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PRESSURE AND TEMPERATURE RESPONSE OF LIQUEFIED GASES IN CONTAINERS AND PRESSURE VESSELS WHICH ARE SUBJECTED TO ACCIDENTAL HEAT INPUT

David Dancer[1] and Dirse W. Sallet[1&2]

[1]Mechanical Engineering Department, University of Maryland, College Park, Maryland 20742 (The United States)
[2]Lehrstuhl A fur Thermodynamik, Technische Universität Munchen, Munich, West Germany

SUMMARY

A new numerical code is presented for the prediction of pressure and temperature histories in pressure vessels due to accidental internal heat production (exothermic reactions) or external heat addition (fire). The paper discusses the main features of the new numerical code which can be run on most desk sized computers. In addition, comparisons between experiments and calculated results are discussed. Two large scale experimental fire test programs were selected for such comparisons, namely the U.S. Army fire tests (1974) of a full scale, 33,000 gallons LPG tank car tank and the U.K. fire tests (1987) of a 5 tonne LPG tank. The calculated pressure and temperature histories are in good agreement with the experimental histories.

INTRODUCTION

In specifying a containment system for the storage or transportation of a hazardous material, an important consideration is what would be the consequences if the containment system were engulfed in an accidental fire. Unfortunately there have been several serious accidents (refs. 1-7) in which tanks containing hazardous materials have been engulfed in fires and have subsequently violently ruptured, resulting in deaths, injuries, and extensive property damage.

Past research in this area has been concerned with developing predictive computer programs (refs. 8-14), conducting laboratory scale experiments (ref.15), conducting field fire tests on small tanks (refs. 13, 16-19), and conducting field fire tests on large tanks (refs. 20-22). A discussion of this past research can be found in (ref. 23). Despite the extensive past research, the effects of the various parameters, such as tank size, initial outage (i.e. the fraction by volume by which a vessel falls short of being liquid full), and radiative properties of the lading

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vapor are still not well understood. Most of the experimental studies have been concerned with small tanks and large outages and therefore, may not be relevant to the usual industrial practice of using large tanks and small outages.

In section 2 of this paper, mathematical models for predicting the response of hazardous materials containment systems to fire engulfment are developed and a computer program incorporating the mathematical models is described. In section 3, the computer program is exercised for two situations for which experimental data is available and the numerical results are compared with the experimental results. The computer program is also exercised for four additional situations which are variations of one of the experimental test cases. In section 4, several conclusions and recommendations are presented. Further details on the modelling and validation of the computer program can be found in (ref. 23).

MATHEMATICAL MODELLING

A computer program, TAC7, has been developed to calculate the transient heat, mass, and momentum transfer of liquids and gases in infinitely long horizontal cylinders which are externally heated (e.g. a fire) or internally heated (e.g. exothermic decomposition). The program is capable of considering either (1) a single phase condition in which the vessel contains only a liquid phase or only a vapor phase, or (2) a two-phase condition in which the vessel contains both a liquid phase and a vapor phase. The program assumes that initially the contents of the vessel are at rest, at a uniform temperature, and, for two phase systems, in equilibrium. The program may be used for either for laminar flow conditions or for turbulent flow conditions. However, the program is not valid for pure conduction or weak convection (i.e. low Rayleigh number) situations. For those situations, a companion program TAC6 should be used. TAC7 does not permit the flow of mass into the container, but outflow of mass (e.g. through a safety relief valve) is permitted. TAC7 assumes that the mass flow rates through the valve are low enough so that rapid depressurization effects and forced convection effects are negligible.

TAC7 is written in standard Basic and has been run on GW-Basic 3.20 and IBM Basic 2.0. The program has 648 statements. The program requires a personal computer with at least 64k of RAM and one diskette drive. There are no specific requirements for ROM, but for large problems it is not uncommon for the data output to exceed the storage capacity of a standard double-side, double density diskette. The computer time required by TAC7 for a particular problem will depend greatly on the computer used and the characteristics of the problem. To simulate a 24 minute fire test conducted by the U.S. Army on a 3 m diameter horizontal tank required 3 hours and 14 minutes on an IBM AT Personal Computer. In that problem a time step of 1 second was used and the tank and lading were broken down into 20 liquid phase elements and 20 vapor phase elements. All properties (except for the vapor pressure and the liquid and vapor viscosities) were assumed constant.

TAC7 requires that a user supply a program to provide input and initialization data for TAC7. TAC7 uses the user supplied data to calculate the transient phenomena occurring in the container and to "dump" the data on a specified disk or diskette drive. At the end of a numerical experiment, the user then may retrieve the data and present the results in an appropriate fashion. The program does not attempt to directly predict when or if the container will fail or the lading will explode. Rather, the program calculates the data needed by the user to interpret the phenomena.

TAC7 employs three heat transfer models to simulate the heating of a container. The first model is the heat transfer from the surroundings to the wall. It is assumed that the heat flux from the surroundings to the container wall is a known function of time, position, and tank wall temperature. In (ref.23) are some guidelines on the heat fluxes to be expected for four commonly occuring situations - (1) the container is engulfed in a pool fire, (2) the container is near a fire source, (3) the container is heated by intense solar radiation, and (4) the container contains a cryogenic liquid and loses its vacuum insulation system. Also included in (ref. 23) are guidelines for the thermal modeling of insulation systems. In this paper, we simulate two experimental test cases by using the experimental heat fluxes measured in each test.

The second heat transfer model is the heat transfer within the container wall. It is assumed that the container wall is such a good thermal conductor that temperature differences across the wall thickness are negligible. However, circumferential conduction heat transfer within the container wall is permitted.

The third heat transfer model is the heat transfer to the lading. As shown in Figure 1, TAC7 divides the lading into various nodes.

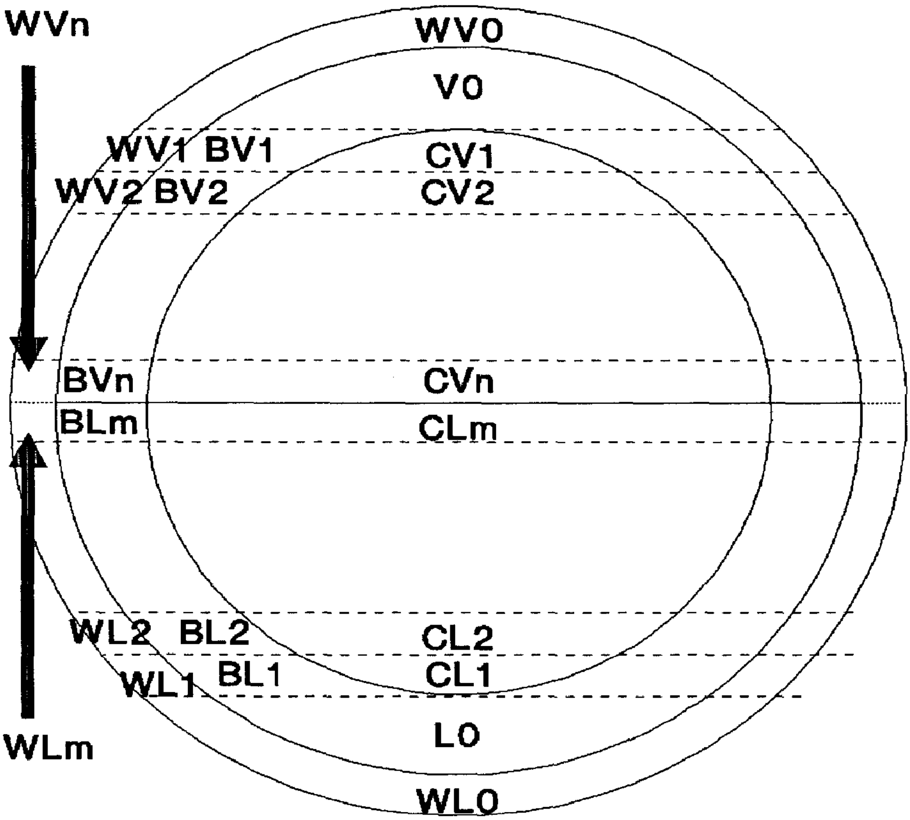

Fig. 1. Diagram showing the nodal arrangement used by TAC7.
Nodes WL0, WV0, WL1 ... WLm, and WV1 ... WVn are wall nodes.
Nodes L0, BL1 ... BLm, and CL1 ... CLm are liquid phase nodes.
Nodes V0, BV1 ... BVn, and CV1 ... CVn are vapor phase nodes.

It is further assumed that the system pressure is equal to the equilibrium vapor pressure evaluated at the temperature of node CLm.

The integral equation method is used to calculate the temperatures and velocities in the lading. Depending on the mode of heat transfer in the lading, appropriate profiles are assumed for the velocities, temperatures, and pressure as functions of x, the horizontal distance from the wall. For example, for laminar natural convection, it is assumed that the vertical velocity, v, in a liquid or vapor boundary layer node is given by:

$$v = V\ (x/\delta)\ (1-x/\delta)^2 + V_c \qquad (1a)$$

and the vertical velocity in a liquid or vapor core node is given by:

$$v = V_c \qquad (1b)$$

In eqns. (1) and (2), the parameters V, δ, and V_c are allowed to vary with time and with the node location. The continuity, momentum, and energy equations are integrated with respect to x. For turbulent natural convection, the wall shear stresses and heat transfer coefficients are based upon recent experimental results of (ref. 24) for turbulent natural convection along a vertical plate. Specifically, the empirical correlations for the shear stress and heat transfer coefficient are given by equations (1) and (2), respectively,

$$\frac{\tau_w}{PU_b^2} = .70\ Gr^{1/12} \qquad (1)$$

$$Nu = .12\ (Gr\ Pr)^{1/3} \qquad (2)$$

where U_b is = $(Gr\ N^3/x^3)^{1/3}$, x is the circumferential distance from the tank bottom, P is the lading density, N is the dynamic lading viscosity, Gr is the local Grashof number, Pr is the Prandtl number, and Nu is the local Nusselt number.

The detailed derivation of the boundary layer and core equations used in this paper are presented in (ref. 23).

NUMERICAL CALCULATIONS

The computer program described in the previous section has been extensively tested by solving problems for which experimental data, analytical solutions, or numerical solutions are available in the literature. These validation studies are described in (ref. 23). This paper presents two of these validation studies.

The two validation test cases were selected because they are well documented and they most closely simulate actual industrial practice. In addition, the two validation test cases appear to be contradictory as to liquid thermal stratification. Also presented in this paper are four additional test cases which are variations of the first test case.

The first test case is a simulation of a fire test of a full scale LPG tank car tank conducted in 1974 by the U. S. Army (refs. 20-21). The tank used in the fire test was a horizontal cylinder, 18.3 m (60 ft) long and 3.0 m (10 ft) in diameter, with 1.6 cm (5/8 in) thick carbon steel walls. The tank was equipped with one Midland Manufacturing A-3180-N relief valve, with a nominal start-to-discharge pressure setting of 280.5 psig, a nominal vapor tight pressure setting of 224 psig, and a throat area of 6.2 square inches. The tank essentially conformed to a U. S. Department of Transportation Specification 112A340W tank car tank. The tank was filled to 27.9 cm (11.0 in) from the top of the car, resulting in an initial outage of approximately 4.6% by volume. The composition of the LPG was 98.0% propane and 2.0% ethane. At the start of the test, the temperature of the LPG was 21 C (70 F) and the gauge vapor pressure was 963 KPa (125 psig). The fire test was conducted in a large excavation, 45.7 m long, 30. 5 m wide, and 7.9 m deep (150 ft by 100 ft by 26 ft). During the fire test, JP-4 jet fuel was continuously supplied to the excavation and the temperatures at various locations in the tank wall and in the lading were continuously monitored. The pressure in the tank was also continuously monitored. The fire characteristics were measured by means of thermocouples, radiometers, and calorimeters. The fire temperatures ranged from 650 to 990 degrees Centigrade and the average cold wall heat flux from the fire to a small calorimeter was 138 KW per square meter. The relief valve was essentially closed for the first three minutes of the fire test (the valve did briefly open at 2.2 minutes and 2.6 minutes after the start of the test). Until the relief valve opened, it was observed that (1) there was considerable temperature stratification in both the liquid and vapor phases and (2) the vapor temperatures were considerably higher than the liquid temperatures. Even after the relief valve opened, it took another seven minutes until the lading became essentially isothermal. After 24.5 minutes, the tank violently ruptured.

Figures 2 - 5 compare the experimental results of test case 1 with the results predicted by the computer program. As can be seen in the figures, the agreement between the experimental results and the computer results is good.

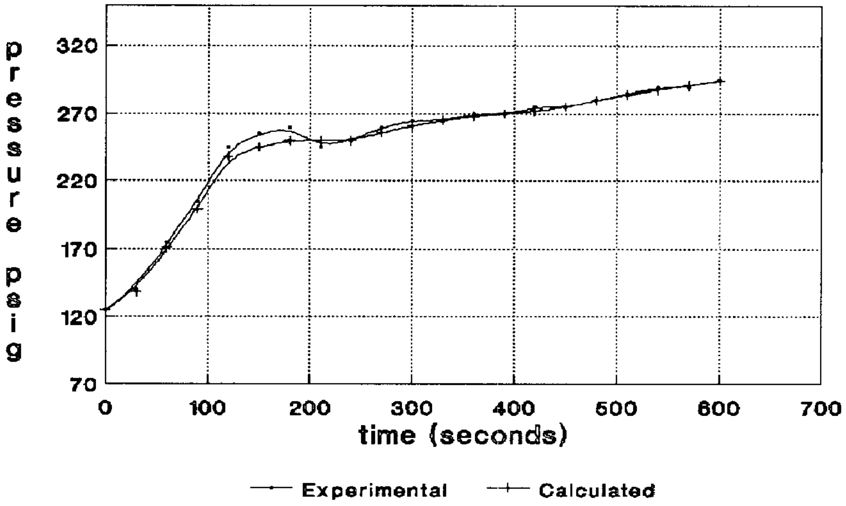

Fig. 2. A comparison of experimental (refs. 20-21) pressures with predictions of TAC7.

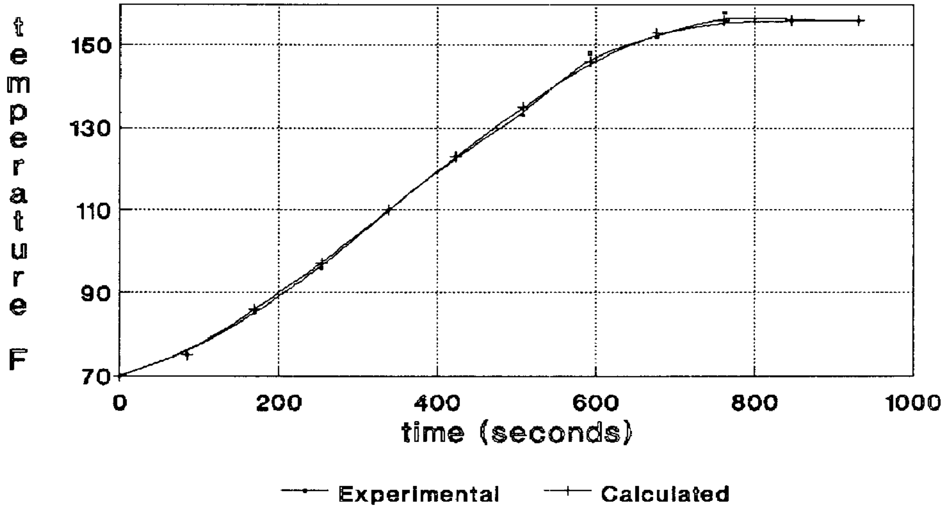

Fig. 3. A comparison of experimental (refs. 20-21) lading temperatures, measured in the core at the horizontal centerline, with the predictions of TAC7.

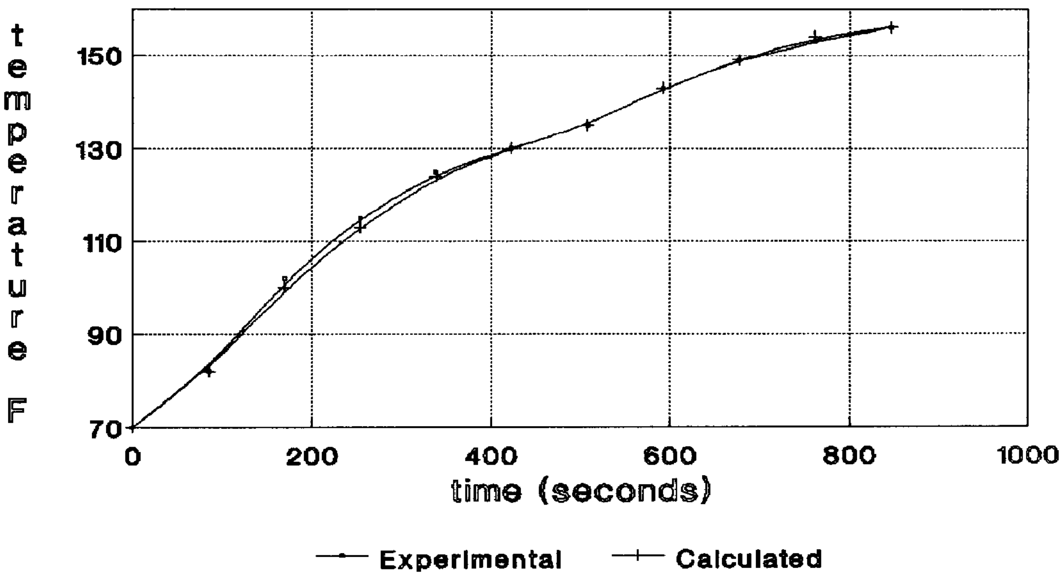

Fig. 4. A comparison of experimental (refs. 20-21) lading temperatures, measured in the core 3.5 feet above the horizontal centerline, with the predictions of TAC7.

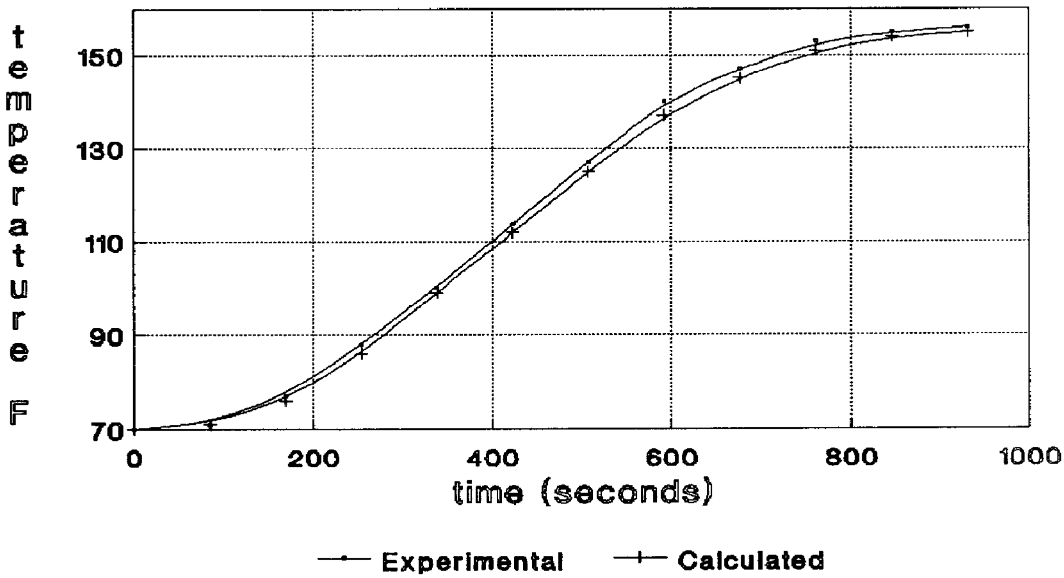

Fig. 5. A comparison of experimental (refs. 20-21) lading temperatures, measured in the core 3.5 feet below the horizontal centerline, with the predictions of TAC7.

The second case study is a simulation of a full scale fire test of a 5 tonne LPG tank that was conducted by the United Kingdom Health & Safety Executive, Research & Laboratory Services Division, and Shell Research Limited (ref. 22). The tank conformed to United Kingdom standard BS 1500 and was a horizontal cylinder, 4 m long and 1.7 m in diameter, with 1.8 cm thick carbon steel walls. The tank was equipped with two standard external pressure relief valves, each with an effective throat area of 8.87 x 10^{-4} square meters and set to open at 14.3 bar guage. The tank was filled with commercial propane and the initial outage was 28% by volume. The composition of the commercial propane was not reported. The initial temperature of the commercial propane was 6.4 C. The fire tests were conducted in a refractory brick lined pit. Kerosine for the fire tests was added to pit (with no replenishment) and was ignited. During the fire test, the temperatures at various locations in the tank wall and in the lading were continuously monitored. The pressure in the tank was also continuously monitored. The fire characteristics were also measured by means of thermocouples and calorimeters. The average cold wall heat flux from the fire to a small calorimeter was estimated to be about 105 KW per square meter. In the fire test, the relief valve opened after 5.2 minutes. Both before and after the pressure relief valve opened, it was observed that (1) there was considerable temperature stratification in the vapor phase, but not in the liquid phase, (2) the vapor temperatures were considerably higher than the liquid temperatures, and (3) the lading thermal boundary layer was very thin.

Figures 6 - 8 compare the experimental results of test case 2 with the results predicted by TAC7. As can be seen in the figures, the agreement between the experimental results and the computer results is good.

The third test case is the same as test case 1, except that the outage is increased to 28%. The computer results for test cases 1 and 3 are presented in Figure 9. As can be seen in Figure 9, the thermal stratification is less in test case 3 than in test case 1.

The fourth test case is the same as test case 1, except that the tank diameter is reduced to 1.7 meters. The computer results for the test cases 1 and 4 are presented in Figure 10. As can be seen in Figure 10, the thermal stratification is less in test case 4 than in test case 1.

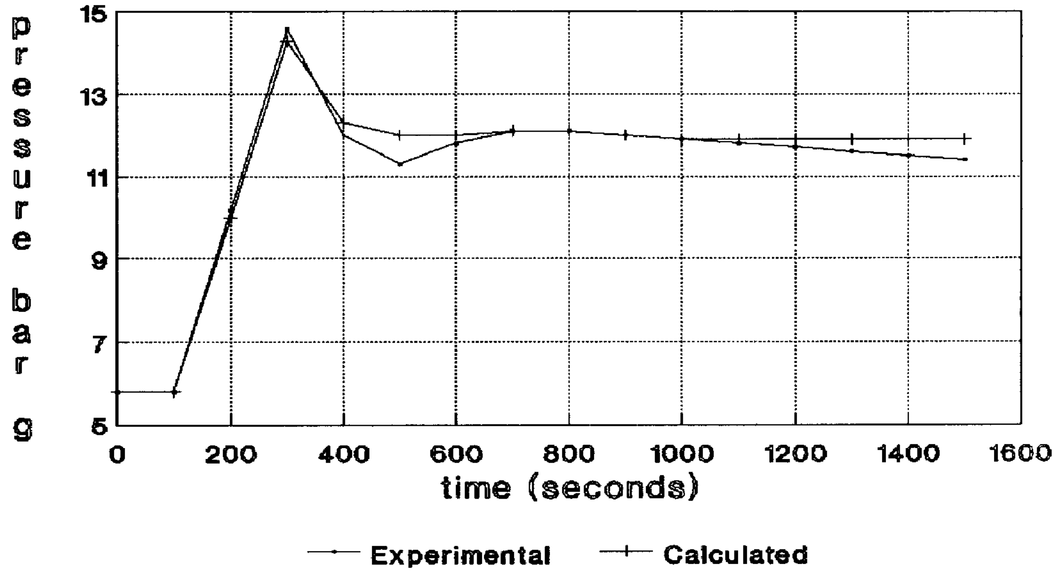

Fig. 6. A comparison of experimental (ref. 22) pressures with the predictions of TAC7.

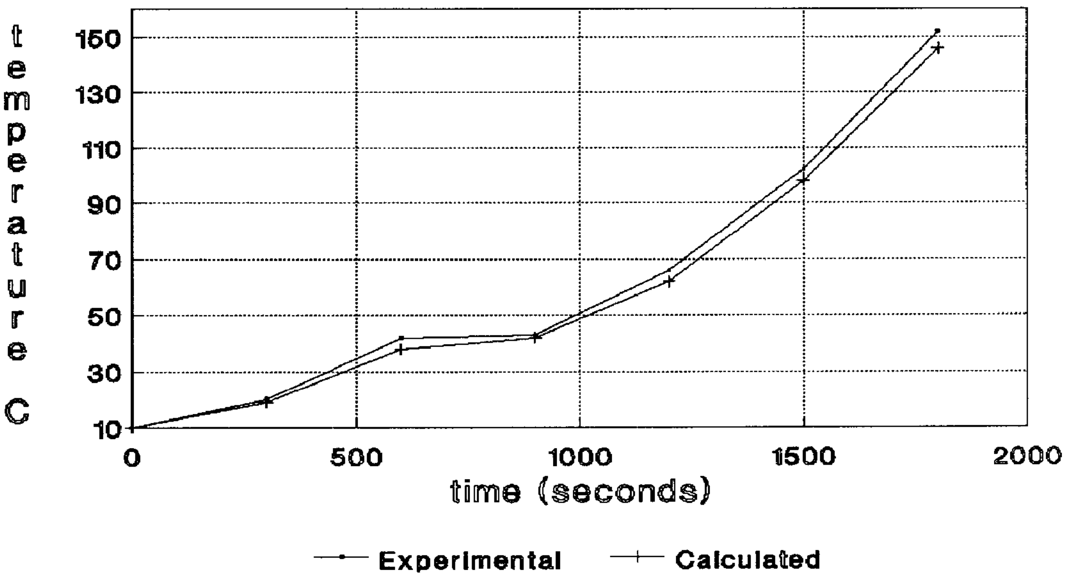

Fig. 7. A comparison of experimental (ref. 22) lading temperatures, measured in the core 0.4 meters above the horizontal centerline, with the predictions of TAC7.

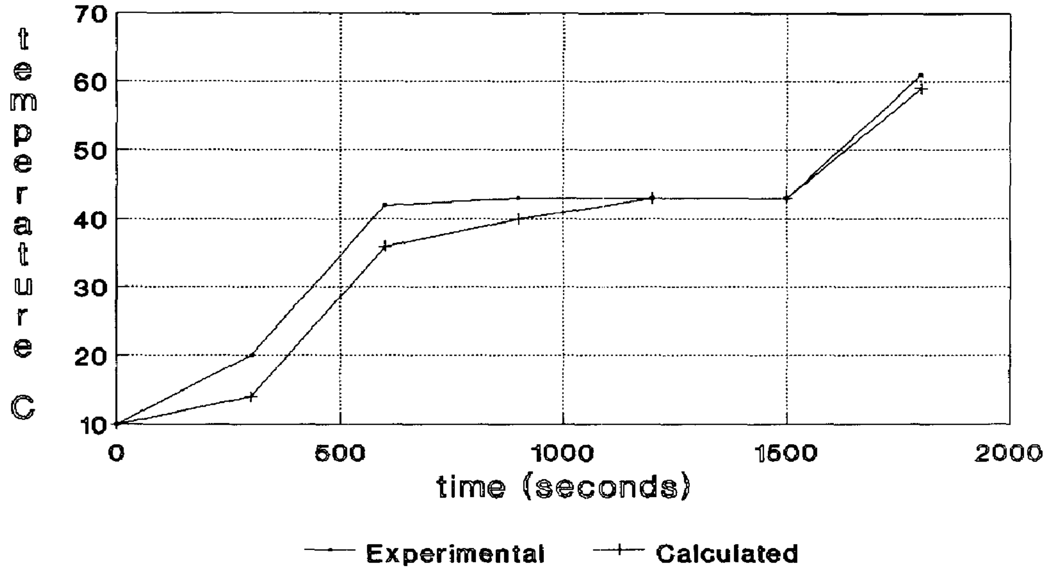

Fig. 8. A comparison of experimental (ref. 22) lading temperatures, measured in the core 0.1 meters below the horizontal centerline, with the predictions of TAC7.

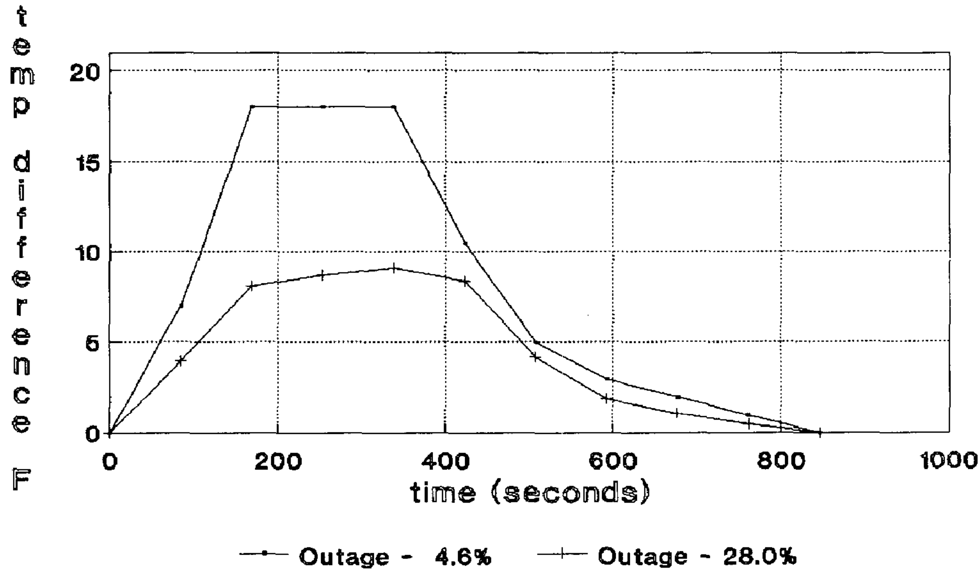

Fig. 9. The difference, predicted by TAC7, between the liquid core temperature at the liquid-vapor interface and the average liquid temperature, as a function of outage and time. Tank is a 10 feet diameter horizontal tank. Heat input to the tank is as measured in (refs. 20-21).

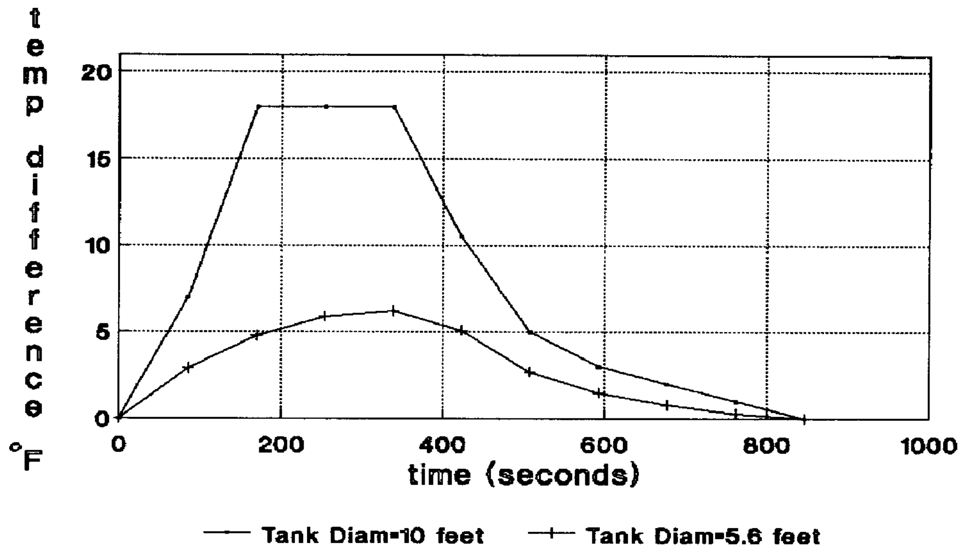

Fig. 10. The difference, predicted by TAC7, between the liquid core temperature at the liquid-vapor interface and the average liquid temperature, as a function of tank diameter and time. Tank is a 10 feet diameter horizontal tank. Heat input to the tank is as measured in (refs. 20-21).

The fifth test case is the same as test case 1, except that both the outage is increased to 28% and the tank diameter is reduced to 3.0 feet (1.7 meters). It should be noted that the fifth test case corresponds to the second test case, except that the fire heat flux in the fifth test case is higher than the fire heat flux in the second test case. The computer results for test cases 1 and 5 are presented in Figure 11. As can be seen in Figure 11, the thermal stratification is less in test case 5 than in test case 1, test case 3, and test case 4 and is comparable to test case 2.

The sixth test case is the same as test case 1, except that in calculating radiative heat transfer, the vapor phase was considered to be isothermal. In both test case 6 and test case 1, convective heat transfer was calculated allowing for nonisothermal conditions. The purpose of test case 6 was to assess the importance of accuracy in the calculation of radiation heat transfer in the vapor phase. The computer results for test cases 1 and 6 are presented in Figure 12. As can be seen in Figure 12, the isothermal approximation can result in appreciable errors at high temperatures.

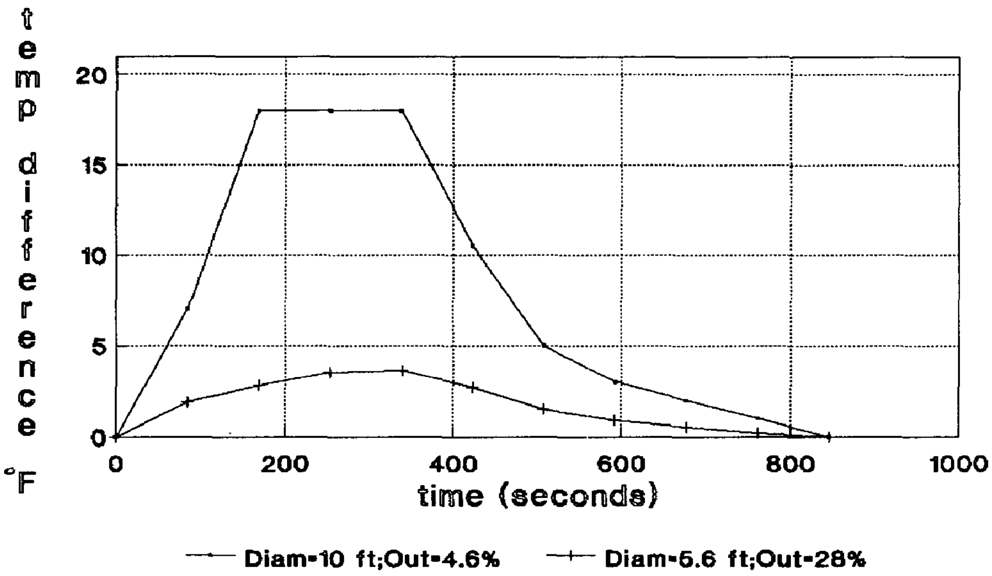

Fig. 11. The difference, predicted by TAC7, between the liquid core temperature at the liquid-vapor interface and the average liquid temperature, as a function of tank diameter, outage, and time. Heat input to the tank is as measured in (refs. 20-21).

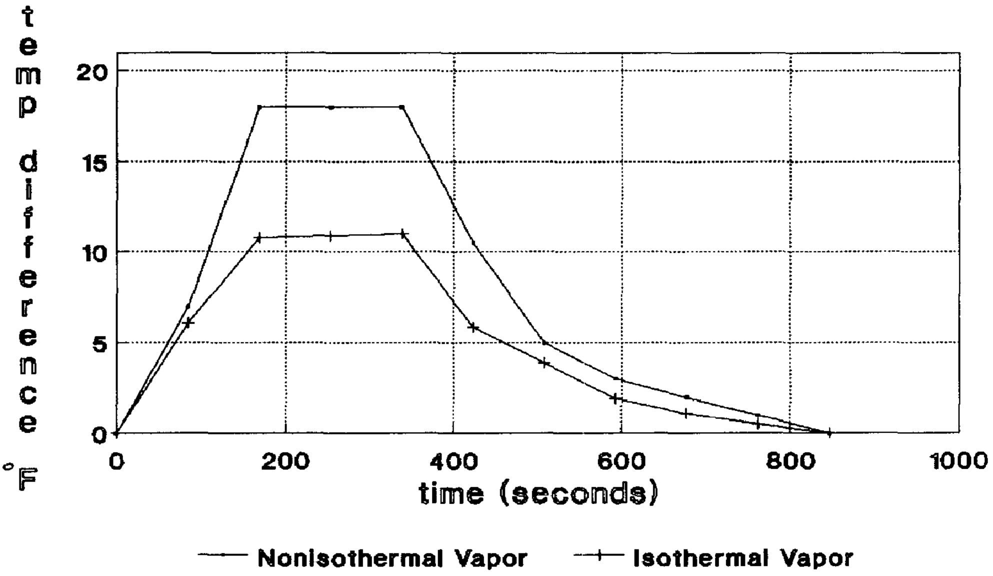

Fig. 12. The difference, predicted by TAC7, between the liquid core temperature at the liquid-vapor interface and the average liquid temperature, as a function of time and which approximation (isothermal vapor or nonisothermal vapor) is used in radiation calculations. Tank diameter is 10 feet and outage is 4.6%. Heat input to the tank is as measured in (refs. 20-21).

CONCLUSIONS AND RECOMMENDATIONS

Calculations using the mathematical model developed in this paper are in good agreement with experimental results.

The amount of outage in a tank significantly affects the lading's response to an external fire. As the outage approaches zero, (1) internal recirculation in the liquid phase becomes inhibited causing increased temperature stratification in the liquid phase, (2) interfacial mass transfer between the liquid and vapor becomes significant, and (3) the thermal expansion of the liquid phase (and corresponding contraction of the vapor phase) causes a sharp increase in the rate of pressure rise. Therefore, the authors recommend that care be taken when extrapolating experimental or analytical results valid for tanks with large outages to tanks with small outages.

The size of the tank also significantly affects the lading's response to an external fire. As the tank's diameter increases, the internal recirculation of the liquid phase decreases and there is more thermal stratification. Therefore, the authors recommend that care be taken when extrapolating experimental or analytical results for small tanks to predict what would occur in large tanks.

Radiation from the unwetted tank wall can be the predominant mode of heat transfer to the vapor phase. Radiation from the unwetted wall is usually an insignificant mode of heat transfer to the overall liquid phase. However, radiation can significantly affect the temperature of the liquid phase near the vapor-liquid interface which in turn will affect the system pressure. In general, assuming the vapor phase is isothermal will overpredict the heat transfer to the vapor phase and will underpredict the heat transfer to the liquid phase near the interface. Therefore, the authors recommend that care be taken when calculating the heat transfer by radiation from the unwetted wall to the vapor phase and to the liquid phase near the interface.

The turbulent natural convection model developed in this paper is consistent with all available experimental velocity and heat flux data. However, most of the relevant data are for air at Rayleigh numbers less than 10^{14}. Therefore, the authors recommend that care be taken when using the model for Prandtl numbers less than 0.5 or greater than 2.0 and for Rayleigh numbers greater than 10^{14}.

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