for the treatment of radiative heat transfer. The task of calculating the heat fluxes is simplified by solving where possible time independent equations and inserting their solutions into the necessary time dependent equations. The effects of wall curvature and temperature variations along it on the convective heat transfer are not treated - average values are calculated instead.

The vapour and liquid phases are each separately well mixed with one vapour and one liquid temperature. The internal pressure is the equilibrium vapour pressure of the bulk liquid.

The PRV may have one of several modes of operation depending on design. Discharge is single phase, critical orifice flow.

COMPARISON OF MODEL PREDICTIONS WITH EXPERIMENTS

The experiments[1,2] were two 0.25 tonne tank tests with a fill of 36%, three 1 tonne tank tests of 16%, 36% and 64% fill and five 5 tonne tank tests of 22%, 36%, 38%, 58% and 72% fill. The fill levels are the percentage of the total tank volume occupied by liquid.

In simulating experiments, only two quantities were fitted; these were the fire flux and the PRV open and close pressures. We used the actual PRV pressures and fire fluxes consistent with those estimated from the experiments.

Pressure prediction: Figure 1 shows experimental and calculated pressure histories for 0.25, 1 and 5 tonne tanks with a fill of 36%. The time to PRV opening and subsequent behaviour for the test duration are very well predicted. Note the different PRV behaviour between the 0.25 and 1 and 5 tonne results (HEATUP contains several models of PRV operation). The 0.25 tonne results were produced with minimal fitting of valve parameters. Figure 2 shows pressures in the 5 tonne tank for different fills (for clarity the pressure curves have been successively displaced by 5 bar). Multiple openings of the PRV in the 22% fill test were after the fire was extinguished and we have not attempted to model these.

PRV discharges: the good prediction of pressures after PRV opening is a partial indication of the ability of HEATUP to predict mass discharge rates for a variety of conditions. Actual and predicted discharges are compared in Figure 3 for 1 tonne tank tests (again for clarity, successive pairs of curves are displaced by 150 kg). The agreement between tests and predictions indicate that both PRV operation and evaporation rates are adequately described. We therefore have confidence in the validity of the assumptions for heat transfer to the liquid, heat and mass transfer between liquid and vapour and for single phase critical flow through the PRV.

Liquid and vapour temperatures: Figure 4 shows a comparison between model and test for the 5 tonne 72% fill test. The numbers against individual curves are thermocouple numbers - their positions are given in reference 1. The liquid immersed thermocouples show essentially similar temperatures until they become uncovered and enter the vapour space. The agreement with the model prediction and the ability to predict the internal pressure from

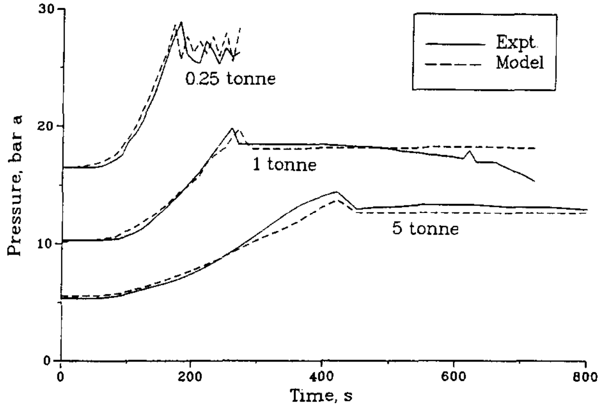

Figure 1: Pressure histories of 0.25 to 5 tonne LPG tanks with a 36% fill. Time is measured from fire ignition (successive plots are displaced for clarity by 5 bar)

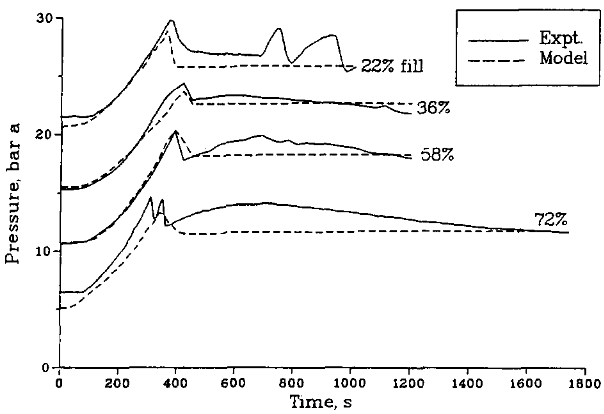

Figure 2: Pressure histories for a 5 tonne tank with a variety of initial fill levels (successive plots are displaced by 5 bar)

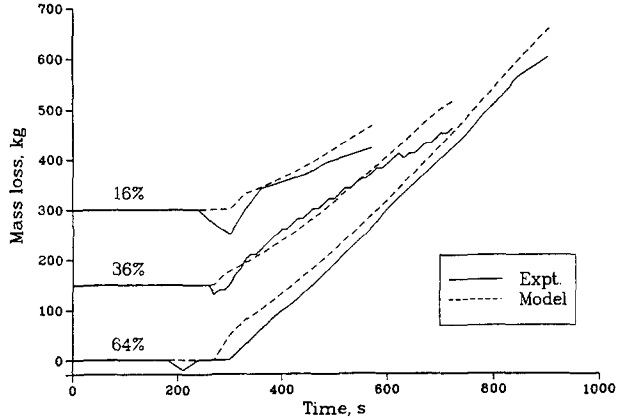

Figure 3: PRV mass loss for 1 tonne tank at various initial fill levels. (successive plots are displaced for clarity by 150kg)

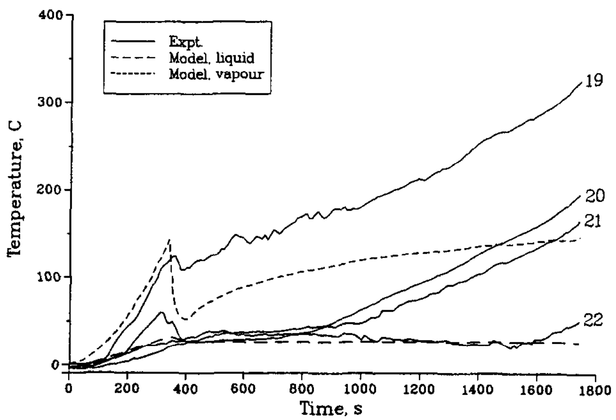

Figure 4: Liquid and vapour temperatures for 5 tonne tank with 72% initial fill

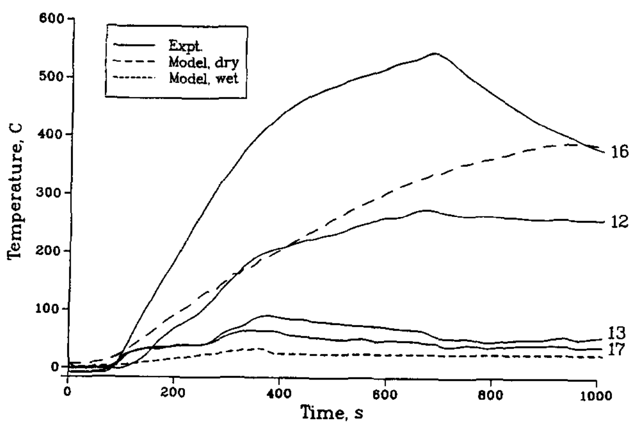

Figure 5: Wall temperatures for 5 tonne tank with 22% initial fill

the computed bulk liquid temperature shows the adequacy of the assumption that the liquid can be considered isothermal and therefore well mixed. The vapour space temperatures indicate considerable stratification even during PRV operation. Whilst the model predicts a realistic mean vapour temperature the assumption of good vapour space mixing is unrealistic. Wall temperatures for a 5 tonne 22% fill are illustrated in Figure 5. The overall agreement in this and the other tests is reasonable although there is some tendency to underpredict wet wall temperatures. The experimental vapour space wall temperatures are non uniform with the hot spot usually at the tank top. The mean temperatures predicted by the model fall within the range of actual values. It is clearly an over simplification to represent the inner surfaces of the wet and dry walls with single temperatures and to ignore vapour space temperature variations. Furthermore, two-dimensional models cannot predict wall temperature variations along the tank length but test results show that these are sometimes significant. The combination of these factors suggests that predictions of the onset and mode of any loss of containment require sharper definition of fire characteristics and wall temperatures.

While noting these limitations, a comparison of HEATUP predictions with experiments over a range of tank sizes and fill levels leads to a degree of confidence in its ability to predict the overall behaviour of cylindrical, pressurised LPG vessels engulfed in fire. With the very minimum of fitting it predicts well pressure histories, PRV performance, fluid and wall temperatures and the effects of fill level and scale.

MODEL DETAILS

Tank Wall Heat Transfer - HEATUP allows definition of multilayered walls to permit calculations on the effect of fire protective coatings. However, to simplify the description only a single layer wall only is treated here.

Temperatures in the tank skin are described by:

$$\sigma_w \frac{\partial T}{\partial t} = \frac{1}{r} \cdot \frac{\partial}{\partial r} (rk \frac{\partial T}{\partial r}) + \frac{1}{r^2} \cdot \frac{\partial}{\partial \phi} (k \frac{\partial T}{\partial \phi}), \; t > 0, \; R_1 < r < R_2, \; 0 < \phi < \pi \quad (1)$$

$$T (0, r, \phi) = T_0 \quad (2)$$

$$\frac{\partial T}{\partial \phi} = 0, \; t > 0, \; R_1 > r > R_2, \; \phi = 0, \pi \quad (3)$$

$$k \frac{\partial T}{\partial r} = \sigma \epsilon_w (T_f^4 - T^4), \; t > 0, \; r = R_2, \; 0 < \phi < \pi \quad (4)$$

$$k \frac{\partial T}{\partial r} = Q_r + Q_c, \; t > 0, \; r = R_1, \; \theta < \phi < \pi \qquad (5)$$

$$k \frac{\partial T}{\partial r} = q_r + q_c, \; t > 0, \; r = R_1, \; 0 < \phi \le \theta \qquad (6)$$

Polar coordinates are used. The tank skin lies between R_1 and R_2. The angular variable ϕ is zero at the tank base. $\phi = \theta$ corresponds to the position of the liquid surface at the inner tank wall. Other quantities are defined in the Notation section at the end.

Equation 1 is a non-steady heat flow equation with a temperature dependent conductivity k and constant heat capacity σ_W. The initial temperature distribution is given by equation 2. Equation 3 is a symmetry condition.

Equation 4 is the outer radius boundary condition for heat exchanged between the wall and fire by radiation. The inner radius boundary conditions are in equations 5 and 6 which equate the heat conducted to the inner surface and the convective and radiative fluxes to the liquid and vapour.

The fire heat flux is defined by an effective fire temperature, T_f, which to allow modelling of a non-uniform flux is given a Gaussian distribution. The position and value of the maximum temperature and the distribution width are adjustable. The fire is assumed to build up to a maximum value over a given time.

Heat transfer to the liquid and vapour

1) The convective flux density to the liquid ,q_C, is calculated by treating the wall as a plate of uniform temperature:

$$T_w = \int_0^\theta \left(\frac{1}{\theta}\right) T\,(t,\, R_1,\, \phi).\, d\phi \qquad (7)$$

Different heat transfer correlations are employed for specific ranges of $(T_2 - T_W)$, corresponding to regimes of free convection, nucleate boiling and transition to film boiling. The general forms of the convective heat flux density are:

$$\psi_1 (T_w - T_2)^{5/4} \qquad 0 < (T_w - T_2) < \delta_1 \qquad (8)$$

$$\psi_2 (T_w - T_2)^3 \qquad \delta_1 \le (T_w - T_2) < \delta_2 \qquad (9)$$

$$\psi_3 + \psi_4 \;(T_w - T_2) \qquad \delta_2 \le (T_w - T_2) < \delta_3 \qquad (10)$$

$$\psi_5 \;(T_w - T_2)^{3/4} \;(1 + \psi_6 (T_w - T_2)^{1/2}) \;(T_w - T_2) \ge \delta_3 \qquad (11)$$

Where the ψ_i and δ_i are functions[6,7] of T_2 and T_w.

2) Q_r and q_r - the radiative heat flux densities. An effective dry wall radiative temperature is given by:

$$T_1^* = \{ \int_{\theta}^{\pi} (\pi - \theta)^{-1} . T^4(t, R_1, \phi) \, d\phi \}^{1/4} \tag{12}$$

Part of the wall radiation will be absorbed by vapour and part by the liquid. Both the dry walls and the liquid surface are treated as grey bodies. The vapour is assumed to absorb and emit radiation in specified wavebands. This simplifies the calculation of absorption in the vapour which will depend on vapour pressure and on the pathlength travelled by the radiation as well as on the temperature of the radiation source. The proportions of the flux from the dry wall which contribute to the vapour and liquid heating are calculated from the radiation balance equations at the dry wall and liquid/vapour interface. There is also a small radiative component from the wet wall (considered as a uniform temperature plate) to the liquid.

3) Q_c - the convective flux density to the vapour. Free convective heat transfer is assumed with the form:

$$\psi_7 \; (T_d - T_1)^{5/4} \tag{13}$$

where T_d is a uniform effective convective temperature given by the dry wall analogue of equation 7.

<u>Liquid and Vapour Heat and Mass Exchange</u>

Global energy and mass balances are imposed on the vapour and liquid spaces and include PRV discharges. The balances are:

$$C_{p2} . m_2 \frac{\partial T_2}{\partial t} = (q_r + q_c) R_1 \theta - M_e(h_s - h_2) \tag{14}$$

$$C_{v1} . m_1 . \frac{\partial T_1}{\partial t} = (Q_r + Q_c) R_1 (\pi - \theta) - M_e (h_1 - h_s) - P \{ \frac{\partial}{\partial t} (\frac{m_1}{\rho_1}) - \frac{M_e}{\rho_2} \} - \frac{PR}{\rho_1} \tag{15}$$

$$\dot{m}_2 = - M_e \tag{16}$$

$$m_1 + m_2 = m_o - S \tag{17}$$

$$\dot{S} = R \tag{18}$$

$$m_2 / \rho_2 + m_1 / \rho_1 = V_0 \tag{19}$$

The required liquid density is given by the Yen Woods[8] correlation as a function of temperature, while the vapour density is calculated from the vapour temperature and pressure assuming ideal gas behaviour. The pressure is taken as the saturated vapour pressure of commercial propane at the liquid temperature.

Non-steady liquid heating arises from any inbalance between convective and radiative heat transfer and heat loss by evaporation. The enthalpy change due to evaporation is represented by the term $(h_s - h_2).M_e$, where h_s is the enthalpy of the vapour at the bulk liquid temperature. Non-steady vapour heating arises from the sum of radiative and convective heat transfer, heat required to bring vapour from the bulk liquid temperature to that of the bulk vapour and work done in compression or expansion and energy lost as vapour is discharged through the valve.

The liquid, vapour and discharged masses are related as follows: the liquid mass decreases at the net evaporation rate (equation 16) while, after the opening of the PRV, mass is lost at a discharge rate R (equation 18). The liquid and vapour remaining in the tank is the original mass minus that discharged (equation 17), and it must fill the tank volume (equation 19).

<u>The pressure relief valve</u>

The maximum flow rate at any given temperature and pressure is:

$$R_v = \chi(P).\ A_v.EPT^{-1/2} \tag{20}$$

where,

$$E = \sqrt{\frac{\gamma M}{R_g}\left(\frac{2}{1+\gamma}\right)^{\left(\frac{\gamma+1}{\gamma-1}\right)}} \tag{21}$$

A_v and $\chi(P)$ define the effective area at a given pressure P. A_v is the effective area when the valve is fully open i.e. the physical area times the discharge coefficient, while the opening function, $\chi(P)$, determines the percentage of this area actually discharging. In its simplest form $\chi(P) = 0$ until a set pressure, P^* is reached and $\chi = 1$ thereafter. However, by varying the form of $\chi(P)$, we can simulate various forms of PRV behaviour e.g. hysteresis where a valve sticks open or one which recloses at a pressure lower than that at which it first opens.

<u>The solution method</u>

A solution is required for the wall temperatures, $T(t,r,\phi)$, the liquid and vapour temperatures, T_2 and T_1 and the mass discharged S(t). All other quantities such as pressure, liquid and vapour mass, evaporation rate and interface height are prescribed functions of T, T_2, T_1 and S.

The wall temperature equations form a set of nonlinear parabolic partial differential equations The boundary conditions at the inner radius link them to the ordinary differential equations for T_1, T_2 and S through radiative and convective losses.

The space derivatives in the wall temperature p.d.e.s are replaced by finite difference approximations resulting in a system of o.d.e.s for the wall temperatures at fixed grid points within the wall. The grid spacing is uniform in the azimuthal and radial directions. The wall temperatures at the intersections of the grid lines obey global energy balances obtained by integrating equation 1 over a control volume around the grid point. The discontinuity at $\phi = \theta$ in the flux conditions at the interface of the internal boundary R_1 is smoothed out by the discretisation.

The resulting system of o.d.e.s (wall temperatures, T_1, T_2, S) is solved using a stiff integration method. In the case of multilayered walls the nonlinear equations for the temperatures at interlayer boundaries are solved using Newton iteration.

CONCLUSIONS

HEATUP has succesfully predicted pressure relief valve opening times, discharge rates, pressure histories and average liquid and vapour temperatures for a range of different tank sizes and fill levels. Predicted mean wall temperatures in both liquid and vapour zones were also in good agreement with measurements. Having been extensively validated in this way, HEATUP can be used as a predictive tool for examining the performance of tanks with variation of scale, fill, PRV characteristics, heat flux and protective coatings. As an example of scaling possibilities, in scaling up from .25 to 5 tonne the tank diameter increases by a factor of over three (from 510mm to 1680mm). In cylindrical tanks, increased tank capacity is obtained by increasing both length and diameter e.g. 5 and 12 tonne tanks have the same diameter. A further increase in diameter of a factor of 3 would allow the model to describe the behaviour of 100-200 tonne tanks.

NOTATION

Units are SI. Where pressures are quoted in bar we take 1 bar = 100 kN/m^2.

A_v	effective PRV area
c_{p2}	specific heat of liquid propane at temperature T_2
c_{v1}, c_{p1}	specific heats of propane vapour at temperature T_1
h_1	enthalpy of vapour at T_1
h_2	enthalpy of liquid at T_2
h_s	enthalpy of vapour at T_2

k	local wall conductivity, T and r dependent
m_1	vapour mass
m_2	liquid mass
m_0	initial total mass of liquid and vapour
M	molecular weight of propane
M_e	net evaporation rate
P	tank pressure
Q_r, q_r	radiative heat flux density at dry/wet wall
Q_c, q_c	convective heat flux density at dry/wet wall
r	radial ordinate
R_1	inner tank radius
R_2	outer tank radius
R_g	gas constant
R_v	maximum mass flow rate through pressure relief valve
R	instantaneous mass flow rate through PRV
S	cumulative mass discharged through PRV
t	time
T	local wall temperature
T_1, T_2	vapour/liquid temperature
T^*_1	average radiative temperature of dry wall
T_d, T_w	average convective temperature of dry/wet wall
T_0	initial wall temperature
T_f	flame temperature
V_0	tank volume
ϵ_w	emissivity of outer tank surface
γ	ratio of specific heats
$\rho_{1,2}$	vapour/liquid density
σ_W	wall specific heat
σ	Stefan-Boltzmann constant
ϕ	azimuthal ordinate
$\chi(P)$	opening characteristic of valve

REFERENCES

1 Moodie K. Cowley L.T. Denny R.B. Small L.M. and Williams I. 'Fire engulfment test on a 5 tonne LPG tank', Conference on Major Hazards in the Transport and Storage of Pressure Liquified Gases, New Brunswick, Canada, August 1987.

2 Moodie K., Billinge K. and Cutler D.P. 'The fire engulfment of LPG. storage tanks' I. Chem. E. Symp. - Assessment and Control of Major Hazards. UMIST. April 1985.

3 Ramskill P.K. Hunt D.L.M. 'The behaviour of tanks engulfed in fire - the development of a computer programme' I. Chem. Symp. - Assessment and Control of Major Hazards UMIST, April 1985

4 Sousa A.C.M. Venart J.E.S. 'Thermal modelling of LPG. rail tank cars exposed to fire environment' 4th Int. Conf. on Mathematical Modelling, Zurich, 1983

6 Perry's Chemical Engineers Handbook 4th edition McGraw Hill, 1950.

7 Cichelli M. Bonilla C. 'Heat transfer to liquids boiling under pressure' Trans.A.I.Ch.E. 41 1945.

8 Reid R.C., Prausnitz J.M. and Sherwood T.K. 'Properties of Gases and Liquids 3rd Edition, McGraw Hill, 1977.