TANK CAR THERMAL ANALYSIS, VOLUME I, USER'S MANUAL FOR ANALYSIS PROGRAM

U.S.Department
of Transportation

Federal Railroad
Administration

Office of Research and
Development
Washington, D.C. 20590

M. R. JOHNSON
IIT Research Institute
Chicago, IL 60616

DOT/FRA/ORD-98/09A

November 1998
FINAL REPORT

This document is available to the U.S. public through the National Technical Information Service Springfield, Virginia 22161

Technical Report Documentation Page

Title

Tank Car Thermal Analysis,
Volume I, Users Manual for Analysis Program

Report Date

November 1998

Author(s)

Milton R. Johnson

Performing Organization Name and Address

IIT Research Institute
10 W. 35th Street
Chicago, IL 60646

Abstract

The computer program AFFTAC is described. The program can be used to analyze the behavior of railroad tank cars when subjected to fire. It is designed to perform the analyses which are required to determine if a tank car meets the requirements of the Code of Federal Regulations, Title 49, Part 179, Section 179.18. The conditions associated with two types of fires are built into the program, the pool fire environment, where the car is fully engulfed by flame, and the torch fire environment, where only a small area of the tank is subjected to a high intensity flame. Other fire conditions can also be analyzed. A wide variety of tank car types can also be considered including cars equipped with safety relief valves or safety vent closed with a frangible disc. The program is described in two volumes. This volume describes the manner in which data is entered to describe the initial analysis conditions. The thermal properties of the product contained in the tank car are also required for the analysis. Properties of 16 commodities are contained in the program. For other commodities, the thermal properties can be entered as part of the initial analysis conditions. Several options are also provided for the output of the results of an analysis.

Key Words

railroad tank car, tank car failure, hazardous material release, fire effects

Distribution Statement

Document is available to the public through the National Technical Information Service, Springfield, Virginia 22161

PREFACE

The work described in this report was conducted by IIT Research Institute (IITRI) under authorization of Federal Railroad Administration (FRA) Contract Nos. DTFR53-90-C-00042, Task Order No. 6, and DTFR53-97-P-00325.

The work was directed at the further development of a program to analyze the effects of fire on a tank car and the product contained in the tank. The final report on this project is presented in two volumes. This volume, Volume I, describes the use of the analysis program and presents example analyses. A second volume, Volume II, is the technical documentation report for the program.

The first period of performance was from September 1994 to March 1995. The program was then distributed to selected users for comment. The FRA reviewed these comments and requested several changes be made in the program and the documentation. Authorization to proceed with the work was received in May 1997. A test version of the software and the draft of the final report was delivered in October 1997. Authorization to deliver the final software and report was received in September 1998.

Dr. Milton R. Johnson was the IITRI Project Manager for this work. Mr. Jose Pena was the FRA Technical Monitor for this project. Mr. Garold R. Thomas was the FRA Contracting Officer's Technical Representative. The contributions of these individuals throughout the course of the work are gratefully acknowledged.

Respectfully submitted,

Milton R. Johnson

EXECUTIVE SUMMARY

This report describes the use of the computer program AFFTAC (Analysis of Fire eFfects on TAnk Cars) which can be used to analyze the behavior of tank cars and the products they contain when subjected to fire. It describes procedures for entering data to provide the initial conditions of the analysis and the options for obtaining the output data, which present the results of the analysis. A separate Technical Documentation Report presents and explains the assumptions and procedures used in the analysis and provides listings of the source codes. The program is designed for interactive use with a video monitor. The results can be displayed at the monitor or written to a file.

There are two parts for the entry of data into the program, the first dealing with the entry of the variables describing the initial conditions for the analysis and the second dealing with the entry of thermal property data. The initial analysis data can be entered at the monitor or read from an existing computer file. Regardless of whether the initial data is read into the program from a file, or entered at the keyboard, the data is sent to a "Report File" so that there is a permanent record of the data.

The next step in the program is the entry of the thermal property data. This can be done by entering the data at the keyboard, by reading a previously developed file of property data, or by using the data for one of the commodities which are stored in the program. Two types of commodities are considered, substances and two-component solutions. After all of the thermal property data have been entered, they are written to a file in a special format so that the data can be read as needed by the analysis program. A copy of the file can be saved for future use so that the thermal property data would not have to be re-entered when additional analyses are conducted.

After all of the initial data have been entered into the program, the options for presenting the results of the analysis are presented. Three alternatives are offered, output data displayed on the monitor, output data written to a file, and output data both displayed on the monitor and written to a file.

After the analysis has ended, either by predicting the failure of the tank, by reaching the time limit, or by reaching some other critical condition, options are presented for terminating the program or for restarting it with the same or modified initial analysis conditions.

Three examples are presented illustrating the use of the program.

TABLE OF CONTENTS

TABLE OF CONTENTS (CONTINUED)

USER'S MANUAL FOR PROGRAM AFFTAC

1. INTRODUCTION

1.1 SCOPE OF PROGRAM

This report describes the use of the program AFFTAC (Analysis of Fire eFfects on TAnk Cars) which can be used to analyze the behavior of tank cars and the products they contain when subjected to fire. It describes procedures for entering data to provide the initial conditions of the analysis and the options for obtaining the output data, which present the results of the analysis. A separate Technical Documentation Report presents and explains the assumptions and procedures used in the analysis and provides listings of the source codes.

The program has been written in FORTRAN using Microsoft Version 5.0 FORTRAN and is intended for use on a personal computer. It has been compiled using the /FPi option which does not require the use of a 8087/80287/80387 math coprocessor to perform floating point operations, but will use it if present in the computer. The program is designed for interactive use with a video monitor. The results can be displayed at the monitor or written to a file.

Fig. 1.1 illustrates the basic phenomena which must be taken into consideration in the analysis of fire effects on tank cars. The car may be in the upright position venting vapor or overturned venting liquid. Most of the heat is conducted into the car through the wetted area of the tank. The properties of the thermal shield (insulation system) determine the rate of heat transfer into the liquid product. Some heat is also conducted through the thermal shield over the vapor space. This increases the temperature of the tank wall in this region more than in the wetted area of the tank. The burst pressure 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 pressure within the tank, failure is assumed, which would cause the sudden release of the product remaining within the car.

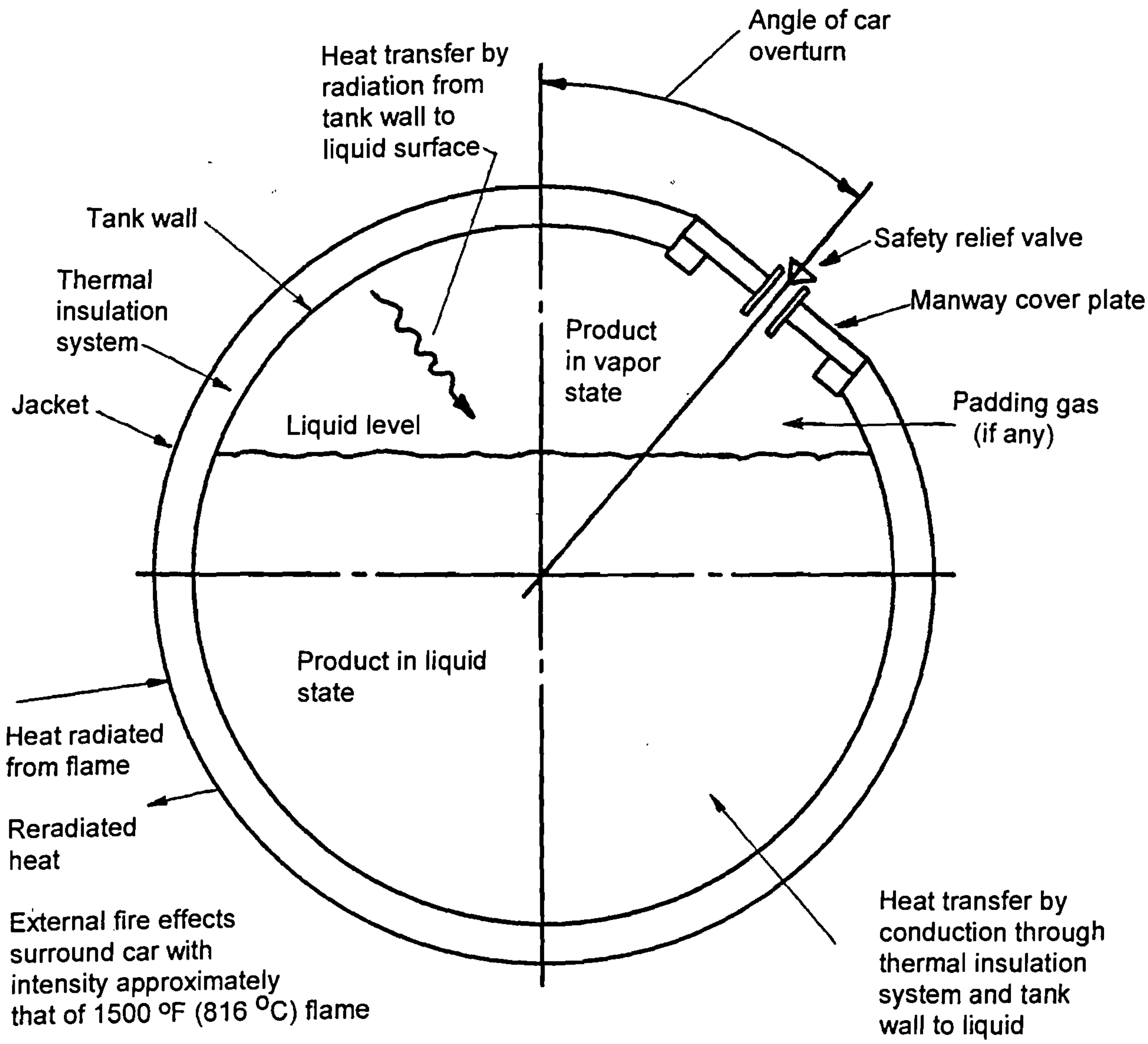

FIG. 1.1 CONDITIONS CONSIDERED IN THE ANALYSIS OF TANK CARS SUBJECTED TO FIRE

1.2 LIMITATIONS OF ANALYSIS

Several assumptions are made in the analytic procedure which limit the scope of the types of situations that can be considered. First, it is assumed that the liquid product within the tank is at a uniform temperature. This implies that the liquid product has low viscosity because this would lead to rapid mixing of the liquid as heat is transferred to it through the tank wall and insulation. Rapid mixing would not take place if the liquid had a high viscosity and this would lead to a nonuniform temperature which would influence the effects of the fire on the tank and the product within the tank.

While the present version of the analytic procedure allows one to consider products which are solutions, it is limited to two-component solutions. Entry of thermal property data for a two-component solution involves considerably more effort than for a substance. Entry of thermal property data for a solution with additional constituents would require considerably greater effort.

A third limitation is that the present analytic procedure does not permit consideration of chemical reactions or changes in phase within the product which would result in the liberation or absorption of heat (except, of course, for the vaporization of product). As certain products are heated beyond a temperature limit, they may undergo a reaction which liberates heat. This would tend to increase the rate of increase of temperature and pressure within the tank.

The analytic procedure considers the effect of discontinuities such as the manway nozzle, jacket spacers, and body bolsters when computing the total heat flow into the tank, but it does not predict the temperature of the tank wall at these locations. The effect of heat flow through discontinuities might lead to local "hot spots" at these locations particularly if the discontinuity were in the vapor space region of the tank, and could be of concern with commodities where a chemical reaction may be initiated if they are raised to a certain temperature.

2. INITIATION OF PROGRAM AND DATA ENTRY

2.1 OVERALL DESCRIPTION

Fig. 2.1 presents a flow chart showing the options and logic for the initiation of the program and the entry of data. There are two parts for this process, the first dealing with the entry of the variables describing the initial conditions for the analysis and the second dealing with the entry of thermal property data. The program is initiated by entering the command AFFTAC*

2.1.1 <u>Entry of Analysis Data</u>

The first decision point is whether the initial values are to be entered at the monitor or read from an existing computer file. If a file is used it must be in the specific format described in Section 2.3.7. A statement then appears on the monitor asking for the name of the file to be entered. If the values are to be entered, one at a time, at the monitor, subroutine ENTRDAT.FOR is called and the values are entered as described in Section 2.3. After all the values have been entered, a statement appears on the monitor asking whether the entered data should be saved in a special file. If so, another statement appears asking for the name of this file to be entered. The data in this file are also stored in the format described in Section 2.3.7, so that they can be used in the future as an input file to run the same type of analysis again. If one decides to run a slightly different case, it is convenient to use an editor to modify the file and then use it as the input file. This will save the effort of entering the values, one at a time, at the monitor.

The flow chart, Fig. 2.1 shows that regardless of whether the initial data is read into the program from a file, or entered at the keyboard, the data is sent to a "Report File", which is named by the user, so that there is a permanent record of the data. This file can be printed to obtain a permanent record.

---

* The program can be run from Windows 95 by using Windows Explorer to find the AFFTAC icon and then double clicking the icon.

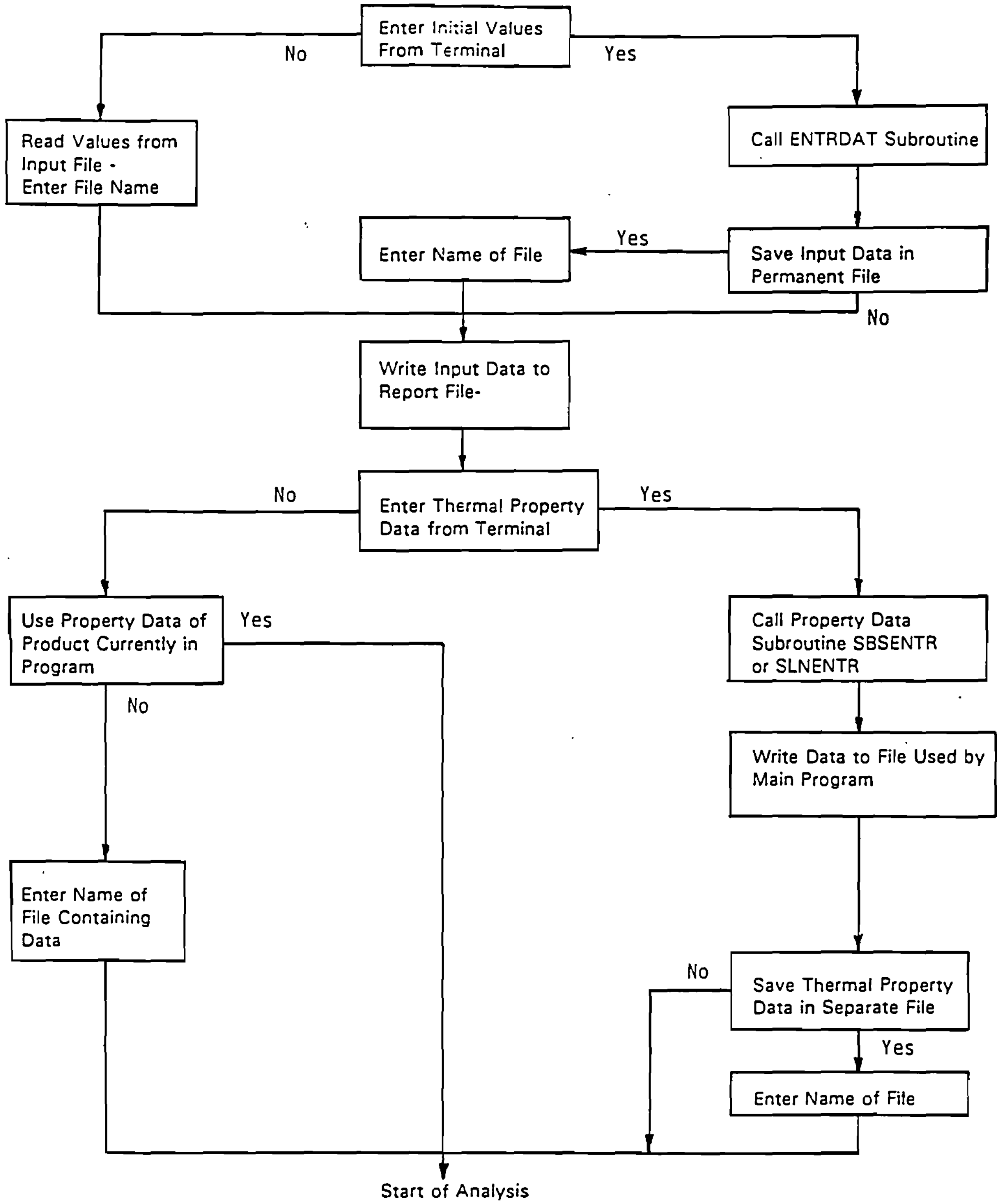

FIG. 2.1 FLOW CHART OF DATA ENTRY FOR PROGRAM 'AFFTAC'

2.1.2 Entry of Thermal Property Data

The next step in the program is the entry of the thermal property data. As indicated by the flow chart, this can be done by entering the data at the monitor, by reading a previously developed file of property data, or by using the data for one of the commodities which are stored in the program. Two types of commodities are considered, substances and two-component solutions.

The procedures for entering thermal property at the monitor are given in Section 3. After all of the data have been entered, they are written to a file in a special format so that the data can be read as needed by the analysis program. This file is named NEWSBS.DAT, if the product is a substance, or NEWSLN.DAT, if the product is a solution. These files are closed and deleted at the end of the analysis. A copy of the file can be saved for future use so that the thermal property data would not have to be reentered for a future analysis. A statement appears on the monitor asking if the data are to be saved. If so, another statement appears asking for the name of the file to be entered. If the thermal property data are entered at the monitor, the data are added to the report file described in the preceding section. This provides a permanent record of the thermal property data entered into the program. If thermal property data stored in the program are used, a summary of the data is added to the report file described in the preceding section. The flow chart indicates that another method of entering the thermal property data is to read a file containing the data. The file must be in the proper format (See Section 3). If this method of data entry is selected a statement appears on the monitor asking for the name of the file to be entered.

The third method of running the analysis program is to use thermal property data stored in the program. If this option is selected, a statement appears on the monitor requesting that the code number of the product be entered. Data for 16 different commodities are available. They are listed in Section 2.3.

2.2 INITIATION OF PROGRAM

The program is initiated by entering the command AFFTAC*. A statement then appears on the monitor asking whether the initial analysis values are to be entered, one at a time, at the monitor or read from a file, as follows:

> ENTER CODE DESIGNATING PROCEDURE FOR ENTERING ANALYSIS DATA (integer number):
>
> (1) Data entry at monitor
> (2) Data read from existing file

If the code for data entry at the monitor is entered, the program goes to the series of interactive steps described in the next section, Section 2.3. If the code for data read from an existing file is entered, the program asks for the entry of the name of the file, as follows:

> ENTER NAME OF FILE CONTAINING DATA (Maximum of 12 Characters):

It then asks for the name of the product to be entered if it is not one of the 16 products which have their thermal properties stored in the program.

> ENTER NAME OF PRODUCT (Maximum of 30 Characters):

2.3 KEYBOARD ENTRY OF ANALYSIS CONDITIONS

This section describes the entry of the initial analysis conditions at the monitor. The name of the variable that is entered at each step in the interactive process is given in this description so that it can be identified in the source code. (The variable names do not appear on the monitor screen.) The prompts for the data indicate whether the value should be entered as a decimal number (a number with a decimal point included) or as an integer number (a number without a decimal point).

---

* The program can be run from Windows 95 by using Windows Explorer to find the AFFTAC icon and then double clicking the icon.

2.3.1 Tank Parameters

The program first calls for the entry of parameters describing the tank as follows:

ENTER NOMINAL CAPACITY OF TANK (decimal number, gallons): SIZE

ENTER TANK INSIDE DIAMETER (decimal number, ins.): DIAI

ENTER TANK WALL THICKNESS (decimal number, ins.): WTKI

Next the program asks for the entry of a code number which designates the type of material used to construct the tank. Three options are offered: carbon and low alloy manganese steel, stainless steel, and aluminum, as follows:

ENTER FOLLOWING CODE NUMBER FOR TYPE OF MATERIAL
(integer number): MCLASS

(1) Carbon and low alloy manganese steel
(2) Stainless Steel
(3) Aluminum

Appendix A of this document lists the materials authorized for tank car construction by the Code of Federal Regulations (CFR) along with their minimum required tensile strengths. If the first option (1) is chosen, a list of the 15 types of carbon and low alloy manganese steel appear on the monitor along with a code number designating each specification. If the second option (2) is chosen, a list of the 4 types of stainless steel appear on the monitor along with a code number designating each specification. If the third option (3) is chosen, a list of the 7 types of aluminum appear on the monitor along with a code number designating each specification. Following any of these lists a statement appears on the monitor requesting the entry of the code number for the specific type of material used to construct the tank, as follows:

ENTER CODE NUMBER FOR SPECIFIC TYPE OF MATERIAL
(Integer number): IMT

The program then automatically reads the appropriate tensile strength (TNSRTH) for the type of material.

At this point the burst pressure of the tank is calculated based on the tensile strength of the material, the inside tank diameter, and the tank wall thickness. This variable is named PCBRS. Next, the nominal burst pressure of the tank based on the DOT specification number is entered as follows:

> ENTER TANK NOMINAL BURSTING PRESSURE (decimal number, psig): PNBRS

A check is then made to insure the calculated burst pressure (PCBRS) is equal to or greater than the nominal burst pressure (PNBRS). If not, the following message will appear on the screen:

> INCONSISTENT BURST PRESSURE

The appropriate tank variables should then be determined, the data entry process stopped, and the data entry begun over again with the correct values.

2.3.2 Product Data

The program calls for the following data describing the product contained in the tank. First, three alternatives are presented for the entry of thermal property data. These alternatives are identified by code numbers as follows:

(1) Use property data for products contained in the program,
(2) Enter new property data at monitor, or
(3) Use property data contained in a separate file.

The appropriate code number is then entered into the program:

> ENTER CODE FOR METHOD OF ENTRY OF THERMAL PROPERTY DATA (integer number): IPTYP

If the first alternative is selected a list of products is displayed on the monitor which have their thermal properties stored in the program. These products along with their identification numbers are listed as follows:

1 - Water
2 - Propane
3 - Ethylene Oxide
4 - Propylene
5 - 1,3 Butadiene
6 - Vinyl Chloride
7 - Monomethylamine
8 - Propylene Oxide
9 - Anhydrous Ammonia
10 - Sulfuric Acid, permissible concentration range 92-94% by weight
11 - Hydrochloric Acid, permissible concentration range 32-38% by weight
12 - Sodium Hydroxide, permissible concentration range 50-60% by weight
13 - Phosphoric Acid, permissible concentration range 75-85% by weight
14 - Superphosphoric Acid (76%P_20_5)
15 - Potassium Hydroxide, permissible concentration range 44-50% by weight
16 - Hydrogen Peroxide Solution, permissible concentration range 66-82% by weight

The program then calls for the entry of the appropriate product identification number:

ENTER PRODUCT NUMBER (integer number): IPR

If the second alternative is selected, the program calls for the entry of the name of the product as follows:

ENTER NAME OF PRODUCT (Maximum of 30 characters): CPRD(20)

After all of the analysis data is entered, the program calls Subroutine SBSENTR.FOR for the entry of thermal property data for a substance, or Subroutine SLNENTR.FOR for the entry of thermal property for a solution (See Section 3). If the third alternative is selected, the program calls for the entry of the name of the product, and then the name of the file containing the data as follows:

ENTER NAME OF PRODUCT (Maximum of 30 characters): CPRD(21)

ENTER NAME OF FILE CONTAINING DATA (Maximum of 12 characters): PNAME

The file must be in the proper format as described in Section 3.

Next, a code is entered for specifying whether the product is a substance or solution.

ENTER CODE FOR TYPE OF PRODUCT (integer number): ISBSL

(1) for substance
(2) for solution

If the alternative was chosen for the entry of product data not in the program the program then asks if there is a critical temperature associated with the product. This would be the temperature at which a self-reaction of the product would begin leading to a rapid increase in temperature and pressure within the tank. It is not the critical temperature above which a substance can only exist in a gaseous state. The following statement appears on the monitor screen:

DOES PRODUCT HAVE A CRITICAL TEMPERATURE?
ENTER Y OR N (FOR YES OR NO): LRESP

If the answer is yes (Y), the program then calls for the entry of the critical temperature, as follows:

ENTER CRITICAL TEMPERATURE (decimal number, °F): TCRIT

The next step in the entry of product data is to enter the initial fraction of the tank volume which is filled with liquid product, as follows:

ENTER INITIAL FRACTION OF TANK FILLED (decimal fraction): FRAT

Then the program calls for the entry of the initial temperature of the product as follows:

ENTER INITIAL TEMPERATURE OF PRODUCT (decimal number, °F): TEMC

If the product is a solution, the program calls for its concentration to be entered, as follows:

ENTER CONCENTRATION OF PRODUCT (decimal fraction): CONC

The final entry under product data deals with the presence or absence of a padding gas. Three alternatives are presented. They are identified by code numbers as follows:

(1) A padding gas is used to bring the internal tank pressure up to atmospheric pressure if the vapor pressure of the product at its initial temperature is below atmospheric pressure.

(2) No padding gas is used.
(3) A padding gas is added to the tank bringing the pressure in the tank up to a specific gage pressure (psig) at the beginning of the analysis.

The appropriate code number is then entered into the program:

ENTER CODE FOR PRESENCE OF PADDING GAS (integer number): IPAD

If the third alternative is selected the program calls for the entry of the final gage pressure of an air or nitrogen pad.

ENTER GAGE PRESSURE WITHIN TANK AFTER ADDITION OF PADDING GAS (decimal number, psig): PPID

If this alternative is selected and the target gage pressure is less than the vapor pressure of the product at the initial temperature, no padding gas will be added.

2.3.3 Safety Relief Device Parameters

The next step in the entry of data deals with the type and characteristics of the safety relief device. Two altematives are presented. They are identified by code numbers as follows:

(1) Safety relief valve is used.
(2) Safety vent with frangible disc is used.

The appropriate code number is then entered into the program.

ENTER CODE FOR TYPE OF SAFETY RELIEF DEVICE (integer number): IVLTYP

If a safety vent with a frangible disc is used, the program calls for the entry of the cross sectional area of the vent and the pressure at which the disc fractures, as follows:

ENTER DISCHARGE AREA OF VENT (decimal number, in.^{2}): AVENT

ENTER FRANGIBLE DISC RUPTURE PRESSURE (decimal number, psig): VGTD

If a safety relief valve is used, the program calls for the entry of the rated flow capacity, the flow rating pressure, and the start-to-discharge pressure, as follows:

ENTER SAFETY VALVE RATED FLOW CAPACITY (decimal number, SCFM, air): SCFM

ENTER SAFETY VALVE FLOW RATING PRESSURE (decimal number, psig): PGSD

ENTER SAFETY VALVE START-TO-DISCHARGE PRESSURE (decimal number, psig): PGTD

The next step in the entry of data related to the safety relief device is entry of the discharge coefficients for vapor and liquid flow through the valve or vent. If the specific coefficients for the valve are not available, 0.8 can be entered for the vapor discharge coefficient and 0.6 for the liquid discharge coefficient as conservative estimates. The program calls for the entry of these data as follows:

ENTER SAFETY RELIEF DEVICE VAPOR DISCHARGE COEFFICIENT (decimal fraction): CVAD

ENTER SAFETY RELIEF DEVICE LIQUID DISCHARGE COEFFICIENT (decimal fraction): CDLQ

The final entry under safety relief device data calls for the entry of the rollover angle of the tank by indicating the orientation angle of the tank car with respect to the vertical (See Fig. 1.1). The data is entered as follows:

ENTER ROLLOVER ORIENTATION ANGLE OF TANK CAR WITH RESPECT TO VERTICAL (decimal number, degs): TILT

For the upright car condition 0.0 would be entered. (Note: A rollover angle of 120 degrees has been used by the FRA to evaluate the rollover condition.)

2.3.4 Thermal Protection System Characteristics

The next step in the entry of analysis data deals with the characteristics of the thermal insulation system on the tank, if any. First, five alternatives are presented. They are identified by code numbers as follows:

(1) Bare, uninsulated tank.

(2) Insulation system which meets FRA high-temperature requirements. Tank cars equipped with such a system would have the letter "J" or "T" in their DOT specification number. (Note: Selection of this option does not preclude the need to consider the effect of tank car discontinuities. See page 19.)

(3) A steel jacketed insulation system where the insulation will lose its effectiveness at high temperature. Initially, the system will have a low conductance. Over a fixed period of time the insulation will deteriorate so that only the presence of the jacket will serve to resist heat flow into the tank. (For example, tests have shown that fiberglass insulation will lose its effectiveness in a pool fire environment over a period of about 15 minutes.)

(4) Other insulation systems where the thermal conductivity of the insulation is assumed to be independent of the temperature of the insulation.

(5) Other insulation systems where the thermal conductivity of the insulation is assumed to be a function of the temperature of the insulation. The temperature dependence of the conductivity is assumed to be a quadratic function of the form:

$$K = A_1 + A_2 T + A_3 T^2$$

where: K is conductivity (BTU/hr-ft^2)/(°F/ft)
T is temperature (°F/1000),
A_1, A_2 and A_3 are constants.

(6) A steel jacketed, two component insulation system where the outer layer of insulation may or may not lose its effectiveness at high temperature [like (3) above] and the inner layer adjacent to the tank wall is a high temperature insulation having a thermal conductivity which is a function of temperature. An example of such a system would be 0.5 inches of Fiberfrax adjacent to the tank wall covered by 3.5 inches of fiberglass and a steel jacket.

The appropriate code is then entered into the program:

ENTER CODE FOR TYPE OF THERMAL INSULATION SYSTEM
(integer number): INS

If the first alternative is selected, a bare uninsulated tank, the thermal resistance to heat flow into the tank is limited to the effect of the tank wall thickness and the film coefficient in the liquid region at the inside surface of the tank.

If the second alternative is selected, an approved high-temperature insulation system, the conductance of the thermal insulation system is assumed to be 4.0 BTU/hr-ft^2-°F. This is the maximum conductance implied by the performance tests prescribed in Appendix B to Part 179 of the CFR. (See Section 6 of Ref. 1, Volume I, listed in the Technical Documentation Report of this project (Volume II) for a discussion of how this value is estimated from performance test results.)

If the third alternative is selected, a jacketed non-high-temperature system, the program calls for the entry of the initial conductance of the system and the period of time over which the insulation is assumed to lose its effectiveness.

> ENTER INITIAL CONDUCTANCE OF THERMAL INSULATION (decimal number, BTU/hr-ft^2-°F): CNDI
>
> ENTER TIME INTERVAL FOR CHANGE IN CONDUCTANCE (decimal number, minutes): CINTV

If the fourth alternative is selected, a system where the conductance is independent of temperature, two additional alternatives are offered, one where the conductance of the system is constant with time and the other where the conductance changes linearly over a fixed time period from an initial value to a steady state value. This provides a method of representing deterioration in the performance of the insulation system as it is exposed to the effects of a fire. The program calls for the entry of a code number to specify the selection of the appropriate case as follows:

(1) Conductance changes with time, or
(2) Conductance constant with time.

> ENTER CODE FOR CONSTANT CONDUCTANCE OR LINEAR CHANGE WITH TIME FROM INITIAL VALUE TO FINAL VALUE (integer number): KINDX

In either case, the program then calls for the entry of the final conductance of the system.

> ENTER THERMAL INSULATION FINAL CONDUCTANCE (decimal number, BTU/hr-ft^2-°F): CNDD

If the option for a linear change in conductance with time is selected the program calls for the entry of the initial conductance and the time interval for the change from the initial value to the final value.

> ENTER INITIAL CONDUCTANCE (decimal number, BTU/hr-ft^2-°F): CNDI
>
> ENTER TIME INTERVAL FOR CHANGE IN CONDUCTANCE (decimal number, minutes): CINTV

If the fifth alternative is selected, conductivity of the insulation is a function of temperature, the program calls for the entry of the thickness of the insulation and the three parameters (as defined earlier in this section) which define its dependence on temperature.

> ENTER THICKNESS OF INSULATION (decimal nurnber, ins.): THIC
>
> ENTER FIRST CONDUCTIVITY PARAMETER (decimal number): A1
>
> ENTER SECOND CONDUCTIVITY PARAMETER (decimal number): A2
>
> ENTER THIRD CONDUCTIVITY PARAMETER (decimal number): A3

If the sixth alternative is selected, the program first calls for the entry of the initial conductance of the outer layer of insulation:

> ENTER INITIAL CONDUCTANCE OF OUTER INSULATION LAYER (decimal number, BTU/hr-ft^2-°F): CNDI

The program then asks if the conductivity of the outer layer of insulation changes linearly with time and calls for the entry of a code number to specify the selection of the appropriate case as follows:

(1) Conductance of outer layer changes with time, or
(2) Conductance of outer layer constant with time.

ENTER CODE FOR CONSTANT CONDUCTANCE OR LINEAR CHANGE OF CONDUCTANCE OF OUTER LAYER OF INSULATION WITH TIME FROM INITIAL VALUE TO FINAL VALUE (integer number): KINDX

If the option for a linear change in conductance is selected the program calls for the entry of the time interval for the change from the initial value to the final value:

ENTER TIME INTERVAL FOR CHANGE IN CONDUCTANCE (decimal number): CINTV

The program then asks if after the period of linear change in conductance, the effectiveness of the outer layer has been completely lost or whether it maintains a final steady state value (For example, if fiberglass were used for the outer layer of insulation, its effectiveness can be assumed to be completely lost after a period of about 15 minutes.):

DOES OUTER INSULATION LAYER MAINTAIN FINAL STEADY STATE VALUE AFTER LINER CHANGE (Y OR N)? RESPNS

Enter Y or N for yes or no. If the answer is yes, the program calls for the entry of the final conductance of the system:

ENTER FINAL CONDUCTANCE OF OUTER LAYER OF INSULATION (decimal number, BTU/hr-ft^2-°F): CNDD

If the answer is no, the program assumes a final conductance for the outer layer of insulation of 40.0 BTU/hr-ft^2-°F. This represents the effect of the residual ash following the deterioration of the insulation.

Next, the program asks for the characteristics of the layer of insulation adjacent to the tank wall which is assumed to function up to the temperature found in the fire environment. Its conductivity is assumed to be a quadratic function of temperature as in the fifth insulation alternative. The program first calls for the entry of its thickness in inches as follows:

ENTER THICKNESS OF INNER LAYER OF INSULATION (decimal number, ins.): THIC

Finally, the three parameters which define the conductivity of this layer of insulation as a function of temperature are entered. The representation of the conductivity as a function of temperature is the same as in the fifth alternative, namely:

$$K = A_1 + A_2T + A_3T^2$$

where: K is conductivity (BTU/hr-ft^2)/(°F/ft),
T is temperature (°F/1000),
A_1, A_2 and A_3 are constants.

The program states:

ENTER FIRST CONDUCTIVITY PARAMETER (decimal number): A_1

ENTER SECOND CONDUCTIVITY PARAMETER (decimal number): A_2

ENTER THIRD CONDUCTIVITY PARAMETER (decimal number): A_3

This completes the entry of data for the sixth type of insulation system.

The next step in the entry of data related to the thermal protection system concerns discontinuities in the thermal protection system which could increase the heat flow into the tank. The effect of discontinuities in the insulation around the tank should be considered on insulated tank cars. Two alternatives are presented. They are identified by code numbers as follows:

(1) Discontinuities not considered in analysis.
(2) Discontinuities considered in analysis.

The appropriate code number is then entered into the program.

ENTER CODE FOR CONSIDERATION OF HEAT TRANSFER THROUGH DISCONTINUITIES (integer number): IDSC

If the second alternative is selected the program calls for the entry of the sum total of all of the "U" factors* represented by the discontinuities. The following list presents typical U factors for the metal fittings on a jacketed tank car with a 4 inch thick insulation:

---

*A "U" factor is defined as an overall heat transfer coefficient (BTU/hr-°F) in the equation:

$$Q = U\Delta T$$

where: Q is a heat flux (BTU/hr), and
ΔT is a temperature differential between inside and outside of tank (°F).

Manway Nozzle and Manway Cover	14.6 BTU/hr-°F
Siphon and Air Vent Nozzle	6.1
Safety Relief Valve Nozzle	3.2
Jacket Spacers	15.5
Bottom Outlet Saddle	13.1
Draft Sills (2, one each end of car)	72.9
Body Bolsters (2, one each end of car)	65.0
Brake Cylinder Support	4.6
Brake Rod Lever Support	3.2

The use of special insulation on some of these components would reduce their U factor. For example, the U factor for a boxed in manway nozzle would be about 5.0 BTU/hr-°F. For jacketed cars with a 6 inch thickness of insulation, the above component values can be reduced by 15 percent because of the longer heat loss path.

Select and sum the component U factors appropriate for the tank car being analyzed and enter the resultant value in response to the following prompt:

> ENTER SUM TOTAL OF "U" FACTORS (decimal number, BTU/hr-°F):
> USUM

The next step in the entry of data related to the thermal protection system is the consideration of tank linings. Two alternatives are presented. They are identified by code numbers as follows:

(1) Tank linings are not considered in analysis
(3) Tank linings are considered in analysis

The appropriate code number is then entered into the program:

> ENTER CODE FOR CONSIDERATION OF TANK LININGS (integer number): LLNG

If the second alternative is selected the program calls for the entry of the code number describing the type of lining. Two alternatives are presented which are identified by code numbers as follows:

(1) Six (6) mil organic liner
(2) 3/16 inch thick rubber liner

The appropriate code number is then entered into the program.

ENTER CODE FOR TYPE OF LINING (integer number): ILN

The program then asks if the lining would deteriorate with time during the exposure to fire because of the increase in temperature of the tank wall, as follows:

DOES LINING DETERIORATE OVER FIXED TIME PERIOD?
ENTER Y OR N (FOR YES OR NO): LRESP

If the answer is yes (Y), the program then calls for the entry of the time period over which the lining deteriorates, as follows:

ENTER TIME INTERVAL FOR DETERIORATION OF LINING (decimal number, minutes): LINTV

2.3.5 Fire Conditions

The next step in the entry of data deals with the conditions of the fire to which the tank is subjected. Three alternatives are present. They are identified by code numbers as follows:

(1) Standard pool fire analysis. This option subjects the entire surface of the tank to the effects of a fire with a 1500 °F flame temperature.
(2) Standard torch fire analysis. This option subjects a 16 ft^2 (4 by 4 ft) surface of the tank to the effects of a fire with a 2200 °F flame temperature.
(3) Special conditions fire analysis.

The appropriate code number is then entered into the program.

ENTER CODE FOR TYPE OF FIRE ANALYSIS (integer number): IFRTYP

If the third alternative is selected the program calls for the entry of the flame temperature and the fraction of the total surface of the tank subjected to fire as follows:

ENTER FLAME TEMPERATURE (decimal number, °F): TEMF

ENTER FRACTION OF TANK SURFACE SUBJECTED TO FIRE (decimal fraction): CFRA

The final item related to the fire conditions calls for the entry of the emissivity/absorptivity of the surface of the thermal insulation system. A typical value for this parameter would be 0.8.

ENTER EMISSIVITY/ABSORPTIVITY OF SURFACE (decimal fraction): ERAD

2.3.6 Analysis Conditions

The final data entered into the program deals with the conditions under which the analysis is conducted. The first is the time increment between steps in the analysis. It must be expressed in terms of a decimal fraction of a minute, the smallest allowable increment being 0.01 minutes. A time increment of 0.1 minutes is the recommended time increment and is the maximum time increment that should be used.

ENTER TIME INCREMENT (e.g. 0.1) FOR ANALYSIS
(decimal number, minutes): DELT

The next entry calls for the number of time increments between the display of output data (e.g. if DELT is 0.1 min, entry of the number 10 would mean that output data is displayed at one minute intervals).

ENTER NUMBER OF TIME INCREMENTS BETWEEN DISPLAY OF OUTPUT DATA (integer number): INTV

The final entry calls for the time limit of the analysis. If the analysis does not predict failure of the tank within this time period, the analysis will be terminated.

ENTER TIME LIMIT OF ANALYSIS (decimal number, minutes): TLIMIT

2.3.7 Option to Save Analysis Data in File

After all of the required data have been entered into the program, a statement appears on the monitor asking if the data should be saved in a new file so that it could be used or modified for future analyses.

DO YOU WISH TO WRITE ANALYSIS DATA TO A NEW FILE (Y OR N)?

Enter Y or N for yes or no. If the answer is yes, the program asks for the name of this new file.

ENTER NAME OF FILE (maximum of 12 characters): BNAME

Each item of data is allocated 8 character spaces in the file arranged into 11 rows as follows:

SIZE, DIAI, WTKI
IMT, TNSRTH, PNBRS, PCBRS
IPTYP, ISBSL, IPR, ICR, TCRIT
FRAT, TEMC, CONC, IPAD, PPID
IVLTYP, AVENT, VGTD, SCFM
PGSD, PGTD, CVAD, CVLQ, TILT
INS, CNDD, KINDX, CNDI, CINTV
THIC, A1, A2, A3
IDSC, USUM, LLNG, ILN, ILD, LINTV
IFRTYP, TEMF, CFRA, CATR, ERAD
TLIMIT, DELT, INTV

The format statements for this file are given as follows:

Row 1	FORMAT (F8.0, F8.2, F8.4,)
Row 2	FORMAT (I8, F8.0, 2F8.1)
Row 3	FORMAT (4I8, F8.2)
Row 4	FORMAT (F8.3, F8.2, F8.3, I8, F8.3)
Row 5	FORMAT (I8, 2F8.2, F8.0)
Row 6	FORMAT (5F8.2)
Row 7	FORMAT (I8, F8.2, I8, 2F8.2)
Row 8	FORMAT (F8.2, 3F8.3)
Row 9	FORMAT (I8, F8.2, 3I8, F8.2)
Row 10	FORMAT (I8, F8.1, 3F8.2)
Row 11	FORMAT (2F8.2, I8)

An example of a file of analysis data is given in Fig. 2.2. Descriptive material below the data explains the meaning of each entry in the file. Note that some of the entries have no relevance to the type of analysis that is to be conducted (e.g., the discharge area of a safety vent for a tank equipped with a safety relief valve). However, there must be an entry in the file for every variable to permit proper reading of the file. Therefore, a dummy number must be included in the file for variables which are not used in the analysis. When data is entered at the monitor, the program automatically enters dummy numbers (either

1.0 or 1 depending whether the number is a floating point or integer number) for the variables which are not used in the analysis.

Note the following restrictions. If keyboard entry of the thermal property data is used (IPTYP=2), IPR must equal 20. If the thermal property data is used from an existing file (IPTYP=3), IPR must equal 21.

33000.	119.00	.7500			
12	81000.	850.0	1021.0		
1	1	2	1	1.00	
.950	60.00	1.000	2	.000	
1	1.00	1.00	25800.		
280.50	255.00	.80	.60	.00	
5	.43	2	.43	1.00	
.50	.017	.019	.042		
2	234.	1	0	1	1.00
1	1500.0	1.00	1.00	.80	
100.00	.10	20			

Explanation of variables in file:

Row 1: Capacity of tank (33,000 gal)
Inside diameter of tank (119.0 ins.)
Tank wall thickness (0.75 ins.)

Row 2: Code number for tank material (TC128 carbon steel)
Tensile strength of tank material (81,000 psi)
Nominal tank burst pressure (850 psig)
Calculated tank burst pressure (1021 psig)

Row 3: Code for thermal property data (use data in program)
Code for type of product in tank (substance)
Product code number (2 for propane)
Code for critical temperature entry (none)
Critical temperature (not used, dummy number)

Row 4: Initial fraction of tank filled with product (0.95)
Initial temperature of product (60 degrees F)
Concentration of product (not used, dummy number)
Code for presence of padding gas (none)
Tank pressure after padding gas added (not used, dummy number)

Row 5: Code for type of safety relief device (safety relief valve)
Discharge area of safety vent (not used, dummy number)
Frangible disc rupture pressure (not used, dummy number)
Safety relief valve rated flow capacity (25,800 SCFM)

Row 6: Safety relief valve flow rating pressure (280.5 psig)
Safety relief valve start-to-discharge pressure (255 psig)
Relief device vapor discharge coefficient (0.8)
Relief device liquid discharge coefficient (0.6)
Tank orientation with respect to vertical (0 degrees)

FIG. 2.2 EXAMPLE OF FILE OF ANALYSIS INPUT DATA

Row 7: Code number for type of thermal insulation (temperature dependent conductivity)
Thermal insulation final conductance (initial value is calculated for this code only, 0.43, BTU/hr-sqft-degF)
Code for conductance change with time (not used, dummy number)
Thermal insulation initial conductance (initial value is calculated for this code only, 0.43, BTU/hr-sqft-degF)
Time interval for change in conductance (not used, dummy number)

Row 8: Thickness of insulation (0.50 ins.)
First temperature dependant conductivity constant (0.017)
Second temperature dependant conductivity constant (0.019)
Third temperature dependant conductivity constant (0.042)

Row 9: Code number for presence of heat transfer discontinuties (2, yes)
Discontinuity heat transfer coefficient (234 BTU/hr-degF)
Code number for consideration of tank liner (none)
Code number for type of liner (not used, dummy number)
Code number for deterioration of liner (not used, dummy number)
Time interval for deterioration of liner (not used, dummy number)

Row 10: Code number for type of fire analysis (pool fire)
Flame temperature (1500 deg F)
Fraction of tank surface engulfed by fire (1.00)
Tank surface area subject to fire (not used, dummy number)
Tank surface emissivity/absorptivity factor (0.8)

Row 11: Time limit of analysis (100 min)
Time increment used in analysis (0.10 min)
Number of time steps between display of output data (20)

FIG. 2.2 EXAMPLE OF FILE OF ANALYSIS INPUT DATA (CONTINUED)

3. ENTRY OF THERMAL PROPERTY DATA

After all of the analysis data have been entered into the program, the program automatically prompts for the entry of thermal property data if this option has been selected during the entry of the analysis data. There are two different procedures for entering the data, one dealing with the entry of data for a substance, the other dealing with the entry of data for a two-component solution.

3.1 ENTRY OF SUBSTANCE DATA

The data entered includes the specific heat, the specific volume, and the heat of vaporization of the liquid substance. This is followed by the vapor pressure, the compressibility factor, and the ratio of specific heats of the substance vapor, all as a function of temperature. The process for the entry of each of these properties is similar, calling for the entry of data at a specific number of temperatures. When planning the number of points to be entered it should be recognized that values in the analysis program are obtained by linear interpolation between the entered data, except for vapor pressure where quadratic functions are developed between data points and used for the interpolation of data. The data must be entered for ascending values of temperature.

The program first calls for the entry of specific heat data. Values of specific heat are entered at a series of specific temperatures. A minimum of 2 and a maximum of 8 such data points are allowed. The following statement appears on the monitor:

> Enter number of data points to be provided
> (integer number), minimum of 2, maximum of 8: NSPEC

Type in the number and then press the enter key to proceed.

After the entry of this number a statement appears on the monitor screen directing the entry of the first set of data. The statement reads:

> Enter TEMPERATURE and corresponding SPECIFIC HEAT
> (separated by a comma) for data point: 1   SPCTMP(I), ESPEC(I)

Type in the two numbers (temperature, °F, and specific heat, BTU/LB-°F) and then press the enter key to proceed. The above statement then appears again for the entry of the next data point. Enter the next pair of values. The statement will continue to appear for the number of data points that were entered for specific heat data.

When the last data point is entered, a summary of the specific heat data will be displayed on the monitor. Examine the data to see if it is accurate. Below the data a statement appears:

> Do you wish to reenter Specific Heat Data?
> (Enter Y for yes, or N for no):

This gives the option for reentering the specific heat data if an error is noted in the displayed data. Note that if Y is entered the entire set of data for specific heat must be reentered. It is not possible to change individual numbers in the data set. If N (or any other response) is entered the statement:

> SPECIFIC HEAT data entry is completed.

will be displayed on the monitor. The program will then move on to the entry of data for the next thermal property.

Similar data entry procedures are used for the other parameters. A minimum of 3 and maximum of 15 data points are required for the entry of vapor pressure data and the number of points must be an odd number. This restriction results from the use of quadratic functions for the interpolation of vapor pressure data. Some substances may have a negligible vapor pressure (i.e., less than 0.1 psia) over the entire temperature range of interest. In this case, it is still necessary to enter data (e.g., 0.0) for at least 3 temperatures, which should cover the temperature range of interest.

It may be difficult to obtain the compressibility factor* and the ratio of specific heats for the vapor of a substance. These variables have little or no significance in the analysis

---

* The compressibility factor is defined as Z in the gas law equation $pv = ZRT$. It represents the deviation from the perfect gas law relationship.

if the vapor pressure is low. If the data are unavailable, a default value of 0.90 can be used for the compressibility factor and value of 1.1 for the ratio of specific heats. These values must be entered for at least two temperatures which cover the temperature range of interest. Finally, the molecular weight of the vapor of the substance is entered.

The thermal property data entered into the program are then written to a file which is used by the main analysis program. An option is then presented to allow the data to be written to a permanent file, which can be used in subsequent analyses. The data are written to this file in the same format as the file used in the main analysis program so that it can be properly read by the main program. The user is prompted by the question:

> DO YOU WANT TO SAVE THERMAL PROPERTY DATA IN A SEPARATE FILE? (ENTER Y OR N FOR YES OR NO):

If the response is Y for yes, the program prompts for the name of the file as follows:

> ENTER NAME OF FILE (maximum of 12 characters):

The format of this file is given in Fig. 3.1.

Another option for the entry of the thermal property data, is the construction of a file like that shown in Fig. 3.1 by using an editor rather than going through the interactive process described in this section.

An example of the entry of thermal property data for a substance is illustrated in Figs. 3.2, and 3.3. The data are for butane. Fig. 3.2 shows a worksheet which has been prepared to facilitate the entry of the data. Fig. 3.3 shows the file that corresponds to Fig. 3.1 which gives the thermal property data in the form used by the main analysis program.

3.2 ENTRY OF SOLUTION DATA

The data entered includes the specific heat, the specific volume, and the heat of vaporization of the liquid solution as a function of temperature. The data entered also includes the vapor pressure, the compressibility factor and the ratio of specific heats of both the solution vapor and the solvent vapor as a function of temperature. The process for the entry of each of these properties is similar to that for substance data which was

NSPEC SPCTMP(1), ESPEC(1) SPCTMP(2), ESPEC(2) ...... SPCTMP(NSPEC), ESPEC (NSPEC)	FORMAT (I10) FORMAT (F10.2, F10.4) FORMAT (F10.2, F10.4) ...... FORMAT (F10.2, F10.4)
NSPLQ SPLTMP(1), ESPLQ(1) SPLTMP(2), ESPLQ(2) ...... SPLTMP(NSPLQ), ESPLQ (NSPLQ)	FORMAT (I10) FORMAT (F10.2, F10.4) FORMAT (F10.2, F10.4) ..... FORMAT (F10.2, F10.4)
NHFLV HFLTMP(1), EHFLV(1) HFLTMP(2), EHFLV(2) ...... HFLTMP(NHFLV), EHFLV (NHFLV)	FORMAT (I10) FORMAT (F10.2, F10.1) FORMAT (F10.2, F10.1) ...... FORMAT (F10.2, F10.1)
NPSBS PSBTMP(1), EPSBS(1) PSBTMP(2), EPSBS(2) ...... PSBTMP(NPSBS), EPSBS (NPSBS)	FORMAT (I10) FORMAT (2F10.2) FORMAT (2F10.2) .... FORMAT (2F10.2)
NZPRO ZPRTMP(1), EZPRO(1) ZPRTMP(2), EZPRO(2) ...... ZPRTMP(NZPRO), EZPRO (NRPRO)	FORMAT (I10) FORMAT (2F10.2) FORMAT (2F10.2) ...... FORMAT (2F10.2)
NGMMP GMPTMP(1), EGMMP(1) GMPTMP(2), EGMMP(2) .... GMPTMP(NGMMP), EGMMP (NGMMP)	FORMAT (I10) FORMAT (2F10.2) FORMAT (2F10.2) ...... FORMAT (2F10.2)
MLWSBS	FORMAT (F10.2)

FIG. 3.1 FORMAT FOR DATA FILE OF THERMAL PROPERTY DATA FOR A SUBSTANCE

Temperature (°F)	30.0	120.0	210.0	260.0	
Specific Heat of Liquid (BTU/lb-°F)	0.5546	0.5946	0.7141	0.9619	
Temperature (°F)	30.0	120.0	210.0	260.0	
Specific Volume of Liquid (ft^3/lb)	0.02684	0.02921	0.03296	0.03375	
Temperature (°F)	30.0	120.0	210.0	260.0	
Heat of Vaporization (BTU/lb)	164.7	143.3	114.4	85.7	
Temperature (°F)	30.0	120.0	180.0	220.0	260.0
Compressibility Factor of Vapor	0.957	0.877	0.790	0.710	0.599
Temperature (°F)	30.0	180.0	220.0	260.0	
Ratio of Specific Heats of Vapor	1.12	1.22	1.31	1.62	

Temperature (°F)	30.0	60.0	90.0	120.0	150.0	180.0	210.0	240.0	270.0
Vapor Pressure (psia)	14.43	25.89	44.05	69.12	105.00	153.07	215.21	295.30	397.10

Molecular Weight of Substance: 44.0

FIG. 3.2 WORKSHEET FOR THERMAL PROPERTY DATA FOR BUTANE

4	
30.00	.5546
120.00	.5946
210.00	.7141
260.00	.9619
4	
30.00	.02684
120.00	.02921
210.00	.03296
260.00	.03375
4	
30.00	164.7
120.00	143.3
210.00	114.4
260.00	85.7
9	
30.00	14.43
60.00	25.89
90.00	44.05
120.00	69.12
150.00	105.00
180.00	153.07
210.00	215.21
240.00	295.30
270.00	397.10
5	
30.00	.96
120.00	.88
180.00	.79
220.00	.71
260.00	.60
4	
30.00	1.12
180.00	1.22
220.00	1.31
260.00	1.62
44.00	

FIG. 3.3 THERMAL PROPERTY DATA FOR BUTANE

described in the preceding section. It calls for the entry of data at a specific number of temperatures. The major difference is that data for specific heat, specific volume, heat of vaporization and vapor pressure are entered for two different concentrations of the solution. These concentrations then become the limits for valid data when the tank car fire analysis is performed. When planning the number of points to be entered it should be recognized that values in the analysis program are obtained by linear interpolation between the entered data, except for vapor pressure where quadratic functions are developed between data points and used for interpolation of data. The data must be entered for ascending values of temperature, and the lower concentration value data must be entered first.

The program first calls for the entry of specific heat of liquid solution data. Values of specific heat are entered at a series of specific temperatures. A minimum of 2 and a maximum of 8 such data points are allowed. The following statement appears on the monitor:

> Enter number of data points to be provided
> (integer number), minimum of 2, maximum of 8: NSPEC

Type in the number and then press the enter key to proceed.

After the entry of this number a statement appears on the monitor screen directing the entry of the concentration level (the lower concentration level) of the first set of specific heat data. The statement reads:

> Enter Lower Concentration Level (decimal fraction): CNCSLN(1,1)

After the entry of this value the specific heat data is entered as follows:

> Enter TEMPERATURE and corresponding SPECIFIC HEAT
> (separated by a comma) for data point: 1 SPCTMP(I,J), ESPEC(I,J)

Type in the two numbers (temperature, °F, and specific heat, BTU/lb.-°F) and then press the enter key to proceed. The above statement then appears again for the entry of the next data point. Enter the next pair of values. The statement will continue to appear for the number of data points that were entered for specific heat data.

When the last data point is entered for the first concentration level, a summary of the specific heat data will be displayed on the monitor. Examine the data to see if it is accurate. Below the data a statement appears:

> Do you wish to reenter Specific Heat Data?
> (Enter Y for yes, or N for no):

This gives the option for reentering the specific heat data if an error is noted in the displayed data. Note the if Y is entered the entire set of data for specific heat must be reentered. It is not possible to change individual numbers in the data set. If N (or any other response) is entered the statement:

> SPECIFIC HEAT data entry is completed.

will be displayed on the monitor. The process is repeated twice, once for each concentration level. The program will then move on to the entry of data for the next thermal property. Similar data entry procedures are used for the entry of the specific volume and the heat of vaporization of the liquid solution.

Data for vapor pressure are then entered into the program. A minimum of 3 and maximum of 15 data points are again allowed for the entry of the vapor pressure data and the number of points must be an odd number. Some solutes may have a negligible vapor pressure (i.e., less than 0.1 psia) over the entire temperature range of interest. In this case, it is still necessary to enter data (e.g., 0.0) for at least 3 temperatures, which should cover the expected temperature range of interest.

Data for the compressibility factor, and the ratio of specific heats for both solute and solvent vapor are then entered into the program. These values would be independent of concentration.

It may be difficult to obtain compressibility factors and ratios of specific heats for the vapor of both the solute and the solvent. These variables have little or no significance in the analysis if the vapor pressures are low. If the data are unavailable, a default value of 0.90 can be used for the compressibility factor and value of 1.1 for the ratio of specific heats. These values must be entered for at least two temperatures which cover the temperature range of interest. Finally, the molecular weights of both the solute vapor and the solvent vapor are entered into the program.

The thermal property data entered into the program are then written to a file which is used by the main analysis program. An option is then presented to allow the data to be written to a permanent file, which can be used in subsequent analyses. It is written to this file in the same format as the file used in the main analysis program so that it can be properly read by the main program. The user is prompted by the question:

> DO YOU WANT TO SAVE THERMAL PROPERTY DATA IN A SEPARATE FILE? (ENTER Y OR N for yes or no):

If the response is yes, the program prompts for the name of the file as follows:

> ENTER NAME OF FILE (maximum of 12 characters):

The format of this file is given in Fig. 3.4.

Another option for the entry of the thermal property data is the construction of a file like that shown in Fig. 3.4 by using an editor rather than going through the interactive process described in this section.

An example of the entry of thermal property data for a solution of hydrochloric acid is illustrated in Figs. 3.5, and 3.6. The concentration of the solution in the analysis is 0.295 by weight, so data are given to bracket this concentration. Fig. 3.5 shows a worksheet which has been prepared to facilitate the entry of the data. Fig. 3.6 shows the file that corresponds to Fig. 3.4 which gives the thermal property data in the form used by the main analysis program.

3.3 EXCEEDANCE OF TEMPERATURE OR CONCENTRATION LIMITS

The first time the thermal property data is used in the analysis the maximum and minimum temperature limits are established for the thermal property data entered into the program. If the product is a solution, the maximum and minimum concentration limits are also established.

During the operation of the program the temperature and concentration (if the product is a solution) are checked to determine if the limits are exceeded. If the temperature range for which thermal property data are entered into the program is exceeded during the analysis, the following statement will appear on the monitor and be written to the output file:

> OUTSIDE TEMPERATURE RANGE OF THERMAL PROPERTY DATA

The calculations will continue, but will be based on extrapolated, rather than interpolated thermal property data.

If the concentration range for which thermal property data for a solution are entered into the program is exceeded during the analysis, the following statement will appear on the monitor and be written to the output file:

OUTSIDE CONCENTRATION RANGE OF THERMAL PROPERTY DATA

The calculations will continue, but will be based on extrapolated, rather than interpolated thermal property data.

NSPEC SPCTMP(1,1), ESPEC(1,1) SPCTMP(1,2), ESPEC(1,2) ..... SPCTMP(1,NSPEC(1), ESPEC(1,NSPEC(1)	FORMAT (I10) FORMAT (F10.2, F10.4) FORMAT (F10.2, F10.4) ...... FORMAT (F10.2, F10.4)
NSPEC SPCTMP (2,1), ESPEC(2,1) SPCTMP (2,2), ESPEC(2,2) ..... SPCTMP(2,NSPEC(2)), ESPEC(2,NSPEC(2))	FORMAT (I10) FORMAT (F10.2, F10.4) FORMAT (F10.2, F10.4) ...... FORMAT (F10.2, F10.5)
NSPLQ SPLTMP(1,1), ESPLQ(1,1) SPLTMP(1,2), ESPLQ(1,2) ..... SPLTMP(1,NSPLQ91)), ESPLQ(1,NSPLQ(1))	FORMAT (I10) FORMAT (F10.2, F10.5) FORMAT (F10.2, F10.5 ...... FORMAT (F10.2, F10.5)
NSPLQ SPLTMP(2,1), ESPLQ(2.1) SPLTMP(2,2), ESPLQ(2,2) ..... SPLTMP(2,NSPLQ(2)), ESPLQ(2,NSPLQ(2))	FORMAT (I10) FORMAT (F10.2, F10.5) FORMAT (F10.2, F10.5) ...... FORMAT (F10.2, F10.5)
NHFLV HFLTMP(1,1,EHFLV(1,1) HFLTMP(1,2), EHFLV(1,2) ..... HFLTMP(1,NHFLV(1)), EHFLV(1,NHFLV(1))	FORMAT (I10) FORMAT (F10.2, F10.4) FORMAT (F10.2, F10.1) ..... FORMAT (F10.2, F10.1)
NHFLV HFLTMP(2,1), EHFLV(2,1) HFLTMP(2,2), EHFLV(2,1) ..... HFLTMP(2,NHFLV(2)), EHFLV(2,NHFLV(2))	FORMAT (I10) FORMAT (F10.2, F10.1) FORMAT (F10.2, F10.1) ..... FORMAT (F10.2, F10.1)

FIG. 3.4 FORMAT FOR DATA FILE OF THERMAL PROPERTY DATA FOR A SOLUTION

NPSLV PSVTMP(2,1),EPSLV(2,1) PSVTMP(2,2), EPSLV(2,2) ..... PSVTMP(2,NPSLV(2)),EPSLV(2,NPSLV(2))	FORMAT (I10) FORMAT (2F10.2) FORMAT (2F10.2) ..... FORMAT (2F10.2)
NZSLT ZSTTMP(1),EZSLT(1) ZSTTMP(2),EZSLT(2) ..... ZSTTMP(NZSLT),EZSLT(NZSTL)	FORMAT (I10) FORMAT (2F10.2) FORMAT (2F10.2) ..... FORMAT (2F10.2)
NZSLV ZSVTMP(1),EZSLV(1) ZSVTMP(2),EZSLV(2) ...... ZSVTMP(NZSLV)EZSLV(NZSLV)	FORMAT (I10) FORMAT (2F10.2) FORMAT (2F10.2) ..... FORMAT (2F10.2)
NGSLT GSTTMP(1),EGSLT(1) GSTTMP(2),EGSLT(2) ...... GSTTMP(NGSLT),EGSLT(NGSLT)	FORMAT (I10) FORMAT (2F10.2 FORMAT (2F10.2) ...... FORMAT (2F10.2)
NGSLV GSVTMP(1),EGSLV(1) GSVTMP(2),EGSLV(2) ...... GSVTMP(NGSLVT),EGSLV(NGSLV)	FORMAT (I10) FORMAT (2F10.2) FORMAT (2F10.2) ..... FORMAT (2F10.2)
MLWTST	FORMAT (F10.2)
MLWTSV	FORMAT (F10.2)

FIG. 3.4 FORMAT FOR DATA FILE OF THERMAL PROPERTY DATA FOR A SOLUTION (CONTINUED)

Concentration (%):	28	
Temperature (^{o}F)	50.0	212.0
Specific Heat of Liquid (BTU/lb-^{o}F)	0.624	0.714

Concentration (%):	32	
Temperature (^{o}F)	50.0	212.0
Specific Heat of Liquid (BTU/lb-^{o}F)	0.600	0.690

Concentration (%):	20					
Temperature (^{o}F)	50.0	68.0	86.0	122.0	167.0	212.0
Specific Volume of Liquid (ft^3/lb)	0.01453	0.01459	0.01465	0.01478	0.01496	0.01515

Concentration (%):	30					
Temperature (^{o}F)	50.0	68.0	86.0	122.0	167.0	212.0
Specific Volume of Liquid (ft^3/lb)	0.01387	0.01394	0.01401	0.01415	0.01433	0.01452

Concentration (%):	25	
Temperature (^{o}F)	50.0	212.0
Heat of Vaporization (BTU/lb)	847.	771.

Concentration (%):	30	
Temperature (^{o}F)	50.0	212.0
Heat of Vaporization (BTU/lb)	803.	731.

FIG. 3.5 WORKSHEET FOR THERMAL PROPERTY DATA FOR HYDROCHLORIC ACID

Temperature (°F)	60.0	260.0
Compressibility Factor of Solute Vapor	0.95	0.95

Temperature (°F)	60.0	260.0
Compressibility Factor of Solvent Vapor	1.00	0.97

Temperature (°F)	60.0	260.0
Ratio of Specific Heats of Solute Vapor	1.30	1.30

Temperature (°F)	60.0	260.0
Ratio of Specific Heats of Solvent Vapor	1.31	1.27

Concentration (%): 28

Temperature (°F)	50.0	68.0	86.0	104.0	122.0	140.0	158.0	176.0	194.0	212.0	230.0
Vapor Pressure of Solute (psia)	0.04	0.10	0.19	0.37	0.69	1.24	2.17	3.64	5.98	9.54	14.70

Concentration (%): 30

Temperature (°F)	50.0	68.0	86.0	104.0	122.0	140.0	158.0	176.0	194.0	212.0	230.0
Vapor Pressure of Solute (psia)	0.10	0.21	0.41	0.76	1.37	2.40	4.02	6.58	10.48	16.34	24.68

FIG. 3.5 (continued) WORKSHEET FOR THERMAL PROPERTY DATA FOR HYDROCHLORIC ACID