AFFTAC

Analysis of Fire Effects
on Tank Cars

Users Manual

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For: The RSI-AAR Railroad Tank Car Safety Research & Test Project

February 10, 2008

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Introduction

Overview

The AFFTAC computer program, originally developed by Dr. Milton Johnson at IITRI circa 1984 under funding from the FRA, predicts the effects of fire on railroad tank cars. Specifically, it makes a prediction of whether the tank fails, computes the time to failure if relevant, computes the amount of product remaining in the tank at failure, and the maximum pressure in the tank as well as the time to reach that pressure. In the years following its initial development, AFFTAC was expanded to provide more information and handle more types of vents, as well as be more accessible to users. Eventually in 1992, it was ported to the PC.

Beginning in 2000, AFFTAC entered a new phase of development with Scott Runnels as its custodian. The first task undertaken in this new phase was the development of a graphical user interface (GUI) to assist the user in managing data and analysis. An overview of how the AFFTAC software package components interact is shown in Figure 1.1. The user interacts with the GUI, which writes an ASCII computational file that the computational module reads. The GUI manages the execution of the computational module and the displaying of the results from the computations. User interaction is eased through the use of databases that store different aspects of the analysis as named datasets. For example, a user can create a thermal protection system, give it a name, store it in the "Insulations" database, and then apply the system to multiple analyses, which are stored in the "Analysis" database.

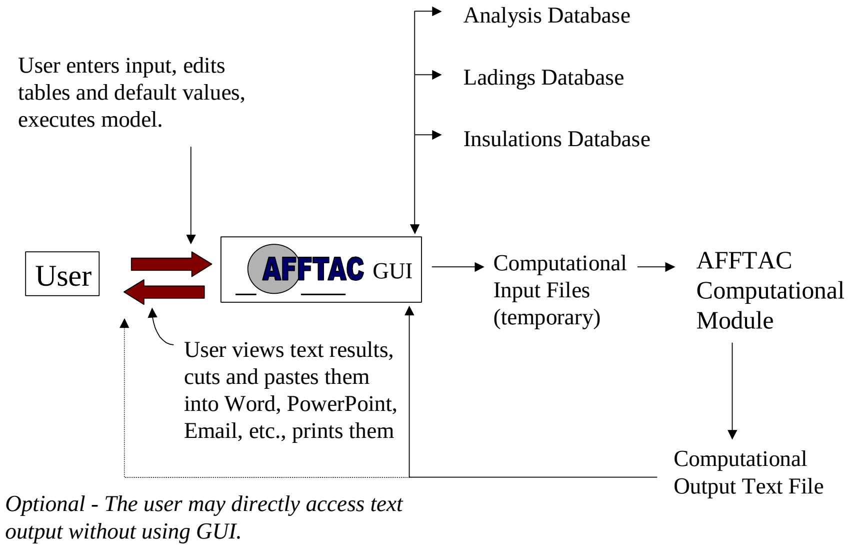


Figure 1.1: Overview of AFFTAC operations.

Essential Elements of Running AFFTAC

The operation of AFFTAC revolves around the management of the analyses. Shown in Figure 1.2 is the AFFTAC Main Window, which displays the database of previous analyses. After selecting an analysis, you may click one of the other two tabs and immediately see the results of that simulation; **AFFTAC Input Summary** displays the input file that is echoed by the computational module and **AFFTAC Output** displays the output file generated by the computational module. Also, as seen in Figure 1.2, you may edit the analysis, copy it to create a new one, delete it, or create a completely new simulation from scratch.

Editing or Creating New Simulations

The process of editing or creating a simulation is divided into four steps which are conducted using four sequential windows: **Analysis Conditions**, **Tank Car Properties**, **Insulation Choices**, and **Lading Properties**. These four windows are shown in Figure 1.3 and are described in more detail in the next chapter. Here an overview is provided.

Analysis Conditions Window

In this window, you may set basic analysis conditions, including the flame type and the length of the simulation. From this window you can also set the frequency of printouts.

Tank Car Properties Window

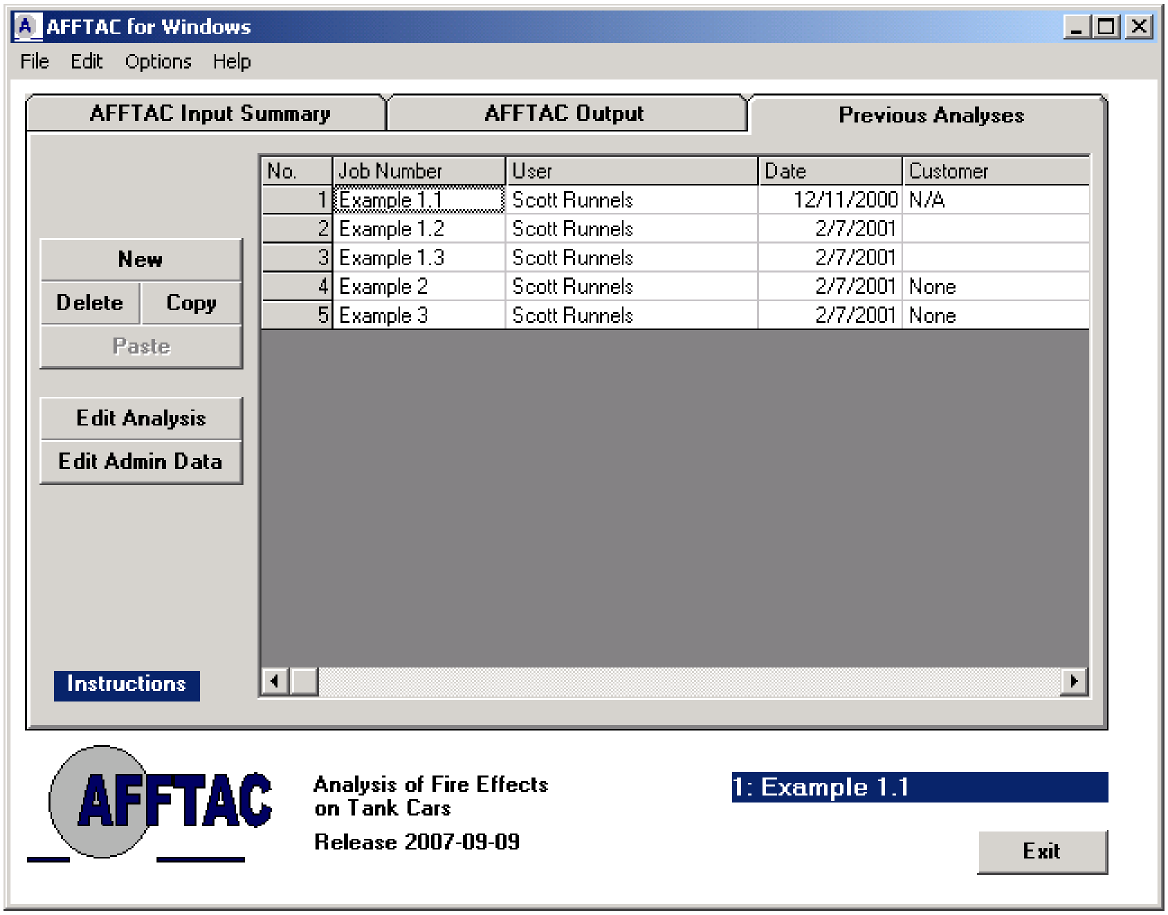
In this window, you set up the properties of the tank car, including the material from which the tank is made and the safety relief device properties.

Insulation Choices Window

In this window, you choose the type of thermal protection system on the tank car by selecting one of the systems that is displayed in a list that represents the database of insulation types. The thermal protection system database may be edited to create new types of systems by clicking on the **Manage Insulation Database** button.

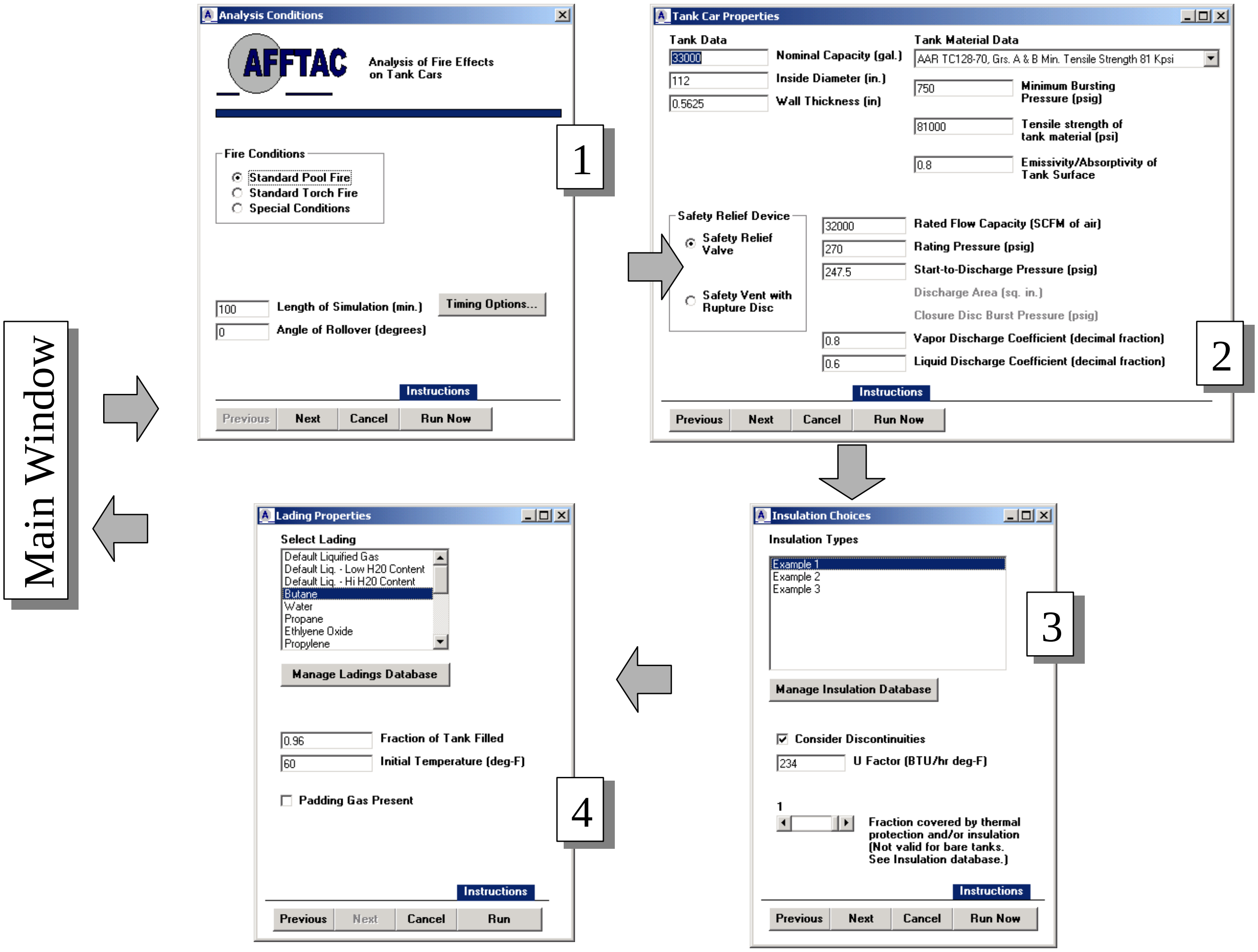
Ladings Properties Window

In this window, you select the lading from a list of ladings stored in the ladings database. You may edit this database to create new ladings by clicking the **Manage Ladings Database** button. Also in the window, you specify the fraction of tank filled by the lading and the initial temperature.



No.	Job Number	User	Date	Customer
1	Example 1.1	Scott Runnels	12/11/2000	N/A
2	Example 1.2	Scott Runnels	2/7/2001	
3	Example 1.3	Scott Runnels	2/7/2001	
4	Example 2	Scott Runnels	2/7/2001	None
5	Example 3	Scott Runnels	2/7/2001	None

Figure 1.2: AFFTAC's Main Window.



Analysis Conditions

Fire Conditions
● Standard Pool Fire
○ Standard Torch Fire
○ Special Conditions

100 Length of Simulation (min.)
0 Angle of Rollover (degrees)

Tank Car Properties

Tank Data
33000 Nominal Capacity (gal.)
112 Inside Diameter (in.)
0.5625 Wall Thickness (in)

Tank Material Data
AAR TC128-70, Grs. A & B Min. Tensile Strength 81 Kpsi
750 Minimum Bursting Pressure (psig)
81000 Tensile strength of tank material (psi)
0.8 Emissivity/Absorptivity of Tank Surface

Safety Relief Device
● Safety Relief Valve
○ Safety Vent with Rupture Disc

32000 Rated Flow Capacity (SCFM of air)
270 Rating Pressure (psig)
247.5 Start-to-Discharge Pressure (psig)
Discharge Area (sq. in.)
Closure Disc Burst Pressure (psig)
0.8 Vapor Discharge Coefficient (decimal fraction)
0.6 Liquid Discharge Coefficient (decimal fraction)

Insulation Choices

Insulation Types
Example 1 (selected)
Example 2
Example 3

☑ Consider Discontinuities
234 U Factor (BTU/hr deg-F)
1 Fraction covered by thermal protection and/or insulation (Not valid for bare tanks. See Insulation database.)

Lading Properties

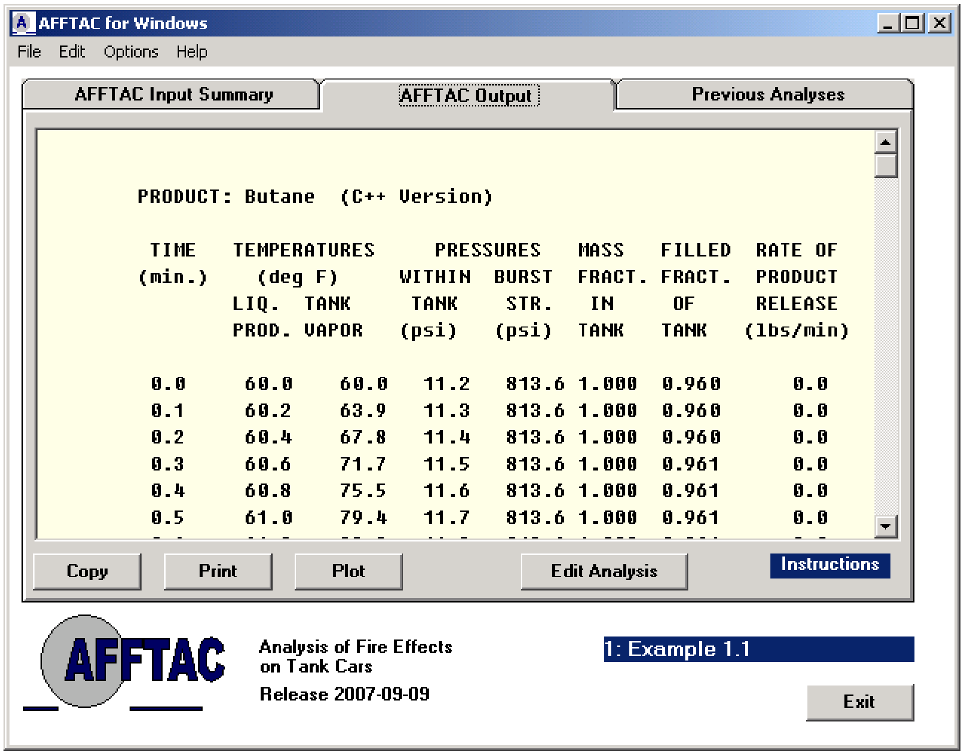
Select Lading
Default Liquified Gas
Default Liq. - Low H20 Content
Default Liq. - Hi H20 Content
Butane
Water
Propane
Ethlyene Oxide
Propylene

0.96 Fraction of Tank Filled
60 Initial Temperature (deg-F)
☐ Padding Gas Present

Figure 1.3: Illustration of the four-step editing process for creating new or changing existing AFFTAC simulations.

Viewing and Using Results

You do not have to go through all four editing windows shown in Figure 1.3 every time. At any time during the four-step process described above, you may choose to run the simulation. When you do, you will be returned to the Main Window's **View AFFTAC Output** tab, which displays the AFFTAC output file, as shown in Figure 1.4. You may also switch to the **AFFTAC Input Summary** tab to verify the inputs that you entered. The results of previously developed analyses, which are stored in the database, may be viewed at any time as well. To do so, switch to the **Previous Analysis** tab (in the Main Window), highlight the analysis of interest, and then switch back to either the **AFFTAC Output** or **AFFTAC Input Summary Tab.**



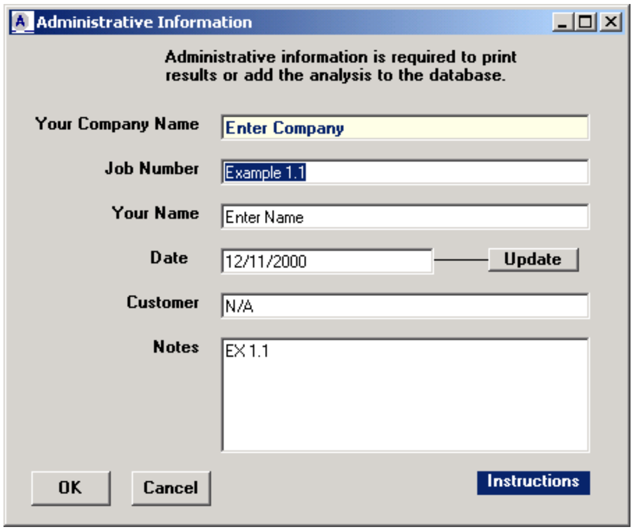
```
PRODUCT: Butane  (C++ Version)

 TIME   TEMPERATURES     PRESSURES    MASS   FILLED  RATE OF
(min.)    (deg F)     WITHIN  BURST  FRACT. FRACT.  PRODUCT
        LIQ.  TANK     TANK   STR.    IN     OF     RELEASE
        PROD. VAPOR   (psi)  (psi)   TANK   TANK   (lbs/min)

 0.0     60.0    60.0    11.2    813.6 1.000  0.960      0.0
 0.1     60.2    63.9    11.3    813.6 1.000  0.960      0.0
 0.2     60.4    67.8    11.4    813.6 1.000  0.960      0.0
 0.3     60.6    71.7    11.5    813.6 1.000  0.961      0.0
 0.4     60.8    75.5    11.6    813.6 1.000  0.961      0.0
 0.5     61.0    79.4    11.7    813.6 1.000  0.961      0.0
```

Figure 1.4: AFFTAC's Main Window, displaying the results of an analysis.

To print results or an input summary, you may click the **Print** button under the respective tabs. Also, you may copy the contents to the Microsoft clipboard by clicking the **Copy** button. These contents may then be pasted into a variety of Microsoft Windows applications such as Word or PowerPoint.

Administrative Information

Administrative information is required in order to print the results of an analysis or to save it in the database. To add the administrative information, highlight the analysis and click the **Edit Admin Data** button in the Main Window. The window used for entering that



Administrative information is required to print results or add the analysis to the database.

Your Company Name: Enter Company
Job Number: Example 1.1
Your Name: Enter Name
Date: 12/11/2000
Customer: N/A
Notes: EX 1.1

Figure 1.5: Administrative Information window that must be completed for a simulation to be printed or added to the analysis database.

administrative information is shown in Figure 1.5. Your name and company name are set by selecting the menu option **Options-User** in the Main Window. The rest of the user-specific information you add in the window shown in Figure 1.5.

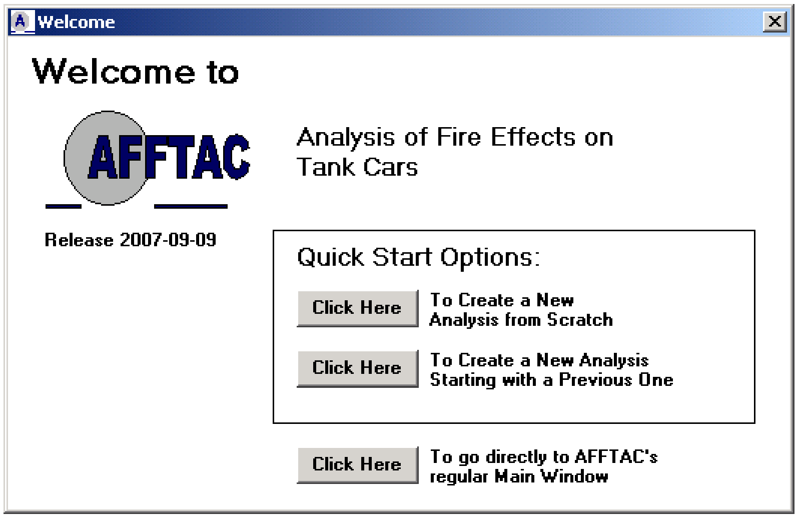
The Quick Start Procedure

It is anticipated that many AFFTAC users will prefer to move quickly through the analysis setup steps, then view and print the results, without necessarily using the other database-driven features of AFFTAC. Because of that, AFFTAC starts up by displaying the Welcome window, shown in Figure 1.6. From this window, the user may choose to move directly through the simulation setup, using a previous analysis or default values as a start.

The Quick Start mode executes only when AFFTAC starts up. After that, new analyses can be created by using the **New** button or the **Copy** then **Paste** buttons under the **Previous Analysis** tab in the Main Window.

Installation and System Requirements

AFFTAC for Windows can be run on a personal computer with a 486 or later processor, at least 8 Mb of RAM, and at least 2 Mb of free disk space. The installation package consists of three files. To install AFFTAC, run the one named **setup** and follow the instructions on the screen.


Welcome

Welcome to

AFFTAC

Analysis of Fire Effects on
Tank Cars

Release 2007-09-09

Quick Start Options:

Figure 1.6: The Welcome window, which is displayed when AFFTAC starts up.

Technical Assistance

The AFFTAC graphical user interface was developed in Microsoft Visual Basic, version 6.0, Visual Studio Service Pack 4. The computational module was compiled under Compaq Visual Fortran 6. Assistance can be obtained from:

Scott Runnels
Scott Runnels Consulting
630 Camino Encantado
Los Alamos, NM 87544
505-695-9241
SRunnels@srconsult.com
www.srconsult.com

Acknowledgements

The original development of AFFTAC for windows and the associated databases was funded by the RPI-AAR Railroad Tank Car Safety Research & Test Project and was performed under Southwest Research Institute project number 18-6965. Development past 2000 was continued by Scott Runnels Consulting.

Special thanks go to Tom Dalrymple for his advice during the designing of the graphical user interface and databases, and the overall project management during 2000-2002.

Thanks also to those who tested the earlier versions, including Bill Bitting, Al Henzi, Thomas Petrunich, and Andy Rohrich.

The late Dr. Milton Johnson’s contributions to the earlier versions of this manual, especially in explaining the models represented in the AFFTAC computational module is gratefully acknowledged. Much of his contributions remain in this revision, in particular the “Aside” comments and Appendix A. Likewise, Mr. Joe Cardinal also provided helpful input on earlier versions of this manual, much of which remains in tact with this revision.

Managing the Databases

AFFTAC comes with three database files to increase the speed and effectiveness of the input process. Each of them are described in detail in this chapter.

Analysis Database

AFFTAC's analysis database allows you to store analyses for later retrieval and use. As mentioned in the previous chapter, the analysis database is central to AFFTAC. Therefore, it is displayed in AFFTAC's Main Window, under the **Analysis Database** tab. To create a new analysis from scratch using the default values, click on the **New** button. To create a new analysis that is based on an existing one, highlight the analysis, click **Copy** and then click **Paste**. When you do, a new analysis will be created that is identical to the one you copied. Then, you may edit that analysis by highlighting it and clicking **Edit**.

Insulation Database

Insulation types may be described, named, and saved in the insulation database. Then when setting up an analysis, the insulation is selected by name. The insulation database may be edited by choosing the **Edit-Insulation Data** menu option in the Main Window, or by clicking the **Manage Insulation Database** button in the Insulation Choices window, which is displayed during the creation or editing of an analysis.

When you choose to manage the insulation database, the window shown in Figure 2.1 is displayed. In this window, insulation types can be edited by double clicking them, or by highlighting them and clicking the **Edit** button. New insulation types can be created by either highlighting an existing one and clicking **Copy** then **Paste**, which creates a copy of the highlighted insulation, or by clicking **New**, which creates a new insulation using default values.

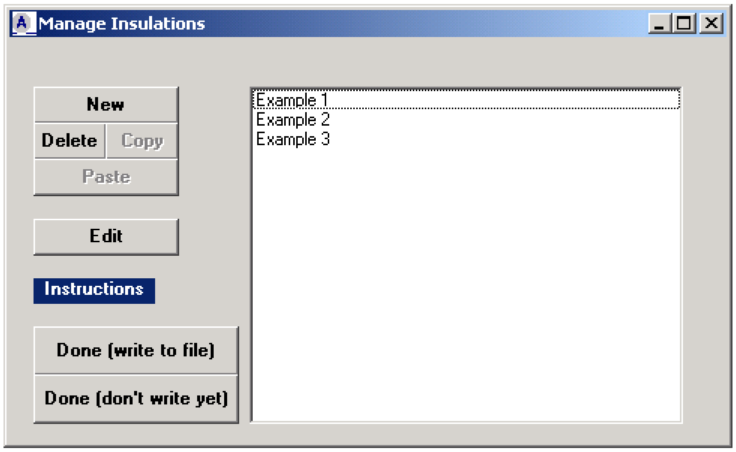


Figure 2.1: The Manage Insulations window.

When you double-click an insulation type or highlight it and then click the **Edit** button, the Thermal Protection System window appears, like that shown in Figure 2.2. This multi-faceted window provides opportunities to create six different insulation types. Its appearance changes depending upon which type of insulation is chosen. Note that there are two ways to exit the Manage Insulations window. One way saves the changes made in the window described below to the database file. The other keeps the changes for use in the current session but does not yet save the changes to the database file. This option is important because sometimes it is helpful to try a modification to an existing thermal protection system without committing to it. If you choose not to write the changes to the file, AFFTAC will ask you again when you try to exit.

And now, described below are the various insulation types in the Thermal Protection Window (refer again to Figure 2.2).

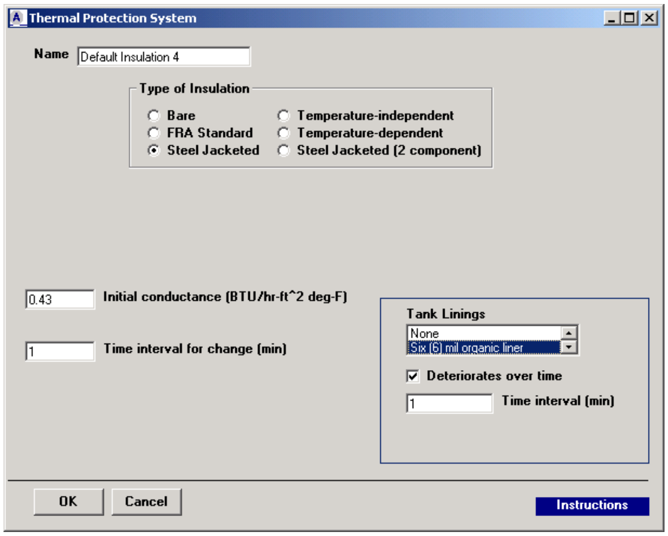
Bare

The Bare option simply means that there is no thermal protection system.

FRA Standard

This insulation system assumes an overall conductance of 4.0 BTU/hr-ft^2-deg-F, which is the maximum conductance that will pass the FRA performance test specified in Appendix B to CFR 179. Insulation systems that pass the test would likely have conductances that are less than this value.

Steel Jacketed


Thermal Protection System

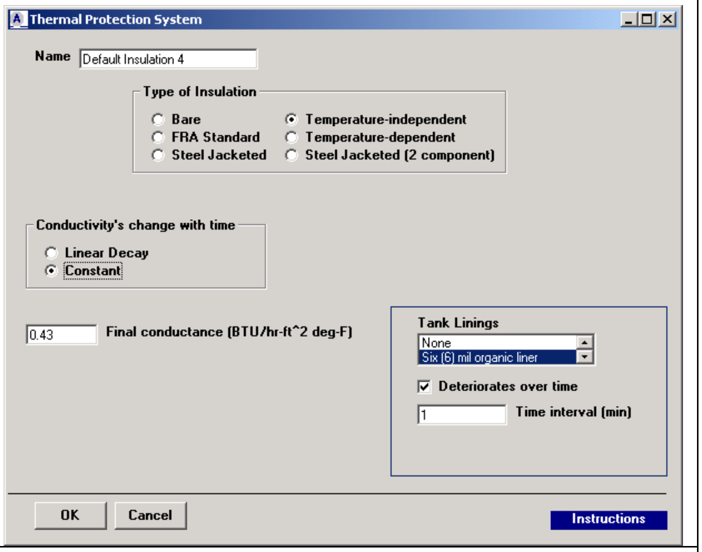
Name: Default Insulation 4

Type of Insulation
○ Bare ○ Temperature-independent
○ FRA Standard ○ Temperature-dependent
● Steel Jacketed ○ Steel Jacketed (2 component)

0.43 Initial conductance (BTU/hr-ft^2 deg-F)
1 Time interval for change (min)

Tank Linings
None
Six (6) mil organic liner
☑ Deteriorates over time
1 Time interval (min)

Temperature-Independent


Thermal Protection System

Name: Default Insulation 4

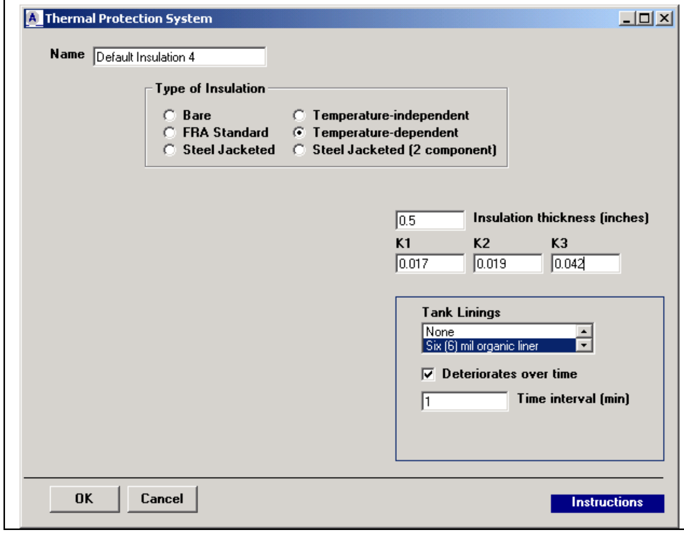
Type of Insulation
○ Bare ● Temperature-independent
○ FRA Standard ○ Temperature-dependent
○ Steel Jacketed ○ Steel Jacketed (2 component)

Conductivity's change with time
○ Linear Decay
● Constant

0.43 Final conductance (BTU/hr-ft^2 deg-F)

Tank Linings
None
Six (6) mil organic liner
☑ Deteriorates over time
1 Time interval (min)

Temperature-Dependent


Thermal Protection System

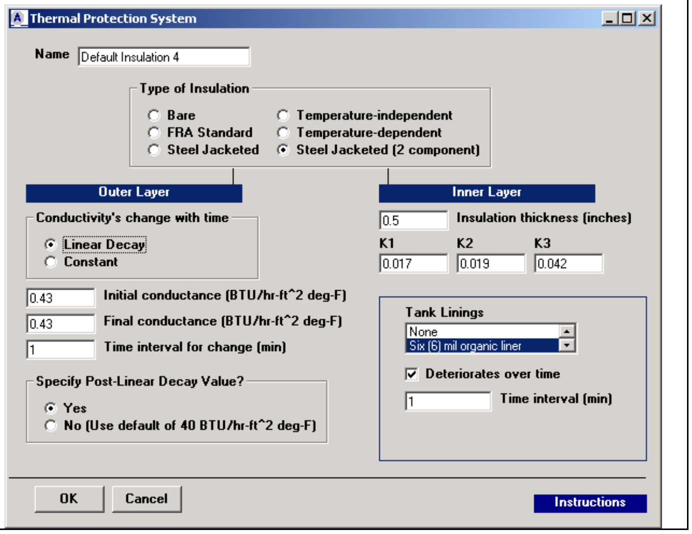
Name: Default Insulation 4

Type of Insulation
○ Bare ○ Temperature-independent
○ FRA Standard ● Temperature-dependent
○ Steel Jacketed ○ Steel Jacketed (2 component)

0.5 Insulation thickness (inches)
K1: 0.017
K2: 0.019
K3: 0.042

Tank Linings
None
Six (6) mil organic liner
☑ Deteriorates over time
1 Time interval (min)

Steel Jacketed (2 component)


Thermal Protection System

Name: Default Insulation 4

Type of Insulation
○ Bare ○ Temperature-independent
○ FRA Standard ○ Temperature-dependent
○ Steel Jacketed ● Steel Jacketed (2 component)

Outer Layer

Conductivity's change with time
● Linear Decay
○ Constant

0.43 Initial conductance (BTU/hr-ft^2 deg-F)
0.43 Final conductance (BTU/hr-ft^2 deg-F)
1 Time interval for change (min)

Specify Post-Linear Decay Value?
● Yes
○ No (Use default of 40 BTU/hr-ft^2 deg-F)

Inner Layer

0.5 Insulation thickness (inches)
K1: 0.017
K2: 0.019
K3: 0.042

Tank Linings
None
Six (6) mil organic liner
☑ Deteriorates over time
1 Time interval (min)

Figure 2.2 The four types of insulations that require user input.

Temperature-Independent Insulation

This type of insulation is constant with temperature but is allowed to change with time. Two alternatives are offered, one where the conductance of the system is constant and the other where the conductance changes linearly over a given time period from an initial value to a steady-state value.

Temperature-Dependent Insulation

If this option is chosen, you may enter three coefficients that are used in the following equation to describe how the thermal conductivity of the tank wall varies as a function of temperature.

$$k = k_1 + k_2T + k_3T^2 \tag{2.1}$$

Note that conductivity typically has units of $\frac{BTU}{hr-ft^2-\deg F/ft}$. When conductivity is computed using the temperature-dependent form, temperature is in thousands of deg *F* and length is in feet. So the units of conductivity are, in the code,

$\frac{BTU}{hr-ft^2-\text{thousands of deg}\,F/ft}$. The k_1 parameter has those units while the other two parameters have units that accommodate the temperature function that multiplies them. In summary:

Parameter	**Units**
k_1	$\frac{BTU}{hr-ft^2-\text{thousands of deg}\,F/ft}$
k_2	$\frac{BTU}{hr-ft^2-(\text{thousands of deg}\,F)^2/ft}$
k_3	$\frac{BTU}{hr-ft^2-(\text{thousands of deg}\,F)^3/ft}$

Steel Jacketed (2 component) Insulation

As the name implies, this insulation option has two layers. For the inner layer, you may enter an initial and final thermal conductivity value and a time interval over which AFFTAC will interpolate between those values (just as in the temperature-independent option described above). For the outer layer, you may specify its thickness and also make its conductivity a function of temperature.

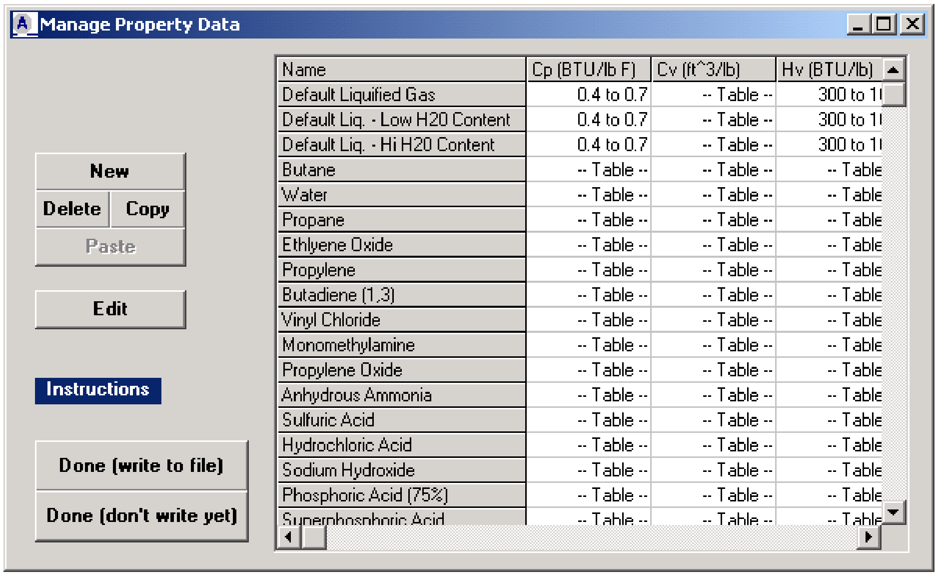
Ladings Database

Ladings may be described, named, and saved in the ladings database. Then when setting up an analysis, the lading is selected by name. The ladings database may be edited by choosing the **Edit-Lading Data** menu option in the Main Window, or by clicking the **Manage Ladings Database** button in the Ladings Properties window, which is displayed during the editing of an analysis.

When you choose to manage the ladings database, a window like that shown in Figure 2.3 is displayed. In this window, ladings can be edited by double clicking them, or by highlighting them and clicking the **Edit** button. New ladings can be created by either highlighting an existing one and clicking **Copy** then **Paste**, which creates a copy of the highlighted lading, or by clicking **New**, which creates a new lading from scratch. As with the thermal protection system database window, you can exit the window with or without saving your changes to the database file. If you choose not to save them to the file, they will still be available for the current AFFTAC session and AFFTAC will ask you if you want to save them when you try to exit.

Using Default Ladings

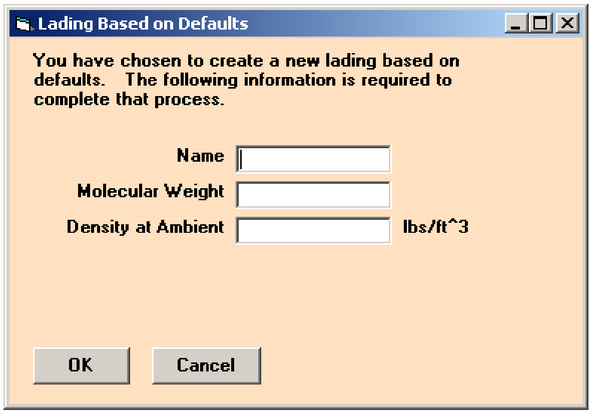
The first entries in the database are default ladings. These cannot be used for an analysis but instead serve as a template from which new ladings can be created when not all of the thermodynamic properties are known. The process for creating a new lading from a default lading is similar to creating one from any other existing lading. Simply highlight the default lading of interest, click **Copy** and then click **Paste**. However, when pasting from a default lading, the dialog box shown in Figure 2.4 appears. This window asks for the name of the new lading, the molecular weight, and the density at ambient. These values are required. The creation of the new lading cannot proceed without them.



Name	Cp (BTU/lb F)	Cv (ft^3/lb)	Hv (BTU/lb)
Default Liquified Gas	0.4 to 0.7	-- Table --	300 to 1
Default Liq. - Low H20 Content	0.4 to 0.7	-- Table --	300 to 1
Default Liq. - Hi H20 Content	0.4 to 0.7	-- Table --	300 to 1
Butane	-- Table --	-- Table --	-- Table
Water	-- Table --	-- Table --	-- Table
Propane	-- Table --	-- Table --	-- Table
Ethlyene Oxide	-- Table --	-- Table --	-- Table
Propylene	-- Table --	-- Table --	-- Table
Butadiene (1,3)	-- Table --	-- Table --	-- Table
Vinyl Chloride	-- Table --	-- Table --	-- Table
Monomethylamine	-- Table --	-- Table --	-- Table
Propylene Oxide	-- Table --	-- Table --	-- Table
Anhydrous Ammonia	-- Table --	-- Table --	-- Table
Sulfuric Acid	-- Table --	-- Table --	-- Table
Hydrochloric Acid	-- Table --	-- Table --	-- Table
Sodium Hydroxide	-- Table --	-- Table --	-- Table
Phosphoric Acid (75%)	-- Table --	-- Table --	-- Table
Superphosphoric Acid	-- Table --	-- Table --	-- Table

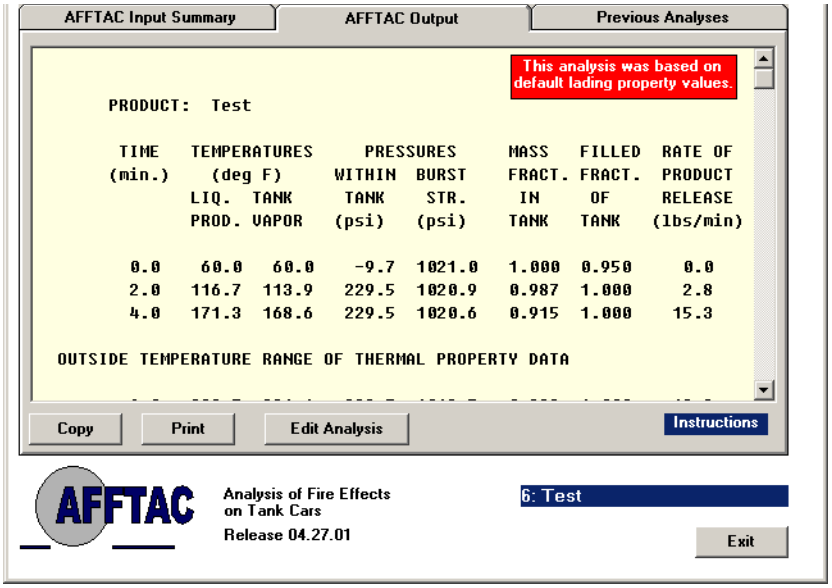
Figure 2.3: The window used for managing the ladings database.

The use of default ladings is not recommended. If they are used, you should understand how their thermodynamic properties were chosen, as described in Appendix A. If you run an analysis using a lading that has been created from a default lading, AFFTAC will remind you when the results are displayed or printed. For example, shown in Figure 2.5 is the Main Window's **AFFTAC Output** tab with the reminder message shown.



You have chosen to create a new lading based on defaults. The following information is required to complete that process.

Figure 2.4: Dialogue box asking for additional information when creating a new lading from a default template.



This analysis was based on default lading property values.

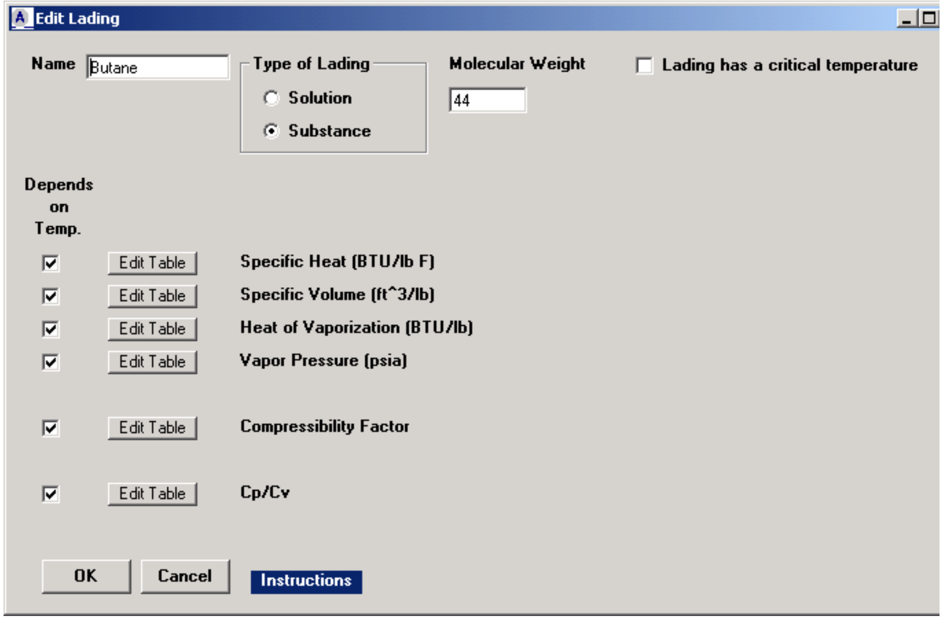
```
     PRODUCT:  Test

      TIME   TEMPERATURES     PRESSURES     MASS   FILLED  RATE OF
     (min.)    (deg F)     WITHIN  BURST   FRACT. FRACT.  PRODUCT
             LIQ.  TANK     TANK    STR.     IN     OF    RELEASE
             PROD. VAPOR   (psi)   (psi)    TANK   TANK  (lbs/min)

       0.0    60.0   60.0    -9.7  1021.0   1.000  0.950     0.0
       2.0   116.7  113.9   229.5  1020.9   0.987  1.000     2.8
       4.0   171.3  168.6   229.5  1020.6   0.915  1.000    15.3

 OUTSIDE TEMPERATURE RANGE OF THERMAL PROPERTY DATA
```

6: Test

Figure 2.5: AFFTAC results displayed with the reminder that the results were obtained using a lading created from one of the default lading templates.

Editing Ladings

When you double-click a lading or highlight it and then click the **Edit** button, the Edit Lading window like those shown in Figure 2.6 appears. This multi-faceted window allows for the input of the thermal properties of the lading.



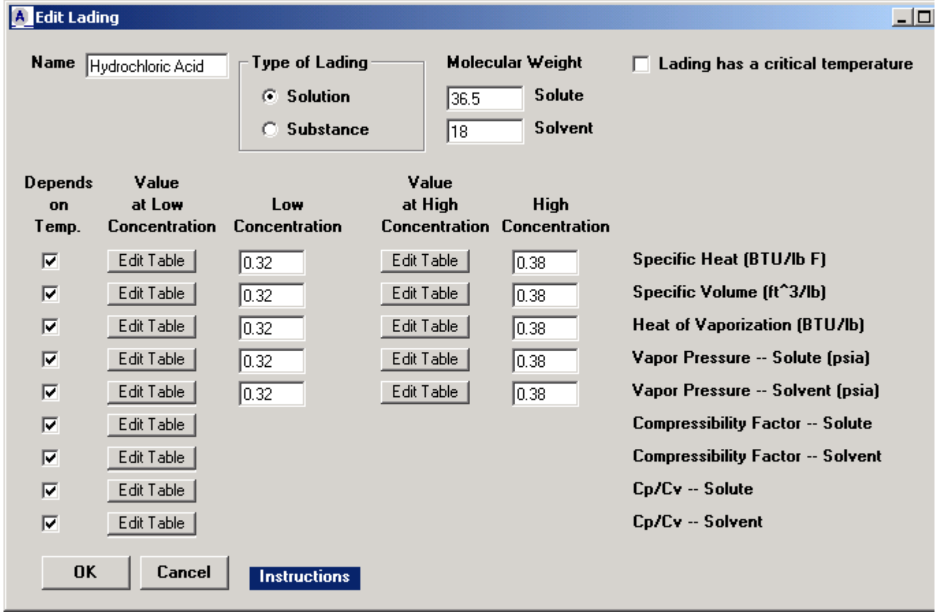
Name: Butane

Type of Lading: ○ Solution ● Substance

Molecular Weight: 44

☐ Lading has a critical temperature

Depends on Temp.		
☑	Edit Table	Specific Heat (BTU/lb F)
☑	Edit Table	Specific Volume (ft^3/lb)
☑	Edit Table	Heat of Vaporization (BTU/lb)
☑	Edit Table	Vapor Pressure (psia)
☑	Edit Table	Compressibility Factor
☑	Edit Table	Cp/Cv



Name: Hydrochloric Acid

Type of Lading: ● Solution ○ Substance

Molecular Weight: 36.5 Solute; 18 Solvent

☐ Lading has a critical temperature

Depends on Temp.	Value at Low Concentration	Low Concentration	Value at High Concentration	High Concentration	
☑	Edit Table	0.32	Edit Table	0.38	Specific Heat (BTU/lb F)
☑	Edit Table	0.32	Edit Table	0.38	Specific Volume (ft^3/lb)
☑	Edit Table	0.32	Edit Table	0.38	Heat of Vaporization (BTU/lb)
☑	Edit Table	0.32	Edit Table	0.38	Vapor Pressure -- Solute (psia)
☑	Edit Table	0.32	Edit Table	0.38	Vapor Pressure -- Solvent (psia)
☑	Edit Table				Compressibility Factor -- Solute
☑	Edit Table				Compressibility Factor -- Solvent
☑	Edit Table				Cp/Cv -- Solute
☑	Edit Table				Cp/Cv -- Solvent

Figure 2.6: Example Edit Lading window where the thermodynamics properties of the lading are entered for a substance (top) or solution (bottom).

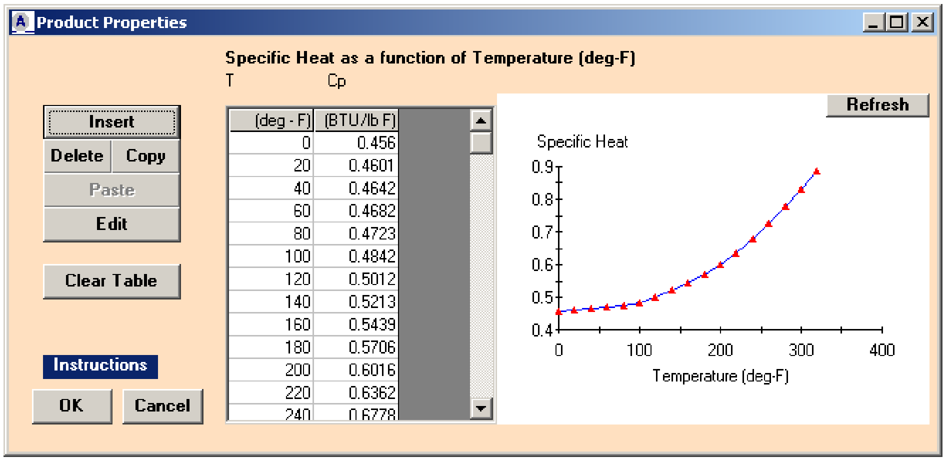
Like the Thermal Protection System window, the Edit Lading window changes its appearance depending upon the options chosen. The most significant change is when you determine if the lading is a substance or a solution[1]. In the upper window of Figure 2.6, the **Substance** option is chosen. In this mode, you need only enter thermodynamic properties for the substance. In the lower window of Figure 2.6, the **Solution** option is chosen, thereby requiring you to enter some of the thermodynamic properties for the solvent and solute at high and low concentrations that bracket, as close as possible, the lading used in the analysis. Inaccuracies can result from the bracketing being too wide.

Any of the lading's thermodynamic properties can be either constant or a function of temperature. If they are constant, the values are simply typed into an entry box. For those properties that are a function of temperature, you must type in the data by clicking the appropriate **Edit Table** button that appears next to the property name.

Shown in Figure 2.7 is the **Product Properties** window for one of the lading's specific heat. The table may be edited by typing in the values as a function of temperature. The recommended method is to clear the table first using the **Clear Table** button, enter the temperature values, using the **ENTER** key to create new rows as you go, and then to enter the property values, using the **ENTER** key to move down the rows (see also, Tutorial 2).

Clicking **Refresh** will update the chart using the values you enter into the table. By clicking on the chart itself and then pressing Control-C on your keyboard, the plot is copied to the Microsoft clipboard and can then be pasted into a variety of Microsoft Windows applications such as PowerPoint and Word.

It is important to remember that the AFFTAC computational module allows only 8 data points for each property except for vapor pressure, which may have between 3 and 15 data points. Also, there must be an odd number of data points entered for vapor pressure.



Specific Heat as a function of Temperature (deg-F)

T (deg - F)	Cp (BTU/lb F)
0	0.456
20	0.4601
40	0.4642
60	0.4682
80	0.4723
100	0.4842
120	0.5012
140	0.5213
160	0.5439
180	0.5706
200	0.6016
220	0.6362
240	0.6778

Figure 2.7: Product Properties window where temperature-dependent data can be entered and charted.

---

[1] A *substance* is matter that is comprised of only one type of molecule. A *solution* is a mixture of two or more substances that is homogenous at the molecular level. AFFTAC allows two-component solutions.

Tutorial 1: A Simple Analysis

To begin this tutorial, run the AFFTAC GUI. When you do, a help screen like that shown in Figure 3.1 will appear describing AFFTAC's auto-recovery feature. Read this important informational window and then click **Close**. The next window that appears is the Welcome window. For this standard analysis, we will bypass the Quick Start option, so on the Welcome screen, click **Go Directly to AFFTAC's Regular Main Window**. When you do, another informational window will appear. Like the first help window, this one also may be disabled by clicking "Do not show this message again." The informational

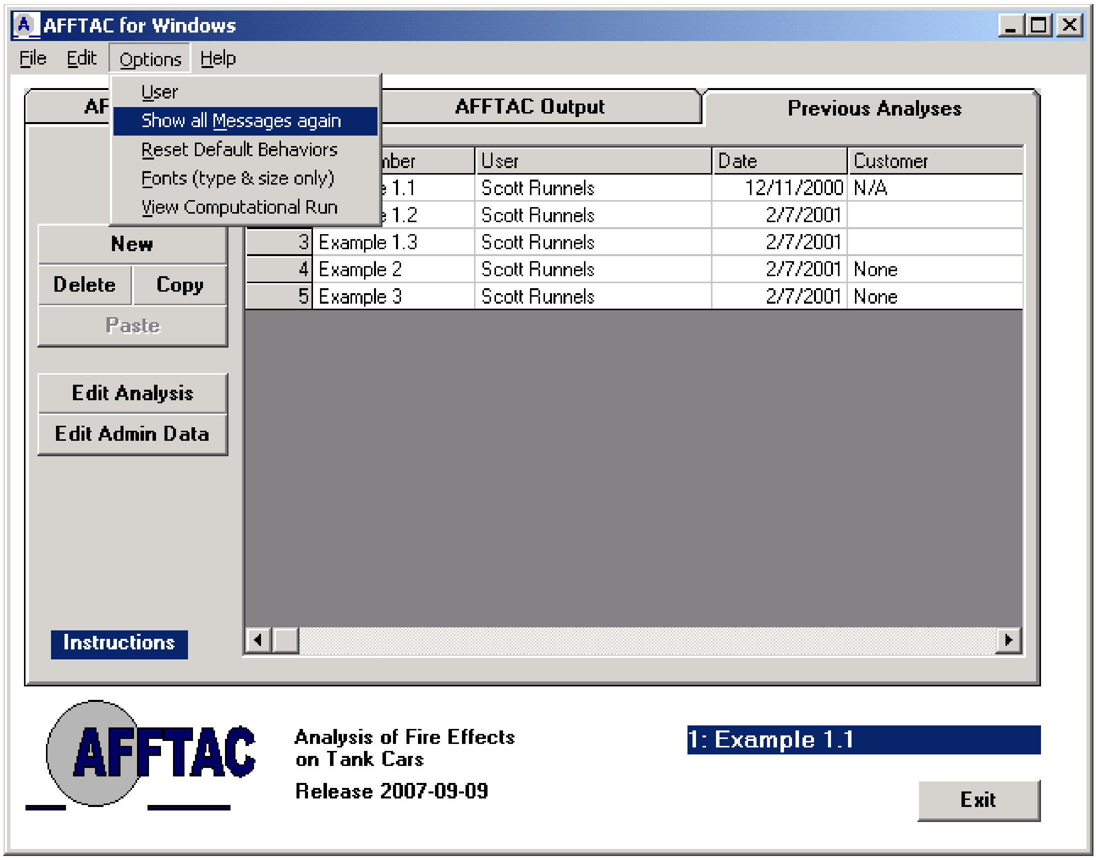
AFFTAC Help

Each time you open AFFTAC, a backup is made of your Analyses.db file in the directory F:\User\AFFTAC_2004\AutoRecovery. If something goes wrong with your AFFTAC session, you can copy it to the F:\User\AFFTAC_2004 directory. Previous versions are also kept and are date+time stamped. The most recent copy is Analyses.db

☐ Do not show this message again.

Figure 3.1: Typical automatic help pop-up window. On each window, the option "Do not show this message again" appears. All messages can be re enabled from the Main Window under the Options menu option. See Figure 3.2.

windows such as the two you have just encountered are part of a proactive help system that will guide you through each step in the AFFTAC usage. Each help window will continue to reappear at the appropriate time unless you disable it. If you feel you need the windows re-enabled after you have disabled them, in the Main Window select the menu option **Options-Show all Messages again** (see Figure 3.2).



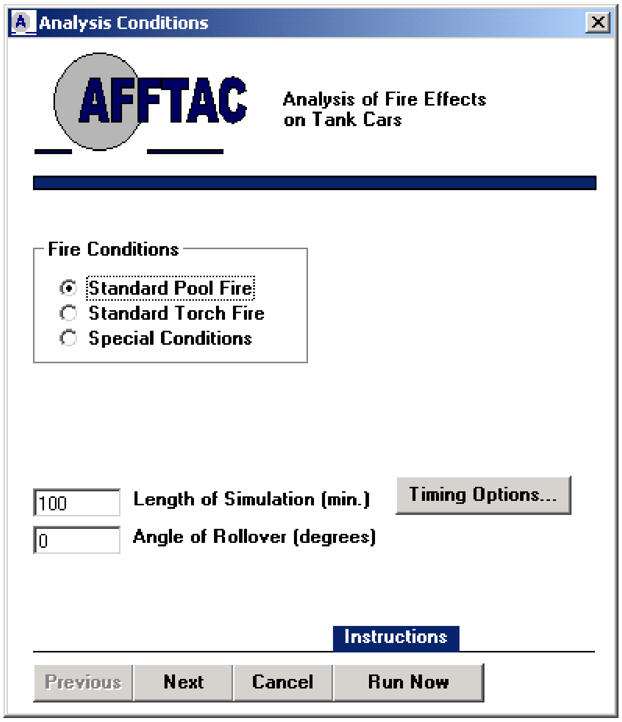
	nber	User	Date	Customer
	e 1.1	Scott Runnels	12/11/2000	N/A
	e 1.2	Scott Runnels	2/7/2001	
3	Example 1.3	Scott Runnels	2/7/2001	
4	Example 2	Scott Runnels	2/7/2001	None
5	Example 3	Scott Runnels	2/7/2001	None

Figure 3.2: Illustration of how to enable all help messages.

After closing the information help window, the Main Window should appear, where the analysis database is displayed. In its distributed version, AFFTAC's analysis database comes preloaded with four example problems that correspond to the example problems in [1]. For this tutorial, one of these example problems (Example 1.1) will be recreated from scratch.

Click **New** in AFFTAC's Main Window. Doing so will display another informational message. Clicking **OK** closes the message window and displays the first in a series of four editing windows.

In the first editing window, select the **Standard Pool Fire** option and enter 100 for the **Length of the Simulation** entry. Leave zero as the entry for the rollover angle. When you are finished making those adjustments, the window should look like that shown in Figure 3.3.



Fire Conditions
● Standard Pool Fire
○ Standard Torch Fire
○ Special Conditions

100 Length of Simulation (min.)
0 Angle of Rollover (degrees)

Figure 3.3: Completed Analysis Conditions window for Tutorial 1.

When it does, click **Next**. Doing so displays the Tank Car Properties window. Enter the following information:

Nominal Capacity: 33000
Inside Diameter: 112
Wall Thickness: 0.5625

Then select **AAR TC128-70, Grs. A & B Min. Tensile Strength 81 Kpsi** from the pull-down arrow. Enter the following data for the material:

Nominal Burst Strength: 750
Tensile Strength: 81000
Emmissivity: 0.8

Select the **Safety Relief Valve** option and enter the following information:

Rated Flow Capacity: 32000
Rating Pressure: 270
Start-to-Discharge Pressure: 247.5
Vapor Discharge Coefficient: 0.8
Liquid Discharge Coefficient:0.6

When you have finished making these entries, the window should look like that shown in Figure 3.4. When it does, click **Next**, read the informational message that appears, and click **Close** on the help window. Doing so will leave you in the Insulation Choices window.

For this tutorial, highlight Example 1, which is a pre-loaded insulation type. To see the data describing the insulation named “Example 1,” double click on it. Doing so displays a help window and after that, the window shown in Figure 3.5.

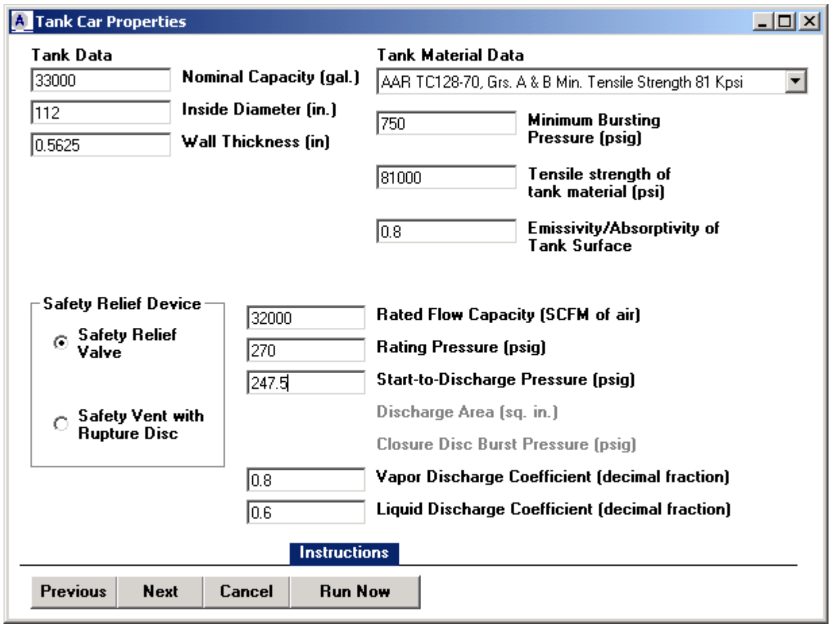
The Example 1 insulation type is a temperature-independent thermal protection system that is constant in time. The value of the conductance is 5.4 BTU/hr-ft^2 deg-F. Now, click **OK** to return to the Insulation Options window. To add or delete insulation types in the insulation database, the database can be accessed by clicking the **Manage Insulation Database** button in the Insulation Options window. It can also be accessed through the Main Window under the **Edit-Insulation Data** menu option.

Highlight Example 1 in the Insulation Options window and click **Next**, which, after a help window, will display the fourth in the series of four editing windows. Select the lading named Butane and enter the following data:

Fraction of Tank Filled: 0.96
Initial Temperature: 60.

The ladings database can be accessed through the **Manage Ladings Database** button, or the menu option **Edit-Lading Property Data** in the Main Window.

The inputs you have provided in the past three windows may be reviewed using the **Previous** and **Next** buttons that are shown at the bottom of each of the four editing



Tank Data
33000 Nominal Capacity (gal.)
112 Inside Diameter (in.)
0.5625 Wall Thickness (in)

Tank Material Data
AAR TC128-70, Grs. A & B Min. Tensile Strength 81 Kpsi
750 Minimum Bursting Pressure (psig)
81000 Tensile strength of tank material (psi)
0.8 Emissivity/Absorptivity of Tank Surface

Safety Relief Device
● Safety Relief Valve
○ Safety Vent with Rupture Disc

32000 Rated Flow Capacity (SCFM of air)
270 Rating Pressure (psig)
247.5 Start-to-Discharge Pressure (psig)
Discharge Area (sq. in.)
Closure Disc Burst Pressure (psig)
0.8 Vapor Discharge Coefficient (decimal fraction)
0.6 Liquid Discharge Coefficient (decimal fraction)

Figure 3.4: Completed Tank Car Properties window for Tutorial 1.

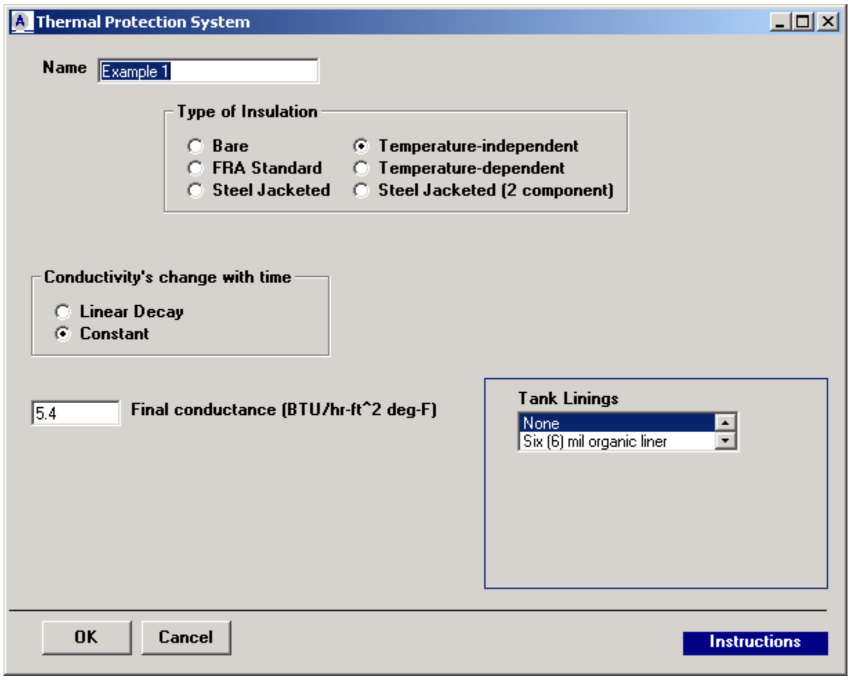
windows. Clicking **Cancel** would erase these changes and return you to the Main Window. At this point, the Ladings Properties window should look like that shown in Figure 3.6. When it does, click **Run**, which will execute the analysis and return you to the **AFFTAC Output** tab of the Main Window (first you will see a help window). To review the input as echoed by the computational module, click the AFFTAC **Input Summary** tab.

Now click the **Previous Analysis** tab in the Main Window. Notice that this analysis is listed with the other previous analysis. However, it has not yet been saved to the analysis database file. Before it can be saved there, the administrative information must be added. Likewise, to print the results of this analysis, the administrative information must be added. Return to the **AFFTAC Output** tab and click **Print.** Doing so displays the administrative data input window. Enter the following information:

Job Number:	My First Turn
Customer:	N/A

Then, click **OK** and the results will be printed.

Note that the default information for your name and your company name may be defined through the Main Window, under the menu option **Options-User**.
While still in the AFFTAC Output window, click Plot. Doing so displays the plot window shown in Figure 3.7. These plots can be cut and pasted into other Microsoft Office applications. Click the Instructions button to learn how to do that, and also to learn how to zoom and pan.



Name: Example 1

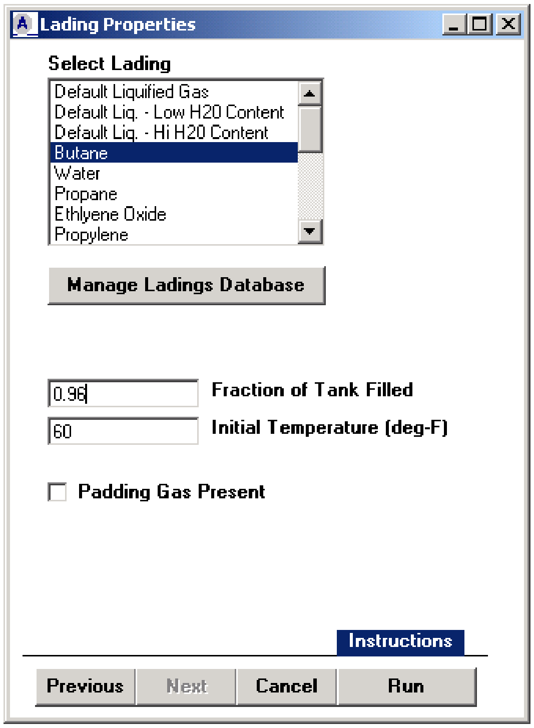
Type of Insulation
○ Bare
○ FRA Standard
○ Steel Jacketed
● Temperature-independent
○ Temperature-dependent
○ Steel Jacketed (2 component)

Conductivity's change with time
○ Linear Decay
● Constant

5.4 Final conductance (BTU/hr-ft^2 deg-F)

Tank Linings
None
Six (6) mil organic liner

Figure 3.5: Thermal Protection System editing window.



Select Lading: Butane

0.96 Fraction of Tank Filled

60 Initial Temperature (deg-F)

☐ Padding Gas Present

Figure 3.6: The Lading Properties window for Tutorial 1.

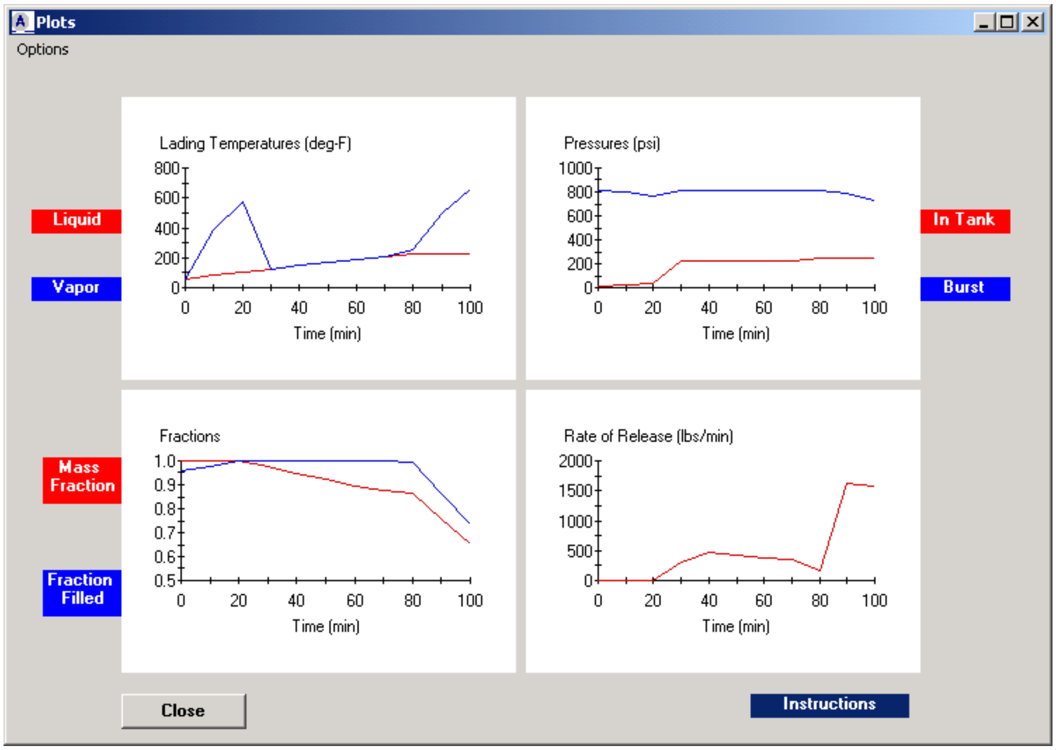
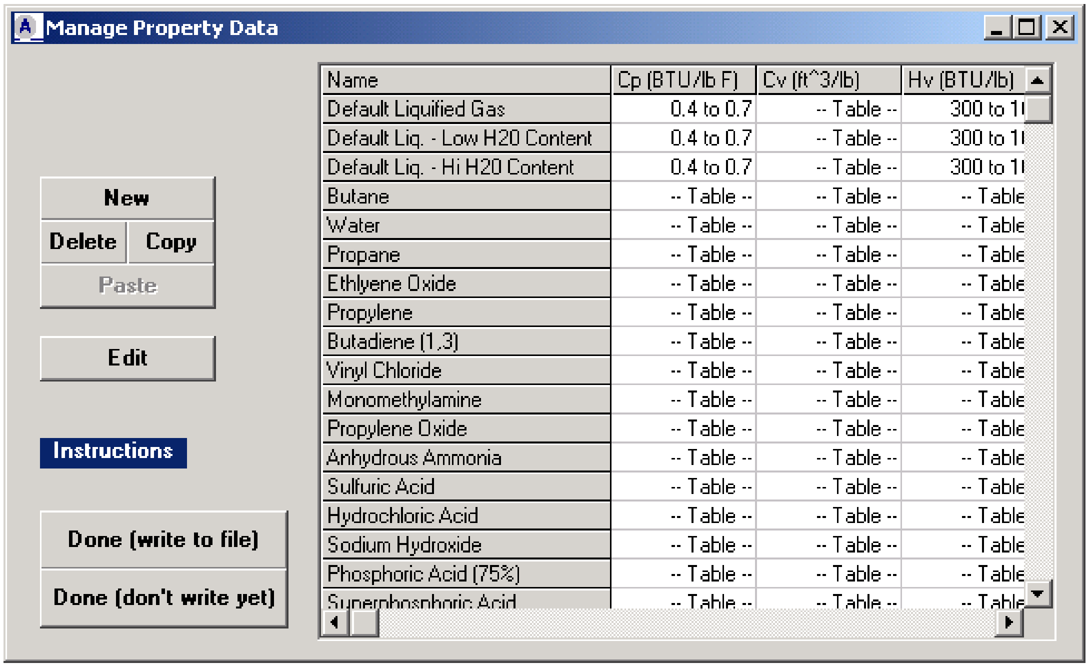


Figure 3.7: Plot window. Cutting-and-pasting, zoom, pan, etc. instructions can be obtained by clicking the “Instructions” button on the lower right part of the window.

Tutorial 2: Adding a Lading

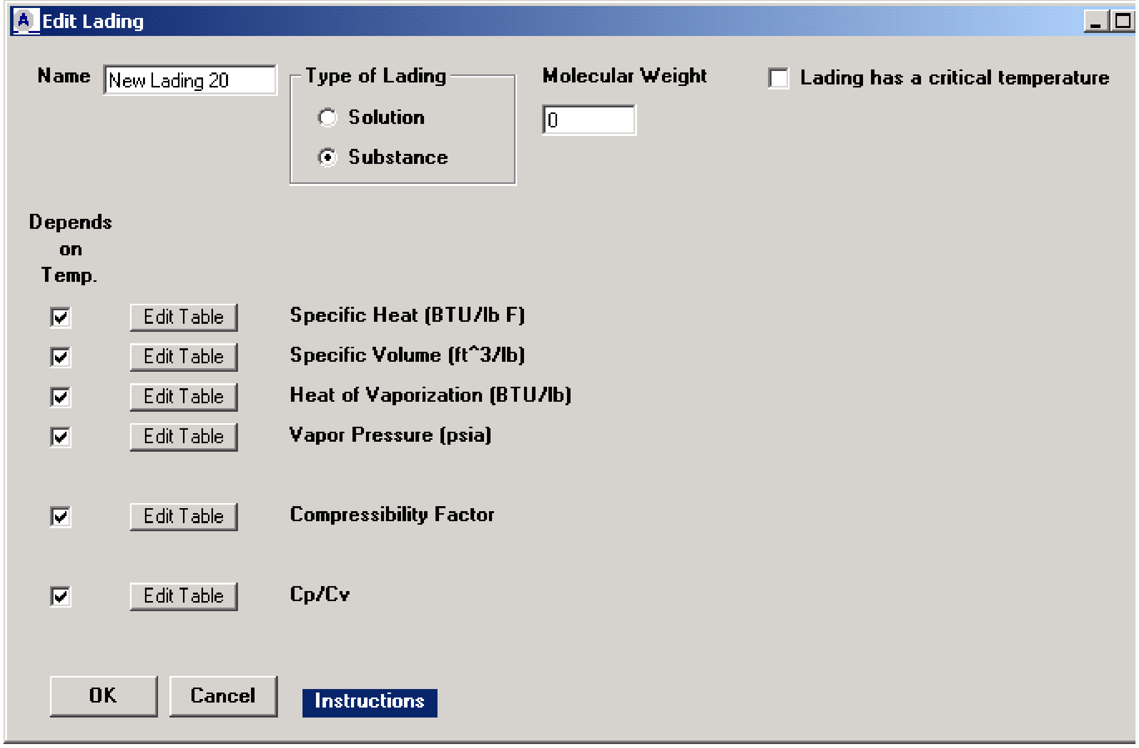
In this tutorial, you will be guided through the process of adding a new lading to the ladings database. Help windows will continue to appear as you work through these instructions, but they will not be mentioned in this text any further. Run AFFTAC and select **Go Directly to AFFTAC's Regular Main Window** from the Welcome window. Once in the Main Window, select the menu option **Edit-Lading Property Data.** Upon doing so, a window like that shown in Figure 4.1 will appear. In that window are listed the various ladings that are already contained in the database file.



Name	Cp (BTU/lb F)	Cv (ft^3/lb)	Hv (BTU/lb)
Default Liquified Gas	0.4 to 0.7	-- Table --	300 to 1
Default Liq. - Low H20 Content	0.4 to 0.7	-- Table --	300 to 1
Default Liq. - Hi H20 Content	0.4 to 0.7	-- Table --	300 to 1
Butane	-- Table --	-- Table --	-- Table
Water	-- Table --	-- Table --	-- Table
Propane	-- Table --	-- Table --	-- Table
Ethlyene Oxide	-- Table --	-- Table --	-- Table
Propylene	-- Table --	-- Table --	-- Table
Butadiene (1,3)	-- Table --	-- Table --	-- Table
Vinyl Chloride	-- Table --	-- Table --	-- Table
Monomethylamine	-- Table --	-- Table --	-- Table
Propylene Oxide	-- Table --	-- Table --	-- Table
Anhydrous Ammonia	-- Table --	-- Table --	-- Table
Sulfuric Acid	-- Table --	-- Table --	-- Table
Hydrochloric Acid	-- Table --	-- Table --	-- Table
Sodium Hydroxide	-- Table --	-- Table --	-- Table
Phosphoric Acid (75%)	-- Table --	-- Table --	-- Table
Superphosphoric Acid	-- Table --	-- Table --	-- Table

Figure 4.1: The Manage Property Data window.

Click **New**. When you do, a new lading is added to the list and is displayed as the last entry. This new lading is merely a placeholder. It does not yet have any real data associated with it. To provide the necessary data, either double click on the new entry, or highlight it and click the **Edit** button.



Edit Lading

Name: New Lading 20

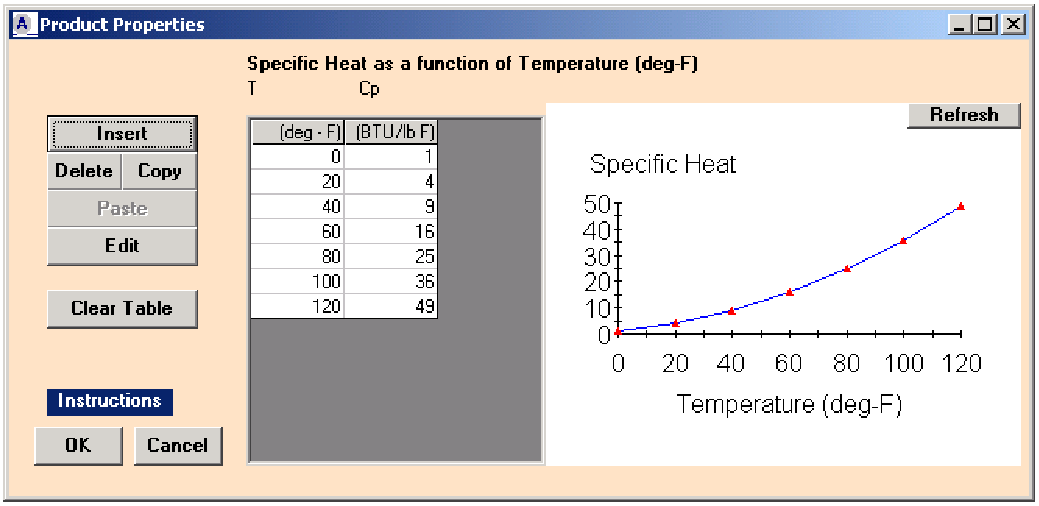
Type of Lading
○ Solution
● Substance

Molecular Weight: 0

☐ Lading has a critical temperature

Depends on Temp.		
☑	Edit Table	Specific Heat (BTU/lb F)
☑	Edit Table	Specific Volume (ft^3/lb)
☑	Edit Table	Heat of Vaporization (BTU/lb)
☑	Edit Table	Vapor Pressure (psia)
☑	Edit Table	Compressibility Factor
☑	Edit Table	Cp/Cv

Figure 4.2: Window for setting up a new lading.



Product Properties

Specific Heat as a function of Temperature (deg-F)

T (deg - F)	Cp (BTU/lb F)
0	1
20	4
40	9
60	16
80	25
100	36
120	49

Figure 4.3: Window displayed when setting up a thermodynamic property for the first time.

Doing so displays the window shown in Figure 4.2. In this window, the various properties required by the AFFTAC computational module are displayed. First, type in the name “My Lading” in the **Name** entry box. Next, make sure that the **Substance** button is selected. Note that if **Solution** is selected (try it) there are some properties that require values for both the solvent and solute, and some values are required at two concentration levels.

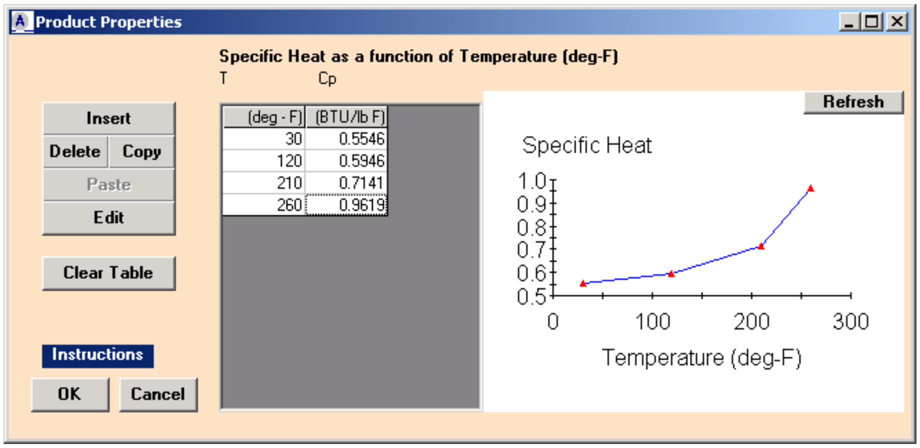
Now it will be demonstrated how to provide the data for one of the properties. Click on the **Edit Table** button next to the **Specific Heat** label. When you do, the window shown in Figure 4.3 appears.

Although there are values supplied in the window, they are not to be taken as legitimate, but rather, placeholders to demonstrate how the window should look once data is entered. For now, click **Clear Table**, which will remove these entries and prepare the table for fresh data.

After you have cleared the placeholder data, click on the left cell, in the temperature column. Using the numeric keypad on your keyboard, type the value 30 and press **ENTER**. Next type 120 and press **ENTER**. Repeat this process to enter 210 and 260 (do not press **ENTER** after 260).

Now, click on the top right cell, under the Cp column. Type 0.5546 and press **ENTER**. Type 0.5946 and press **ENTER** again. Continue, entering 0.7141 and 0.9619 (do not press **ENTER** after 0.9619).

Click **Refresh** to view the updated graph. You may edit the data by clicking directly over the cell you wish to change. Use the **BACKSPACE** key to erase characters. You can also copy, cut, and paste rows using the buttons provided. When you are finished, the window should look like that shown in Figure 4.4.



Specific Heat as a function of Temperature (deg-F)

T Cp

(deg - F)	(BTU/lb F)
30	0.5546
120	0.5946
210	0.7141
260	0.9619

Figure 4.4: Completed Specific Heat window for Tutorial 2.

Once the data has been entered correctly, click **OK**. This same process may be repeated for all of the properties listed. Note that the current version of the computational module has certain requirements regarding the number of data points that should be provided for each property. If those requirements are not met, the AFFTAC GUI will inform you when you click **OK** in the Edit Lading window.

Theory

Scope of the Simulation

The AFFTAC simulation includes heat conduction, stress, and a failure model of the tank, a thermodynamic model of its fluid contents, and a flow model for the lading flowing through the safety relief device. It is essentially a model that enforces the conservation of thermal energy and mass. The bulk geometry of the tank car is considered in terms of quantities like diameter, volume, wall thickness, and the rollover angle[2] as opposed to a detailed geometric description. Therefore, although the simulation is transient and gives a time-dependent prediction, it does not provide spatial resolution. It is assumed that the liquid and vapor parts of the lading are at the same uniform temperature.

Heat is added to the system on the outside of the tank car wall to represent the fire. This heat is conducted to the inside of the tank and eventually transported into the lading by contact with the wall and by radiation from the surfaces not in contact. The lading responds by heating up; the liquid evaporates and thermally expands and the vapor pressure increases. As a result of the vapor's pressure or geometric expansion of the liquid in a shell full[3] condition, the pressure on the inside of the tank car increases. When it reaches a sufficient level, the tank's safety relief device opens and allows lading to be released. A supporting model for the safety relief device is provided as part of the AFFTAC simulator. In simple terms, the model uses the current and past pressures inside the tank to predict the current cross sectional area in the relief device available for lading release. The flow through that area is modeled using sets of separate supporting fluid flow equations, depending on whether vapor, liquid, or a mixture of the two is being expelled. Those equations are developed in detail in Appendix B.

The simulation is carried out starting at time = 0 and, under normal circumstances, ending at a user-specified time. However, as the simulation proceeds, the lading could

---

[2] If the tank has tilted along its longitudinal axis with respect to the ground, it has a nonzero "rollover" angle.

[3] Car completely filled with liquid

eventually be completely expelled, causing the simulation to end earlier. Another possibility for early termination occurs when the safety relief device is not able to accommodate the expulsion of lading quickly enough. In that case, the pressure inside the tank car builds up to be high enough to rupture the tank.

In addition to the models for the safety relief device and the flow through it, AFFTAC has other supporting models that play key roles in the simulation. There are models for how the insulating layers of the tank wall change with time and temperature. There are also auxiliary models, including a stress model that computes the strain in the tank wall and subsequent change in the tank volume. Finally, there is a temperature-dependent failure model for the tank wall's structural layer.

An overview of the AFFTAC simulation is shown in Figure 5.1. Each of the models are linked and executed in a time-marching loop that proceeds through the simulation in small time increments. These models are discussed in the following sections. After that, important aspects of their implementation in the time-marching loop are discussed.

Thermal Transport Model

Below are some important introductory facts regarding AFFTAC's thermal transport model:

1. The liquid and vapor phases of the lading are assumed to be at the same temperature, and the part of the tank wall adjacent to the liquid phase is also

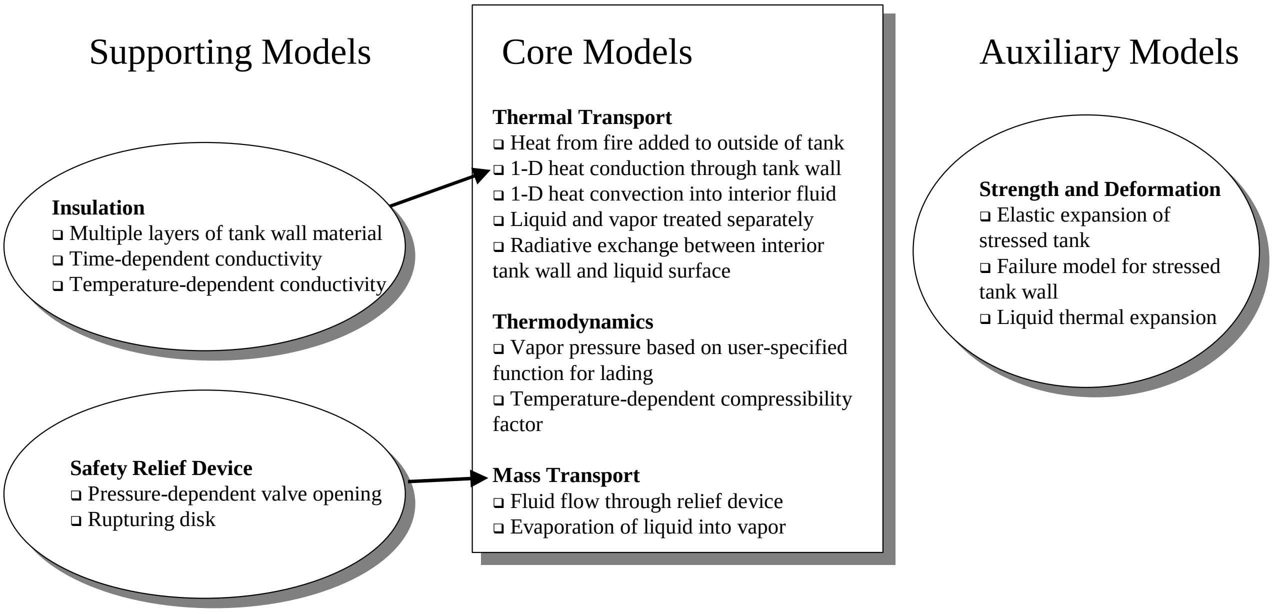


Figure 5.1: AFFTAC physics model summary.

assumed to be at that same temperature. The temperature of these three components is referred to as T_{lading}.

2. The interior of the tank wall adjacent to the vapor is at a separate temperature, $T_{wall\text{-}vapor}$.

3. The tank's outer surface has four different temperatures. First, partial insulation coverage is modeled, and so different outer temperatures exist for the regions with and without insulation. Also, different outer temperatures exist for the parts adjacent to liquid and vapor. Thus the four outer temperatures are $T_{outer\text{-}Ins\text{-}liquid}$, $T_{outer\text{-}noIns\text{-}liquid}$, $T_{outer\text{-}Ins\text{-}vapor}$, $T_{outer\text{-}noIns\text{-}vapor}$.

To solidify these definitions, the temperatures are defined in Figures 5.2 and 5.3 for the two different cases (jacketed and unjacketed). Notice in both cases that there is one temperature for the lading, both vapor and liquid, and that same temperature is the temperature of the interior tank wall adjacent to the liquid.

The thermal model tracks heat for the following three entities:

1. *Temperature evolution of the lading:* The heat flowing into the lading is modeled and this heat is used to determine the changes in the lading temperature. Also considered are the thermodynamic effects of ejecting the lading through the pressure relief device.
2. *Temperature evolution of the wall above the vapor space:* Since the wall above

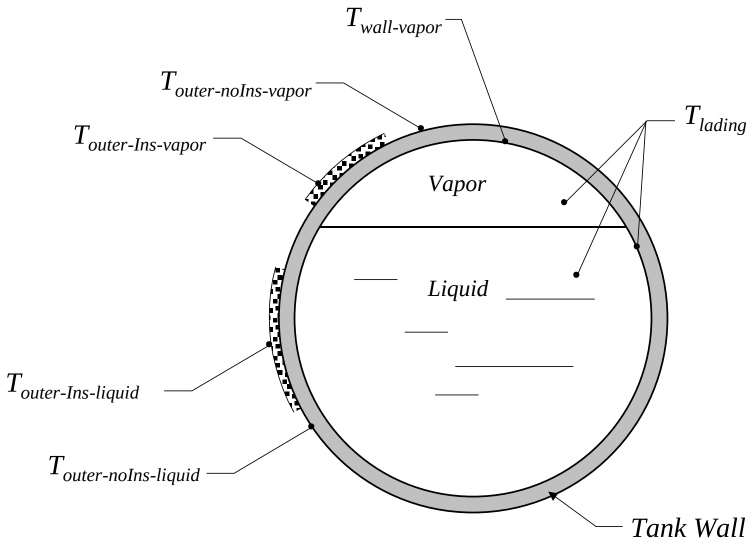


Figure 5.2: Temperature definitions for the case of an unjacketed tank.

the vapor space is considered to have its own temperature, the overall heat balance on that part of the wall is modeled and used to evolve the temperature.

3. *Heat balance on outer surfaces:* The outer surfaces of the tank are modeled using separate heat balance equations.

The models for these three entities will be discussed in greater detail shortly. But first, background material concerning radiative exchange is needed.

Radiative Heat Exchange Computations

Radiative heat exchange occurs between the flame and outer tank wall, as well as the inner tank wall and liquid surface. AFFTAC models all radiative exchange using a classical law [18], and represents every surface as being gray with a single value of emissivity.

For radiative exchange between two surfaces, the emissive powers of the two surfaces are

$$\begin{aligned} E_1 &= \varepsilon_1 \sigma T_1^4 \\ E_2 &= \varepsilon_2 \sigma T_2^4 \end{aligned} \qquad 5.2.1$$

where σ is the Stefan-Boltzmann constant. As shown in [18] a heat flux balance between two gray surfaces connected in the logical configuration indicated in Figure 5.4 results in the following relationship:

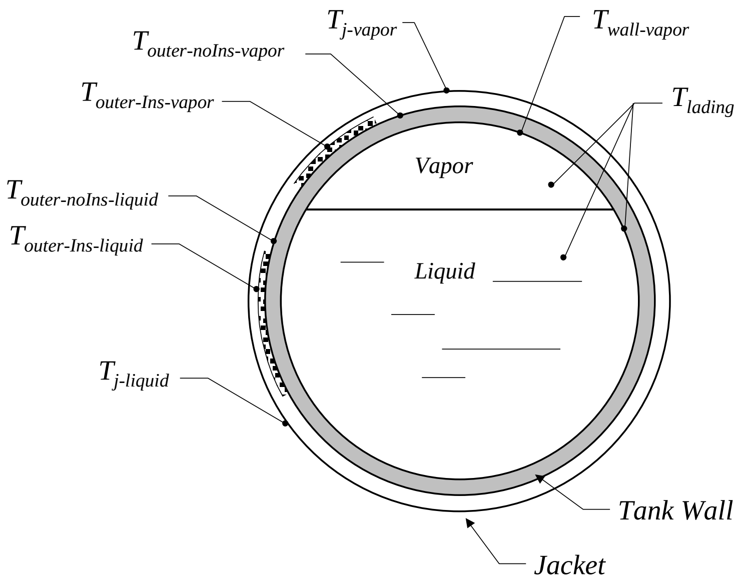


Figure 5.3: Temperature definitions for the case of a jacketed tank with partial insulation coverage.

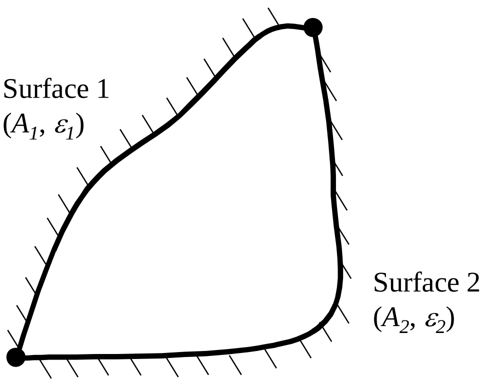


Figure 5.4: Gray body configuration used in AFFTAC.

$$Q_{1-2} = \frac{\sigma\left(T_1^4 - T_2^4\right)}{\frac{1-\varepsilon_1}{A_1\varepsilon_1} + \frac{1}{A_1F_{1-2}} + \frac{1-\varepsilon_2}{A_2\varepsilon_2}} \tag{5.2.2}$$

where

Q_{1-2} is the net heat flux from surface 1 to surface 2
F_{1-2} is the geometric view factor, which represents the line-of-sight exposure between surfaces 1 and 2 as defined in [18], and
A_i is the area of the surfaces i (i = 1,2).

Rearranging, the above equation becomes

$$\frac{Q_{1-2}}{A_1} \equiv q_{1-2} = \frac{\sigma\left(T_1^4 - T_2^4\right)}{\frac{1}{F_{1-2}} + \left(\frac{1}{\varepsilon_1} - 1\right) + \frac{A_1}{A_2}\left(\frac{1}{\varepsilon_1} - 1\right)} \tag{5.2.3}$$

Through this equation the "surface configuration factor," f_{1-2}, is defined and used in AFFTAC to scale the radiative flux exchange. That factor,

$$f_{1-2} \equiv \frac{1}{\frac{1}{F_{1-2}} + \left(\frac{1}{\varepsilon_1} - 1\right) + \frac{A_1}{A_2}\left(\frac{1}{\varepsilon_2} - 1\right)} \tag{5.2.4}$$

is used in combination with the surface areas, Stefan-Boltzmann constant, and temperatures of the exchanging surfaces to predict the radiant heat flux, i.e.,

$$q_{1-2} = f_{1-2}\sigma\left(T_1^4 - T_2^4\right) \qquad 5.2.5$$

In computing the radiative exchange between the inside tank wall and the liquid surface, 1 becomes "*liquid*" and 2 becomes "*wall*" to represent the tank wall. 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. A reciprocal relationship is used to compute $f_{wall\text{-}liquid}$.

To compute the view factor, $F_{liquid\text{-}wall}$, and areas A_{liquid}, A_{wall}, used in the above equation, the geometry of the liquid surface relative to the tank wall must be computed. Figure 5.5 shows a cross-section of the tank. The area of the bottom quadrant is $\pi r^2/4$. The area of the arc region above that is $\pi\theta^2/2$. The area of the shaded rectangle is $r^2 \sin\theta \cos\theta/2$. Twice the sum of these areas represents the entire area under the liquid surface. Therefore,

$$A_{liquid} = 2\times\left[\frac{1}{4}\pi r^2 + \frac{1}{2}\pi\theta^2 + \frac{1}{2}r^2\sin\theta\cos\theta\right] = \frac{1}{2}\pi r^2 + \pi\theta^2 + r^2\sin\theta\cos\theta \qquad 5.2.6$$

The ratio of this quantity to the total cross-sectional area (πr^2) is the same as the fraction of the tank volume occupied by the liquid, i.e.,

$$\frac{V_{liquid}}{V_{total}} = \frac{1}{\pi}\left[\frac{\pi}{2} + \theta + \sin\theta\cos\theta\right] \qquad 5.2.7$$

This equation is solved through trial and error during the simulation to determine θ at each point in time. From this value, the surface area of the liquid can be computed. In

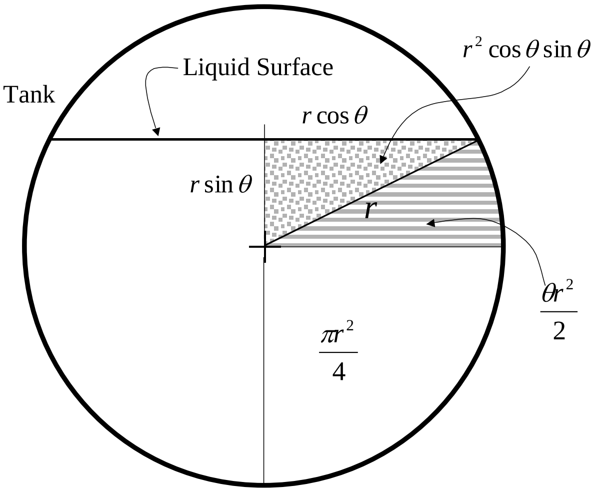


Figure 5.5: Geometry used to derive the equation relating the angle to the liquid surface endpoint to the fraction of tank filled with liquid.

addition, this value is used to determine whether or not liquid or vapor is adjacent to the safety relief device.

Three-Entity Thermal Model

In the following sub-sections, the details will be given for the three-entity thermal model. Note that all three of these entities are intimately connected. Therefore, the equations that are written for them are mathematically linked. In the AFFTAC numerical procedures, a method often called “operator splitting” (or “nonlinear lagging”) is employed to solve these linked equations. In the operator splitting process, one sub-set of the set of governing equations are solved while setting the other variables to their value from the previous time-step. So, for example, when solving for the outer surface temperatures, which is the first entity to be discussed, the interior temperatures from the previous time step are considered good enough approximations for the outer surface heat balance equations. Then, when solving the equations for the lading temperature increase, the newly-computed outer surface temperatures are used. Again, in principle, these equations should be solved simultaneously at each time step. But, if the time steps are sufficiently small, using values for some of the variables from the previous time step produces acceptable error. Even with the use of operator splitting, there are nonlinear equations (sometimes multiple nonlinear equations) that still must be solved. But the problem is made much more tractable through the use of this simple, and time-tested technique known as operator splitting.

Entity 1 of 3: Outer Surface Temperatures

The first entity considered at each time step is the outer surface temperatures. As already mentioned, there are two configurations that are considered. They are shown in Figure 5.6. Those two cases are considered separately, below.

Case A: Bare Tank or Tank with Partial Insulation Coverage

Although a bare tank may perform and appear very different than a tank with insulation, from a modeling standpoint, the two cases are identical. Specifically, the heat transfer from the inside of the tank wall to the outermost surface is equal to the temperature difference on those two surfaces times a thermal conductivity. Granted, the conductivity in the bare tank case will be much higher than in the insulation case, but that does not change the fact that the equations are the same form.

And so, in AFFTAC, the bare tank and insulation packed inside a jacket are treated exactly the same way, with different values for conductivity. The treatment is a heat balance on the outermost surface that accommodates areas with and without insulation, which is as follows:

$$\sigma\varepsilon f T_f^4 - \sigma\varepsilon T_{outer-noIns}^4 + c_{Ins}\left(T_{outer-Ins} - T_i\right) = 0$$
$$\sigma\varepsilon f T_f^4 - \sigma\varepsilon T_{outer-noIns}^4 + c_{noIns}\left(T_{outer-noIns} - T_i\right) = 0 \qquad 5.2.8$$

These nonlinear equations are solved for $T_{outer\text{-}Ins}$ and $T_{outer\text{-}noIns}$ in the routine SolveRadConduct, twice, once for the wall adjacent to the liquid and once for the wall adjacent to the vapor. The first time, T_i is set to T_{lading} (considered known) so that $T_{outer\text{-}Ins}$ can be used as the solution for $T_{outer\text{-}Ins\text{-}liquid}$ and $T_{outer\text{-}noIns}$ is the solution for $T_{outer\text{-}noIns\text{-}liquid}$. The second time, T_i is set to $T_{wall\text{-}vapor}$ (considered known) so that $T_{outer\text{-}Ins}$ can be used as the solution for $T_{outer\text{-}Ins\text{-}vapor}$ and $T_{outer\text{-}noIns}$ is the solution for $T_{outer\text{-}noIns\text{-}vapor}$.

Case B: Partial Insulation Coverage Inside Jacket

In this case, the model accommodates a variable amount of coverage from the insulation that is sandwiched between the steel jacket and the tank wall.

The model assumes that the steel jacket is so thin that it does not support a temperature gradient, i.e., it is a constant temperature T_j. The inner temperature of the tank wall is either T_{lading}, or $T_{wall\text{-}vapor}$ depending on which region is being considered. Thus, the equations below, which govern the heat flow through the wall and insulation, are solved twice: Once for the wall adjacent to the liquid and once for the wall adjacent to the

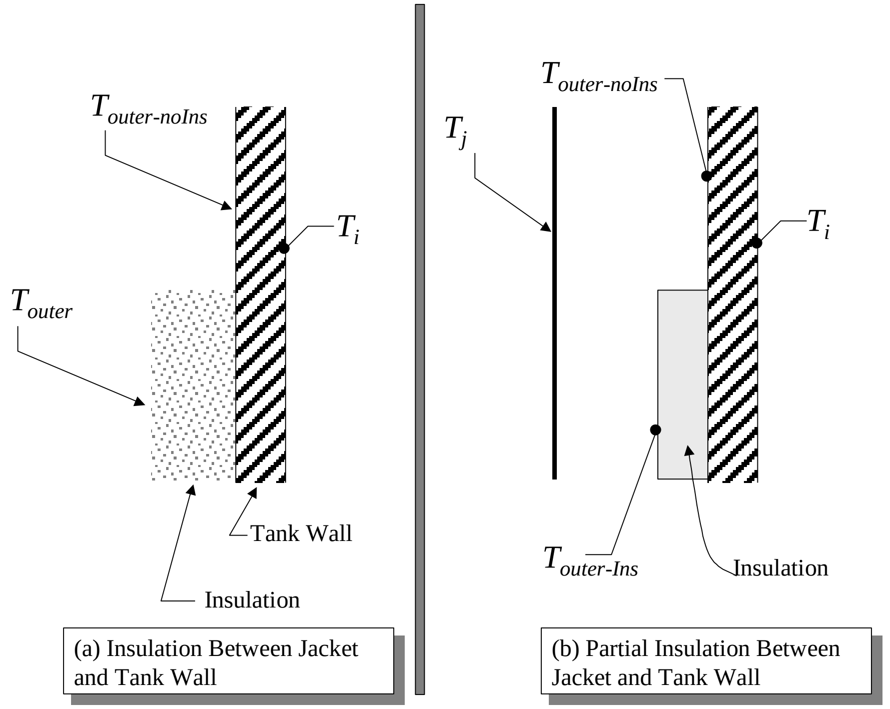


Figure 5.6: Heat exchange diagram showing relevant nomenclature.

vapor. When solving for the liquid region, the solution obtained for $T_{outer\text{-}Ins}$ is used for $T_{outer\text{-}Ins\text{-}liquid}$ and the solution obtained for $T_{outer\text{-}noIns}$ is used for $T_{outer\text{-}noIns\text{-}liquid}$. The exact analogy is used for the vapor region. F_{sp} is the fraction of insulation coverage.

Heat Balance on Jacket:

$$\sigma\varepsilon f T_f^4 - \sigma\varepsilon T_j^4 - \sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_j^4 + \sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_{outer-noIns}^4\left(1-F_{SP}\right) + \sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_{outer-Ins}^4 F_{SP} = 0 \qquad 5.2.9$$

Heat Balance on Bare Tank Surface:

$$\sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_j^4 - \sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_{outer-noIns}^4 - C_w\left(T_{outer-noIns} - T_i\right) = 0 \qquad 5.2.10$$

Heat Balance on Insulation/Thermal Protection Surface:

$$\sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_j^4 - \sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_{outer-Ins}^4 - \overline{C}\left(T_{outer-Ins} - T_i\right) = 0 \qquad 5.2.11$$

In the above equations, σ is the Stefan-Boltzmann constant, and the f parameters are the surface configuration factors. The surface configuration factors rely upon the emissivities, geometric view factors, and areas of the surfaces involved (see Equations 5.2.1-5.2.5). The C_w and $\overline{C}$ are thermal conductances.

The unknowns in the above Equations are T_j, $T_{outer\text{-}Ins}$, and $T_{outer\text{-}noIns}$. To solve the equations using the Newton-Raphson method, first the left-hand-side of the equations are given names, f_1, f_2, and f_3:

$$f_1 \equiv \sigma\varepsilon f T_f^4 - \sigma\varepsilon T_j^4 - \sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_j^4 + \sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_{outer-noIns}^4\left(1-F_{SP}\right) + \sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_{outer-Ins}^4 F_{SP} \qquad 5.2.12$$

$$f_2 \equiv \sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_j^4 - \sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_{outer-noIns}^4 - C_w\left(T_{outer-noIns} - T_i\right) \qquad 5.2.13$$

$$f_3 \equiv \sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_j^4 - \sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_{outer-Ins}^4 - \overline{C}\left(T_{outer-Ins} - T_i\right) \qquad 5.2.14$$

Second, an array containing the three unknown temperatures and an array containing the three functions are defined:

$$\mathbf{T} \equiv \begin{bmatrix} T_j \\ T_{outer-noIns} \\ T_{outer-Ins} \end{bmatrix} \quad \text{and} \quad \mathbf{f}(\mathbf{T}) \equiv \begin{bmatrix} f_1(\mathbf{T}) \\ f_2(\mathbf{T}) \\ f_3(\mathbf{T}) \end{bmatrix} \tag{5.2.15}$$

The nonlinear system of three equations may now be expressed as follows:

$$\mathbf{f}(\mathbf{T}) = \mathbf{0} \tag{5.2.16}$$

The Newton-Raphson method of solving a nonlinear system such as that in Equation (5.2.16) is to start with an initial guess, $\mathbf{T}^0$ and then update that guess as follows:

$$\mathbf{T}^{i+1} = \mathbf{T}^i + \boldsymbol{\delta}^i \tag{5.2.17}$$

Where $\boldsymbol{\delta}^i$ is the solution to the following linear system of equations:

$$\begin{bmatrix} \frac{\partial f_1}{\partial T_j} & \frac{\partial f_1}{\partial T_{outer-noIns}} & \frac{\partial f_1}{\partial T_{outer-Ins}} \\ \frac{\partial f_2}{\partial T_j} & \frac{\partial f_2}{\partial T_{outer-noIns}} & \frac{\partial f_2}{\partial T_{outer-Ins}} \\ \frac{\partial f_3}{\partial T_j} & \frac{\partial f_3}{\partial T_{outer-noIns}} & \frac{\partial f_3}{\partial T_{outer-Ins}} \end{bmatrix}_{\mathbf{T}^i} \boldsymbol{\delta}^i = -\mathbf{f}(\mathbf{T}^i) \tag{5.2.18}$$

The right hand side is an array of three entries, which are the **f** functions evaluated at the previous guess. The matrix is comprised of partial derivatives of the three functions with respect to the different temperatures, also evaluated at the previous guess.

Working from Equations 5.2.12-5.2.14, the partial derivatives are as follows:

$$\begin{aligned} \frac{\partial f_1}{\partial T_j} &= -4\sigma\varepsilon T_j^3 - 4\sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_j^3 \\ \frac{\partial f_1}{\partial T_{outer-noIns}} &= 4\sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_{outer-noIns}^3\left(1-F_{SP}\right) \\ \frac{\partial f_1}{\partial T_{outer-Ins}} &= 4\sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_{outer-Ins}^3 F_{SP} \end{aligned} \tag{5.2.19}$$

$$\frac{\partial f_2}{\partial T_j} = 4\sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_j^3$$
$$\frac{\partial f_2}{\partial T_{outer-noIns}} = -4\sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_{outer-noIns}^3 - C_w$$
$$\frac{\partial f_2}{\partial T_{outer-Ins}} = 0 \tag{5.2.20}$$

$$\frac{\partial f_3}{\partial T_j} = 4\sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_j^3$$
$$\frac{\partial f_3}{\partial T_{outer-noIns}} = 0$$
$$\frac{\partial f_3}{\partial T_{outer-Ins}} = -4\sigma\left(\frac{\varepsilon}{2-\varepsilon}\right)T_{outer-Ins}^3 - \overline{C} \tag{5.2.21}$$

An initial guess is required to start the Newton-Raphson iterations. For all but the first time step, the solution from the previous time step is sufficient. But for the first time step, the initial guess is provided using an approximation.

The geometric view factor for the flame-tank exchange is assumed to be unity except in the case of a torch fire where it is assumed to be 0.536. The geometric view factor for the jacket-wall exchange is unity. The system is solved by the NewtonRaphson routine, which is called from surfacet.

Entity 2 of 3: Heat Flow into Lading

AFFTAC assumes the vapor and liquid temperatures are equal but that the temperature on the outside of the wall adjacent to the vapor is different than the temperature of the outside of the wall adjacent to the liquid. In determining the heat transported into the lading, AFFTAC considers the heat into the liquid and the tank wall adjacent to it as a single system and denotes their collective temperature as T_{lading}. The thermal mass of the vapor is negligible in comparison. The mechanisms of heat transfer into the liquid-wall system includes the following:

1.) Heat convected to the vapor part of the lading,
2.) Heat radiated to the liquid surface directly from the part of the wall over the vapor, and
3.) Heat conducted through the wall touching the liquid.

Figure 5.7 shows these three heat fluxes. A heat balance on the liquid-wall system sums the three arrows in Figure 5.7 as follows:

$$\begin{aligned}&A_{wall-liquid}\left[F_{SP}C_{Ins}(T_{outer-Ins-liquid}-T_{lading})+(1-F_{SP})C_{noIns}(T_{outer-noIns-liquid}-T_{lading})\right]\times(\text{Fraction Engulfed})+\\&A_{wall-vapor}\times f_{wall-liquid}(T^{4}_{wall-vapor}-T^{4}_{lading})+\\&A_{liquidsurface}h(T_{wall-vapor}-T_{lading})+\\&=Q_{net}\end{aligned} \quad 5.2.22$$

The first square-bracketed term is the conductive exchange between the tank wall and the liquid. The temperatures in that term are obtained for either Case A or Case B described in the previous section. Keeping in mind that the thermal model is one-dimensional, the "Fraction Engulfed" term is used to represent the fact that some of the tank may not be engulfed in the flame. It changes depending upon whether a pool fire or a torch fire is being considered. The second term is the radiative exchange between the interior of the wall adjacent to the vapor and the liquid surface. It uses the radiative surface configuration factor described earlier along with the area of the wall over the vapor, $A_{wall-vapor}$. The third term is the convective exchange between the wall and the liquid part of the lading, which is accomplished through the fluid flow of the vapor. It uses a heat transfer coefficient h that is a function of the fraction of tank volume occupied by the liquid and the flow rate through the safety relief device. Its value has been deduced, in part, from the full-scale fire tests and is discussed more fully in the section on conduction models. The imbalance between these three heat fluxes, denoted as Q_{net} above, will cause the liquid to heat up.

During times when the safety relief device is open and vapor is being expelled, the amount of work, W_{vapor}, performed by pushing part of itself through the device is subtracted from Q_{net}. Also, the latent heat of vaporization for the expelled lading is subtracted. Thus the temperature change is given by

$$M_{liquid+adjacentwall}\frac{dT_{lading}}{dt}=Q_{net}+W-\dot{m}H_{f} \quad 5.2.23$$

Here the thermal mass ($M_{liquid\ +\ adjacent\ wall}$) is taken to be the thermal mass of the liquid and the part of the tank wall adjacent to it; the thermal mass of the vapor is neglected. H_f is the latent heat of vaporization.

Entity 3 of 3: Heat Into Wall Over Vapor Space

The temperature of the inner wall of the tank over the vapor is determined without assuming that it is in equilibrium with its surroundings. At any point in time, there may be a net flux of heat into the tank wall over the vapor causing its temperature to increase. The net heat flux is the heat entering the wall from the outside minus the heat leaving the wall and going into the lading. The equation below represents what is currently coded in AFFTAC:

$$M_{wall-vapor}\frac{dT_{wall-vapor}}{dt}= \qquad (5.2.24)$$
$$F_{SP}(T_{outer-Ins-vapor}-T_{wall-vapor})\mathrm{C}_1+(1-F_{SP})(T_{outer-noIns\_vapor}-T_{wall-vapor})\mathrm{C}_2$$
$$-\sigma f_{wall-liquid}(T^4_{wall-vapor}-T^4_{lading})-h(T_{wall-vapor}-T_{lading})$$

where $M_{wall\text{-}vapor}$ is the thermal mass per area of the tank wall over the vapor space, which is a product of its mass and specific heat, $f_{wall\text{-}liquid}$ is the surface configuration factor for the liquid lading surface and the tank wall above it, and C_1 and C_2 represent the conductivities for the regions with and without insulation. The $f_{wall\text{-}liquid}$ value is a function of the liquid surface angle θ, and is computed in the routine RadiationFactor. This equation is marched through time using values for the previous time step for $T_{wall\text{-}vapor}$ on the right hand side, as part of the operator splitting approach. It is solved incrementally at each time step in the routine WallTemperatureOverLading.

Aside

Modeling the tank wall over the vapor space and liquid each as having a single temperature is based on the assumption that the conditions are uniform on the inside surface of the tank. This assumption is not strictly without consequence because the temperature of the inner wall surface could be colder for regions close to the liquid's surface. 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 difference in temperature may be larger when the liquid level is near the center of the tank, calculations show that the difference would only have a small effect on the total heat transfer.

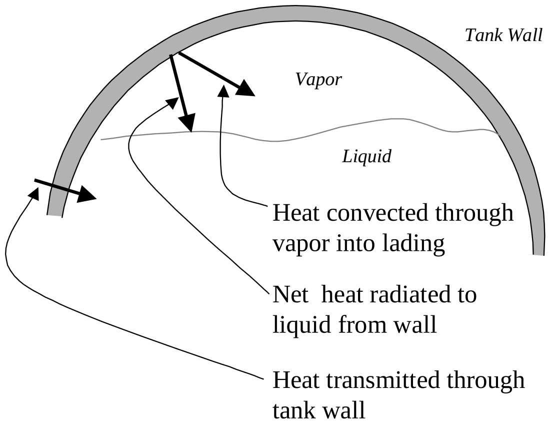


Figure 5.7: Heat balance on the liquid part of the lading.

Insulation Models

One-Dimensional Bulk Conductance

The thermal transport models described in the previous section rely heavily on composite conductances. Considering one-dimensional heat conduction through several layers, it is well known that the effective conductance, C, of the composite layer is related to the conductance, C_i, of each layer as follows:

$$\frac{1}{C} = \sum_{i=1}^{n} \frac{1}{C_i} \qquad 5.2.25$$

where n is the number of layers. Here, each C_i represents a layer in a composite system. Those layers include the tank wall itself, but also insulation, and tank linings.

AFFTAC accommodates different models for how the insulation layers and linings behave. For example, the user can specify an amount of time during which some layers deteriorate. Also, the user can specify a temperature-dependent conductivity. In that case, a nonlinear system must be solved to determine the effective conductance of the entire layer. Specifically, the conductivity may be expressed by the user as follows:

$$K(T) = K_1 + K_2 T + K_3 T^2 \qquad 5.2.26$$

Here, T is in units of ^{o}F/1000, and the conductivity K has units of (BTU/hr-ft^2)/(^{o}F/ft). The algorithm divides the insulation layer into 50 elements. It then starts at the inside of the layer and using the previous value for the effective conductance and the heat flux that it allows, it marches through the 50 elements computing the temperature distribution as it proceeds. When it arrives at the outside of the insulation, it checks to see if the temperature matches that predicted by using the previous effective conductance. If it does not, the effective conductance is adjusted and the process is repeated until convergence is achieved.

The other various insulation models in AFFTAC are a result of the different insulations used in tank cars. For example, 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-deg-F. This value would imply a conductance of 6.4 BTU/hr-ft^2-deg-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 that do not have any exterior insulation because the adjacent steel tank wall would soon be heated to over 1000 deg-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^2-deg-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-deg-F, which implies a thermal conductance of 500 BTU/hr-ft^2-deg-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.

Each of the layers discussed above are represented by a C_i in Equation (5.2.25). The approach of conductances is extended one step further by representing the heat convected across the solid-fluid boundary using the classical heat convection model,

$$Q_{wall-fluid} = A_{sharedsurface} h\left(T_{wall} - T_{fluid}\right) \qquad 5.2.27$$

where h is the film coefficient. The above relationship is couched as a conductance since it involves a linear temperature difference.

The h film coefficient is difficult to estimate since it represents fluid flow. Film coefficients 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 [5]). 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 [6]. The results of this test indicated that the average conductance over the surface of the car was 300 BTU/hr-ft^2-deg-F. The conductance of the 5/8 in. thick steel wall can be estimated at approximately 500 BTU/hr-ft^2-deg-F, which implies that the conductance for the film would be about 750 BTU/hr-ft^2-deg-F. A value of 1000 BTU/hr-ft^2-deg-F is recommended as a conservative representative value. When only vapor is present, the convection coefficient is set to 1.0 BTU/hr –ft^2-deg-F.

Mass Transport Models

The four different scenarios in which the tank car can lose lading through the safety relief device are illustrated in Figure 5.8. In the two cases where vapor alone is being ejected, the classical model for choked vapor flow, described in a subsequent section, is used. In the two cases where liquid is being ejected, it is assumed that some of the liquid might evaporate during the process resulting in two-phase flow. Therefore, a two-phase isentropic, inviscid flow model is used in some of those cases.

The flow models for choked flow and two-phase flow are discussed in the following sections. A summary of the mass transport scenarios is tabulated below.

Tank Contents	Flowing Out	Supporting Model
Liquid and Vapor	Vapor	Choked Flow or Low-Speed Flow
Liquid and Vapor	Liquid	Two-Phase Flow
Liquid	Liquid	Liquid or Two-Phase Flow
Vapor	Vapor	Choked Flow or Low-Speed Flow

Choked Flow Model

If the total pressure within the tank is greater than 27.0 psia, 12.3 psig, the flow of vapor through the relief device can be modeled as choked flow. The value of 12.3 psig is the pressure required to sustain choked flow. The classical equation for choked flow of a compressible gas flow through a nozzle is therefore used. That model is derived in detail in Appendix B and is

$$w = 144 C_d A_v P \sqrt{\frac{g\gamma}{ZRT}\left[\frac{2}{\gamma+1}\right]^{\frac{\gamma+1}{\gamma-1}}} \tag{5.3.1}$$

where

w = mass flow rate (lbs/sec)
A_v = minimum cross-sectional area of the valve (ft^2)
C_d = valve discharge coefficient
P = upstream gas pressure (psia)
T = upstream gas temperature (absolute, deg-R)
g = gravitational constant (ft/sec^2)
Z = gas compressibility factor
R = gas constant, equal to 1,545/(molecular weight) (ft/deg –R)
γ = ratio of specific heats

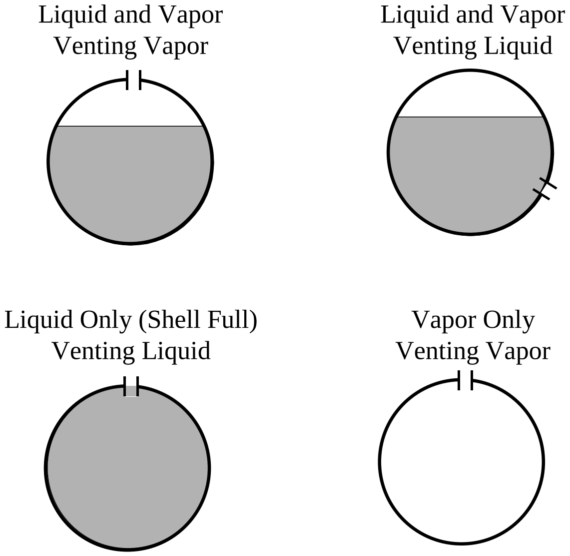


Figure 5.8: Illustration of the four different scenarios for lading release.

Most of the terms in this equation are constants and are therefore separated into a single value. Specifically, the constant V_{con} is defined as follows:

$$V_{con} \equiv 144\sqrt{\frac{g\gamma}{R}\left[\frac{2}{\gamma+1}\right]^{\frac{\gamma+1}{\gamma-1}}} \qquad 5.3.2$$

so that the first equation for the mass flow rate may be written

$$w = V_{con}\frac{C_d A_v p}{\sqrt{ZT}} \qquad 5.3.3$$

For air it is assumed that $Z = 1.0$, $\gamma = 1.4$, $R = 53.3$, $T = 519.7$ R (60 deg-F). Given the current pressure and temperature, the gas compressibility factor can be computed from user-specified tabular data. The valve discharge coefficient is a user input.

The above equation is used for each constituent in the vapor, where p becomes the constituent's partial pressure, p_i. The effect of the padding gas on the mass flow rate becomes negligible after a short period of time, because its mass is small compared to that of the lading.

The minimum cross-sectional area, A_v, is computed to be 0.0763 lbs/ft^3 using the density of air at standard conditions (60 deg-F and 14.7 psia). Substituting that into the above equation and rearranging terms allows for the minimum cross sectional area to be computed as

$$A_v = \frac{m_r}{C_d p_s 2644} \qquad 5.3.4$$

Low Speed Vapor Flow

If the total pressure within the tank is greater than atmospheric pressure (14.7 psia), but less than 12.3 psig, the flow can no longer be considered choked. In these cases, the amount of vapor flow produced during a choked condition is computed and then scaled downward accordingly.

Two-Phase Flow

When liquid escapes through the safety relief device, its pressure and temperature drops, leading to the creation of some vapor from the liquid state. The resulting situation is known as "two-phase flow" and can occur any time liquid is being ejected.

The model for two-phase flow assumes that the flow is inviscid, which means that the Bernoulli equation can be applied along any streamline. The streamline that flows through the middle of the relief device is chosen for the analysis. For any two points, 1 and 2, on the streamline, the Bernoulli equation states that

$$V_2^2(p_2) = V_1^2 + 2g\int_{p_1}^{p_2} \frac{dp}{\rho} \tag{5.3.5}$$

where V is the speed at those points and p is the pressure. Since the pressure is a function of temperature, the above integral may be rewritten as

$$V_2^2(p_2(T)) = V_1^2 + 2g\int_{p(T_1)}^{p(T_2)} \left(\frac{dp}{dT}\right)\frac{dT}{\rho(T)} \tag{5.3.6}$$

For this analysis, Point 1 is assumed to be located far from the opening so that, when there is no padding gas present, V_1 can be assumed to be zero. When padding gas is present, the saturated condition of the liquid flow through the valve will be reached after the fluid has been given some velocity. In this circumstance, the initial velocity is approximated as

$$V_1 = \sqrt{\frac{2gp}{\rho}} \tag{5.3.7}$$

In either case, V_1 is known and so is $p(T_1)$, the bulk pressure inside the tank.

For any value T_2, which corresponds to some unknown position along the streamline, the above integral can therefore be used to compute the speed $V_2(p_2)$ at a second point. The objective is to find the temperature T_2 that corresponds to the point along the streamline where the cross-sectional area of the flow is a minimum. When that point is found, it is used to compute the mass flow rate.

Point 2 is found using the above integral with the help of an additional constraint, which is that the entropy of the liquid-vapor mixture is constant. The integral form of the Bernoulli equation, plus the constraint of isentropy provides the theoretical backbone of the algorithm to compute two-phase flow through the relief device. The integral in Equation 5.3.6 is approximated as this summation:

$$V_2^2 = V_1^2 + 2g\sum_{i=1}^{?} \frac{1}{\rho(T_1 + i\Delta T)} \frac{dp}{dT}\Delta T \tag{5.3.8}$$

The summation is not carried out at once, but instead in a step-by-step fashion. Because of the temperature-pressure relationship, each addition of a term in the summation represents a small step along the streamline. At each step, the specific entropies (recall $\Delta S = \Delta Q/T$) of the liquid and vapor are computed as follows:

$$\text{Liquid State: } S_L(T) = S_{L1} - c_{p-liq}\frac{T - T_1}{(T + T_1)/2} \tag{5.3.9}$$

$$\text{Vapor State: } S_V(T) = S_L(T) + \frac{H_v}{(T + T_1)/2}$$

Where $c_{p\text{-}liq}$ is the liquid's specific heat. Based on the assumption of isentropy, the

$$\text{Combined total entropy: } S(T) = \lambda S_L(T) + (1 - \lambda)S_V(T) \tag{5.3.10}$$

must remain constant. Therefore requiring

$$S(T_{\text{`}}) = \lambda S_L(T_i) + (1 - \lambda)S_V(T_i) \tag{5.3.11}$$

at each step allows the ratio λ to be computed at each step. With the value obtained for $V(T_i)$ and the ratio λ , which allows for the density to be computed, the cross-sectional area at step i can be computed.

Calculations proceed for $i = 1, 2, \ldots,$ at each step computing λ and the cross-sectional area. When the cross-sectional area reaches a minimum value, the computations are stopped. That cross-sectional area is used with the speed and density computed at that point to provide the estimate for the mass flow rate for the two-phase flow.

This calculation is performed in the routine named Avflow.

Liquid Expansion in the Shell Full Condition

It is assumed that when the liquid expands in the shell full condition the safety relief device will open to allow for liquid to be expelled. So, that aspect is not in question and the amount of flow required to accommodate the expansion is granted by the model. However, the model attempts to determine if any *additional* lading is expelled during the current time step.

The specific volume, which is specified as a function of temperature by the user, is used to compute the expansion that would occur if completely unconstrained. Then, the Bernoulli equation is used to provide an estimate of the pressure required to expel that amount during the current time step. For this situation, which is depicted in Figure 5.9, the Bernoulli equation is

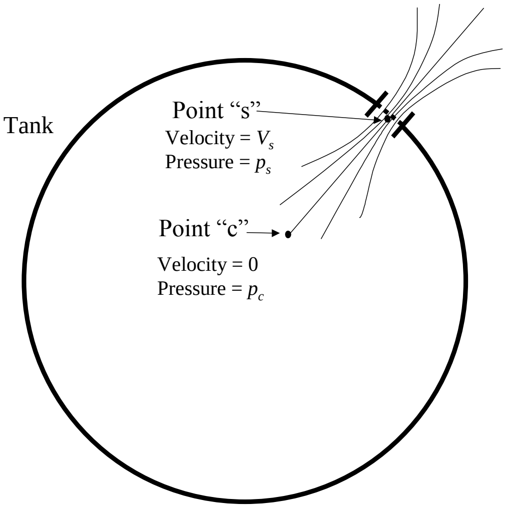


Figure 5.9: Configuration representing the expulsion of liquid due to thermal expansion while in the shell full condition.

$$\frac{1}{2}\rho V_s^2 = g(p_c - p_s) \qquad 5.3.12$$

The velocity V_s is related to the mass flow rate through the following relationship[4]

$$V_s = \frac{\text{Mass Flow Rate (lbs/sec)}}{\text{Liquid Discharge Coefficient} \times \text{Device Opening Area} \times \text{Density (lbs/ft}^3\text{)}} \qquad 5.3.13$$

all of which are known. Therefore, the Bernoulli equation can be used to determine p_c, the upstream pressure, in terms of p_s. To provide an estimate[5], p_s is assigned the value of the saturated vapor pressure or the atmospheric pressure, whichever is higher. Once p_c is computed, it is used to determine what type of flow conditions exist.

In one case, if p_s is not sufficiently high, the flow through the relief device is assumed to be in the liquid phase. It is assumed that the device will accommodate the amount of mass flow, but no more than that will leave. Therefore, the tank will remain shell full having expelled exactly the amount that is due to thermal expansion. This situation occurs for a vent if $p_s < p_{atm}$ (atmospheric pressure) and as a result, the total pressure inside the tank is set to p_{atm}. Likewise, this situation occurs for a valve if $p_s < P_{close}$ (valve closing pressure) and a result, the total pressure in the tank is set to P_{close}.

---

[4] See Appendix B for a discussion on the use of the liquid and vapor discharge coefficients.

[5] Consideration of two-phase flow effects for high vapor pressure ladings might result in a slightly lower tank pressure, but the difference would be small.

If p_s is sufficiently high (greater than p_{atm} for a vent or greater than P_{close} for a valve), it is assumed that two-phase flow occurs. In this situation, the two-phase flow model discussed previously is invoked to determine the mass flow rate. If, in the case of an upright car, enough lading can be expelled in the vapor phase so that the tank will not be shell full at the end of the time step, the tank is no longer considered to be shell full and a logical flag in the program is set to record that fact. Otherwise, the tank remains shell full.

Pressure Model

The pressure of the vapor is computed using the partial pressures of the vapor's constituents. For ladings that are a pure substance, the total vapor pressure is the sum of the vaporized lading's partial pressures plus that of the padding gas, if present. For a solution, it is the sum of the partial pressures of the solution's vaporized constituents plus the pressure of the padding gas.

When the quantity of liquid in the tank is very small, the remaining vapor is treated as an ideal gas. The temperature from the previous time step is used, thereby immediately allowing the computation of the vapor pressure p_i.

When the quantity of liquid in the tank is not small, the vapor is assumed to be saturated. The partial pressures of the lading's constituents are computed using pressure-versus-temperature data, entered in tabular form by the user. That data is queried through quadratic interpolation during the simulation.

It is assumed that the padding gas first achieves an initial state of equilibrium before the fire, but after that no further mass exchange occurs between the padding gas in the vapor and the liquid lading, which is to say that the padding gas is assumed to never diffuse into or out of the liquid, regardless of the pressure. Once the relief device has opened, the padding gas pressure is calculated from the mass of the padding gas remaining in the tank and its temperature.

> Aside:
>
> The assumption described above is believed to have little or no impact on the simulation results. The primary reason for it is the little likelihood that equilibrium conditions could ever be attained during the course of the fire. There would not be sufficient time for the effect of the padding gas' partial pressure to be communicated to all portions of the liquid within the tank for the gas to be absorbed or liberated quickly enough.
>
> Additionally, the assumption is believed to produce a conservative estimate for the padding gas pressure even though it has counteracting impacts. Specifically, during the initial stages of heating, allowing mass exchange to maintain equilibrium would cause there to be an increase in

> the amount of gas in the liquid phase caused by the initial expansion of the liquid phase due to heating. That dissolution into the liquid phase would lead to a decrease in the padding gas' partial pressure. However, counteracting that effect is the fact that, if mass exchange were allowed, then after the initial opening of the safety relief device, the decrease in pressure would lead to liberation of the padding gas from the liquid phase, causing an increase in vapor pressure and an increase flow rate through the valve.
>
> Therefore, no mass exchange of the padding gas between the vapor and liquid phases would on the one hand delay the time at which the relief device opens, but on the other hand increase the pressure after the lading begins to flow through it. To some extent, these effects would probably counteract each other. Regardless, when the space occupied by the vapor reaches approximately 10%, the effect of the padding gas becomes insignificant on the prediction of flow through the relief device.

Once the amount of liquid is small, the pressure of the padding gas is computed using the ideal gas law, still holding to the assumption of no mass exchange between the liquid and vapor phases. The user's inputs for the padding gas' initial pressure, initial volume occupied by the vapor, and initial temperature are used in conjunction with the current volume and current temperature to compute the current pressure. The embodiment of this law is expressed in:

$$p_{pad}(t) = p_{pad}(0) \times \frac{1 - f(0)}{1 - f(t)} \times \frac{T_{lading}(t)}{T_{lading}(0)} \times \frac{w_{pad}(t)}{w_{pad}(0)} \qquad 5.4.1$$

where $p_{pad}(t)$ is the pressure of the padding gas at time, t, $f(t)$ is the fraction of the tank filled with liquid at time, t, and $w(t)$ is the weight of the padding gas at time, t. In all cases, the pad gas pressure is never allowed to be negative.

Safety Relief Device Models

AFFTAC accommodates two different types of pressure relief devices. The models for these two types both have the same purpose, which is to provide an estimate for the area available for flow used in the flow models previously described. These two models are described below.

Spring-Loaded Valve

The valve-type safety relief device is spring loaded so that it remains closed unless a sufficient amount of pressure builds up inside the tank. If a certain pressure is exceeded, the valve opens an amount that is approximately proportional to the excess pressure. As lading is released and the pressure differential decreases, the valve's spring begins to close it again.

There are some subtleties to how the valve performs, most notably, hysteresis. This subtlety and others are captured in Figure 5.10. The path followed during opening is indicated by the arrows that point towards the right. Once the "Start-to-Discharge" pressure P_s is reached, the valve begins to open in proportion to the amount that pressure is exceeded. If the pressure continues to increase, the valve will eventually be fully open.

There are two paths that the valve can follow when closing. If the valve is fully open and the pressure drops below the full open pressure (103% of P_s), the valve will begin to close an amount that is proportional to the difference between the full open pressure and a reference closing pressure (88% of P_s). Once that pressure is reached, the valve will become more sensitive; the rate of closure with respect to the pressure increases until it is fully closed at 82% of P_s. That path is marked "A". The other path, marked "B", is followed if the pressure begins to drop before the valve is fully open.

Frangible Disk

The model for the frangible disk is straightforward. If the pressure differential across the disk is less than the user-specified disk burst pressure, there is no opening. However, once the pressure increases beyond that burst pressure, the disk is destroyed and the release area defined by the user is present for the remainder of the simulation.

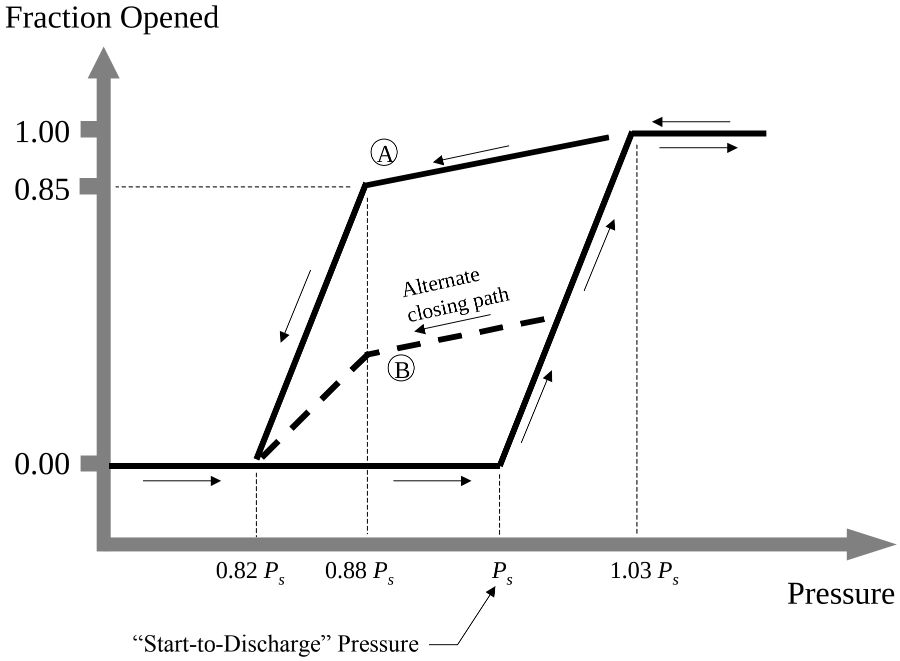


Figure 5.10: Model for the spring-loaded safety relief valve.

Strength and Deformation Models

Tank Expansion

When the tank heats up, its volume increases due to thermal expansion of the tank wall. Although this expansion is relatively small, in a shell-full condition it has an impact because as the liquid heats, it also expands and needs more room. A linear thermal expansion law is used as the basis for the tank expansion computation. It is that

$$L(T) = L_{ref}\left[1 + \alpha\left(T - T_{ref}\right)\right] \tag{5.5.1}$$

where $L(T)$ is length as a function temperature T, L_{ref} is the length at a reference temperature T_{ref}, and α is the coefficient of thermal expansion. The ratio of lengths at two different temperatures is therefore

$$\frac{L(T_2)}{L(T_1)} = \frac{1 + \alpha\left(T_2 - T_{ref}\right)}{1 + \alpha\left(T_1 - T_{ref}\right)} \tag{5.5.2}$$

T_{ref} can be taken to be zero with no loss of generality. Therefore, the relationship reduces to

$$\frac{L_2}{L_1} = \frac{1 + \alpha T_2}{1 + \alpha T_1} \tag{5.5.3}$$

If T_1 is taken to be the initial temperature of the tank, then the above ratio represents the thermal strain,

$$\varepsilon_T(T) = \frac{1 + \alpha T}{1 + \alpha T_{init}} \tag{5.5.4}$$

The tank can also expand due to internal stresses imposed through the pressure build up inside. As shown in Figure 5.11, the pressure differential represented as p in the figure is balanced by the circumferential stress inside the tank wall. Through geometrical considerations the following stress balance in the radial direction can be written:

$$2\sigma_c t_w \frac{\Delta\theta}{2} = pr\frac{\Delta\theta}{2} \tag{5.5.5}$$

Canceling terms and using half the diameter ($d/2$) instead of radius, r, produces

$$\sigma_c = \frac{pd}{2t_w} \tag{5.5.6}$$

In a similar way, the axial strain can be related to the internal pressure by writing a stress balance in the axial direction. Referring to Figure 5.12, the balance of stresses requires that

$$\left(\pi r^2\right)p = \sigma_a t_w \left(2\pi r\right) \tag{5.5.7}$$

In terms of diameter, *d*, the result is

$$\sigma_a = \frac{dp}{4t_w} \tag{5.5.8}$$

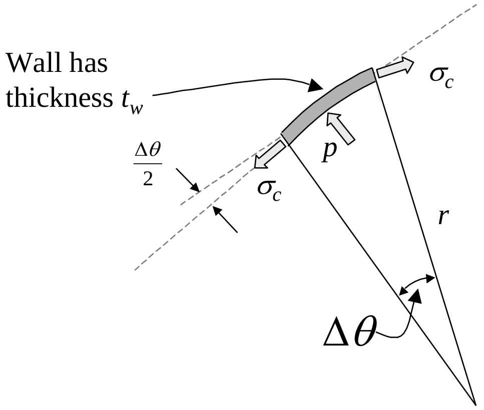


Figure 5.11: Circumferential stress in the tank wall and its relationship to the pressure differential.

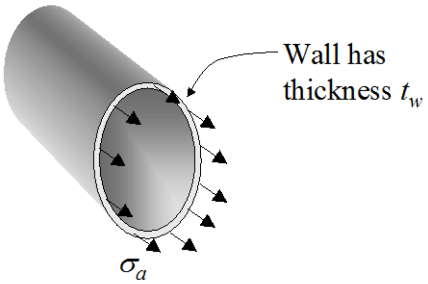


Figure 5.12: Axial stress in the tank wall.

The axial and circumferential stresses derived above are related to the corresponding strains through Hooke's law of elasticity

$$\varepsilon_c = \frac{\sigma_c}{E} - \nu \frac{\sigma_a}{E}$$
$$\varepsilon_a = \frac{\sigma_a}{E} - \nu \frac{\sigma_c}{E} \tag{5.5.9}$$

where E is Young's modulus and ν is Poisson's ratio.

The thermal strain, circumferential strain, and axial strains all contribute to a change in volume of the tank car. The thermal strain acts in all three directions and so the change in volume depends on it to the third power. The circumferential strain will act only on the circular cross section and so the change in volume depends on it to the second power. The axial strain only acts in one direction. Therefore, the new volume is due to these effects is modeled as

$$V = V_{init}(1+\varepsilon_c)^2(1+2\varepsilon_a)\left(\frac{1+\alpha T}{1+\alpha T_{init}}\right)^3 \tag{5.5.10}$$

Failure Model

Using the tensile strength of the tank and the relationship between pressure and circumferential stress derived in the previous section, the pressure at which the tank will fail can be estimated. This pressure is known as the burst pressure, and is

$$p_{burst} = \frac{2\sigma_{to} f_\sigma(T) t_{wall}}{d} \tag{5.5.11}$$

where σ_{to} is the tensile strength of the tank wall material entered by the user and $f_\sigma(T)$ is a temperature-dependent function that represents the reduction of strength with increasing temperature. This function is hard-coded inside the AFFTAC computational module for different tank wall materials. The sources for those functions are as follows:

Carbon Steel (based on TC128)	Ref. 15
Stainless Steel	Refs. 16 and 17
Aluminum Allows	Ref. 12

At the end of each time step in the time marching scheme, the tank's internal pressure is compared to the burst pressure of the tank. If the burst pressure is exceeded, then the tank is said to have failed and the simulation is terminated.

Numerics

Some of core conservation models in AFFTAC manifest themselves as first order ordinary differential equations. For example, Equation (5.2.23) is the transient equation for the lading temperature. Likewise, the mass of constituent *i* in the vapor phase is

$$\frac{dm_{vapor}}{dt} = -w + R \tag{5.6.1}$$

where *w* is the mass flow rate through the valve (zero unless discharging vapor) and *R* is the rate of evaporation of liquid.

AFFTAC uses a step-wise transient approach known as the Forward Euler with nonlinear lagging method to solve this transient equation, as well as the other transient heat and mass conservation equations. In the Euler method, the derivative is estimated as follows, for example:

$$\frac{dT_{lading}}{dt} \approx \frac{T_{lading}^{new} - T_{lading}^{old}}{\Delta t} \tag{5.6.2}$$

By substituting this approximate derivative, an equation for T_{lading}^{new} is obtained. That equation uses values of the other temperatures from the previous time step, e.g., $T_{outer-vapor}^{old}$, etc. The overall conceptual flow chart of the AFFTAC computations is shown in Figure 5.13, which illustrates the presence of the Forward Euler method.

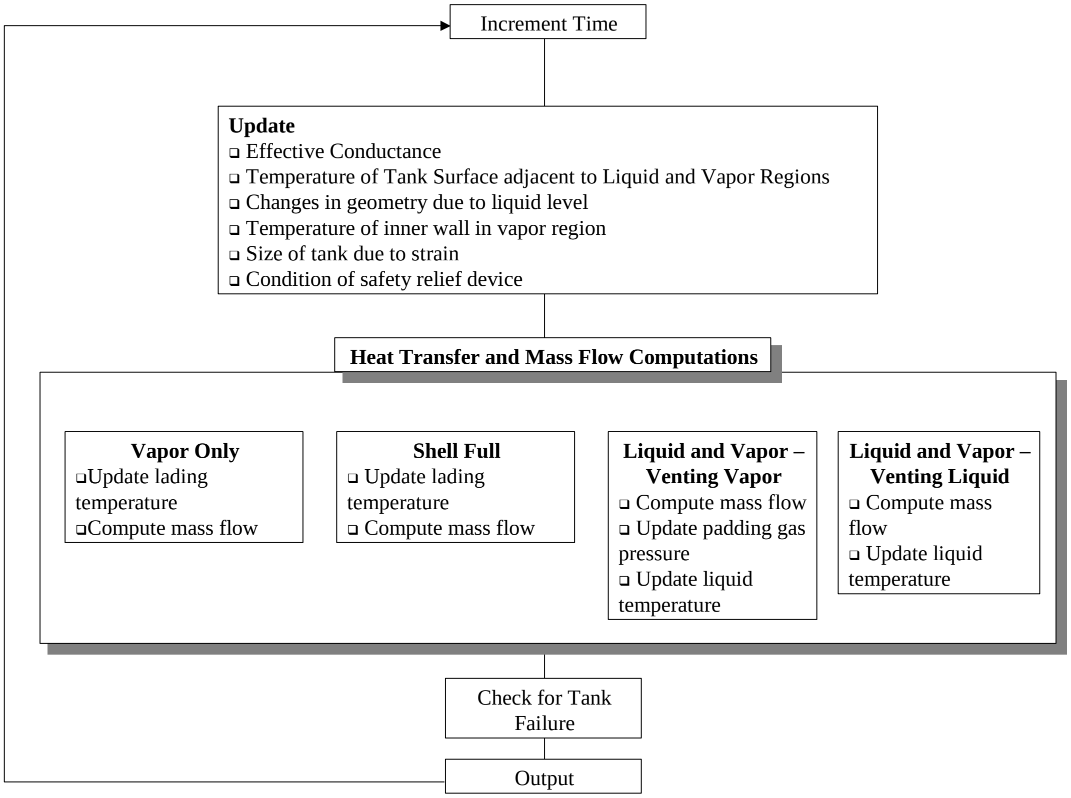


Figure 5.13: Conceptual flow chart of the AFFTAC model computations.

Dampening

The advantages and disadvantages of the Forward Euler method have been clearly discussed in the literature. The advantages are that it eliminates the need to solve nonlinear equations. Specifically, at each time step, the previous time step's solution is used to extrapolate forward in time. The disadvantage is that if the time step is too large, the extrapolation can cause the solution to overshoot acceptable bounds.

As a simple example of this phenomenon, consider two stacked blocks of wood, A and B, where A is hotter than B. Because A is hotter, heat flux will flow from it to B. The amount of heat flux is proportional to their temperature difference. So, in reality, as B warms up and A cools off, the heat flux falls off to zero. In a Forward Euler scheme, the initial temperature difference would be used to compute an initial flux between them. That flux would be multiplied by a time step and used to extrapolate to determine the temperatures at the end of the time step. If the time step is not too big, the result will be that B is a little warmer and A is a little cooler. In that case, the method works fine. But if the time step is too big, the initial flux will be extrapolated out in time too long, causing B to actually become warmer than A, and A cooler than B.

This scenario is unstable and causes the simulation to fail miserably. One approach to solving this problem is to continue to use a larger time step but arbitrarily reduce the flux used for extrapolation. The effect is to dampen the transient behavior. Although there are errors associated with this approach, often an appropriate dampening factor can be used that causes the solution to be stable. Although the transient solution will be in error, the steady state solution will still be correct, unless nonlinear effects play a dominant role.

AFFTAC makes heavy use of this approach. It is manifested in the source code as a weighted average between the previous time step's solution for, say, temperature, and the prediction for the temperature at the new time step, e.g.,

$$T^{new} = \alpha T^{old} - (1-\alpha)\hat{T}^{new} \tag{5.6.3}$$

where $\hat{T}^{new}$ is the value predicted without dampening. Typically, $0.25 < \alpha < 0.5$. In addition to the thermal solution values, dampening is also used for the auxiliary models. For example, in computing the change in volume due to thermal expansion and the pressure differential, the new value for the volume is dampened using $\alpha = 1/3$.

Overshoot

A problem similar to the instability problem discussed above is that of overshoot. For example, during the choked flow computations, if the resulting pressure after discharge during the time step 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, the out-flows are arbitrarily reduced. This compensation is required because of the consequences due to the 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.

Testing

Partial Insulation Coverage Tests

The AFFTAC computational module has three regression tests, which are Examples 6.1.1,. 6.1.2, 6.1.3, 6.2 and 6.3 in [1]. In addition to these tests, more tests have been developed to test the more sophisticated models for partial coverage of insulation inside the steel jacket. These tests are documented here.

Extreme Values Tests

Test cases 6.1.1, 6.1.2, 6.1.3, 6.2, and 6.3 [1] are modified so that they all use the “Steel Jacketed” (Option 3) thermal protection system, with an initial conductance of 0.22 Btu/hr-ft^2 deg-F and a near-infinite interval for change (e.g., 999999 min for “Time interval for change”). However, the fraction of the tank covered by that system is set to zero. These cases are then renamed as follows:

6.1.1 → 1.1a
6.1.2 → 1.2a
6.1.3 → 1.3a
6.2 → 2a
6.3 → 3a

Duplicates of these cases are made, except the insulation system is changed so that it has an instantaneous decay time but 100% coverage of the tank. The test cases are named as follows:

6.1.1 → 1.1b
6.1.2 → 1.2b
6.1.3 → 1.3b
6.2 → 2b
6.3 → 3b

Since there should be no difference between an insulation that does not decay but also does not cover the tank at all and an insulation that decays instantly but covers the tank fully, the results for the "a" and "b" versions should be identical.

In a similar way, two more sets of test cases are developed and named as follows:

6.1.1 → 1.1c and 1.1d
6.1.2 → 1.2c and 1.2d
6.1.3 → 1.3c and 1.3d
6.2 → 2c and 2d
6.3 → 3c and 3d

The "c" cases use Option 5, "Temperature Dependent" thermal protection system with K_1 = 0.017, K_2 = 0.014, and K_3 = 0.011. In case "c", the coverage is set to zero and the thickness of the insulation is set to 1 inch. In case "d", the "Bare Tank" option (Option 1) is chosen. The results should be the same.

The same test used above is also used for the temperature-independent (Option 4) system and the FRA-standard (Option 2) system.

Lastly, two more test case sets, "e" and "f" are created in an analogous way. Sets "e" use the 2-component Steel Jacketed system (Option 6) with zero coverage. Sets "f" use the Steel Jacketed system (Option 3) with 100% coverage, but with instantaneous decay (i.e., the "Time interval for change" is set to zero). These results should also be the same. Note: In testing version 04.02.04, the results are close but were not identical.

Contrived Values Test

A more rigorous test of the partial coverage capability requires the following modifications:

1. `SurfaceT` – At the end of the routine, artificially set $T_w = T_{outer\_liquid}$ and $T_w = T_{outer\_vapor}$.
2. `GetWallConductance` – Artificially set the composite conductivity for the liquid and vapor regions equal for both the bare tank case (Option 1) and the temperature-independent insulation case (Option 4).

Then, two versions "g" and "h" of the original test cases discussed above are created. Both use temperature-independent insulation (Option 4) with time-constant insulation. The parameters for Option 4 are obtained by making reference to Figure 6.1, with the modifications described above in mind. A unit of the tank is considered, wherein the outer surfaces of the insulated and non-insulated surfaces are forced to be the same temperature. A fraction F_i is covered by insulation with conductivity c_i. The tank conductivity is C_T, and is the same in the liquid and the vapor regions (again, via code modification). The heat flux q_i is

$$q_i = \frac{c_i c_T}{c_i + c_T} \Delta T F_i + c_T \Delta T (1 - F_i) \tag{6.1.1}$$

The heat fluxes for cases "g" and "h", q_g and q_h, can be expressed using the above equation. Furthermore, by equating them and setting $c_h = Mc_g$, the following equation results:

$$F_h = F_g \left(\frac{Mc_g + c_T}{c_g + c_T} \right) \tag{6.1.2}$$

Next, M is arbitrarily chosen to be 10 and F_g to be 100%. The result is the following:

Case "g": Constant conductivity of 54 BTU/hr-ft^2 deg F at 100% coverage
Case "h": Constant conductivity of 5.4 BTU/hr-ft^2 deg F at 88% coverage

The results for these two sets of cases (1.1g, 1.2g, 1.3g, 2g and 3g and the corresponding "h" versions) should be identical. When run in AFFTAC, the results are close but not identical because of numerical aspects. Specifically, the higher conductivity used in case "h" requires a smaller time step. By reducing the time step from the original test cases, the results for "g" and "h" can be brought into acceptably close agreement.

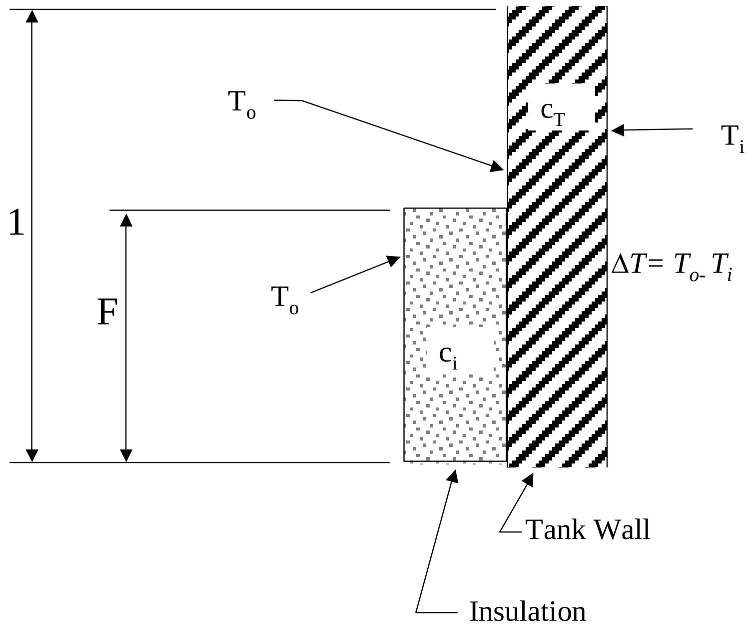


Figure 6.1: Contrived test case for testing partial coverage of insulation/thermal protection.

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Appendix A: Default Ladings

By Milton Johnson, Ph.D.

The use of default values for the thermal properties is not recommended. If at all possible, a search for the thermal properties of a lading should be conducted and the values that are obtained entered into the AFFTAC database. If this is not feasible, then the default lading templates may be used, keeping in mind the following guidelines that have been followed to estimate their thermal properties. These guidelines do not apply to tank cars transporting cryogenic liquids, compressed gases such as helium, or slurries/products, such as liquid sulfur, which solidify upon heating. If the product being considered is a solution, it should be treated as though it were a substance for the purpose of obtaining default values and the following guidelines should be used.

Vapor Pressure

The test pressure of the tank car class authorized to transport a product is often an indication of the vapor pressure of the product. Therefore, two sets of values for default vapor pressure data are provided, one for products that would be shipped in non-pressure cars having a test pressure of 100 psi and the other for products that must be shipped in pressure tank cars having a test pressure of 300 psi or greater. Some products that have low vapor pressures, e.g. products classified as poison by inhalation, must be shipped in pressure tank cars even though they may have low vapor pressures. This is done to require the use of a stronger tank car providing added safety in the shipment of the product. The suggested vapor pressures given below could be substantially over estimated for those ladings.

Assuming that liquefied gases are shipped in pressure cars and liquids are shipped in non-pressure cars, the vapor pressure property values are estimated as follows:

Liquids (non-pressure cars)

Temperature (°F)	Vapor Pressure (psia)
60	5
150	40
240	125

Liquefied gasses (pressure cars)

Temperature (°F)	Vapor Pressure (psia)
60	140
120	300
180	570

Some products, such as bromine, chlorine and hydrogen cyanide, must be shipped in tank cars having a test pressure of 500 psi or greater. This is done not because they have high vapor pressures, but to insure they are shipped in stronger, safer cars. The vapor pressures given above for pressure tank cars would be conservative for these products.

Specific Heat

There is a wide range of values for the specific heat of the liquid for products shipped in tank cars. Values can range from over 1.00 BTU/lb-°F, for solutions containing a large percentage of water, to as low as 0.10 BTU/lb-°F for bromine at about 200 °F. Also, for most products the specific heat tends to rise with increasing temperature, but for some products (e.g. bromine) it decreases. This makes it difficult to suggest default properties for specific heat that are conservative, but not overly conservative. Since the specific heat of the liquid determines the rate of temperature increase of the product with a given heat input, it is obvious that lower values for this parameter will lead to more conservative analyses. The following default values are suggested, although they may not always lead to conservative results:

Temperature (°F)	Specific Heat (BTU/lb-°F)
60	0.40
300	0.70

Specific Volume

It is assumed that the density of the product is known. The specific volume is simply the inverse of this value expressed in ft^3/lb. Since the density of materials tend to decrease with increasing temperature, the specific volume will increase with increasing temperature.

Again, there is a considerable variation of this rate of increase among products shipped in tank cars making it difficult to suggest default properties. Values range from an increase in specific volume of 13 percent for chlorosulfonic acid in the temperature range from 50 to 302 °F to a 70 percent increase for hydrogen fluoride in the same temperature range. The rate of increase in specific volume with temperature is an important parameter when the tank car becomes shell full and liquid is being expelled through the valve, a larger valve capacity for liquid flow being required when the rate of increase is higher. Tentative values are suggested as follows.

Liquids (non-pressure cars) or Liquefied Gases Containing at least 50% water

Temperature (°F)	Percentage increase in Specific Volume from Ambient Value
60	Ambient Value
180	10%
300	30%

Liquefied gasses (pressure cars)

Temperature (°F)	Percentage increase in Specific Volume from Ambient Value
60	Ambient Value
150	20%
240	50%

Heat of Vaporization

There is also considerable variation in the heat of vaporization among products shipped in tank cars ranging from about 1000 BTU/lb for solutions containing a high percentage of water to less than 100 BTU/lb, for products such as bromine, methyltrichlorosilane, titanium tetrachloride and phosphorus trichloride. Other factors being equal, a lower heat of vaporization will result in the generation of greater volume of vaporized product requiring a larger capacity pressure relief valve. The heat of vaporization decreases with increasing temperature. The following default values are suggested although they may not be conservative in all cases:

Temperature (°F)	Heat of Vaporization BTU/lb
60	300
240	100

If the product is a solution containing at least 50 percent water as the solvent, the following values are suggested:

Temperature (^{o}F)	Heat of Vaporization BTU/lb
60	800
240	300

Compressibility Factor

This parameter does not have a major influence on the calculations. A default value of 0.9 is suggested for the compressibility factor of product vapor. It would be entered into the program at two values for temperature (e.g. 60 and 300 ^{o}F).

Ratio of Specific Heats

This parameter does not have a major influence on the calculations. A default value of 1.1 is suggested for the ratio of specific heats of product vapor. It would be entered into the program at two values for temperature (e.g. 60 and 300 ^{o}F).

Appendix B: Vapor Flow Derivation

The primary reference for these derivations is given in [19].

Applications of the First Law of Thermodynamics

Application to Quasi-Static Process

In this section, thermodynamic relationships are derived that describe intrinsic responses of the fluid, without consideration of a system. To derive these relationships, consider fluid in a quasi-static process, where p is uniform. The differential form of the First Law of Thermodynamics (hereafter, "First Law") reduces to

$$dq - dw = du \qquad \text{B.1}$$

where u is the internal energy of the fluid, q is the heat transferred into the fluid, and w is the work done by the fluid.

If this process is adiabatic, reversible (isentropic), $dq = 0$. Also, fluid alone can only do work intrinsically through expansion, so $dw = pdv$. Therefore, the First Law for the fluid is

$$du = -pdv\,. \qquad \text{B.2}$$

The specific heat at constant volume, c_v, is defined as

$$c_v \equiv \frac{du}{dT} \qquad \text{B.2}$$

or

$$du = c_v dT \tag{B.4}$$

so that

$$c_v dT = -pdv\,. \tag{B.5}$$

Returning to Equation B.2 and adding *pdv* to both sides,

$$du + pdv + vdp = vdp \tag{B.6}$$

which means that

$$d(u + pv) = vdp \tag{B.7}$$

or

$$dh = vdp \tag{B.8}$$

where $h = u + pv$ is enthalpy. The specific heat at constant pressure, c_p, is defined as

$$c_p \equiv \frac{dh}{dT} \tag{B.9}$$

or

$$dh = c_p dT \tag{B.10}$$

so that

$$c_p dT = vdp\,. \tag{B.11}$$

Divide Equation B.11 by B.5, to get

$$\frac{c_p}{c_v} = -\frac{vdp}{pdv}\,. \tag{B.12}$$

Rearrange,

$$-\frac{c_p dv}{c_v v} = -\frac{dp}{p}\,, \tag{B.13}$$

and define the ratio of specific heats as $k=c_p/c_v$, so that

$$-k\frac{dv}{v}=\frac{dp}{p}\,. \qquad \text{B.14}$$

Assume a constant ratio (k) of specific heats, and integrate:

$$-\int k\frac{dv}{v}=\int\frac{dp}{p} \qquad \text{B.15}$$

$$pv^k=\text{constant}\,. \qquad \text{B.16}$$

The above equation means that the product of pressure and specific volume is everywhere constant in the quasi-static process. Introducing "*i*" to denote an inlet and "*o*" to denote and outlet, the above equation implies that

$$p_i v_i^k = p_o v_o^k \qquad \text{B.17}$$

$$\frac{p_i}{p_o}=\left(\frac{v_o}{v_i}\right)^k \qquad \text{B.18}$$

For an ideal gas, $pv=RT$ so that the above equation may be written as

$$\frac{T_i v_o}{T_o v_i}=\left(\frac{v_o}{v_i}\right)^k \qquad \text{B.19}$$

or

$$\frac{T_i}{T_o}=\left(\frac{v_o}{v_i}\right)^{k-1} \qquad \text{B.20}$$

The ideal gas law, $pv=RT$, can be applied again, to produce

$$\frac{T_i}{T_o}=\left(\frac{RT_o/p_o}{RT_i/p_i}\right)^{k-1}=\left(\frac{T_o p_i}{T_i p_o}\right)^{k-1} \qquad \text{B.21}$$

Manipulation of the above equation results in

$$\frac{T_i}{T_o}=\left(\frac{p_i}{p_o}\right)^{k-1\!\!\not\,k} \qquad \text{B.22}$$

Application to a Control Volume

The differential form of the First Law of Thermodynamics for a system ("First Law") is as follows,

$$dQ - dW = dE \qquad \text{B.23}$$

where

$$\begin{aligned} Q &= \text{heat transferred in to the system} \qquad \text{B.24} \\ W &= \text{work done by the system} \\ E &= \text{energy in the system} \end{aligned}$$

The right-hand side has to do with the state of the fluid in the system. Since fluid can move through the system, it is helpful to highlight that fact when writing the First Law as time derivatives. In particular, the energy time derivative must be a "substantial" derivative (i.e., follows the substance which is the fluid). Capital "*D*" is used for that purpose, and the time-derivative form of the First Law may be written as

$$\frac{dQ}{dt} - \frac{dW}{dt} = \frac{DE}{Dt} \qquad \text{B.25}$$

It is necessary at this point to more firmly establish the notion of a control volume, which will be denoted here by Ω. The Reynolds Transport Theorem accounts for the fact that the substance (fluid) flows through the control volume. In taking the flow into account, the First Law, which is meant to apply to a system, can be made to handle the situation where fluid flows through the system. The derivation of the Reynold's Transport Theorem can be made from geometrical considerations and can be applied to any material state variable. For energy, it is stated as follows:

$$\frac{DE}{Dt} = \int_{\partial\Omega} e\rho\mathbf{V}\cdot\hat{\mathbf{n}}dA + \frac{\partial}{\partial t}\int_{\Omega} e\rho dv \qquad \text{B.26}$$

where $\partial\Omega$ is the boundary of Ω, *e* is the material-intensive energy, **V** is the velocity vector at the boundary, and $\hat{\mathbf{n}}$ is the outward normal at the boundary.

For steady-state flow, the second term on the right-hand side is zero. Using the resulting expression for *DE/Dt* in the First Law,

$$\frac{dQ}{dt} - \frac{dW}{dt} = \int_{\partial\Omega} e\rho\mathbf{V}\cdot\hat{\mathbf{n}}dA. \qquad \text{B.27}$$

It is helpful to separate the work term on the left-hand side into two parts:

$$\frac{dW}{dt} = \frac{dW_s}{dt} + \int_{\partial\Omega} \mathbf{T} \cdot \mathbf{V} dA = \text{"Shaft work rate"} + \text{"Flow work rate"} \tag{B.28}$$

where **T** is the stress tensor. The product of **T** and **V** represent stress through a distance, per time. When integrated over an area, it represents the rate of work done by the fluid.

The first term is the rate of work done on the fluid by moving parts inside the control volume (e.g., a fan). For flow through the safety relief device, there are no moving parts that do any appreciable work on the fluid, so the “shaft work rate” is zero, which leaves only the flow work rate, so that

$$\frac{dW}{dt} = \int_{\partial\Omega} \mathbf{T} \cdot \mathbf{V} dA. \tag{B.29}$$

In flow through the safety relief device, it is assumed the flow is frictionless, so the only stress at the surface is normal stress. In other words,

$$\mathbf{T} = p\hat{\mathbf{n}} \tag{B.30}$$

So, the flow work rate is

$$\frac{dW}{dt} = \int_{\partial\Omega} \mathbf{T} \cdot \mathbf{V} dA = \int_{\partial\Omega} p\mathbf{V} \cdot \hat{\mathbf{n}} dA. \tag{B.31}$$

Substituting this expression for the work term on the left-hand side of the First Law produces the following form of the First Law:

$$\frac{dQ}{dt} - \int_{\partial\Omega} p\mathbf{V} \cdot \hat{\mathbf{n}} dA = \int_{\partial\Omega} e\rho\mathbf{V} \cdot \hat{\mathbf{n}} dA \tag{B.32}$$

In the release of vapor through the safety relief device, the flow is sufficiently fast to completely neglect any heat exchanged between the fluid and the valve. Hence, the flow is adiabatic/isentropic and the *dQ/dt* term is zero, and the First Law becomes

$$-\int_{\partial\Omega} p\mathbf{V} \cdot \hat{\mathbf{n}} dA = \int_{\partial\Omega} e\rho\mathbf{V} \cdot \hat{\mathbf{n}} dA. \tag{B.33}$$

The term on the left-hand side can be combined with the term on the right-hand side by inserting ρv, which is unity. Doing so produces

$$-\int_{\partial\Omega} pv\rho\mathbf{V} \cdot \hat{\mathbf{n}} dA = \int_{\partial\Omega} e\rho\mathbf{V} \cdot \hat{\mathbf{n}} dA. \tag{B.34}$$

Then, combining the two integrals,

$$\int_{\partial\Omega} \rho(e + pv)\mathbf{V} \cdot \hat{\mathbf{n}} dA = 0 \qquad \text{B.35}$$

The energy of the material is comprised of kinetic, gravitational potential, and internal energy. In other words,

$$e = \frac{V^2}{2} + gz + u \qquad \text{B.36}$$

where g is the acceleration due to gravity, z is the height above a datum, and u is the internal energy. Inserting this expression for energy into the preceding equation produces the following form of the First Law:

$$\int_{\partial\Omega} \rho\left(\frac{V^2}{2} + gz + u + pv\right)\mathbf{V} \cdot \hat{\mathbf{n}} dA = 0 . \qquad \text{B.37}$$

In flow through the safety relief device, there is no appreciable altitude change. Therefore, the total surface integral of gz can be neglected. And so the First Law becomes

$$\int_{\partial\Omega} \rho\left(\frac{V^2}{2} + u + pv\right)\mathbf{V} \cdot \hat{\mathbf{n}} dA = 0 . \qquad \text{B.38}$$

Using enthalpy, which is defined as $h = u + pv$, the First Law can be expressed as

$$\int_{\partial\Omega} \rho\left(\frac{V^2}{2} + h\right)\mathbf{V} \cdot \hat{\mathbf{n}} dA = 0 . \qquad \text{B.39}$$

At this point, the surface integral can be simplified in two ways:

1. In the present application, the surface area is comprised of only one inlet and one outlet. The areas for the inlet and outlet are A_i and A_o, respectively.
2. An approximation is made concerning the direction of the flow at the inlet and outlet. It is assumed that the flow is normal to the control volume (A_i and A_o), which means that the dot product between velocity and the surface normal vector is simply the magnitude of the velocity (V).

Under these assumptions,

$$\left(\frac{V_o^2}{2}+h_o\right)\rho_o A_o V_o=\left(\frac{V_i^2}{2}+h_i\right)\rho_i A_i V_i\,. \tag{B.40}$$

The products of density, area, and velocity that appear on both sides of the above equation are expressions of mass flow rate. Conservation of mass therefore means that these two products must be equal and therefore cancel. And so the First Law becomes,

$$\frac{V_o^2}{2}+h_o=\frac{V_i^2}{2}+h_i\,. \tag{B.41}$$

The control volume for this application is chosen to be such that the velocity at the inlet is very small such that V_i^2 is negligible. Under that assumption, the First Law is

$$\frac{V_o^2}{2}+h_o=h_i\,. \tag{B.42}$$

Next, it is assumed that the specific heats are constant, i.e., that

$$c_p\equiv\frac{dh}{dT} \tag{B.43}$$

is a constant. With c_p being a constant, the above equation may be integrated such that

$$h-h_d=c_p\left(T-T_d\right). \tag{B.44}$$

Here, h_d-T_d is an arbitrary datum. Substituting this expression into the First Law produces

$$\frac{V_o^2}{2}+c_p\left(T_o-T_d\right)=c_p\left(T_i-T_d\right). \tag{B.45}$$

The T_d terms cancel, and thus

$$\frac{V_o^2}{2}+c_pT_o=c_pT_i\,. \tag{B.46}$$

Dividing by T_o,

$$\frac{V_o^2}{2T_o}+c_p=c_p\frac{T_i}{T_o} \tag{B.47}$$

and then by c_p,

$$\frac{V_o^2}{2c_pT_o}+1=\frac{T_i}{T_o}\,. \qquad \text{B.48}$$

In Appendix C, it is shown that for an ideal gas, $c_p=\left(\frac{k}{k-1}\right)R$. Using that fact, the First Law becomes

$$\frac{V_o^2}{kRT_o}\frac{(k-1)}{2}+1=\frac{T_i}{T_o}\,. \qquad \text{B.49}$$

Also, for an ideal gas, $c^2=kRT$, and this term appears in the above equation. Therefore, the ratio $\frac{V_o^2}{kRT_o}=\frac{V_o^2}{c^2}=M^2$, where M is the Mach number (the ratio of speed to the speed of sound). The First Law in terms of M is

$$M^2\frac{(k-1)}{2}+1=\frac{T_i}{T_o} \qquad \text{B.50}$$

Inverting the above equation,

$$\frac{T_o}{T_i}=\frac{1}{1+M^2\frac{(k-1)}{2}} \qquad \text{B.51}$$

Using Equation B.22, the First Law may be written as

$$\left(\frac{p_o}{p_i}\right)^{k-1/k}=\frac{1}{1+\frac{(k-1)}{2}M^2} \qquad \text{B.52}$$

or

$$\frac{p_o}{p_i}=\frac{1}{\left(1+\frac{(k-1)}{2}M^2\right)^{k/k-1}} \qquad \text{B.53}$$

Mass Flow for an Ideal Gas

The mass flow rate is

$$G = \rho VA \qquad \text{B.54}$$

where

$$\begin{aligned}\rho &= \text{density} \\ V &= \text{average velocity} \\ A &= \text{area of flow}\end{aligned} \qquad \text{B.55}$$

For an ideal gas,

$$\rho = p / RT \qquad \text{B.56}$$

where

$$\begin{aligned}p &= \text{pressure} \\ R &= \text{gas constant}\end{aligned} \qquad \text{B.57}$$

By substitution of the ideal gas law into the mass flow rate equation,

$$G = \frac{p}{RT} VA \qquad \text{B.58}$$

The following step is simple algebra. The *RT* term is split into two square roots and a form of unity (*k/k*) is introduced. The value *k* is the ratio of the vapor's specific heats, and will be described more fully later.

$$G = pA \frac{V}{\sqrt{kRT}} \sqrt{\frac{k}{RT}} \qquad \text{B.59}$$

For an ideal gas, the speed of sound, *c*, is

$$c = \sqrt{kRT}\,. \qquad \text{B.60}$$

For an ideal gas the Mach number is

$$M = \frac{V}{c} = \frac{V}{\sqrt{kRT}} \qquad \text{B.61}$$

The Mach number can therefore be used in the expression for the mass flow rate as follows:

$$G = pAM\sqrt{\frac{k}{RT}} \qquad \text{B.62}$$

Introducing the subscript "*o*" for "outlet," the above equation may be used to express the mass flow rate at the outlet of a control volume,

$$G = p_o AM\sqrt{\frac{k}{RT_o}} \qquad \text{B.63}$$

Into this equation, pressures and temperatures at the inlet (subscript "*i*") will be introduced in ratios that equal unity. Then the terms are rearranged:

$$G = p_o AM\sqrt{\frac{k}{RT_o}}\left(\sqrt{\frac{T_i}{T_i}}\,\frac{p_i}{p_i}\right) \qquad \text{B.64}$$

or

$$G = \frac{p_o}{p_i} AM\sqrt{\frac{k}{R}}\sqrt{\frac{T_i}{T_o}}\,\frac{p_i}{\sqrt{T_i}} \qquad \text{B.65}$$

Into this equation, the relationships derived earlier for p_o/p_i and T_o/T_i (Equations B.51 and B.53) are substituted:

$$G = \frac{MA}{\left(1+\frac{(k-1)}{2}M^2\right)^{(k+1)/2(k-1)}}\sqrt{\frac{k}{R}}\,\frac{p_i}{\sqrt{T_i}} \qquad \text{B.66}$$

For $M=1$,

$$G\big|_{M=1} = p_i A\left(\frac{2}{(k+1)}\right)^{(k+1)/2(k-1)}\sqrt{\frac{k}{RT_i}} \qquad \text{B.67}$$

Or, combining terms,

$$G\big|_{M=1} = p_i A\sqrt{\frac{k}{RT_i}\left(\frac{2}{(k+1)}\right)^{k+1/k-1}} \qquad \text{B.68}$$

Use of Discharge Coefficient for Flow through Relief Device

AFFTAC's Choked Vapor Flow Model

Equation B.68 is an idealized model and therefore has to be adjusted for use with real relief devices. This adjustment is made by measuring the flow rate of a real device at critical flow (i.e., choked flow, where $M = 1$) and using that experimental result to adjust the prediction of the model through a fitting parameter, which is called the "vapor discharge coefficient," C_{Dv}. Therefore, Equation B.68 becomes

$$G_{AFFTAC-\text{ChokedFlow}} = p_i A C_{Dv} \sqrt{\frac{k}{RT_i}\left(\frac{2}{(k+1)}\right)^{k+1/k-1}} \qquad \text{B.69}$$

The flow path through a safety relief device does not have a single representative cross-sectional area. In other words, A in Equation B.69 is not a value that can simply be taken from the geometry a real device. Therefore, in practice, instead of determining C_{Dv} from experimental data, the product AC_{Dv} is determined [20].

If $G_{\exp}$ represents the mass flow rate at critical (choked) flow, then from Equation B.69,

$$G_{\exp} = p_{\exp} A C_{Dv} \sqrt{\frac{k}{RT_{\exp}}\left(\frac{2}{(k+1)}\right)^{k+1/k-1}} \qquad \text{B.70}$$

where the subscript "exp" refers to known, experimental conditions. Solving for AC_{Dv},

$$AC_{Dv} = \frac{G_{\exp}}{p_{\exp}\sqrt{\frac{k}{RT_{\exp}}\left(\frac{2}{(k+1)}\right)^{k+1/k-1}}} \qquad \text{B.71}$$

To recapitulate, the *idea* behind AFFTAC's vapor flow model through the safety relief device is to use experimental conditions to compute AC_{Dv}. It then uses AC_{Dv} in Equation B.69 to compute the mass flow rate for choked flow. AFFTAC assumes that choked flow occurs when the pressure differential is greater than a hard-coded value of 12.3 psig.

Although the *idea* behind the calculations is fairly straightforward, as implemented in AFFTAC they are slightly more complex. First, as will be discussed in a later section, the *liquid* flow model borrows from the vapor flow model an effective area, A. Therefore, although in principle a value of A, separate from C_{Dv} is not required for the vapor flow model, it is nevertheless computed. Rearranging Equation B.71 to represent the computation produces

$$A = \frac{G_{\exp}}{C_{Dv} p_{\exp} \sqrt{\frac{k}{RT_{\exp}} \left(\frac{2}{(k+1)} \right)^{k+1/k-1}}} \qquad \text{B.72}$$

If one were to substitute Equation B.72 into Equation B.69, the C_{Dv} terms would cancel, thereby reinforcing the fact that C_{Dv} is not needed in the vapor flow calculation itself. However, for the purposes of computing an area used in the liquid flow model, it is needed. Equation B.72 corresponds to the source code line in AFFTAC,

```
avlv = ValveFlowCapacity /(DischargeCoef_Vap*pasd*2644.0);
```

This value is scaled further because of how the relief device may only be partially open. Specifically, the experimental valve flow capacity is scaled, depending on the state of the relief valve. For example,

```
tcfm = ValveFlowCapacity *(0.85+0.15*(ptot-prtn)/(popn-prtn)) ;
```

is a type of computation used to compute a new valve flow capacity that depends on the state of the valve. Then, finally, `avlv` and `tcfm` are combined to compute an effective valve area, using this line of source code,

```
EffectiveValveArea = avlv*tcfm/ ValveFlowCapacity;
```

In the above three lines of source code, note that the variable `ValveFlowCapacity` appears three times, eventually canceling in such a way that only one remains. The `EffectiveValveArea` is then used in Equation B.69, which in the AFFTAC source code appears as

```
wsbout = psbs*EffectiveValveArea*DischargeCoef_Vap*vlsbcn*60.0*delt/sqrt(tempr*zsbs);
```

Notice here that `DischargeCoef_Vap` appears in the denominator of `avlv`, but in the numerator of `wsbout`, thereby canceling computationally.

The value `EffectiveValveArea` is used in AFFTAC's mixed-phase flow model, along with the liquid discharge coefficient, to compute the mass flow rate when the tank is overturned.

AFFTAC's Sub-Sonic Vapor Flow Model

If the pressure is not sufficiently high, then it is assumed choked flow has not occurred, and so $M<1$. Therefore, the applicable equation is not Equation B.68, but rather its predecessor, Equation B.66, which modified to include the vapor discharge coefficient results in

$$G_{\text{sub-sonic}} = \frac{M\left(AC_{Dc}\right)}{\left(1+\frac{\left(k-1\right)}{2}M^{2}\right)^{(k+1)/2(k-1)}}\sqrt{\frac{k}{R}}\frac{p_i}{\sqrt{T_i}} \tag{B.73}$$

However, it is noted here that AFFTAC instead uses a simplified linear model for sub-sonic flow. Specifically, AFFTAC computes the flow rate as if the flow is choked, and then linearly scales it according to pressure. This simplification in AFFTAC is probably unneeded, since the compact analytical form is readily available in Equation B.72.

Appendix C: Thermodynamic Identities for an Ideal Gas

By definition,

$$c_p = \frac{dh}{dT} = \frac{d}{dT}\left(u + pv\right) \tag{C.1}$$

For an ideal gas,

$$pv = RT \tag{C.2}$$

And so

$$c_p = \frac{d}{dT}\left(u + RT\right) = c_v + R \tag{C.3}$$

Therefore,

$$c_p - c_v = R \tag{C.4}$$

Dividing both sides by c_v,

$$\frac{c_p}{c_v} - 1 = \frac{R}{c_v} \tag{C.5}$$

The ratio of specific heats appears often and is defined here as k,

$$k \equiv \frac{c_p}{c_v} \tag{C.6}$$

Therefore, using this definition,

$$\begin{aligned} k - 1 &= \frac{R}{c_v} \\ &= \frac{Rk}{c_p} \end{aligned} \tag{C.7}$$

so that

$$c_p = \left(\frac{k}{k-1} \right) R \tag{C.8}$$