

**TANK CAR THERMAL ANALYSIS,  
VOLUME II, TECHNICAL  
DOCUMENTATION REPORT FOR  
ANALYSIS PROGRAM**

**U.S. Department  
of Transportation**

**Federal Railroad  
Administration**

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FINAL REPORT**

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<p><b>Title</b>          Tank Car Thermal Analysis,          Volume II, Technical Documentation Report for Analysis Program</p>
<p><b>Report Date</b>          November 1998</p>
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<p><b>Abstract</b></p> <p>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 a safety relief valve or a safety vent closed with a frangible disc. The program is described in two volumes. This volume describes the assumptions and procedures used in the analysis. Four main conditions must be considered, an upright car orientation where vapor is vented, an overturned car condition where liquid is vented, a shell full condition where the tank contains only product in the liquid phase, and the condition where the tank contains only product in the vapor phase. The source codes of the main program and the subroutines are presented in a series of appendices.</p>
<p><b>Key Words</b></p> <p>railroad tank car, tank car failure, hazardous material release, fire effects</p>
<p><b>Distribution Statement</b></p> <p>Document is available to the public through the National Technical Information Service, Springfield, Virginia 22161</p>

## PREFACE

The work described in this report was conducted by IIT Research Institute (IITRI) under authorization of Federal Railroad Administration (FRA) Contract No. 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 II, describes the technical background for the analysis program. A second volume, Volume I, is the user's manual 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,

A handwritten signature in cursive script that reads "Milton R. Johnson".

Milton R. Johnson

## EXECUTIVE SUMMARY

This report describes the technical background for 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. The assumptions and procedures used in the analysis are described in this report and the source codes of the main program and subroutines are presented in a series of appendices.

The first version of the program was developed for the Federal Railroad Administration in 1984. Since that time certain features have been added to the program such as the thermal properties of additional commodities and the ability to consider a tank with a safety vent as well as the safety relief valve. The thermal properties of 16 commodities are now contained in the program.

Originally, the program accepted entry of input variables at the monitor. This has been modified so that input data can be read from a file or entered in an interactive way at the monitor. The interactive process at the monitor has been expanded with prompts added to provide added instructions for the entry of data.

Another feature that has been added in this version of the program is the entry of thermal property data. Now one can enter thermal property data for products by creating and reading a file of data or by entering the data at the keyboard of the monitor following the instructions given by a series of prompts on the screen.

Several different conditions must be recognized when analyzing the effects of fire on a tank car. First, the car may be 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 (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 which increases the temperature of the liquid product, increasing as its temperature increases. The presence of a pad of inert gas must be considered for cars containing certain commodities.

The analysis considers whether the car is equipped with a safety relief valve or a safety vent with a frangible disc. If the car is equipped with a safety relief valve the valve opens allowing the vapor to exhaust from the car when the pressure within the tank

exceeds the start-to-discharge pressure of the valve. 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 exhausted from the tank. If 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. If the car is equipped with a safety vent, the vent opens and stays open for the remainder of the calculation when the rupture pressure of the frangible disc is reached.

Another condition is the overturned car case. The car is assumed to be partially rolled over so that when the safety relief device 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 is calculated assuming homogenous isentropic two-phase flow (liquid and vapor). Two-phase effects are significant only when the product has a high vapor pressure.

Still another condition is where the tank is "shell full" (of liquid) and for all practical purposes there is no vapor space left within the tank. This occurs when the car is initially filled with only a small empty volume (outage) 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. When the car becomes shell full, any further increase in temperature of the product will cause liquid flow through the safety relief device. If the capacity of the device is small and the rate of increase in the specific volume of the liquid is large, very high pressures can be developed.

A fourth condition is 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. The tank wall temperature also increases fairly rapidly because there is no cooling effect from the vaporization of liquid product within the tank.

For each of these four conditions, 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 causing the sudden release of the remaining product within the car.

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 /Fi 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 monitor. The results can be displayed at the monitor or written to a report file.

## TABLE OF CONTENTS

SECTION	PAGE NO.
1. Introduction	1
2. Background	3
3. General Considerations	5
3.1 Description of Phenomena	5
3.2 Standard Fire Conditions	8
3.3 Use of Subroutines	10
3.4 Variables Used to Describe Conditions of the Analysis	10
3.5 Exceedance of Temperature or Concentration Limits	12
3.6 Limitations of Analysis	12
4. Analytical Procedure	15
4.1 Initialization	15
4.1.1 Data Entry	15
4.1.2 Calculate Other Initial Values	18
4.2 Preliminary Calculations of Fire Effects	20
4.2.1 Determine Effective Conductance of Thermal Insulation and Thermal Protection Systems	20
4.2.2 Calculate Temperature of Tank Surface Outside of Liquid Region	21
4.2.3 Calculate Temperature of Tank Surface Outside of Vapor Region	21
4.2.4 Establish Geometry of Liquid Levels	22
4.2.5 Radiation Surface Configuration Factor	22
4.2.6 Calculate Temperature of Inner Wall Surface in Vapor Region	23
4.2.7 Adjust Tank Size for Temperature and Strain Effects	23
4.2.8 Determine Vent Opening or Degree of Valve Opening	25
4.2.9 Determine Conditions in the Tank	25
4.3 Calculation of Effects with Liquid and Vapor within Tank with Vapor adjacent to Safety Relief Device	27
4.3.1 Calculate Heat Transfer to Liquid Product	27
4.3.2 Calculate Mass Flow Rate Through Safety Relief Device	27
4.3.3 Calculate Change in Mass of Product	28
4.3.4 Calculate Temperature Rise of Liquid	28



## TABLE OF CONTENTS (continued)

SECTION NO.		PAGE
4.4	Calculation of Liquid and Vapor within Tank with Liquid Adjacent to Safety Relief Device	28
4.4.1	Calculate Heat Input to Liquid Product	29
4.4.2	Calculate Liquid Flow Rate Through Safety Relief Device	29
4.4.3	Calculate Change in Temperature	29
4.4.4	Determine New Properties	29
4.4.5	Calculate Remaining Mass of Product and Padding Gas	29
4.4	Calculation of Effects with Shell Full Conditions	30
4.4.3	Calculate Heat Transferred to Liquid Product	30
4.4.4	Calculate Change in Temperature	31
4.4.5	Determine New Properties	31
4.4.6	Calculate Required Volume of Flow	31
4.4.7	Calculate Pressure Required to Generate Sufficient Flow	31
4.4.8	Calculate Mass of Product Remaining in Tank	32
4.5	Calculation of Effects with Vapor Phase only Within Tank	32
4.5.3	Calculate Heat Transfer to Vapor Product	32
4.5.4	Calculate Change in Pressure	32
4.5.5	Calculate Mass Flow Out	33
4.5.6	Calculate Change in Tank Temperature	33
4.6	Output Data	33
4.7	Compare Tank Bursting Pressure and Internal Pressure	34
4.8	Check for Time Limit	35
4.9	Program Termination or Restart	35
4.10	Program Listings	35
5.	References	36
	APPENDIX A SOURCE CODE FOR MAIN PROGRAM: AFFTAC	
	APPENDIX B SUBROUTINE ENTRDAT	
	APPENDIX C SUBROUTINE ANLYRPT	
	APPENDIX D SUBROUTINE SBSENTR	
	APPENDIX E SUBROUTINE SLNENTR	
	APPENDIX F SUBROUTINE SBSPROP	
	APPENDIX G SUBROUTINE SLNPROP	
	APPENDIX H SUBROUTINE FPRPSBS	
	APPENDIX I SUBROUTINE FPRPSLV	
	APPENDIX J SUBROUTINE SURFACET	
	APPENDIX K SUBROUTINE AVFLOW	
	APPENDIX L SUBROUTINE TSHIELD	

## TABLE OF CONTENTS (continued)

<b>LIST OF FIGURES</b>		<b>PAGE NO.</b>
3.1	Conditions Considered in the Analysis of Tank Cars Subjected to Fire	6
4.1	Flow Chart for Program 'AFFTAC'	16
4.2	Flow Chart of Data Entry for Program 'AFFTAC'	17
4.3	Relationship Between Degree of Valve Opening and Pressure	26

# **TECHNICAL DOCUMENTATION REPORT FOR PROGRAM AFFTAC**

## **1. INTRODUCTION**

This report describes the technical details for the computer program AFFTAC (Analysis of Fire eEffects on TAnk Cars). The program is used to analyze the behavior of tank cars and the products they contain when subjected to fire. The assumptions and procedures used in the analysis are described in this report and the source codes of the main program and subroutines are presented in a series of appendices.



## 2. BACKGROUND

In 1984, IIT Research Institute (IITRI) developed a computer program for analytic procedure which could be used to calculate the effects of fire on a railroad tank car. The work was sponsored by the Federal Railroad Administration (FRA). The procedure was developed so that the consequences of using different conductances of thermal insulation systems on the tank and different flow capacities of the safety relief valve could be determined. It was used to predict various effects of the fire, such as the time to tank failure, the amount of product remaining in the tank at the time of failure, the maximum pressure in the tank, the time to reach certain pressure levels, etc. Both upright and overturned car cases were considered. Tank cars containing the following products were analyzed: ethylene oxide, propane, propylene, 1,3-butadiene, vinyl chloride, monomethylamine, and propylene oxide. A report describing the procedure and presenting the source code of the computer program was published in 1984 by the FRA (Ref. 1).

In subsequent years IITRI modified the procedure to include additional commodities and different conditions, such as the use of safety vents closed by frangible discs instead of safety relief valves, the use of linings in the tank, the expansion of the tank due to internal pressure, etc. This was done so that it could be used to analyze different situations where tank cars are engulfed by fire.

The thermal properties of other commodities were also entered into the program. Some of these commodities were solutions, such as hydrochloric acid, where consideration had to be given to a change in the concentration of the solution as vaporization and venting of the product takes place.

In November 1992 a project was initiated with the Association of American Railroads (AAR) to make the computer program more accessible to the tank car industry. The purpose of this project was to document the changes and describe the operation of the program so that it could be used by others. The work included modification of the program to run on a personal computer.

The results of this work were published in April 1993 in a draft report. The executable program was distributed to selected users by the AAR for evaluation. Comments on the program were not transmitted to IITRI until October 1994. The program was revised and resubmitted to the AAR in November 1994 (Ref. 2).

As mentioned in the Preface to this report, the present efforts to expand the capabilities of the analysis program were initiated in September 1994.

### 3. GENERAL CONSIDERATIONS

The analytic procedure allows the conditions within the tank to be determined as a function of time for different initial conditions, which include characteristics of the tank, product contained in the tank, the safety relief device, thermal insulation and fire. The computer 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 monitor. The results can be displayed at the monitor or written to a file.

#### 3.1 DESCRIPTION OF PHENOMENA

Fig. 3.1 illustrates the basic phenomena which must be taken into consideration. Four different conditions are recognized. The first is 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 (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 which increases the temperature of the tank wall. As the temperature rises, heat is radiated from the wall to the liquid below. The amount of radiated heat depends on both the radiation surface configuration factor of the surface of the liquid and the temperatures of the wall and liquid.

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 causing the sudden release of the remaining product within the car.

The pressure within the tank is a function of the temperature of the liquid product, increasing as its temperature increases. The presence of a pad of inert gas, must be considered for cars containing certain commodities.

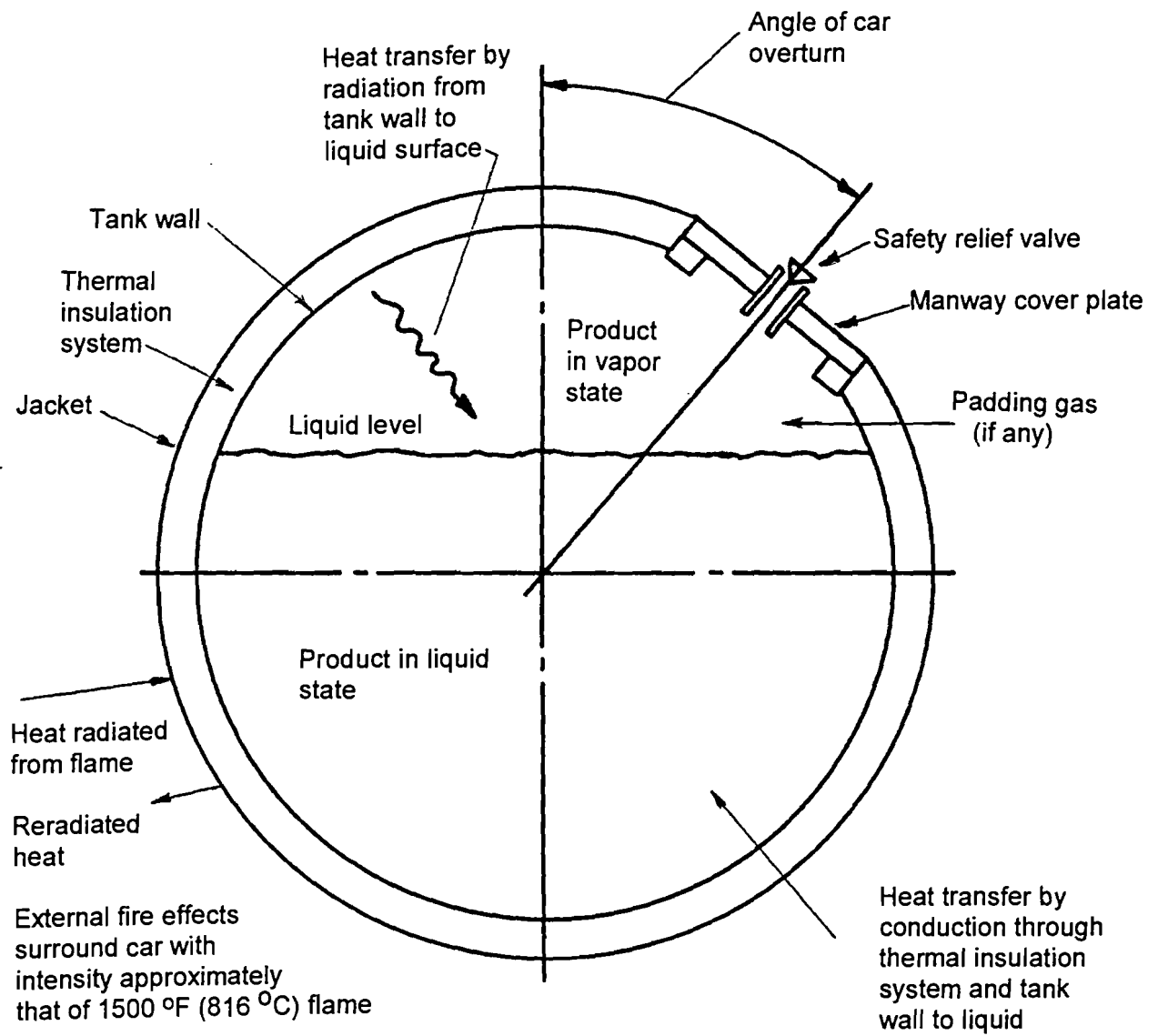


FIG. 3.1 CONDITIONS CONSIDERED IN THE ANALYSIS OF TANK CARS SUBJECTED TO FIRE



The calculation considers whether the car is equipped with a safety relief valve or a safety vent with a frangible disc. If the car is equipped with a safety relief valve the valve opens allowing the vapor to exhaust from the car when the pressure within the tank exceeds the start-to-discharge pressure of the valve. 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 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. If the car is equipped with a safety vent, the vent opens and stays open for the remainder of the calculation when the rupture pressure of the frangible disc is reached.

The second condition is the overturned car case. The car is assumed to be partially rolled over so that when the safety relief device 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 is calculated assuming homogenous isentropic two-phase flow (liquid and vapor). Two-phase effects are significant only when the product has a high vapor pressure.

The third condition is where the tank is "shell full" (of liquid) and for all practical purposes there is no vapor space left within the tank. This condition is more likely to occur when the car is initially filled with only a small empty volume (outage) 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. When the car becomes shell full, any further increase in temperature of the product will cause liquid flow through the safety relief device. If the capacity of the device is small and the rate of increase in the specific volume of the liquid is large, very high pressures can be developed.

The fourth condition is 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 device is capable of relieving any increases in pressure as the vapor becomes hotter. For a valve, the pressure would be maintained near the valve closing pressure. The tank wall temperature also increases fairly rapidly because there is no cooling effect from the vaporization of liquid product within the tank.

The calculational procedure assumes that each of the parameters remains 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 found to be adequate for the calculations.

### **3.2 STANDARD FIRE CONDITIONS**

Two standard fire conditions are built into the analytic procedure. They are the pool fire condition and the torch fire condition. They are based on the requirements of Appendix B to Part 179 of the Code of Federal Regulations (CFR).

The pool fire simulation test described in the CFR calls for a sample insulation system to be subjected to a  $1600\text{ }^{\circ}\text{F} \pm 100\text{ }^{\circ}\text{F}$  flame. Analysis of the full scale fire tests on tank cars containing propane indicated that the effects of the fire could be represented by complete engulfment of the car in a fire with approximate flame temperature  $1500\text{ }^{\circ}\text{F}$ . (See Refs. 1 and 4.)

A torch fire is defined as a high intensity flame that will heat and weaken the tank wall in a localized area. The effect will be much more pronounced if the flame impinges on the tank wall over the vapor space because the cooling effect of the liquid product will not be present. It will have a minimal effect, when compared to a pool fire, in raising

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\* This critical temperature has a different meaning than the "critical temperature" entered into the program. "critical temperature" here refers to the maximum temperature at which the product can exist in the liquid state.

the temperature of the contents of the tank, because heat is transmitted into the tank only in a localized area.

The heat input used to analyze the effects of a torch fire on a tank car is based on the requirements for a simulated torch fire test which are also given in Appendix B to Part 179 of the CFR. The requirements state that the flame shall have a temperature of  $2200 \pm 100$  °F and shall be directed at the test specimen at a velocity of  $40 \pm 10$  mph. The intensity of the heat input from this flame is to be verified by directing it at a 4 by 4 ft steel plate 5/8 in. thick, which is initially between 32 and 100 °F. When the flame is directed at the plate, the plate is to reach a temperature of 800 °F in  $4.0 \pm 0.5$  minutes.

Torch fire simulation test has been analyzed to determine the heat input required to raise the temperature of the plate to 800 °F in four minutes. The result is a thermal input of approximately 37,000 BTU/hr-ft<sup>2</sup> to a cold plate surface. This equivalent to the radiant energy from a flame with a temperature of 2200 °F, but with a factor of 0.536 to account for the fact that the flame does not completely surround the plate. In the analytic procedure a flame with this intensity is directed at the outer surface of the tank wall (for a bare uninsulated tank) or the jacket of an insulated tank. The heat input to the tank will be reduced, as the surface temperature is raised.

The above calculated value of thermal input has been used in the tank car torch fire analysis. It is assumed to be applied to a 4 ft square section of the surface of the tank adjacent to the liquid for the calculation of heat input to the tank. For purposes of determining the reduction of in burst pressure of the tank, it is assumed that the heat input is directed at the tank wall adjacent to the vapor space.

The assumption is made for the purpose of analysis that all of the heat is transferred to the surface of the tank by radiation. Under actual test conditions, heat transfer by convection would also be present because of the 40 mph flow velocity specified for the flame. However, there is no way to separate out the relative effects of the two mechanisms of heat transfer. Assuming the heat transfer is by radiation is a conservative assumption because it results a significant level of heat transfer even when there is only a small difference in temperature between the flame and the outside surface of the tank.

### 3.3 USE OF SUBROUTINES

The computer program is named AFFTAC and makes use of subroutines which are listed as follows:

ENTRDAT permits entry of variables used in the analysis interactively at the computer terminal,

SURFACET calculates the surface temperature of the outside of the tank insulation system,

AVFLOW calculates the liquid flow through a safety relief device, and

TSHIELD calculates the effective conductance of an insulation system, where temperature dependent conductivity is assumed.

Two different subroutines are used for the entry of thermal property data. These are:

SBSENTR for the entry of thermal property data for a substance, and

SLNENTR for the entry of thermal property data for a solution.

The analysis requires establishing the current values for the thermal properties of the product at various steps through the calculations. The values are found by calling one of four subroutines. Two subroutines, FPRPSBS and FPRPSLV, are used to obtain data for products where the thermal properties are stored in the program. FPRPSBS contains data for products which are substances. FPRPSLV contains data for products which are solutions. The other two subroutines are used for cases where the property data are entered into the program either by reading a file or by entering at the monitor. One of these subroutines, SBSPROP, is used for products which are substances. The other, SLNPROP, is used for products which are solutions.

The subroutine ANLYRPT is used to prepare a file describing the analysis conditions for any given run of the program.

### 3.4 VARIABLES USED TO DESCRIBE CONDITIONS OF THE ANALYSIS

The following variables are entered into the program to establish the conditions of the analysis.

### **Tank Characteristics**

Capacity of Tank (gal)  
Inside Tank Diameter (ins.)  
Tank Wall Thickness (ins.)  
Tank Material Type  
Tensile Strength of Tank Material (psi)  
Nominal Burst Pressure (psig)  
Tank Orientation with Respect to Vertical (deg)

### **Product Characteristics**

Type of Product in Tank: Substance or Solution  
Procedure for Entry of Thermal Property Data  
Name of Product  
Fraction of Tank Filled with Product  
Initial Temperature of Product (deg F)  
Concentration of Product (if solution)  
Padding Gas Pressure (if present, psig)

### **Safety Relief Device Characteristics**

Type of Safety Relief Device; Valve or Vent  
Discharge Area for Vent (if used, in<sup>2</sup>)  
Frangible Disc Rupture Pressure for Vent (if used, psig)  
Flow Capacity of Safety Relief Valve (if used, SCFM)  
Flow Rating Pressure of Safety Relief Valve (if used, psig)  
Start-to-Discharge Pressure of Safety Relief Valve (if used, psig)  
Vapor Discharge Coefficient  
Liquid Discharge Coefficient

### **Thermal Insulation System Characteristics**

Type of Thermal Insulation System  
Initial Conductance of Thermal Insulation (BTU/hr-ft<sup>2</sup>-°F)  
Final Conductance of Thermal Insulation (BTU/hr-ft<sup>2</sup>-°F)  
Time Interval for Change from Initial to Final Conductance (if any, min)  
Thickness of Thermal Insulation (only for temperature dependent conductivity cases, ins.)  
Constants Defining Thermal Conductivity (only for temperature dependent conductivity cases)  
Effect of Discontinuities Increasing Heat Transfer (if any)  
Type of Lining (if any)

### **Fire Characteristics**

Type of Fire (pool, torch, or special conditions)  
Flame Temperature (deg F)  
Fraction of Tank Surface Subjected to Fire  
Emissivity/Absorptivity of Tank Surface

### **Analysis Conditions**

Time Increment Used in Analysis (min)

Number of Time Increments Between Display of Output Data

Time Limit Analysis (min)

The manner in which these data are entered into the program is described in the User's Manual.

### **3.5 EXCEEDENCE OF TEMPERATURE OR CONCENTRATION LIMITS**

During the operation of the program the temperature and concentration (if the product is a solution) are checked to determine if certain 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 terminal screen and 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 terminal screen 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.

### **3.6 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 a 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 the 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.





## 4. ANALYTICAL PROCEDURE

The program is initiated by entering the command: AFFTAC.\* The steps in the analysis are described in this section. Additional explanatory notes are contained in the listing of the source code, which is presented in Appendix A. A flow chart for the program is presented in Fig. 4.1.

### 4.1 INITIALIZATION

The first part of the program deals with the entry of data.

#### 4.1.1 Data Entry

Fig. 4.2 presents a flow chart showing the options and logic for the entry of data. There are two parts to this process, the first dealing with the entry of the variables describing the initial conditions of the analysis and the second dealing with the entry of thermal property data.

The first decision point is whether the initial values are to be entered at the monitor or from an existing computer file. If a file is used, the name of the file must be entered. If the values are to be entered, one at a time, at the terminal, subroutine ENTRDAT.FOR is called. See the User's Manual, Section 2, for a detailed description of this part of the program. The source code for subroutine ENTRDAT.FOR is presented in Appendix B of this report. A report of the initial data is prepared by subroutine ANLYRPT.FOR. The source code for this subroutine is presented in Appendix C of this report.

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 property data at the monitor, reading a previously developed file or property data, or by using the property 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 described in Section 3 of the User's Manual. The source codes for the two subroutines for the entry of thermal property data, SBSENTR.FOR and SLNENTR.FOR are presented in Appendices D and E of this report.

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

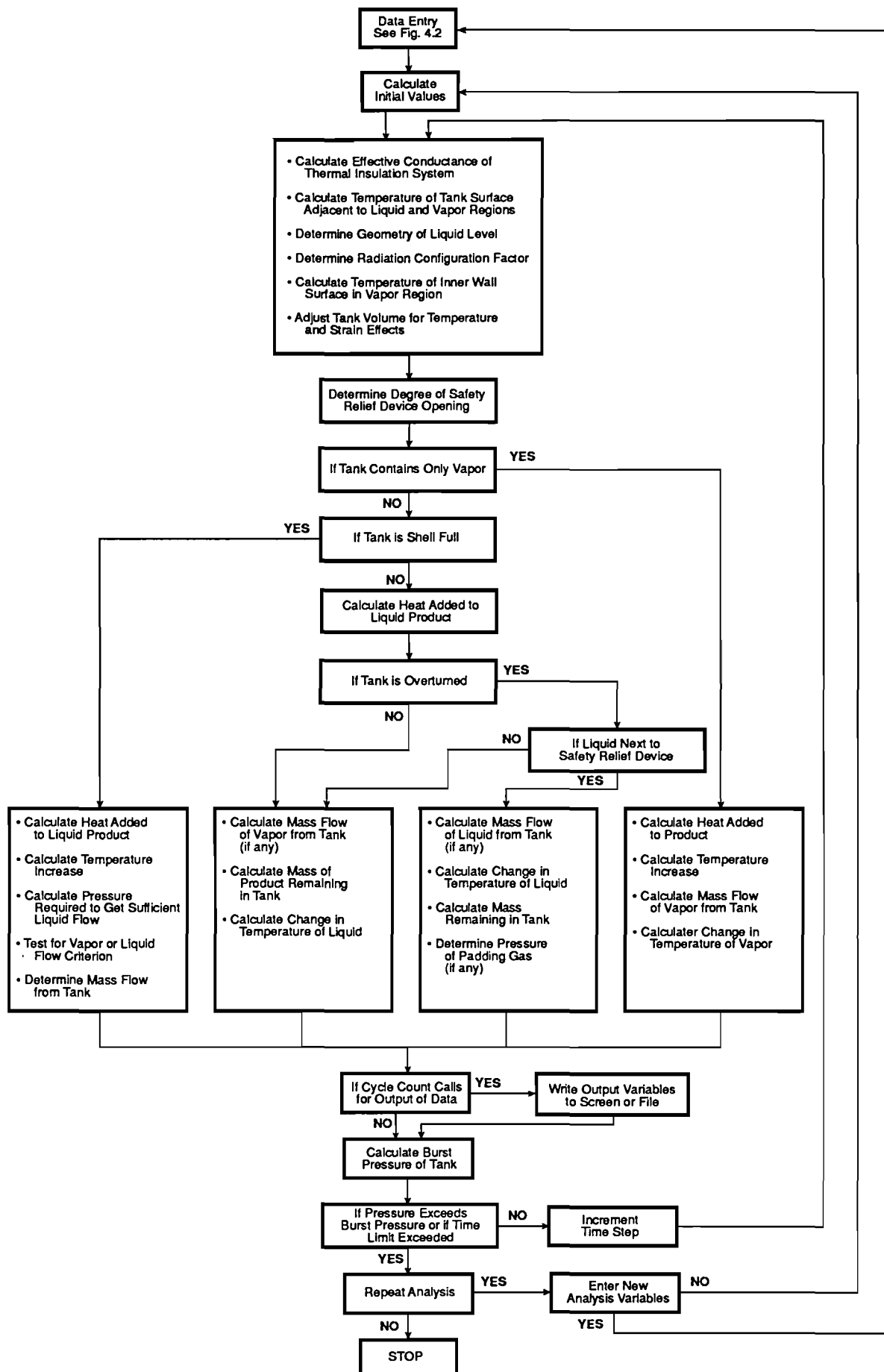


FIG. 4.1 FLOW CHART FOR PROGRAM 'AFFTAC'

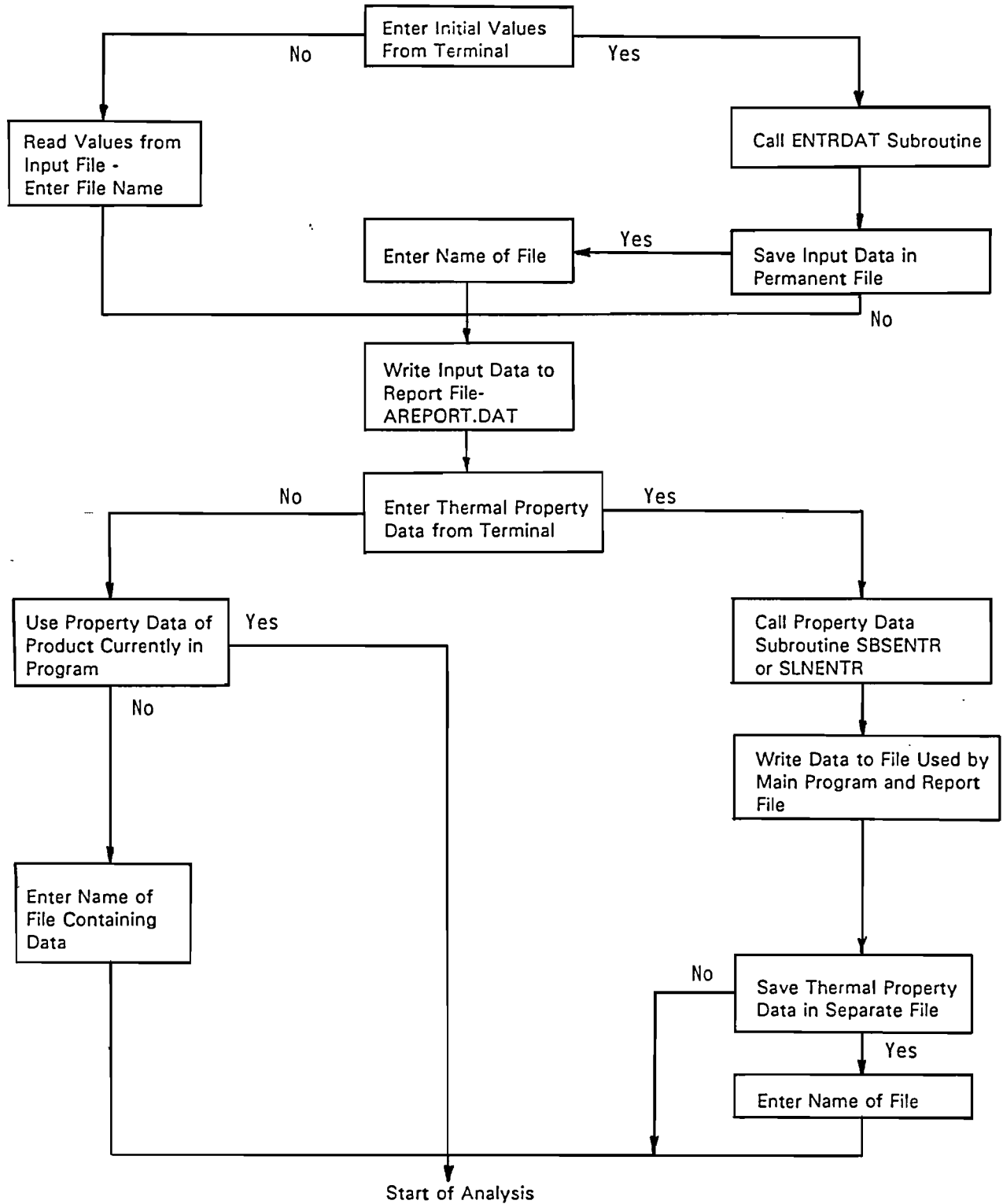


FIG. 4.2 FLOW CHART OF DATA ENTRY FOR PROGRAM 'AFFTAC'

A statement then appears on the screen asking definition of the type of data output desired. The alternatives are data written to the monitor screen, data written to a file, or both. If data is to be written to a file, a statement appears on the screen asking the name of the output file. Type in the name of the file and press the return key.

#### 4.1.2 Calculate Other Initial Values

After the entry of initial analysis and thermal property data the program then proceeds with the calculation of other parameters.

First, conductances are calculated for the tank wall and the tank wall in combination with a film coefficient between the liquid and tank wall. The thermal resistance offered by the film coefficient is difficult to estimate. Conductances ranging from several hundred to several thousand are reported in the literature depending on the properties of the liquid, whether or not boiling is present at the interface, and the geometry of the interface (e.g., see Ref. 3). An indication of a representative value to use for this parameter can be inferred from the results\* of the full scale fire test on a tank car filled with propane (Ref. 4). A value of 1000 BTU/hr-ft<sup>2</sup>-°F is recommended as a conservative representative value of the film coefficient.

Next, other parameters, such as the volume of the tank, tank length, tank surface area, weight of tank shell, initial weight of liquid product, initial weight of padding gas, if any, weight of product in the vapor space, etc., are determined. The appropriate product subroutine is called to get the product data for these calculations. Pressures related to the safety relief valve are converted to absolute values. Pressures defining the degree of opening of a safety relief valve are also established.

If a safety relief valve is used, its cross sectional area is calculated from the standard equation for compressible gas flow through a nozzle:

$$w = 144C_d A_v P \sqrt{\frac{g \gamma}{ZRT} \left[ \frac{2}{\gamma + 1} \right]^{\frac{\gamma + 1}{\gamma - 1}}} \quad (1)$$

---

\* The results of this test indicated that the average conductance over the surface of the car was 300 BTU/hr-ft<sup>2</sup>-°F. The conductance of the 5/8 in. thick steel wall can be estimated at approximately 500 BTU/hr-ft<sup>2</sup>-°F, which implies that the conductance of the film coefficient would be about 750 BTU/hr-ft<sup>2</sup>-°F.

where :  $w$  is mass flow rate (lbs/sec),  
 $A_v$  is minimum cross sectional area of valve (ft<sup>2</sup>),  
 $C_d$  is the valve discharge coefficient,  
 $P$  is upstream gas pressure (psia),  
 $T$  is upstream gas temperature (absolute temperature, °R\*),  
 $g$  is the gravitational constant (ft/sec<sup>2</sup>),  
 $Z$  is the gas compressibility factor,  
 $R$  is the gas constant, equal to 1545/(molecular weight)(ft°R), and  
 $\gamma$  is the ratio of specific heats.

For air it is assumed that  $Z$  equals 1.0,  $\gamma$  equals 1.4, and  $R$  equals 53.3.  $T$  is assumed to be 519.7 or 60 °F.

Equation (1) then becomes:

$$w = 3.3958 PC_d A_v \quad (2)$$

The density of air at standard conditions (60° F and 14.7 psia) is 0.0763 lbs/ft<sup>3</sup>. Substituting and rearranging terms, the minimum cross sectional area of the valve can be expressed as follows:

$$A_v = (\text{SCFM}) / (C_d P_s 2644) \quad (3)$$

where: SCFM is the rated flow capacity (ft<sup>3</sup>/min), and  
 $P_s$  is the valve flow rating pressure (psia).

If a safety relief valve is used, constants related to the equation for vapor flow through a valve (VLPCON), are calculated so that they can be used later in the analysis when vapor mass flow through the valve is determined. The constants are calculated, as appropriate, for vapor flow of the substance, solvent and padding gas as follows:

$$\text{VLPCON} = 144 \sqrt{\frac{g \gamma}{R} \left[ \frac{2}{\gamma + 1} \right]^{\frac{\gamma + 1}{\gamma - 1}}} \quad (4)$$

---

\* The notation °R is used to refer to absolute temperature in degrees Rankine.

## 4.2 PRELIMINARY CALCULATIONS OF FIRE EFFECTS

### 4.2.1 Determine Effective Conductance of Thermal Insulation and Thermal Protection System(s)

Once all the initial value calculations have been completed, the program begins the analysis of the effects of the fire on the tank car. The first step in this process is to integrate the effects of any linings, if present, into the conductance's previously determined for the tank wall and the tank wall combined with the film coefficient. This calculation also takes into account any deterioration in the thermal resistance afforded by the lining which may take place over time. This option is provided in the entry of data (see Section 2.3.4 in the User's Manual). Two options are provided, the use of a rubber liner or an organic coating.

Rubber liners are used on some acid cars. They would initially offer a high value of insulation. A typical value for the conductivity of rubber is 0.1 BTU/hr-ft-°F. This would imply a conductance of 6.4 BTU/hr-ft<sup>2</sup>-°F for a 3/16 in. thick rubber liner, which would provide a high degree of resistance to heat flow into the tank. It is likely, however, that the effectiveness of the rubber as a thermal insulator would soon be destroyed on cars which do not have any exterior insulation because the adjacent steel tank wall would soon be heated to over 1000 °F which would melt the surface of the rubber in contact with it. Therefore, in an analysis of this condition, it is recommended that the rubber liner be considered to have an initial conductance of 6.4 BTU/hr-ft<sup>2</sup>-°F, but that this would be degraded linearly over a 15 minute period. The rubber liner on an insulated car is likely to remain effective for a much longer time because the exterior insulation would keep the tank wall at a moderate temperature.

Some cars have an organic coating on the inside of the tank. It would offer less resistance to heat flow than a rubber liner because of its small thickness. An estimate of its conductivity is 0.25 BTU/hr-ft-°F which implies a thermal conductance of 500 BTU/hr-ft<sup>2</sup>-°F for a 6 mil thickness. Its effectiveness would be expected to be retained for a fairly long period of time because, its conductance is high, which means the temperature of the inside of the tank wall would be close to the temperature of the product within the tank. Thus, it is less likely to be damaged by high temperature.

The overall value for the conductance of the tank (CNDLQ in liquid region or CNDVD in vapor region) is determined from the conductances of the component parts by the following formula:

$$\frac{1}{\text{CNDLQ or CNDVD}} = \sum \frac{1}{C_i} \quad (5)$$

where:  $C_i$  is the conductance of a component of the system (e.g., tank wall, insulation, etc.)

#### **4.2.2 Calculate Temperature of Tank Surface Outside of Liquid Region**

Next, the temperature of the outer surface of the tank in the liquid region is calculated. This calculation is carried out in subroutine SURFACET. (See Appendix J.) 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 except in the case of a torch fire where it is assumed to be 0.536. The surface emissivity factor is as entered with the input parameters. 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 heat balance under these conditions.

#### **4.2.3 Calculate Temperature of Tank Surface Outside of Vapor Region**

The calculation of the temperature of the outer wall surface in the vapor region is also made using subroutine SURFACET. The conservative assumption is made, if a padding gas was initially present, 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 contact 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.

#### 4.2.4 Establish Geometry of Liquid Levels

The calculation requires the establishment of the angle from the horizontal (THET), in radians, of a radial line to the liquid level at the surface of 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:

$$\text{FRAC} = 1/\pi [\pi/2 + \text{THET} + \sin(\text{THET}) \cos(\text{THET})] \quad (6)$$

#### 4.2.5 Radiation Surface Configuration Factor

First, the area of the surface of the liquid (AREALQ) within the tank is calculated. 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:

$$A_1 F_{12} = A_2 F_{21} \quad (7)$$

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:

$$F_{12} = \frac{1}{1/f_{12} + (1/\epsilon_1 - 1) + (A_1/A_2)(1/\epsilon_2 - 1)} \quad (8)$$

where:  $f_{12}$  is the radiation surface configuration factor for a black body,  
and  
 $\epsilon_1$  and  $\epsilon_2$  are emissivities of surfaces 1 and 2.

In using this equation it is assumed that  $f_{i\text{q},\text{tk}} = 1$  since the liquid surface sees only the tank wall.



The radiation surface configuration factor for the liquid to the tank is designated FLQT, and the factor for the tank to the liquid is designated FTLQ. FTLQ is calculated from FLQT using the reciprocal relationship. The emissivity of the inside tank wall is assumed to be 0.8. The emissivity of the liquid surface is assumed to be 0.9.

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. Although the transient differences may be larger when the liquid level is near the center of the tank, calculations show that they would only have a small effect on the total heat transfer.

#### **4.2.6 Calculate Temperature of Inner Wall Surface in Vapor Region**

The next step is to calculate the temperature of the tank wall in the vapor region. This is done by taking the value for the outer tank wall surface temperature 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. The calculation also considers that there is small amount of convected heat loss. Various values for the convection coefficient are assumed depending on the orientation of the car, the fraction of tank volume occupied by liquid and the flow rate through the safety relief device. This characteristic has been deduced, in part, from the full scale fire tests.

#### **4.2.7 Adjust Tank Size for Temperature and Strain Effects**

Next, the size of the tank is adjusted for temperature and strain effects. The temperature of the tank adjacent to the liquid is used to determine the expansion of the volume of the tank due to its rise in temperature. The use of the liquid temperature is a reasonable assumption because the effect is only significant when the product is near the shell full condition. Calculation of the expansion of the tank is based on the following equation:

$$l_1 = l_0 [ 1 + \alpha (T_1 - T_2)] \quad (9)$$

where:  $l_1$  is length dimension at temperature  $T_1$  (1/°F),  
 $l_0$  is length dimension at temperature  $T_0$  (1/°F), and  
 $\alpha$  is a constant, which depends on the type of material (1/°F).

The ratio of any dimension on the tank at elevated temperature to the original dimension is then:

$$\frac{1 + \alpha T_2}{1 + \alpha T_1} \quad (10)$$

where:  $T_2$  is the elevated temperature of the tank, and  
 $T_1$  is the initial temperature of the tank.

Since this ratio applies to each of the three spatial dimensions, the ratio of volume expansion would be the cube of the ratio.

The size of the tank is also adjusted to account for the membrane stresses in the tank caused by the circumferential and axial stresses.

The circumferential and axial strains associated with these stress are given as follows:

$$\epsilon_c = \sigma_c/E - \mu(\sigma_a/E) \quad (11)$$

$$\epsilon_a = \sigma_a/E - \mu(\sigma_c/E) \quad (12)$$

where:  $\epsilon_c$  is the circumferential strain,  
 $\epsilon_a$  is the axial strain,  
 $E$  is the Modulus of Elasticity of tank material (psi),  
 $\mu$  is Poisson's ratio assumed to be 0.3 for all tank materials,  
 $\sigma_c$  is circumferential stress, equal to  $pd/2t$  (psi),  
 $\sigma_a$  is the axial stress, equal to  $pd/4t$  (psi),  
 $p$  is the internal pressure (psig),  
 $d$  is the tank inside diameter (ins.), and  
 $t$  is tank wall thickness (ins.).

Substituting the values for stresses in the strain equations leads to the following relationships:

$$\epsilon_c = 0.425 \frac{pd}{E t} \quad (13)$$

$$\epsilon_a = 0.100 \frac{pd}{E t}$$

The cross sectional area of the tank would increase by a factor  $(1 + \epsilon_c)^2$ . The volume of the tank would then increase by the following factor:

$$[ (1 + \epsilon_c)^2 (1 + \epsilon_a) ] \quad (14)$$

#### **4.2.8 Determine Vent Opening or Degree of Valve Opening**

The next step in the calculation is to determine the degree to which the safety relief valve has opened, when this type of device is used. 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 percent of the start-to-discharge pressure, the valve closing pressure, which is assumed to be 82 percent of the start-to-discharge pressure, and a reference pressure on the closing stroke of the valve which is 88 percent of the start-to-discharge pressure. The degree to which the valve is opened depends on whether the pressure is increasing or decreasing. The relationship between the degree of valve opening and the pressure is shown in Fig. 4.3. Note that an alternate closing path is shown, which represents the condition where the valve starts to close before it has fully opened.

#### **4.2.9 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 been previously defined as:

- Liquid and vapor within the tank with vapor adjacent to safety relief device,
- Liquid and vapor within the tank with liquid adjacent to safety relief device,
- Shell full of liquid product, and
- Containing only product in the vapor phase.

The calculational procedure is divided at this point so that each of these cases is 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 or vent.

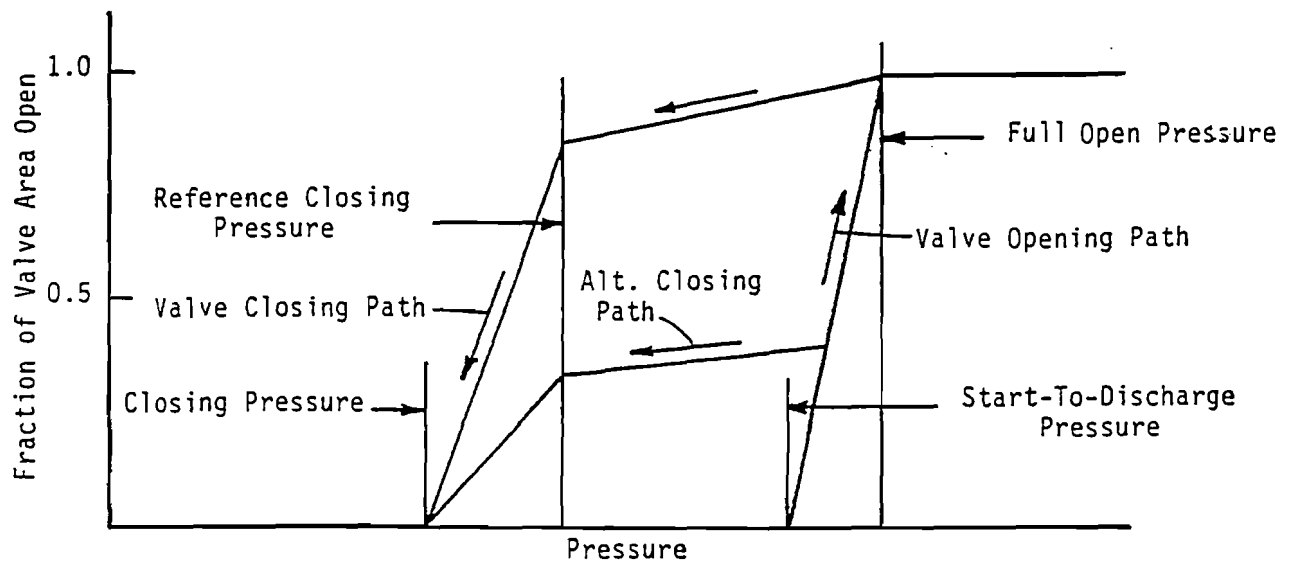


FIG. 4.3 RELATIONSHIP BETWEEN DEGREE OF VALVE OPENING AND PRESSURE

### 4.3 CALCULATION OF EFFECTS WITH LIQUID AND VAPOR WITHIN TANK WITH VAPOR ADJACENT TO SAFETY RELIEF DEVICE

#### 4.3.1 Calculate Heat Transfer to Liquid Product

If the type of fire is not a torch fire, 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 a jacket, if present, and insulation materials can be neglected. If the effect of discontinuities on heat transfer is considered, the heat transfer through these discontinuities is added to the heat input calculated for the insulated part of the tank.

If the type of fire is a torch fire the heat input is calculated for a 16 ft<sup>2</sup> portion of the tank wall adjacent to the liquid. The effect of discontinuities are not included.

The radiant exchange of energy between the tank shell above the liquid and the liquid surface has been discussed in Section 4.2.5.

#### 4.3.2 Calculate Mass Flow Rate Through Safety Relief Device

The mass flow rate through the safety relief device is computed for vapor flow, if the pressure is sufficient to open the valve or to have ruptured the frangible disc. The calculation is first made by using the standard compressible gas flow equation, for flow through a nozzle, which was previously given in Equation 1. The calculation makes use of the VLPCON constants calculated at the beginning of the analysis. The formula for the mass flow rate becomes.

$$W = (\text{VLPCON}) C_d A P \sqrt{\frac{1}{ZT}} \quad (15)$$

Where there is more than one component in the vapor, such as a padding gas, or vapor from the solvent of a commodity that is in solution, it is assumed that the mass flow of each component is proportional to the partial pressure of each gas. The effect of the padding gas on the mass flow rate becomes negligible after a short period of time,

because its mass in relation to the mass of the product is quite small. Examination of the logic in the calculation will show that the out-flows are arbitrarily reduced if the resulting pressure would be less than atmospheric in the case of a vent, or less than the valve closing pressure in the case of a safety relief valve. This compensates for the consequences of using a finite time step which may not be sufficiently accurate for rapidly changing conditions. The effect is significant only as the shell full condition is approached.

If the total pressure within the tank is greater than atmospheric pressure (14.7 psia), but less than 27.0 psia, the calculated outflow of vapor is reduced because a critical flow condition would not be reached at the minimum area cross section of the valve or vent.

If less than 2.5 percent of the tank is filled with liquid, rapid changes in the outflow are limited by adding one-half of the newly calculated outflow to one-half of the outflow calculated in the previous step.

After these calculations are completed, additional checks are made, if a padding gas was initially present, to determine if the outflow is such that the pressure within the tank would be below atmospheric pressure in the case of a vent or below the closing pressure in the case of a relief valve. If the pressure is below the appropriate limit, the calculated outflow of vapor is reduced further to keep the vapor pressure in the tank at the limit.

#### **4.3.3 Calculate Change in Mass of Product**

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

#### **4.3.4 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 between the total heat flow to the product and the heat absorbed by the vaporization of the product.

### **4.4 CALCULATION OF LIQUID AND VAPOR WITHIN TANK WITH LIQUID ADJACENT TO SAFETY RELIEF DEVICE**

This case represents the overturned car condition.

#### **4.4.1 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.

#### **4.4.2 Calculate Liquid Flow Rate Through Safety Relief Device**

The liquid flow rate through the safety relief device, if it is open is calculated using subroutine AVFLOW, (see Appendix K) which assumes homogenous, isentropic, two-phase flow (liquid and vapor). Two-phase flow effects will be a significant factor only if the product has a high vapor pressure.

#### **4.4.3 Calculate Change in Temperature**

The change in temperature of the liquid of the 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.

#### **4.4.4 Determine New Properties**

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

#### **4.4.5 Calculate Remaining Mass of Product and Padding Gas**

The remaining mass of the product within the tank, and its division between liquid and vapor states, is recalculated under the new temperature and pressure conditions.

The following assumptions are made for the cases where a padding gas is used. First, it is assumed that initially the padding gas in the vapor space is in equilibrium with the gas dissolved in the liquid product. Because of the small outage volume in which the gas is contained, there may be more gas dissolved in the product than present in the vapor phase. It is also assumed that there is no exchange between the padding gas dissolved in the fluid and the gas in the vapor phase during the course of the exposure to the fire environment. If equilibrium were to be maintained between the padding a gas in the vapor phase and the gas dissolved in the product, there would first be an increase in the amount of the dissolved gas and a corresponding decrease in the amount of padding gas 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 padding gas would be less than that predicted by the assumption of no exchange between the vapor and the dissolved state. After the safety relief device opens and the product starts to flow from the car, the outage volume would increase and the corresponding decrease in the vapor pressure would cause more padding gas to be liberated from the fluid. Also, as the liquid product is heated, more of the padding gas would be liberated from the fluid. Thus, there would be a tendency to maintain the partial pressure of the gas above that predicted by the assumption of no exchange between the vapor and the dissolved states. The assumption that equilibrium is maintained would delay slightly the time at which the safety relief device 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 outage gets to approximately 10 percent, the effect of the padding gas becomes insignificant on the prediction of flow through the relief device.

The major reason that the exchange of padding gas 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 padding gas in the vapor state to be communicated to all portions of the liquid within the tank and for gas to be absorbed in the early phases of the predicted effects. Similarly, the effect of the decrease in the partial pressure of the padding gas once the device is opened, would not be immediately communicated to all portions of the liquid in the tank so a non-equilibrium condition would likely exist. Consequently, the assumption that there is no exchange of the padding gas from the vapor phase to the dissolved state is believed to have minimal significance in the predicted events associated with the flow of the product from the tank car.

#### **4.5 CALCULATION OF EFFECTS WITH SHELL FULL CONDITIONS**

This case considers the condition where the tank is completely filled with liquid.

##### **4.5.1 Calculate Heat Transferred to Liquid Product**

The total heat transmitted to the liquid product of the tank in the time increment is calculated.



#### **4.5.2 Calculate Change in Temperature**

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

#### **4.5.3 Determine New Properties**

The new properties of the product at the higher temperature are determined by calling the appropriate property subroutine.

#### **4.5.4 Calculate Required Volume of Flow**

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

#### **4.5.5 Calculate Pressure Required to Generate Sufficient Flow**

The pressure that must be developed within the tank so that the required volume will be discharged through the valve is calculated. This pressure is calculated by assuming that the pressure difference driving the fluid out through the device will have as the lower pressure the maximum of the saturated vapor pressure or atmospheric pressure. This is a conservative assumption. Consideration of two-phase flow effects for high vapor pressure products might result in a slightly lower tank pressure, but the difference would be small. The following formula is utilized:

$$w = C_d A \rho \sqrt{(2g/\rho) (p_c - p_s)} \quad (16)$$

where:  $w$  is the mass flow rate, (lbs/sec),  
 $C_d$  is the liquid discharge coefficient of the valve,  
 $A$  is the cross sectional area of the valve (ft<sup>2</sup>),  
 $\rho$  is the density of the liquid (lbs/ft<sup>3</sup>),  
 $p_c$  is the upstream fluid pressure (lbs/ft<sup>2</sup>), and  
 $p_s$  is the saturated vapor pressure at the temperature of the fluid, or atmospheric pressure, whichever is greater (lbs/ft<sup>2</sup>).

If the vapor pressure is less than atmospheric pressure, in the case of a vent, or less than the valve closing pressure, in the case of a valve, the pressure is reset to one of these values. The tank remains full.

If sufficient vapor flow can be generated with the pressure at saturated conditions, in the case of an upright car, enough product may be passed through the

relief device so that the tank will not be shell full the next time through the calculational cycle. The liquid flow calculation is made using subroutine AVFLOW so that two-phase flow effects are considered. If these calculations indicate that the mass flow is less than the minimum required for the shell full condition, an index is set so that a shell full condition will be recognized the next time through the calculational cycle. If the calculations show that the mass flow is greater than the minimum required for the shell full condition, the index is set so that a non-shell full condition will be recognized.

#### **4.5.6 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 or the mass flow calculated from saturated vapor flow for an upright car or liquid flow for an overturned car.

### **4.6 CALCULATION OF EFFECTS WITH VAPOR PHASE ONLY WITHIN TANK**

This condition occurs after the critical temperature\* is reached (a condition obtained only at high temperatures for the products: propane, ethylene oxide, propylene, or propylene oxide, which have their properties contained in the program) 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 condition the pressure within the tank may increase due to the increased pressure of the product, but the increased pressure will be relieved by flow through the safety valve closing pressure.

#### **4.6.1 Calculate Heat Transfer to Vapor Product**

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

#### **4.6.2 Calculate Change in Pressure**

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

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\* See note on page 8.

#### **4.6.3 Calculate Mass Flow Out**

The mass out through the safety relief device is calculated using the equation previously presented for vapor flow (Equation 1). A compressibility factor of 0.7 is assumed for all commodities except for propane where it is represented as a function of the total pressure within the tank, the temperature and specific volume.

#### **4.6.4 Calculate Change in Tank Temperature**

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

### **4.7 OUTPUT DATA**

The program provides two different types of format for displaying the results of the calculations. The first format writes data to a file at selected time intervals during the course of analysis. The interval is selectable as a multiple of the time increments used during the analysis. The second format displays a more limited set of data on the monitor screen at selected intervals. The output variables displayed at the monitor are: time, the pressure within the tank, the burst pressure of the tank, the temperature of the product, the fraction of the tank filled with liquid, the fraction of the original mass of product remaining in the tank, and the rate of product out-flow through the safety relief device. The output to the monitor pauses after 20 lines of data have been displayed on the screen. The calculation can be restarted by pressing the ENTER key.

The output variables which are written to the computer file include all of the above along with the temperature of the tank over the vapor space. The rate of product out-flow that is displayed in each of these cases is the average out-flow over the number of time increments between the display of data.

If during the course of the analysis the temperature of the product exceeds the temperature for which thermal property data have been entered into the program, the following message will appear in the output data:

#### **OUTSIDE TEMPERATURE RANGE OF THERMAL PROPERTY DATA**

The analysis program will still run if a temperature limit is exceeded, but reduced accuracy should be anticipated because the property values would be determined by extrapolation rather than by interpolation.

If during the course of the analysis of a solution, the concentration of the solution goes outside the range for which thermal property data have been entered into the program, the following message will appear in the output data:

#### OUTSIDE CONCENTRATION RANGE OF THERMAL PROPERTY DATA

The analysis program will still run if the concentration range has been exceeded, but reduced accuracy should be anticipated because the property values would be determined by extrapolation rather than interpolation.

If a critical temperature has been entered into the program, the program will terminate the analysis if the critical temperature is exceeded. A message will appear in the output data stating:

#### CRITICAL TEMPERATURE EXCEEDED

### 4.8 COMPARE TANK BURSTING PRESSURE AND INTERNAL PRESSURE

The final step in the calculation is to compare the internal pressure in the tank with its bursting pressure. The bursting pressure is determined from the tensile strength of the tank material, which is a function of its maximum temperature. If the internal pressure exceeds the burst pressure it is assumed that the tank will fail and the calculation is stopped. The burst pressure is calculated by substituting the tensile strength in the formula for the membrane circumferential stress in the tank as follows:

$$P_b = 2\sigma_t t / d \quad (17)$$

where:  $P_b$  is the burst pressure (psig),  
 $\sigma_t$  is the tensile strength (psi),  
 $t$  is the tank wall thickness (ins.), and  
 $d$  is the inside diameter of the tank (ins.).

A number of functions are contained in the program which define the reduction in strength of tank materials with increasing temperature. These functions reduce the value of the tensile strength of the tank material, which is entered into the program at the beginning of the analysis, as the temperature of the tank increases. The reduced strength is then used to calculate the burst pressure. One function is used for carbon

steel. It is based on data for TC128 steel given in Ref. 14. Two functions are used for stainless steel. They are based on data in Refs. 15 and 16. Three functions are used for aluminum alloys. They are based on data in Ref. 13. The program uses the identification number for the tank material, IMT, to select the appropriate function.

#### **4.9 CHECK FOR TIME LIMIT**

If the burst pressure has not been exceeded, a check is made to determine if the time limit has been exceeded. If so, the calculation is halted. Otherwise, the time is incremented and the calculation returns to the point where the effective conductance of the thermal shield is determined (see Section 4.2.1).

#### **4.10 PROGRAM TERMINATION OR RESTART**

After the analysis has been completed an option is provided to terminate the operation of the program or conduct a repeat analysis. If a repeat analysis is desired, an option is provided to begin the analysis using the same initial conditions and thermal properties as the preceding analysis, or to change the initial conditions.

##### **4.1.1 PROGRAM LISTINGS**

The source code for the main program AFFTAC.FOR is presented in Appendix A. The source codes for the subroutines are presented in Appendices B through L.



## 5. REFERENCES

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APPENDIX A

SOURCE CODE FOR MAIN PROGRAM: AFFTAC

C AFFTAC.FOR IS A PROGRAM FOR THE ANALYSIS OF TANK CARS IN THE  
 C POOL OR TORCH FIRE ENVIRONMENTS VENTING LIQUID OR VAPOR. THE  
 C PROGRAM USES SUBROUTINES FPRPSBS, FPRPSLV, AVFLOW, ASETUP, SURFACET,  
 C TSHIELD, ENTRDAT, ALYRPT, SBSENTR, SLNENTR, SBSPROP, AND SLNPROP.  
 C.....Version 3.0, November 11, 1998

```

REAL CNDLQ, CNDVP, TWAL, TWAV, ATEM, WLET
REAL NETQ, LENG, K WALL, WOUT, CONC, TEMP, CINTV, FLFAC
REAL LINTV, MLWSBS, MLWSLV, SCFM, CNDD, ERAD, TFLA
REAL THIC, A1, A2, A3, TTNK, TTNV, CDJNT, CNDWL
REAL WOUT2, DELT, CVLQ, PNIT, TIME
INTEGER*4 NTIME
INTEGER*2 INTYPE, OTYPE, NALYSS, IPFST
INTEGER*2 IMT, IPTYP, ISBSL, IPR, ICR, IPAD, IVLTYP
INTEGER*2 INS, KINDX, IDSC, LLNG, ILN, ILD, IFRTYP, INTV
CHARACTER*1 RESPNS
CHARACTER*12 FNAME, ANAME, PNAME
CHARACTER*30 QNAME, CPRD (21)
DIMENSION CDLIN (2)

```

C

```

COMMON/TANK/SIZE, DIAI, WTKI
COMMON/MATL/IMT, TNSRTH, PNBR, PCBRS
COMMON/PRDCT1/IPTYP, ISBSL, IPR, ICR, TCRIT
COMMON/PRDCT2/FRAT, TEMC, CONC, IPAD, PPID
COMMON/SRELF1/IVLTYP, AVENT, VGTD, SCFM
COMMON/SRELF2/PGSD, PGTD, CVAD, CVLQ, TILT
COMMON/THRML1/INS, CNDD, KINDX, CNDI, CINTV
COMMON/THRML2/THIC, A1, A2, A3
COMMON/THRML3/IDSC, USUM, LLNG, ILN, ILD, LINTV
COMMON/FIRE/IFRTYP, TEMF, CFRA, CATR, ERAD
COMMON/ITIME/TLIMIT, DELT, INTV

```

C

```

COMMON/PROP1/SPEC, SPLQ, HFLV, PSBS, PSLV, ZSBS, ZSLV, VVAP
COMMON/PROP2/GAMSBS, GAMSLV, MLWSBS, MLWSLV
COMMON/PROP3/TLMTMN, TLMTMX, CNCMIN, CNCMAX

```

C

```

COMMON/NAME/CPRD

```

C

```

WRITE (*,*)
1 WRITE (*,*) 'VERSION 3.0 OF PROGRAM AFFTAC, November 11, 1998'
WRITE (*,*) ' '
WRITE (*,*) ' Press Enter to Proceed'
READ (*,*)
WRITE (*,*) ' '

```

C

```

NALYSS=0 ! identifier for repeat analysis
QNAME='BLANK'
WRITE (*,*)
1 'ENTER CODE DESIGNATING PROCEDURE FOR ENTERING ANALYSIS DATA'
WRITE (*,*) ' (enter integer number):'
WRITE (*,*) ' 1 - Data entry at monitor'
WRITE (*,*) ' 2 - Data read from existing file'
READ (*,*) INTYPE
403 CONTINUE

```

```

IF (INTYPE.EQ.1) CALL ENTRDAT(QNAME, NALYSS)
IF (INTYPE.EQ.2) THEN
WRITE (*,*) 'ENTER NAME OF FILE CONTAINING ANALYSIS DATA'
WRITE (*,*) ' (Maximum of 12 Characters):'
READ (*,519) ANAME
OPEN (UNIT=11, FILE=ANAME, STATUS='OLD')
READ (11,501) SIZE, DIAI, WTKI

```

```

        READ (11,502) IMT, TNSRTH, PNBRS, PCBRS
        READ (11,503) IPTYP, ISBSL, IPR, ICR, TCRIT
        READ (11,504) FRAT, TEMC, CONC, IPAD, PPID
        READ (11,505) IVLTYP, AVENT, VGTD, SCFM
        READ (11,507) PGSD, PGTD, CVAD, CVLQ, TILT
        READ (11,509) INS, CNDD, KINDX, CNDI, CINTV
        READ (11,511) THIC, A1, A2, A3
        READ (11,513) IDSC, USUM, LLNG, ILN, ILD, LINTV
        READ (11,515) IFRTYP, TEMF, CFRA, CATR, ERAD
        READ (11,517) TLIMIT, DELT, INTV
    ENDIF
501    FORMAT (F8.0, F8.2, F8.4)
502    FORMAT (I8, F8.0, 2F8.1)
503    FORMAT (4I8, F8.2)
504    FORMAT (F8.3, F8.2, F8.3, I8, F8.3)
505    FORMAT (I8, 2F8.2, F8.0)
507    FORMAT (5F8.2)
509    FORMAT (I8, F8.2, I8, 2F8.2)
511    FORMAT (F8.2, 3F8.3)
513    FORMAT (I8, F8.2, 3I8, F8.2)
515    FORMAT (I8, F8.1, 3F8.2)
517    FORMAT (2F8.2, I8)
519    FORMAT (A12)
521    FORMAT (A30)
    AVHOLD=AVENT
    CNHOLD=CONC
    IPHOLD=IPAD
C
    IF (INTYPE.EQ.2.AND.IPR.GT.16) THEN
        WRITE (*,*)
    1    'ENTER NAME OF PRODUCT (Maximum of 30 Characters):'
        READ (*,521) QNAME
    ENDIF
C.....Write input data to a report file.....
C
    CALL ANLYRPT (QNAME)
C
C.....Select method for entering thermal property data.....
C
    IF (NALYSS.EQ.0.AND.IPTYP.EQ.2) THEN
        IF (ISBSL.EQ.1) THEN
            OPEN (UNIT=16, FILE='NEWSBS.DAT', STATUS='NEW')
            CALL SBSENTR (QNAME)
        ENDIF
        IF (ISBSL.EQ.2) THEN
            OPEN (UNIT=16, FILE='NEWSLN.DAT', STATUS='NEW')
            CALL SLNENTR (QNAME)
        ENDIF
    ENDIF
    IF (NALYSS.EQ.0.AND.IPTYP.EQ.3) THEN
        WRITE (*,*)
    1    'ENTER NAME OF FILE CONTAINING THERMAL PROPERTY DATA'
        WRITE (*,*) ' (File must be in proper format; see'
        WRITE (*,*) ' Users Manual; maximum of 12 characters)'
        READ (*,519) PNAME
        OPEN (UNIT=13, FILE=PNAME, STATUS='OLD')
    ENDIF
C
405    CONTINUE
        WRITE(*,*)

```

```

1  'ENTER CODE FOR DESIGNATION OF TYPE OF DATA OUTPUT'
WRITE(*,*)' 1 - for data display at monitor'
WRITE(*,*)' 2 - for writing data to file'
WRITE(*,*)' 3 - for both types of output'
READ(*,*) OTYPE
IF (OTYPE.EQ.2.OR.OTYPE.EQ.3) THEN
  WRITE(*,*)'ENTER OUTPUT FILE NAME maximum 12 characters'
  READ(*,519) FNAME
  OPEN(UNIT=19,FILE=FNAME,STATUS='NEW')
ENDIF
C.....Set up conductances for tank wall and film coefficient.....
IF (IMT.LE.15) KWALL=26.0 ! conductivity of carbon steel
IF (IMT.GE.16.AND.IMT.LE.19)KWALL=10.0 ! cond. of stainless steel
IF (IMT.GE.20) KWALL=100.0 ! conductivity of aluminum
CWALI=12.0*KWALL/WTKI
CFILM=1000.0
CJNTI=CWALI*CFILM/(CWALI+CFILM)
CDLIN(1)=500.0
CDLIN(2)=6.4
C
IPAD=IPHOLD
CONC=CNHOLD
AVENT=AVHOLD
WSBOUT=0.0
WSVOUT=0.0
PASD=PGSD+14.7
PATD=PGTD+14.7
DHTK=DAI/12.0
ITEMP=0 ! index for temperature range message
ICONC=0 ! index for concentration range message
IFRAC=0 ! index for shell full (1 is shell full)
IF (FRAT.GE.(1.0)) THEN
  FRAT=1.0 ! Vs 3.0
  IFRAC=1 ! Vs 3.0
ENDIF
NVLV=0 ! valve opening index (0 is closed)
NFRST=0 ! index for first time valve opens
NTIME=0 ! time counting index
IPFST=0 ! changed first time thru property SUBROUTINE
NREFTM=INT(100.0*DELT+0.0001)
TEMP=TEMC
WAVOUT=0.0 ! average product outflow for data output
C
C...INITIALIZATION OF THERMAL PROPERTIES AT START OF ANALYSIS
C
IF (IPTYP.EQ.1) THEN
  IF (IPR.GE.1.AND.IPR.LE.9) CALL FPRPSBS (IPR,TEMP)
  IF (IPR.GE.10.AND.IPR.LE.16) CALL FPRPSLV (IPR,CONC,TEMP)
ENDIF
IF (IPTYP.EQ.2.OR.IPTYP.EQ.3) THEN
  IF (ISBSL.EQ.1) CALL SBSPROP (IPFST,IPR,TEMP)
  IF (ISBSL.EQ.2) CALL SLNPROP (IPFST,IPR,CONC,TEMP)
ENDIF
SZGL=SIZE/7.48 ! size in cubic feet
TPSZGL=SZGL ! size adjusted for expansion
LENG=SZGL/(0.7854*DHTK*DHTK) ! length of tank (ft)
AREA=3.1416*DHTK*(LENG+0.5*DHTK) ! surface area of tank (sq ft)
WTWL=WTKI*0.283*144.0 ! weight of tank wall (lbs/sq-ft)
C
IF (IPAD.EQ.1) PPAD=14.7-PSBS-PSLV

```

```

IF (IPAD.EQ.2) PPAD=0.0
IF (IPAD.EQ.3) PPAD=PPID+14.7-PSBS-PSLV
IF (IPAD.EQ.1.AND.PPAD.LE.(0.0)) PPAD=0.0
IF (IPAD.EQ.3.AND.PPAD.LE.(0.0)) THEN
  IPAD=2
  PPAD=0.0
ENDIF
1  WGNT=(1.0-FRAT)*SZGL*2.61*PPAD/  ! weight of padding gas
   (460.0+TEMC)                    ! at start of analysis (lbs)
  WPAD=WGNT
  WLIQ=SZGL*FRAT/SPLQ              ! weight of liquid prdct in tank (lbs)
  WVAP=(1.0-FRAT)*SZGL/VVAP       ! wght of prdct vap in tank (lbs)
  WGHT=WLIQ+WVAP                  ! weight of product (lbs)
  WSBS=WGHT*CONC
  WSLV=WGHT*(1.0-CONC)
  AVLV=SCFM/(CVAD*PASD*2644.0)    ! discharge area of safety
  C                                ! relief valve (sq ft)

  KDCNT=0
  FRAC=FRAT
  TIME=0.0
  WOUT=0.0
  AVENT=AVENT/144.0               ! convert to square feet
  ATEM=0.0                        ! vent or valve closed
  FMSS=WGHT
  PNIT=PPAD
  PTOT=PSBS+PSLV+PNIT
  PSIG=PTOT-14.7
  CNDLQ=CNDI
  CNDVP=CNDI
  CLINT=A1*12.0/THIC              ! initialization
  CVINT=A1*12.0/THIC             ! for INS=6
  TEMH=TEMC
  FMAT=1.0
  KCNT=INTV                       ! count for display interval
  KPAGE=0
  KCNTRL=21
  WOLST=0.0
  RQLST=0.0
  TCLST=0.0                       ! value of TCFM from prior time step; TCFM
  C                                ! is flow capacity of partially open valve.
  TFLA=(TEMF+460.0)/1000.0       ! flame temperature (0.001 deg R)
  C                                ! inner tank wall temp. next to
  TTNK=(TEMC+460.0)/1000.0       ! liquid (0.001 deg R)
  C                                ! hold initial value of TTNK
  TTNV=(TEMC+460.0)/1000.0       ! inner tank wall temp. next to
  C                                ! vapor space (0.001 deg R)
  TWAL=TFLA-0.001                ! outer jacket (or tank) surface temp.
  C                                ! next to liquid (0.001 deg R)
  C                                ! outer jacket (or tank) surface temp.
  TWAV=TFLA-0.001                ! next to vapor (0.001 deg R)
  C                                ! initialization for INS=6
  TMIV=TTNV+0.25*(TWAV-TTNV)     ! initialization for INS=6
  TMIL=TTNK+0.25*(TWAL-TTNK)     ! initialization for INS=6
  PLST=0.0                        ! value of PTOT from prior time step
  POPN=1.03*PGTD+14.7            ! valve fully open pressure (psia)
  PRTN=0.88*PGTD+14.7           ! valve 85% open closing press (psia)
  PCLS=0.82*PGTD+14.7           ! valve closed pressure (psia)
  TEMP=TEMC
  PCOM=0.0
  REQL=0.0
  TRLT=3.1416*(0.5-TILT/180.0)   ! angle (rad) with ref. to horz.

```

```

KIDN=0                                ! analysis type, e.g. shell full, etc.
VLPPCN=75.31                          ! padding gas (air)
ZPAD=0.98                              ! compressibility, air

C
IF (INS.EQ.5) THEN                    ! initialization needed when
  CNDLQ=0.2                            ! considering variable
  CNDVP=0.2                            ! conductivity
ENDIF

C
IF (IFRTYP.EQ.2) THEN                ! view factor for
  FLFAC=0.536                          ! torch fire
ELSE
  FLFAC=1.00
ENDIF

C
C.....BEGINNING OF CALCULATIONS.....
IF (NTIME.EQ.0) GO TO 153
211 CONTINUE
NTIME=NTIME+1

C
C.....following is calculation of valve flow constants.....
GSBFCT=GAMSBS*((2.0/(GAMSBS+1.0))**((GAMSBS+1.0)/(GAMSBS-1.0)))
GSLFCT=GAMSLV*((2.0/(GAMSLV+1.0))**((GAMSLV+1.0)/(GAMSLV-1.0)))
VLSBCN=144.0*SQRT(32.2*MLWSBS*GSBFCT/1545.0)
VLSLCN=144.0*SQRT(32.2*MLWSLV*GSLFCT/1545.0)

C.....Calculation of Effective Conductance.....
C.....Make adjustments in wall conductances to account for linings.....
CNDWL=CWALI
CDJNT=CJNTI
IF (LLNG.EQ.2) THEN
  IF (ILD.EQ.2.AND.TIME.LT.LINTV) THEN
    CTEMPJ=CDLIN(ILN)*CJNTI/(CDLIN(ILN)+CJNTI)
    CTEMPW=CDLIN(ILN)*CWALI/(CDLIN(ILN)+CWALI)
    CNDWL=CTEMPW-(CTEMPW-CWALI)*TIME/LINTV
    CDJNT=CTEMPJ-(CTEMPJ-CJNTI)*TIME/LINTV
  ENDIF
ENDIF

C.....Consider Effects of Various Thermal Insulation Options....
C.....Bare uninsulated tank case.....
IF (INS.EQ.1) THEN
  CNDLQ=CDJNT
  CNDVP=CNDWL
ENDIF

C.....Constant conductance high temperature insulation.....
IF (INS.EQ.2) THEN
  CNDLQ=CNDD*CDJNT/(CNDD+CDJNT)
  CNDVP=CNDD*CNDWL/(CNDD+CNDWL)
ENDIF

C.....Determine outer surface temperatures for jacket only case.
IF (INS.EQ.3) THEN
  CTMPVP=40.0*CNDWL/(40.0+CNDWL)
  CTMPLQ=40.0*CDJNT/(40.0+CDJNT)
  IF (TIME.LT.CINTV) THEN
    CNDVP=CNDI+(CTMPVP-CNDI)*(TIME/CINTV)
    CNDLQ=CNDI+(CTMPLQ-CNDI)*(TIME/CINTV)
  ELSEIF (TIME.GE.CINTV) THEN
    CNDVP=CTMPVP
    CNDLQ=CTMPLQ
  ENDIF
ENDIF
ENDIF

```

```

C.....Non-temperature dependent conductivity.....
  IF (INS.EQ.4) THEN
    IF (KINDX.EQ.1) THEN
      CNDVP=CNDI+(CNDD-CNDI)*(TIME/CINTV)
      CNDVP=CNDVP*CNDWL/(CNDVP+CNDWL)
      CNDLQ=CNDI+(CNDD-CNDI)*(TIME/CINTV)
      CNDLQ=CNDLQ*CDJNT/(CNDVP+CDJNT)
    ENDIF
    IF (KINDX.NE.1) THEN
      CNDLQ=CNDD*CDJNT/(CNDD+CDJNT)
      CNDVP=CNDD*CNDWL/(CNDD+CNDWL)
    ENDIF
  ENDIF
C.....Establish effective conductance adjacent to vapor and liquid
C.....for temperature dependent conductivity
C
  IF (INS.EQ.5) THEN
    CALL TSHIELD(TWAL,TTNK,CNDLQ,THIC,A1,A2,A3,CDJNT)
    CALL TSHIELD(TWAV,TTNV,CNDVP,THIC,A1,A2,A3,CNDWL)
  ENDIF
C
  IF (INS.EQ.6) THEN
    IF (TIME.LT.CINTV) THEN
      CNDVP=CNDI+(CNDD-CNDI)*(TIME/CINTV)
      CNDLQ=CNDI+(CNDD-CNDI)*(TIME/CINTV)
    ELSEIF (TIME.GE.CINTV) THEN
      CNDVP=CNDD
      CNDLQ=CNDD
    ENDIF
C
    CALL TSHIELD(TMIL,TTNK,CLINT,THIC,A1,A2,A3,CDJNT)
    CALL TSHIELD(TMIV,TTNV,CVINT,THIC,A1,A2,A3,CNDWL)
C
    CVTEMP=CNDVP
    CLTEMP=CNDLQ
    CNDLQ=(CNDLQ*CLINT)/(CNDLQ+CLINT)
    CNDVP=(CNDVP*CVINT)/(CNDVP+CVINT)
    TMIL=(TWAL*CLTEMP+TTNK*CLINT)/(CLINT+CLTEMP)
    TMIV=(TWAV*CVTEMP+TTNV*CVINT)/(CVINT+CVTEMP)
  ENDIF
C
C-----
C..Determine effective outer surface temps; adjacent to the liquid:
  CALL SURFACET(TWAL,TTNK,ERAD,CNDLQ,TFLA,INS,TIME,CINTV,FLFAC)
C.....adjacent to vapor space:
  CALL SURFACET(TWAV,TTNV,ERAD,CNDVP,TFLA,INS,TIME,CINTV,FLFAC)
C-----
C.....Determine angle THET (radians) between horizontal reference line
C.....through center of tank and radius line to surface of liquid at
C.....tank wall; use iterative solution for THET as function of FRAC.
  THOU=0.10
  THEM=1.5708
  IF (FRAC.LE.0.0001) THEN
    THET=-1.5708
  ELSE
222  CONTINUE
      FTST=(1.5708+THEM+COS(THEM)*SIN(THEM))/3.1416
      IF (ABS(FTST-FRAC).LT.0.0001) THEN
        THET=THEM
      ELSE

```

```

                IF (FTST.LT.FRAC) GO TO 224
                THEM=THEM-THOU
                IF (THEM.LE.(-1.5708)) GO TO 224
                GO TO 222
224             CONTINUE
                THEM=THEM+0.8*THOU
                THOU=THOU/5.0
                GO TO 222
            ENDIF
        ENDIF
C-----
C             Determine radiation surface configuration factor.
C
                AREALQ=DHTK*COS(THET)*LENG+1.0           ! area liquid surface
                ATANK=LENG*DHTK*(1.5708-THET)
                1   +1.5708*(1.0-FRAC)*DHTK*DHTK+1.0     ! tank area over vapor
                IF (ATANK.LE.0.0) THEN
                    FLTQ=0.9
                    GO TO 369
                ENDIF
                FLQT=1.0/(1.10+0.25*(AREALQ/ATANK))
                FTLQ=FLQT*AREALQ/ATANK
369           CONTINUE
C-----
C             Readjust vapor tank temperatures for shell full condition.
C
                IF (WGNT.LT.(0.1).AND.IFRAC.EQ.1) THEN
                    TTNV=TTNK
                    TWAV=TWAL
                    GO TO 371
                ENDIF
C-----
C             Determine inner wall temperature next to vapor space.
C
                HCNV=0.0
                IF (KIDN.EQ.2.OR.KIDN.EQ.3) THEN
                    IF (FRAC.GT.0.99) HCNV=2.0
                    IF (FRAC.GT.0.95.AND.FRAC.LE.0.99) HCNV=0.5
                ENDIF
                IF (KIDN.EQ.1) THEN
                    IF (WOUTDL.GT.1500.0) THEN
                        IF (FRAC.GT.0.9) HCNV=6.0
                        IF (FRAC.GT.0.4.AND.FRAC.LE.0.9) HCNV=1.5
                    ELSEIF (WOUTDL.GT.200.0.AND.WOUTDL.LE.1500.0) THEN
                        IF (FRAC.GT.0.9) HCNV=2.0
                        IF (FRAC.GT.0.6.AND.FRAC.LE.0.9) HCNV=0.50
                        IF (FRAC.GT.0.4.AND.FRAC.LE.0.6) HCNV=0.25
                    ENDIF
                ENDIF
C
C.....Heat radiated and convected from tank wall to liquid surface.
                QOUT=0.48*FTLQ*(TTNV**4-TTNK**4)+HCNV*(TTNV-TTNK)/3.6
C.....Heat conducted through insulation to tank wall (BTU/sq.ft-sec).....
C.....Calculate temperature of tank wall over vapor space.....
                NETQ=(TWAV-TTNV)*(CNDVP/3.6)-QOUT ! Net heat input to wall
                TDEL=(NETQ/WTWL)*(60.0/125.0)*DELT ! Incremental temperature increase
                TTNV=TTNV+TDEL
371           CONTINUE
C-----
C             Adjust volume of tank for temperature and stress effects.....

```



```

TPSLST=TPSZGL
IF (IMT.GE.20) THEN
    EMOD=10.0*(10.0**6.0)           ! aluminum
ELSE
    EMOD=30.0*(10.0**6.0)         ! steel
ENDIF
IF (IMT.LE.15) ALPHA=6.0/(10.0**6.0)
IF (IMT.GE.16.AND.IMT.LE.19) ALPHA=10.0/(10.0**6.0)
IF (IMT.GE.20) ALPHA=13.0/(10.0**6.0)
RATIO=(1.0+ALPHA*TEMP)/(1.0+ALPHA*TEMC)
STRN=(0.5*(PTOT-14.7)*DHTK*12.0)/(WTKI*EMOD)
TPSZGL=0.33*(SZGL*((1.0+0.850*STRN)**2.0)*(1.0+0.200*STRN)
1      *(RATIO**3.0))+0.67*TPSLST
C-----
C.....Determine the degree of safety relief device opening.....
IF (IVLTYP.EQ.2) GO TO 322
C.....Calculation for valve, first determine valve opening index number....
IF (NVLV.EQ.0.AND.PTOT.GT.PATD) THEN
    NFRST=1
    IF (PTOT.LT.POPN) NVLV=1
    IF (PTOT.GE.POPN) NVLV=2
    GO TO 320
ENDIF
IF (NVLV.EQ.1.AND.PTOT.LT.PCLS) THEN
    NVLV=0
    GO TO 320
ENDIF
IF (NVLV.EQ.1.AND.PTOT.LT.PLST) THEN
    PKEEP=PLST
    NVLV=4
    GO TO 320
ENDIF
IF (NVLV.EQ.1.AND.PTOT.GE.PLST) THEN
    IF (PTOT.GE.POPN) NVLV=2           ! NVLV stays at 1 if PTOT<POPN
    GO TO 320
ENDIF
IF (NVLV.EQ.2) THEN
    IF (PTOT.LT.POPN.AND.PTOT.GT.PCLS) NVLV=3
    IF (PTOT.LE.PCLS) NVLV=0
    GO TO 320
ENDIF
IF (NVLV.EQ.3) THEN
    IF (PTOT.GE.POPN) NVLV=2
    IF (PTOT.LE.PCLS) NVLV=0
    GO TO 320
ENDIF
IF (NVLV.EQ.4) THEN
    IF (PTOT.LT.POPN.AND.PTOT.GE.PKEEP) NVLV=1
    IF (PTOT.GE.POPN) NVLV=2
    IF (PTOT.LE.PCLS) NVLV=0
    GO TO 320
ENDIF
320 CONTINUE
C.....determine flow rate based on valve opening index.....
IF (NVLV.EQ.0) TCFM=0
IF (NVLV.EQ.1) TCFM=SCFM*(PTOT-PATD)/(POPN-PATD)
IF (NVLV.EQ.2) TCFM=SCFM
IF (NVLV.EQ.3.AND.PTOT.GE.PRTN) THEN
    TCFM=SCFM*(0.85+0.15*(PTOT-PRTN)/(POPN-PRTN))
ENDIF

```

```

IF (NVLV.EQ.3.AND.PTOT.LT.PRTN) THEN
  TCFM=SCFM*0.85*(PTOT-PCLS)/(PRTN-PCLS)
ENDIF
IF (NVLV.EQ.4.AND.PTOT.GE.PRTN) THEN
  TCFM=SCFM*(0.85+0.15*(PTOT-PRTN)/(POPN-PRTN))
1   * ((PKEEP-PATD)/(POPN-PATD))
ENDIF
IF (NVLV.EQ.4.AND.PTOT.LT.PRTN) THEN
  TCFM=SCFM*0.85*((PTOT-PCLS)/(PRTN-PCLS))
1   * ((PKEEP-PATD)/(POPN-PATD))
ENDIF
C
TCLST=TCFM
ATEM=AVLV*TCFM/SCFM
322 CONTINUE
IF (IVLTYP.EQ.2) THEN
  IF (NVLV.EQ.0.AND.PTOT.GT.VGTD) THEN
    ATEM=AVENT
    NVLV=5
    NFRST=1
  ENDIF
ENDIF
C-----
C      Sort out conditions in the tank.
C...If contents are above critical temperature, analyze as vapor in tank.
IF (TTNK.GT.0.6659.AND.IPR.EQ.2) GO TO 430 ! temperature greater
IF (TTNK.GT.0.830.AND.IPR.EQ.3) GO TO 430 ! than critical temp.
IF (TTNK.GT.0.6567.AND.IPR.EQ.4) GO TO 430 ! for
IF (TTNK.GT.0.8681.AND.IPR.EQ.8) GO TO 430 ! product
IF (FRAC.LT.0.0005) GO TO 430 ! no liquid left in tank
IF (IFRAC.EQ.1) GO TO 410 ! tank filled with liquid
C-----
C      Both liquid and vapor within tank. . . . .
C      Determine heat in through wetted area and radiated to surface.
C
THEA=0.0
IF (THET.LT.(-1.0)) THEA=0.10
C
IF (IFRTYP.NE.2) HTINR=(0.48*FLQT*((TTNV)**4-(TTNK)**4)+
1 (TTNV-TTNK)*HCNV/3.6)*AREALQ*DELT*60.0
IF (IFRTYP.EQ.2) HTINR=(0.48*1.0*((TTNV)**4-(TTNK)**4)+
1 (TTNV-TTNK)*HCNV/3.6)*16.0*DELT*60.0 ! Note 16.0 put in
C
STDA=AREA*(1.5708+THEA+THET)/3.1416
IF (IFRTYP.EQ.2) THEN
  HTIN=HTINR ! No heat to liquid
ELSE ! because torch over vap
  HTIN=CFRA*((TWAL-TTNK)*CNDLQ*STDA*DELT*60.0/3.6+HTINR)
  IF (IDSC.EQ.2) HTIN=HTIN+USUM*(TWAL-TTNK)*DELT*
1 (60.0/3.6)*(0.5+THET/3.1416)
ENDIF
C
THRML=SPEC*WLIQ+0.125*WTWL*STDA
TLST=TTNK
SLST=VVAP
PLST=PTOT
IF (THET.LE.TRLT) GO TO 420
C*****
C      Liquid and vapor in tank, venting liquid..(KIDN=2). . . . .
C      .....Calculate mass flow out through valve.....

```

```

C
PTOT=PSBS+PSLV+PNIT
1 IF (NVLV.NE.0) CALL AVFLOW(TTNK,WOUT,ATEM,DELT,CVLQ,PNIT,
C     CONC,IPR,IPFST,ISBSL,IPTYP,TIME)
C
IF (IPTYP.EQ.1) THEN
  IF (IPR.GE.1.AND.IPR.LE.9) CALL FPRPSBS (IPR,TEMP)
  IF (IPR.GE.10.AND.IPR.LE.16) CALL FPRPSLV (IPR,CONC,TEMP)
ENDIF
IF (IPTYP.EQ.2.OR.IPTYP.EQ.3) THEN
  IF (ISBSL.EQ.1) CALL SBSPROP (IPFST,IPR,TEMP)
  IF (ISBSL.EQ.2) CALL SLNPROP (IPFST,IPR,CONC,TEMP)
ENDIF
C
WSBOUT=WOUT*CONC
WSVOUT=(1.0-CONC)*WOUT
QWRK=WOUT*SPLQ*PTOT*144.0/778.0
C
C     .....Determine temperature increase.....
C
TELTV=(HTIN-QWRK-WOUT*SPLQ*HFLV/VVAP)/THRML
TTNK=TTNK+TELT/1000.0
C
C     .....Calculate mass remaining in tank.....
C
FMSS=FMSS-WOUT
WSBS=WSBS-WSBOUT
WSLV=WSLV-WSVOUT
TEMP=(TTNK-0.46)*1000.0
C
IF (IPTYP.EQ.1) THEN
  IF (IPR.GE.1.AND.IPR.LE.9) CALL FPRPSBS (IPR,TEMP)
  IF (IPR.GE.10.AND.IPR.LE.16) CALL FPRPSLV (IPR,CONC,TEMP)
ENDIF
IF (IPTYP.EQ.2.OR.IPTYP.EQ.3) THEN
  IF (ISBSL.EQ.1) CALL SBSPROP (IPFST,IPR,TEMP)
  IF (ISBSL.EQ.2) CALL SLNPROP (IPFST,IPR,CONC,TEMP)
ENDIF
C
PTOT=PSBS+PSLV+PNIT
WLIQ=(FMSS-TPSZGL/VVAP)/(1.0-SPLQ/VVAP)
WVAP=FMSS-WLIQ
VLIQ=WLIQ*SPLQ
FRAC=VLIQ/TPSZGL
IF (VLIQ.GE.TPSZGL.AND.PPAD.LT.(0.001)) THEN
  FRAC=1.0
  IFRAC=1
ELSE
  IFRAC=0
ENDIF
IF (VLIQ.GE.TPSZGL.AND.PPAD.LT.(0.001)) THEN
  PNIT=1.1*PNIT
  VLIQ=TPSZGL-0.01
  GO TO 329
ENDIF
C
IF (VLIQ.LE.0.0) FRAC=0.0
C
C     .....Determine pressure of padding gas (if present).....
C

```

```

1      IF (IFRAC.EQ.0) PNIT=
          PPAD*(TTNK/TNKHLD)*(1.0-FRAT)*(SZGL/TPSZGL)/(1.0-FRAC)
C
329    CONTINUE
        PTOT=PSBS+PSLV+PNIT
        IF (NVLV.LE.1.AND.WGNT.GT.(0.0)) THEN
          IF (PTOT.GT.POPN) PNIT=POPN-PSBS-PSLV
          IF (PNIT.LT.(0.0)) PNIT=0.0
        ENDIF
        PTOT=PSBS+PSLV+PNIT
        IF (PTOT.LT.14.7) PTOT=14.7
        KIDN=2
        GO TO 153
C*****
C      Shell full case.....( KIDN=3 ). . . . .
C.....Calculate heat in and change in temperature.....
C
410    CONTINUE
        IF (IFRTYP.EQ.2) THEN
          HTIN=CATR*(TWAL-TTNK)*CNDLQ*DELT*60.0/3.6
        ELSE
          HTIN=(TWAL-TTNK)*CFRA*CNDLQ*AREA*DELT*60.0/3.6
          IF (IDSC.EQ.2) HTIN=HTIN+USUM*(TWAL-TTNK)*DELT*60.0/3.6
        ENDIF
        TELT=HTIN/(SPEC*WLIQ*1000.0+125.0*WTWL*AREA)
        TLST=TTNK
        SLST=VVAP
        PLST=PTOT
        TTNK=TTNK+TELT
        IPAD=0
        NFRST=1
C
        TEMP=(TTNK-0.46)*1000.0
C
        IF (IPTYP.EQ.1) THEN
          IF (IPR.GE.1.AND.IPR.LE.9) CALL FPRPSBS (IPR,TEMP)
          IF (IPR.GE.10.AND.IPR.LE.16) CALL FPRPSLV (IPR,CONC,TEMP)
        ENDIF
        IF (IPTYP.EQ.2.OR.IPTYP.EQ.3) THEN
          IF (ISBSL.EQ.1) CALL SBSPROP (IPFST,IPR,TEMP)
          IF (ISBSL.EQ.2) CALL SLNPROP (IPFST,IPR,CONC,TEMP)
        ENDIF
C.....Calculate pressure required to get sufficient flow.....
        REQL=0.5*REQL+0.5*(FMSS*SPLQ-TPSZGL)/DELT
        IF (REQL.LT.0.0) REQL=0.0
        WOUT1=REQL*DELT/SPLQ
C
        IF (IVLTYP.EQ.1) AREQ=AVLV
        IF (IVLTYP.EQ.2) AREQ=AVENT
        PTOT=PSBS+PSLV
        PMIN=AMAX1(PTOT,(14.7))
        PCOM=PMIN+((REQL/(720.0*CVLQ*AREQ))**2)/(64.4*SPLQ)
C
        IF (IVLTYP.EQ.1.AND.PTOT.LT.PCLS) THEN
          PTOT=AMAX1(PCLS,PCOM)
          WOUT=WOUT1
          FMSS=FMSS-WOUT
          FRAC=1.0
          IFRAC=1
          GO TO 416

```

```

ENDIF
IF (IVLTYP.EQ.2.AND.PTOT.LT.(14.7)) THEN
  PTOT=PCOM
  WOUT=WOUT1
  FMSS=FMSS-WOUT
  FRAC=1.0
  IFRAC=1
  GO TO 416
ENDIF
C
IF (TILT.GE.10.0) GO TO 411
TEMPR=1000.0*TTNK
WSBOUT=PSBS*ATEM*CVAD*VLSBCN*60.0*DELT/SQRT(TEMPR*ZSBS)
WSVOUT=PSLV*ATEM*CVAD*VLSLCN*60.0*DELT/SQRT(TEMPR*ZSLV)
IF (PTOT.LT.(27.0)) THEN
  WSBOUT=WSBOUT*(PTOT-14.7)/12.3
  WSVOUT=WSVOUT*(PTOT-14.7)/12.3
ENDIF
IF (WSBOUT.LT.0.0) WSBOUT=0.0
IF (WSVOUT.LT.0.0) WSVOUT=0.0
WOUT2=WSBOUT+WSVOUT
GO TO 413
411 CONTINUE
1 CALL AVFLOW(TTNK,WOUT2,ATEM,DELT,CVLQ,PNIT,
C CONC,IPR,IPFST,ISBSL,IPTYP,TIME)
IF (IPTYP.EQ.1) THEN
  IF (IPR.GE.1.AND.IPR.LE.9) CALL FPRPSBS (IPR,TEMP)
  IF (IPR.GE.10.AND.IPR.LE.16) CALL FPRPSLV (IPR,CONC,TEMP)
ENDIF
IF (IPTYP.EQ.2.OR.IPTYP.EQ.3) THEN
  IF (ISBSL.EQ.1) CALL SBSPROP (IPFST,IPR,TEMP)
  IF (ISBSL.EQ.2) CALL SLNPROP (IPFST,IPR,CONC,TEMP)
ENDIF
C
413 CONTINUE
C
IF (WOUT2.GT.WOUT1) THEN
  WOUT=WOUT2
  FMSS=FMSS-WOUT
  FRAC=FMSS*SPLQ/TPSZGL
  IF (FRAC.GT.1.000) FRAC=0.9999 ! v3.0 rev
  IFRAC=0
  GO TO 416
ENDIF
C
PTOT=PCOM
WOUT=WOUT1
FMSS=FMSS-WOUT
FRAC=1.0
IFRAC=1
C
416 CONTINUE
VLIQ=FMSS*SPLQ
WVAP=0.0
IF (IPR.NE.1) THEN
  WSBOUT=WOUT*CONC
  WSVOUT=WOUT*(1.0-CONC)
ELSEIF (IPR.EQ.1) THEN
  WSBOUT=0.0

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      WSVOUT=WOUT
    ENDIF
    WNTOUT=0.0
    PNIT=0.0
    WPAD=0.0
    WLIQ=FMSS
    WSBS=FMSS*CONC
    WSLV=FMSS*(1.0-CONC)
    SLST=TPSZGL/FMSS
C
    KIDN=3
    GO TO 153
C*****
C      Liquid and vapor in car, but venting vapor..( KIDN=1) . . .
C      .....Calculate mass flow rate through valve.....
C
420    CONTINUE
      IF (IFRAC.EQ.0.AND.WGNT.NE.(0.0)) THEN
        PNIT=((1.0-FRAT)/(1.0-FRAC))*PPAD*(TTNK/TNKHLD)*WPAD/WGNT
      ELSE
        PNIT=0.0
      ENDIF
C
      PTOT=PSBS+PSLV+PNIT
      IF (IVLTYP.EQ.1.AND.NVLV.LE.1.AND.WGNT.GT.(0.0)) THEN
        IF (PTOT.GT.POPN) PNIT=POPN-PSBS-PSLV
        IF (PNIT.LT.(0.0)) PNIT=0.0
      ENDIF
      PTOT=PSBS+PSLV+PNIT
C
      IF (NFRST.EQ.0) GO TO 424
      WSBOLD=WSBOUT
      WTROLD=WSVOUT
      WNTOLD=WNTOUT
      TEMPR=1000.0*TTNK
      WSBOUT=PSBS*ATEM*CVAD*VLSBCN*60.0*DELT/SQRT(TEMPR*ZSBS)
      WSVOUT=PSLV*ATEM*CVAD*VLSLCN*60.0*DELT/SQRT(TEMPR*ZSLV)
      WNTOUT=PNIT*ATEM*CVAD*VLPPCN*60.0*DELT/SQRT(TEMPR*ZPAD)
      IF (PTOT.GT.(14.7).AND.PTOT.LT.(27.0)) THEN
        WSBOUT=WSBOUT*(PTOT-14.7)/12.3
        WSVOUT=WSVOUT*(PTOT-14.7)/12.3
        WNTOUT=WNTOUT*(PTOT-14.7)/12.3
      ENDIF
      IF (FRAC.LE.0.040) THEN
        WSBOUT=0.5*(WSBOUT+WSBOLD)
        WSVOUT=0.5*(WSVOUT+WTROLD)
        WNTOUT=0.5*(WNTOUT+WNTOLD)
      ENDIF
C
      IF (IPAD.EQ.0) GO TO 424
      WNTHLD=WPAD
      PNTHLD=PNIT
      WPAD=WPAD-WNTOUT
      IF (WPAD.LT.(0.0)) WPAD=0.0
      PTOT=PSBS+PSLV+PNIT
      IF (IVLTYP.EQ.2.AND.PTOT.LT.14.7) THEN
        PNIT=14.71-PSBS-PSLV
        IF (PNTHLD.LE.(0.0)) THEN
          WPAD=0.0
        ELSE

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        WPAD=WNTHLD*PNIT/PNTHLD
    ENDIF
    IF (WNTOUT.LE.(0.0)) THEN
        RATIO=1.0
    ELSE
        RATIO=(WNTHLD-WPAD)/WNTOUT
        IF(RATIO.LE.0.0)RATIO=0.1      ! v3.0 rev
    ENDIF
    WNTOUT=WNTHLD-WPAD
    IF (WNTOUT.LT.(0.0)) WNTOUT=0.0  ! v3.0 rev
    WSVOUT=WSVOUT*RATIO
    WSBOUT=WSBOUT*RATIO
ENDIF
IF (IVLTYP.EQ.1.AND.PTOT.LT.PCLS) THEN
    PNIT=PCLS-PSBS-PSLV+1.0
    IF (PNTHLD.LE.(0.0)) THEN
        WPAD=0.0
    ELSE
        WPAD=WNTHLD*PNIT/PNTHLD
    ENDIF
    IF (WNTOUT.LE.(0.0)) THEN
        RATIO=1.0
    ELSE
        RATIO=(WNTHLD-WPAD)/WNTOUT
        IF (RATIO.LE.0.0) RATIO=0.1
    ENDIF
    WNTOUT=WNTHLD-WPAD
    WSVOUT=WSVOUT*RATIO
    WSBOUT=WSBOUT*RATIO
ENDIF
PTOT=PSBS+PSLV+PNIT
CONTINUE
424
C
    FMSS=FMSS-WSVOUT-WSBOUT
C
C
    Calculate change in temperature.
C
    QVAL=(WSBOUT+WSVOUT)*HFLV
    TELT=(HTIN-QVAL)/(THRML*1000.0)
    TLST=TTNK
    TTNK=TTNK+TELT
    IF(FRAC.LT.0.025)TTNK=0.2*TTNK+0.8*TLST
C
    TEMP=(TTNK-0.46)*1000.0
C
    IF (IPTYP.EQ.1) THEN
        IF (IPR.GE.1.AND.IPR.LE.9) CALL FPRPSBS (IPR,TEMP)
        IF (IPR.GE.10.AND.IPR.LE.16) CALL FPRPSLV (IPR,CONC,TEMP)
    ENDIF
    IF (IPTYP.EQ.2.OR.IPTYP.EQ.3) THEN
        IF (ISBSL.EQ.1) CALL SBSPROP (IPFST,IPR,TEMP)
        IF (ISBSL.EQ.2) CALL SLNPROP (IPFST,IPR,CONC,TEMP)
    ENDIF
C
    WLIQ=(FMSS-TPSZGL/VVAP)/(1.0-SPLQ/VVAP)
    WVAP=FMSS-WLIQ
    VLIQ=WLIQ*SPLQ
    FRAC=VLIQ/TPSZGL
    SLST=TPSZGL/FMSS
    IF(VLIQ.GE.TPSZGL) THEN

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        FRAC=1.0
        IFRAC=1
    ELSE
        IFRAC=0
    ENDIF
    IF (VLIQ.LE.0.0) FRAC=0.0
C
    WSBS=WSBS-WSBOUT
    WSLV=WSLV-WSVOUT
    CONC=WSBS/(WSBS+WSLV)
C
    KIDN=1
    GO TO 153
C*****
C    Tank filled only with vapor (nitrogen pad neglected)...( KIDN=4)...
C
430    CONTINUE
        IF (IFRTYP.EQ.2) THEN
            HTIN=(TTNV-TTNK)*CATR*1000.0*1.0*DELT/60.0
        ELSE
            HTIN=(TTNV-TTNK)*AREA*1000.0*1.0*DELT/60.0
        ENDIF
        PLST=PTOT
        ZSBS=0.7
        PNIT=0.0
        IPAD=0
        SVLV=TPSZGL/FMSS
        PTOT=(PLST*SLST/SVLV*TTNK/TLST)*0.3+0.7*PLST
        SLST=SVLV
        IF (IVLTYP.EQ.1.AND.PTOT.LE.PCLS) PTOT=PCLS+0.001
        TEMPR=1000.0*TTNK
        WSBOUT=PSBS*ATEM*CVAD*VLSBCN*60.0*DELT/SQRT(TEMPR*ZSBS)
        WSVOUT=PSLV*ATEM*CVAD*VLSLCN*60.0*DELT/SQRT(TEMPR*ZSLV)
        IF (PTOT.LT.(27.0)) THEN
            WSBOUT=WSBOUT*(PTOT-14.7)/12.3
            WSVOUT=WSVOUT*(PTOT-14.7)/12.3
        ENDIF
        WLET=WOUT
        WOUT=WSBOUT+WSVOUT
        IF ((FMSS/WGHT).LE.0.0100) THEN
            ALFA=0.5
            IF (SCFM.GT.15000.0) ALFA=0.05
            WOUT=WOUT*ALFA+WLET*(1.0-ALFA)
        ENDIF
        QWRK=WOUT*SVLV*PTOT*144.0/778.0
C
C    Calculate change in temperature.
C
        TELT=(HTIN-QWRK)/(FMSS*0.40*1000.0)
        TLST=TTNK
        TTNK=TTNK+TELT
        FMSS=FMSS-WOUT
        WLIQ=0.0
        WVAP=FMSS
        FRAC=0.000
        IFRAC=0
        IF ((FMSS/WGHT).LT.(0.0005)) GO TO 470
        KIDN=4
        GO TO 153
C*****

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C .....Burst strength of tank.....
C
153 CONTINUE
    FCTR=1.0
C.....Carbon Steels.....
    IF (IMT.GE.1.AND.IMT.LE.15) THEN
        IF (TTNV.LT. (1.260)) FCTR=1.0-(0.54)*(TTNV-0.460)**4
        IF (TTNV.GE. (1.260)) FCTR=1.74-1.17*(TTNV-0.460)
        IF (TTNV.GE. (1.947)) FCTR=0.0
    ENDIF
C.....Stainless Steels.....
    IF (IMT.EQ.16.OR.IMT.EQ.17) THEN
        IF (TTNV.GE. (0.860).AND.TTNV.LT. (1.760))
1          FCTR=1.0-0.45*(TTNV-0.86)/0.90
        IF (TTNV.GE. (1.760).AND.TTNV.LT. (2.160))
1          FCTR=0.55-0.55*(TTNV-1.76)/0.40
        IF (TTNV.GE. (2.160)) FCTR=0.0
    ENDIF
    IF (IMT.EQ.18.OR.IMT.EQ.19) THEN
        IF (TTNV.GE. (0.860).AND.TTNV.LT. (1.760))
1          FCTR=1.0-0.55*(TTNV-0.86)/0.90
        IF (TTNV.GE. (1.760).AND.TTNV.LT. (2.160))
1          FCTR=0.45-0.45*(TTNV-1.76)/0.40
        IF (TTNV.GE. (2.160)) FCTR=0.0
    ENDIF
C.....Aluminum Alloys.....
    IF (IMT.GE.20.AND.IMT.EQ.25) THEN
        IF (TTNV.GE. (0.610).AND.TTNV.LT. (1.260))
1          FCTR=1.0-(TTNV-0.61)/0.65
        IF (TTNV.GE. (1.260)) FCTR=0.0
    ENDIF
    IF (IMT.EQ.26) THEN
        IF (TTNV.GE. (0.610).AND.TTNV.LT. (0.860))
1          FCTR=1.0-0.48*(TTNV-0.61)/0.25
        IF (TTNV.GE. (0.860).AND.TTNV.LT. (1.260))
1          FCTR=0.52-0.52*(TTNV-0.86)/0.40
        IF (TTNV.GE. (0.860)) FCTR=0.0
    ENDIF
    IF (IMT.EQ.27) THEN
        IF (TTNV.GE. (0.610).AND.TTNV.LT. (0.960))
1          FCTR=1.0-0.83*(TTNV-0.61)/0.35
        IF (TTNV.GE. (0.960).AND.TTNV.LT. (1.260))
1          FCTR=0.17-0.17*(TTNV-0.96)/0.30
        IF (TTNV.GE. (0.860)) FCTR=0.0
    ENDIF
C
    PBR=PCBR*S*FCTR
C
C.....Set output parameters.....
C
    PSIG=PTOT-14.7
    TEMP=1000.0*TTNK-460.0
    TEMW=1000.0*TWAL-460.0
    TEMH=1000.0*TTNV-460.0
    FMAT=FMSS/WGHT
    FRCLQ=WLIQ/WGHT
    KCNT=KCNT+1
C
    TIME=(FLOAT(NTIME*NREFTM))/100.0
C

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155 CONTINUE
C
C HEADINGS FOR OUTPUTS
C
IF(PBRS.LT.PSIG)GO TO 470
IF (NTIME.GT.0.OR.OTYPE.EQ.1) GO TO 465
IF(IPR.EQ.1)WRITE(19,57)'PRODUCT: WATER'
IF(IPR.EQ.2)WRITE(19,57)'PRODUCT: PROPANE'
IF(IPR.EQ.3)WRITE(19,57)'PRODUCT: ETHLYENE OXIDE'
IF(IPR.EQ.4)WRITE(19,57)'PRODUCT: PROPYLENE'
IF(IPR.EQ.5)WRITE(19,57)'PRODUCT: 1,3-BUTADIENE'
IF(IPR.EQ.6)WRITE(19,57)'PRODUCT: VINYL CHLORIDE'
IF(IPR.EQ.7)WRITE(19,57)'PRODUCT: MONOMETHYLAMINE'
IF(IPR.EQ.8)WRITE(19,57)'PRODUCT: PROPYLENE OXIDE'
IF(IPR.EQ.9)WRITE(19,57)'PRODUCT: ANHYDROUS AMMONIA'
IF(IPR.EQ.10)WRITE(19,57)'PRODUCT: SULFURIC ACID'
IF(IPR.EQ.11)WRITE(19,57)'PRODUCT: HYDROCHLORIC ACID'
IF(IPR.EQ.12)WRITE(19,57)'PRODUCT: SODIUM HYDROXIDE'
IF(IPR.EQ.13)WRITE(19,57)'PRODUCT: PHOSPHORIC ACID (75%)'
IF(IPR.EQ.14)WRITE(19,57)'PRODUCT: SUPERPHOSPHORIC ACID'
IF(IPR.EQ.15)WRITE(19,57)'PRODUCT: POTASSIUM HYDROXIDE'
IF(IPR.EQ.16)WRITE(19,57)'PRODUCT: HYDROGEN PEROXIDE SOLUTION'
C
IF (IPR.EQ.20.OR.IPR.EQ.21)
1 WRITE(19,59)'PRODUCT:',QNAME
C
57 FORMAT(T8,A/)
59 FORMAT(T8,A,T18,A/)
WRITE(19,73)' TIME TEMPERATURES PRESSURES',
1 'MASS FILLED RATE OF'
WRITE(19,73)'(min.) (deg F) WITHIN BURST',
1 'FRACT. FRACT. PRODUCT '
WRITE(19,73)' LIQ. TANK TANK STR.',
1 ' IN OF RELEASE '
WRITE(19,73)' PROD. VAPOR (psi) (psi)',
1 'TANK TANK (lbs/min) '
WRITE (19,971) ' '
73 FORMAT(T8,A,T47,A)
465 CONTINUE
C
C....Outside temperature range of thermal property data message.....
IF (ITEMP.EQ.1) GO TO 466
IF (TEMP.GT.(TLMTMX+0.01).OR.TEMP.LT.(TLMTMN-0.01)) THEN
1 IF (OTYPE.EQ.1.OR.OTYPE.EQ.3) WRITE (*,577)
1 'OUTSIDE TEMPERATURE RANGE OF THERMAL PROPERTY DATA'
1 IF (OTYPE.EQ.2.OR.OTYPE.EQ.3) WRITE (19,577)
1 'OUTSIDE TEMPERATURE RANGE OF THERMAL PROPERTY DATA'
ITEMP=1
ENDIF
466 CONTINUE
C
C....Outside concentration range of thermal property data message.....
IF (ICONC.NE.0) GO TO 467
IF (ISBSL.NE.2) GO TO 467 ! corrected 11/1/97 was NE.0
IF (CONC.GT.(CNCMAX+0.001).OR.CONC.LT.(CNCMIN-0.001)) THEN
1 IF (OTYPE.EQ.1.OR.OTYPE.EQ.3) WRITE (*,577)
1 'OUTSIDE CONCENTRATION RANGE OF THERMAL PROPERTY DATA'
1 IF (OTYPE.EQ.2.OR.OTYPE.EQ.3) WRITE (19,577)
1 'OUTSIDE CONCENTRATION RANGE OF THERMAL PROPERTY DATA'
ICONC=1

```

```

      ENDIF
467  CONTINUE
577  FORMAT (/T3,A/)
C
C.....Outside range of critical temperature message.....
      IF (ICR.EQ.2.AND.TEMP.GE.TCRIT) THEN
          IF (OTYPE.EQ.2.OR.OTYPE.EQ.3)
1      WRITE (19,577) 'CRITICAL TEMPERATURE EXCEEDED'
          IF (OTYPE.EQ.1.OR.OTYPE.EQ.3)
1      WRITE (*,577) 'CRITICAL TEMPERATURE EXCEEDED'
          GO TO 470
      ENDIF
C
      WOUTDL=WSBOUT+WSVOUT+WNTOUT      ! used for control on HCNV
      WAVOUT=WAVOUT+WOUTDL             ! cummlate
      WOUTDL=WOUTDL/DELT               ! change to rate
C
      IF (KCNT.LT.INTV.AND.TIME.LT.TLIMIT) GO TO 211
      IF (TIME.GE.TLIMIT) GO TO 470
C
      WAVOUT=WAVOUT/(FLOAT(INTV)*DELT)
      IF (OTYPE.EQ.2.OR.OTYPE.EQ.3) WRITE (19,980) TIME, TEMP,
1      TEMH, PSIG, PBRs, FMAT, FRAC, WAVOUT
C
980  FORMAT(F12.1,F8.1,F7.1,2F8.1,F8.3,F7.3,F8.1)
C.....write to monitor.....
C
      IF (OTYPE.EQ.2) GO TO 917
      KDCNT=KDCNT+1
      IF (KDCNT.EQ.1) WRITE(*,969)' TIME    TEMP    PRESSURE',
1      ' TANK BURST    LIQUID    MASS    OUT-FLOW'
      IF (KDCNT.EQ.1) WRITE(*,969)' (min.) (deg F)    (psi)',
1      ' PRESSURE    FRACTION    FRACTION    (lbs/min)'
      WRITE(*,967) TIME, TEMP, PSIG, PBRs, FRAC, FMAT, WAVOUT
      IF (KDCNT.EQ.KCNTRL) THEN
          WRITE (*,*) 'Type "ENTER" to proceed'
          READ(*,*)
          KDCNT=0
          KPAGE=KPAGE+1
          IF (KPAGE.GE.1) KCNTRL=20
      ENDIF
967  FORMAT(F8.2,F8.1,F9.1,F11.1,F11.3,F11.3,F11.1)
969  FORMAT(T4,A,T29,A)
      KCNT=0
917  CONTINUE
      WAVOUT=0.0
      IF (TIME.LT.TLIMIT) GO TO 211
C
470  CONTINUE
C
      PENDT=PSIG
      PENDB=PBRs
      IF (KCNT.NE.0) WAVOUT=WAVOUT/(FLOAT(KCNT)*DELT)
      IF (PSIG.GT.PBRs) PENDT=AMIN1(PSIG,PBRs)
      IF (PSIG.GT.PBRs) PENDB=AMIN1(PSIG,PBRs)
      IF (OTYPE.EQ.2.OR.OTYPE.EQ.3) WRITE (19,980) TIME, TEMP, TEMH,
1      PENDT, PENDB, FMAT, FRAC, WAVOUT
      IF (OTYPE.EQ.1.OR.OTYPE.EQ.3)
1      WRITE (*,967) TIME, TEMP, PENDT, PENDB, FRAC, FMAT, WAVOUT
977  FORMAT(F8.2,F8.1,F9.1,F11.1,F11.3,F11.3,F11.1,F5.2)

```

C

```
WRITE (*,971)
1 'DO YOU WISH TO TERMINATE OPERATION OF PROGRAM ?'
WRITE (*,971) ' (Enter Y or N):'
READ (*,973) RESPNS
IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 473
```

C

```
IF (IPTYP.EQ.3) REWIND 13 ! old file of thermal property data
IF (IPTYP.EQ.2) REWIND 16 ! new file of thermal property data
WRITE (*,971)
1 'DO YOU WISH TO CHANGE INITIAL ANALYSIS CONDITIONS?'
WRITE (*,971) ' (Enter Y or N):'
READ (*,973) RESPNS
IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') THEN
    NALYSS=1
    INTYPE=1
    GO TO 403
ELSE
    GO TO 405
ENDIF
```

C

```
473 CONTINUE
971 IF (IPTYP.EQ.2) CLOSE (16, STATUS='DELETE')
973 FORMAT (T3,A)
    FORMAT (A1)
    STOP
    END
```

## APPENDIX B

### SUBROUTINE ENTRDAT

Subroutine ENTRDAT.FOR is used to enter the initial analysis data into the program. See the User's Manual for a detailed description for the use of this subroutine. After all of the data have been entered, the program presents the option of storing the data in a separate file, which can be used for data input, if desired, on succeeding analyses.

The source code for the subroutine is presented on the following pages.

C.....Subroutine ENTRDAT.FOR is developed for the entry of data.  
 C.....All entered data is placed in COMMON.  
 C.....Version 3.0, November 11, 1998

C  
 SUBROUTINE ENTRDAT(QNAME,NALYSS)  
 C  
 CHARACTER\*30 CPRD(21),QNAME  
 CHARACTER\*12 BNAME  
 CHARACTER\*1 RESPNS,LRESP  
 REAL LINTV  
 INTEGER\*2 IMT,IPTYP,ISBSL,IPR,ICR,IPAD,IVLTYP,NALYSS  
 INTEGER\*2 INS,KINDX,IDSC,LLNG,ILN,ILD  
 INTEGER\*2 IFRTYP,INTV

C.....  
 COMMON/TANK/SIZE,DIAI,WTKI  
 COMMON/MATL/IMT,INSRTH,PNBR,PCBR  
 COMMON/PRDCT1/IPTYP,ISBSL,IPR,ICR,TCRIT  
 COMMON/PRDCT2/FRAT,TEMC,CONC,IPAD,PPID  
 COMMON/SRELF1/IVLTYP,AVENT,VGTD,SCFM  
 COMMON/SRELF2/PGSD,PGTD,CVAD,CVLQ,TILT  
 COMMON/THRML1/INS,CNDD,KINDX,CNDI,CINTV  
 COMMON/THRML2/THIC,A1,A2,A3  
 COMMON/THRML3/IDSC,USUM,LLNG,ILN,ILD,LINTV  
 COMMON/FIRE/IFRTYP,TEMF,CFRA,CATR,ERAD  
 COMMON/ITIME/TLIMIT,DELT,INTV

C  
 CPRD(1)='WATER'  
 CPRD(2)='PROPANE'  
 CPRD(3)='ETHYLENE OXIDE'  
 CPRD(4)='PROPYLENE'  
 CPRD(5)='1,3 BUTADIENE'  
 CPRD(6)='VINYL CHLORIDE'  
 CPRD(7)='MONOMETHYLAMINE'  
 CPRD(8)='PROPYLENE OXIDE'  
 CPRD(9)='ANHYDROUS AMMONIA'  
 CPRD(10)='SULFURIC ACID'  
 CPRD(11)='HYDROCHLORIC ACID'  
 CPRD(12)='SODIUM HYDROXIDE'  
 CPRD(13)='PHOSPHORIC ACID (75%)'  
 CPRD(14)='SUPERPHOSPHORIC ACID'  
 CPRD(15)='POTASSIUM HYDROXIDE'  
 CPRD(16)='HYDROGEN PEROXIDE SOLUTION'  
 CPRD(17)='BLANK'  
 CPRD(18)='BLANK'  
 CPRD(19)='BLANK'

C  
 C.....TANK PARAMETERS.....  
 C

WRITE(\*,\*)  
 1 'ENTER NOMINAL CAPACITY OF TANK (decimal number, gallons):'  
 READ(\*,\*) SIZE

C  
 WRITE(\*,\*)  
 1 'ENTER INSIDE TANK DIAMETER (decimal number, inches):'  
 READ(\*,\*) DIAI

C  
 WRITE(\*,\*)  
 1 'ENTER TANK WALL THICKNESS (decimal number, inches):'  
 READ(\*,\*) WTKI

C

```

WRITE(*,*)
1 'ENTER FOLLOWING CODE NUMBER FOR TYPE OF MATERIAL'
WRITE(*,*)
1 '(integer number):'
WRITE(*,*)
1 ' 1 - Carbon Steel or Carbon Steel Alloys'
WRITE(*,*)
1 ' 2 - Stainless Steel'
WRITE(*,*)
1 ' 3 - Aluminum'
READ(*,*) MCLASS

```

C

```

IF (MCLASS.EQ.1) THEN
  WRITE(*,*)
  1 ' CODE SPECIFICATION MINIMUM TENSILE'
  WRITE(*,*)
  1 ' NUMBER NUMBER STRENGTH (psi)'
  WRITE(*,*)
  1 ' 1 ASTM A 515-70, Gr. 55 55,000'
  WRITE(*,*)
  1 ' 2 ASTM A 515-70, Gr. 60 60,000'
  WRITE(*,*)
  1 ' 3 ASTM A 515-70, Gr. 65 65,000'
  WRITE(*,*)
  1 ' 4 ASTM A 515-70, Gr. 70 70,000'
  WRITE(*,*)
  1 ' 5 ASTM A 285-70a, Gr. A 45,000'
  WRITE(*,*)
  1 ' 6 ASTM A 285-70a, Gr. B 50,000'
  WRITE(*,*)
  1 ' 7 ASTM A 286-70a, Gr. C 55,000'
  WRITE(*,*)
  1 ' 8 ASTM A 516-70a, Gr. 55 55,000'
  WRITE(*,*)
  1 ' 9 ASTM A 516-70a, Gr. 60 60,000'
  WRITE(*,*)
  1 ' 10 ASTM A 516-70a, Gr. 65 65,000'
  WRITE(*,*)
  1 ' 11 ASTM A 516-70a, Gr. 70 70,000'
  WRITE(*,*)
  1 ' 12 AAR TC128-70, Grs. A & B 81,000'
  WRITE(*,*)
  WRITE(*,*)
  1 ' Low Alloy Manganese Carbon Steels'
  WRITE(*,*)
  WRITE(*,*)
  1 ' 13 ASTM A 537-80, Class 1 70,000'
  WRITE(*,*)
  1 ' 14 ASTM A 302-69a, Gr. B 80,000'
  WRITE(*,*)
  1 ' 15 ASTM A 302-70a, Gr. B 80,000'
  WRITE(*,*)
  1 'ENTER CODE NUMBER FOR SPECIFIC TYPE OF STEEL'
  WRITE(*,*)
  1 '(integer number):'
  READ(*,*) IMT
ENDIF

```

C

```

IF (MCLASS.EQ.2) THEN
  WRITE(*,*)

```

```

1   ' CODE                SPECIFICATION                MINIMUM TENSILE'
   WRITE(*,*)
1   ' NUMBER                NUMBER                STRENGTH (psi)'
   WRITE(*,*)
1   ' 16                ASTM A 240-70, Type 304                75,000'
   WRITE(*,*)
1   ' 17                ASTM A 240-70, Type 304L                70,000'
   WRITE(*,*)
1   ' 18                ASTM A 240-70, Type 316                75,000'
   WRITE(*,*)
1   ' 19                ASTM A 240-70, Type 316L                70,000'
   WRITE(*,*)
1   'ENTER CODE NUMBER FOR SPECIFIC TYPE OF STAINLESS STEEL'
   WRITE(*,*)
1   '(integer number):'
   READ(*,*) IMT
   ENDIF

```

C

```

IF (MCLASS.EQ.3) THEN
   WRITE(*,*)
1   ' CODE                SPECIFICATION                MINIMUM TENSILE'
   WRITE(*,*)
1   ' NUMBER                NUMBER                STRENGTH (psi)'
   WRITE(*,*)
1   ' 20                ASTM B 209-70, Alloy 5052                25,000'
   WRITE(*,*)
1   ' 21                ASTM B 209-70, Alloy 5083                38,000'
   WRITE(*,*)
1   ' 22                ASTM B 209-70, Alloy 5086                35,000'
   WRITE(*,*)
1   ' 23                ASTM B 209-70, Alloy 5154                30,000'
   WRITE(*,*)
1   ' 24                ASTM B 209-70, Alloy 5254                30,000'
   WRITE(*,*)
1   ' 25                ASTM B 209-70, Alloy 5454                31,000'
   WRITE(*,*)
1   ' 26                ASTM B 209-70, Alloy 5652                25,000'
   WRITE(*,*)
1   ' 27                ASTM B 209-70, Alloy 6061                24,000'
   WRITE(*,*)
1   'ENTER CODE NUMBER FOR SPECIFIC TYPE OF ALUMINUM'
   WRITE(*,*)
1   '(integer number):'
   READ(*,*) IMT
   ENDIF

```

C

```

IF (IMT.EQ.1.OR.IMT.EQ.7.OR.IMT.EQ.8) TNSRTH=55000.0
IF (IMT.EQ.2.OR.IMT.EQ.9) TNSRTH=60000.0
IF (IMT.EQ.3.OR.IMT.EQ.10) TNSRTH=65000.0
IF (IMT.EQ.4.OR.IMT.EQ.11.OR.IMT.EQ.13) TNSRTH=70000.0
IF (IMT.EQ.17.OR.IMT.EQ.19) TNSRTH=70000.0
IF (IMT.EQ.5) TNSRTH=45000.0
IF (IMT.EQ.6) TNSRTH=50000.0
IF (IMT.EQ.12) TNSRTH=81000.0
IF (IMT.EQ.14.OR.IMT.EQ.15) TNSRTH=60000.0
IF (IMT.EQ.16.OR.IMT.EQ.18) TNSRTH=75000.0
IF (IMT.EQ.20.OR.IMT.EQ.26) TNSRTH=75000.0
IF (IMT.EQ.21) TNSRTH=38000.0
IF (IMT.EQ.22) TNSRTH=35000.0
IF (IMT.EQ.23.OR.IMT.EQ.24) TNSRTH=30000.0

```



```

IF(IMT.EQ.25)TNSRTH=31000.0
IF(IMT.EQ.27)TNSRTH=34000.0
C
C.....Determine Calculated Burst Strength.....
PCBRs=2.0*TNSRTH*WTKI/DIAI
C
WRITE(*,*)'ENTER NOMINAL TANK BURSTING STRENGTH'
WRITE(*,*)' (decimal number, psig):'
READ(*,*) PNBRs
C
IF (PNBRs.GT.PCBRS) WRITE(*,*)
1 'INCONSISTENT BURST PRESSURE'
C
C.....PRODUCT DATA.....
C
IF (NALYSS.NE.0) GO TO 101
WRITE (*,*)
1 'ENTER CODE FOR METHOD OF ENTRY OF THERMAL PROPERTY'
WRITE (*,*) ' DATA OF PRODUCT (enter integer number):'
WRITE (*,*) ' (1) Use product property data'
WRITE (*,*) ' contained in program'
WRITE (*,*) ' (2) Enter new property data at monitor'
WRITE (*,*) ' (3) Read property data from existing'
WRITE (*,*) ' separate file'
READ (*,*) IPTYP
C
IF (IPTYP.EQ.1) THEN
WRITE(*,*) ' SELECT PRODUCT FROM FOLLOWING LIST'
WRITE(*,*)
WRITE(*,*) '1-WATER 9 -ANHYDROUS AMMONIA'
WRITE(*,*) '2-PROPANE 10-SULFURIC ACID'
WRITE(*,*) '3-ETHYLENE OXIDE 11-HYDROCHLORIC ACID'
WRITE(*,*) '4-PROPYLENE 12-SODIUM HYDROXIDE'
WRITE(*,*) '5-1,3 BUTADIENE 13-PHOSPHORIC ACID (75%)'
WRITE(*,*) '6-VINYL CHLORIDE 14-SUPERPHOSPHORIC ACID'
WRITE(*,*) '7-MONOMETHYLAMINE 15-POTASSIUM HYDROXIDE'
WRITE(*,*) '8-PROPYLENE OXIDE 16-HYDROGEN PEROXIDE SOLUTION'
WRITE(*,*) ' '
WRITE(*,*) ' ENTER PRODUCT NUMBER (integer number):'
READ(*,*) IPR
CPRD(20)='BLANK'
CPRD(21)='BLANK'
IF (IPR.LE.9) ISBSL=1
IF (IPR.GE.10.AND.IPR.LE.16) ISBSL=2
ELSEIF (IPTYP.EQ.2) THEN ! keyboard entry of property data
IPR=20
WRITE (*,*) 'ENTER NAME OF PRODUCT:'
WRITE (*,*) ' (Maximum of 30 Characters)'
READ (*,201) CPRD(20)
ELSEIF (IPTYP.EQ.3) THEN ! read file of property data
IPR=21
WRITE (*,*) 'ENTER NAME OF PRODUCT:'
WRITE (*,*) ' (Maximum of 30 Characters)'
READ (*,201) CPRD(21)
ENDIF
QNAME=CPRD(IPR)
C
IF (IPTYP.NE.1) THEN
1 WRITE (*,*)
'ENTER CODE FOR TYPE OF PRODUCT (integer number):'

```

```

        WRITE (*,*) ' (1) for substance'
        WRITE (*,*) ' (2) for solution'
        READ (*,*) ISBSL
    ENDIF
C
    IF (IPR.GE.1.AND.IPR.LE.16) THEN
        ICR=1
        TCRIT=1.0
    ENDIF
C
    IF(IPR.GT.16) THEN
        WRITE (*,*)
1      'DOES PRODUCT HAVE A CRITICAL TEMPERATURE?'
        WRITE (*,*) ' ENTER Y or N (for yes or no):'
        READ (*,205) LRESP
        IF (LRESP.EQ.'Y') THEN
            ICR=2
            WRITE (*,*)
1          'ENTER CRITICAL TEMPERATURE (decimal number, deg F):'
            READ (*,*) TCRIT
        ELSE
            ICR=1
            TCRIT=1.0
        ENDIF
    ENDIF
C
101  CONTINUE
C
        WRITE(*,*)
1      'ENTER INITIAL FRACTION OF TANK FILLED (decimal fraction):'
        READ(*,*) FRAT
C
        WRITE (*,*) 'ENTER INITIAL TEMPERATURE OF PRODUCT'
        WRITE (*,*) ' (decimal number, deg F):'
        READ (*,*) TEMC
C
        IF (ISBSL.EQ.2) THEN
            WRITE (*,*)
1          'ENTER CONCENTRATION OF PRODUCT (decimal fraction):'
            READ(*,*) CONC
        ELSE
            CONC=1.0
        ENDIF
C
        WRITE (*,*) 'ENTER CODE FOR PRESENCE OF PADDING GAS'
        WRITE (*,*) ' (Enter integer number):'
        WRITE (*,*) ' (1) Padding gas used to bring internal tank'
        WRITE (*,*) ' pressure to atmospheric pressure if'
        WRITE (*,*) ' vapor pressure of product is'
        WRITE (*,*) ' below atmospheric pressure'
        WRITE (*,*) ' (2) No padding gas is used'
        WRITE (*,*) ' (3) Padding gas added to give specific'
        WRITE (*,*) ' gage pressure within tank '
        READ(*,*) IPAD
        IF (IPAD.EQ.1.OR.IPAD.EQ.2) THEN
            PPID=0.0 ! Pressure adjusted in main program for IPAD=1
        ELSE
            WRITE(*,*)
1          'ENTER GAGE PRESSURE WITHIN TANK AFTER ADDITION OF'
            WRITE (*,*) 'PADDING GAS (decimal number, psig):'

```

```

        READ(*,*) PPID
    ENDIF
C
C.....SAFETY RELIEF DEVICE PARAMETERS.....
C
    WRITE (*,*)
1   'ENTER CODE FOR TYPE OF SAFETY RELIEF DEVICE'
    WRITE (*,*) ' (integer number):'
    WRITE (*,*) ' (1) Safety relief valve'
    WRITE (*,*) ' (2) Safety vent with rupture disc'
    READ(*,*) IVLTYP
C
    IF (IVLTYP.EQ.2) THEN
        WRITE (*,*) 'ENTER DISCHARGE AREA OF VENT'
        WRITE (*,*) ' (decimal number, square inches):'
        READ(*,*) AVENT
        WRITE (*,*) 'ENTER FRANGIBLE DISC RUPTURE PRESSURE'
        WRITE (*,*) ' (decimal number, psig):'
        READ (*,*) VGTD
        SCFM=1.0
        PGSD=1.0
        PGTD=1.0
    ENDIF
C
    IF (IVLTYP.EQ.1) THEN
        WRITE (*,*)
1   'ENTER SAFETY VALVE RATED FLOW CAPACITY'
        WRITE (*,*) ' (decimal number, SCFM of air):'
        READ(*,*) SCFM
        WRITE (*,*)
1   'ENTER SAFETY VALVE FLOW RATING PRESSURE'
        WRITE (*,*) ' (decimal number, psig):'
        READ (*,*) PGSD
        WRITE (*,*) 'ENTER SAFETY VALVE START-TO-DISCHARGE PRESSURE'
        WRITE (*,*) ' (decimal number, psig):'
        READ (*,*) PGTD
        AVENT=1.0
        VGTD=1.0
    ENDIF
C
    WRITE (*,*) 'ENTER SAFETY RELIEF DEVICE DISCHARGE COEFFICIENTS'
    WRITE (*,*) ' (as decimal fractions),'
    WRITE (*,*) ' VAPOR DISCHARGE COEFFICIENT:'
    READ (*,*) CVAD
    WRITE (*,*) ' LIQUID DISCHARGE COEFFICIENT:'
    READ (*,*) CVLQ
C
    WRITE (*,*) 'ENTER ROLLOVER ORIENTATION ANGLE OF TANK CAR'
    WRITE (*,*)
1   ' WITH RESPECT TO VERTICAL (decimal number, deg):'
    READ (*,*) TILT
C
C.....THERMAL PROTECTION SYSTEM CHARACTERISTICS.....
C
    WRITE (*,*)
1   'ENTER CODE FOR TYPE OF THERMAL INSULATION SYSTEM'
    WRITE (*,*) ' (integer number):'
    WRITE (*,*) ' (1) Bare, Uninsulated Tank'
    WRITE (*,*)
1   ' (2) Approved High Temperature Insulation System'

```

```

WRITE (*,*)
1 ' (3) Jacketed Insulation System Not Resistant to High'
WRITE (*,*) ' Temperature Effects'
WRITE (*,*)
1 ' (4) Other Systems, Conductivity Independent of Temperature'
WRITE (*,*) ' (5) Other Systems, Conductivity is a'
WRITE (*,*) ' Function of Temperature'
WRITE (*,*) ' (6) Jacketed, Two Component Insulation with'
WRITE (*,*) ' Conductivity a Function of Temperature'
WRITE (*,*) ' for Insulation Adjacent to Tank Wall'
READ (*,*) INS
C
CNDD=1.0
KINDX=2
CNDI=1.0
CINTV=1.0
THIC=1.0
A1=1.0
A2=1.0
A3=1.0
C
IF (INS.EQ.2) THEN
CNDD=4.0
CNDI=4.0
ENDIF
C
IF (INS.EQ.3) THEN
WRITE (*,*)
1 'ENTER INITIAL CONDUCTANCE OF THERMAL INSULATION'
WRITE (*,*) ' (decimal number, BTU/hr-sqft-degF):'
READ (*,*) CNDI
CNDD=CNDI
WRITE (*,*)
1 'ENTER TIME INTERVAL FOR CHANGE IN CONDUCTANCE'
WRITE (*,*) ' (decimal number, minutes):'
READ (*,*) CINTV
ENDIF
C
IF (INS.EQ.4) THEN
WRITE (*,*)
1 'ENTER CODE FOR CONSTANT CONDUCTANCE OR LINEAR CHANGE'
WRITE (*,*)
1 ' WITH TIME FROM INITIAL VALUE TO FINAL VALUE'
WRITE (*,*) ' (integer number):'
WRITE (*,*) ' (1) Conductance changes with time'
WRITE (*,*) ' (2) Conductance constant with time'
READ(*,*) KINDX
C
WRITE (*,*)
1 'ENTER THERMAL INSULATION FINAL CONDUCTANCE'
WRITE (*,*) ' (decimal number, BTU/hr-sq.ft-deg F):'
READ (*,*) CNDD
CNDI=CNDD
C
IF (KINDX.EQ.1) THEN
WRITE (*,*) 'ENTER INITIAL CONDUCTANCE'
WRITE (*,*) ' (decimal number, BTU/hr-sqft-DegF):'
READ (*,*) CNDI
WRITE (*,*)
1 'ENTER TIME INTERVAL FOR CHANGE IN CONDUCTANCE'

```

```

        WRITE (*,*) ' (decimal number, minutes):'
        READ (*,*) CINTV
    ENDIF
ENDIF
C
IF (INS.EQ.5) THEN
    WRITE (*,*)
1   'ENTER THICKNESS OF INSULATION (decimal number, inches):'
    READ (*,*) THIC
    WRITE (*,*)
1   'ENTER FIRST CONDUCTIVITY PARAMETER (decimal number):'
    READ (*,*) A1
    WRITE (*,*)
1   'ENTER SECOND CONDUCTIVITY PARAMETER (decimal number):'
    READ (*,*) A2
    WRITE (*,*)
1   'ENTER THIRD CONDUCTIVITY PARAMETER (decimal number):'
    READ (*,*) A3
    TEMPC=TEMPC/1000.0
    CNDD=12.0*(A1+A2*TEMPC+A3*TEMPC*TEMPC)/THIC
    CNDI=CNDD
ENDIF
C
IF (INS.EQ.6) THEN
    WRITE (*,*)
1   'ENTER INITIAL CONDUCTANCE OF OUTER INSULATION LAYER'
    WRITE (*,*) ' (decimal number, BTU/hr-sqft-DegF):'
    READ (*,*) CNDI
    CNDD=CNDI
C
    WRITE (*,*)
1   'ENTER CODE FOR CONSTANT CONDUCTANCE OR LINEAR CHANGE'
    WRITE (*,*)
1   ' OF CONDUCTANCE OF OUTER LAYER OF INSULATION WITH'
    WRITE (*,*)
1   ' TIME FROM INITIAL VALUE TO FINAL VALUE'
    WRITE (*,*) ' (integer number):'
    WRITE (*,*)
1   ' (1) Conductance of outer layer changes with time'
    WRITE (*,*)
1   ' (2) Conductance of outer layer constant with time'
    READ(*,*) KINDX
C
    IF (KINDX.EQ.1) THEN
        WRITE (*,*)
1   'ENTER TIME INTERVAL FOR CHANGE IN CONDUCTANCE'
        WRITE (*,*) ' (decimal number, minutes):'
        READ (*,*) CINTV
        WRITE (*,*)
1   'DOES OUTER INSULATION LAYER MAINTAIN FINAL STEADY STATE'
        WRITE (*,*) ' VALUE AFTER LINEAR CHANGE (Y OR N)?'
        READ (*,205) RESPNS
        IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') THEN
            WRITE (*,*)
1   'ENTER FINAL CONDUCTANCE OF OUTER LAYER OF INSULATION'
            WRITE (*,*) ' (decimal number, BTU/hr-sq.ft-deg F):'
            READ (*,*) CNDD
        ELSE
            CNDD=40.0
        ENDIF
    ENDIF

```

```

        ENDIF
C
        WRITE (*,*)
1      'ENTER THICKNESS OF INNER LAYER OF INSULATION'
        WRITE (*,*) '(decimal number, inches):'
        READ (*,*) THIC
        WRITE (*,*)
1      'ENTER FIRST CONDUCTIVITY PARAMETER (decimal number):'
        READ (*,*) A1
        WRITE (*,*)
1      'ENTER SECOND CONDUCTIVITY PARAMETER (decimal number):'
        READ (*,*) A2
        WRITE (*,*)
1      'ENTER THIRD CONDUCTIVITY PARAMETER (decimal number):'
        READ (*,*) A3
        ENDIF
C
C.....Heat transfer through discontinuities.....
C
        WRITE (*,*) 'ENTER CODE FOR CONSIDERATION OF HEAT TRANSFER'
        WRITE (*,*) ' THROUGH DISCONTINUITIES (integer number):'
        WRITE (*,*) ' (1) Discontinuities not considered in analysis'
        WRITE (*,*) ' (2) Discontinuities considered in analysis'
        READ(*,*) IDSC
        IF (IDSC.EQ.2) THEN
1      'ENTER SUM TOTAL OF "U" FACTORS (Overall heat transfer'
        WRITE (*,*) ' coefficient, decimal number, BTU/hr-deg F):'
        READ (*,*) USUM
        ELSE
            USUM=1.0
        ENDIF
C
C.....Use of tank linings.....
C
        WRITE (*,*)
1      'ENTER CODE FOR CONSIDERATION OF TANK LININGS'
        WRITE (*,*) ' (integer number):'
        WRITE (*,*) ' (1) Tank linings not considered in analysis'
        WRITE (*,*) ' (2) Tank linings considered in analysis'
        READ(*,*) LLNG
        IF (LLNG.EQ.2) THEN
            WRITE (*,*) 'ENTER CODE FOR TYPE OF LINING (integer number):'
            WRITE (*,*) ' (1) Six (6) mil organic liner'
            WRITE (*,*) ' (2) 3/16 inch thick rubber liner'
            READ (*,*) ILN
            WRITE (*,*)
1      'DOES LINING DETERIORATE OVER FIXED TIME PERIOD?'
            WRITE (*,*) ' ENTER Y or N (for yes or no):'
            READ (*,205) LRESP
            IF (LRESP.EQ.'Y') THEN
                ILD=2
                WRITE (*,*)
1      'ENTER TIME INTERVAL FOR DETERIORATION OF LINING'
                WRITE (*,*) ' (decimal number, minutes):'
                READ (*,*) LINTV
            ELSE
                ILD=1
                LINTV=1.0
            ENDIF
        ENDIF

```

```

ELSE
  ILN=0
  ILLD=1
  LINTV=1.0
ENDIF
C
C.....FIRE CONDITIONS.....
C
  WRITE (*,*)
  1 'ENTER CODE FOR TYPE OF FIRE ANALYSIS (integer number):'
  WRITE (*,*) ' (1) Standard Pool Fire Analysis'
  WRITE (*,*) ' (2) Standard Torch Fire Analysis'
  WRITE (*,*) ' (3) Special Conditions Fire Analysis'
  READ(*,*) IFRTYP
C
  IF (IFRTYP.EQ.1) THEN
    TEMF=1500.0
    CFRA=1.0
    CATR=1.0          ! Dummy value
  ELSEIF (IFRTYP.EQ.2) THEN
    TEMF=2200.0
    CFRA=1.0          ! Dummy value
    CATR=16.0
  ELSEIF (IFRTYP.EQ.3) THEN
    WRITE (*,*) 'ENTER FLAME TEMPERATURE (decimal number, deg F):'
    READ (*,*) TEMF
    WRITE (*,*)
  1 'ENTER FRACTION OF TANK SURFACE SUBJECTED TO FIRE'
    WRITE (*,*) ' (decimal fraction):'
    READ (*,*) CFRA
    CATR=1.0          ! Dummy value
  ENDIF
C
  WRITE (*,*) 'ENTER EMISSIVITY/ABSORPTIVITY OF TANK SURFACE'
  WRITE (*,*) ' (decimal fraction):'
  READ (*,*) ERAD
C
C.....ANALYSIS CONDITIONS.....
C
  WRITE (*,*) 'ENTER TIME INCREMENT (must be given in tenths of'
  WRITE (*,*) ' a minute as a decimal number, minimum value is'
  WRITE (*,*) ' 0.01, recommended value is 0.1):'
  READ (*,*) DELT
C
  WRITE (*,*)
  1 'ENTER NUMBER OF TIME INCREMENTS BETWEEN DISPLAY'
  WRITE (*,*) ' OF OUTPUT DATA (integer number):'
  READ (*,*) INTV
C
  WRITE (*,*)
  1 'ENTER TIME LIMIT OF ANALYSIS (decimal number, minutes):'
  READ (*,*) TLIMIT
C
  WRITE (*,*)
  1 'DO YOU WISH TO WRITE ANALYSIS DATA TO A NEW FILE? (Y or N)'
  READ (*,205) RESPNS
  IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') THEN
    WRITE (*,*)
  1 'ENTER NAME OF FILE (Maximum of 12 Characters)'
    READ (*,203) BNAME

```

```
OPEN (UNIT=14, FILE=BNAME, STATUS= 'NEW' )
```

```
C
```

```
WRITE (14, 501) SIZE, DIAI, WTKI  
WRITE (14, 502) IMT, TNSRTH, PNBR, PCBR  
WRITE (14, 503) IPTYP, ISBSL, IPR, ICR, TCRIT  
WRITE (14, 504) FRAT, TEMC, CONC, IPAD, PPID  
WRITE (14, 505) IVLTYP, AVENT, VGTD, SCFM  
WRITE (14, 507) PGSD, PGTD, CVAD, CVLQ, TILT  
WRITE (14, 509) INS, CNDD, KINDX, CNDI, CINTV  
WRITE (14, 511) THIC, A1, A2, A3  
WRITE (14, 513) IDSC, USUM, LLNG, ILN, ILD, LINTV  
WRITE (14, 515) IFRTYP, TEMF, CFRA, CATR, ERAD  
WRITE (14, 517) TLIMIT, DELT, INTV  
ENDIF
```

```
C
```

```
201 FORMAT (A30)  
203 FORMAT (A12)  
205 FORMAT (A1)  
501 FORMAT (F8.0, F8.2, F8.4)  
502 FORMAT (I8, F8.0, 2F8.1)  
503 FORMAT (4I8, F8.2)  
504 FORMAT (F8.3, F8.2, F8.3, I8, F8.3)  
505 FORMAT (I8, 2F8.2, F8.0)  
507 FORMAT (5F8.2)  
509 FORMAT (I8, F8.2, I8, 2F8.2)  
511 FORMAT (F8.2, 3F8.3)  
513 FORMAT (I8, F8.2, 3I8, F8.2)  
515 FORMAT (I8, F8.1, 3F8.2)  
517 FORMAT (2F8.2, I8)
```

```
C
```

```
RETURN  
END
```



## **APPENDIX C**

### **SUBROUTINE ANLYRPT**

Subroutine ANLYRPT.FOR is used to prepare a report of the initial analysis data entered into the program. The report describes the nature and value of each variable required by the conditions of the analysis. The report is contained in a file which is named by the user. It may be printed to provide a permanent record.

The source code for this subroutine is presented on the following pages.

```

C.....ANLYRPT.FOR prepares a report of the data entered into
C.....the program describing the conditions of the analysis.
C.....(Version 1.0, April 4, 1995) Modified to add thermal
C.....properties from FPRPSBS, FPRPSLV, SBSENTR, and SLNENTR.
C.....Version 3.0, November 11, 1998
C
      SUBROUTINE ANLYRPT(QNAME)
C
      REAL LINTV,MLWSBS,MLWSLV,SCFM,CNDD
      INTEGER*2 IMT,IPTYP,ISBSL,IPR,ICR,IPAD,IVLTYP,INS
      INTEGER*2 KINDX,IDSC,LLNG,ILN,ILD,IFRTYP,INTV
      CHARACTER*13 BNAME
      CHARACTER*30 CPRD(21),CMATYP(15),CLNTYP(10),QNAME
      CHARACTER*40 CINTYP(10)
C
      COMMON/TANK/SIZE,DIAI,WTKI
      COMMON/MATL/IMT, TNSRTH,PNBR,PCBR
      COMMON/PRDCT1/IPTYP,ISBSL,IPR,ICR,TCRIT
      COMMON/PRDCT2/FRAT,TEMC,CONC,IPAD,PPID
      COMMON/SRELF1/IVLTYP,AVENT,VGTD,SCFM
      COMMON/SRELF2/PGSD,PGTD,CVAD,CVLQ,TILT
      COMMON/THRML1/INS,CNDD,KINDX,CNDI,CINTV
      COMMON/THRML2/THIC,A1,A2,A3
      COMMON/THRML3/IDSC,USUM,LLNG,ILN,ILD,LINTV
      COMMON/FIRE/IFRTYP,TEMF,CFRA,CATR,ERAD
      COMMON/ITIME/TLIMIT,DELT,INTV
C
      COMMON/PROP1/SPEC,SPLQ,HFLV,PSBS,PSLV,ZSBS,ZSLV,VVAP
      COMMON/PROP2/GAMSBS,GAMSLV,MLWSBS,MLWSLV
      COMMON/PROP3/TLMTMN,TLMTMX,CNCMIN,CNCMAX
C
      COMMON/NAME/CPRD
C
      WRITE (*,*)
      1   'Enter Name of File Which is Used to Present Analsis Data,'
      WRITE (*,*)
      1   ' Maximum of 12 Characters Including ".DAT" Extension,'
      WRITE (*,*)
      1   ' For Example: REPORT.DAT'
      READ (*,447) BNAME
      OPEN (UNIT=12,FILE=BNAME,STATUS='NEW')
C
C.....Initialization of Character Variables.....
      CPRD(1)='WATER'
      CPRD(2)='PROPANE'
      CPRD(3)='ETHLYENE OXIDE'
      CPRD(4)='PROPYLENE'
      CPRD(5)='1,3-BUTADIENE'
      CPRD(6)='VINYL CHLORIDE'
      CPRD(7)='MONOMETHYLAMINE'
      CPRD(8)='PROPYLENE OXIDE'
      CPRD(9)='ANHYDROUS AMMONIA'
      CPRD(10)='SULFURIC ACID'
      CPRD(11)='HYDROCHLORIC ACID'
      CPRD(12)='SODIUM HYDROXIDE'
      CPRD(13)='PHOSPHORIC ACID (75%)'
      CPRD(14)='SUPERPHOSPHORIC ACID'
      CPRD(15)='POTASSIUM HYDROXIDE'
      CPRD(16)='HYDROGEN PEROXIDE SOLUTION'
      CPRD(17)='BLANK'

```

```

CPRD(18)='BLANK'
CPRD(19)='BLANK'

C
CLNTYP(1)='6 mil ORGANIC LINER'
CLNTYP(2)='3/16 in. RUBBER LINER'

C
CMATYP(1)='CARBON STEEL'
CMATYP(2)='STAINLESS STEEL'
CMATYP(3)='ALUMINUM ALLOY'

C
CINTYP(1)='Bare Uninsulated Tank'
CINTYP(2)='"J" (DOT Approved High Temperature)'
CINTYP(3)='Jacketed, Non-High Temperature'
CINTYP(4)='Conductivity Independent of Temperature'
CINTYP(5)='Conductivity Function of Temperature'
CINTYP(6)='Jacketed, Two Component Insulation'

C
WRITE (12,305)
1 'DATA ENTERED INTO AFFTAC PROGRAM FOR ANALYSIS'
WRITE (12,305) ' Program Version 3.0, November 11, 1998'
WRITE (12,303) ' '

C
WRITE (12,301) 'TANK PARAMETERS'
WRITE (12,303) ' '
WRITE (12,323) 'Capacity (gal):',SIZE
WRITE (12,331) 'Inside Diameter (ins.):',DIAI
WRITE (12,329) 'Wall Thickness (ins.):',WTKI
IF (IMT.GE.1.AND.IMT.LE.15) IWRT=1
IF (IMT.GE.16.AND.IMT.LE.19) IWRT=2
IF (IMT.GE.20.AND.IMT.LE.27) IWRT=3
WRITE (12,383) 'Tank Material Type:',CMATYP(IWRT)
WRITE (12,346)
1 'Tensile Strength of Tank Material (psi):',TNSRTH
WRITE (12,345) 'Nominal Burst Strength (psig):',PNBRS
WRITE (12,345) 'Calculated Burst Strength (psig):',PCBRS
WRITE (12,363)
1 'Tank Car Orientation with Respect'
WRITE (12,367) 'to Vertical (deg):',TILT
WRITE (12,303) ' '

C
WRITE (12,301) 'PRODUCT DATA'
WRITE (12,303) ' '
IF (IPTYP.EQ.1) WRITE (12,303)
1 'Product Thermal Property Data Contained in Program'
IF (IPTYP.EQ.2) WRITE (12,303)
1 'Product Thermal Property Data Entered in Program'
IF (IPTYP.EQ.3) WRITE (12,303)
1 'Product Thermal Property Data Read from File'
IF (IPR.EQ.20.OR.IPR.EQ.21)
1 WRITE (12,381) 'Product Name:',QNAME
IF (IPR.GE.1.AND.IPR.LE.16)
1 WRITE (12,381) 'Product Name:',CPRD(IPR)
IF (ISBSL.EQ.1) WRITE (12,303) 'Product Type: Substance'
IF (ISBSL.EQ.2) WRITE (12,303) 'Product Type: Solution'
IF (ICR.EQ.2) WRITE (12,355)
1 'Product Has Critical Temperature (deg F):',TCRIT
WRITE (12,343) 'Initial Fraction of Tank Filled:',FRAT
WRITE (12,341) 'Initial Temperature of Product:',TEMC
IF (ISBSL.EQ.2) WRITE (12,321) 'Concentration:',CONC
IF (IPAD.EQ.1.OR.IPAD.EQ.3)

```

```

1          WRITE (12,303) 'Padding Gas Used'
  IF (IPAD.EQ.1) WRITE (12,303)
1  'Atmospheric Pressure in Tank at Beginning of Analysis'
  IF (IPAD.EQ.3) WRITE (12,303)
1  'Target Gage Pressure Within Tank'
  IF (IPAD.EQ.3) WRITE (12,337)
1  'After Addition of Padding Gas (psig):',PPID
  IF (IPAD.EQ.3) WRITE (12,337)
1  '(Note: Padding gas pressure will be 0.0 if target gage'
  IF (IPAD.EQ.3) WRITE (12,337)
1  ' pressure is less than initial product vapor pressure.)'
  IF (IPAD.EQ.2) WRITE (12,303) 'No Padding Gas Used'
  WRITE (12,303) ' '
C
  WRITE (12,301) 'SAFETY RELIEF DEVICE PARAMETERS'
  WRITE (12,303) ' '
  IF (IVLTYP.EQ.2) THEN
    WRITE (12,303) 'Safety Vent Used'
    WRITE (12,341) 'Cross Sectional Area (sq.ins.):',AVENT
    WRITE (12,351)
1    'Frangible Disc Rupture Pressure (psig):',VGTD
  ENDIF
C
  IF (IVLTYP.EQ.1) THEN
    WRITE (12,303) 'Safety Relief Valve Used'
    WRITE (12,333) 'Rated Flow Capacity (SCFM):',SCFM
    WRITE (12,335) 'Flow Rating Pressure (psig):',PGSD
    WRITE (12,349) 'Start-to-Discharge Pressure (psig):',PGTD
  ENDIF
  WRITE (12,359)
1  'Vent or Valve Vapor Flow Discharge Coefficient:',CVAD
  WRITE (12,363)
1  'Vent or Valve Liquid Flow Discharge Coefficient:',CVLQ
  WRITE (12,303) ' '
C
  WRITE (12,301) 'THERMAL PROTECTION SYSTEM CHARACTERISTICS'
  WRITE (12,303) ' '
C
  IF (INS.EQ.1) THEN
    WRITE (12,303) 'Bare, Uninsulated Tank'
    WRITE (12,303) ' '
  ENDIF
C
  IF (INS.EQ.2) THEN
    WRITE (12,303)
1    '"J" Type Insulation, Approved High Temperature System'
    WRITE (12,357)
1    'Steady State Conductance (BTU/hr-sq.ft-deg F):',CNDD
    WRITE (12,303) ' '
  ENDIF
C
  IF (INS.EQ.3) THEN
    WRITE (12,303) 'Jacketed Insulation System Not Resistant'
    WRITE (12,303) ' to High Temperature Effects'
    WRITE (12,355)
1    'Initial Conductance (BTU/hr-sq.ft-deg F):',CNDI
    WRITE (12,303)
1    'Time Interval for Linear Change from Initial Conductance'
    WRITE (12,369) 'to Final Conductance (min):',CINTV
    WRITE (12,303) ' '

```

```

ENDIF
C
IF (INS.EQ.4) THEN
WRITE (12,303) 'Other Insulation System, Conductivity'
WRITE (12,303) ' Independent of Temperature'
WRITE (12,357)
1 'Final Conductance (BTU/hr-sq.ft-deg F):',CNDD
IF (KINDX.EQ.1) THEN
WRITE (12,303)
1 'Change from Initial to Final Conductance'
WRITE (12,355)
1 'Initial Conductance (BTU/hr-sq.ft-deg F):',CNDI
WRITE (12,303)
1 'Time Interval for Linear Change from Initial Conductance'
WRITE (12,369) 'to Final Conductance (min):',CINTV
ENDIF
WRITE (12,303) ' '
ENDIF
C
IF (INS.EQ.5) THEN
WRITE (12,303) 'Other Insulation System, Conductivity'
WRITE (12,303) ' is a Function of Temperature'
WRITE (12,341) 'Thickness of Insulation (ins.):',THIC
WRITE (12,337) 'First Conductivity Parameter:',A1
WRITE (12,339) 'Second Conductivity Parameter:',A2
WRITE (12,337) 'Third Conductivity Parameter:',A3
WRITE (12,303) ' '
ENDIF
C
IF (INS.EQ.6) THEN
WRITE (12,303)
1 'Jacketed, Two Component Insulation System, where '
WRITE (12,303)
1 ' Conductivity of Inner Layer is a '
WRITE (12,303) ' Function of Temperature'
WRITE (12,303)
1 'Initial Conductance of Outer Layer'
WRITE (12,331) ' (BTU/hr-sq.ft-deg F):',CNDI
IF (KINDX.EQ.1) THEN
WRITE (12,303)
1 'Change from Initial to Final Conductance of Outer Layer'
WRITE (12,303)
1 'Time Interval for Linear Change from Initial Conductance'
WRITE (12,369) 'to Final Conductance (min):',CINTV
WRITE (12,303)
1 'Final Conductance of Outer Layer'
WRITE (12,331) ' (BTU/hr-sq.ft-deg F):',CNDD
ENDIF
IF (KINDX.EQ.2) WRITE(12,303)
1 'Conductance of Outer Layer Stays Constant'
WRITE (12,357)
1 'Thickness of Inner Layer of Insulation (ins.):',THIC
WRITE (12,337) 'First Conductivity Parameter:',A1
WRITE (12,339) 'Second Conductivity Parameter:',A2
WRITE (12,337) 'Third Conductivity Parameter:',A3
WRITE (12,303) ' '
WRITE (12,303) ' '
ENDIF
C
IF (IDSC.EQ.1) WRITE (12,303)

```

```

1      'Discontinuities in Insulation Not Considered'
      IF (IDSC.EQ.2) THEN
          WRITE (12,303)
1      'Discontinuities Considered in Insulation'
          WRITE (12,351)
1      'Sum Total of "U" Factors (BTU/deg F):',USUM
      ENDIF
      WRITE (12,303) ' '
C
      IF (LLNG.EQ.2) THEN
          WRITE (12,303) 'Tank Lining Used'
          WRITE (12,385) 'Type of Lining:',CLNTYP(ILN)
          IF (ILD.EQ.2) WRITE (12,345)
1          'Lining Deterioration Time (min):',LINTV
          IF (ILD.EQ.1) WRITE (12,303)
1          'Lining Does Not Deteriorate'
      ENDIF
      IF (LLNG.EQ.1) WRITE (12,303) 'No Tank Lining Used'
      WRITE (12,303) ' '
C
      WRITE (12,301) 'FIRE CONDITIONS'
      WRITE (12,303) ' '
      IF (IFRTYP.EQ.1) WRITE (12,303)
1      'Standard Pool Fire Simulation Analysis'
      IF (IFRTYP.EQ.2) WRITE (12,303)
1      'Standard Torch Fire Simulation Analysis'
      IF (IFRTYP.EQ.3) WRITE (12,303)
1      'Special Fire Simulation Analysis'
      WRITE (12,327) 'Flame Temperature (deg F):',TEMP
      IF (IFRTYP.EQ.1.OR.IFRTYP.EQ.3) WRITE (12,359)
1      'Fraction of Tank Surface Subject to Heat Input:',CFRA
      IF (IFRTYP.EQ.2) WRITE (12,365)
1      'Area of Tank Surface Subject to Heat Input (sq.ft):',CATR
      WRITE (12,351) 'Tank Radiation Emissivity Coefficient:',ERAD
      WRITE (12,303) ' '
C
      WRITE (12,301) 'ANALYSIS CONDITIONS'
      WRITE (12,303) ' '
      WRITE (12,325) 'Time Limit (min):',TLIMIT
      WRITE (12,347) 'Time Increment for Analysis (min):',DELT
      WRITE (12,361)
1      'Time Increments Between Display of Output Data:',INTV
C
301     FORMAT (T6,A)
303     FORMAT (T8,A)
305     FORMAT (T20,A)
321     FORMAT (T8,A,T23,F8.3)
323     FORMAT (T8,A,T24,F8.0)
325     FORMAT (T8,A,T26,F8.2)
327     FORMAT (T8,A,T35,F8.1)
329     FORMAT (T8,A,T31,F8.4)
331     FORMAT (T8,A,T32,F8.2)
333     FORMAT (T8,A,T36,F8.0)
335     FORMAT (T8,A,T37,F8.2)
337     FORMAT (T8,A,T38,F8.3)
339     FORMAT (T8,A,T39,F8.3)
341     FORMAT (T8,A,T40,F8.2)
343     FORMAT (T8,A,T41,F8.3)
345     FORMAT (T8,A,T42,F8.1)
346     FORMAT (T8,A,T49,F8.0)

```

```

347  FORMAT (T8,A,T43,F8.2)
349  FORMAT (T8,A,T44,F8.2)
351  FORMAT (T8,A,T48,F8.2)
355  FORMAT (T8,A,T50,F8.2)
357  FORMAT (T8,A,T55,F8.2)
359  FORMAT (T8,A,T56,F8.2)
361  FORMAT (T8,A,T56,I8)
363  FORMAT (T8,A,T57,F8.2)
365  FORMAT (T8,A,T60,F8.2)
367  FORMAT (T10,A,T29,F8.2)
369  FORMAT (T10,A,T39,F8.2)
381  FORMAT (T8,A,T22,A30)
383  FORMAT (T8,A,T30,A30)
385  FORMAT (T8,A,T24,A30)
443  FORMAT (A12)
445  FORMAT (A1)
447  FORMAT (A13)
C*****
      IF (IPTYP.NE.1) GO TO 999
      IF (IPR.GE.10) GO TO 131
C.....Thermal Property Data for Substances.....
      WRITE (12,715) ' '
      WRITE (12,301)
1  'THERMAL PROPERTY DATA CONTAINED IN PROGRAM'
      WRITE (12,719)
1  'FOR',CPRD(IPR)
      WRITE (12,715) ' '
      WRITE (12,711)
1  'Temperature (degrees F), Vapor Pressure (psia), Specific'
      WRITE (12,711)
1  'Heat (BTU/lb-deg F), Specific Volume (cu. ft/lb), Heat of'
      WRITE (12,711)
1  'Vaporization (BTU/lb), Compressibility Factor of Vapor,'
      WRITE (12,711) 'and Ratio of Specific Heats of Vapor'
      WRITE (12,711) ' '
      WRITE (12,711)
1  '
      WRITE (12,711)
1  '
      WRITE (12,711)
1  '
      WRITE (12,711)
1  'Temp.  Pres.  Heat  Volume  Vap.  Fact.  Heats'
      WRITE (12,711) ' '
C
      IF (IPR.NE.1.OR.IPR.NE.9) DGRF=0.0
      IF (IPR.EQ.1) DGRF=40.0
      IF (IPR.EQ.9) DGRF=-20.0
      DSTEP=20.0
      IF (IPR.EQ.1) NTEMP=24
      IF (IPR.EQ.2) NTEMP=11
      IF (IPR.EQ.3) NTEMP=17
      IF (IPR.EQ.4.OR.IPR.EQ.9) NTEMP=10
      IF (IPR.EQ.5) NTEMP=15
      IF (IPR.EQ.6) NTEMP=14
      IF (IPR.EQ.7) NTEMP=13
      IF (IPR.EQ.8) NTEMP=20
      DO I=1,NTEMP
      CALL FPRPSBS (IPR,DGRF)
      WRITE (12,713) DGRF,PSBS,SPEC,SPLQ,HFLV,ZSBS,GAMSBS

```

```

      DGRF=DGRF+DSTEP
      ENDDO
      WRITE (12,711) ' '
      -- WRITE (12,717) 'MOLECULAR WEIGHT:',MLWSBS
      GO TO 999
C*****
C.....Thermal Property Data for Solutions.....
131  CONTINUE
      WRITE (12,715) ' '
      WRITE (12,301) 'THERMAL PROPERTY DATA CONTAINED IN PROGRAM'
      WRITE (12,719) 'FOR',CPRD(IPR)
      WRITE (12,715) ' '
      WRITE (12,711)
1  'Temperature (degrees F), Specific Heat of Solution'
      WRITE (12,711)
1  '(BTU/lb-deg F), Specific Volume of Solution (cu. ft/lb),'
      WRITE (12,711)
1  'Heat of Vaporization of Solution (BTU/lb), Vapor Pressure of'
      WRITE (12,711)
1  'Substance (psia), Vapor Pressure of Solvent (psia),'
      WRITE (12,711)
1  'Compressibility Factor for Substance Vapor, Compressibility'
      WRITE (12,711)
1  'Factor for Solvent Vapor, Ratio of Specific Heats for'
      WRITE (12,711)
1  'Substance Vapor, and Ratio of Specific Heats for'
      WRITE (12,711)
1  'Solvent Vapor'
      WRITE (12,715) ' '
729  FORMAT (T1,A,T44,A)
C
      NUMBCNC=2
      IF (IPR.EQ.11) NUMBCNC=4
      IF (IPR.EQ.16) NUMBCNC=3
      DO I=1,NUMBCNC
        DGRF=0.0
        DSTEP=20.0
        WRITE (12,715) ' '
        IF (IPR.EQ.10.AND.I.EQ.1) CONC=0.92
        IF (IPR.EQ.10.AND.I.EQ.2) CONC=0.94
        IF (IPR.EQ.11.AND.I.EQ.1) CONC=0.32
        IF (IPR.EQ.11.AND.I.EQ.2) CONC=0.34
        IF (IPR.EQ.11.AND.I.EQ.3) CONC=0.36
        IF (IPR.EQ.11.AND.I.EQ.4) CONC=0.38
        IF (IPR.EQ.12.AND.I.EQ.1) CONC=0.50
        IF (IPR.EQ.12.AND.I.EQ.2) CONC=0.60
        IF (IPR.EQ.13.AND.I.EQ.1) CONC=0.75
        IF (IPR.EQ.13.AND.I.EQ.2) CONC=0.85
        IF (IPR.EQ.14.AND.I.EQ.1) CONC=0.755
        IF (IPR.EQ.14.AND.I.EQ.2) CONC=0.765
        IF (IPR.EQ.15.AND.I.EQ.1) CONC=0.44
        IF (IPR.EQ.15.AND.I.EQ.2) CONC=0.50
        IF (IPR.EQ.16.AND.I.EQ.1) CONC=0.82
        IF (IPR.EQ.16.AND.I.EQ.2) CONC=0.74
        IF (IPR.EQ.16.AND.I.EQ.3) CONC=0.65
        WRITE (12,735) 'CONCENTRATION:',CONC
        WRITE (12,711) ' '
        WRITE (12,729)
1  ' Solution Properties      Vapor      '
2  ' Compress.      Ratio of Spec.'

```



```

        WRITE (12,729)
1 '      Spec. Spec. Heat of Pressures ',
2 '      Fact. of Vap. Heats of Vap.'
        WRITE (12,729)
1 '      Temp. Heat Volume Vap. Sbs. Solv.',
2 '      Sbs. Solv. Sbs. Solv. '
        WRITE (12,711) ' '
        IF (IPR.EQ.10.OR.IPR.EQ.13) NTEMP=23
        IF (IPR.EQ.11) NTEMP=11
        IF (IPR.EQ.12) NTEMP=16
        IF (IPR.EQ.14.OR.IPR.EQ.15) NTEMP=18
        IF (IPR.EQ.16) NTEMP=13
        DO J=1,NTEMP
            CALL FPRPSLV (IPR,CONC,DGRF)
            WRITE (12,733) DGRF,SPEC,SPLQ,HFLV,PSBS,PSLV,ZSBS,
1            ZSLV,GAMSBS,GAMSLV
            DGRF=DGRF+DSTEP
        ENDDO
        ENDDO
        WRITE (12,715) ' '
        WRITE (12,727) 'MOLECULAR WEIGHT OF SUBSTANCE:',MLWSBS
        WRITE (12,727) 'MOLECULAR WEIGHT OF SOLVENT:',MLWSLV
C*****
733      FORMAT (F7.2,F7.4,F7.5,F7.0,2F7.2,F7.2,F6.2,F9.2,F7.2)
735      FORMAT (T6,A,T21,F6.2)
711      FORMAT (T8,A)
715      FORMAT (/T8,A)
717      FORMAT (T8,A,T26,F6.2)
719      FORMAT (T6,A,T11,A)
713      FORMAT (F12.2,F9.2,F8.4,F9.5,F8.1,2F8.2)
727      FORMAT (T8,A,T38,F6.2)
C*****
999      CONTINUE
        RETURN
        END

```



## APPENDIX D

### SUBROUTINE SBSENTR

Subroutine SBSENTR.FOR is used to enter thermal property data for a substance into the program. See the User's Manual for a detailed discussion of the use of this subroutine.

While the data is being entered into the program, the data is also written to the report file. This file may be printed to provide a permanent record.

After all of the data has been entered, the data is written to a file named NEWSBS.DAT. This file is read by the appropriate property subroutine to get the data into the main program.

Also, after all of the data has been entered, the program presents the option of storing the data in a separate file which can be used, if desired, for data input on succeeding analyses.

The variables used in this subroutine are defined as follows:

NSPEC	Number of data points for specific heat to be entered in program,
SPCTMP(I)	Temperature of the I'th data point for specific heat (°F),
ESPEC(I)	Value of specific heat at temperature of I'th data point (BTU/lb-°F),
NPSLQ	Number of data points for specific volume to be entered into program,
SPLTMP(I)	Temperature of the I'th data point for specific volume (°F),
ESPLQ(I)	Value of specific volume at temperature of I'th data point (ft <sup>3</sup> /lb),
NHFLV	Number of data points for heat of vaporization to be entered into program,
HFLTMP(I)	Temperature of the I'th data point for heat of vaporization (°F),
EHFLV(I)	Value of heat of vaporization at temperature of I'th data point (BTU/lb),
NPSBS	Number of data points for vapor pressure to be entered into program,
PSBTMP(I)	Temperature of the I'th data point for vapor pressure (°F),
EPSBS(I)	Value of vapor pressure at temperature of I'th data point (psia),
NZPRO	Number of data points for compressibility factor of vapor to be entered into program,

ZPRTMP(I) Temperature of the I'th data point for compressibility factor of vapor (°F),  
EZPRO(I) Value of compressibility factor of vapor at temperature of I'th data point,  
NGMMP Number of data points for ratio of specific heats of vapor to be entered into  
program,  
GMPTMP(I) Temperature of the I'th data point for ratio of specific heats of vapor (°F),  
EGMMP(I) Value of ratio of specific heats of vapor at temperature of I'th data point,  
and  
MLWSBS Molecular weight of vapor.

C.....SBSENTR.FOR is a subroutine developed  
 C.....for the entry of thermal property data for a substance  
 C.....by an interactive process at the computer terminal.  
 C.....Version 2.0, August 30, 1997

C

SUBROUTINE SBSENTR(QNAME)

C

DIMENSION ESPEC(8), ESPLQ(8), EHFLV(8), EPSBS(15)  
 DIMENSION SPCTMP(8), SPLTMP(8), HFLTMP(8), PSBTMP(15)  
 DIMENSION EZPRO(8), EGMMP(8), ZPRTMP(8), GMPTMP(8)  
 REAL MLWSBS  
 INTEGER\*2 NSPEC, NSPLQ, NHFLV, NPSBS, NZPRO, NGMMP  
 CHARACTER\*1 RESPNS  
 CHARACTER\*12 FLNAME  
 CHARACTER\*30 QNAME

C

C.....Initialize variables.....

C

```
DO I=1,8
  ESPEC(I)=0.0
  ESPLQ(I)=0.0
  EHFLV(I)=0.0
  EZPRO(I)=0.0
  EGMMP(I)=0.0
  SPCTMP(I)=0.0
  SPLTMP(I)=0.0
  HFLTMP(I)=0.0
  ZPRTMP(I)=0.0
  GMPTMP(I)=0.0
ENDDO
DO I=1,15
  EPSBS(15)=0.0
  PSBTMP(15)=0.0
ENDDO
```

C

```
WRITE (12,202) ' '
WRITE (12,201) ' THERMAL PROPERTY DATA'
WRITE (12,251) 'PRODUCT NAME:',QNAME
WRITE (12,202) ' '
```

C

C\*\*\*\*\* ENTRY OF THERMAL PROPERTY DATA \*\*\*\*\*

111

```
CONTINUE
WRITE (*,201)
1 'Entry of data defining thermal properties of a substance'
WRITE (*,202) ' as a function of temperature (deg F)'
WRITE (*,202) ' GENERAL INSTRUCTIONS '
WRITE (*,201)
1 'Property data is entered at specific temperatures. The'
WRITE (*,202)
1 ' order of entry must be for increasing temperatures.'
WRITE (*,201) 'Temperatures and thermal property data should be'
WRITE (*,201)
1 ' entered as real numbers (i.e. with a decimal point).'
```

C\*\*\*\*\*

C.....Entry of SPECIFIC HEAT Data.....

121

```
CONTINUE
WRITE (*,202)
```

```

1      'Entry of Property data for SPECIFIC HEAT of liquid'
WRITE (*,201) 'SPECIFIC HEAT data (BTU/lb-deg F) is normally'
WRITE (*,202) ' entered to four decimal places (e.g. 0.5432).'
```

```

WRITE (*,201) 'Enter number of data points to be provided'
WRITE (*,201) ' (integer number), minimum of 2, maximum of 8:'
READ (*,203) NSPEC
DO I=1,NSPEC
  WRITE (*,205)
1      'Enter TEMPERATURE and corresponding SPECIFIC HEAT'
  WRITE (*,315) ' (separated by a comma) for data point:',I
  READ (*,311) SPCTMP(I), ESPEC(I)
ENDDO
C.....Review of Data Entered .....
WRITE (*,202)
1      ' DATA ENTERED IN PROGRAM FOR SPECIFIC HEAT'
WRITE (*,202)
1      ' Temperature (deg F) Specific Heat (BTU/lb-deg F)'
DO I=1,NSPEC
  WRITE (*,213) SPCTMP(I),ESPEC(I)
ENDDO
WRITE (*,202) ' '
C.....Check Acceptability of Data Entered.....
WRITE (*,*) 'Do you wish to reenter Specific Heat Data?'
WRITE (*,*) ' (Enter Y for yes, or N for no):'
READ (*,241) RESPNS
IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 121
C.....Write Data to Report File.....
WRITE (12,202)
1      'DATA ENTERED IN PROGRAM FOR SPECIFIC HEAT'
WRITE (12,202)
1      ' Temperature (deg F) Specific Heat (BTU/lb-deg F)'
DO I=1,NSPEC
  WRITE (12,213) SPCTMP(I),ESPEC(I)
ENDDO
WRITE (12,202) ' '
C.....
311  FORMAT (F8.2,F8.4)
315  FORMAT (T3,A,T44,I3)
WRITE(*,204) 'SPECIFIC HEAT data entry is completed.'
C*****
C.....Entry of SPECIFIC VOLUME of Liquid Data.....
131  CONTINUE
WRITE (*,202)
1      'Entry of Property data for SPECIFIC VOLUME of liquid'
WRITE (*,201) 'SPECIFIC VOLUME (cu. ft/lb) data is normally'
WRITE (*,202) ' entered to five decimal places (e.g. 0.01120).'
```

```

WRITE (*,201) 'Enter number of data points to be provided'
WRITE (*,201) ' (integer number), minimum of 2, maximum of 8:'
READ (*,203) NSPLQ
DO I=1,NSPLQ
  WRITE (*,205)
1      'Enter TEMPERATURE and corresponding SPECIFIC VOLUME'
  WRITE (*,315) ' (separated by a comma) for data point:',I
  READ (*,313) SPLTMP(I), ESPLQ(I)
ENDDO
C.....Review of Data Entered .....
WRITE (*,202)
1      'DATA ENTERED IN PROGRAM FOR SPECIFIC VOLUME'
WRITE (*,202)
1      ' Temperature (deg F) Specific Volume (cu.-ft/lb)'
```

```

DO I=1,NSPLQ
  WRITE (*,214) SPLTMP(I),ESPLQ(I)
ENDDO
WRITE (*,202) ' '
C.....Check Acceptability of Data Entered.....
WRITE (*,*) 'Do you wish to reenter Specific Volume Data?'
WRITE (*,*) ' (Enter Y for yes, or N for no):'
READ (*,241) RESPNS
IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 131
C.....Write Data to Report File.....
WRITE (12,202)
1 'DATA ENTERED IN PROGRAM FOR SPECIFIC VOLUME'
WRITE (12,202)
1 ' Temperature (deg F) Specific Volume (cu.-ft/lb)'
DO I=1,NSPLQ
  WRITE (12,214) SPLTMP(I),ESPLQ(I)
ENDDO
WRITE (12,202) ' '
C.....
WRITE(*,204) 'SPECIFIC VOLUME data entry is completed.'
313 FORMAT (F8.2,F8.5)
C*****
C.....Entry of HEAT OF VAPORIZATION Data.....
141 CONTINUE
WRITE (*,202)
1 'Entry of Property data for HEAT OF VAPORIZATION'
WRITE (*,201) 'HEAT OF VAPORIZARION data (BTU/lb) is normally'
WRITE (*,202) ' entered to one decimal place (e.g. 1010.1).'

```

```

C.....
  WRITE(*,204)
  1   'HEAT OF VAPORIZATION data entry is completed.'
317  FORMAT (F8.2,F8.1)
C*****
C.....Entry VAPOR PRESSURE OF SUBSTANCE Data.....
151  CONTINUE
      WRITE (*,202)
      1   'Entry of Property data for VAPOR PRESSURE OF SUBSTANCE'
          WRITE (*,201)
          1   'VAPOR PRESSURE OF SUBSTANCE data (psia) is normally'
              WRITE (*,202) ' entered to two decimal places (e.g. 60.55). '
              WRITE (*,201) 'Enter number of data points to be provided'
              WRITE (*,201) ' (integer number); must be an odd number of'
              WRITE (*,201) ' points, minimum of 3, maximum of 15:'
              READ (*,203) NPSBS
              DO I=1,NPSBS
                  WRITE (*,205)
                  1   'Enter TEMPERATURE and corresponding VAPOR PRESSURE'
                      WRITE (*,315) ' (separated by a comma) for data point',I
                      READ (*,319) PSBTMP(I),EPSBS(I)
              ENDDO
C.....Review of Data Entered .....
      WRITE (*,202)
      1   'DATA ENTERED IN PROGRAM FOR VAPOR PRESSURE OF SUBSTANCE'
          WRITE (*,202)
          1   ' Temperature (deg F)          Vapor Pressure (psia)'
              DO I=1,NPSBS
                  WRITE (*,221) PSBTMP(I),EPSBS(I)
              ENDDO
          WRITE (*,202) ' '
C.....Check Acceptability of Data Entered.....
      WRITE (*,*) 'Do you wish to reenter Vapor Pressure Data?'
      WRITE (*,*) ' (Enter Y for yes, or N for no):'
      READ (*,241) RESPNS
      IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 151
C.....Write Data to Report File.....
      WRITE (12,202)
      1   'DATA ENTERED IN PROGRAM FOR VAPOR PRESSURE OF SUBSTANCE'
          WRITE (12,202)
          1   ' Temperature (deg F)          Vapor Pressure (psia)'
              DO I=1,NPSBS
                  WRITE (12,221) PSBTMP(I),EPSBS(I)
              ENDDO
          WRITE (12,202) ' '
C.....
319  FORMAT(2F8.2)
      WRITE(*,204) 'VAPOR PRESSURE data entry is completed.'
C*****
C.....Entry of COMPRESSIBILITY FACTOR OF SUBSTANCE VAPOR Data.....
161  CONTINUE
      WRITE (*,202)
      1   'Property data for COMPRESSIBILITY FACTOR OF SUBSTANCE VAPOR'
          WRITE (*,201)
          1   'COMPRESSIBILITY FACTOR data is normally entered to two'
              WRITE (*,202) ' decimal places (e.g. 0.97). '
              WRITE (*,201) 'Enter number of data points to be provided'
              WRITE (*,201) ' (integer number), minimum of 2, maximum of 8:'
              READ (*,203) NZPRO
              DO I=1,NZPRO

```



```

        WRITE (*,205)
1   'Enter TEMPERATURE and corresponding COMPRESSIBILITY FACTOR'
    WRITE (*,315) ' (separated by a comma) for data point',I
    READ (*,319) ZPRTMP(I), EZPRO(I)
    ENDDO
C.....Review of Data Entered .....
    WRITE (*,201)
1   'DATA ENTERED IN PROGRAM FOR COMPRESSIBILITY FACTOR'
    WRITE (*,202)
1   '
      OF SUBSTANCE VAPOR'
    WRITE (*,202)
1   ' Temperature (deg F)    Compressibility Factor'
    DO I=1,NZPRO
        WRITE (*,221) ZPRTMP(I),EZPRO(I)
    ENDDO
    WRITE (*,202) ' '
C.....Check Acceptability of Data Entered.....
    WRITE (*,*) 'Do you wish to reenter Compressibility Factor Data?'
    WRITE (*,*) ' (Enter Y for yes, or N for no):'
    READ (*,241) RESPNS
    IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 161
C.....Write Data to Report File.....
    WRITE (12,201)
1   'DATA ENTERED IN PROGRAM FOR COMPRESSIBILITY FACTOR'
    WRITE (12,202)
1   '
      OF SUBSTANCE VAPOR'
    WRITE (12,202)
1   ' Temperature (deg F)    Compressibility Factor'
    DO I=1,NZPRO
        WRITE (12,221) ZPRTMP(I),EZPRO(I)
    ENDDO
    WRITE (12,202) ' '
C.....
    WRITE(*,204)
1   'COMPRESSIBILITY FACTOR data entry is completed.'
C*****
C.....Entry of RATIO OF SPECIFIC HEATS OF SUBSTANCE VAPOR Data.....
171 CONTINUE
    WRITE (*,202)
1   'Property data for RATIO OF SPECIFIC HEATS OF SUBSTANCE VAPOR'
    WRITE (*,201)
1   'RATIO OF SPECIFIC HEATS data is normally entered to two'
    WRITE (*,202) ' decimal places (e.g. 1.37).'

```

```

1      ' Temperature (deg F)      Ratio of specific heats'
WRITE (*,201) '      '
DO I=1,NGMMP
  WRITE (*,221) GMPTMP(I),EGMMP(I)
ENDDO
WRITE (*,202) '      '
C.....Check Acceptability of Data Entered.....
WRITE (*,*) 'Do you wish to reenter Specific Heat Ratio Data?'
WRITE (*,*) ' (Enter Y for yes, or N for no):'
READ (*,241) RESPNS
IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 171
C.....Write Data to Report File.....
WRITE (12,201)
1      'DATA ENTERED IN PROGRAM FOR RATIO OF SPECIFIC HEATS'
WRITE (12,201)
1      '      OF SUBSTANCE VAPOR'
WRITE (12,201)
1      ' Temperature (deg F)      Ratio of specific heats'
WRITE (12,201) '      '
DO I=1,NGMMP
  WRITE (12,221) GMPTMP(I),EGMMP(I)
ENDDO
WRITE (12,202) '      '
C.....
WRITE(*,204)
1      'RATIO OF SPECIFIC HEATS data entry is completed.'
C*****
C.....Entry of MOLLECLULAR WEIGHT OF SUBSTANCE VAPOR Data.....
181    CONTINUE
WRITE (*,201)
1      'Property data for MOLLECLULAR WEIGHT OF SUBSTANCE VAPOR'
WRITE (*,201) 'MOLLECLULAR WEIGHT data is normally entered'
WRITE (*,201) ' to two decimal places (e.g. 18.00).'
WRITE (*,201) '      '
WRITE (*,201) 'Enter Molleclular Weight:'
READ (*,209) MLWSBS
WRITE (*,201) '      '
C.....Review of Data Entered .....
WRITE (*,201)
1      'DATA ENTERED IN PROGRAM FOR MOLECULAR WEIGHT'
WRITE (*,202)
1      '      OF SUBSTANCE VAPOR'
WRITE (*,245) MLWSBS
WRITE (*,202) '      '
C.....Check Acceptability of Data Entered.....
WRITE (*,*) 'Do you wish to reenter Molleclular Weight Data?'
WRITE (*,*) ' (Enter Y for yes, or N for no):'
READ (*,241) RESPNS
IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 181
C.....Write Data to Report File.....
WRITE (12,201)
1      'DATA ENTERED IN PROGRAM FOR MOLECULAR WEIGHT'
WRITE (12,202)
1      '      OF SUBSTANCE VAPOR'
WRITE (12,245) MLWSBS
WRITE (12,202) '      '
C.....
WRITE(*,204)
1      'MOLLECLULAR WEIGHT OF VAPOR data entry is completed.'
C*****

```

C.....If desired, save thermal property data by writing it.....  
 C.....to a separate file.....  
 C

```

  ISTART=16
  WRITE (*,*) 'Do you want to save Thermal Property Data in'
  WRITE (*,*) ' a separate file? (Enter Y or N):'
  READ (*,241) RESPNS
  IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') THEN
    WRITE (*,*) 'Enter name of file (maximum of 12 characters):'
    READ (*,243) FLNAME
    OPEN ( UNIT=17,FILE=FLNAME,STATUS='NEW')
    ISTART=17
  ENDIF

```

C  
 C.....Write data to NEWSBS.DAT file (and above optional file).....  
 C

```

  DO I=16,ISTART
    WRITE (I,223) NSPEC
    DO J=1,NSPEC
      WRITE (I,225) SPCTMP(J),ESPEC(J)
    ENDDO
    WRITE (I,223) NSPLQ
    DO J=1,NSPLQ
      WRITE (I,226) SPLTMP(J),ESPLQ(J)
    ENDDO
    WRITE (I,223) NHFLV
    DO J=1,NHFLV
      WRITE (I,227) HFLTMP(J),EHFLV(J)
    ENDDO
    WRITE (I,223) NPSBS
    DO J=1,NPSBS
      WRITE (I,229) PSBTMP(J),EPSBS(J)
    ENDDO
    WRITE (I,223) NZPRO
    DO J=1,NZPRO
      WRITE (I,229) ZPRTMP(J),EZPRO(J)
    ENDDO
    WRITE (I,223) NGMMP
    DO J=1,NGMMP
      WRITE (I,229) GMPTMP(J),EGMMP(J)
    ENDDO
    WRITE (I,247) MLWSBS
  ENDDO
  REWIND 16
  CONTINUE

```

```

411
C*****
201  FORMAT (T3,A)
202  FORMAT (T3,A/)
203  FORMAT (I8)
204  FORMAT (T3,A//)
205  FORMAT (/T3,A)
209  FORMAT (F8.2)
212  FORMAT (F10.5)
213  FORMAT (T10,F8.2,T27,F10.4)
214  FORMAT (T10,F8.2,T27,F10.5)
219  FORMAT (T10,F8.2,T27,F10.1)
221  FORMAT (T10,F8.2,T27,F10.2)
223  FORMAT (I10)
225  FORMAT (F10.2,F10.4)
226  FORMAT (F10.2,F10.5)

```

```
227   FORMAT (F10.2, F10.1)
229   FORMAT (2F10.2)
241   FORMAT (A1)
243   FORMAT (A12)
245   FORMAT (T10, F8.2)
247   FORMAT (F10.2)
251   FORMAT (T10, A, T25, A)
C
      RETURN
      END
```

## APPENDIX E

### SUBROUTINE SLNENTR

Subroutine SLNENTR.FOR is used to enter thermal property data for a solution into the program. See the User's Manual for a detailed discussion of the use of this subroutine.

While the data is being entered into the program, the data is written to the report file. This file may be printed to provide a permanent record.

After all of the data has been entered, the data is written to a file named NEWSLN.DAT. This file is read by the appropriate property subroutine to get the data into the main program.

Also, after all of the data has been entered, the program presents the option of storing the data in a separate file which can be used, if desired, for data input on succeeding analyses.

The variables used in this subroutine are defined as follows:

NSPEC	Number of data points for specific heat to be entered in program,
SPCTMP(I,J)	Temperature of the J'th data point for specific heat of liquid at I'th value of concentration (°F),
ESPEC(I,J)	Value of specific heat of liquid at temperature of J'th data point for the I'th value of concentration (BTU/lb-°F),
NPSLQ	Number of data points for specific volume of liquid to be entered into program,
SPLTMP(I)	Temperature of the J'th data point for specific volume of liquid at the I'th value of concentration (°F),
ESPLQ(I,J)	Value of specific volume of liquid at temperature of J'th data point for the I'th value of concentration (ft <sup>3</sup> /lb),
NHFLV	Number of data points for heat of vaporization to be entered into program,
HFLTMP(I,J)	Temperature of the J'th data point for heat of vaporization at the I'th value of concentration (°F),
EHFLV(I,J)	Value of heat of vaporization at temperature of J'th data point for the I'th value of concentration (BTU/lb),

NPSLT	Number of data points for vapor pressure to be entered into program,
PSTTMP(I,J)	Temperature of the J'th data point for vapor pressure of solute at the I'th value of concentration (°F),
EPSLT(I,J)	Value of vapor pressure of solute at temperature of J'th data point for the I'th value of concentration (psia),
NPSLV	Number of data points for vapor pressure of solvent to be entered into program,
PSVTMP(I,J)	Temperature of the J'th data point for vapor pressure of solvent at the I'th value of concentration (°F)
EPSLV(I,J)	Value of vapor pressure of solvent at temperature of J'th data point for the I'th value of concentration (psia),
NZSLT	Number of data points for compressibility factor of solute vapor to be entered into program,
ZSTTMP(I)	Temperature of the I'th data point for compressibility factor of solute vapor (°F),
EZSLT(I)	Value of compressibility factor of solute vapor at temperature of I'th data point,
NZSLV	Number of data points for compressibility factor of solvent vapor to be entered into program,
ZSVTMP(I)	Temperature of the I'th data point for compressibility factor of solvent vapor (°F),
EZSLV(I)	Value of compressibility factor of solvent vapor at temperature of I'th data point,
NGSLT	Number of data points for ratio of specific heats of solute vapor to be entered into program,
GSTTMP(I)	Temperature of the I'th data point for ratio of specific heats of solute vapor (°F),
EGSLT(I)	Value of ratio of specific heat of solute vapor at temperature of I'th data point,
NGSLV	Number data points for ratio of specific heats of solvent vapor to be entered into the program,

GSVTMP(I)	Temperature of the I'th data point for ratio of specific heats of solvent vapor (°F),
EGSLV(I)	Value of ratio of specific heats of solvent vapor at temperature of I'th data point,
MLWSBS	Molecular weight of solute vapor, and
MLWSLV	Molecular weight of solvent vapor.

C.....SLNENTR.FOR is a program developed  
 C.....for the entry of thermal property data for a two-component  
 C.....solution (solvent and solute) by an interactive process  
 C.....at the computer terminal.

C.....Version 2.0, August 30, 1997  
 C

SUBROUTINE SLNENTR(QNAME)

C

```

DIMENSION ESPEC(2,8), ESPLQ(2,8), EHFLV(2,8), EPSLT(2,15)
DIMENSION EPSLV(2,15), EZSLT(8), EZSLV(8)
DIMENSION EGSLT(8), EGSLV(8), CNCSLN(7,2)
DIMENSION SPCTMP(2,8), SPLTMP(2,8), HFLTMP(2,8), PSTTMP(2,15)
DIMENSION PSVTMP(2,15), ZSTTMP(8), ZSVTMP(8)
DIMENSION GSTTMP(8), GSVTMP(8)
REAL MLWSBS, MLWSLV
INTEGER*2 NSPEC, NSPLQ, NHFLV, NPSLT, NPSLV
INTEGER*2 NZSLT, NZSLV, NGSLT, NGSLV
CHARACTER*1 RESPNS
CHARACTER*12 FLNAME
CHARACTER*30 QNAME

```

C

C.....Initialize variables.....

C

```

DO I=1,2
  DO J=1,8
    ESPEC(I,J)=0.0
    ESPLQ(I,J)=0.0
    EHFLV(I,J)=0.0
    SPCTMP(I,J)=0.0
    SPLTMP(I,J)=0.0
    HFLTMP(I,J)=0.0
  ENDDO
ENDDO
DO I=1,2
  DO J=1,15
    EPSLT(I,J)=0.0
    PSTTMP(I,J)=0.0
    EPSLV(I,J)=0.0
    PSVTMP(I,J)=0.0
  ENDDO
ENDDO
DO I=1,5
  DO J=1,2
    CNCSLN(I,J)=1.000
  ENDDO
ENDDO
DO I=1,8
  EZSLT(I)=0.0
  EZSLV(I)=0.0
  EGSLT(I)=0.0
  EGSLV(I)=0.0
  ZSTTMP(I)=0.0
  ZSVTMP(I)=0.0
  GSTTMP(I)=0.0
  GSVTMP(I)=0.0
ENDDO

```

C

```

WRITE (12,202) ' '
WRITE (12,201) ' THERMAL PROPERTY DATA'
WRITE (12,259) 'PRODUCT NAME',QNAME

```



```

WRITE (12,202) ' '
C
C***** ENTRY OF THERMAL PROPERTY DATA *****
WRITE (*,201)
1 'Entry of data defining thermal properties of a solution'
WRITE (*,201) ' as a function of temperature (deg F)'
WRITE (*,202) ' GENERAL INSTRUCTIONS '
WRITE (*,202)
1 'Property data is entered at two levels of concentration'
WRITE (*,201)
1 ' of the solution for specific heat, specific volume,'
WRITE (*,201)
1 ' heat of vaporization, vapor pressure of solute, and'
WRITE (*,201)
1 ' vapor pressure of solvent data.'
WRITE (*,202)
1 'Property data is entered at specific temperatures. The'
WRITE (*,201)
1 ' order of entry must be for increasing temperatures.'
WRITE (*,201)
1 ' (Note: the same number of data points are to be provided'
WRITE (*,201) ' at each concentration level.)'
WRITE (*,201) 'Temperatures and thermal property data should be'
WRITE (*,201)
1 ' entered as real numbers (i.e. with a decimal point).'
WRITE (*,201)
1 ' Temperatures (degs F) are normally entered to two decimal'
WRITE (*,201) ' places (e.g. 70.50).'

```

```

        WRITE (*,205)
1      'Enter TEMPERATURE and corresponding SPECIFIC HEAT'
        WRITE (*,315) ' (separated by a comma) for data point:',J
        READ (*,311) SPCTMP(I,J), ESPEC(I,J)
        ENDDO
C.....Review of Data Entered .....
        WRITE (*,202)
1      ' DATA ENTERED IN PROGRAM FOR SPECIFIC HEAT'
        WRITE (*,252) ' AT CONCENTRATION OF:',CNCSLN(1,I)
        WRITE (*,202)
1      ' Temperature (deg F) Specific Heat (BTU/lb-deg F)'
        DO J=1,NSPEC
            WRITE (*,213) SPCTMP(I,J),ESPEC(I,J)
        ENDDO
        WRITE (*,201) ' '
C.....Check Acceptability of Data Entered.....
        WRITE (*,*) 'Do you wish to reenter Specific Heat Data?'
        WRITE (*,*) ' (Enter Y for yes, or N for no):'
        READ (*,241) RESPNS
        IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 117
115    CONTINUE
C.....
C.....Write Data to Report File.....
        DO 119 I=1,2
            WRITE (12,201)
1          'DATA ENTERED IN PROGRAM FOR SPECIFIC HEAT OF LIQUID'
            IF (I.EQ.1) WRITE (12,253)
1          ' AT FIRST CONCENTRATION:',CNCSLN(1,1)
            IF (I.EQ.2) WRITE (12,253)
1          ' AT SECOND CONCENTRATION:',CNCSLN(1,2)
            WRITE (12,201) ' '
            WRITE (12,201)
1          ' Temperature (deg F) Specific Heat (BTU/lb-deg F)'
            WRITE (12,201) ' '
C
            DO J=1,NSPEC
C.....Write Data to Report File.....
                WRITE (12,213) SPCTMP(I,J),ESPEC(I,J)
                ENDDO
                IF (I.EQ.1) WRITE (12,201) ' '
119    CONTINUE
C
        WRITE (*,201) 'SPECIFIC HEAT data entry is completed.'
        WRITE (*,201) ' Type ENTER to proceed'
        READ (*,*)
        WRITE (*,202) ' '
        WRITE (12,202) ' '
C
C*****
C.....Entry of SPECIFIC VOLUME of Liquid Data.....
121    CONTINUE
        WRITE (*,202)
1      'Entry of Property data for SPECIFIC VOLUME of liquid'
        WRITE (*,201)
1      ' at two levels of concentration of the solution.'
        WRITE (*,202)
1      'SPECIFIC VOLUME data (cu.-ft/lb) is normally'
        WRITE (*,201) ' entered to five decimal places (e.g. 0.01234).'
        WRITE (*,202) 'Enter number of data points to be provided'
        WRITE (*,201) ' (integer number), minimum of 2, maximum of 8:'

```

```

      READ (*,203) NSPLQ
C
      DO 125 I=1,2
127     CONTINUE
          WRITE (*,201) 'Property Data for SPECIFIC VOLUME of liquid at'
          IF (I.EQ.1) THEN
              WRITE (*,201) ' Lower Concentration Level'
              WRITE (*,201)
1              'Enter Lower Concentration Value (decimal fraction):'
              READ (*,249) CNCSLN(2,1)
          ENDIF
          IF (I.EQ.2) THEN
              WRITE (*,201) ' Upper Concentration Level'
              WRITE (*,201)
1              'Enter Upper Concentration Value (decimal fraction):'
              READ (*,249) CNCSLN(2,2)
          ENDIF
C.....
      DO J=1,NSPLQ
          WRITE (*,205)
1          'Enter TEMPERATURE and corresponding SPECIFIC VOLUME'
          WRITE (*,315) ' (separated by a comma) for data point:',J
          READ (*,313) SPLTMP(I,J), ESPLQ(I,J)
      ENDDO
C.....Review of Data Entered .....
      WRITE (*,202)
1      ' DATA ENTERED IN PROGRAM FOR SPECIFIC VOLUME'
      WRITE (*,252) ' AT CONCENTRATION OF:',CNCSLN(2,I)
      WRITE (*,202)
1      ' Temperature (deg F) Specific Volume (cu.-ft/lb)'
      DO J=1,NSPLQ
          WRITE (*,214) SPLTMP(I,J),ESPLQ(I,J)
      ENDDO
      WRITE (*,201) ' '
C.....Check Acceptability of Data Entered.....
      WRITE (*,*) 'Do you wish to reenter Specific Volume Data?'
      WRITE (*,*) ' (Enter Y for yes, or N for no):'
      READ (*,241) RESPNS
      IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 127
125     CONTINUE
C.....
C.....Write Data to Report File.....
      DO 129 I=1,2
          WRITE (12,201)
1          'DATA ENTERED IN PROGRAM FOR SPECIFIC VOLUME OF LIQUID'
          IF (I.EQ.1) WRITE (12,253)
1          ' AT FIRST CONCENTRATION:',CNCSLN(2,1)
          IF (I.EQ.2) WRITE (12,253)
1          ' AT SECOND CONCENTRATION:',CNCSLN(2,2)
          WRITE (12,201) ' '
          WRITE (12,201)
1          ' Temperature (deg F) Specific Volume (cu.-ft/lb)'
          WRITE (12,201) ' '
C
          DO J=1,NSPLQ
C.....Write Data to Report File.....
              WRITE (12,214) SPLTMP(I,J),ESPLQ(I,J)
              ENDDO
              IF (I.EQ.1) WRITE (12,201) ' '
129     CONTINUE

```

```

C
WRITE(*,201) 'SPECIFIC VOLUME data entry is completed.'
WRITE (*,201) ' Type ENTER to proceed'
READ (*,*)
WRITE (*,202) ' '
WRITE (12,202) ' '

C
C*****
C.....Entry of HEAT OF VAPORIZATION Data.....
131 CONTINUE
WRITE (*,202)
1 'Entry of Property data for HEAT OF VAPORIZATION'
WRITE (*,201)
1 ' at two levels of concentration of the solution.'
WRITE (*,202)
1 'HEAT OF VAPORIZATON data (BTU/lb) is normally'
WRITE (*,201) ' entered to two decimal places (e.g. 345.67).'

```

```

C.....Write Data to Report File.....
C.....Write Data to Report File.....
    DO 139 I=1,2
    WRITE (12,201)
1   'DATA ENTERED IN PROGRAM FOR HEAT OF VAPORIZATION'
    IF (I.EQ.1) WRITE (12,253)
1   ' AT FIRST CONCENTRATION:',CNCSLN(3,1)
    IF (I.EQ.2) WRITE (12,253)
1   ' AT SECOND CONCENTRATION:',CNCSLN(3,2)
    WRITE (12,201) ' '
    WRITE (12,201)
1   ' Temperature (deg F) Heat of Vaporization (BTU/lb) '
    WRITE (12,201) ' '

C
    DO J=1,NHFLV
C.....Write Data to Report File.....
        WRITE (12,219) HFLTMP(I,J),EHFLV(I,J)
        ENDDO
        IF (I.EQ.1) WRITE (12,201) ' '
139    CONTINUE
C
    WRITE(*,201)
1   'HEAT OF VAPORIZATION data entry is completed.'
    WRITE (*,201) ' Type ENTER to proceed'
    READ (*,*)
    WRITE (*,202) ' '
    WRITE (12,202) ' '

C
C*****
C.....Entry VAPOR PRESSURE OF SOLUTE Data.....
141    CONTINUE
    WRITE (*,202)
1   'Entry of Property data for VAPOR PRESURE OF SOLUTE'
    WRITE (*,201)
1   ' at two levels of concentration of the solution.'
    WRITE (*,202)
1   'VAPOR PRESSURE OF SOLUTE data (psia) is normally'
    WRITE (*,201) ' entered to two decimal places (e.g. 35.67). '
    WRITE (*,202) 'Enter number of data points to be provided,'
    WRITE (*,201) ' must be an odd number (integer number), '
    WRITE (*,201) ' minimum of 3, maximum of 15:'
    READ (*,203) NPSLT

C
    DO 145 I=1,2
147    CONTINUE
        WRITE (*,201) 'Property Data for VAPOR PRESSURE OF SOLUTE at'
        IF (I.EQ.1) THEN
            WRITE (*,201) ' Lower Concentration Level'
            WRITE (*,201)
1         'Enter Lower Concentration Value (decimal fraction):'
            READ (*,249) CNCSLN(4,1)
        ENDIF
        IF (I.EQ.2) THEN
            WRITE (*,201) ' Upper Concentration Level'
            WRITE (*,201)
1         'Enter Upper Concentration Value (decimal fraction):'
            READ (*,249) CNCSLN(4,2)
        ENDIF
C.....
    DO J=1,NPSLT

```

```

        WRITE (*,205)
1  'Enter TEMPERATURE and corresponding VAPOR PRESSURE OF SOLUTE'
    WRITE (*,315) ' (separated by a comma) for data point:',J
    READ (*,319) PSTTMP(I,J), EPSLT(I,J)
ENDDO
C.....Review of Data Entered .....
    WRITE (*,202)
1  ' DATA ENTERED IN PROGRAM FOR VAPOR PRESSURE OF SOLUTE'
    WRITE (*,252) ' AT CONCENTRATION OF:',CNCSLN(4,I)
    WRITE (*,202)
1  ' Temperature (deg F) Vapor Pressure of Solute (psia)'
    DO J=1,NPSLT
        WRITE (*,221) PSTTMP(I,J),EPSLT(I,J)
    ENDDO
    WRITE (*,201) ' '
C.....Check Acceptability of Data Entered.....
    WRITE (*,*)
1  'Do you wish to reenter Vapor Pressure of Solute Data?'
    WRITE (*,*) ' (Enter Y for yes, or N for no):'
    READ (*,241) RESPNS
    IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 147
145 CONTINUE
C.....
C.....Write Data to Report File.....
    DO 149 I=1,2
    WRITE (12,201)
1  'DATA ENTERED IN PROGRAM FOR VAPOR PRESSURE OF SOLUTE'
    IF (I.EQ.1) WRITE (12,253)
1  ' AT FIRST CONCENTRATION:',CNCSLN(4,1)
    IF (I.EQ.2) WRITE (12,253)
1  ' AT SECOND CONCENTRATION:',CNCSLN(4,2)
    WRITE (12,201) ' '
    WRITE (12,201)
1  ' Temperature (deg F) Solute Vapor Pressure (psia)'
    WRITE (12,201) ' '
C
    DO J=1,NPSLT
C.....Write Data to Report File.....
        WRITE (12,221) PSTTMP(I,J),EPSLT(I,J)
    ENDDO
    IF (I.EQ.1) WRITE (12,201) ' '
149 CONTINUE
C
    WRITE(*,201)
1  'VAPOR PRESSURE OF SOLUTE data entry is completed.'
    WRITE (*,201) ' Type ENTER to proceed'
    READ (*,*)
    WRITE (*,202) ' '
    WRITE (12,202) ' '
C
C*****
C.....Entry VAPOR PRESSURE OF SOLVENT Data.....
151 CONTINUE
    WRITE (*,202)
1  'Entry of Property data for VAPOR PRESURE OF SOLVENT'
    WRITE (*,201)
1  ' at two levels of concentration of the solution.'
    WRITE (*,202)
1  'VAPOR PRESSURE OF SOLVENT data (psia) is normally'
    WRITE (*,201) ' entered to two decimal places (e.g. 35.67).'
```

```

WRITE (*,202) 'Enter number of data points to be provided,'
WRITE (*,201) ' must be an odd number (integer number),'
WRITE (*,201) ' minimum of 3, maximum of 15:'
READ (*,203) NPSLV
C
DO 155 I=1,2
157 CONTINUE
    WRITE (*,201) 'Property Data for VAPOR PRESSURE OF SOLUTE at'
    IF (I.EQ.1) THEN
        WRITE (*,201) ' Lower Concentration Level'
        WRITE (*,201)
        1 'Enter Lower Concentration Value (decimal fraction):'
        READ (*,249) CNCSLN(5,1)
    ENDIF
    IF (I.EQ.2) THEN
        WRITE (*,201) ' Upper Concentration Level'
        WRITE (*,201)
        1 'Enter Upper Concentration Value (decimal fraction):'
        READ (*,249) CNCSLN(5,2)
    ENDIF
C.....
    DO J=1,NPSLV
        WRITE (*,205)
        1 'Enter TEMPERATURE and corresponding VAPOR PRESSURE OF SOLVENT'
        WRITE (*,315) ' (separated by a comma) for data point:',J
        READ (*,319) PSVTMP(I,J), EPSLV(I,J)
    ENDDO
C.....Review of Data Entered .....
    WRITE (*,202)
    1 ' DATA ENTERED IN PROGRAM FOR VAPOR PRESSURE OF SOLUTE'
    WRITE (*,252) ' AT CONCENTRATION OF:',CNCSLN(5,I)
    WRITE (*,202)
    1 ' Temperature (deg F) Vapor Pressure of Solvent (psia)'
    DO J=1,NPSLV
        WRITE (*,221) PSVTMP(I,J),EPSLV(I,J)
    ENDDO
    WRITE (*,201) ' '
C.....Check Acceptability of Data Entered.....
    WRITE (*,*)
    1 'Do you wish to reenter Vapor Pressure of Solvent Data?'
    WRITE (*,*) ' (Enter Y for yes, or N for no):'
    READ (*,241) RESPNS
    IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 157
155 CONTINUE
C.....
C.....Write Data to Report File.....
    DO 159 I=1,2
        WRITE (12,201)
        1 'DATA ENTERED IN PROGRAM FOR VAPOR PRESSURE OF SOLVENT'
        IF (I.EQ.1) WRITE (12,253)
        1 ' AT FIRST CONCENTRATION:',CNCSLN(5,1)
        IF (I.EQ.2) WRITE (12,253)
        1 ' AT SECOND CONCENTRATION:',CNCSLN(5,2)
        WRITE (12,201) ' '
        WRITE (12,201)
        1 ' Temperature (deg F) Solvent Vapor Pressure (psia)'
        WRITE (12,201) ' '
C
    DO J=1,NPSLV
C.....Write Data to Report File.....

```

```

        WRITE (12,221) PSVTMP(I,J),EPSLV(I,J)
        ENDDO
        IF (I.EQ.1) WRITE (12,201) ' '
159 CONTINUE
C
    WRITE(*,201)
    1 'VAPOR PRESSURE OF SOLVENT data entry is completed.'
    WRITE (*,201) ' Type ENTER to proceed'
    READ (*,*)
    WRITE (*,202) ' '
    WRITE (12,202) ' '
C
C*****
C.....Entry of COMPRESSIBILITY FACTOR OF SOLUTE VAPOR Data.....
161 CONTINUE
    WRITE (*,202) 'Entry of Property data for COMPRESSIBILITY'
    WRITE (*,201) ' FACTOR OF SOLUTE VAPOR'
    WRITE (*,202)
    1 'COMPRESSIBILITY FACTOR data is normally'
    WRITE (*,201) ' entered to two decimal places (e.g. 0.95).'
    WRITE (*,202) 'Enter number of data points to be provided'
    WRITE (*,201) ' (integer number), minimum of 2, maximum of 8:'
    READ (*,203) NZSLT
C
167 CONTINUE
    WRITE (*,201)
    1 'Property Data for COMPRESSIBILITY FACTOR OF SOLUTE VAPOR'
C.....
    DO I=1,NZSLT
        WRITE (*,205)
    1 'Enter TEMPERATURE and corresponding COMPRESSIBILITY FACTOR'
        WRITE (*,315) ' (separated by a comma) for data point:',I
        READ (*,319) ZSTTMP(I), EZSLT(I)
    ENDDO
C.....Review of Data Entered .....
    WRITE (*,202) ' DATA ENTERED IN PROGRAM FOR COMPRESSIBILITY'
    WRITE (*,201) ' FACTOR OF SOLUTE VAPOR'
    WRITE (*,202)
    1 ' Temperature (deg F) Compresibility Factor of Solute Vapor'
    DO I=1,NZSLT
        WRITE (*,221) ZSTTMP(I), EZSLT(I)
    ENDDO
    WRITE (*,201) ' '
C.....Check Acceptibility of Data Entered.....
    WRITE (*,*)
    1 'Do you wish to reenter Compressibility Factor Data?'
    WRITE (*,*) ' (Enter Y for yes, or N for no):'
    READ (*,241) RESPNS
    IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 167
C.....
C.....Write Data to Report File.....
    WRITE (12,201) 'DATA ENTERED IN PROGRAM FOR COMPRESSIBILITY'
    WRITE (12,201) ' FACTOR OF SOLUTE VAPOR'
    WRITE (12,201) ' '
    WRITE (12,201)
    1 ' Temperature (deg F) Compressibility Factor'
    WRITE (12,201) ' '
C
    DO I=1,NZSLT
C.....Write Data to Report File.....

```



```

        WRITE (12,221) ZSTTMP(I),EZSLT(I)
    ENDDO
    WRITE (12,201) ' '
C
    WRITE (*,201) 'COMPRESSIBILITY FACTOR OF SOLUTE VAPOR'
    WRITE (*,201) ' data entry is completed.'
    WRITE (*,201) ' Type ENTER to proceed'
    READ (*,*)
    WRITE (*,202) ' '
    WRITE (12,202) ' '
C
C*****
C.....Entry of COMPRESSIBILITY FACTOR OF SOLVENT VAPOR Data.....
171 CONTINUE
    WRITE (*,202) 'Entry of Property data for COMPRESSIBILITY'
    WRITE (*,201) ' FACTOR OF SOLVENT VAPOR'
    WRITE (*,202)
    1 'COMPRESSIBILITY FACTOR data is normally'
    WRITE (*,201) ' entered to two decimal places (e.g. 0.95).'
    WRITE (*,202) 'Enter number of data points to be provided'
    WRITE (*,201) ' (integer number), minimum of 2, maximum of 8:'
    READ (*,203) NZSLV
C
177 CONTINUE
    WRITE (*,201)
    1 'Property Data for COMPRESSIBILITY FACTOR OF SOLVENT VAPOR'
C.....
    DO I=1,NZSLV
        WRITE (*,205)
    1 'Enter TEMPERATURE and corresponding COMPRESSIBILITY FACTOR'
        WRITE (*,315) ' (separated by a comma) for data point:',I
        READ (*,319) ZSVTMP(I), EZSLV(I)
    ENDDO
C.....Review of Data Entered .....
    WRITE (*,202) ' DATA ENTERED IN PROGRAM FOR COMPRESSIBILITY'
    WRITE (*,201) ' FACTOR OF SOLVENT VAPOR'
    WRITE (*,202)
    1 ' Temperature (deg F) Compresibility Factor of Solvent Vapor'
    DO I=1,NZSLV
        WRITE (*,221) ZSVTMP(I), EZSLV(I)
    ENDDO
    WRITE (*,201) ' '
C.....Check Acceptability of Data Entered.....
    WRITE (*,*)
    1 'Do you wish to reenter Compressibility Factor Data?'
    WRITE (*,*) ' (Enter Y for yes, or N for no):'
    READ (*,241) RESPNS
    IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 177
C.....
C.....Write Data to Report File.....
    WRITE (12,201) 'DATA ENTERED IN PROGRAM FOR COMPRESSIBILITY'
    WRITE (12,201) ' FACTOR OF SOLVENT VAPOR'
    WRITE (12,201) ' '
    WRITE (12,201)
    1 ' Temperature (deg F) Compressibility Factor'
    WRITE (12,201) ' '
C
    DO I=1,NZSLV
C.....Write Data to Report File.....
        WRITE (12,221) ZSVTMP(I),EZSLV(I)

```

```

        ENDDO
        WRITE (12,201) ' '
C
        WRITE(*,201) 'COMPRESSIBILITY FACTOR OF SOLVENT VAPOR'
        WRITE(*,201) ' data entry is completed.'
        WRITE (*,201) ' Type ENTER to proceed'
        READ (*,*)
        WRITE (*,202) ' '
        WRITE (12,202) ' '
C
C*****
C.....Entry of RATIO OF SPECIFIC HEATS OF SOLUTE VAPOR Data.....
181 CONTINUE
        WRITE (*,202) 'Entry of Property data for RATIO OF SPECIFIC'
        WRITE (*,201) ' HEATS OF SOLUTE VAPOR'
        WRITE (*,202)
1 'RATIO OF SPECIFIC HEATS data is normally'
        WRITE (*,201) ' entered to two decimal places (e.g. 1.30).. '
        WRITE (*,202) 'Enter number of data points to be provided'
        WRITE (*,201) ' (integer number), minimum of 2, maximum of 8:'
        READ (*,203) NGSLT
C
187 CONTINUE
        WRITE (*,201)
1 'Property Data for RATIO OF SPECIFIC HEATS OF SOLUTE VAPOR'
C.....
        DO I=1,NGSLT
            WRITE (*,205)
1 'Enter TEMPERATURE and corresponding RATIO OF SPECIFIC HEATS'
            WRITE (*,315) ' (separated by a comma) for data point:',I
            READ (*,319) GSTTMP(I), EGSLT(I)
        ENDDO
C.....Review of Data Entered .....
        WRITE (*,202) ' DATA ENTERED IN PROGRAM FOR RATIO OF SPECIFIC'
        WRITE (*,201) ' HEATS OF SOLUTE VAPOR'
        WRITE (*,202)
1 ' Temperature (deg F) Ratio of Specific Heats'
        DO I=1,NGSLT
            WRITE (*,221) GSTTMP(I), EGSLT(I)
        ENDDO
        WRITE (*,201) ' '
C.....Check Acceptability of Data Entered.....
        WRITE (*,*)
1 'Do you wish to reenter Ratio of Specific Heat Data?'
        WRITE (*,*) ' (Enter Y for yes, or N for no):'
        READ (*,241) RESPNS
        IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 187
C.....
C.....Write Data to Report File.....
        WRITE (12,201) 'DATA ENTERED IN PROGRAM FOR RATIO OF SPECIFIC'
        WRITE (12,201) ' HEATS OF SOLUTE VAPOR'
        WRITE (12,201) ' '
        WRITE (12,201)
1 ' Temperature (deg F) Ratio of Specific Heats'
        WRITE (12,201) ' '
C
        DO I=1,NGSLT
C.....Write Data to Report File.....
            WRITE (12,221) GSTTMP(I),EGSLT(I)
        ENDDO

```

```

WRITE (12,201) ' '
C
WRITE(*,201) 'RATIO OF SPECIFIC HEATS OF SOLUTE VAPOR'
WRITE(*,201) ' data entry is completed.'
WRITE (*,201) ' Type ENTER to proceed'
READ (*,*)
WRITE (*,202) ' '
WRITE (12,202) ' '
C
C*****
C.....Entry of RATIO OF SPECIFIC HEATS OF SOLVENT VAPOR Data.....
191 CONTINUE
WRITE (*,202) 'Entry of Property data for RATIO OF SPECIFIC'
WRITE (*,201) ' HEATS OF SOLVENT VAPOR'
WRITE (*,202)
1 'RATIO OF SPECIFIC HEATS data is normally'
WRITE (*,201) ' entered to two decimal places (e.g. 1.30).'

```

```

WRITE(*,201) 'RATIO OF SPECIFIC HEATS OF SOLVENT VAPOR'
WRITE(*,201) ' data entry is completed.'
WRITE(*,201) ' Type ENTER to proceed'
READ(*,*)
WRITE(*,202) ' '
WRITE(12,202) ' '

C
C*****
C.....Entry of MOLLECULAR WEIGHT OF SOLUTE VAPOR Data.....
611 CONTINUE
      WRITE(*,201)
      1 'Property Data for MOLLECULAR WEIGHT OF SOLUTE VAPOR'
        WRITE(*,201) ' '
        WRITE(*,201) 'Enter MOLLECULAR WEIGHT data to two decimal'
        WRITE(*,201) ' places (e.g. 18.00)'
        WRITE(*,201) ' '
        WRITE(*,201) 'Enter Mollecular Weight:'
        READ(*,209) MLWSBS
        WRITE(*,201) ' '
C.....Review of Data Entered .....
      WRITE(*,202) ' DATA ENTERED IN PROGRAM FOR MOLECULAR WEIGHT'
      WRITE(*,201) ' OF SOLUTE VAPOR'
      WRITE(*,245) MLWSBS
      WRITE(*,202) ' '
C.....Check Acceptability of Data Entered.....
      WRITE(*,*)
      1 'Do you wish to reenter Molecular Weight Data?'
        WRITE(*,*) ' (Enter Y for yes, or N for no):'
        READ(*,241) RESPNS
        IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 611
C.....Write Data to Report File.....
      WRITE(12,201)
      1 'DATA ENTERED IN PROGRAM FOR MOLECULAR WEIGHT OF SOLUTE VAPOR'
        WRITE(12,201) ' '
        WRITE(12,245) MLWSBS
        WRITE(12,201) ' '

C
C*****
C.....Entry of MOLLECULAR WEIGHT OF SOLVENT VAPOR Data.....
621 CONTINUE
      WRITE(*,201)
      1 'Property Data for MOLLECULAR WEIGHT OF SOLVENT VAPOR'
        WRITE(*,201) ' '
        WRITE(*,201) 'Enter MOLLECULAR WEIGHT data to two decimal'
        WRITE(*,201) ' places (e.g. 18.00)'
        WRITE(*,201) ' '
        WRITE(*,201) 'Enter Mollecular Weight:'
        READ(*,209) MLWSLV
        WRITE(*,201) ' '
C.....Review of Data Entered .....
      WRITE(*,202) ' DATA ENTERED IN PROGRAM FOR MOLECULAR WEIGHT'
      WRITE(*,201) ' OF SOLVENT VAPOR'
      WRITE(*,245) MLWSLV
      WRITE(*,202) ' '
C.....Check Acceptability of Data Entered.....
      WRITE(*,*)
      1 'Do you wish to reenter Molecular Weight Data?'
        WRITE(*,*) ' (Enter Y for yes, or N for no):'
        READ(*,241) RESPNS
        IF (RESPNS.EQ.'Y'.OR.RESPNS.EQ.'y') GO TO 621

```

```

C.....Write Data to Report File.....
  WRITE (12,201)
1  'DATA ENTERED IN PROGRAM FOR MOLECULAR WEIGHT OF SOLVENT VAPOR'
  WRITE (12,201) ' '
  WRITE (12,245) MLWSLV
C
  WRITE(*,201)
1  'MOLECULAR WEIGHT data entry is completed.'
  WRITE (*,201) ' '
  WRITE (*,201) ' '
  WRITE (12,201) ' '
  WRITE (12,201) ' '
C
C*****
C.....If desired, save thermal property data by writing it.....
C.....to a separate file.....
C
  ISTART=16
  WRITE (*,*) 'Do you want to save Thermal Property Data in'
  WRITE (*,*) ' a separate file? (Enter Y or N):'
  READ (*,241) RESPNS
  IF (RESPNS.EQ.'Y') THEN
    WRITE (*,*) 'Enter name of file (maximum of 12 characters):'
    READ (*,243) FLNAME
    OPEN ( UNIT=17,FILE=FLNAME,STATUS='NEW')
    ISTART=17
  ENDIF
C.....Write data to NEWSLN.DAT file (and above optional file).....
C
  DO I=16,ISTART
    WRITE (I,255) CNCSLN(1,1),CNCSLN(1,2)
    DO J=1,2
      WRITE (I,223) NSPEC
      DO K=1,NSPEC
        WRITE (I,225) SPCTMP(J,K),ESPEC(J,K)
      ENDDO
    ENDDO
    WRITE (I,255) CNCSLN(2,1),CNCSLN(2,2)
    DO J=1,2
      WRITE (I,223) NSPLQ
      DO K=1,NSPLQ
        WRITE (I,226) SPLTMP(J,K),ESPLQ(J,K)
      ENDDO
    ENDDO
    WRITE (I,255) CNCSLN(3,1),CNCSLN(3,2)
    DO J=1,2
      WRITE (I,223) NHFLV
      DO K=1,NHFLV
        WRITE (I,227) HFLTMP(J,K),EHFLV(J,K)
      ENDDO
    ENDDO
    WRITE (I,255) CNCSLN(4,1),CNCSLN(4,2)
    DO J=1,2
      WRITE (I,223) NPSLT
      DO K=1,NPSLT
        WRITE (I,229) PSTTMP(J,K),EPSLT(J,K)
      ENDDO
    ENDDO
    WRITE (I,255) CNCSLN(5,1),CNCSLN(5,2)
    DO J=1,2

```

```

WRITE (I,223) NPSLV
DO K=1,NPSLV
  WRITE (I,229) PSVTMP(J,K),EPSLV(J,K)
ENDDO
ENDDO

```

C

```

WRITE (I,223) NZSLT
DO J=1,NZSLT
  WRITE (I,229) ZSTTMP(J),EZSLT(J)
ENDDO
WRITE (I,223) NZSLV
DO J=1,NZSLV
  WRITE (I,229) ZSVTMP(J),EZSLV(J)
ENDDO
WRITE (I,223) NGSLT
DO J=1,NGSLT
  WRITE (I,229) GSTTMP(J),EGSLT(J)
ENDDO
WRITE (I,223) NGSLV
DO J=1,NGSLV
  WRITE (I,229) GSVTMP(J),EGSLV(J)
ENDDO
WRITE (I,247) MLWSBS
WRITE (I,247) MLWSLV
ENDDO
REWIND 16

```

C

```

.....
201  FORMAT (T3,A)
202  FORMAT (/T3,A)
203  FORMAT (I8)
205  FORMAT (T3,A,T30,I3)
207  FORMAT (T3,A,T40,I3)
209  FORMAT (F8.2)
211  FORMAT (F10.4)
212  FORMAT (F10.5)
213  FORMAT (T10,F8.2,T27,F10.4)
214  FORMAT (T10,F8.2,T27,F10.5)
215  FORMAT (F10.1)
217  FORMAT (T3,A,T47,I3)
219  FORMAT (T10,F8.2,T27,F10.1)
221  FORMAT (T10,F8.2,T27,F10.2)
222  FORMAT (T10,F8.3,T27,F10.3)
223  FORMAT (I10)
225  FORMAT (F10.2,F10.4)
226  FORMAT (F10.2,F10.5)
227  FORMAT (F10.2,F10.1)
229  FORMAT (2F10.2)
241  FORMAT (A1)
243  FORMAT (A12)
245  FORMAT (T10,F8.2)
247  FORMAT (F10.2)
249  FORMAT (F10.3)
251  FORMAT (T3,A,T20,F8.3)
252  FORMAT (T3,A,T25,F7.3)
253  FORMAT (T3,A,T30,F6.3)
255  FORMAT (2F10.3)
257  FORMAT (T3,A,T45,F6.3)
259  FORMAT (T10,A,T25,A)
311  FORMAT (F8.2,F8.4)
313  FORMAT (F8.2,F8.5)

```

```
315     FORMAT (T3,A,T44,I3)
317     FORMAT (F8.2,F8.1)
319     FORMAT (2F8.2)
C
```

```
RETURN
END
```





## APPENDIX F

### SUBROUTINE SBSPROP

Subroutine SBSPROP.FOR is called by the main program to obtain the current thermal properties of a substance at a specific temperature. This is done by interpolating between values entered into the program. These values are read from the file NEWSBS.DAT on the first call of the subroutine. The variables in SBSPROP are the same as those listed for subroutine SBSEINTR.

After all the data has been entered, the maximum and minimum temperature limits are established. The minimum value is established by determining the maximum temperature of the first data points entered for each of the properties. The maximum value is established by determining the minimum temperature of the final data points entered for each of the properties. The analysis program will still run if these limits are exceeded, but reduced accuracy should be anticipated because the values of the properties would be determined by extrapolation rather than by interpolation.

```

C.....SBSPROP.FOR is a subroutine for obtaining the thermal properties
C.....of a SUBSTANCE at a given temperature from a generalized
C..... file of data at specific temperatures.
C.....Version 2.0, October 20, 1997
C
C      SUBROUTINE SBSPROP(IPFST, IPR, TEMP)
C
C      REAL MLWSBS, MLWSLV, TEMP
C      DIMENSION ESPEC(8), ESPLQ(8), EHFLV(8), EPSBS(15)
C      DIMENSION SPCTMP(8), SPLTMP(8), HFLTMP(8), PSBTMP(15)
C      DIMENSION EZPRO(8), EGMP(8)
C      DIMENSION ZPRTMP(8), GMPTMP(8)
C      INTEGER*2 NSPEC, NSPLQ, NHFLV, NPSBS, NZPRO, NGMMP, IPR
C      INTEGER*2 IPFST
C
C      COMMON/PROP1/SPEC, SPLQ, HFLV, PSBS, PSLV, ZSBS, ZSLV, VVAP
C      COMMON/PROP2/GAMSBS, GAMSLV, MLWSBS, MLWSLV
C      COMMON/PROP3/TLMTMN, TLMTMX, CNCMIN, CNCMAX
C
C      IF (IPFST.EQ.0) THEN
C          IF (IPR.EQ.20) IP=16      ! keyboard entry of data
C          IF (IPR.EQ.21) IP=13    ! read data in existing file
C
C          READ (IP,223) NSPEC
C          DO I=1,NSPEC
C              READ (IP,225) SPCTMP(I), ESPEC(I)
C          ENDDO
C          READ (IP,223) NSPLQ
C          DO I=1,NSPLQ
C              READ (IP,226) SPLTMP(I), ESPLQ(I)
C          ENDDO
C          READ (IP,223) NHFLV
C          DO I=1,NHFLV
C              READ (IP,227) HFLTMP(I), EHFLV(I)
C          ENDDO
C          READ (IP,223) NPSBS
C          DO I=1,NPSBS
C              READ (IP,229) PSBTMP(I), EPSBS(I)
C          ENDDO
C          READ (IP,223) NZPRO
C          DO I=1,NZPRO
C              READ (IP,229) ZPRTMP(I), EZPRO(I)
C          ENDDO
C          READ (IP,223) NGMMP
C          DO I=1,NGMMP
C              READ (IP,229) GMPTMP(I), EGMP(I)
C          ENDDO
C          READ (IP,247) MLWSBS
C.....Initialize variables not used with substance.....
C          PSLV=0.0
C          ZSLV=1.0
C          CNCMIN=1.0
C          CNCMAX=1.0
C          GAMSLV=1.1
C          MLWSLV=1.0
C.....Establish lower and upper temperature limits of data
C.....entered into program.....
C          TLMTMN=AMAX1 (SPCTMP(1), SPLTMP(1), HFLTMP(1), PSBTMP(1),
C              ZPRTMP(1), GMPTMP(1))
C          TLMTMX=AMIN1 (SPCTMP(NSPEC), SPLTMP(NSPLQ), HFLTMP(NHFLV),

```

1

```

1          PSBTMP (NPSBS) , ZPRTMP (NZPRO) , GMPTMP (NGMMP)
C
      IPFST=1
      ENDIF
C.....CALCULATION OF PROPERTIES.....
C.....Specific Heat.....
C
      IF (TEMP.LT.SPCTMP(1)) THEN
        ISPCUP=2
        ISPCLW=1
        GO TO 111
      ENDIF
C
      DO I=2, NSPEC
      IF (TEMP.GE.SPCTMP(I-1) .AND. TEMP.LT.SPCTMP(I)) THEN
        ISPCUP=I
        ISPCLW=I-1
        GO TO 111
      ENDIF
      ENDDO
C
      IF (TEMP.GE.SPCTMP(NSPEC)) THEN
        ISPCUP=NSPEC
        ISPCLW=NSPEC-1
        GO TO 111
      ENDIF
C
111     CONTINUE
      IF (SPCTMP(ISPCUP) .EQ. SPCTMP(ISPCLW)) THEN
        WRITE(*,*) 'Bad temperature data; program run terminated'
        GO TO 399
      ENDIF
      SPEC=ESPEC (ISPCLW) + (ESPEC (ISPCUP) - ESPEC (ISPCLW))
1          * (TEMP-SPCTMP (ISPCLW)) / (SPCTMP (ISPCUP) - SPCTMP (ISPCLW))
C
C.....Specific Volume.....
C
      IF (TEMP.LT.SPLTMP(1)) THEN
        ISPLUP=2
        ISPLLW=1
        GO TO 121
      ENDIF
C
      DO I=2, NSPLQ
      IF (TEMP.GE.SPLTMP(I-1) .AND. TEMP.LT.SPLTMP(I)) THEN
        ISPLUP=I
        ISPLLW=I-1
        GO TO 121
      ENDIF
      ENDDO
C
      IF (TEMP.GE.SPLTMP(NSPEC)) THEN
        ISPCUP=NSPLQ
        ISPCLW=NSPLQ-1
        GO TO 121
      ENDIF
C
121     CONTINUE
      IF (SPLTMP(ISPLUP) .EQ. SPLTMP(ISPLLW)) THEN
        WRITE(*,*) 'Bad temperature data; program run terminated'

```

```

        GO TO 399
    ENDIF
    SPLQ=ESPLQ (ISPLLW) + (ESPLQ (ISPLUP) - ESPLQ (ISPLLW) )
1      * (TEMP-SPLTMP (ISPLLW) ) / (SPLTMP (ISPLUP) - SPLTMP (ISPLLW) )
C
C.....Heat of Vaporization.....
C
    IF (TEMP.LT.HFLTMP(1)) THEN
        IHFLUP=2
        IHFLLW=1
        GO TO 131
    ENDIF
C
    DO I=2,NHFLV
    IF (TEMP.GE.HFLTMP(I-1) .AND. TEMP.LT.HFLTMP(I) ) THEN
        IHFLUP=I
        IHFLLW=I-1
        GO TO 131
    ENDIF
    ENDDO
C
    IF (TEMP.GE.HFLTMP(NHFLV) ) THEN
        IHFLUP=NHFLV
        IHFLLW=NHFLV-1
        GO TO 131
    ENDIF
C
131  CONTINUE
    IF (HFLTMP (IHFLUP) .EQ. HFLTMP (IHFLLW) ) THEN
        WRITE (*,*) 'Bad temperature data; program run terminated'
        GO TO 399
    ENDIF
    HFLV=EHFLV (IHFLLW) + (EHFLV (IHFLUP) - EHFLV (IHFLLW) )
1      * (TEMP-HFLTMP (IHFLLW) ) / (HFLTMP (IHFLUP) - HFLTMP (IHFLLW) )
C
C.....Vapor Pressure of Product.....
C
    IF (TEMP.LT.PSBTMP(1)) THEN
        IPSBUP=3
        IPSBMD=2
        IPSBLW=1
        GO TO 141
    ENDIF
C
    DO I=3,NPSBS,2
    IF (TEMP.GE.PSBTMP(I-2) .AND. TEMP.LT.PSBTMP(I) ) THEN
        IPSBUP=I
        IPSBMD=I-1
        IPSBLW=I-2
        GO TO 141
    ENDIF
    ENDDO
C
    IF (TEMP.GE.PSBTMP(NPSBS) ) THEN
        IPSBUP=NPSBS
        IPSBMD=NPSBS-1
        IPSBLW=NPSBS-2
        GO TO 141
    ENDIF
C

```

```

141 CONTINUE
DELTO=PSBTMP(IPSBLW) - PSBTMP(IPSBLW)
DELT1=PSBTMP(IPSBUY) - PSBTMP(IPSBLW)
DELT2=PSBTMP(IPSBUY) - PSBTMP(IPSBLW)
IF (DELTO.EQ.0.OR.DELT1.EQ.0.OR.DELT2.EQ.0) THEN
  WRITE(*,*) 'Bad temperature data; program run terminated'
  GO TO 399
ENDIF
BCON=(EPSBS(IPSBLW)*DELT1-EPSBS(IPSBLW)*DELT2
1 +EPSBS(IPSBUY)*DELTO)/(DELTO*DELT1*DELT2)
ACON=(EPSBS(IPSBLW) - EPSBS(IPSBLW))/DELTO - BCON*DELTO
PSBS=EPSBS(IPSBLW) + ACON*(TEMP - PSBTMP(IPSBLW))
1 +BCON*((TEMP - PSBTMP(IPSBLW))**2.0)
C
C.....Compressibility Factor.....
C
  IF (TEMP.LT.ZPRTMP(1)) THEN
    IZPRUP=2
    IZPRLW=1
    GO TO 151
  ENDIF
C
  DO I=2,NZPRO
  IF (TEMP.GE.ZPRTMP(I-1).AND.TEMP.LT.ZPRTMP(I)) THEN
    IZPRUP=I
    IZPRLW=I-1
    GO TO 151
  ENDIF
  ENDDO
C
  IF (TEMP.GE.ZPRTMP(NZPRO)) THEN
    IZPRUP=NZPRO
    IZPRLW=NZPRO-1
    GO TO 151
  ENDIF
C
151 CONTINUE
IF (ZPRTMP(IZPRUP).EQ.ZPRTMP(IZPRLW)) THEN
  WRITE(*,*) 'Bad temperature data; program run terminated'
  GO TO 399
ENDIF
1 ZSBS=EZPRO(IZPRLW) + (EZPRO(IZPRUP) - EZPRO(IZPRLW))
  *(TEMP - ZPRTMP(IZPRLW)) / (ZPRTMP(IZPRUP) - ZPRTMP(IZPRLW))
C
C.....Ratio of Specific Heats for Vapor.....
C
  IF (TEMP.LT.GMPTMP(1)) THEN
    IGMPUP=2
    IGMPPLW=1
    GO TO 161
  ENDIF
C
  DO I=2,NGMMP
  IF (TEMP.GE.GMPTMP(I-1).AND.TEMP.LT.GMPTMP(I)) THEN
    IGMPUP=I
    IGMPPLW=I-1
    GO TO 161
  ENDIF
  ENDDO
C

```

```

      IF (TEMP.GE.GMPTMP(NGMMP)) THEN
        IGMPUP=NGMMP
        IGMPPLW=NGMMP-1
        GO TO 161
      ENDIF
C
161  CONTINUE
      IF (GMPTMP(IGMPUP).EQ.GMPTMP(IGMPLW)) THEN
        WRITE(*,*) 'Bad temperature data; program run terminated'
        GO TO 399
      ENDIF
      GAMSBS=EGMMP(IGMPLW)+(EGMMP(IGMPUP)-EGMMP(IGMPLW))
1      *(TEMP-GMPTMP(IGMPLW))/(GMPTMP(IGMPUP)-GMPTMP(IGMPLW))
C
C.....Specific Volume of Substance Vapor.....
C
      VVAP=1545.4*ZSBS*(TEMP+460.0)/(144.0*PSBS*MLWSBS)
C
399  CONTINUE
C
223  FORMAT (I10)
225  FORMAT (F10.2,F10.4)
226  FORMAT (F10.2,F10.5)
227  FORMAT (F10.2,F10.1)
229  FORMAT (2F10.2)
247  FORMAT (F10.2)
251  FORMAT (A12)
C
      RETURN
      END

```

## APPENDIX G

### SUBROUTINE SLNPROP

Subroutine SLNPROP.FOR is called by the main program to obtain the current thermal properties of a solution at a specific temperature. This is done by interpolating between values entered into the program. These values are read from the file NEWSLN.DAT on the first call of the subroutine. The variables in SLNPROP are the same as those listed for subroutine SLNENTR.

After all the data have been entered, the maximum and minimum temperature and concentration limits are established. The minimum temperature value is established by determining the maximum temperature of the first data points entered for each of the properties. The maximum value is established by determining the minimum temperature of the final data points entered for each of the properties. The minimum concentration is established by determining the maximum value of the lower level concentration for the properties and the maximum concentration is established by determining the minimum value of the upper level concentration for the properties. The analysis program will still run if these limits are exceeded, but reduced accuracy should be anticipated because the values of the properties would be determined by extrapolation rather than by interpolation.

C....SLNPROP.FOR is a routine for obtaining the thermal properties  
 C.....of a SOLUTION, at a given temperature from a generalized  
 C.....file of data, which defines the properties at specific points.  
 C.....Version 2.0, October 20, 1997

C

```
      SUBROUTINE SLNPROP(IPFST,IPR,CONC,TEMP)
```

C

```
      DIMENSION ESPEC(2,8),ESPLQ(2,8),EHFLV(2,8),EPSLT(2,15)
      DIMENSION EPSLV(2,15),EZSLT(8),EZSLV(8)
      DIMENSION EGSLT(8),EGSLV(8)
      DIMENSION SPCTMP(2,8),SPLTMP(2,8),HFLTMP(2,8),PSTTMP(2,15)
      DIMENSION PSVTMP(2,15),ZSTTMP(8),ZSVTMP(8)
      DIMENSION GSTTMP(8),GSVTMP(8),CNCSLN(5,2)
      DIMENSION TSPEC(2),TSPLQ(2),THFLV(2),TPSLT(2),TPSLV(2)
      INTEGER*2 NSPEC(2),NSPLQ(2),NHFLV(2),NPSLT(2),NPSLV(2)
      INTEGER*2 NZSLT,NZSLV,NGSLT,NGSLV,IPR,IPFST
      REAL MLWSBS,MLWSLV,CONC,TEMP
```

C

```
      COMMON/PROP1/SPEC,SPLQ,HFLV,PSBS,PSLV,ZSBS,ZSLV,VVAP
      COMMON/PROP2/GAMSBBS,GAMSLV,MLWSBS,MLWSLV
      COMMON/PROP3/TLMTMN,TLMTMX,CNCMIN,CNCMAX
```

C

```
      IF (IPFST.EQ.0) THEN
        IF (IPR.EQ.20) IP=16      ! keyboard entry of data
        IF (IPR.EQ.21) IP=13      ! read data in existing file
```

C

```
      READ (IP,255) CNCSLN(1,1),CNCSLN(1,2)
      DO I=1,2
        READ (IP,223) NSPEC(I)
        DO J=1,NSPEC(I)
          READ (IP,225) SPCTMP(I,J),ESPEC(I,J)
        ENDDO
      ENDDO
      READ (IP,255) CNCSLN(2,1),CNCSLN(2,2)
      DO I=1,2
        READ (IP,223) NSPLQ(I)
        DO J=1,NSPLQ(I)
          READ (IP,226) SPLTMP(I,J),ESPLQ(I,J)
        ENDDO
      ENDDO
      READ (IP,255) CNCSLN(3,1),CNCSLN(3,2)
      DO I=1,2
        READ (IP,223) NHFLV(I)
        DO J=1,NHFLV(I)
          READ (IP,227) HFLTMP(I,J),EHFLV(I,J)
        ENDDO
      ENDDO
      READ (IP,255) CNCSLN(4,1),CNCSLN(4,2)
      DO I=1,2
        READ (IP,223) NPSLT(I)
        DO J=1,NPSLT(I)
          READ (IP,229) PSTTMP(I,J),EPSLT(I,J)
        ENDDO
      ENDDO
      READ (IP,255) CNCSLN(5,1),CNCSLN(5,2)
      DO I=1,2
        READ (IP,223) NPSLV(I)
        DO J=1,NPSLV(I)
          READ (IP,229) PSVTMP(I,J),EPSLV(I,J)
        ENDDO
      ENDDO
```



```

ENDDO
C
    READ (IP,223) NZSLT
    DO I=1,NZSLT
        READ (IP,229) ZSTTMP(I),EZSLT(I)
    ENDDO
    READ (IP,223) NZSLV
    DO I=1,NZSLV
        READ (IP,229) ZSVTMP(I),EZSLV(I)
    ENDDO
    READ (IP,223) NGSLT
    DO I=1,NGSLT
        READ (IP,229) GSTTMP(I),EGSLT(I)
    ENDDO
    READ (IP,223) NGSLV
    DO I=1,NGSLV
        READ (IP,229) GSVTMP(I),EGSLV(I)
    ENDDO
    READ (IP,247) MLWSBS
    READ (IP,247) MLWSLV
C.....Establish lower and upper temperature and concentration
C          limits of data entered into program
    TLMTMN=AMAX1 (SPCTMP(1,1),SPLTMP(1,1),HFLTMP(1,1),
1      PSTTMP(1,1),PSVTMP(1,1),ZSTTMP(1),ZSVTMP(1),
1      GSTTMP(1),GSVTMP(1),SPCTMP(2,1),SPLTMP(2,1),
1      HFLTMP(2,1),PSTTMP(2,1),PSVTMP(2,1))
    TLMTMX=AMIN1 (SPCTMP(1,NSPEC(1)),SPLTMP(1,NSPLQ(1)),
1      HFLTMP(1,NHFLV(1)),PSTTMP(1,NPSLT(1)),PSVTMP(1,NPSLV(1)),
1      ZSTTMP(NZSLT),ZSVTMP(NZSLV),GSTTMP(NGSLT),
1      GSVTMP(NGSLV),SPCTMP(2,NSPEC(2)),SPLTMP(2,NSPLQ(2)),
1      HFLTMP(2,NHFLV(2)),PSTTMP(2,NPSLT(2)),PSVTMP(2,NPSLV(2)))
C
    CNCMIN=AMAX1 (CNCSLN(1,1),CNCSLN(2,1),CNCSLN(3,1),
1      CNCSLN(4,1),CNCSLN(5,1))
    CNCMAX=AMIN1 (CNCSLN(1,2),CNCSLN(2,2),CNCSLN(3,2),
1      CNCSLN(4,2),CNCSLN(5,2))
C
    IPFST=1
    ENDIF
C
C.....Specific Heat.....
C
    DO 115 I=1,2
    IF (TEMP.LT.SPCTMP(I,1)) THEN
        JSPCUP=2
        JSPCLW=1
        GO TO 111
    ENDIF
C
    DO J=2,NSPEC(I)
    IF (TEMP.GE.SPCTMP(I,J-1).AND.TEMP.LT.SPCTMP(I,J)) THEN
        JSPCUP=J
        JSPCLW=J-1
        GO TO 111
    ENDIF
    ENDDO
C
    IF (TEMP.GE.SPCTMP(I,NSPEC(I))) THEN
        JSPCUP=NSPEC(I)
        JSPCLW=NSPEC(I)-1

```

```

        GO TO 111
    ENDIF
C
111  CONTINUE
    IF (SPCTMP(I,JSPCUP).EQ.SPCTMP(I,JSPCLW)) THEN
        WRITE(*,*) 'Bad temperature data; program run terminated'
        GO TO 399
    ENDIF
C
    TSPEC(I)=ESPEC(I,JSPCLW)+(ESPEC(I,JSPCUP)-ESPEC(I,JSPCLW))
1    *(TEMP-SPCTMP(I,JSPCLW))/(SPCTMP(I,JSPCUP)-SPCTMP(I,JSPCLW))
115  CONTINUE
C
    SPEC=TSPEC(1)+(TSPEC(2)-TSPEC(1))
1    *(CONC-CNCSLN(1,1))/(CNCSLN(1,2)-CNCSLN(1,1))
C
C.....Specific Volume.....
C
    DO 125 I=1,2
    IF (TEMP.LT.SPLTMP(I,1)) THEN
        JSPLUP=2
        JSPLLW=1
        GO TO 121
    ENDIF
C
    DO J=2,NSPLQ(I)
    IF (TEMP.GE.SPLTMP(I,J-1).AND.TEMP.LT.SPLTMP(I,J)) THEN
        JSPLUP=J
        JSPLLW=J-1
        GO TO 121
    ENDIF
    ENDDO
C
    IF (TEMP.GE.SPLTMP(I,NSPEC(I))) THEN
        JSPCUP=NSPLQ(I)
        JSPCLW=NSPLQ(I)-1
        GO TO 121
    ENDIF
C
121  CONTINUE
    IF (SPLTMP(I,JSPLUP).EQ.SPLTMP(I,JSPLLW)) THEN
        WRITE(*,*) 'Bad temperature data; program run terminated'
        GO TO 399
    ENDIF
C
    TSPLQ(I)=ESPLQ(I,JSPLLW)+(ESPLQ(I,JSPLUP)-ESPLQ(I,JSPLLW))
1    *(TEMP-SPLTMP(I,JSPLLW))/(SPLTMP(I,JSPLUP)-SPLTMP(I,JSPLLW))
125  CONTINUE
C
    SPLQ=TSPLQ(1)+(TSPLQ(2)-TSPLQ(1))
1    *(CONC-CNCSLN(2,1))/(CNCSLN(2,2)-CNCSLN(2,1))
C
C.....Heat of Vaporization.....
C
    DO 135 I=1,2
    IF (TEMP.LT.HFLTMP(I,1)) THEN
        JHFLUP=2
        JHFLW=1
        GO TO 131
    ENDIF

```

```

C
DO J=2,NHFLV(I)
IF (TEMP.GE.HFLTMP(I,J-1).AND.TEMP.LT.HFLTMP(I,J)) THEN
  JHFLUP=J
  JHFLW=J-1
  GO TO 131
ENDIF
ENDDO

C
IF (TEMP.GE.HFLTMP(I,NHFLV(I))) THEN
  JHFLUP=NHFLV(I)
  JHFLW=NHFLV(I)-1
  GO TO 131
ENDIF

C
131 CONTINUE
IF (HFLTMP(I,JHFLUP).EQ.HFLTMP(I,JHFLW)) THEN
  WRITE(*,*) 'Bad temperature data; program run terminated'
  GO TO 399
ENDIF

C
1 THFLV(I)=EHFLV(I,JHFLW)+(EHFLV(I,JHFLUP)-EHFLV(I,JHFLW))
1 * (TEMP-HFLTMP(I,JHFLW))/(HFLTMP(I,JHFLUP)-HFLTMP(I,JHFLW))
135 CONTINUE

C
1 HFLV=THFLV(1)+(THFLV(2)-THFLV(1))
1 * (CONC-CNCSLN(3,1))/(CNCSLN(3,2)-CNCSLN(3,1))

C
C.....Vapor Pressure of Solute.....
C
DO 145 I=1,2
IF (TEMP.LT.PSTTMP(I,1)) THEN
  JPSBUP=3
  JPSBMD=2
  JPSBLW=1
  GO TO 141
ENDIF

C
DO J=3,NPSLT(I),2
IF (TEMP.GE.PSTTMP(I,J-2).AND.TEMP.LT.PSTTMP(I,J)) THEN
  JPSBUP=J
  JPSBMD=J-1
  JPSBLW=J-2
  GO TO 141
ENDIF
ENDDO

C
IF (TEMP.GE.PSTTMP(I,NPSLT(I))) THEN
  JPSBUP=NPSLT(I)
  JPSBMD=NPSLT(I)-1
  JPSBLW=NPSLT(I)-2
  GO TO 141
ENDIF

C
141 CONTINUE
DELTO=PSTTMP(I,JPSBMD)-PSTTMP(I,JPSBLW)
DELT1=PSTTMP(I,JPSBUP)-PSTTMP(I,JPSBMD)
DELT2=PSTTMP(I,JPSBUP)-PSTTMP(I,JPSBLW)
IF (DELTO.EQ.0.OR.DELT1.EQ.0.OR.DELT2.EQ.0) THEN
  WRITE(*,*) 'Bad temperature data; program run terminated'

```

```

        GO TO 399
    ENDIF
    BCON=(EPSLT(I,JPSBLW)*DELT1-EPSLT(I,JPSBMD)*DELT2
1      +EPSLT(I,JPSBUP)*DELT0)/(DELT0*DELT1*DELT2)
    ACON=(EPSLT(I,JPSBMD)-EPSLT(I,JPSBLW))/DELT0-BCON*DELT0
    TPSLT(I)=EPSLT(I,JPSBLW)+ACON*(TEMP-PSTTMP(I,JPSBLW))
1      +BCON*((TEMP-PSTTMP(I,JPSBLW))**2.0)
145  CONTINUE
C
    PSBS=TPSLT(1)+(TPSLT(2)-TPSLT(1))
1      *(CONC-CNCSLN(4,1))/(CNCSLN(4,2)-CNCSLN(4,1))
C
C.....Vapor Pressure of Solvent.....
C
    DO 149 I=1,2
    IF (TEMP.LT.PSVTMP(I,1)) THEN
        JPSBUP=3
        JPSBMD=2
        JPSBLW=1
        GO TO 146
    ENDIF
C
    DO J=3,NPSLV(I),2
    IF (TEMP.GE.PSVTMP(I,J-2).AND.TEMP.LT.PSVTMP(I,J)) THEN
        JPSBUP=J
        JPSBMD=J-1
        JPSBLW=J-2
        GO TO 146
    ENDIF
    ENDDO
C
    IF (TEMP.GE.PSVTMP(I,NPSLV(I))) THEN
        JPSBUP=NPSLV(I)
        JPSBMD=NPSLV(I)-1
        JPSBLW=NPSLV(I)-2
        GO TO 146
    ENDIF
C
146  CONTINUE
    DELT0=PSVTMP(I,JPSBMD)-PSVTMP(I,JPSBLW)
    DELT1=PSVTMP(I,JPSBUP)-PSVTMP(I,JPSBMD)
    DELT2=PSVTMP(I,JPSBUP)-PSVTMP(I,JPSBLW)
    IF (DELT0.EQ.0.OR.DELT1.EQ.0.OR.DELT2.EQ.0) THEN
        WRITE(*,*) 'Bad temperature data; program run terminated'
        GO TO 399
    ENDIF
1      BCON=(EPSLV(I,JPSBLW)*DELT1-EPSLV(I,JPSBMD)*DELT2
1      +EPSLV(I,JPSBUP)*DELT0)/(DELT0*DELT1*DELT2)
    ACON=(EPSLV(I,JPSBMD)-EPSLV(I,JPSBLW))/DELT0-BCON*DELT0
1      TPSLV(I)=EPSLV(I,JPSBLW)+ACON*(TEMP-PSVTMP(I,JPSBLW))
1      +BCON*((TEMP-PSVTMP(I,JPSBLW))**2.0)
149  CONTINUE
C
    PSLV=TPSLV(1)+(TPSLV(2)-TPSLV(1))
1      *(CONC-CNCSLN(5,1))/(CNCSLN(5,2)-CNCSLN(5,1))
C
C.....Compressibility Factor of Solute Vapor.....
C
    IF (TEMP.LT.ZSTTMP(1)) THEN
        IZPRUP=2

```

```

        IZPRLW=1
        GO TO 151
    ENDIF
C
    DO I=2,NZSLT
        IF (TEMP.GE.ZSTTMP(I-1).AND.TEMP.LT.ZSTTMP(I)) THEN
            IZPRUP=I
            IZPRLW=I-1
            GO TO 151
        ENDIF
    ENDDO
C
    IF (TEMP.GE.ZSTTMP(I)) THEN
        IZPRUP=NZSLT
        IZPRLW=NZSLT-1
        GO TO 151
    ENDIF
C
151    CONTINUE
        IF (ZSTTMP(IZPRUP).EQ.ZSTTMP(IZPRLW)) THEN
            WRITE(*,*) 'Bad temperature data; program run terminated'
            GO TO 399
        ENDIF
        ZSBS=EZSLT(IZPRLW)+(EZSLT(IZPRUP)-EZSLT(IZPRLW))
    1    *(TEMP-ZSTTMP(IZPRLW))/(ZSTTMP(IZPRUP)-ZSTTMP(IZPRLW))
C
C.....Compressibility Factor of Solvent Vapor.....
C
        IF (TEMP.LT.ZSVTMP(1)) THEN
            IZPRUP=2
            IZPRLW=1
            GO TO 156
        ENDIF
C
    DO I=2,NZSLV
        IF (TEMP.GE.ZSVTMP(I-1).AND.TEMP.LT.ZSVTMP(I)) THEN
            IZPRUP=I
            IZPRLW=I-1
            GO TO 156
        ENDIF
    ENDDO
C
    IF (TEMP.GE.ZSVTMP(NZSLV)) THEN
        IZPRUP=NZSLV
        IZPRLW=NZSLV-1
        GO TO 156
    ENDIF
C
156    CONTINUE
        IF (ZSVTMP(IZPRUP).EQ.ZSVTMP(IZPRLW)) THEN
            WRITE(*,*) 'Bad temperature data; program run terminated'
            GO TO 399
        ENDIF
        ZSLV=EZSLV(IZPRLW)+(EZSLV(IZPRUP)-EZSLV(IZPRLW))
    1    *(TEMP-ZSVTMP(IZPRLW))/(ZSVTMP(IZPRUP)-ZSVTMP(IZPRLW))
C
C.....Ratio of Specific Heats for Solute Vapor.....
C
        IF (TEMP.LT.GSTTMP(1)) THEN
            IGMPUP=2

```

```

        IGMPLW=1
        GO TO 161
    ENDIF
.C
    DO I=2,NGSLT
        IF (TEMP.GE.GSTTMP(I-1).AND.TEMP.LT.GSTTMP(I)) THEN
            IGMPUP=I
            IGMPLW=I-1
            GO TO 161
        ENDIF
    ENDDO
C
    IF (TEMP.GE.GSTTMP(NGSLT)) THEN
        IGMPUP=NGSLT
        IGMPLW=NGSLT-1
        GO TO 161
    ENDIF
C
161    CONTINUE
        IF (GSTTMP(IGMPUP).EQ.GSTTMP(IGMPLW)) THEN
            WRITE(*,*) 'Bad temperature data; program run terminated'
            GO TO 399
        ENDIF
        GAMSBS=EGSLT(IGMPLW) + (EGSLT(IGMPUP) - EGSLT(IGMPLW))
1    *(TEMP-GSTTMP(IGMPLW)) / (GSTTMP(IGMPUP) - GSTTMP(IGMPLW))
C
C.....Ratio of Specific Heats for Solvent Vapor.....
C
        IF (TEMP.LT.GSVTMP(1)) THEN
            IGMPUP=2
            IGMPLW=1
            GO TO 166
        ENDIF
C
        DO I=2,NGSLV
            IF (TEMP.GE.GSVTMP(I-1).AND.TEMP.LT.GSVTMP(I)) THEN
                IGMPUP=I
                IGMPLW=I-1
                GO TO 166
            ENDIF
        ENDDO
C
        IF (TEMP.GE.GSVTMP(NGSLV)) THEN
            IGMPUP=NGSLV
            IGMPLW=NGSLV-1
            GO TO 166
        ENDIF
C
166    CONTINUE
        IF (GSVTMP(IGMPUP).EQ.GSVTMP(IGMPLW)) THEN
            WRITE(*,*) 'Bad temperature data; program run terminated'
            GO TO 399
        ENDIF
        GAMSLV=EGSLV(IGMPLW) + (EGSLV(IGMPUP) - EGSLV(IGMPLW))
1    *(TEMP-GSVTMP(IGMPLW)) / (GSVTMP(IGMPUP) - GSVTMP(IGMPLW))
C
C.....Specific Volume of Combined Solute and Solvent Vapor.....
C
1    VVAP=1545.4*(TEMP+459.7) /
        (144.0*(PSBS*MLWSBS/ZSBS+PSLV*MLWSLV/ZSLV))

```

C  
399 CONTINUE

C.....

223 FORMAT (I10)  
225 FORMAT (F10.2, F10.4)  
226 FORMAT (F10.2, F10.5)  
227 FORMAT (F10.2, F10.1)  
229 FORMAT (2F10.2)  
247 FORMAT (F10.2)  
255 FORMAT (2F10.3)

C  
RETURN  
END





## APPENDIX H

### SUBROUTINE FPRPSBS

Subroutine FPRPSBS.FOR contains the thermal property data for the commodities available in the program. The following are input data to the subroutine.

KPRD Identification number for commodity contained in tank. (See Section 2.3.2 of the User's Manual for product designations), and

TEMP Temperature (°F).

The following properties of a product are then calculated at saturated vapor condition as a function of temperature:

PSBS Vapor pressure of product (psia),

SPEC Specific heat of the liquid (BTU/lb-°F),

SPLQ Specific volume of liquid (ft<sup>3</sup>/lb),

HFLV Heat of vaporization (BTU/lb-°F),

GAMSBS Ratio of specific heats of substance vapor,

ZSBS Compressibility factor of substance vapor,

MLWSBS Molecular weight of substance vapor, and

VVAP Specific volume of vapor (ft<sup>3</sup>/lb).

The thermal properties of the products listed in Section 2.3.2 of the User's Manual are contained in this subroutine.

The thermal property data are represented as quadratic functions of temperature within given temperature ranges. A sufficient number of temperature ranges are used with each commodity to give an accurate representation of the property data. The subroutine is called with a given value of temperature (TEMP) in °F.

The thermal property data are based on the following sources: propane (Ref. 5), ethylene oxide (Ref. 5), propylene (Ref. 5), 1,3-butadiene (Refs. 5 and 6), vinyl chloride (Refs. 5 and 6), monomethylamine (Refs. 5 and 7), and propylene oxide (Ref. 8).

```

C THIS SUBROUTINE, FPRPSBS.FOR, CONTAINS THE THERMAL PROPERTIES OF
C WATER(1), PROPANE(2), ETHYLENE OXIDE(3), PROPYLENE(4),
C 1,3-BUTADIENE(5), VINYL CHLORIDE(6), MONOMETHYLAMINE(7),
C PROPYLENE OXIDE(8), AND ANHYDROUS AMMONIA(9), UNDER SATURATED
C VAPOR CONDITIONS AS A FUNCTION OF TEMPERATURE. PROPERTIES ARE:
C PSBS-VAPOR PRESSURE OF SUBSTANCE (PSIA)
C SPEC-SPECIFIC HEAT OF LIQUID (BTU/LB-DEG F)
C SPLQ-SPECIFIC VOLUME LIQUID (CU FT/LB)
C HFLV-HEAT OF VAPORIZATION (BTU/LB)
C VVAP-SPECIFIC VOLUME VAPOR (CU FT/LB)
C ZSBS-COMPRESSIBILITY FACTOR OF SOLUTE VAPOR
C GAMSBS-RATIO OF SPECIFIC HEATS OF SOLUTE
C MLWSBS-MOLLECULAR WEIGHT OF SOLUTE VAPOR
C.....Version 2.1, November 11, 1998
C SUBROUTINE FPRPSBS (KPRD,TEMP)

```

```

C
C REAL MLWSBS,MLWSLV
C INTEGER*2 KPRD
C
C COMMON/PROP1/SPEC,SPLQ,HFLV,PSBS,PSLV,ZSBS,ZSLV,VVAP
C COMMON/PROP2/GAMSBS,GAMSLV,MLWSBS,MLWSLV
C COMMON/PROP3/TLMTMN,TLMTMX,CNCMIN,CNCMAX

```

```

C
C PSLV=0.0
C ZSLV=1.0
C GAMSLV=1.1
C MLWSLV=1.0
C CNCMIN=1.0
C CNCMAX=1.0
C GO TO (101,102,103,104,105,106,107,108,109) KPRD

```

```

C
C.....PROPERTIES OF WATER.....
101 CONTINUE

```

```

1 IF (TEMP.LE.100.0) PSBS=0.089+0.000706*(TEMP-32.0)
1 +0.000176*((TEMP-32.0)**2.0)
IF (TEMP.GT.100.0.AND.TEMP.LE.160.0) PSBS=0.949
1 +0.021733*(TEMP-100.0)+0.000691*((TEMP-100.0)**2.0)
IF (TEMP.GT.160.0.AND.TEMP.LE.280.0) THEN
TDELT=TEMP-160.0
PSBS=4.74+0.0459*TDELT+0.00269*TDELT*TDELT
ENDIF
IF (TEMP.GT.280.0.AND.TEMP.LE.400.0) THEN
TDELT=TEMP-280.0
PSBS=49.2+0.643*TDELT+0.00840*TDELT*TDELT
ENDIF
IF (TEMP.GT.400) THEN
TDELT=TEMP-400.0
PSBS=247.31+3.390*TDELT+0.01099*TDELT*TDELT
ENDIF

```

```

C
IF (TEMP.LE.300.0) SPEC=1.0+0.000112*(TEMP-32.0)
IF (TEMP.GT.300.0) SPEC=1.03+0.000864*(TEMP-300.0)
IF (TEMP.LE.300.0) SPLQ=0.01602+0.00000534*(TEMP-32.0)
IF (TEMP.GT.300.0) SPLQ=0.01745+0.00001568*(TEMP-300.0)
IF (TEMP.LE.300.0) HFLV=1075.8-0.618*(TEMP-32.0)
IF (TEMP.GT.300.0) HFLV=910.1-1.0168*(TEMP-300.0)
IF (TEMP.LE.300.0) GAMSBS=1.32-0.0000373*(TEMP-32.0)
IF (TEMP.GT.300.0) GAMSBS=1.31-0.0001818*(TEMP-300.0)
IF (TEMP.LE.300.0) ZSBS=0.998-0.000157*(TEMP-32.0)
IF (TEMP.GT.300.0) ZSBS=0.956-0.000809*(TEMP-300.0)

```

MLWSBS=18.0  
TLMTMN=32.0  
TLMTMX=520.0  
GO TO 999

C  
C.....PROPERTIES OF PROPANE.....  
102 CONTINUE  
C

```
IF (TEMP.LE.56.75) THEN
  PSBS=38.32+0.711*TEMP+0.00751*TEMP*TEMP
  SPLQ=0.029456+0.0000327*TEMP
  HFLV=170.38-0.3105*TEMP
ENDIF
IF (TEMP.GT.56.75.AND.TEMP.LE.81.12) THEN
  PSBS=44.809+0.47317*TEMP+0.0096905*TEMP*TEMP
  SPLQ=(31.312+
1   .05029*(TEMP-56.75)+.0002*((TEMP-56.75)**2))/1000.
  HFLV=166.67-0.12991*TEMP-0.00203103*TEMP*TEMP
ENDIF
IF (TEMP.GT.81.12.AND.TEMP.LE.135.59) THEN
  PSBS=63.705+0.026189*TEMP+0.012329*TEMP*TEMP
  SPLQ=(32.656+.05999*(TEMP-81.12)+.0003307*((TEMP-81.12)**2)
1  )/1000.
  HFLV=164.54-0.10958*TEMP-0.00195787*TEMP*TEMP
ENDIF
IF (TEMP.GT.135.59.AND.TEMP.LE.172.54) THEN
  PSBS=123.25-0.8776297*TEMP+0.015756*TEMP*TEMP
  SPLQ=(36.905+.085936*(TEMP-135.59)+0.001399*((TEMP-135.59)**2)
1  )/1000.
  HFLV=105.00+0.7376607*TEMP-0.00496746*TEMP*TEMP
ENDIF
IF (TEMP.GT.172.54.AND.TEMP.LE.201.25) THEN
  PSBS=193.32-1.723723*TEMP+0.0183058*TEMP*TEMP
  SPLQ=(41.991+.13595*(TEMP-172.54)+.00901*((TEMP-172.54)**2))
1  /1000.
  IF (TEMP.LE.187.63) HFLV=84.39-(TEMP-172.54)*1.226
  IF (TEMP.GT.187.63) HFLV=65.88-(TEMP-187.63)*2.472
ENDIF
IF (TEMP.GT.201.25) THEN
  PSBS=587.84+6.0748*(TEMP-201.25)
  SPLQ=0.053324+(TEMP-201.25)*0.003496
  HFLV=32.21-(TEMP-201.25)*6.341
ENDIF
```

```
C
IF (TEMP.LE.40.0)
1  SPEC=0.5539+0.00065*TEMP+0.0000035*(TEMP**2.0)
IF (TEMP.GT.40.0.AND.TEMP.LE.80.0) SPEC=0.5855
1  +0.000920*(TEMP-40.0)+0.00000675*((TEMP-40.0)**2.0)
IF (TEMP.GT.80.0.AND.TEMP.LE.123.64) SPEC=0.6331
1  +0.001207*(TEMP-80.0)+0.00002637*((TEMP-80.0)**2.0)
IF (TEMP.GT.123.64.AND.TEMP.LE.163.975) THEN
  TDELT=TEMP-123.64
  SPEC=0.736+0.0019923*TDELT+0.00005325*(TDELT**2)
ENDIF
IF (TEMP.GT.163.975.AND.TEMP.LE.201.25) THEN
  TDELT=TEMP-163.975
  SPEC=0.903+0.00033931*TDELT+0.0006224*(TDELT**2)
ENDIF
IF (TEMP.GT.201.25) SPEC=3.976
```

C

```

IF (TEMP.LT.80.0) THEN
  GAMSBS=1.21+0.00133*(TEMP-20.0)
  ZSBS=0.920-0.00105*TEMP-0.00000438*TEMP*TEMP
ENDIF
IF (TEMP.GE.80.0.AND.TEMP.LT.140.0) THEN
  GAMSBS=1.29+0.00383*(TEMP-80.0)
  ZSBS=0.810-0.002200*(TEMP-80.0)
ENDIF
IF (TEMP.GE.140.0.AND.TEMP.LT.196.0) THEN
  GAMSBS=1.52+0.00564*(TEMP-140.0)
  ZSBS=0.678-0.004107*(TEMP-140.0)
ENDIF
IF (TEMP.GE.196.0.AND.TEMP.LT.206.3) THEN
  GAMSBS=1.84 ! 2.1 rev
  ZSBS=0.448-0.0173*(TEMP-196.0)
ENDIF
IF (TEMP.GE.206.3) THEN
  GAMSBS=1.20+0.68*(10.0/(10.0+(603.0-PSBS)**2.0)) ! 2.1 rev
  ZSBS=0.700-0.252*(10.0/(10.0+(603.0-PSBS)**2.0))
ENDIF
MLWSBS=44.0
TLMTMN=0.0
TLMTMX=1000.0
GO TO 999

```

```

C
C.....PROPERTIES OF ETHYLENE OXIDE.....
103 CONTINUE
C

```

```

IF(TEMP.LE.70.0) PSBS=3.73
1 +0.0846*(TEMP+4.0)+0.002194*((TEMP+4.0)**2.0)
IF(TEMP.GT.70.0.AND.TEMP.LE.130.0) PSBS=22.00
1 +0.4135*(TEMP-70.0)+0.004650*((TEMP-70.0)**2.0)
IF(TEMP.GT.130.0.AND.TEMP.LE.190.0) PSBS=63.55
1 +0.9692*(TEMP-130.0)+0.007861*((TEMP-130.0)**2.0)
IF(TEMP.GT.190.0.AND.TEMP.LE.250.0) PSBS=150.00
1 +1.9145*(TEMP-190.0)+0.011506*((TEMP-190.0)**2.0)
IF(TEMP.GT.250.0.AND.TEMP.LE.310.0) PSBS=306.29
1 +3.3008*(TEMP-250.0)+0.015317*((TEMP-250.0)**2.0)
IF(TEMP.GT.310.0.AND.TEMP.LE.370.0) PSBS=559.48
1 +5.1473*(TEMP-310.0)+0.018989*((TEMP-310.0)**2.0)
IF(TEMP.GT.370.0) PSBS=936.68+7.383*(TEMP-370.0)

```

```

C
IF(TEMP.LT.85.0) SPEC=0.4560+0.000204*TEMP
IF(TEMP.GT.85.0.AND.TEMP.LE.145.0) SPEC=0.4733
1 +0.00067*(TEMP-85.0)+0.00000367*((TEMP-85.0)**2.0)
IF(TEMP.GT.145.0.AND.TEMP.LE.205.0) SPEC=0.5267
1 +0.001065*(TEMP-145.0)+0.00000539*((TEMP-145.0)**2.0)
IF(TEMP.GT.205.0.AND.TEMP.LE.265.0) SPEC=0.6100
1 +0.001610*(TEMP-205.0)+0.00000933*((TEMP-205.0)**2.0)
IF(TEMP.GT.265.0.AND.TEMP.LE.325.0) SPEC=0.7402
1 +0.002435*(TEMP-265.0)+0.00000383*((TEMP-265.0)**2.0)
IF(TEMP.GT.325.0.AND.TEMP.LE.355.0) SPEC=
1 0.9001+0.00010733*((TEMP-325.0)**2.0)
IF(TEMP.GT.355.0.AND.TEMP.LE.375.0)
1 SPEC=0.9967+0.13*(TEMP-355.0)
IF(TEMP.GT.375.0) SPEC=2.7+4.4*(TEMP-375.0)

```

```

C
IF (TEMP.LE.70.0) SPLQ=0.01744+0.00001086*TEMP
IF (TEMP.GT.70.0.AND.TEMP.LE.130.0) SPLQ=
1 (18.200+0.01195*(TEMP-70.)+0.0000672*(TEMP-70.)**2)/1000.0

```

```

IF (TEMP.GT.130.0.AND.TEMP.LE.190.0) SPLQ=
1 (19.159+0.02108*(TEMP-130.0)+0.000065*(TEMP-130.0)**2)/1000.0
IF (TEMP.GT.190.0.AND.TEMP.LE.250.0) SPLQ=
1 (20.658+0.02888*(TEMP-190.0)+0.0000828*(TEMP-190.0)**2)/1000.0
IF (TEMP.GT.250.0.AND.TEMP.LE.310.0) SPLQ=
1 (22.689+0.03543*(TEMP-250.0)+0.000273*(TEMP-250.0)**2)/1000.0
IF (TEMP.GT.310.0.AND.TEMP.LE.370.0) SPLQ=
1 (25.799+0.060*(TEMP-310.0)+0.001*(TEMP-310.0)**2)/1000.0
IF (TEMP.GT.370.0)
1 SPLQ=0.032999+0.0012499*(TEMP-370.0)

```

C

```

IF (TEMP.LE.70.0) HFLV=261.4-0.2586*TEMP
IF (TEMP.GT.70.0.AND.TEMP.LE.250.0)
1 HFLV=261.04-0.2219*TEMP-0.000451*TEMP*TEMP
IF (TEMP.GT.250.0.AND.TEMP.LE.310.0) HFLV=177.4
1 -0.4474*(TEMP-250.0)-0.003182*((TEMP-250.0)**2.0)
IF (TEMP.GT.310.0.AND.TEMP.LE.370.0) HFLV=139.1
1 -0.7517*(TEMP-310.0)-0.003944*((TEMP-310.0)**2.0)
IF (TEMP.GT.370.0)
1 HFLV=79.8-5.542*(TEMP-370.0)

```

C

```

IF (TEMP.LE.100.0) ZSBS=0.9522-0.00044167*TEMP
IF (TEMP.GT.100.0.AND.TEMP.LE.220.0) ZSBS=0.908
1 -0.00044167*(TEMP-100.0)-0.00000542*((TEMP-100.0)**2.0)
IF (TEMP.GT.220.0.AND.TEMP.LE.340.0) ZSBS=0.777
1 -0.00073327*(TEMP-220.0)-0.00000889*((TEMP-220.0)**2.0)
IF (TEMP.GT.340.0.AND.TEMP.LE.370.0) ZSBS=0.561
1 -0.002867*(TEMP-340.0)
IF (TEMP.GT.370.0) ZSBS=0.475-0.017*(TEMP-370.0)

```

C

```

GAMSBS=1.2
MLWSBS=44.05
TLMTMN=-20.0
TLMTMX=1000.0
GO TO 999

```

C

C.....PROPERTIES OF PROPYLENE.....

104

CONTINUE

C

```

IF(TEMP.LE.40.0) THEN
  PSBS=47.97+1.2138*TEMP
  SPEC=0.5552+0.00046*TEMP+0.00000375*TEMP*TEMP
  SPLQ=0.028032+0.00004*TEMP
  HFLV=173.0-0.3225*TEMP
ENDIF
IF(TEMP.GT.40.0.AND.TEMP.LE.80.0) THEN
  F=TEMP-40.0
  PSBS=96.52+1.5303*F+0.0106*F*F
  SPEC=0.5796+0.000743*F+0.00000713*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
ENDIF
IF(TEMP.GT.80.0.AND.TEMP.LE.120.0) THEN
  F=TEMP-80.0
  PSBS=174.71+2.3750*F+0.01343*F*F
  SPEC=0.6207+0.001235*F+0.000018*F*F
  SPLQ=(31716.0+56.03*F+0.4*F*F)/10.0**6
  HFLV=141.91-0.475250*F-0.001263*F*F
ENDIF
IF (TEMP.GT.120.0.AND.TEMP.LE.160.0) THEN

```

```

F=TEMP-120.0
PSBS=291.19+3.4445*F+0.01750*F*F
SPEC=0.6989+0.001870*F+0.0000945*F*F
SPLQ=(34599.0+100.15*F+1.0*F*F)/10.0**6
HFLV=120.88-0.479250*F-0.006388*F*F
ENDIF
IF (TEMP.GT.160.0.AND.TEMP.LE.180.0) THEN
F=TEMP-160.0
PSBS=456.97+4.8570*F+0.02160*F*F
SPEC=0.9249+0.02555*F
SPLQ=(40205.0+128.15*F+4.81*F*F)/10.0**6
HFLV=91.49-1.038500*F-0.013550*F*F
ENDIF
IF (TEMP.GT.180.0.AND.TEMP.LE.190.0) THEN
SPEC=1.4915+0.0237*((TEMP-180.0)**2.0)
SPLQ=0.044690+0.0005126*(TEMP-180.0)
HFLV=65.3-1.803*(TEMP-180.0)
ENDIF
IF (TEMP.GT.190.0) THEN
SPEC=3.865
SPLQ=0.049816+0.00319*(TEMP-190.0)
HFLV=47.27-6.593*(TEMP-190.0)
ENDIF
IF (TEMP.GT.180.0) THEN
F=TEMP-180.0
PSBS=562.75+5.6680*F+0.03460*F*F
ENDIF

```

C

```

IF (TEMP.LE.100.0)
1 ZSBS=0.805-0.00111*TEMP-0.0000038*TEMP*TEMP
IF (TEMP.GT.100.0) ZSBS=0.656
1 -0.0011375*(TEMP-100.0)-0.00002344*((TEMP-100.0)**2.0)

```

C

```

IF (TEMP.LE.50.0) GAMSBS=1.32+0.0006*TEMP
IF (TEMP.GT.50.0.AND.TEMP.LE.100.0)
1 GAMSBS=1.35+0.0026*(TEMP-50.0)
IF (TEMP.GT.100.0.AND.TEMP.LE.140.0)
1 GAMSBS=1.48+0.0075*(TEMP-100.0)
IF (TEMP.GT.140.0.AND.TEMP.LE.180.0)
1 GAMSBS=1.78+0.0425*(TEMP-140.0)
IF (TEMP.GT.180.0) GAMSBS=3.48+0.088*(TEMP-180.0)
MLWSBS=42.08
TLMTMN=0.0
TLMTMX=1000.0
GO TO 999

```

C

C.....PROPERTIES OF 1,3-BUTADIENE.....

105 CONTINUE

C

```

IF (TEMP.LE.40.0) THEN
PSBS=8.46+0.19825*TEMP+0.002563*TEMP*TEMP
SPEC=0.5026+0.000485*TEMP
SPLQ=0.024060+0.00002428*TEMP
HFLV=184.0-0.22775*TEMP
ENDIF
IF (TEMP.GT.40.0.AND.TEMP.LE.80.0) THEN
F=TEMP-40.0
PSBS=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
ENDIF
IF (TEMP.GT.80.0.AND.TEMP.LE.120.0) THEN
  F=TEMP-80.0
  PSBS=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
ENDIF
IF (TEMP.GT.120.0.AND.TEMP.LE.160.0) THEN
  F=TEMP-120.0
  PSBS=80.11+1.14975*F+0.007063*F*F
  SPEC=0.583+0.000875*F+0.0000013*F*F
  SPLQ=(27470.0+35.50*F+0.1250*F*F)/10.0**6
  HFLV=153.60-0.30825*F-0.000613*F*F
ENDIF
IF (TEMP.GT.160.0.AND.TEMP.LE.200.0) THEN
  F=TEMP-160.0
  PSBS=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=140.29-0.36275*F-0.001113*F*F
ENDIF
IF (TEMP.GT.200.0.AND.TEMP.LE.240.0) THEN
  F=TEMP-200.0
  PSBS=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
ENDIF
IF (TEMP.GT.240.0) THEN
  F=TEMP-240.0
  PSBS=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
ENDIF
IF (TEMP.LE.100.0) ZSBS=1.00-0.00097*TEMP
IF (TEMP.GT.100.0.AND.TEMP.LE.200.0)
1  ZSBS=0.903-0.00151*(TEMP-100.0)
IF (TEMP.GT.200.0) ZSBS=0.752-0.00274*(TEMP-200)
MLWSBS=54.09
GAMSBS=1.3
TLMTMN=0.0
TLMTMX=280.0
GO TO 999

```

```

C
C.....PROPERTIES OF VINYL CHLORIDE.....
106 CONTINUE
C

```

```

IF (TEMP.LE.40.0) THEN
  PSBS=12.2+0.25*TEMP+0.0045*TEMP*TEMP
  SPEC=0.276+0.000675*TEMP
  SPLQ=0.01666+0.000011*TEMP
  HFLV=142.3-0.16*TEMP
ENDIF
IF (TEMP.GT.40.0.AND.TEMP.LE.100.0) THEN
  F=TEMP-40.0
  PSBS=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=135.9-0.2017*(TEMP-40.0)
    ENDIF
    IF (TEMP.GT.100.0.AND.TEMP.LE.140.0) THEN
      F=TEMP-100.0
      PSBS=82.00+0.92500*F+0.008750*F*F
      SPEC=0.3445+0.000678*F
      SPLQ=(18080.0+22.50*F+0.0250*F*F)/10.0**6
      HFLV=123.80-0.17500*F-0.001000*F*F
    ENDIF
    IF (TEMP.GT.140.0.AND.TEMP.LE.180.0) THEN
      F=TEMP-140.0
      PSBS=133.00+1.57500*F+0.008750*F*F
      SPEC=0.3718+0.000688*F
      SPLQ=(19020.0+23.25*F+0.1880*F*F)/10.0**6
      HFLV=115.20-0.25000*F-0.000500*F*F
    ENDIF
    IF (TEMP.GT.180.0.AND.TEMP.LE.220.0) THEN
      F=TEMP-180.0
      PSBS=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
    ENDIF
    IF (TEMP.GT.220.0) THEN
      F=TEMP-220.0
      PSBS=329.00+3.52500*F+0.023750*F*F
      SPEC=0.4265+0.000678*F
      SPLQ=(21970.0+52.25*F+0.4130*F*F)/10.0**6
      HFLV=90.20-0.27500*F-0.004250*F*F
    ENDIF
    ZSBS=0.900-0.00146*TEMP
    MLWSBS=62.5
    GAMSBS=1.3
    TLMTMN=0.0
    TLMTMX=260.0
    GO TO 999

```

```

C
C.....PROPERTIES OF MONOMETHYLAMINE.....
107 CONTINUE
C

```

```

    IF(TEMP.LE.50.0) THEN
      PSBS=8.78+0.223*TEMP+0.003976*TEMP*TEMP
      SPEC=0.730+0.00084*TEMP
      SPLQ=0.02264+0.0000204*TEMP+0.00000003*TEMP*TEMP
      HFLV=367.8-0.416*TEMP
    ENDIF
    IF(TEMP.GT.50.0.AND.TEMP.LE.86.0) THEN
      F=TEMP-50.0
      PSBS=29.87+0.6372*F+0.006728*F*F
      SPEC=0.772+0.000806*F+0.0000077*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
    ENDIF
    IF (TEMP.GT.86.0.AND.TEMP.LE.122.0) THEN
      F=TEMP-86.0
      PSBS=61.53+0.9669*F+0.013627*F*F
      SPEC=0.811+0.001167*F+0.0000031*F*F
      SPLQ=(24640.0+26.11*F+0.0620*F*F)/10.0**6
      HFLV=329.9-0.5083*F-0.000463*F*F
    ENDIF

```



```

ENDIF
IF (TEMP.GT.122.0.AND.TEMP.LE.150.0) THEN
  F=TEMP-122.0
  PSBS=114.00+1.89250*F+0.009451*F*F
  SPEC=0.857+0.001132*F+0.0000016*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
ENDIF
IF (TEMP.GT.150.0.AND.TEMP.LE.180.0) THEN
  F=TEMP-150.0
  PSBS=174.40+2.4267*F+0.015111*F*F
  SPEC=0.890+0.001467*F
  SPLQ=(26540.0+32.67*F+0.0440*F*F)/10.0**6
  HFLV=293.1-0.6933*F-0.003111*F*F
ENDIF
IF (TEMP.GT.180.0.AND.TEMP.LE.210.0) THEN
  F=TEMP-180.0
  PSBS=260.80+3.2867*F+0.016444*F*F
  SPEC=0.934+0.001367*F+0.0000022*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
ENDIF
IF (TEMP.GT.210.0) THEN
  F=TEMP-210.0
  PSBS=374.20+4.568*F+0.024960*F*F
  SPEC=0.977+0.001300*F+0.0000067*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
ENDIF
ZSBS=0.980-0.00041*TEMP
GAMSBS=1.3
TLMTMN=50.0
TLMTMX=240.0
MLWSBS=31.06
GO TO 999

```

```

C
C.....PROPERTIES OF PROPYLENE OXIDE.....
108 CONTINUE
C

```

```

IF (TEMP.LE.40.0) THEN
  PSBS=1.4+0.075*TEMP
  SPEC=0.442+0.001*TEMP
  SPLQ=0.01836+0.00001225*TEMP
  HFLV=223.0-0.175*TEMP
ENDIF
IF (TEMP.GT.40.0.AND.TEMP.LE.160.0) THEN
  F=TEMP-40.0
  PSBS=4.4+0.05667*F+0.002417*F*F
  SPEC=0.482+0.001167*F+0.0000017*F*F
  SPLQ=(18850.0+14.667*F+0.014*F*F)/10.0**6
  HFLV=216.0-0.24*F
ENDIF
IF (TEMP.GT.160.0.AND.TEMP.LE.280.0) THEN
  F=TEMP-160.0
  PSBS=46.0+0.55000*F+0.007500*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
ENDIF
IF (TEMP.GT.280.0.AND.TEMP.LE.370.0) THEN

```

```

      F=TEMP-280.0
      PSBS=220.0+1.55556*F+0.018519*F*F
      SPEC=0.991+0.0021944*F+0.0000076*F*F
      SPLQ=(23990.0+11.556*F+0.752*F*F)/10.0**6
      HFLV=151.2-0.19*F-0.006333*F*F
    ENDIF
    IF (TEMP.GT.370.0) THEN
      IF (TEMP.LE.400.0) PSBS=510.0+4.667*(TEMP-370.0)
      IF (TEMP.GT.400.0) PSBS=650.0+7.529*(TEMP-370.0)
      SPEC=1.25+0.01*(TEMP-370.0)
      SPLQ=0.03112+0.000147*(TEMP-370.0)
1      +0.0000061*((TEMP-370.0)**2.0)
      HFLV=82.8-2.151*(TEMP-370.0)
    ENDIF
  C
    IF (TEMP.LE.100.0) ZSBS=0.9522-0.00044167*TEMP
    IF (TEMP.GT.100.0.AND.TEMP.LE.220.0) ZSBS=0.908
1    -0.00044167*(TEMP-100.0)-0.00000542*((TEMP-100.0)**2.0)
    IF (TEMP.GT.220.0.AND.TEMP.LE.340.0) ZSBS=0.777
1    -0.00073327*(TEMP-220.0)-0.00000889*((TEMP-220.0)**2.0)
    IF (TEMP.GT.340.0.AND.TEMP.LE.370.0) ZSBS=0.561
1    -0.002867*(TEMP-340.0)
    IF (TEMP.GT.370.0) ZSBS=0.475-0.006415*(TEMP-370.0)
  C
    TLMTMN=0.0
    TLMTMX=1000.0
    GAMSBS=1.3
    MLWSBS=58.08
    GO TO 999
  C
  C.....PROPERTIES OF ANHYDROUS AMMONIA.....
109 CONTINUE
  C
    IF (TEMP.LT.20.0) PSBS=18.30
1    +0.46425*(TEMP+20.0)+0.007088*((TEMP+20.0)**2.0)
    IF (TEMP.GE.20.0.AND.TEMP.LT.60.0) PSBS=48.21
1    +1.02625*(TEMP-20.0)+0.01146*((TEMP-20.0)**2.0)
    IF (TEMP.GE.60.0.AND.TEMP.LT.100.0) PSBS=107.6
1    +1.93250*(TEMP-60.0)+0.01688*((TEMP-60.0)**2.0)
    IF (TEMP.GE.100.0.AND.TEMP.LT.140.0) PSBS=211.9
1    +3.26975*(TEMP-100.0)+0.02276*((TEMP-100.0)**2.0)
    IF (TEMP.GE.140.0) PSBS=379.1+5.08861*(TEMP-140.0)
1    +0.02995*((TEMP-140.0)**2.0)
  C
    SPEC=1.100+0.001*(TEMP-20.0)
  C
    IF (TEMP.LT.20.0) HFLV=583.6-0.7625*(TEMP+20.0)
    IF (TEMP.GE.20.0.AND.TEMP.LT.80.0) HFLV=553.1
1    -0.8133*(TEMP-20.0)-0.001556*((TEMP-20.0)**2.0)
    IF (TEMP.GE.80.0) HFLV=498.7-0.9952*(TEMP-80.0)
1    -0.002489*((TEMP-80.0)**2.0)
  C
    IF (TEMP.LT.20.0) SPLQ=0.02369+0.00002625*(TEMP+20.0)
    IF (TEMP.GE.20.0.AND.TEMP.LT.80.0) SPLQ=0.02473
1    +(28.2*(TEMP-20.0)+0.072*((TEMP-20.0)**2.0))/(10.0**6.0)
    IF (TEMP.GE.80.0) SPLQ=0.02668
1    +(37.0*(TEMP-80.0)+0.125*((TEMP-80.0)**2.0))/(10.0**6.0)
  C
    IF (TEMP.LT.50.0) ZSBS=0.967-0.000786*(TEMP+20.0)
    IF (TEMP.GE.50.0) ZSBS=0.912-0.00135*(TEMP-50.0)

```

```
GAMSBS=1.32
MLWSBS=17.0
TLMTMN=-20.0
TLMTMX=176.0
```

C

```
GO TO 999
```

C.....

999

```
CONTINUE
IF (PSBS.LE.(0.01)) THEN
  VVAP=20000.0
ELSE
  VVAP=ZSBS*(1545.0/MLWSBS)*(TEMP+460.0)/(PSBS*144.0)
ENDIF
RETURN
END
```



## APPENDIX I

### SUBROUTINE FPRPSLV

Subroutine FPRPSLV.FOR contains the thermal property data for the commodities available in the program which are solutions. The following are input data to the subroutine.

KPRD	Identification number for commodity contained in tank. (See Section 2.3.2 of the User's Manual for product designations),
CONC	Product concentration, (decimal fraction), and
TEMP	Temperature (°F).

The following properties of a product are then calculated at saturated vapor condition as a function of temperature:

PSBS	Vapor pressure of product (psia),
PSLV	Vapor pressure of solvent (psia),
SPEC	Specific heat of the liquid (BTU/lb-°F),
SPLQ	Specific volume of liquid (ft <sup>3</sup> /lb),
HFLV	Heat of vaporization (BTU/lb-°F),
GAMSBS	Ratio of specific heats of substance vapor,
GAMSLV	Ratio of specific heats of solvent vapor,
ZSBS	Compressibility factor of substance vapor,
MLWSBS	Molecular weight of substance vapor, and
VVAP	Specific volume of vapor (ft <sup>3</sup> /lb).

The thermal properties of the products listed in Section 2.3.2 of the User's Manual are contained in this subroutine.

The thermal property data are represented as quadratic functions of temperature within given temperature ranges. A sufficient number of temperature ranges are used with each commodity to give an accurate representation of the property data. The subroutine is called with a given value of temperature (TEMP) in °F.

The thermal property data for the acids and caustic soda were obtained from various sources (Refs. 9 to 12). A listing of the subroutine is presented on the following pages.

```

C      THIS SUBROUTINE, FPRPSLV.FOR, CONTAINS THE THERMAL PROPERTIES
C      OF SULFURIC ACID(10), HYDROCHLORIC ACID(11), SODIUM
C      HYDROXIDE(12), PHOSPHORIC ACID-75%(13), SUPER
C      PHOSPHORIC ACID(14) POTASSIUM HYDROXIDE(15), AND HYDROGEN
C      PEROXIDE SOLUTIONS (16), UNDER SATURATED VAPOR
C      CONDITIONS AS A FUNCTION OF TEMPERATURE.
C      PROPERTIES ARE:
C          PSBS-VAPOR PRESSURE OF SUBSTANCE (PSIA)
C          PSLV-VAPOR PRESSURE OF WATER (FOR SOLUTIONS, PSIA)
C          SPEC-SPECIFIC HEAT OF LIQUID (BTU/LB-DEG F)
C          SPLQ-SPECIFIC VOLUME LIQUID (CU FT/LB)
C          HFLV-HEAT OF VAPORIZATION (BTU/LB)
C          VVAP-SPECIFIC VOLUME VAPOR (CU FT/LB)
C          ZSBS-COMPRESSIBILITY FACTOR OF SOLUTE VAPOR
C          ZSLV-COMPRESSIBILITY FACTOR OF SOLVENT VAPOR
C          GAMSBS-RATIO OF SPECIFIC HEATS OF SOLUTE
C          GAMSLV-RATIO OF SPECIFIC HEATS OF SOLVENT
C          MLWSBS-MOLLECULAR WEIGHT OF SOLUTE VAPOR
C          MLWSLV-MOLLECULAR WEIGHT OF SOLVENT VAPOR
C.....Version 2.1, November 11, 1998
C      SUBROUTINE FPRPSLV (KPRD,CONC,TEMP)
C
C      REAL MLWSBS,MLWSLV
C      INTEGER*2 KPRD
C
C      COMMON/PROP1/SPEC,SPLQ,HFLV,PSBS,PSLV,ZSBS,ZSLV,VVAP
C      COMMON/PROP2/GAMSBS,GAMSLV,MLWSBS,MLWSLV
C      COMMON/PROP3/TLMTMN,TLMTMX,CNCMIN,CNCMAX
C
C      ZSLV=0.95
C      GAMSLV=1.26
C      TLMTMN=0.0
C      MLWSLV=18.0
C      JPRD=KPRD-9
C
C      GO TO (101,102,103,104,105,106,107) JPRD
C.....PROPERTIES OF SULFURIC ACID.....
101 CONTINUE
C
C      IF (TEMP.LE.50.0) THEN
C          PSLV=0.0
C          PSBS=0.0
C      ENDIF
C      IF (TEMP.GT.50.0.AND.TEMP.LE.230.0) THEN
C          TDELT=TEMP-50.0
C          PWTR92=2.736*(TDELT**4.0)/(10.0**11.0)
C          PWTR94=1.478*(TDELT**4.0)/(10.0**11.0)
C          PSLF92=0.0
C          PSLF94=0.0
C          PSLV=PWTR92+(CONC-0.92)*(PWTR94-PWTR92)*50.0
C          PSBS=PSLF92+(CONC-0.92)*(PSLF94-PSLF92)*50.0
C      ENDIF
C      IF (TEMP.GT.230.0.AND.TEMP.LE.410.0) THEN
C          TD=TEMP-230.0
C          PWTR92=0.02872+(9.0*TD*TD+0.3081*(TD**3.0))/(10.0**6.0)
C          PWTR94=0.01552+(3.2*TD*TD+0.2020*(TD**3.0))/(10.0**6.0)
C          PSLF92=1.015*(TD**3.0)/(10.0**8.0)
C          PSLF94=1.219*(TD**3.0)/(10.0**8.0)
C          PSLV=PWTR92+(CONC-0.92)*(PWTR94-PWTR92)*50.0
C          PSBS=PSLF92+(CONC-0.92)*(PSLF94-PSLF92)*50.0

```

```

ENDIF
IF (TEMP.GT.410.0) THEN
  TD=TEMP-410.0
  PWTR92=2.1176+0.001127*TD+0.000863*(TD**2.0)
  PWTR94=1.2966+0.000561*TD+0.1302*(TD**2.0)/(10.0**6.0)
  PSLF92=0.0592+(27.5*TD*TD+0.09074*(TD**3.0))/(10.0**6.0)
  PSLF94=0.0711+(33.1*TD*TD+0.09000*(TD**3.0))/(10.0**6.0)
  PSLV=PWTR92+(CONC-0.92)*(PWTR94-PWTR92)*50.0
  PSBS=PSLF92+(CONC-0.92)*(PSLF94-PSLF92)*50.0
ENDIF
C
IF (PSLV.LT.(0.01).AND.PSBS.LT.(0.01)) THEN
  VVAP=40000.0
ELSE
  VVAP=0.95*(TEMP+459.0)/(144.0*(PSLV/85.8+PSBS/86.2))
ENDIF
HFLV=1550.0+(CONC-0.900)*4540.0
SPLQ=0.0087+2.778*(TEMP-104.0)/(10.0**6.0)
SPEC=0.36
GAMSBS=1.2
MLWSBS=98.0
TLMTMX=450.0
CNCMIN=0.920
CNCMAX=0.940
ZSBS=.950
C
GO TO 999
C.....PROPERTIES OF HYDROCHLORIC ACID.....
102 CONTINUE
C
SPEC=0.561+0.000573*(TEMP-32.0)
SPLQ=0.0140*(1.0+0.000282*(TEMP-68.0))
HFLV=1000.0
C
EXPN=9.4670-2094.0/(255.38+TEMP/1.8)
PHCL38=0.0193337*(10.0**EXPN)
EXPN=9.5262-2229.0/(255.38+TEMP/1.8)
PHCL36=0.0193337*(10.0**EXPN)
EXPN=9.6061-2316.0/(255.38+TEMP/1.8)
PHCL34=0.0193337*(10.0**EXPN)
EXPN=9.7523-2457.0/(255.38+TEMP/1.8)
PHCL32=0.0193337*(10.0**EXPN)
C
EXPN=9.20783-2579.0/(255.38+TEMP/1.8)
PH2O38=0.0193337*(10.0**EXPN)
EXPN=9.11815-2526.0/(255.38+TEMP/1.8)
PH2O36=0.0193337*(10.0**EXPN)
EXPN=9.07143-2487.0/(255.38+TEMP/1.8)
PH2O34=0.0193337*(10.0**EXPN)
EXPN=9.03317-2453.0/(255.38+TEMP/1.8)
PH2O32=0.0193337*(10.0**EXPN)
C
IF (CONC.GE.(0.36)) THEN
  PSBS=PHCL36+(PHCL38-PHCL36)*(CONC-0.36)/(0.02)
  PSLV=PH2O36+(PH2O38-PH2O36)*(CONC-0.36)/(0.02)
ENDIF
IF (CONC.LE.(0.36).AND.CONC.GE.(0.34)) THEN
  PSBS=PHCL34+(PHCL36-PHCL34)*(CONC-0.34)/(0.02)
  PSLV=PH2O34+(PH2O36-PH2O34)*(CONC-0.34)/(0.02)
ENDIF

```

```

IF (CONC.LE.(0.34)) THEN
  PSBS=PHCL32+(PHCL34-PHCL32)*(CONC-0.32)/(0.02)
  PSLV=PH2O32+(PH2O34-PH2O32)*(CONC-0.32)/(0.02)
ENDIF
C
IF (PSLV.LT.(0.01).AND.PSBS.LT.(0.01)) THEN
  VVAP=20000.0
ELSE
  VVAP=0.95*(TEMP+459.0)/(144.0*(PSLV/85.8+PSBS/86.2))
ENDIF
GAMSBS=1.41
MLWSBS=36.5
ZSBS=0.95
TLMTMX=200.0
CNCMIN=0.320
CNCMAX=0.380
C
GO TO 999
C.....PROPERTIES OF SODIUM HYDROXIDE.....
103 CONTINUE
PSBS=0.0
IF (TEMP.LE.212.0) THEN
  EXPN=9.0349-2413.0/(255.2+TEMP/1.8)
  PH2O50=0.0193337*(10.0**EXPN)
  EXPN=9.1517-2492.9/(255.2+TEMP/1.8)
  PH2O60=0.0193337*(10.0**EXPN)
ENDIF
IF (TEMP.GT.212.0) THEN
  EXPN=8.7309-2299.6/(255.2+TEMP/1.8)
  PH2O50=0.0193337*(10.0**EXPN)
  EXPN=8.9058-2401.2/(255.2+TEMP/1.8)
  PH2O60=0.0193337*(10.0**EXPN)
ENDIF
C
PSLV=PH2O50+(PH2O60-PH2O50)*(CONC-0.50)/0.10
C
IF (PSLV.LT.(0.01).AND.PSBS.LT.(0.01)) THEN
  VVAP=30000.0
ELSE
  VVAP=0.95*(TEMP+459.0)/(144.0*(PSLV/85.8))
ENDIF
C
SPLQ50=0.010326*(1.0+0.000252*TEMP)
SPLQ60=0.009725*(1.0+0.000243*TEMP)
SPLQ=SPLQ50+(SPLQ60-SPLQ50)*(CONC-0.50)/0.10
C
SPEC=0.783
HFLV=1071.3-0.64*(TEMP-40.0)
ZSBS=0.900
GAMSBS=1.2
MLWSBS=40.0
TLMTMX=300.0
CNCMIN=0.500
CNCMAX=0.600
GO TO 999
C.....PROPERTIES OF 75% PHOSPHORIC ACID.....
104 CONTINUE
C
PSBS=0.0
IF (TEMP.LE.86.0) THEN

```



```

EXPN=8.3798-2236.08/(255.2+TEMP/1.8)
PH2O75=0.0193337*(10.0**EXPN)
EXPN=8.3047-2335.554/(255.2+TEMP/1.8)
PH2O85=0.0193337*(10.0**EXPN)
ENDIF
IF (TEMP.GT.86.0.AND.TEMP.LE.230.0) THEN
EXPN=8.25245-2191.13/(255.2+TEMP/1.8)
PH2O75=0.0193337*(10.0**EXPN)
EXPN=8.2724-2324.161/(255.2+TEMP/1.8)
PH2O85=0.0193337*(10.0**EXPN)
ENDIF
IF (TEMP.GT.230.0.AND.TEMP.LE.284.0) THEN
EXPN=8.3176-2216.09/(255.2+TEMP/1.8)
PH2O75=0.0193337*(10.0**EXPN)
EXPN=8.3198-2342.314/(255.2+TEMP/1.8)
PH2O85=0.0193337*(10.0**EXPN)
ENDIF
IF (TEMP.GT.284.0.AND.TEMP.LE.370.0) THEN
EXPN=8.2067-2170.273/(255.2+TEMP/1.8)
PH2O75=0.0193337*(10.0**EXPN)
EXPN=7.8042-2129.348/(255.2+TEMP/1.8)
PH2O85=0.0193337*(10.0**EXPN)
ENDIF
IF (TEMP.GT.370.0) THEN
EXPN=7.8952-2026.744/(255.2+TEMP/1.8)
PH2O75=0.0193337*(10.0**EXPN)
EXPN=7.5828-2027.346/(255.2+TEMP/1.8)
PH2O85=0.0193337*(10.0**EXPN)
ENDIF
C
PSLV=PH2O75+(PH2O85-PH2O75)*(CONC-0.75)/0.10
IF (PSLV.LT.(0.01).AND.PSBS.LT.(0.01)) THEN
VVAP=25000.0
ELSE
VVAP=0.95*(TEMP+459.0)/(144.0*(PSLV/85.8))
ENDIF
C
HFLV=1071.3-0.64*(TEMP-40.0)
C
SPC75=0.4844+0.000306*(TEMP-59.0)
SPC85=0.4380+0.000267*(TEMP-59.0)
SPEC=SPC75+(SPC85-SPC75)*(CONC-0.75)/0.10
C
SPL75=0.01019+2.83*(TEMP-77.0)/(10.0**6.0)
SPL85=0.00951+2.53*(TEMP-77.0)/(10.0**6.0)
SPLQ=SPL75+(SPL85-SPL75)*(CONC-0.75)/0.10
C
MLWSBS=142.0
ZSBS=0.7
GAMSBS=1.2
TLMTMX=450.0
CNCMIN=0.750
CNCMAX=0.850
GO TO 999
C.....PROPERTIES OF SUPERPHOSPHORIC ACID.....
105 CONTINUE
C
PSBS=0.0
PSLV=0.0
HFLV=1000.0

```

```

SPEC=0.352+0.000197*TEMP
SPLQ=0.00811*(1.0+0.000300*TEMP)
MLWSBS=142.0
TLMTMN=0.0
TLMTMX=350.0
CNCMIN=0.755
CNCMAX=0.765
ZSBS=0.7
GAMSBS=1.2
VVAP=20000.0
GO TO 999

```

C.....PROPERTIES OF POTASSIUM HYDROXIDE.....

```

106 CONTINUE
PSBS=0.0
EXPN=-1.0706+0.015264*(TEMP-68.0)-0.0000217*((TEMP-68.0)**2.0)
PH2O44=10.0**EXPN
EXPN=-1.3010+0.015405*(TEMP-68.0)-0.0000191*((TEMP-68.0)**2.0)
PH2O50=10.0**EXPN

```

```

C PSLV=PH2O50+(PH2O50-PH2O44)*(CONC-0.50)/0.0556
C

```

```

C IF (PSLV.LT.(0.01).AND.PSBS.LT.(0.01)) THEN
  VVAP=25000.0
  ELSE
    VVAP=0.95*(TEMP+459.0)/(144.0*(PSLV/85.8))
  ENDIF

```

```

C SPLQ50=0.01602*(0.6528+0.000132*TEMP)
SPLQ44=0.01602*(0.6812+0.000150*TEMP)
SPLQ=SPLQ50+(SPLQ50-SPLQ44)*(CONC-0.50)/0.0556
C

```

```

C SPEC50=0.6374
SPEC44=0.6710
SPEC=SPEC50+(SPEC50-SPEC44)*(CONC-0.50)/0.0556
C

```

```

C HFLV50=1066.0+.4694*TEMP
HFLV44=1129.0-0.2389*TEMP
HFLV=HFLV50+(HFLV50-HFLV44)*(CONC-0.50)/0.0556
MLWSBS=56.11
GAMSBS=1.2
ZSBS=0.7
TLMTMX=350.0
CNCMIN=0.440
CNCMAX=0.500
GO TO 999

```

C.....PROPERTIES OF HYDROGEN PEROXIDE SOLUTIONS.....

```

107 CONTINUE
C
SPEC=0.757-0.065*(CONC-0.6)/0.2
DENS=64.295+22.5*CONC-0.0134*TEMP+6.35*CONC*CONC-0.031*CONC*TEMP
SPLQ=1.0/DENS
HFLV=(828.0-83.0*(CONC-0.6)/0.2)*(1.0-0.0006*(TEMP-77.0))

```

```

C IF (TEMP.LT.158.0) THEN
  ATEMP=TEMP-68.0
  PH2O5=0.12+0.00544*ATEMP+1.50*(ATEMP**3.0)/(10.0**6.0)
  PH2O6=0.09+0.00262*ATEMP+1.52*(ATEMP**3.0)/(10.0**6.0)
  PH2O7=0.05+0.00269*ATEMP+0.73*(ATEMP**3.0)/(10.0**6.0)
  PH2O25=0.01+0.000650*ATEMP+0.22*(ATEMP**3.0)/(10.0**6.0)

```

```

PH2026=0.01+0.000792*ATEMP+0.30*(ATEMP**3.0)/(10.0**6.0)
PH2027=0.02+0.000646*ATEMP+0.41*(ATEMP**3.0)/(10.0**6.0)
PH2021=0.03+0.001213*ATEMP+0.60*(ATEMP**3.0)/(10.0**6.0)
ENDIF

```

C

```

IF (TEMP.GE.158.0.AND.TEMP.LT.230.0) THEN
ATEMP=TEMP-158.0
PH205=1.70+0.0333*ATEMP+0.000787*ATEMP*ATEMP
PH206=1.23+0.0236*ATEMP+0.000586*ATEMP*ATEMP
PH207=0.82+0.0156*ATEMP+0.000409*ATEMP*ATEMP
PH2025=0.23+0.00444*ATEMP+0.000177*ATEMP*ATEMP
PH2026=0.30+0.00611*ATEMP+0.000224*ATEMP*ATEMP
PH2027=0.38+0.00667*ATEMP+0.000285*ATEMP*ATEMP
PH2021=0.58+0.01080*ATEMP+0.000417*ATEMP*ATEMP
ENDIF

```

C

```

IF (TEMP.GE.230.0) THEN
ATEMP=TEMP-230.0
PH205=8.18+0.1396*ATEMP+0.001902*ATEMP*ATEMP
PH206=5.97+0.1036*ATEMP+0.001420*ATEMP*ATEMP
PH207=4.06+0.0711*ATEMP+0.000995*ATEMP*ATEMP
PH2025=1.47+0.0275*ATEMP+0.000540*ATEMP*ATEMP
PH2026=1.90+0.0353*ATEMP+0.000687*ATEMP*ATEMP
PH2027=2.34+0.0429*ATEMP+0.000837*ATEMP*ATEMP
PH2021=3.52+0.0661*ATEMP+0.001219*ATEMP*ATEMP
ENDIF

```

C

```

IF (CONC.GE.(0.815)) THEN
PSBS=PH2027+(PH2021-PH2027)*(CONC-0.815)/(0.185)
PSLV=PH207+(0.0-PH207)*(CONC-0.815)/(0.185)
ENDIF
IF (CONC.GE.(0.739).AND.CONC.LT.(0.815)) THEN
PSBS=PH2026+(PH2027-PH2026)*(CONC-0.739)/(0.076)
PSLV=PH206+(PH207-PH206)*(CONC-0.739)/(0.076)
ENDIF
IF (CONC.LT.(0.739)) THEN
PSBS=PH2025+(PH2026-PH2025)*(CONC-0.6537)/(0.0853)
PSLV=PH205+(PH206-PH205)*(CONC-0.6537)/(0.0853)
ENDIF
IF (PSBS.LT.0.0) PSBS=0.0
IF (PSLV.LT.0.0) PSLV=0.0

```

C

```

IF (PSLV.LT.(0.01).AND.PSBS.LT.(0.01)) THEN
VVAP=20000.0
ELSE
VVAP=0.95*(TEMP+459.0)/(144.0*(PSLV/85.8+PSBS/40.7))
ENDIF
GAMSBS=1.3
MLWSBS=38.0
ZSBS=0.95
TLMTMX=250.0
CNCMIN=0.654
CNCMAX=0.815

```

C

```

GO TO 999

```

C\*\*\*\*\*

```

999 RETURN
END

```

→



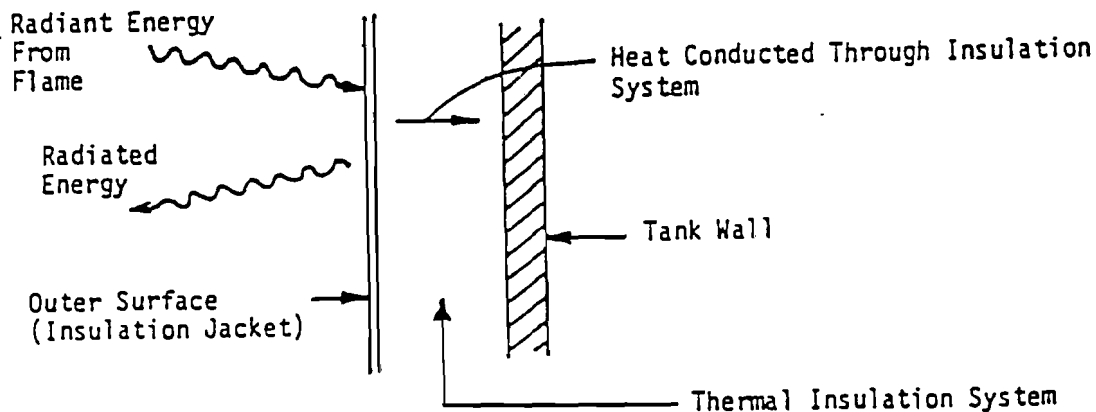
## APPENDIX J

### SUBROUTINE SURFACET

Subroutine SURFACET.FOR 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.

There are two parts to the subroutine. The first set of calculations deals with the case where there is functioning insulation between the outer surface (or jacket) and the tank wall. This calculational procedure is used for the bare, uninsulated tank case by considering the conductivity of the tank wall itself as providing the thermal resistance. The second set of calculations deals with the case where there is a jacket, but where the insulation between the jacket and tank wall has lost its effectiveness because it is not capable of functioning at high temperature. In this case the jacket acts as a thermal radiation barrier and heat is transferred from the jacket to the tank wall by radiation.

The heat balance for the first set of calculations is illustrated as follows:

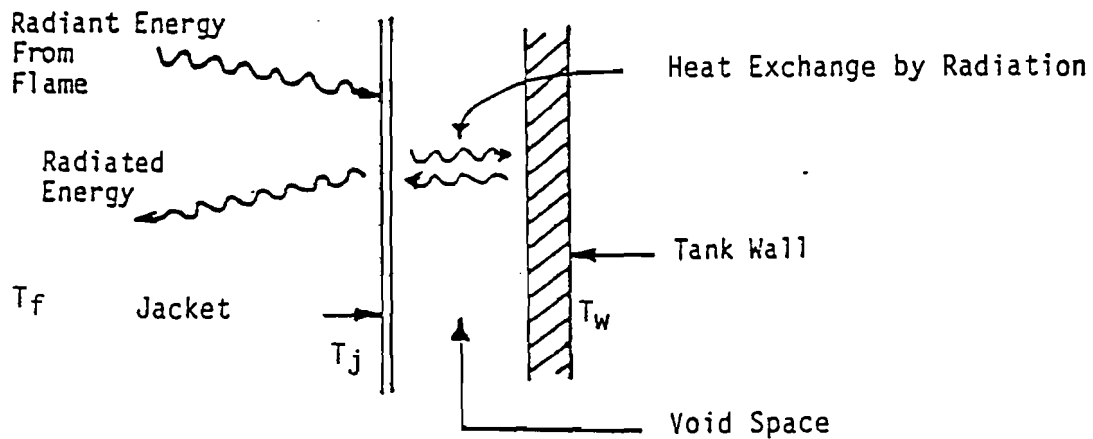


The following equation represents a heat balance at the outer surface of the insulation system.

$$0.48 [ T_f^4 \epsilon_r - T_s^4 \epsilon_r ] = [ T_s - T_t ] C_d / 3.6 \quad (18)$$

where:  $T_f$  is flame temperature ( $^{\circ}R/1000$ ),  
 $T_s$  is surface temperature ( $^{\circ}R/1000$ ),  
 $T_t$  is tank wall temperature ( $^{\circ}R/1000$ ),  
 $C$  is conductance of thermal shield (BTU/hr-ft<sup>2</sup>°F), and  
 $\epsilon_r$  is the emmissivity/absorptivity of the outer surface.

The heat balance for the second set of calculations illustrated as follows:



The following equation represents a heat balance at the jacket:

$$0.48 [ T_f^4 \epsilon_r ] - 0.48 [ T_j^4 \epsilon_r ] = [ \epsilon_r / ( 2 - \epsilon_r ) ] ( 0.48 ) ( T_j^4 - T_w^4 ) \quad (19)$$

where:  $T_j$  is the jacket temperature ( $^{\circ}R/1000$ ),  
and other variables have the same definition as in Equation 18.

The subroutine calculates an effective value for the conductance of heat flow into the tank, which is returned to the main program for heat flow calculations.

When calculating the heat flow to the tank, it is assumed that the effective conductance changes from an initial value at the beginning of the fire exposure to a final value which only considers the thermal resistance of the jacket. The transition takes place over a time period which is an input variable to the main program. This accounts for the deterioration of a non high-temperature insulation. The final value of conductance includes an allowance for the residue of the charred insulation which is assumed to have a conductance of 40 BTU/hr- ft<sup>2</sup>-°F).

The source code for this subroutine is presented on the following page.

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

TFLA is flame temperature (°R/1000),

TCAL is surface temperature (°R/1000),

TINS is tank wall temperature (°R/1000),

COND is conductance of thermal shield (BTU/hr- ft<sup>2</sup>-°F), and

ERAD is the emmissivity/absorptivity of outer surface.

```

SUBROUTINE SURFACET(TSURF,TINSD,ERAD,
1      COND,TFLA,INS,TIME,CINTV,FLFAC)
C
C      Determine the temperature of the outer surface of the
C      wall of the tank, TSURF, by an iterative
C      solution of the equation formed by taking a heat balance
C      at this point. Note, TINSD is inside wall temperature
C      at this location. TSURF is the outside surface
C      temperature which is calculated by the routine.
C.....Version 3.1, November 11, 1998
C
      REAL TSURF,TINSD,ERAD,COND,TFLA,TIME,CINTV,FLFAC
      INTEGER*2 INS
C
      IF (INS.NE.3.OR.INS.NE.6) TFLA1=TFLA
C.....Jacket with only annular air space.....
C      (original insulation destroyed by high temperature)
      IF (INS.EQ.3.OR.INS.EQ.6) TFLA1=(((2.0-ERAD)*FLFAC
1      *(TFLA**4)+(TINSD**4))/(3.0-ERAD)**0.25
C.....Iteration to Find Surface Temperature.....
50      CONTINUE
      TTEST=0.400
      IF (INS.NE.3.OR.INS.NE.6)
1      REFT=FLFAC*(TFLA1**4)*0.48*ERAD+TINSD*COND/3.6
      IF (INS.EQ.3.OR.INS.EQ.6)
1      REFT=(TFLA1**4)*0.48*ERAD/(2.0-ERAD)+TINSD*COND/3.6
      AFDW=0.100
35      TTEST=TTEST+AFDW
      IF (INS.NE.3.OR.INS.NE.6)
1      GNCT=(TTEST**4)*0.48*ERAD+TTEST*COND/3.6
      IF (INS.EQ.3.OR.INS.EQ.6)
1      GNCT=(TTEST**4)*0.48*ERAD/(2.0-ERAD)+TTEST*COND/3.6
      IF (ABS(REFT-GNCT).LT.0.0001)GO TO 39
      IF (GNCT.GT.REFT) THEN
          TTEST=TTEST-AFDW
          AFDW=AFDW/10.0
      ENDIF
      GO TO 35
39      CONTINUE
      TSURF=TTEST
C
100     CONTINUE
      RETURN
      END

```



## APPENDIX K

### SUBROUTINE AVFLOW

Subroutine AVFLOW.FOR is used to calculate the liquid flow through a safety relief valve. The liquid flow through the valve is calculated assuming homogenous 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:

$$V_1^2 - V_0^2 = 2g \int_0^1 dp/\rho \quad (20)$$

where:  $V_1$  is the flow velocity (ft/sec),  
 $V_0$  is the entry flow velocity at the valve (ft/sec),  
 $p$  is pressure (lbs/ft<sup>2</sup>),  
 $\rho$  is fluid density (lbs/ft<sup>3</sup>), and  
 $g$  is the gravitational constant (ft/sec<sup>2</sup>).

The integration is carried out along an isentropic path where an integration step equivalent to a ½ °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 or vent to determine the mass flow rate.

The entropies of products in the liquid and vapor states are 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 can be estimated from the following relationships:

$$SL_{t2} = SL_{t1} - CP (T_2 - T_1) / (T_2 + T_1) \quad (21)$$

$$SV_{t2} = SL_{t2} + 2 (HFLV_{t2}) / (T_2 + T_1) \quad (22)$$

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-°R),  
 $C_p$  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, and  
 $T_1$  and  $T_2$  are temperatures (°R).

Where there is no padding gas present, the velocity,  $V_0$ , at the entry to the valve would be assumed to be zero. However, when there is padding gas 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:

$$V_0 = \sqrt{2gp/\rho} \quad (23)$$

where:  $\rho$  is the density of the liquid product (lbs/ft<sup>3</sup>),  
 $p$  is the padding gas pressure (lbs/ft<sup>2</sup>), and  
 $g$  is the gravitational constant (ft/sec<sup>2</sup>).

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

```

C.....THIS SUBROUTINE IS USED FOR THE ANALYSIS OF TWO-PHASE
C.....FLOW THROUGH A TANK CAR SAFETY VALVE OR VENT.....
SUBROUTINE AVFLOW(TTNK,WOUT,ATEM,DELT,CDLQ,PNIT,
1      CONC,IPR,IPFST,ISBSL,IPTYP,TIME)
C.....Version 3.0, October 20, 1997
C      This subroutine is used to calculate the liquid mass flow
C      rate through a safety relief valve. Homogeneous isentropic
C      flow is assumed. The presense of a nitrogen pad pressure
C      is also taken into account.
C
REAL WOUT,TTNK,ATEM,DELT,CDLQ,PNIT,CONC,TIME
INTEGER*2 IPR,ISBSL,IPTYP,IPFST
COMMON/PROP1/SPEC,SPLQ,HFLV,PSBS,PSLV,ZSBS,ZSLV,VVAP
C
DEGF=1000.0*TTNK-460.0
TBEG=DEGF
KCNT=0
C
GO TO 896      ! get initial value of entropy
C
Start with initial conditions; drop temperature by 1/2 degree
C      and calculate the cross sectional valve area for a one
C      lb per sec mass flow rate.
C
898  KCNT=1
SSTND=SLIQ
VLONE=0.0
ARONE=1000.0
HTEST=0.0
C
PTEST=PSBS+PSLV
PTOT=PSBS+PSLV+PNIT
IF (PTOT.LE.(14.7)) THEN
WOUT=0.0
GO TO 823
ENDIF
IF (PTEST.LE.(14.7)) THEN
PDRV=PTOT-14.7
ELSE
PDRV=PNIT
ENDIF
C
IF (PDRV.LT.(0.001)) THEN
VLONE=0.0
ELSE
VLONE=96.24*SQRT(SPLQ*PDRV)
ARONE=SPLQ/VLONE
ENDIF
C
ATEST=ARONE
895  CONTINUE
DEGF=DEGF-0.5
C
896  CONTINUE
C
IF (IPTYP.EQ.1) THEN
IF (IPR.GE.1.AND.IPR.LE.9) CALL FPRPSBS (IPR,DEGF)
IF (IPR.GE.10.AND.IPR.LE.16) CALL FPRPSLV (IPR,CONC,DEGF)
ENDIF
IF (IPTYP.EQ.2.OR.IPTYP.EQ.3) THEN

```

```

        IF (ISBSL.EQ.1) CALL SBSPROP (IPFST,IPR,DEGF)
        IF (ISBSL.EQ.2) CALL SLNPROP (IPFST,IPR,CONC,DEGF)
    ENDIF
C
C.....Entropies of commodities.....
    IF (KCNT.EQ.0) THEN
        SLIQ=1.000
        DGLST=TBEG
        GO TO 898
    ENDIF
C
    SLIQ=SLIQ+SPEC*(DEGF-DGLST)/((DGLST+DEGF)*0.5+459.6)
    SVAP=SLIQ+HFLV/(DEGF+459.6)
    DGLST=DEGF
C.....
    PREF=PSBS+PSLV
    IF (PREF.LE.(14.7)) GO TO 821
C
    X=(SSTND-SVAP)/(SLIQ-SVAP)
    VLTST=X*SPLQ+(1.0-X)*VVAP
    HTEST=HTEST+(PTEST-PREF)*144.0*VLTST*64.4
C
    VELOCB=SQRT(VLONE**2+HTEST)
    ARTWO=VLTST/VELOCB
    PTEST=PREF
C
    IF (ARTWO.LT.ATEST) THEN
        ATEST=ARTWO
        GO TO 895
    ENDIF
C
C    Repeat calculations until area becomes minimum; then calculate
C    mass flow rate.
C
821    CONTINUE
    WOUT=60.0*DELT*CDLQ*ATEM/ATEST
823    CONTINUE
C
    RETURN
    END

```

## APPENDIX L

### SUBROUTINE TSHIELD

Subroutine TSHIELD.FOR is used to determine the effective conductance of a 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.

$$K = A_1 + A_2T + A_3T^2 \quad (24)$$

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

The subroutine requires as input the thickness of the insulation under consideration (THIC), in inches, the outer and inner temperature of the insulation system (TOTSD and TINSO, 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 close to TOTSD a new value for the heat flux is assumed and the calculation is repeated. When a sufficiently close value to TOTSD 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 listed as follows:

TOTSD	Temperature of outside of insulation system ( $^{\circ}\text{R}/1000$ ),
CNDCT	Effective conductance of insulation system ( $\text{BTU}/\text{hr}\text{-ft}^2$ ),
THIC	Thickness of insulation system (ins.),
CKND	Conductivity of thermal insulation material ( $\text{BTU}/\text{hr}\text{-ft}^2/(\text{^{\circ}\text{F}}/\text{ft})$ ), and
QFLX	Heat flux through insulation system ( $\text{BTU}/\text{hr}\text{-ft}^2$ ).

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

```

SUBROUTINE TSHIELD (TOTSD, TINS, CN, TH, A1, A2, A3, CDAUX)
C
C   This subroutine calculates the effective conductance of a
C   given thickness of insulation where the conductivity of
C   the material is a quadratic function of temperature and the
C   inner and outer temperatures of the insulation are known.
C   Start with estimate of heat flux from last time step.
C.....Version 3.0, October 20, 1997
C
REAL TOTSD, TINS, CN, TH, A1, A2, A3, CDAUX
C
QFLX=CN*(TOTSD-TINS)*1000.0
KQT=0 ! check for first pass through calculation
TFINS=TINS*1000.0-460.0 ! convert to deg F
TFOTS=TOTSD*1000.0-460.0 ! convert to deg F
TFLAS=TFOTS
DELX=TH/(12.0*50.0) ! Divide insulation into 50
! layers and convert to feet.
C....With the assumed heat flux, start with inside wall temperature
C and determine temperature of outside wall.
100 CONTINUE
TFEMP=TFINS+QFLX/CDAUX
DO I=1,50
TTEMP=TFEMP/1000.0
CKND=A1+A2*TTEMP+A3*TTEMP*TTEMP
TFEMP=TFEMP+QFLX*DELX/CKND
ENDDO
C
C....Compare TFEMP with TFOTS, if too far off modify heat flux
C and recalculate.
C
IF (ABS (TFEMP-TFOTS) .LT. (0.1)) GO TO 103
C
C....Calculate new QFLX on first pass through calculation....
C
IF (KQT.EQ.0) THEN
QDEL=ABS (QFLX* (TFEMP-TFOTS) /TFEMP)
IF (TFEMP.GT.TFOTS) QFLX=QFLX-QDEL
IF (TFEMP.LT.TFOTS) QFLX=QFLX+QDEL
TFLAS=TFEMP
KQT=1
GO TO 100
ENDIF
C
C.....Calculate new QFLX on subsequent passes through calculation.
C
IF (TFLAS.LT.TFOTS.AND.TFEMP.GT.TFOTS) QDEL=QDEL/3.0
IF (TFLAS.GT.TFOTS.AND.TFEMP.LT.TFOTS) QDEL=QDEL/3.0
IF (TFEMP.GT.TFOTS) QFLX=QFLX-QDEL

```

```
IF (TFTEMP.LT.TFOTSD) QFLX=QFLX+QDELTA  
TFLAST=TFTEMP  
GO TO 100
```

C

C.....Last step; new calculate effective conductance.

C

```
103 CONTINUE  
CNDCT=QFLX/((TOTSD-TINSD)*1000.0)  
RETURN  
END
```

→



