DRAFT FINAL REPORT

DESCRIPTION OF COMPUTER PROGRAM FOR CALCULATION OF TEMPERATURES, PRESSURES AND LIQUID LEVELS OF TANK CARS ENGULFED IN FIRES

Contract No. DTFR53-81-C-00016: Task VC-4

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1. INTRODUCTION

This report describes work that has been carried out under Federal Railroad Administration Contract No. DTFR53-81-C-00016, Task Order VC-4, entitled "Temperatures, Pressures and Liquid Levels of Tank Cars Engulfed in Fires".

The objective of this task order was the further development and utilization of a procedure for calculating the fire effects on a tank car containing certain hazardous materials. This report describes the analytical procedure and the computer program which was used to analyze the effects of safety relief valve flow capacities and thermal shield conductances on the vulnerability of cars containing liquids and liquified gases in the pool fire environment (complete fire engulfment). Results from the use of the program to calculate the effects on cars containing ethylene oxide and propane are described in Ref. 1. Results from the use of the program to calculate the effects on cars containing propylene, 1,3-butadiene, vinyl chloride, monomethylamine or propylene oxide are described in Ref. 2.

The program has been written in FORTRAN and has been run on a Data General ECLIPSE computer. The program is designed for interactive use with a terminal. The initial conditions are entered at the terminal. The results can be displayed at the terminal or printed at a line printer. Another option is to provide plots of pressure, tank wall temperature over the vapor space and liquid fraction as a function of time.

Section 2 of this report gives an overview of the modeling procedure. Section 3 presents a flow chart of the program and discusses the technical background for specific steps in the calculation. Program listings are presented in Section 4. A sample problem with results is presented in Section 5.

2. ANALYTICAL PROCEDURE

The calculational procedure, which has been developed under this program to model fire effects on tank cars, allows the conditions within the tank to be determined as a function of time for arbitrary characteristics of the thermal insulation system and the flow capacity of the safety relief valve. The assumption is made that the car is fully engulfed by the fire so that the fire is of uniform intensity all over the tank. The calculational procedure begins by assuming that the car has been loaded in accordance with allowable filling density tables so that there is an outage volume which is occupied by the product in the vapor state. Figure 1 illustrates the basic phenomena which must be taken into consideration. Four different sets of conditions are recognized. The first deals with the situation where the car is in the upright position venting vapor. Most of the heat is conducted into the car through the wetted area of the tank. The properties of the thermal shield determines the rate of heat transfer into the liquid product. Some heat is also conducted through the thermal shield over the vapor space which increases the temperature of the tank wall. As the temperature rises, some heat is radiated from the wall to the liquid below. The amount of heat radiated depends on both the radiation surface configuration factor of the surface of the liquid and the temperatures of the wall and liquid. This factor decreases as the liquid level drops.

The burst strength of the tank is estimated as a function of the wall temperature over the vapor space. When the tank is no longer capable of containing the vapor pressure, failure is assumed causing the sudden release of the remaining product within the car.

The vapor pressure within the tank is a function of the temperature of the liquid product, increasing as its temperature increases. The presence of nitrogen, which is used as a pad of inert gas, must be considered for cars containing certain commodities. When the vapor pressure within the tank exceeds the start-to-discharge pressure of the valve, the valve opens allowing the vapor to exhaust from the car. A slight rise in the pressure above this value causes the valve to move to the fully open position. If the valve flow capacity is adequate, the liquid will tend to remain at a nearly constant temperature as it is vaporized and is exhausted from the tank. If

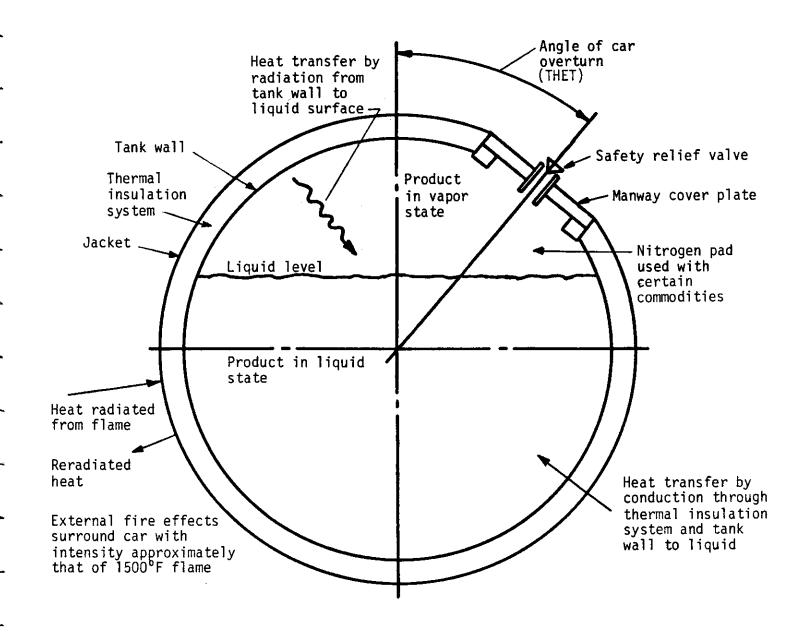


FIGURE 1. CONDITIONS CONSIDERED IN THE ANALYSIS OF TANK CARS SUBJECTED TO FIRE

the valve flow capacity is not large enough, the pressure in the tank will rise allowing the temperature of the liquid to increase and also resulting in a somewhat larger mass flow rate through the valve.

The second set of conditions which must be considered is the over-turned car case. The conditions are similar to those of the upright car case except that the car is assumed to be partially rolled over so that when the safety relief valve opens it will vent liquid instead of vapor. The volumetric flow rate for liquid discharge is less than for the vapor case at any given pressure, but the mass flow rate may be larger because of the greater density of the fluid. Liquid flow through the valve is calculated assuming homogeneous isentropic two phase flow (liquid and vapor) and a liquid discharge coefficient of 0.7.

The third set of conditions is the case where the tank car is "shell full" (of liquid) and for all practical purposes there is no vapor space left within the tank. This condition occurs when the car is initially filled with only a small empty volume above the liquid surface. When the car is exposed to the fire, the temperature of the product rises and its specific volume increases so that eventually all of the tank is filled with liquid. DOT requirements, for example, allow some products within Class 105 tank cars to be filled so that the car becomes shell full when the product temperature rises to 105°F. When the car becomes shell full, any further increase in temperature of the product will cause liquid flow through the safety relief valve. An increase of the pressure within the tank above the saturated vapor pressure may be necessary to cause a sufficient flow rate. If the capacity of the valve is small and the rate of increase in the specific volume of the liquid is large, very high pressures can be developed. The calculation of the fire effects under these conditions assumes the heat is transferred to the liquid over the entire area of the tank shell.

The fourth set of conditions is the case where all the liquid has been vaporized. This condition is also associated with the case where the critical temperature of the product is exceeded before all the liquid is vaporized so that the vapor state is the only phase in which the product can exist. The temperature of the vapor will increase at a fairly rapid rate because heat is both convected and radiated to the product and because

the mass of the product within the tank is relatively small. Under almost all conditions, the safety relief valve is fully capable of relieving any increases in pressure as the vapor becomes hotter. The pressure would be maintained near the valve closing pressure. The tank wall temperature also increases fairly rapidly during this phase because there is no cooling effect from liquid product within the tank.

The calculational procedure assumes that each of the parameters remain constant over a given time step. The parameters are then updated at the end of the time step. An integration time step of 0.1 minutes has been used for the parametric analyses conducted under this study. This time step has been found to be fully adequate for describing the various phenomena. The computer program contains an optional time period for printing out intermediate results.

3. DESCRIPTION OF COMPUTER PROGRAM

The computer program is described in this section. Five subroutines are used with the basic program:

SURFACET to calculate the surface temperature of the outside of the tank insulation system,

PROPERTIES to establish the thermal properties of the product as a function of temperature,

VCAP to calculate the liquid flow capacity of the safety relief valve as a function of the fluid properties,

 $\overline{\text{TSHIELD}}$ to calculate the effective conductance of a thermal shield system where temperature dependent conductivity is assumed as a function of the temperature on the inside and outside faces of the system, and

<u>PLT3</u> to construct plots of tank wall temperature over the vapor space, liquid fraction remaining, and pressure versus time.

Figure 2 shows a flow chart for the steps which are carried out during each calculational cycle.

3.1 ESTABLISHMENT OF INITIAL VALUES

The first step is to enter initial values for the analysis into the computer terminal. The following information must be provided:

Display Type: Whether the results are to be displayed at a terminal or line printer

Plot or Print Data: Whether a plot of temperature, pressure and liquid fraction versus time is desired or tabulated results

Product Within Tank

Angle of Rollover for Safety Valve Orientation

Tank Diameter

Tank Wall Thickness

Volumetric Capacity of Tank

Volumetric Fraction of Tank Initially Filled with Liquid

Safety Relief Valve Flow Rating Pressure

Safety Relief Valve Start-to-Discharge Pressure

Net Absorptivity of Tank Wall Surface

Net Emissivity of Tank Wall Surface

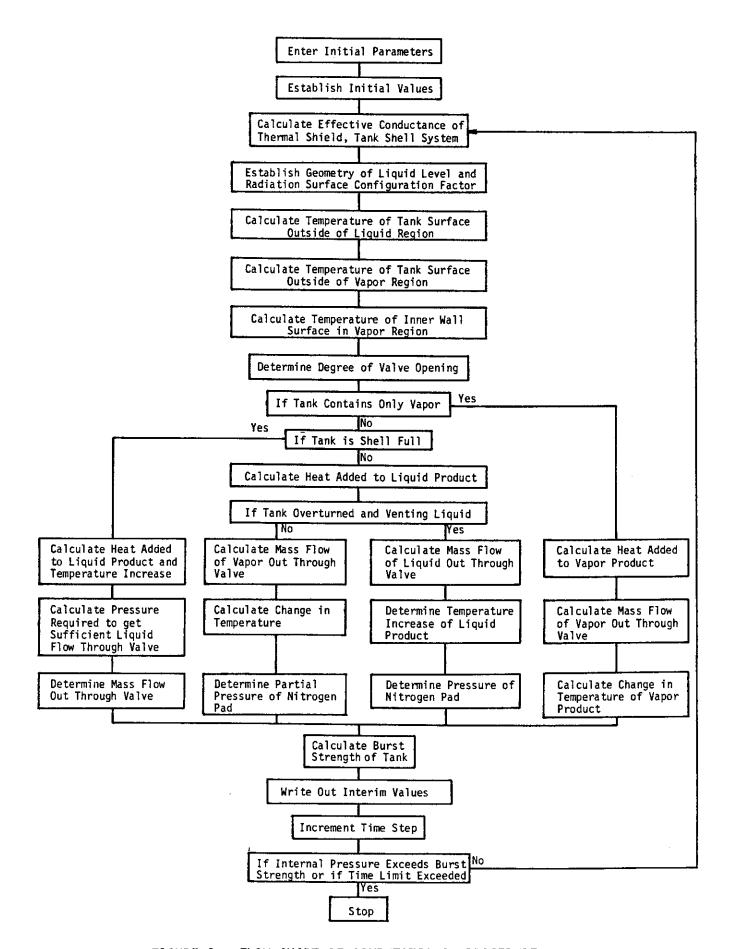


FIGURE 2. FLOW CHART OF COMPUTATIONAL PROCEDURE

Bursting Strength of Tank

Thermal Shield Conductance

Safety Relief Valve Rated Flow Capacity

Constant Conductivity or Temperature Dependent Conductivity of Tank Insulation Material: If temperature dependent conductivity is selected, the thickness of the insulation material is also entered.

Consideration of Initial Conductance: This option permits entry of an initial value for conductance of the thermal insulation system which is different than the value of conductance previously entered. If this option is selected the desired initial value is also entered.

Flame Temperature

Nitrogen Padding Pressure

Area Exponent: This is an exponent which is applied to the surface area of the tank to determine the effective area subjected to the fire. Normally it would be 1.0. It is included in the calculation so that comparisons can be made to AAR valve design criteria where an exponent of 0.82 is used (Ref. 3).

Initial Temperature of Tank and Contents

Time Increment

Number of Time Steps Between Display of Data

Gas Compressibility Factor (Z)

Safety Relief Valve Gas Flow Constant: This constant (VLCON) is explained in Section 3.11.3.

Typical values which have been used for the tank car design parameters are listed below:

<u>Parameter</u>	105A100W Car Containing Ethylene Oxide	105A300W Car Containing Propane	112A340W Car Containing Propane
Tank diameter (ft)	9.5	9.9	10.0
Tank wall thickness (in.)	0.562	0.562	0.625
Nominal capacity (gals)	25,000	33,600	33,600
Safety valve flow rating pressure (psia)	99.7	284.7	320.7
Safety valve start- to discharge pressure (psia)	89.7	262.2	295.2
Burst Strength of Tank (psi)	500	750	850

3.2 ESTABLISH INITIAL VALUES

The program proceeds with the calculation of other parameters such as the volume of the tank, tank length, tank surface area, weight of tank shell, weight of liquid product, weight of nitrogen gas pad, weight of product in the vapor space, etc. Subroutine PROPERTIES is called to get the product data for these calculations.

An estimate is made of the cross sectional area of the safety valve. It is based on an assumed discharge coefficient of 0.9 for the passage of air. The equation is given as follows:

$$A_v = (SCFM)/(C_d P_s 2638) \tag{1}$$

where A_v is the cross sectional area of the valve (ft²) C_d is the discharge coefficient, and P_s is the valve flow rating pressure (psia)

3.3 DETERMINE CONDUCTANCE OF THERMAL SHIELD

The calculational cycle which is carried out each time step begins with the establishment of the conductance of the thermal shield. Two options are provided: one where constant conductivity is assumed (except for the first thirty minutes as indicated below) and the other where temperature dependent conductivity of the thermal insulation material is assumed. This has the effect of allowing the conductance to change as a function of time because the average temperature through the insulation changes with time. If temperature dependent conductivity is assumed the calculation of the effective conductance of the shield is carried out in subroutine TSHIELD. This subroutine utilizes an algebraic relationship for defining the conductivity as a function of temperature. An iterative solution is used to determine the effective conductance of the system when operating between the temperature limits on the inside and outside of the faces of the material at this point in the calculational cycle.

A second option is provided, which allows one to consider that there is an initial value of conductance and that there is a linear relationship between this value and the value which normally would be reached after a 30 minute period. This option is included to represent conditions that have

been observed for some types of 105 car insulation materials when they are exposed to a fire environment. The initial value of these conductances is quite low and is based on the allowable conductance in the AAR tank car specifications. It has been found that these materials lose their effectiveness as they become heated and that the period of the breakdown of the insulation typically can be assumed to take place over an approximate 30 minute period. Therefore, when calculating the effects on a 105 tank car it is reasonable to give the final value of the conductance as the high temperature value of the thermal insulation and the initial value as called for in the AAR specification. This value is $0.30~(BTU/hr-ft^2-{}^oF)$ and is based on the assumptions described in the AAR Tank Car Specifications (Ref. 3).

3.4 CALCULATE TEMPERATURE OF TANK SURFACE OUTSIDE OF LIQUID REGION

The next step is the calculation of the temperature of the outer surface of the tank in the liquid region. This calculation is carried out in subroutine SURFACET. It is assumed that a quasi-steady temperature distribution exists through the tank wall thermal insulation system and that the inside wall temperature maintains the value which has been established in the last calculational cycle. The heat input to the outside surface is assumed to be the radiant energy from the flame at the flame temperature. The radiation surface configuration factor is assumed to be unity and the surface emissivity factor is assumed to be 0.8. A heat balance then exists between the heat radiated to the outside surface of the shell, the heat that is being conducted through the insulation, and the heat being radiated away back to the fire from the outside surface of the tank. The solution for the temperature of the outside wall is carried out in an iterative manner to find the solution for the heat balance under these conditions.

3.5 ESTABLISH GEOMETRY OF LIQUID LEVELS

The calculation requires the establishment of the angle (THET), as defined in Figure 1 associated with the liquid level in the tank. The angle THET is a function of the fraction of tank volume occupied by the liquid, which is defined as FRAC. The determination of THET requires an iterative solution of the equation:

$$FRAC = \frac{1}{\pi} \left[\frac{\pi}{2} + THET + \sin \left(THET \right) \cos \left(THET \right) \right]$$
 (2)

The area of the surface of the liquid (AREALQ) is also calculated at this point.

3.6 RADIATION SURFACE CONFIGURATION FACTOR

Next the radiation surface configuration factor for the transfer of radiant energy from the tank wall over the vapor space to the surface of the liquid is established. The view factor is estimated from the relationship:

$$A_1 F_{12} = A_2 F_{21} \tag{3}$$

where F_{ij} is the radiation surface configuration factor for a gray body. F_{12} can be calculated taking into account the emissivities of the two surfaces by using the following equation:

$$F_{12} = \frac{1}{\frac{1}{f_{12}} + (\frac{1}{\epsilon_1} - 1) + \frac{A_1}{A_2} (\frac{1}{\epsilon_2} - 1)}$$
(4)

where f_{12} is the radiation surface configuration for a black body, and ϵ_1 and ϵ_2 are the emissivities of surfaces 1 and 2.

In using this equation it is assumed that $f_{1iq,tk} = 1$ since the area of the liquid surface sees only the tank wall.

The radiation surface configuration for the liquid to the tank is designated FLQT, and the coefficient for the tank to the liquid is designated FTLQ. FTLQ is calculated from FLQT using the recircular relationship.

These equations are used with the assumption that the conditions are uniform on the inside surface of the tank. This is not strictly correct because the temperature of the inner wall surface would be cooler for regions closer to the surface of the liquid. The temperature would depend on the length of time the wall has been exposed to the vapor and also the amount of radiant energy that has been received from the hotter part of the wall. Uniform conditions will be closely approached when the liquid level

is near the top of the tank, because a slight drop in the liquid level will expose a large area of the inner surface of the tank. Uniform conditions will also be approached when the level of the liquid is low. To make an adjustment for the condition when the angle THET of the liquid is between approximately 60° and 120°, where the temperature of the tank wall immediately above the liquid surface would not be as high as at the top of the tank, the black body radiation surface configuration factor is assumed to be only 0.75.

3.7 CALCULATION OF TEMPERATURE OF OUTER WALL SURFACE IN VAPOR REGION

The calculation of the temperature of the outer wall surface in the vapor region is also made using subroutine SURFACET. The assumption is made that even when the tank is shell full, there is a small volume of vapor between the top of the shell and the surface of the liquid so that the tank wall is not cooled by conduction with the liquid product. This allows for the fact that the tank might not be completely level allowing a small region of vapor at the high end of the tank.

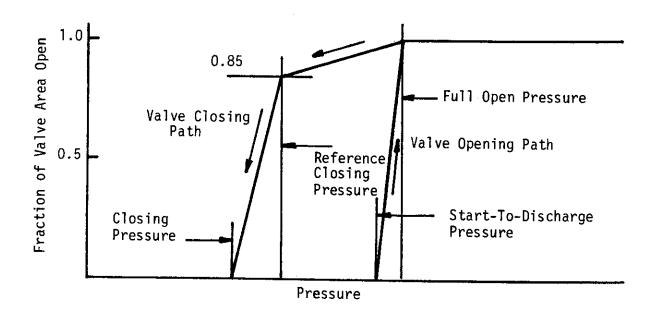
3.8 CALCULATE TEMPERATURE OF INNER WALL SURFACE IN VAPOR REGION

The next step in the procedure is to calculate the temperature of the tank wall in the vapor region. This is done taking the value for the outer tank wall surface previously computed and establishing a heat balance on the inside surface between the heat that is being conducted through the tank wall and insulation system and the heat that is being lost by convection and radiation to the inside of the tank. For radiant heat transfer, a surface emissivity of 0.8 is assumed. The calculation considers that there is a small amount of convected heat loss (0.18 BTU/hr-ft²- $^{\circ}$ F) when the car is more than 0.4 filled, the car is in the upright position and venting vapor through the safety relief valve. A larger convection coefficient is assumed if the flow rate through the valve is greater than 1,500 lbs/min. This characteristic has been deduced from the full scale fire tests.

3.9 DETERMINE THE DEGREE OF VALVE OPENING

The next step in the calculation is to determine the amount to which the safety relief valve has opened. Three pressure levels are defined

with reference to the start-to-discharge pressure. These are the fully opened pressure, which is assumed to be 103% of the start-to-discharge pressure, the valve closing pressure, which is assumed to be 82% of the start-to-discharge pressure, and a reference pressure on the closing stroke of the valve which is 85% of the start-to-discharge pressure. The degree to which the valve is opened depends on whether the pressure is increasing or decreasing. The functional relationship between the degree of valve openings and the pressure is shown in the following figure:



3.10 DETERMINE CONDITIONS IN THE TANK

The next step in the calculation is to determine which of the four conditions exist within the tank. These have previously been defined as:

- Liquid and vapor within the tank venting vapor,
- Liquid and vapor within the tank venting liquid,
- Shell full of liquid product,
- Containing only product in the vapor phase

The calculational procedure is divided at this point so that each of these cases are considered separately. The general procedure is the same in each case, the major difference being associated with the determination of the mass flow rate of the product through the valve.

3.11 LIQUID AND VAPOR WITHIN TANK VENTING VAPOR

3.11.1 Calculate Heat Transfer to Liquid Product

The heat transfer to the liquid product is determined by calculating the heat conducted through the portion of the tank shell which is in contact with the liquid and by estimating the radiant heat transfer to the surface of the liquid from the tank wall above the liquid. In the calculation of the heat conducted through the wetted area of the shell, it is assumed that the heat transfer in the circumferential direction is negligible, a quasi-steady situation exists (transient effects are neglected), and that the heat capacity of the jacket and insulation materials can be neglected.

The radiant exchange of energy between the tank shell above the liquid and the liquid surface has been discussed in Section 3.6.

3.11.2 Calculate Mass Flow Rate Through Safety Relief Valve

The mass flow rate through the safety relief valve is computed for vapor flow by using the standard valve flow equation:

$$\dot{W} = C_{d}Ap \sqrt{\frac{g}{ZRT}} \gamma \left(\frac{2}{\gamma+1}\right)^{\left(\frac{\gamma+1}{\gamma-1}\right)}$$
 (5)

where W is flow rate (lbs/sec)

A is minimum cross sectional area of valve (ft²)

 $\mathbf{C}_{\mathbf{d}}$ is the valve discharge coefficient

p is upstream gas pressure (lbs/ft²)

T is upstream gas temperature (°R)

g is the gravitational constant (ft/sec²)

Z is the gas compressibility factor

R is the gas constant $(ft/^{\circ}R)$

 γ is the ratio of specific heats

For air, the above equation reduces to:

$$\dot{W}_{air} = C_d Ap \sqrt{\frac{g}{ZRT} (.4689)}$$
 (6)

For both ethylene oxide and propane the same equation is obtained for W:

$$\dot{W} = C_d Ap \sqrt{\frac{g}{ZRT} (.4027)}$$
 (7)

Noting that the rated capacity of the valve, SCFM, can be related to \dot{W}_{air} as follows:

$$SCFM = 60 (\dot{W}_{air})/\rho_{sc}$$
 (8)

where $\rho_{\mbox{\scriptsize SC}}$ is the density of air at standard conditions

Dividing Equation 7 by Equation 6 and substituting Equation 8 results in the following equation:

$$\dot{W} = 0.063 \, (p/p_r) \, (SCFM) / \sqrt{TZ}$$
 (9)

where W is mass flow rate (lbs/min),

Pr is the valve flow rating pressure (psia), and

P is the flowing pressure of the gas (psia)

A value of 0.7 is assumed for Z in this equation for the propane, propylene and ethylene oxide cases. The following values of Z are assumed for the other commodities: butadiene, 0.77; vinyl chloride, 0.72; monomethylamine, 0.93; and propylene oxide, 0.99.

The constant 0.063 in Equation 9 is entered separately at the beginning of the analysis. The value 0.063 is satisfactory for propane, ethylene oxide and propylene. For other commodities the following values are used: butadiene, 0.0692; vinyl chloride, 0.0761; monomethylamine, 0.0535; and propylene oxide, 0.0692.

Where a nitrogen pad pressure is present it is assumed that the mass flow of each component (product and nitrogen) is proportional to the partial pressure of each gas. Because the total mass of nitrogen in the car is small in relationship to the product, the effect of the nitrogen on the mass flow rate becomes negligible after a short period of time.

3.11.3 Calculate Temperature Rise of Liquid

The temperature rise of the liquid product is calculated by determining the net heat flow into the liquid product which is the difference of the total heat flow to the product and the heat lost by the vaporization of the product.

3.11.4 Calculate Change in Mass of Product

The next step in the calculation is to determine the change in the mass of the product within the tank and its apportionment between the liquid and vapor state. The change in mass of the nitrogen pad is also determined.

3.12 LIQUID AND VAPOR WITHIN TANK VENTING LIQUID

3.12.1 Calculate Heat Input to Liquid Product

The heat transferred to the liquid product within the time increment is determined by calculating the heat conducted through the wetted area of the tank and the heat radiated to the surface of the liquid from the inner tank shell surface over the vapor space as described in Section 3.6.

3.12.2 Calculate Liquid Flow Rate through Safety Relief Valve

The liquid flow rate through the safety relief valve is calculated in subroutine VCAP. Homogeneous, isentropic, two-phase flow (liquid and vapor) and a liquid discharge coefficient of 0.7 are assumed.

3.12.3 Calculate Change in Temperature

The change in temperature of the liquid product over the time increment is calculated by considering the heat added to the liquid product, the amount of liquid that is vaporized within the time increment and the work done in expelling the fluid from the tank.

3.12.4 Determine New Properties

The properties of the product at the new temperature are determined by calling subroutine PROPERTIES.

3.12.5 Recalculate Remaining Mass of Product Nitrogen Pad Pressure

The remaining mass of the product within the tank, both liquid and vapor components, are recalculated under the new temperature and pressure conditions.

For the cases where nitrogen gas padding is used the following assumptions are made: First, it is assumed that the nitrogen in the vapor phase is in equilibrium with the nitrogen dissolved in the liquid product. Because of the small outage volume in which the nitrogen gas is contained, there may be more nitrogen dissolved in the product than present in the vapor phase. It is also assumed that there is no exchange between the nitrogen dissolved in the fluid and the nitrogen in the vapor phase during the course of the exposure to the fire environment. If equilibrium were to be maintained between the nitrogen in the vapor phase and the nitrogen dissolved in the product there would first be an increase in the amount of the dissolved nitrogen and a corresponding decrease in the amount of nitrogen vapor. This would be caused by the increase in pressure when the outage volume is diminished by the expansion of the product as it is heated. This would mean the pressure of the nitrogen padding gas would be less than that predicted by the assumption of no exchange between the vapor in the dissolved state. After the safety valve opens and the product starts to flow from the car the outage volume would increase and the corresponding decrease in the vapor pressure of the nitrogen would cause more nitrogen to be liberated from the fluid thus tending to maintain the partial pressure of the nitrogen above that predicted by the assumption of no exchange between the vapor and the liquid dissolved states. Thus, the effects of assuming that equilibrium were maintained would be to delay the time at which the safety valve is first opened, but increase the pressure after the product starts to flow through the valve. These effects would counteract one another. In any event, when the liquid level gets to approximately 10-20% outage the effect of the nitrogen padding gas becomes insignificant on the prediction of flow through the valve.

The major reason that the exchange of nitrogen between the vapor state and the dissolved state is not included in the analysis is that one would expect that equilibrium conditions would not be attained during the course of the phenomena predicted by the fire environment. There would not be sufficient time for the effect of the partial pressure of the nitrogen gas in the vapor state to be communicated to all portions of the liquid within the tank and for the gas to be absorbed in the early phases of the predicted effects. Similarly, the effect of the decrease in the partial pressure of the nitrogen gas once the valve is opened, would not be

immediately communicated to all portions of the liquid in the tank so a non-equilibrium situation would exist. Consequently the assumption has been made that there is no exchange of the nitrogen padding gas from the vapor phase to the dissolved state and this assumption is believed to have minimal significance in the predicted events associated with the flow of the product from the tank car.

3.13 SHELL FULL CONDITIONS

3.13.1 Calculate Heat Transferred to Liquid Product

The total heat transmitted to the liquid product of the tank in the time increment is calculated with the assumption that heat is transferred through the entire surface area of the surface of the tank.

3.13.2 Calculate Change in Temperature

The change in temperature of the liquid product is established from the heat transferred into the tank.

3.13.3 <u>Determine New Properties</u>

The new properties of the product at the higher temperature are determined by calling subroutine ${\sf PROPERTIES}$.

3.13.4 Calculate Required Volume of Flow

The volume that must be discharged through the safety relief valve in the time increment is determined by calculating the change in the specific volume of the product over the time increment.

3.13.5 <u>Calculate Pressure Required to Generate Sufficient Flow</u>

The pressure that must be developed within the tank so that the required volume will be discharged through the valve is calculated next. This pressure is calculated in two different ways. First, it is assumed that the critical pressure for the flow through the valve will be the saturated pressure and the excess fluid pressure which will be required to generate sufficient flow is determined. The following formula is utilized:

$$\dot{W} = C_d A_\rho \sqrt{\frac{2g}{\rho} (p_c - p_s)}$$
 (10)

where $\mathbf{C}_{\mathbf{d}}$ is the liquid discharge coefficient of the valve

A is the cross sectional area of the valve (ft²)

- ρ is the density of the liquid (lbs/ft³)
- p_c is the fluid pressure (lbs/ft²)
- ps is the saturated vapor pressure at the temperature of the fluid (lbs/ft2)

The second estimate of the pressure is made by assuming that saturated conditions exist at the entry to the valve and the saturated vapor pressure that would give rise to sufficient flow is determined. Subroutine VCAP could be used for this calculation, but in order to reduce calculational time a linear expression for this pressure as a function of the required flow rate is used. Use of subroutine VCAP as a separate program has shown that the saturated vapor liquid flow rate through the valve can be closely represented by a linear function of the saturated vapor pressure over a wide range of pressures. The minimum of these two pressures is then used as the best estimate of the pressure required to develop sufficient flow through the valve.

If sufficient flow can be generated with a pressure at saturated conditions (the second pressure calculated) sufficient flow may be passed through the valve so that the tank will not be shell full the next time through the calculational cycle. If this condition is not realized, the mass of the fluid remaining in the tank is set so that a shell full condition will be recognized the next time through the calculational cycle.

Two adjustments are made in the calculated pressures to provide a better representation of the behavior of the valve when the vapor is less than the valve start-to-discharge pressure. First, if the calculated pressure is less than the start-to-discharge pressure of the valve and the valve is closed, the pressure is reset to the start-to-discharge pressure and the valve is reset to the open position. Second, if the pressure is less than the closing pressure of the valve and the valve is open, the valve is reset to be closed. This gives a more accurate representation of the valve cycling open and closed.

3.13.6 Calculate Mass of Product Remaining in Tank

The remaining mass in the tank is calculated. The mass flow from the tank will be the larger of the mass flow required to accommodate the increase in specific volume of the product and the mass flow calculated from isentropic flow through the valve starting from the saturated vapor IIT RESEARCH INSTITUTE

pressure of the fluid at its current temperature.

3.14 VAPOR PHASE ONLY WITHIN TANK

This condition occurs after the critical temperature is reached (a condition obtained only for a few cases with propane and propylene while there is still liquid product within the tank) or after the vaporization of all of the liquid within the tank. The temperature of the remaining product within the tank will increase at a fairly rapid rate during this phase because of the relatively low mass of product and the fact that there is no heat absorbed by the vaporization of the liquid. During this phase the pressure within the tank will begin to increase due to the increased pressure of the product, but the increased pressure will be relieved by flow through the safety valve. The pressure within the tank will be maintained near the valve closing pressure.

3.14.1 Calculate Heat Transfer to Vapor Product

The first step in the calculation of this case is to calculate the heat transfer to the vapor product. This is estimated by assuming that there is a convection coefficient of 1.0 BTU/hr-ft 2 - 0 F between the vapor and the inner wall of the tank.

3.14.2 Calculate Change in Pressure

The change in pressure of the vapor within the tank can be calculated using the ideal gas law and considering the change in temperature from the beginning of the time increment.

3.14.3 Calculate Mass Flow Out

The mass out through the safety valve is calculated using the equation previously presented for vapor flow (Equation 5). The compressibility factor, Z, of 0.7 is assumed for all commodities except for propane where Z is represented as a function of the total pressure within the tank, the temperature and specific volume.

3.14.4 <u>Calculate Change in Tank Temperature</u>

The change in the temperature of the product within the tank over the time increment is calculated on the basis of the heat transferred to the product and the work done in expelling the gas from the tank.

3.15 CALCULATE BURST STRENGTH OF TANK

The brust strength of the tank is assumed to be a function of temperature. The temperature used in this calculation is that of the tank shell over the vapor regions.

3.16 DISPLAY DATA

The program provides two different types of format for displaying the results of the calculation. The first format prints out data at selected time intervals during the course of the analysis. The interval is selectable as a multiple of the time increments used during the analysis.

The second format gives a plot of the temperature of the tank wall above the vapor space, the pressure within the tank, and the liquid fraction remaining in the tank as a function of time.

3.17 COMPARE BURST STRENGTH AND INTERNAL PRESSURE

The final step in the calculation is to compare the internal pressure in the tank with the burst strength. If the internal pressure exceeds the burst strength it is assumed that the tank will fail and the calculation is stopped. A comparison is also made to determine if the time limit has been exceeded and if this has occurred the calculation is also halted. Otherwise the time is incremented and the calculation returns to the point where the effective conductance of the thermal shield is determined (Section 3.3).

4. COMPUTER PROGRAM LISTINGS

Listings of the basic computer program and the subroutines are presented in this section. The basic program is designated FEAVIT for Fire Effects Analysis of Vented Insulated Tanks. The principal parameters used in the basic program are indicated as follows:

KPRD	Product type
TILT	Angle of valve overturn from vertical (deg)
PREF	Vapor pressure of product (psia)
PTOT	Total pressure within tank (psia)
PPAD	Partial pressure of nitrogen pad (psi)
PATD	Start-to-discharge pressure of safety relief valve (psia)
HTIN	Heat transmitted to product in time increment (BTU)
FRAC	Fraction of tank volume filled with liquid
FMSS	Mass of product in tank (lbs)
FMAT	Fraction of original mass remaining in tank
WOUT	Mass of product vented through safety relief valve in time increment (lbs)
WLIQ	Weight of liquid product in tank (lbs)
WVAP	Weight of product in vapor plane (lbs)
TFLA	Temperature of flame (°R/1000)
TTNK	Temperature of tank wall adjacent to liquid (°R/1000)
TTNV	Temperature of tank wall adjacent to vapor space (°R/1000)
CNDD	Conductance of thermal insulation system (BTU/hr-ft²-ºF)
DELT	Time increment (min)

Other parameters are defined in the initial section of the program listing and the descriptions of the subroutines.

```
PROGRAM FEAVIT (FIRE EFFECTS ANALYSIS OF VENTED INSULATED
C
           TANKS) FOR ANALYSIS OF CARS CONTAINING PROPANE, ETHYLENE OXIDE,
C
          PROPYLENE, 1,3-BUTADIENE, VINYL CHLORIDE, MONOMETHYLAMINE, OR PROPYLENE OXIDE IN THE POOL FIRE ENVIRONMENT VENTING LIQUID OR VAPOR....TILT ANGLE
C
ċ
C
           OF THE SAFETY RELIEF VALVE IS SPECIFIED (\emptyset-18\emptyset DEGREES).
           THE PROGRAM USES SUBROUTINES SURFACET, PROPERTIES,
C
           VCAP, TSHIELD, AND PLT3.
Ċ
           ACCEPT "DISPLAY TYPE, LPT-12.....CONSOLE-10" ,KW
           IF (KW.EQ.10)GO TO 15
           OPEN 12, "@LPT", ATT="OP"
ACCEPT "PLOT-2 PRINT TERM OR LPT-1" , KPLT
15
           ACCEPT "PROP-1 EO-2 PROPYL-3 BUTA-4 VC-5 MONO-6 POX-7" ,KPRD ACCEPT "ANGLE OF TILT (DEG)" ,TILT
           TRLT=1.5708-TILT/180.0*3.1416
           ACCEPT "TANK DIAMETER (FT)" , DHTK
ACCEPT "TANK WALL THICKNESS (IN.)"
           ACCEPT "TANK WALL THICKNESS(IN.)" , DHTW ACCEPT "NOMINAL CAPACITY (GALLS)" , SIZE
           ACCEPT MOMITAL CATACITY (GALLS), JIAB
ACCEPT "INITIAL FRACTION FILLED", FRAT
ACCEPT "SAFETY VALVE FLOW RATING PRESSURE (PSIA)", PASD
ACCEPT "SAFETY VALVE START TO DISCHARGE PRESS (PSIA)", PATD
           ACCEPT "NET ABSORPTIVITY" , EABS
           ACCEPT "NET EMISSIVITY" , ERAD
ACCEPT "TANK BURSTING STRENGTH (PSI)" , PBRT
           ACCEPT "CAR CONDUCTANCE (BTU/HR SQFT DEG F)"
                                                                           , CNDD
            ACCEPT "SAFETY VALVE RATED FLOW CAPACITY (SCFM, AIR)", SCFM
           ACCEPT "TYPE 1 FOR CONSTANT CONDUCT. OR 2 FOR VAR. CND.", KCND
            IF(KCND.EQ.2)GO TO 14
            ACCEPT "INITIAL CAR CONDUCTANCE (BTU/HR SQFT DEG F)" , CNDI
            GO TO 17
           ACCEPT "THICKNESS OF INSULATION(INS.)", THIC ACCEPT "WISH TO CONSID. INIT. CNDT. YES-1 NO-2", KINDX
 14
            IF(KINDX.EQ.2)GO TO 17
           ACCEPT "INITIAL CAR CONDUCTANCE (BTU/HR SQFT DEG F)" , CNDI ACCEPT "FLAME TEMPERATURE (DEG F)" , TEMF
 17
            ACCEPT "PRESSURE(PSI) OF NITROGEN PAD" , PPAD ACCEPT "AREA EXPONENT" , EXPP
            ACCEPT "INITIAL TEMPERATURE (DEG F)" , TEMC
            ACCEPT "TIME INCREMENT (MIN), (MUST BE EVEN TENTH)" , DELT
            ACCEPT "NUMBER OF TIME STEPS BETWEEN DISPLAY" , INTV ACCEPT "GAS COMPRESSIBILITY FACTOR, 2" , ZPRO
            ACCEPT "VALVE GAS FLOW CONSTANT" , VLCON
            INITIALIZATION OF PARAMETERS AT BEGINNING OF EACH ANALYSIS
 С
            TEMP=TEMC
            PREF=100.
            SPEC=Ø.6
            SPLQ=Ø.Ø3
            HFLV=100.0
            VVAP=1.Ø
            DVDT=1.Ø
            DLDT=1.Ø
            TWAL = \emptyset.5
            TWAV = Ø.5
 C
            CALL PROPERTIES (KPRD, TEMP, PREF, SPEC, SPLO, HFLV, VVAP, DVDT, DLDT)
 C
```

SZGL=SIZE/7.48

```
WGHT=SZGL*(FRAT/SPLQ)+(1.8-FRAT)*SZGL/VVAP
        LENG=SIZE/(5.875*DHTK*DHTK)
        AREA=Ø.535*SIZE/DHTK+1.57Ø8*DHTK*DHTK
        WTWL=DHTW*Ø.283*144.Ø
         WGNT=(1.Ø-FRAT)*SZGL*2.61*PPAD/(46Ø.+TEMC)
        WNIT=WGNT
С
         FRAC=FRAT
         TIME = Ø.Ø
         WOUT=Ø.Ø
         WLET=1.Ø
         WPRT=Ø.Ø
         ATEM=0.0
         FMSS=WGHT
         PTOT=PREF
         PNIT=PPAD
         KTCT=1
         KCNT=Ø
         KIDN=Ø
         WLIQ=SZGL*FRAT/SPLQ
         WVAP=(1.Ø-FRAT)*SZGL/VVAP
         WOLST-Ø.Ø
         PICR=Ø.Ø
         TCLST=Ø.Ø
         TFLA=(TEMF+460.0)/1000.0
         TTNK = (TEMC+460.0)/1000.0
         TTMC = TTNK
         TTNV=(TEMC+460.0)/1000.0
         TTMV = TTNV
         TWAL = TFLA - \emptyset . \emptyset 5 \emptyset
         TWAV = TWAL
         PLST=Ø.Ø
         POPN=1.03*(PATD-14.7)+14.7
         PRTN=Ø.88*(PATD-14.7)+14.7
         PCLS=0.82*(PATD-14.7)+14.7
C
         COMPUTE NOMINAL VALVE AREA; ASSUME DISCHARGE COEF: CVAD
С
С
         CVAD=0.9
         AVLV=SCFM/(CVAD*PASD*2638.)
C
         BEGINNING OF CALCULATION: DETERMINE COND. OF THERMAL SHIELD
C
C
         IF(KCND.EQ.2)GO TO 22
21
         CVP=CNDD
         CLQ=CNDD
         GO TO 23
         CALL TSHIELD (TWAL, TTNK, CLQ, THIC)
CALL TSHIELD (TWAV, TTNV, CVP, THIC)
22
 23
          IF(KINDX.EQ.2.OR.TIME.GT.30.0)GO TO 26
         CNDLQ=CNDI+(CLQ-CNDI)*(TIME/3Ø.)
         CNDVP=CNDI+(CVP-CNDI)*(TIME/38.)
         GO TO 28
         CNDVP=CVP
 26
         CNDLQ=CLQ
 23
         CONTINUE
         DETERMINE OUTER WALL TEMPERATURE ADJACENT TO THE LIQUID.
C
С
          CALL SURFACET (TWAL, TINK, EABS, ERAD, CNDLO, TFLA)
```

```
C
        DETERMINE GEOMETRY OF LIQUID LEVEL.
        IF(FRAC.GT.Ø.ØØØ1)GO TO 521
        THET=-1.57Ø8
        GO TO 55Ø
        THOU=Ø.1Ø
521
         THEM=1.57Ø8
        FTST=(1.5708+THEM+COS(THEM)*SIN(THEM))/3.1416
522
         IF(ABS(FTST-FRAC).LT.Ø.0001)GO TO 545
         IF(FTST.LT.FRAC)GO TO 531
         THEM=THEM-THOU
         IF(THEM.LE.(-1.5708))GO TO 531
         GO TO 522
         THEM=THEM+THOU
531
         THOU=THOU/5.Ø
         THEM=THEM-THOU
         GO TO 522
         THET=THEM
545
· 55Ø
         CONTINUE
         AREALQ=DHTK*COS(THET)*LENG+1.Ø
         ATANK=AREA*(1.57Ø8-THET)/3.1416+1.Ø
C
         DETERMINE RADIATION SURFACE CONFIGURATION FACTOR.
С
         FLQT=1.0/(1.25+0.25*(AREALQ/ATANK))
         FAFTLQ=FLQT*AREALQ/ATANK
         FLOT=1.0/(1.58+0.33*(AREALQ/ATANK))
         FBFTLQ=1.33*FLQT*AREALQ/ATANK
         FCFTLQ=(-THET-Ø.53)*FBFTLQ/Ø.Ø4+(Ø.57+THET)*FAFTLQ/Ø.Ø4
         FTLQ=FAFTLQ
         IF(THET.LT.Ø.55.AND.THET.GE.(-Ø.53))FTLQ=FBFTLQ
         IF(THET.LT.(-0.53).AND.THET.GT.(-0.57))FTLQ=FCFTLQ
C
         DETERMINE OUTER SURFACE TEMPERATURE ADJACENT TO VAPOR SPACE.
C
С
         CALL SURFACET (TWAV, TINV, EABS, ERAD, CNDVP, TFLA)
C
         DETERMINE INNER WALL TEMPERATURE NEXT TO VAPOR SPACE.
C
C
151
         HCNV = \emptyset . \emptyset
         IF(KIDN.NE.1)GO TO 152
         IF(WPRT.GT.1500.0)GO TO 154
         IF(FRAC.GT.Ø.9)HCNV=Ø.Ø5
         IF (FRAC.GT.Ø.4.AND.FRAC.LE.Ø.9) HCNV=Ø.Ø5
         GO TO 152
         IF(FRAC.GT.\emptyset.9)HCNV=6.\emptyset
 154
         IF (FRAC.GT.Ø.4.AND.FRAC.LE.Ø.9) HCNV=1.5
         DELV=Ø.48*FTLQ*(TTNV**4-TTNK**4)
 152
         DELV=DELV+HCNV*(TTNV-TTNK)
         DELV=(TWAV-TINV)*(CNDVP/3.6)-DELV
         DELV=(DELV/WTWL)*(60.0/125.0)*DELT
         TTNV=TTNV+DELV
         TTMV=TTNV
         DETERMINE THE DEGREE OF VALVE OPENING.
 С
 С
 120
         CONTINUE
         IF(PTOT.LT.POPN)GO TO 302
         TCFM=SCFM
```

```
GO TO 350
302
         IF(PTOT.GT.PLST.AND.TCLST.EQ.Ø.Ø)GO TO 32Ø
         IF(PTOT.LE.PRTN)GO TO 3Ø4
         TCFM=SCFM*(Ø.85+.15*(PTOT-PRTN)/(POPN-PRTN))
         GO TO 35Ø
3Ø4
         IF(PTOT.LE.PCLS)GO TO 3Ø6
         TCFM=SCFM*Ø.85*(PTOT-PCLS)/(PRTN-PCLS)
         GO TO 35Ø
3Ø6
         TCFM=Ø.Ø
         GO TO 35Ø
         IF(PTOT.LE.PATD)GO TO 322
320
         TCFM=SCFM*(PTOT-PATD)/(POPN-PATD)
         GO TO 35Ø
322
         TCFM=Ø.Ø
35Ø
         CONTINUE
         TCLST=TCFM
         CDLQ=Ø.7Ø
         ATEM=AVLV*CDLQ*TCFM/SCFM
C
С
         SORT OUT CONDITIONS IN THE TANK.
         IF (TTNK.GT.Ø.6659.AND.KPRD.EQ.1)GO TO 438 :
         IF(TTNK.GT.Ø.83Ø.AND.KPRD.EQ.2)GO TO 43Ø
         IF(TTNK.GT.Ø.6567.AND.KPRD.EQ.3)GO TO 430
         IF(FRAC.LT.Ø.ØØØ5)GO TO 43Ø
C
         IF((FMSS*SPLQ).GT.SZGL)GO TO 410
C
C
         BOTH LIQUID AND VAPOR WITHIN TANK. . . .
С
С
         DETERMINE HEAT IN THROUGH WETTED AREA AND RADIATED TO SURFACE.
         IF(THET.LT.(-1.\emptyset))THEA=\emptyset.1\emptyset
         HTINR=Ø.48*FLQT*((TTMV)**4-(TTNK)**4)*(AREALQ**EXPP)*DELT*6Ø.Ø
         STDA=AREA*(1.57Ø8+THEA+THET)/3.1416
         HTIN=(TWAL-TTNK)*CNDLQ*(STDA**EXPP)*DELT*6Ø.Ø/3.6+HTINR
         THRML=SPEC*WLIQ+Ø.125*WTWL*STDA
         TLST=TTNK
         SLST=VVAP
         PLST=PTOT
         IF (THET.LE.TRLT)GO TO 42Ø
C
C
        LIQUID AND VAPOR IN TANK, VENTING LIQUID. . . . .
C
        CALCULATE MASS FLOW OUT THROUGH VALVE.
C
        CALL VCAP(TINK, PNIT, WOUT, ATEM, KPRD, PREF, SPEC, SPLQ.
        HFLV, VVAP, DVDT, DSDT, DELT)
QWRK=WOUT*SPLQ*PTOT*144./778.
C
        DETERMINE TEMPERATURE INCREASE.
C
C
        AA=THRML*(DVDT-DLDT)
        BB=THRML*(VVAP-SPLQ)-(DVDT-DLDT)*(HTIN-QWRK)
        -(WLIQ*DLDT+WVAP*DVDT)*HFLV
        CC=-(HTIN-QWRK)*(VVAP-SPLQ)+WOUT*SPLQ*HFLV
        TELT=(-BB+SQRT(BB*BB-4.0*AA*CC))/(2.0*AA)
        TTNK=TTNK+TELT/1000.0
С
```

```
C
         CALCULATE MASS REMAINING IN TANK.
         FMSS=FMSS-WOUT
         FMAT=FMSS/WGHT
         IF(KIDN.EQ.2)PICR=14.7
C
         TEMP = (TTNK-Ø.46) * 1000.0
         CALL PROPERTIES (KPRD, TEMP, PREF, SPEC, SPLQ, HFLV, VVAP, DVDT, DLDT)
C
         PTOT=PREF
         WLIQ=(FMSS*VVAP-SZGL)/(VVAP-SPLQ)
         WVAP=FMSS-WLIQ
         VLIQ=WLIQ*SPLQ
         FRAC=VLIQ/SZGL
         IF(VLIQ.GE.SZGL)FRAC=1.Ø
         IT(VLIQ.LE.Ø.Ø)FRAC=Ø.Ø
C
         DETERMINE PRESSURE OF NITROGEN PAD (IF PRESENT).
         IF(KPRD.EQ.1)GO TO 391
         IF(KPRD.GE.3.AND.KPRD.LE.6)GC TO 391
         STEST=SZGL-WLIQ*SPLQ
         IF(STEST.LE.Ø.Ø)STEST=Ø.ØØØ5
         PNIT=PPAD*TTNK/TTMC*(1.Ø-FRAT)*SZGL/STEST
         PTOT=PREF+PNIT
391
         KIDN=2
         CONTINUE
C
         GO TO 153
С
         SHELL FULL CASE. . . . . . .
C
С
C
         CALCULATE CHANGE IN TEMPERATURE.
С
410
         HTIN=(TWAL-TTNK)*CNDLQ*(AREA**EXPP)*DELT*60.0/3.6
         TELT=HTIN/(SPEC*WLIQ*1000.0+125.0*WTWL*AREA)
         TLST=TTNK
         SLST=VVAP
         PLST=PTOT
         TTNK=TTNK+TELT
C
         TEMP = (TTNK - \emptyset.46) * 1000.0
         CALL PROPERTIES(KPRD, TEMP, PREF, SPEC, SPLQ, HFLV, VVAP, DVDT, DLDT)
C
         VLIQ=FMSS*SPLQ
         WVAP=Ø.Ø
         REQL=1000.0*FMSS*DLDT*TELT/DELT
C
         CDLQ=Ø.7
         PTOT=PREF
         IF(KPRD.EQ.1)PISN=REQL/(CDLQ*AVLV*SPLQ*241.Ø)-25Ø.Ø
         IF(KPRD.EQ.2)PISN=REQL/(CDLQ*AVLV*SPLQ*49Ø.Ø)-18.6
         IF(KPRD.EQ.3)PISN=REQL/(CDLQ*AVLV*SPLQ*242.4)-280.0
         IF(KPRD.EQ.4)PISN=REQL/(CDLQ*AVLV*SPLQ*31Ø.5)-135.8
         IF(KPRD.EQ.5)PISN=REQL/(CDLQ*AVLV*SPLQ*507.1)-67.6
         IF(KPRD.EQ.6)PISN=REQL/(CDLQ*AVLV*SPLQ*309.4)-120.2
         IF(KPRD.EQ.7)PISN=REQL/(CDLQ*AVLV*SPLQ*3Ø2.9)-111.Ø
         PCOM=PREF+((REQL/(720.0*CDLQ*AVLV))**2)/(64.4*SPLQ)
         PICR=AMIN1(PISN, PCOM)
         IF(PISN.LT.PREF.AND.PTOT.GT.PCLS)GO TO 87
```

```
IF(PICR.GT.PREF)PTOT=PICR
        IF (PTOT.LT.PATD.AND.TCLST.LT.Ø.ØØ1)GO TO 85
        IF (PICR.LT.PCLS.AND.TCLST.GT.Ø.Ø)PTOT=PREF
        GO TO 84
85
        PTOT=PATD
        GO TO 84
С
87
        PICR=14.7
        IF (KPRD.EQ.1)WOUT=ATEM*60.*DELT*(1004.+4.023*PTOT)
        IF(KPRD.EQ.2)WOUT=ATEM*60.0*DELT*(152.0+8.16*PTOT)
        IF(KPRD.EQ.3)WOUT=ATEM*60.*DELT*(1131.+4.0398*PTOT)
        IF(KPRD.EQ.4)WOUT=ATEM*60.*DELT*(673.0+5.1753*PTOT)
        IF(KPRD.EQ.5)WOUT=ATEM*60.0*DELT*(571.1+8.4515*PTOT)
        IF (KPRD.EQ.6)WOUT=ATEM*6Ø.*DELT*(619.6+5.1563*PTOT)
        IF (KPRD.EQ.7) WOUT=ATEM*60.*DELT*(560.4+5.0475*PTOT)
        WROUT=DELT*REQL/SPLQ
        IF(WROUT.GT.WOUT)GO TO 86
С
        FMSS=FMSS-WOUT
        FMAT=FMSS/WGHT
        FRAC=VLIQ/SZGL
        KIDN=32
        IF(VLIQ.GE.SZGL)FRAC=1.Ø
        GO TO 88
86
        PTOT=PREF
        WOUT=WROUT
84
        FMSS=SZGL/SPLQ+1.Ø
        FRAC=1.Ø
        WOUT=DELT*REQL/SPLQ
        KIDN=31
        IF (PCOM.GT.PISN) KIDN=33
        TCLST=1.Ø
        FMAT=FMSS/WGHT
С
88
        PNIT=Ø.Ø
        WLIQ=FMSS
        PLST=PTOT
        SLST=SZGL/FMSS
        GO TO 153
С
Č
        LIQUID AND VAPOR IN CAR, BUT VENTING VAPOR. . . . . .
C
c
        CALCULATE MASS FLOW RATE THROUGH VALVE.
С
420
        WCHK=WOUT
        WOUT=((PTOT-PNIT)/PASD)*TCFM*VLCON/SQRT(TTNK*ZPRO)*DELT
        IF(FRAC.GT.Ø.Ø25)GO TO 424
        ALFA=Ø.1Ø
        WOUT=WOUT*ALFA+WCHK*(1.Ø-ALFA)
С
C
        CALCULATE CHANGE IN TEMPERATURE.
С
424
        QVAL=WOUT*HFLV
        TELT=(HTIN-QVAL)/(THRML*1000.0)
        TLST=TTNK
        TTNR = TTNK + TELT
        IF(FRAC.LT.Ø.Ø25)TTNK=Ø.2*TTNK+Ø.8*TLST
        FMSS=FMSS-WOUT
        FMAT=FMSS/WGHT
```

```
VOLL=FMSS*SPLQ
 C
         CALCULATE CHANGE IN MASS OF NITROGEN PAD (IF PRESENT).
 С
 С
         WNOUT=WOUT*PNIT/(PTOT-PNIT)
         WNTST=0.4*WNIT
         IF (WNOUT.GT.WNTST)WNOUT=WNTST
         WNIT=WNIT-WNOUT
         IF (WNIT.LT.Ø.Ø)WNIT=Ø.Ø
         IF (WGNT.LE.Ø.Ø.OR.FRAC.GE.1.Ø)GO TO 421
         PNIT=((1.-FRAT)/(1.-FRAC))*PPAD*(TTNK/TTMC)*WNIT/WGNT
         GO TO 422
 421
         PNIT=Ø.Ø
         WNIT=Ø.Ø
C
 422
         TEMP = (TTNK - \emptyset.46) * 1000.0
         CALL PROPERTIES (KPRD, TEMP, PREF, SPEC, SPLQ, HFLV, VVAP, DVDT, DLDT)
C
         PTOT=PREF+PNIT
         IF(PREF.GT.PCLS.OR.PTOT.LT.(PATD+1.Ø))GO TO 423
         PNTEMP=PATD-PREF+Ø.5
         WNIT=WNIT*PNTEMP/PNIT
         PNIT=PNTEMP
         PTOT=PNIT+PREF
423
         IF (KIDN.EQ.1)PICR=Ø.Ø
         WLIQ=(FMSS*VVAP-SZGL)/(VVAP-SPLQ)
         WVAP=FMSS-WLIQ
         VLIQ=WLIQ*SPLQ
         FRAC=VLIQ/SZGL
         SLST=SZGL/FMSS
         IF(VLIQ.GE.SZGL)FRAC=1.0
         IF(VLIQ.LE.Ø.Ø)FRAC=Ø.Ø
        PICR=14.7
        KIDN=1
        GO TO 153
C
C
        CASE OF TANK FILLED ONLY WITH VAPOR (NITROGEN PAD NEGLECTED):
C
430
        HTIN=(TTNV-TTNK)*AREA*1000.0*1.0*DELT/60.0
        PLST=PTOT
        ZPRO=Ø.7
        PNIT=Ø.Ø
        SVLV=SZGL/FMSS
        IF(KPRD.EQ.1)GO TO 501
        PTOT=(PLST*SLST/SVLV*TTNK/TLST)*Ø.3+Ø.7*PLST
        SLST=SVLV
        GO TO 5Ø2
5Ø1
        CONTINUE
        PTOT=243.4*TTNK/(SVLV-Ø.Ø3226)-17.98/(SVLV**2)
        ZPRO=Ø.30411*PTOT*SVLV/TTNK
5Ø2
        CONTINUE
        IF(PTOT.LE.PCLS)PTOT=PCLS+Ø.ØØ1
        WLET-WOUT
        WOUT=(PTOT/PASD)*TCFM*VLCON/SQRT(TTNK*ZPRO)*DELT
        IF (FMAT.GT.Ø.Ø1ØØ)GO TO 5Ø3
        ALFA=Ø.2
        IF (SCFM.GT.15000.0) ALFA=\emptyset.05
        WOUT=WOUT*ALFA+WLET*(1.Ø-ALFA)
5@3
        QWRK=WOUT*SVLV*PTOT*144.Ø/778.Ø
```

1

```
CALCULATE CHANGE IN TEMPERATURE.
C
        TELT=(HTIN-QWRK)/(FMSS*Ø.40*1966.0)
        TLST=TTNK
        TTNK=TTNK+TELT
        FMSS=FMSS-WOUT
        WLIQ=Ø.Ø
        WVAP=FMSS
        FRAC=Ø.ØØØ
        PICR=14.7
        FMAT=FMSS/WGHT
         TEMP=(TTNK-\emptyset.46)*1000.0
        CALL PROPERTIES (KPRD, TEMP, PREF, SPEC, SPLO, HFLV, VVAP, DVDT, DLDT)
        KIDN=4
        GO TO 153
C
        BURST STRENGTH OF TANK
С
С
         IF(TTNV.LT.1.260)FCTR=1.0-(0.54)*(TTNV-0.46)**4"
153
         IF(TTNV.GE.1.260)FCTR=1.74-1.17*(TTNV-0.46)
         PERS=PBRT*FCTR
С
         SET OUTPUT PARAMETERS.
C
         PSIG=PTOT-14.7
         PACR=PICR-14.7
         WPRT=WOUT/DELT
         TEMP = 1000.0 * TTNK - 460.0
         TEMW=1000.0*TWAL-460.0
         TEMH=1000.0*TTNV-460.0
         TEMQ=1000.0*TTMV-460.0
         FRCLQ=WLIQ/WGHT
С
         HFADINGS FOR OUTPUTS
С
         IF(PBRS.LT.PSIG)GO TO 98
         IF(TIME.GT.Ø.Ø)GO TO 65
         IF(KPRD.EQ.1)WRITE(KW,57)
         IF (KPRD.EQ.2) WRITE (KW, 58)
         IF(KPRD.EQ.3)WRITE(KW,55)
         IF (KPRD.EQ.4)WRITE (KW,54)
         IF (KPRD.EQ.5)WRITE (KW,53)
         IF(KPRD.EQ.6)WRITE(KW,52)
         IF (KPRD.EQ.7)WRITE (KW,51)
         FORMAT(5x,7HPROPANE,1x,3HCAR)
 57
         FORMAT(5x,8HETHLYENE,1x,5HOXIDE,1x,3HCAR)
 58
         FORMAT (5x, 9HPROPYLENE, 1x, 3HCAR)
 55
         FORMAT (5X, 13H1, 3-BUTADIENE, 1X, 3HCAR)
 54
         FORMAT(5x,5HVINYL,1x,8HCHLORIDE,1x,3HCAR)
 53
         FORMAT (5X, 15HMONOMETHYLAMINE, 1X, 3HCAR)
 52
         FORMAT (5x, 9HPROPYLENE, 1x, 5HOXIDE, 1x, 3HCAR)
 51
         WRITE(KW, 59)
         FORMAT(2X,4HSVPR,5X,4HINTT,5X,4HCOND,3X,4HSCFM,3X,4HTEMF,
 59
         5x, 4HSIZE, 2x, 4HTILT, 2x, 6HWEIGHT, 2x, 5HTHICK)
         WRITE (KW, 60) PASD, TEMC, CNDD, SCFM, TEMF, SIZE, TILT, WGHT, THIC
         FORMAT (F8.2,F8.2,F8.2,F8.0,F8.2,F8.0,F6.0,F8.0,F7.3)
 6.:
          IF(KW.EQ.10)WRITE(KW,63)
          IF(KW.EQ.12)WRITE(KW,64)
          FORMAT (4X,4HTIME, 3X,4HPSIG,4X,4HTTNK,3X,4HTWAL,3X,4HFRAC,
 63
```

```
2X,4HFMAT,2X,4HTVAP,2X,4HWOUT,2X,4HPBRS,4X,4HPNIT,1X,4HKIDN)
64
         FORMAT (4X,4HTIME,3X,4HPSIG,4X,4HTTNK,3X,4HTWAL,3X,4HFRAC,
         2%,4HFMAT,2X,4HTVAP,2X,4HWOUT,2X,4HPBRS,4X,4HPNIT,1X,4HKIDN,3X,5HTHETA,5X,4HPICR,2X,5HCNDLQ,2X,5HCNDVP,2X,6HFRACLQ)
65
         IF(KCNT.LT.INTV)GO TO 99
С
98
         IF(KPLT.EQ.2)CALL PLT3 ("DATA", FRAC, PSIG, TEMQ, TIME)
         IF (KW.EQ.12)GO TO 66
         WRITE(KW, 67) TIME, PSIG, TEMP, TEMW, FRAC, FMAT, TEMH, WPRT, PBRS,
        PNIT, KIDN
         GO TO 69
         WRITE(KW, 68) TIME, PSIG, TEMP, TEMW, FRAC, FMAT, TEMH, WPRT, PBRS,
66
         PNIT, KIDN, THET, PACR, CNDLQ, CNDVP, FRCLQ
69
         CONTINUE
         FORMAT(F8.2,F8.2,F7.Ø,F8.Ø,F6.3,F6.3,F7.1,F6.Ø,F7.1,F7.1,I3)
67
68
         FORMAT(F8.2,F8.2,F8.0,F8.0,F6.3,F6.3,F6.0,F6.0,F6.0,F9.1,I3,
         F8.3, F9.1, F7.2, F7.2, F7.3)
         KCNT=Ø
         KTCT=KTCT+1
С
         IF(PBRS.LT.PSIG)GO TO 78
C
99
         KCNT=KCNT+1
         IF (KTCT.EQ.18.AND.KW.EQ.10) PAUSE
         IF(KTCT.EQ.18)KTCT=1
С
92
         DITME=TIME*20.0+0.1
         KTIME=IFIX(DTIME)
         DTIME=FLOAT(KTIME)
         TIME=DTIME/20.0
         TIME=TIME+DELT
         IF(TIME.GT.600.0)GO TO 78
77
         GO TO 21
78
         CONTINUE
С
93
         IF(KPLT.EQ.2)CALL PLT3 ("PLOT")
         IF(KPLT.EQ.2)CALL PLT3 ("STOP")
         STOP
         END
```

* #

4.1 SUBROUTINE PROPERTIES

Subroutine PROPERTIES contains the thermal property data for the commodities considered under this program. The following properties of a product are given at saturated vapor conditions as a function of temperature:

PREF	Vapor pressure (psia)
SPEC	Specific heat of the liquid (BTU/lb °F)
SPLQ	Specific volume of liquid (ft³/lb)
HFLV	Heat of vaporization (BTU/lb)
VVAP	Specific volume of vapor (ft³/lb)
DVDT	Rate of change of the function VVAP with temperature (ft³/lb°F)
DLDT	Rate of change of the function SPLQ with temperature (ft3/lb°F)

The thermal property data is represented as quadratic functions of temperature within given temperature ranges. A sufficient number of temperature ranges are used with each commodity to give a sufficiently accurate representation of the property data. The subroutine is called with a given value of temperature (TEMP) in °F. The thermal property data is based on the following sources: propane (Ref. 4), ethylene oxide (Ref. 4), propylene (Ref. 4), 1-3 butadiene (Refs. 4 and 5), vinyl chloride (Refs. 4 and 5), monomethylamine (Refs. 4 and 6), and propylene oxide (Ref 7). A listing of the subroutine is presented on the following pages.

```
SUBROUTINE PROPERTIES (KPRD, TEMP, PREF, SPEC, SPLO, HFLV, VVAP,
        THIS SUBROUTINE CONTAINS REPRESENTATIONS OF THE THERMAL
    1 DVDT, DLDT)
           PROPERTIES OF PROPANE(1), ETHYLENE OXIDE(2), PROPYLENE(3),
           1,3-BUTADIENE(4), VINYL CHLORIDE(5), MONOMETHYLAMINE(6),
           AND PROPYLENE OXIDE(7) UNDER SATURATED VAPOR CONDITIONS
C
           AS A FUNCTION OF TEMPERATURE. PROPERTIES ARE: PREF (VAPOR
C
00000
               PREF-VAPOR PRESSURE (PSIA)
               SPEC-SPECIFIC HEAT OF LIQUID (BTU/LB-DEG F)
               SPLO-SPECIFIC VOLUME LIQUID (CU FT/LB)
               HFLV-HEAT OF VAPORIZATION (BTU/LB)
               VVAP-SPECIFIC VOLUME VAPOR (CU FT/LB)
               DVDT-RATE OF CHANGE OF VVAP WITH TEMP (CU FT/LB-DEF F)
DLDT-RATE OF CHANGE OF SPLQ WITH TEMP (CU FT/LB-DEF F)
CCC
         IF(KPRD.EQ.2)GO TO 391
 C
         IF (KPRD.EQ.3)GO TO 811
          IF(KPRD.EQ.4)GO TO 831
          IF(KPRD.EQ.5)GO TO 841
          IF (KPRD.EQ.6)GO TO 851
          IF(KPRD.EQ.7)GO TO 821
          PROPERTIES OF PROPANE
          IF(TEMP.GT.81.12)GO TO 313
          PREF=44.809+0.47317*TEMP+0.0096905*TEMP*TEMP
          SPLO=(31.312+.05029*(TEMP-56.75)+.0002*((TEMP-56.75)**2))/1000.
          VVAP=2.29511-0.82836*TEMP+8.888111*TEMP*TEMP
          DVDT=-0.02836+0.000222*TEMP
           GO TO 319
           IF(TEMP.GT.135.59)GO TO 314
           PREF=63.705+0.026189*TEMP+0.012329*TEMP*TEMP
  313
           SPLQ=(32.656+.05999*(TEMP-81.12)+.0003307*((TEMP-81.12)**2)
           VVAP=1.86981-0.018250*TEMP+0.000051*TEMP*TEMP
           DVDT=-0.018250+0.000102*TEMP
           GO TO 319
           IF(TEMP.GT.172.54)GO TO 315
           PREF=123.25-Ø.8776297*TEMP+Ø.Ø15756*TEMP*TEMP
   314
           SPLQ=(36.905+.085936*(TEMP-135.59)+0.001399*((TEMP-135.59)**2)
           )/1000.
           VVAP=1.34795-Ø.818288*TEMP+8.888821*TEMP*TEMP
            DVDT=-Ø.Ø1Ø28Ø+Ø.ØØØØ42*TEMP
            GO TO 319
            IF(TEMP.GT.201.25)GO TO 316
            PREF=193.32-1.723723*TEMP+Ø.Ø183Ø58*TEMP*TEMP
   315
            SPLQ=(41.991+.13595*(TEMP-172.54)+.86981*((TEMP-172.54)**2))
            VVAP=0.345139+0.0011835*TEMP-0.0000118*TEMP*TEMP
            /1000.
            DVDT=+Ø.ØØ11835-Ø.ØØ00236*TEMP
            GO TO 319
            PREF=587.84+6.0748*(TEMP-201.25)
    316
            SPLQ=0.053324+(TEMP-201.25)*0.003496
            VVAP=0.107648-(TEMP-201.25)*0.007079
            TVDT=-0.007079
            CONTINUE
    319
    C
            IF(TEMP.GT.77.395)GO TO 321
            SPEC=0.5890+0.002858*(TEMP-61.185)-0.0000165*((TEMP-61.185)**2)
```

```
GO TO 329
321
        IF(TEMP.GT.123.64)GO TO 322
        SPEC=.631-.00006635*(TEMP-77.395)+.00005053*((TEMP-77.395)**2)
        GO TO 329
322
        IF(TEMP.GT.163.975)GO TO 323
        SPEC=.736+.0019923*(TEMP-123.64)+.00005325*((TEMP-123.64)**2)
        GO TO 329
323
        IF(TEMP.GT.201.25)GO TO 324
        SPEC=.903+.00033931*(TEMP-163.975)+.0006224*((TEMP-163.975)**2)
        GO TO 329
324
        SPEC=3.976
        CONTINUE
329
        IF(TEMP.GT.81.12)GO TO 341
        HFLV=166.67-0.12991*TEMP-0.00203103*TEMP*TEMP
        GO TO 349
341
        IF(TEMP.GT.135.59)GO TO 342
        HFLV=164.54-0.10958*TEMP-0.00195787*TEMP*TEMP
        GO TO 349
342
        IF(TEMP.GT.172.54)GO TO 343
        HFLV=185.88+8.7376687*TEMP-8.88496746*TEMP*TEMP*
        GO TO 349
343
        IF(TEMP.GT.187.63)GO TO 344
        HFLV=84.39-(TEMP-172.54)*1.226
        GO TO 349
344
        IF(TEMP.GT.201.25)GO TO 345
        HFLV=65.88-(TEMP-187.63)*2.472
        GO TO 349
345
        HFLV=32.21-(TEMP-201.25)*6.341
349
        CONTINUE
        IF(TEMP.GT.77.395)GO TO 381
        DLDT=(.053+.00009042*(TEMP-61.185)+.00001726*((TEMP-61.185)**2))
        /1000.0
        GO TO 389
381
        IF(TEMP.GT.123.64)GO TO 383
        DLDT=(.059+.00054482*(TEMP-77.395)+.000000178*((TEMP-77.395)**2))
        /1000.
        GO TO 389
383
        IF(TEMP.GT.163.975)GO TO 385
        DLDT=(.088+.00033791*(TEMP-123.64)
        +.00003895*((TEMP-123,64)**2))/1000.00
        GO TO 389
385
        IF(TEMP.GT.201.25)GO TO 386
        DLDT=(.165+.00061313*(TEMP-163.975)+.00037422*((TEMP-163.975)**
        2))/1000.0
        GO TO 389
386
        DLDT=Ø.003496
389
        GO TO 899
С
С
        PROPERTIES OF ELHYLENE OXIDE
391
        IF(TEMP.GE.160.0)GO TO 713
        PREF=12.784-0.2172*TEMP+0.00475*TEMP*TEMP
        VVAP=585.07/TEMP+0.0048*TEMP-3.1188
        DVDT=-585.07/(TEMP*TEMP)+0.0048
        GO TO 72Ø
        IF(TEMP.GE.280.0)GO TO 715
713
        PREF=191.52-2.423*TEMP+0.01156*TEMP*TEMP
        VVAP=541.67/TEMP+Ø.00373*TEMP-2.6762
```

```
DVDT=-541.7/(TEMP*TEMP)+Ø.8837
        GO TO 72Ø
        PREF=658.24-5.8526*TEMP+8.81785*TEMP*TEMP
715
        VVAP=382.63/TEMP+0.001477*TEMP-1.4780
        DVDT=-382.6/(TEMP*TEMP)+0.0015
        CONTINUE
72Ø
C
        IF(TEMP.GE.265.0)GO TO 723
        SPEC=0.46754-.000386*TEMP+0.8666053*TEMP*TEMP
        GO TO 738
        SPEC=0.565079-0.0009733*TEMP+0.0000062*TEMP*TEMP
723
        CONTINUE
73Ø
C
         IF(TEMP.GE.130.0)GO TO 733
         SPLQ=(18.200+0.01195*(TEMP-70.)+0.0000672*(TEMP-70.)**2)/1000.0
        GO TO 740
         IF(TEMP.GE.190.0)GO TO 734
733
         SPLQ=(19.159+8.82188*(TEMP-138.)+8.888865*(TEMP-138.)**2)/1888.
         GO TO 748
         IF(TEMP.GT.250.0)GO TO 735
734
         SPLQ=(20.658+0.02888*(TEMP-190.)+0.0000828*(TEMP-190.)**2)/1000.
         GO TO 740
         IF(TEMP.GT.310.0)GO TO 736
735
         SPLQ=(22.689+$.$3543*(TEMP-25$.)+$.$$$$273*(TEMP-25$.)**2)/18$$.
         GO TO 748
         IF(TEMP.GT.370.0)GO TO 737
736
         SPLQ=(25.799+8.868*(TEMP-318.8)+8.881*(TEMP-318.8)**2)/1888.8
         GO TO 74Ø
         SPLQ = \emptyset.\emptyset32999 + \emptyset.\emptyset\emptyset12499 * (TEMP - 370.0)
737
         CONTINUE
74Ø
         IF(TEMP.GE.250.0)GO TO 743
         HFLV=261.84-8.2219*TEMP-8.888451*TEMP*TEMP
         GO TO 75Ø
         HFLV=110.94+0.995*TEMP-0.002917*TEMP*TEMP
743
         CONTINUE
75Ø
         IF(TEMP.GE.115.8)GO TO 773
         DLDT=(7.95+.1997*(TEMP-51.)-Ø.888668*((TEMP-51.)**2))/(18:**6)
         GO TO 78Ø
         IF(TEMP.GE.175.8)GO TO 774
773
         DLDT=(18.+.1865*(TEMP-115.)-.000628*((TEMP-115.)**2))/(10:**6)
         GO TO 78Ø
         IF(TEMP.GT.235.Ø)GO TO 775
774
         DLDT=(26.93+.1393*(TEMP-175.)+.000289*((TEMP-175.)**2))/
         (10.**6)
         GO TO 780
         IF(TEMP.GT.295.)GO TO 776
 775
         DLDT=(36.33+.891667*(TEMP-235.)+.885856*((TEMP-235.)**2))/
         (10.**6)
         GO TO 78Ø
         IF(TEMP.GT.370.0)GO TO 777
 776
         DLDT=(68.83+.4985*(TEMP-295.)+.816683*((TEMP-295.)**2))/
         (10.**6)
         GO TO 78Ø
 777
         DLDT=\emptyset.\emptyset\emptyset125
         GO TO 899
 708
 C
 C
         PROPERTIES OF PROPYLENE
 C
```

```
IF(TEMP.GT.8Ø.Ø)GO TO 813
811
        F=TEMP-40.0
        PREF=96.52+1.53Ø3*F+Ø.Ø1Ø6*F*F
        SPEC=0.5817-0.0007975*F+0.0000334*F*F
        SPLQ=(29633.0+60.13*F-0.2*F*F)/10.0**6
        HFLV=160.1-0.458250*F+0.000088*F*F
        VVAP=1.141923-8.817456*F+8.888113*F*F
        DVDT=-(18349.Ø-329.625*F+2.36375*F*F)/1Ø.Ø**6
        DLDT=(48.05+0.4005*F)/10.0**6
        GO TO 899
        IF(TEMP.GT.128.8)GO TO 814
813
        F=TEMP-80.0
        PREF=174.71+2.3750*F+0.01343*F*F
        SPEC=0.6032+0.0010350*F-0.0000160*F*F
         SPLQ=(31716.Ø+56.Ø3*F+Ø.4*F*F)/1Ø.Ø**6
        HFLV=141.91-0.475250*F-0.001263*F*F
         VVAP=0.624061-0.008598*F+0.000056*F*F
         DVDT=-(8496.0-138.400*F+0.933*F*F)/10.0**6
         DLDT=(64.87+0.2803*F+0.010013*F*F)/10.6**6
         GO TO 899
C
314
         IF (TEMP.GT.16Ø.Ø)GO TO 815
         F=TEMP-12Ø.Ø
         PREF=291.19+3.4445*F+0.01750*F*F
         SPEC=Ø.619Ø-Ø.ØØØ385*F+Ø.0602Ø6*F*F
         SPLQ=(34599.8+108.15*F+1.8*F*F)/18.8**6
         HFLV=120.88-0.479250*F-0.006388*F*F
         VVAP=8.359924-8.884661*F+8.888818*F*F
         DVDT=-(49\( 2.\theta - 6\theta . 75\( 0 * F + \theta . 553 * F * F ) / 1\( 0 . \theta * * 6 \)
         DLDT=(88.10+2.6025*F-0.610000*F*F)/10.0**6
         GO TO 899
         IF(TEMP.GT.18Ø.Ø)GO TO 816
 815
         P=TEMP-168.8
         PREF=456.97+4.8570*F+0.02160*F*F
         SPEC=0.9328+0.010760*F+0.000432*F*F
         SPLQ=(48285.8+128.15*F+4.81*F*F)/18.8**6
         HFLV=91.49-1.038500*F-0.013550*F*F
         VVAP=0.202948-0.003356*F+0.0000056*F*F
         DVDT=-(3356.0-14.400*F+0.320*F*F)/10.0**6
         DLDT=(176.20-1.2020*F+0.600700*F*F)/10.0**6
         GO TO 899
 816
         F = TEMP - 18\%.6
         PREF=562.75+5.6680*F+0.03460*F*F
         SPEC=1.3208+0.020692*F+0.011466*F*F
         SPLQ=(4469Ø.Ø-1Ø48.19*F+156.Ø8*F*F)/1Ø.Ø**6
         HFLV=65.3Ø+Ø.9866Ø3*F-Ø.27896Ø*F*F
         VVAP=0.138075-0.0023618*F-0.0000842*F*F
         DVDT=-(3196.8-3.832*F+6.883*F*F)/18.8**6
         DLDT=(392.44-92.23676*F+2Ø.519276*F*F)/1Ø.Ø**6
         IF(TEMP.GE.190.0)GO TO 899
         G=TEMP-17Ø.Ø
         SPLQ=(41967.0+152.15*G+12.02*G*G)/10.0**6
         HFLV=79.75-1.266*G-Ø.Ø179*G*G
         DLDT=(224.25-31.2495*G+4.80685*G*G)/10.0**6
         GO TO 899
 C
         PROPERTIES OF PROPYLENE OXIDE
```

1

```
C
821
        IF(TEMP.GT.168.8)GO TO 822
        F = TEMP - 40.0
        PREF=4.4+0.05667*F+0.002417*F*F
        SPEC=0.482+0.001167*F+0.0000017*F*F
        SPLQ=(1885@.@+14.667*F+@.@14*F*F)/1@.@**6
        HFLV=216.Ø-Ø.24*F
        VVAP*19.31187-23.264172*F/(42.585136+F)
        DVDT=-(Ø.36400-0.523542*F/(69.803922+F))
        DLDT=(14.Ø+Ø.Ø3333*F)/18.Ø**6
        GO TO 899
822
        IF(TEMP.GT.280.0)GO TO 823
        F = TEMP - 16\emptyset.\emptyset
        PREF=46.8+8.55888*F+8.887588*F*F
        SPEC=0.646+0.0012583*F+0.0000135*F*F
        SPLQ=(20810.0+16.500*F+0.083*F*F)/10.0**6
        HFLV=187.2-0.24*F-0.000500*F*F
        VVAP=2.14117-2.993435*F/(90.529783+F)
        DVDT=-(0.03300-0.047801*F/(87.079646+F))
        DLDT=(18.Ø+Ø.Ø9167*F+Ø.ØØØ69*F*F)/1Ø.Ø**6
        GO TO 899
823
        F = TEMP - 280.0
        PREF=220.0+1.55556*F+0.018519*F*F
        SPEC=0.991+0.8821944*F+8.8888876*F*F
        SPLQ=(23998.8+11.556*F+8.752*F*F)/18.8**6
        HFLV=151.2-0.19*F-0.006333*F*F
        VVAP=Ø.43494-Ø.899Ø8Ø*F/(188.41Ø256+F)
        DVDT=-(\emptyset.00530-0.014720*F/(324.0+F))
        DLDT={39.Ø+Ø.443567*F+141.867*F**4/10.Ø**8}/10.Ø**6
825
        GO TO 899
С
        PROPERTIES OF 1.3-BUTADIENE
C
C
831
         IF(TEMP.GT.80.0)GO TO 832
         F=TEMP-40.0
         PREF=20.49+0.403250*F+0.003888*F*F
        SPEC=0.522+0.000700*F
         SPLQ=(25030.0+26.25*F+0.0375*F*F)/10.0**6
        HFLV=174.89-0.22900*F-0.000525*F*F
        VVAP=4.61652-6.65973*F/(75.24724+F)
        DVDT=-(\emptyset.0905-0.1305500*F/(59.847328+F))
        DLDT=(26.Ø+Ø.Ø65Ø*F+Ø.ØØ1ØØ*F*F)/1Ø.Ø**6
        GO TO 899
C
832
         IF(TEMP.GT.120.0)GO TO 833
         F = TEMP - 8\emptyset.\emptyset
         PREF=42.84+0.71425*F+0.005438*F*F
         SPEC=0.550+0.000775*F+0.0000013*F*F
         SPLQ=(26140.0+30.75*F+0.0625*F*F)/10.0**6
        HFLV=164.89-0.25775*F-0.000613*F*F
         VVAP=2.30506-3.38068*F/(89.63582+F)
        DVDT=-(Ø.Ø382-Ø.Ø55455Ø*F/(7Ø.9Ø9Ø91+F))
        DLDT=(30.2+0.1500*F+0.000000*F*F)/10.0**6
        GO TO 899
833
         IF(TEMP.GT.160.0)GO TO 834
         F=TEMP-12Ø.Ø
         PREF=80.11+1.14975*F+8.007063*F*F
```

```
SPEC=0.583+0.000875*F+0.0000013*F*F
       SPLQ=(27470.0+35.50*F+0.1250*F*F)/18.0**6
        HFLV=153.60-0.30825*F-0.000613*F*F
        VVAP=1.26193-1.92821*F/(106.71005+F)
        DVDT=-(Ø.Ø182-Ø.Ø26237Ø*F/(82.891566+F))
        DLDT=(36.2+Ø.1975*F+Ø.ØØØ88*F*F)/10.Ø**6
        GO TO 899
        IF(TEMP.GT.200.0)GO TO 835
834
        F = TEMP - 160.0
        PREF=137.40+1.72150*F+0.008900*F*F
        SPEC=0.620+0.001500*F
        SPLQ=(29090.0+45.00*F+0.2000*F*F)/10.0**6
        HFLV=14Ø.29-Ø.36275*F-Ø.ØØ1113*F*F
        VVAP=0.73621-1.20622*F/(126.50152+F)
        DVDT=-(Ø.ØØ966-Ø.Ø1Ø3113*F/(65.217391+F))
        DLDT=(45.5+0.2825*F+0.00088*F*F)/10.0**6
        GO TO 899
835
        IF(TEMP.GT.240.0)GO TO 836
        F=TEMP-200.0
        PREF=220.50+2.51250*F+0.013125*F*F
        SPEC=0.680+0.001325*F+0.0000088*F*F
        SPLQ=(31210.0+52.25*F+0.3625*F*F)/10.0**6
        HFLV=124.00-0.25500*F-0.003850*F*F
        VVAP=0.44643-0.723699*F/(118.45396+F)
        DVDT=-(Ø.ØØ574-Ø.ØØ827Ø7*F/(121.37931+F))
        DLDT=(58.2+Ø.185*F+Ø.Ø1525*F*F)/1Ø.Ø**6
        GO TO 899
836
        F = TEMP - 240.0
        PREF=342.00+3.70000*F+0.007500*F*F
        SPEC=0.747+0.002550*F+0.0000175*F*F
        SPLQ=(33880.0+87.50*F+1.5000*F*F)/10.0**6
        HFLV=107.64-0.58050*F-0.008325*F*F
        VVAP=Ø.26374-1.331294*F/(362.72Ø7Ø+F)
        DVDT=-(Ø.ØØ369-Ø.ØØ299ØØ*F/(133.33333+F))
        DLDT=(90.0+1.525*F+0.04875*F*F)/10.0**6
        GO TO 899
        PROPERTIES OF VINYL CHLORIDE
        IF(TEMP.GT.100.0)GO TO 842
841
        F=TEMP-40.0
        PREF=29.40+0.7100*F+0.002778*F*F
        SPEC=0.3034+0.000688*F
        SPLQ=(17100.0+14.33*F+0.0330*F*F)/10.0**6
        HFLV=135.90-0.21170*F+0.000167*F*F
        VVAP=2.482-2.89440*F/(49.15420+F)
        DVDT=-(Ø.Ø46Ø-Ø.Ø532*F/(27.Ø466+F))
        DLDT=(13.Ø+Ø.Ø93Ø*F+Ø.ØØØ6Ø*F*F)/1Ø.Ø**6
        GO TO 899
C
842
         IF(TEMP.GT.140.0)GO TO 843
         F=TEMP-100.0
        PREF=82.00+0.92500*F+0.008750*F*F
         SPEC=Ø.3445+Ø.000678*F
         SPLQ=(18Ø8Ø.Ø+22.5Ø*F+Ø.Ø25Ø*F*F)/1Ø.Ø**6
        HFLV=123.80-0.17500*F-0.001000*F*F
```

С C

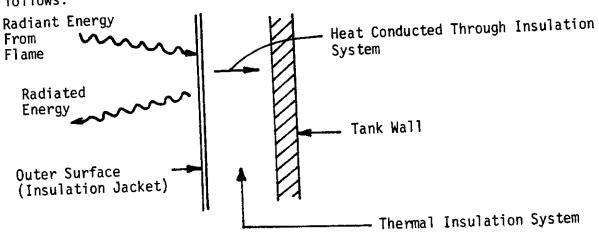
С C

```
VVAP=0.89100-1.91450*F/(179.42860+F)
       DVDT=-(8.8893-8.8156*F/(228.888+F))
       DLDT = (28.6+8.1425*F+8.88818*F*F)/18.8**6
        GO TO 899
        IF(TEMP.GT.188.8)GO TO 844
C
843
        F=TEMP-140.0
        PREF=133.88+1.57588*F+8.888758*F*F
        SFEC=Ø.3718+Ø.000688*F
        SPLQ=(19020.0+23.25*F+0.1880*F*F)/10.0**6
        HFLV=115.20-0.25000*F-0.000500*F*F
        VVAP=0.542-0.84230*F/(122.75860+F)
        DVDT=-(Ø.8869-Ø.8899888*F/(96.88+F))
        DLDT=(26.5+0.1925*F+0.0011*F*F)/10.0**6
         GO TO 899
         IF(TEMP.GT.220.0)GO TO 845
 844
         F=TEMP-180.0
         PREF=210.00+2.32500*F+0.016250*F*F
         SPEC=0.3991+0.000685*F
         SPLQ=(20250.0+34.00*F+0.2250*F*F)/10.0**6
         HFLV=104.40-0.2950*F-0.001500*F*F
         VVAP=0.33508-0.61920*F/(152.00+F)
         DVDT=-(Ø.88488-8.8128*F/(288.88+F))
         DLDT=(36.0+0.2500*F+0.00500*F*F)/10.0**6
         GO TO 899
         F=TEMP-220.0
 -845
          PREF=329.00+3.52500*F+0.023750*F*F
          SPEC=0.4265+0.000678*F
          SPLQ=(21978.8+52.25*F+8.4138*F*F)/18.8**6
          HFLV=90.20-0.27500*F-0.004250*F*F
          VVAP=0.20600-0.386200*F/(155.556+F)
          DVDT=-(0.00250-0.0020*F/(60.00+F))
          DLDT=(54.0+3.200*F-0.080*F*F)/10.0**6
          GO TO 899
  C
  C
          PROPERTIES OF MONOMETHYLAMINE
  Ċ
  Ċ
          IF(TEMP.GT.86.0)GO TO 852
  851
          F=TEMP-5Ø.Ø
          PREF=29.87+0.6372*F+0.006728*F*F
          SPEC=Ø.772+Ø.ØØØ8Ø6*F+Ø.ØØØØØ77*F*F
          SPLQ=(23740.0+23.89*F+0.0310*F*F)/10.0**6
          HFLV=347.00-0.45830*F-0.000463*F*F
           VVAP=5.653-6.95918*F/(57.8977+F)
           DVDT=-(Ø.1020-0.0820*F/(21.913+F))
           DLDT=(23.33+Ø.Ø93*F)/10.Ø**6
           GO TO 899
           IF(TEMP.GT.122.0)GO TO 853
   852
           F=TEMP-86.0
           PREF=61.53+Ø.9669*F+Ø.Ø13627*F*F
           SPEC=0.811+0.001167*F+0.0000031*F*F
           SPIN = (24640.0+26.11*F+0.0620*F*F)/10.0**6
           HFLV=329.9-Ø.5Ø83*F-Ø.ØØØ463*F*F
           VVAP=2.962-3.5983*F/(61.7659+F)
           DVDT=-(Ø.Ø51@-Ø.1167*F/(132.Ø+F))
           DLDT=(26.66+Ø.Ø93Ø*F)/1Ø.Ø**6
```

```
GO TO 899
853
        IF(TEMP.GT.150.0)GO TO 854
        F=TEMP-122.0
        PREF=114.00+1.89250*F+0.009451*F*F
        SPEC=Ø.857+Ø.001132*F+Ø.0000016*F*F
        SPLQ=(25660.0+30.20*F+0.0440*F*F)/10.0**6
        HFLV=311.00-0.5516*F-0.003132*F*F
        VVAP=1.637-2.3389*F/(95.6876+F)
        DVDT = -(\emptyset.0260 - \emptyset.0250 * F/(33.5063 + F))
        DLDT=(38.88+8.8928*F)/18.8**6
        GO TO 899
C
854
        IF(TEMP.GT.180.0)GO TO 855
        F = TEMP - 150.0
        PREF=174.48+2.4267*F+8.815111*F*F
        SPEC=0.898+0.801467*F
        SPLQ=(26540.0+32.67*F+0.0440*F*F)/10.0**6
        HFLV=293.1-Ø.6933*F-Ø.ØØ3111*F*F
        VVAP=1.109-1.6613*F/(116.1538+F)
        DVDT=-(8.8146-8.8224*F/(98.8+F))
        DLDT=(32.59+Ø.Ø93*F)/1Ø.Ø**6
        GO TO 899
C
        IF(TEMP.GT.210.0)GO TO 856
855
        F=TEMP-180.0
        PREF=260.86+3.2867*F+8.016444*F*F
        SPEC=Ø.934+Ø.ØØ1367*F+Ø.ØØØØØ22*F*F
        SPLQ=(27560.0+35.33*F+0.0440*F*F)/10.0**6
        HFLV=269.50-0.870*F-0.002000*F*F
        VVAP=Ø.768-1.1124*F/(125.2174+F)
        DVDT=-(Ø.ØØ9ØØ-Ø.Ø144*F/(1Ø5.Ø+F))
        DLDT=(35.37+0.093*F)/10.0**6
        GO TO 899
856
        F = TEMP - 210.0
        PREF=374.2Ø+4.568*F+Ø.Ø2496Ø*F*F
        SPEC=Ø.977+Ø.ØØ13ØØ*F+Ø.ØØØØØ67*F*F
        SPLQ=(28660.0+32.67*F+0.4*F*F)/10.0**6
        HFLV=241.60-0.9667*F-0.001778*F*F
        VVAP=Ø.553-3.978Ø*F/(75Ø.Ø+F)
        DVDT=-(Ø.88588-8.8891*F/(188.8+F))
        DLDT=(38.14+Ø.Ø93*F)/10.Ø**6
        GO TO 899
899
         RETURN
        END
```

4.2 SUBROUTINE SURFACET

Subroutine SURFACET is used to calculate the surface temperature of the outside of the insulated tank which is engulfed in the fire. It is assumed that the dominant mechanism for the transfer of heat to the outer surface is by radiation from the flame. It is also assumed that a quasi-steady state condition exists for the transfer of heat from the outer surface of the insulation system to the steel wall of the tank. The subroutine uses an iterative solution of the equation defining a heat balance at the outer surface to determine the temperature of the surface. The heat balance is illustrated as follows:



The following equation represents a heat balance at the outer surface of the insulation system:

0.48
$$[T_f^{4} \epsilon_a - T_s^{4} \epsilon_r] = [T_s - T_+] C_d/3.6$$
 (11)

where T_f is flame temperature (${}^{\circ}R/1000$)

 T_s is surface temperature (°R/1000)

 T_{t} is tank wall temperature (°R/1000)

C is conductance of thermal shield (BTU/hr-ft 2 - $^\circ$ F)

 ϵ_a is the absorptivity of outer surface

 ϵ_{r} is the emissivity of outer surface

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The principal parameters used in the subroutine are defined as follows:

TFLA Flame temperature (°R/1000)

TCAL Surface temperature (°R/1000)

TINS Tank wall temperature (°R/1000)

COND Conductance of thermal shield (BTU/hr-ft²-°F)

EABS Absorptivity of outer surface

ERAD Emissivity of outer surface

SUBROUTINE SURFACET (TCAL, TIMS, EABS, ERAD, COND, TFLA) 00000000 DETERMINE THE TEMPERATURE OF THE OUTER SURFACE OF THE WALL OF THE TANK, TCAL, BY AN ITERATIVE SOLUTION OF THE EQUATION FORMED BY TAKING A HEAT BALANCE AT THIS POINT. NOTE, TIMS IS INSIDE WALL TEMPERATURE AT THIS LOCATION. TCAL = 0.500 TCAL=TCAL-8.1 REFT=(TFLA**4)*#.48*EABS+TINS*COND/3.6 FNCT=(TCAL**4)*#.48*ERAD+TCAL*COND/3.6-REFT AFWD=Ø.188 TCAL=TCAL+AFWD 35 GNCT=(TCAL**4)*#.48*ERAD+TCAL*COND/3.6-REPT IF (ABS (FNCT-GNCT) .LT. 8.881)GO TO 39 IF (GNCT.LT. 8.8)GO TO 31 GO TO 37 FNCT=GNCT 31 GO TO 35 TCAL=TCAL-AFWD 37 AFWD=AFWD/10.0 GO TO 35 RETURN 39

. . .

END

4.3 SUBROUTINE VCAP

Subroutine VCAP is used to calculate liquid flow through the safety relief valve. The liquid flow through the valve is calculated assuming homogeneous isentropic two-phase flow (liquid and vapor). The calculation starts with the fluid conditions at the entry to the valve and integrates the conditions as the pressure and temperature drop when the fluid moves through the valve. The following equation is used:

$$V_1^2 - V_0^2 = 2g \int_0^1 \frac{dp}{p}$$
 (12)

where V_1 is the flow velocity (ft/sec)

V is the entry flow velocity at the valve (ft/sec)

p is pressure (lbs/ft²)

 ρ is the fluid density (lbs/ft³)

q is the gravitational constant (ft/sec2)

The integration is carried out along an isentropic path where an integration step equivalent to a 1/2°F drop in temperature of the fluid is used. After each integration step the cross sectional area required to pass a unit mass flow rate is determined. When this area reaches a minimum value in the integration process it is assumed that the critical valve cross section has been reached. This area is related to the cross sectional area of the valve to determine the mass flow rate.

Subroutine VCAP contains algebraic representations of entropy for the liquid and vapor states at saturated conditions for propane, ethylene oxide and propylene. Entropy data was not available for butadiene, vinyl chloride, monomethylamine or propylene oxide. The entropies of these products in the liquid and vapor states were calculated by assuming that the entropy of the liquid under the initial saturated condition had a value of 1.0 and that the entropies at other conditions could be estimated from the following relationships:

$$SL_{t2} = SL_{t1} - 2CP(T_2 - T_1)/(T_2 + T_1)$$
 (13)

$$SV_{t2} = SL_{t2} + 2(HFLV_{t2})/(T_2+T_1)$$
 (14)

where SL_{t2} is the entropy of the liquid at temperature 2 (BTU/lb°R) SL_{t1} is the entropy of the liquid at temperature 1 (BTU/lb°F) CP is the average specific heat between temperatures T_1 and T_2 (BTU/lb°R) SV_{t2} is the entropy of the vapor at temperature 2 HFLV is the heat of vaporization at temperature 2 T_1 and T_2 are temperatures (°R)

Where there is no nitrogen pad present, the velocity, V_0 , at the entry to the valve would be assumed to be 0. However, when there is a nitrogen pressure component the saturated condition of the liquid flow through the valve will be reached after the fluid has been given some velocity. Under these conditions V_0 in Equation 12 will have a finite value which is estimated from the following formula:

$$V_{p} = \sqrt{\frac{p}{\rho} - 2g}$$
 (15)

where ρ is the density of the liquid product (lbs/ft³)

p is the initial pad pressure (lb/ft^2)

g is the gravitational constant (ft/sec2)

A listing of the subroutine is presented on the following pages.

```
SUBROUTINE VCAP(TINK, PRIT, WOUT, ATEM, KPRD, PREF, SPEC, SPLO,
       HFLV, VVAP, DVDT, DSDT, DELT)
        THIS SUBROUTINE IS USED TO CALCULATE THE LIQUID MASS FLOW
C
           RATE THROUGH A SAFETY RELIEF VALVE. HOMOGENEOUS ISENTROPIC
С
           PLOW IS ASSUMED. THE PRESENSE OF A NITROGEN PAD PRESSURE
C
C
           IS ALSO TAKEN INTO ACCOUNT.
¢
        DEGF=1000.0*TTNK-460.0
        TBEG=DEGF
        KCNT=Ø
        GO TO 896
        START WITH INITIAL CONDITIONS; DROP TEMPERATURE BY 1/2 DEGREE
C
            AND CALCULATE THE CROSS SECTIONAL VALVE AREA FOR A ONE
C
C
            LB PER SEC MASS FLOW RATE.
¢
C
        KCNT=1
898
         ARONE=1000.0
         HTEST=Ø.Ø
         PTEST=PREF
         SSTND=SLIQ
         VLONE=Ø.Ø
         IF(PNIT.LT.Ø.ØØ1)GO TO 897
         VLONE=96.24*SORT(SPLO*PNIT)
         ARONE=SPLQ/VLONE
         ATEST=ARONE
 897
         DEGF=DEGF-Ø.5
 895
         CALL PROPERTIES (KPRD, DEGF, PREF, SPEC, SPLO, HFLV, VVAP, DVDT, DSDT)
 C
 896
         IF(KPRD.EQ.1)GO TO 824
         IF(KPRD.EQ.3)GO TO 841
         IF(KPRD.GE.4)GO TO 851
 C
          IF(DEGF.GE.130.0)GO TO 803
         SLIQ=-0.0594222+0.000841111*DEGF+0.0000001111*DEGF*DEGF
          GO TO 81#
          IF(DEGF.GE.190.0)GO TO 805
          SLIQ=-0.05623+0.000794167*DEGF+0.0000002833*DEGF*DEGF
 8Ø3
          GO TO 81Ø
          IF(DEGF.GE.250.0)GO TO 807
          SLIQ=-0.04626556+0.000711111*DEGF+0.0000004444*DEGF*DEGF
  895
          GO TO 810
          SLIQ=0.00984556+0.000250556*DEGF+0.0000013889*DEGF*DEGF
  8Ø7
          CONTINUE
  81Ø
  C
          IF(DEGF.GE.13Ø.Ø)GO TO 813
          SVAP=0.50970333-0.000865*DEGF+0.0000020667*DEGF*DEGF
          GO TO 828
          IF(DEGF.GE.19Ø.Ø)GO TO 815
          SVAP=8.58255333-8.888742833*DEGF+8.88888155*DEGF*DEGF
  813
          GO TO 820
          IF(DEGF.GE.25Ø.Ø)GO TO 817
          SVAP-8.468964-8.888381222*DEGF+8.88888883778*DEGF*DEGF
  815
          GO TO 828
          SVAP=0.483520-0.0004345*DEGF+0.00000055*DEGF*DEGF
  817
          GO TO 823
  828
```

PROPERTIES OF PROPANE

C

```
C
824
        IF(DEGF.GT.81.12)GO TO 825
        SLIQ=0.99838+0.000604*DEGF+0.00000376*DEGF*DEGF
        GO TO 829
        IF(DEGF.GT.135.59)GO TO 826
825
        SLIQ=0.98298+0.001052*DEGF+0.0000005858*DEGF*DEGF
        GO TO 829
        IF(DEGF.GT.172.54)GO TO 827
826
        SLIQ=1.02457+0.000435*DEGF+0.00000287*DEGF*DEGF
        GO TO 829
        IF(DEGF.GT.201.25)GO TO 828
827
        SLIQ=1.62902-0.00641777*DEGF+0.00002228*DEGF*DEGF
        GO TO 829
        SLIQ=1.23985+(DEGF-201.25)*0.006378
828
        CONTINUE
829
C
         IF(DEGF.GT.81.12)GO TO 832
         SVAP=1.35869-8.88828934*DEGF+8.888888837*DEGF*DEGF
         GO TO 839
         IF(DEGF.GT.135.59)GO TO 833
832
         SVAP=1.34298-0.00003735*DEGF-0.00000058*DEGF*DEGF
         GO TO 839
         IF(DEGF.GT.172.54)GO TO 834
833
         SVAP=1.29831+0.0005701*DEGF-0.00000263*DEGF*DEGF
         GO TO 839
         IF(DEGF.GT.281.25)GO TO 835
 834
         SVAP=0.725233+0.00705593*DEGF-0.00002097*DEGF*DEGF
         GO TO 839
         SVAP=1.29605-(DEGF-201.25)*0.004685
 835
         GO TO 823
 839
         IF(DEGF.GT.80.0)GO TO 842
 841
         F=DEGF-40.0
         SLIQ=1.06766+0.0018783*F+8.0000009*F*F
         SVAP=1.38608-0.0003250*F+0.0000013*F*F
         GO TO 849
         IF(DEGF.GT.120.0)GO TO 843
 842
         F=DEGF-80.0
         SLIQ=1.11217+0.0018975*F-8.0000006*F*F
         SVAP=1.37508-0.0001710*F-0.0000026*F*F
         GO TO 849
         IF(DEGF.GT.160.0)GO TO 844
 843
         F=DEGF-128.8
         SLIQ=1.15507+0.00009250*F+0.0000055*F*F
         SVAP=1.36408-0.0003000*F-0.0000025*F*F
         GO TO 849
          IF(DEGF.GT.18Ø.Ø)GO TO 845
 844
          F=DEGF-160.0
          SLIQ=1.20087+0.0013770*F+6.0000114*F*F
          SVAP=1.34808-0.0005500*F-0.0000050*F*F
          GO TO 849
          F=DEGF-180.0
  845
          SLIQ=1.23297+#.##12273*F+#.###1433*F*F
          SVAP=1.33508+0.0012359*F-0.0002036*F*F
          IF(DEGF.GT.190.0)GO TO 849
          G=DEGF-170.0
          SVAP=1.34208-0.0006500*G-0.000656*G*G
          GO TO 823
  849
```

823

GO TO 86Ø

```
C
851
        IF(KCNT.EQ.1)GO TO 853
        SLIQ=1.000
        DGLST=TBEG
        GO TO 868
        SLIQ=SLIQ+SPEC*(DEGF-DGLST)/((DGLST+DEGF)*#.5+459.6)
853
        SVAP=SLIQ+HFLV/(DEGF+459.6)
        DGLST=DEGF
C
86Ø
        IF(KCNT.EQ.Ø)GO TO 898
C
        X = (SSIND-SVAP) / (SLIQ-SVAP)
        VLTST=X*SPLO+(1.Ø-X)*VVAP
        HTEST=HTEST+(PTEST-PREF)*144.8*VLTST*64.4
         VELOCB=SQRT(VLONE**2+HTEST)
        ARTWO-VLTST/VELOCB
         PTEST=PREF
         IF(ARTWO.GT.ATEST.OR.PTEST.LT.14.7)GO TO 821
         ATEST=ARTWO
         GO TO 895
         REPEAT CALCULATIONS UNTIL AREA BECOMES MINIMUM; THEN CALCULA"
č
            MASS FLOW RATE.
Č
821
         WOUT=68.8*DELT*ATEM/ATEST
         CALL PROPERTIES (KPRD, TBEG, PREF, SPEC, SPLQ, HFLV, VVAP, DVDT, DSDT
 C
         RETURN
```

END

4.4 SUBROUTINE TSHIELD

Subroutine TSHIELD is used to determine the effective conductance of the thermal shield system which is constructed of a material with a conductivity which is a function of temperature. The subroutine assumes the following functional dependence of conductivity with temperature:

$$K = 0.2 + 0.1938T + 0.6769T^2$$

where T is the temperature in 1000 $^{\circ}$ F units ($^{\circ}$ F/1000) K is the conductivity (BTU-in./hr-ft²- $^{\circ}$ F)

This relationship gives an approximate tenfold increase in conductivity from 60°F to 1600°F and is representative of the maximum change one would see in a high temperature insulation material used on railroad tank cars. The subroutine requires as input the thickness of the insulation under consideration (THICK) the outer and inner temperature of the insulation system (TOUTR and TINSD, respectively) and the value of the effective conductance that was calculated at the last time step (CNDCT). The output from the subroutine is a calculated value of effective conductance of the thermal shield system which reflects the current temperature distribution through the insulation material.

The subroutine divides the insulation into 50 layers. It then starts at the inside of the shell and using the last value of CNDCT and the heat flux that this implies, it goes through the insulation layer by layer to calculate the outside temperature of the insulation system. If the calculated temperature is not sufficiently a close to TOUTR a new value for the heat flux is assumed and the calculation is repeated. When a sufficiently close value to TOUTR is achieved, it is assumed that the proper heat flux has been established through the insulation material and a new value of the effective conductance (CNDCT) is calculated using the temperature difference across the insulation system.

The principal parameters used in the subroutine are lised as follows:

TOUTR	Temperature of outside of insulation system (°F/1000)
TINSD	Temperature of inside of insulation system (°F/1000)
CNDCT	Effective conductance of insulation system (BTU/hr-ft²-°F)
THICK	Thickness of insulation system (in.)
CKND	Conductivity of thermal insulation material (BTU-in./hr-ft²-°F)
QFLX	Heat flux through insulation system (BTU/hr-ft²)

A listing of the subroutine is presented on the following page.

```
SUBROUTINE TSHIELD (TOUTR, TIMED, CMDCT, THICK)
C
        QFLX=CNDCT*(TOUTR-TIMSD)*1868.8
        KNT-Ø
        KOT-Ø
        START=TINSD*1888.8-468.8
        TWALL=START
        TPAST=TOUTR * 1888 . 8-468 . 8
        TARGET=TOUTR*1888.8-468.8
C
        DELX=THICK/58.
155
        TL=TWALL/1000.0
        CKND=8.2+8.1938*TL+8.6769*TL*TL
        TWALL = TWALL + OFLX * DELX / CKND
        IF (KNT.EQ.50) GO TO 101
        KNT=KNT+1
        GO TO 128
        CONTINUE
181
        KNT=Ø
C
        IF(ABS(TWALL-TARGET).LT.#.1)GO TO 1#3
         IF (KOT.EQ.1)GO TO 112
        ODELT=ABS(OFLX*(TWALL-TARGET)/TWALL)
        KQT=1
112
         CONTINUE
         IF (TPAST.LT.TARGET.AND.TWALL.GT.TARGET)QDELT=QDELT/3.8
         IF(TPAST.GT.TARGET.AND.TWALL.LT.TARGET)QDELT=QDELT/3.8
         IF (TWALL.GT.TARGET)OFLX=OFLX-ODELT
         IF: TWALL.LT.TARGET)QFLX=QFLX+QDELT
         TPAST=TWALL
         TWALL=START
         GO TO 100
С
1#3
         CNDCT=QFLX/((TOUTR-TINSD)*1888.8)
         RETURN
```

END

4.5 SUBROUTINE PLT3

Subroutine PLT3 is a specialized subroutine for constructing plots. It is written solely for use on a Data General Eclipse computer which uses a VERSATEC plotter. A listing of the subroutine is given on the following pages.

```
C PRODUCE ONE PLOT WITH 3 VERTICAL SCALES FORS SATA :
        SUBROUTINE PLT3 (ICOMOAND, Y1, Y2, Y3) X)
                           ECOMMAND (1)
  IF COMMAND EQ 'DATA' THEM PLOT A NEW DATA SET.
EQ 'PLOT' THEM START A NEW PLOT PAGE.
                 'STOP' THEN CLOSE ALL PLOT FILES.
  Y1 IS A DATA SET OF THE FIRST PLOT LINE.
Y2 IS A DATA SET OF THE SECOND PLOT LINE.
  Y3 IS A DATA SET OF THE THIRD PLOT LINE.
  X IS THE COMMON DATA SET FOR ALL Y COORDINATES.
  NOTE: THE PLOT COMMANDS ARE CALCOMP CALLS WHICH ARE COMPATABLEC
          WITH ROUTINES FOR THE VERSATEC AND TEXTRONIX LIBRARIES.
        DIMENSION STORE (4), PLT LAST (4), PLT MEXT (4)
C DEFINE THE RANGES FOR ALL SCALES
        DIMENSION SCALE 1: (6,3), SCALE 2 (6,3), SCALE 3 (6,3),
                   SCALE X (6,6)
  EACH VERTICAL SCALE HAS 5 UNITS (PLUS THE START EQUALS 6) AND :
       MAY HAVE ONE OF THREE POSSIBLE RANGES.
        DATA SCALE 1 /
                                  .2,
        DATA SCALE 2 /
                                        488,
                                              688,
        DATA SCALE 3 /
                                        688,
                                 388,
                                              988,
                                                    1288, 1588,
                                  488,
                                        888, 1288, 1686,
  THE HORIZONTAL SCALE ALSO HAS 5 UNITS (PLUSETHE START EQUAL 6) AND
      MAY HAVE ONE OF SIX POSSIBLE RANGES.
         DATA SCALE X /
                                                      28.
                                                           500
                                  288,
C DEFINE PLOT'S MIN AND MAX STARTING POINTS
         DATA XMIN, XMAX, YMIN, YMAX
              1.5, 6.5, 3.5, 8.6 /
  DEFINE PROGRAM INITIAL VARIABLES Y
         DATA ICURRENT, IUSE 1, IUSE 2, IUSE 3, IUSE X
```

```
TA TOPEN / # /, IUNIT / 7 /
  SEE IF THE PLOT OR STOP COMMAND IS GIVEN
         IF (ICOMMAND (1) .EQ. "PL" .OR. ICOMMAND (1) .EQ.
         GO TO 188
          IF (ICOMMAND (1) .EQ. "ST" .OR. ICOMMAND (1) .EQ. "ST")
C
         GO TO 300
  ON THE FIRST CALL, OPENOUP A SAVE FILE FOR THE DATA SETS.
          IF (IOPEN .NE. 8) GO TO 18
                  IUNIT, "PLT_SAVE.BN"
          REWIND IUNIT
          IOPEN = 1
C STORE THE DATA SETS ON THE SAVE FILE
          STORE (1) = Y1
1#
          STORE (2) = Y2
          STORE (3) = Y3
          STORE (4) = X
C
          WRITE BINARY (IUNIT) STORE
C
           ICURRENT = ICURRENT + 1
 C SEE WHICH RANGE EACH SCALE WILL BE SET TO 8
           J = IUSE 1
          DO 20 I = 3, J, -1
IF (Y1 .LE. SCALE.1 (6,I)) IUSE 1 = I).
 22
          J = IUSE 2
DO 3Ø I = 3, J, -1
IF (Y2 .LE. SCALE 2 (6,I)) IUSE 2 = I(
30
 ·C
           J = IUSE 3
           DO 40 I = 3, J, -1
           IF (Y3 .LE. SCALE.3 (6,1)) IUSE 3 = I!
 48
           J = IUSE X
           DO 50 I = 6, J, -1
IF (X .LE. SCALE.X (6,I)) IUSE X = II
 5Ø
           TYPE "SCALES SELECTED ARE", IUSE 1, IUSE 2, IUSE 3, IUSE X
           TYPE "SCALE 1 MAX =", SCALE 1 (6, IUSE 1)
TYPE "SCALE 2 MAX ==, SCALE 2 (6, IUSE 2)
TYPE "SCALE 3 MAX ==, SCALE 3 (6, IUSE 3)
TYPE "SCALE X MAX ==, SCALE X (6, IUSE X)
           RETURN
  C PLOT THE SAVED DATA SETPONTO THE SELECTED SCALES PANCES.
```

TYPE "MAKING PLOTSFOR", ICURRENT," DATA POINTS"

```
WIND IUNIT
        DO 181 I=1, ICURRENT
         READ BIMARY (IUMIT) STORE
  27
         TYPE I," DATA =", STORE
X181
         CONTINUE
         REWIND IUNIT
X
C FIRST PLOT THE BOX WITH THE THREE VERTICAL AND ONE HORISONTAL SCALES
C
         CALL PLOTS (#, #, #)
C DRAW THE BOX WITH THICK SIDES, PLUS AM EXTER LINE ON THE SIDE
C
         CALL NEWPEN (-3)
c
         CALL PLOT (XMIH, WMIH, 3)
         CALL PLOT (XMIN, YMAX, 2)
         CALL PLOT (XMAX, YMAX, 2)
CALL PLOT (XMAX, YMIN, 2)
         CALL PLOT (XMIN, VMIN, 2)
         CALL PLOT (XMIN - 8.5, YMIN, 3)
         CALL PLOT (XMIN - 8.5, YMAX, 2)
C DRAW TIC MARKS AROUND THE BOX POINTING INMARDS AND ONETHE THIRD SCALE
         CALL NEWPEN (1)
C
         IYTIC = 5
         YDIFF = (YMAX - YMIN) Y IYTIC
C
         DO 128 I = 8, IYTIC
TIC = YMIN + (I * YDIFF)
         CALL PLOT (XMIN,
                                FIC, 3)
         CALL PLOT (XMIN + 8.1, TIC, 2)
         CALL PLOT (XMAX,
                                TIC, 3)
         CALL PLOT (XMAX - 8.1, TIC, 2)
         CALL PLOT (XMIN - #.5, TIC, 3)
         CALL PLOT (XMIN - Ø.57, TIC, 2)
 128
         IXTIC = 5
         XDIFF = (XMAX - XMIN) / IXTIC
         DO 138 I = 8, IXTIC
TIC = XMIN + (I * XDIFF)
          CALL PLOT (TIC, YMIN,
          CALL PLOT (TIC, YMIN + #.1, 2)
          CALL PLOT (TIC, YMAX,
          CALL PLOT (TIC, YMAX - $.1, 2)
 138
 C DRAW THE X AXIS 'TIME' WITH INTEGER MUNBERS SEELOW THE LIME.
          DO 158 I = 1, 6
          CALL NUMBER (XMIN + ((I-1) * XDIPF), THIN - #.27 #.1,
 150
                        SCALE X (I, IUSE X), #.#$ -1)
          CALL SYMBOL (XMIN)+ 1.8, YMIN - $.4, $.15, "TIME (MIN)", $.5, 15)
```

```
Y1 AXIS 'LIQUID LEVEL' WITH DECIMAL MUMBERS OUTSIDE TO
        DO 16# I = 1,
        CALL NUMBER (XMAX + #.2, YMIN + ((I-1) * YDIFF)) #.1,
                       SCALE 1 (I, IUSE 1), 98.8, +1)
        CALL SYMBOL (XMAX + #.5, YMIN + 1.7, #.15,
                       "LIQUID LEVEL", 98.8, 12)
C DRAW THE Y2 AXIS 'PRESURE' WITH INTEGER NUMBERS OUTSIDE THE LINE.
         DO 178 I = 1, 6
         CALL NUMBER (XMIN:- 8.1, YMIN + ((I-1) * YDIFF)) 8.1,
178
                        SCALE 2 (I, IUSE 2), 98.5, -1)
         CALL SYMBOL (XMIN - #.25, YMIN + 1.5, #.15,
                        "PRESURE (PSIG)", 98.8, 14)
C DRAW THE Y3 AXIS 'TANK WALL TEMP' WITH INTEGER NUMBERS OUTSIDE.
C
         DO 188 I = 1, 6
         CALL NUMBER (XMIN'- 8.6, YMIN + ((I-1) * YDIFF)) 8.1,
SCALE 3 (I, IUSE 3), 98.8, -1)
188
C
         CALL SYMBOL (XMIN - #.75, YMIN + 1.8, ) #.15
                         "TANK WALL TEMP (P )", 98.8, 19)
         CALL SYMBOL (XMIN :- 8.85, YMIN + 3.55; 8.85, "O", 98.8, 1)
  NOW PLOT THE DATA AS THREE SEPARATE LINES. TO
          DO 250 NEXT = 1. ICURRENT
          READ BINARY (IUNIT) STORE
          PLT NEXT (1) = STORE (1) / SCALE 1 (60 IUSE 1)
 C
          PLT NEXT (2) = STORE (2) / SCALE 2 (6; IUSE 2)
          PLT NEXT (3) = STORE (3) / SCALE 3 (6) IUSE 3)
PLT NEXT (4) = STORE (4) / SCALE X (6) IUSE X)
 С
          DO 220 J=1,3
          PLT NEXT (J) = YMIN + PLT NEXT (J) * (YMAX - YMIN)
          PLT NEXT (4) = XMIN + PLT MEXT (4) * (XMAX - XMIN)
 228
          IF (NEXT .EQ. 1) GO TO 248
 C
          CALL NEWPEN (1)
          CALL MODE (18, FLOAT (177777K), 9999., 9999.)
CALL PLOT (PLT LAST (4), PLT LAST (1), 3)
           CALL PLOT (PLT NEXT (4), PLT NEXT (1), 2)
  C
           CALL NEWPEN (2)
           CALL MODE (18, FLOAT (878787K), 9999., 9999.)
  C
           CALL PLOT (PLT LAST (4), PLT LAST (2), 3)
CALL PLOT (PLT NEXT (4), PLT NEXT (2), 2)
           CALL NEWPEN (3)
           CALL MODE (18, FLOAT (181184K), 9999.; 9999.)
           CALL PLOT (PLT LAST (4), PLT LAST (3); 3)
           CALL PLOT (PLT MEKT (4), PLT MEXT (3), 2)
  łC
```

maria di Pa

25% J=1.4

PLT LAST (J) - PLT MEXT (J)

25% CONTINUE

C FINISH OFF THE CURRENT PLOT AND SET UP FOR A MEM GME.A

CALL PLOT (S.S., S.S., 999)

C REWIND IUNIT

C ICURRENT - S
IUSE 1 = 1
IUSE 2 = 1
IUSE 3 = 1
IUSE X = 1

C RETURN

C RETURN

C C C STOP ALL PLOTTING PROCESSING.

C STOP TYPE IN 'VCOPY' TO GENERATE A RASTER PLOTA"

RETURN

END

\$

1. 1. 4 11 9.41 1

5. SAMPLE PROBLEM

A sample problem is described in this section to illustrate the use of the program. The problem considers the case of a 33,600 gal. Class 105A100W tank car containing 1,3-butadiene, which is in the pool fire environment. It is assumed that the car is overturned 120° so that initially the safety relief valve would vent liquid product. It is also assumed that the thermal insulation system has an effective conductance of 4.0 BTU/hr-ft²- $^{\circ}$ F and that the safety relief valve has a flow capacity of 20,000 SCFM.

The following table lists the parameters that are entered into the computer to begin the analysis:

TERMINAL PROMPT	ENTERED VALUE
DISPLAY TYPE, LPT-12; CONSOLE-10	12 (10 for second run)
PLOT-2 PRINT TERM OR LPT-1	1 (2 for second run)
PROP-1 EO-2 PROPYL-3 BUTA-4 VC-5 MONO-6 POX-7	4
ANGLE OF TILT (DEG)	120.0
TANK DIAMETER (FT)	9.9
TANK WALL THICKNESS (IN.)	0.5
NOMINAL CAPACITY (GALLS)	33,600.0
INITIAL FRACTION FILLED	0.949
SAFETY VALVE FLOW RATING PRESSURE (PSIA)	99.7
SAFETY VALVE START-TO-DISCHARGE PRESS (PSIA)	89.7
NET ABSORPTIVITY	0.8
NET EMISSIVITY	0.8
TANK BURSTING STRENGTH (PSI)	500.0
CAR CONDUCTANCE (BTU/HR SQFT DEG F)	4.0
SAFETY VALVE RATED FLOW CAPACITY (SCFM,AIR)	20,000.0
TYPE 1 FOR CONSTANT CONDUCT. OR 2 FOR VAR. CND.	1
INITIAL CAR CONDUCTANCE (BTU/HR SQFT DEG F)	0.3
FLAME TEMPERATURE (DEG F)	1,500.0
PRESSURE (PSI) OF NITROGEN PAD	0.0
AREA EXPONENT	1.0
INITIAL TEMPERATURE (DEG F)	60.0
TIME INCREMENT (MIN)	0.1
NUMBER OF TIME STEPS BETWEEN DISPLAY	5 (7 for second run)
GAS COMPRESSIBILITY FACTOR, Z	0.77
VALVE GAS FLOW CONSTANT	0.0692

The problem has been run twice. The first time the output parameters were tabulated every 0.5 minutes. The second time a plot was made of tank wall temperature over vapor space, pressure and liquid fraction remaining as a function of time.

The tabulated output data includes the following information:

Input Conditions

SVPR	Safety valve flow rating pressure (psia)
INIT	Initial temperature (°F)
COND	Input Conductance (BTU/hr-ft²-°F)
SCFM	Valve flow capacity (SCFM)
TEMP	Flame temperature (°F)
SIZE	Car capacity (gallons)
TILT	Angle of safety relief valve from vertical (degrees)
WEIGHT	Initial weight of product (lbs)
THICK	(This parameter applicable only to case of temperature dependent conductivity. Default value of 0.0 is shown.)

Parameters Given as Function of Time

TIME	Time (minutes)
PSIG	Pressure within tank (psig)
TTNK	Temperature of product (°F)
TWAL	Temperature of outside surface of tank in wetted region (°F)
FRAC	Fraction of tank volume occupied by liquid
FMAT	Fraction of original product weight remaining
TVAP	Temperature of tank over vapor space (°F)
WOUT	Mass flow rate through safety valve (lbs/min)
PBRS	Burst strength of tank (psig)
PNIT	Partial pressure of nitrogen padding gas (psi)
KIDN	Identification no. used in program
THETA	Angle of liquid surface from horizontal (radians)
PICR	Parameter associated with liquid flow thorugh valve
CNDLQ	Effective conductance of thermal shield in wetted region (BTU/hr-ft 2 - 0 F)
CNDVP	Effective conductance of thermal shield in vapor region (BTU/hr-ft 2 - $^\circ$ F)
FRACLQ	Fraction of original product weight in liquid state

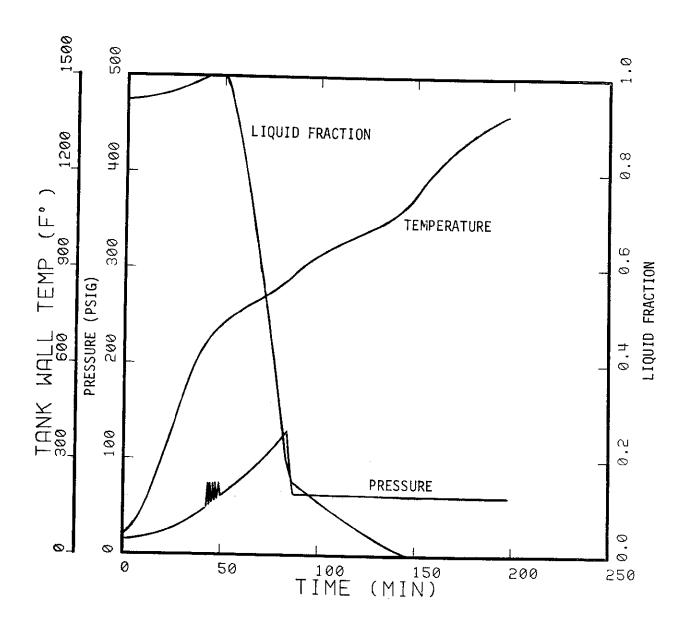
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PRESSURE, TANK WALL TEMPERATURE OVER VAPOR SPACE AND FRACTION OF TANK VOLUME FILLED WITH LIQUID AS FUNCTION OF TIME; 33,600 GAL. 105A100W TANK CAR CONTAINING 1,3-BUTADIENE, OVERTURNED (120°) CAR CASE, SAFETY RELIEF VALVE FLOW CAPACITY 20,000 SCFM, THERMAL SHIELD CONDUCTANCE 4.0 BTU/HR-FT²-°F

6. REFERENCES

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