

Appendix G. ChemSTEER Case Study

Mock PMN Information

EPA primary uses ChemSTEER to assess new chemicals submitted for PMN review under TSCA section 5. This Case Study presents a hypothetical set of input values developed for a “mock” PMN. These values are consistent with information typically submitted for a new chemical review. The ChemSTEER spreadsheet formats of this information is shown on the following pages.

Brief Description of the Scenario

The chemical that is being assessed is a semivolatile liquid used as a chemical intermediate. It is manufactured in formulation at a concentration of 80%. The formulation is then sold to other facilities to be used in other reactions (i.e., the chemical will be destroyed in the reactions).

The manufacturers perform QC sampling of the formulation before it is loaded into drums for distribution to the users. The manufacturers also clean the reactor vessel once every 5 batches.

The users receiving the drums of the intermediate formulation containing the chemical (at a concentration of 80%) pump it from the drums and into the process. When a drum is emptied, the residues are rinsed with a solvent that is subsequently incinerated.

Information on the Chemical to be Assessed

- Production volume (PV) = 100,000 kg/yr
- Name = “Case Study Chemical”
- Molecular weight = 150
- Vapor pressure = 1 torr
- Density = 0.815 g/cm³

Information on the Manufacture

- Performed at one site
- Batch size is 1,000 kg of the formulated product (80% chemical) per batch
- 12 hours per batch; 1 batch per day
- Process description: Reactants are added to reactor -> Formulation (80% chemical) sampled -> Formulation loaded into 40-gallon drums for distribution to user sites -> Reactor vessel is rinsed with water every 5 batches
- 4 workers performing sampling, drumming, and reactor cleaning activities:

Activity	Concentration	# Workers	Hrs/day	Days/yr
Sampling	80%	4	0.02	125
Drumming	80%	4	ChemSTEER will estimate hpd and dpy	
Cleaning reactor	< 80%	4	1.5	25

Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001
Appendix G. ChemSTEER Case Study

Information on the Use

- Use rate = 10 kg formulation per site, per day (formulation contains 80% chemical)
- Use sites operate 250 days per year
- Process description:

Formulation containing 80% chemical is metered from drum into the process -> chemical is destroyed in the reaction/converted to a new substance -> empty drums are rinsed with solvent before disposal -> used solvent is incinerated

- 3 workers per site are involved in handling the formulation containing the chemical:

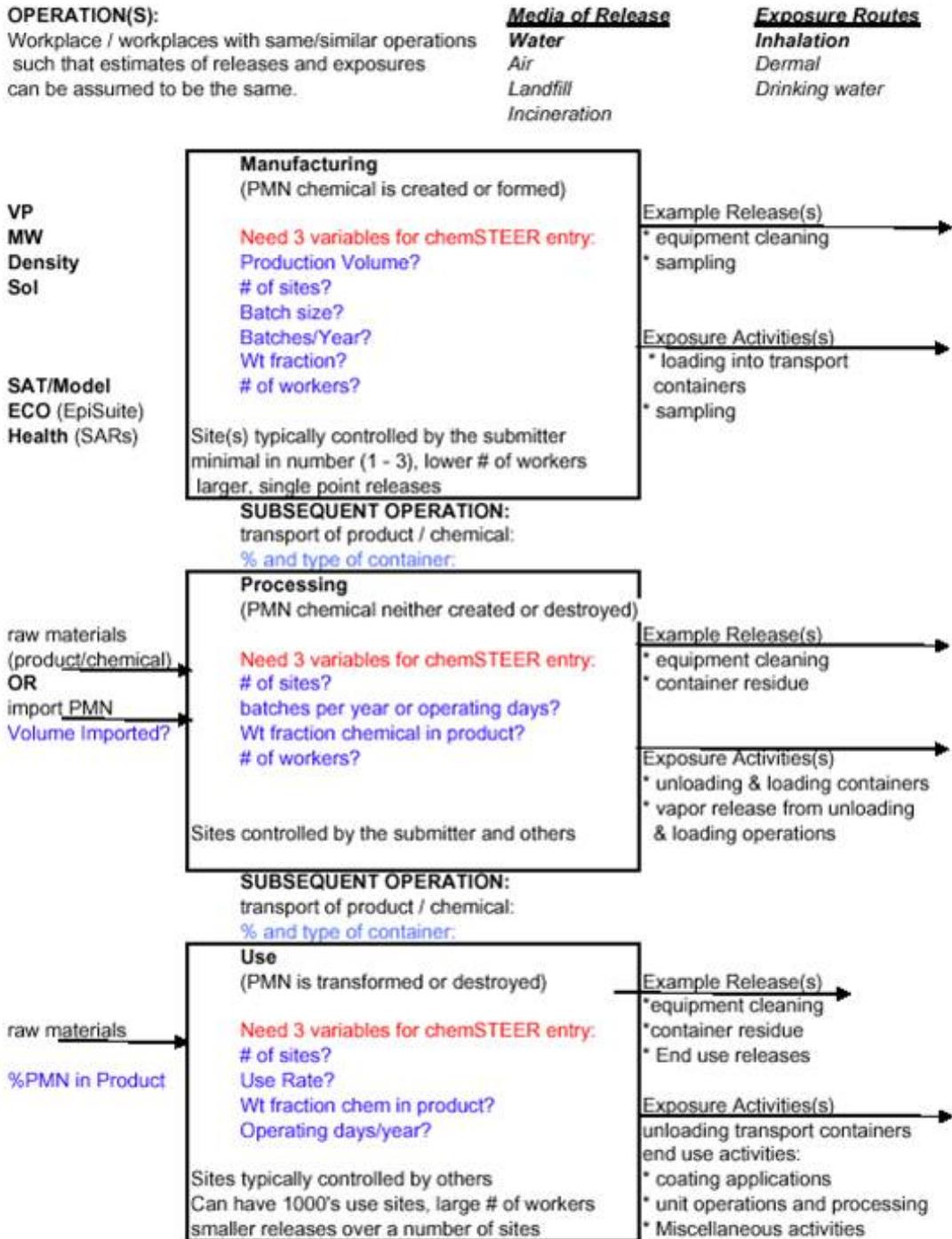
Activity	Concentration	# Workers	Hrs/day	Days/yr
Unloading	80%	3	ChemSTEER will	estimate hpd and dpy
Cleaning reactor	< 80%	3	0.5	ChemSTEER will estimate dpy

The ChemSTEER spreadsheet formats of this information is shown on the following pages.

The images are the **Blank Spreadsheet of Model Inputs**, and the **Completed Spreadsheet of Model Inputs**.

**Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001
Appendix G. ChemSTEER Case Study**

Blank Spreadsheet of Model Inputs



**Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001
Appendix G. ChemSTEER Case Study**

Completed Spreadsheet of Model Inputs

OPERATION(S):

Workplace / workplaces with same/similar operations such that estimates of releases and exposures can be assumed to be the same.

Media of Release

Water
Air
Landfill
Incineration

Exposure Routes

Inhalation
Dermal
Drinking water

VP 1
MW 150
Density 0.815
Sol

SAT/Model
ECO (EpiSuite)
Health (SARs)

Manufacturing
(PMN chemical is created or formed)
semi volatile liquid
Need 3 variables for chemSTEER entry:
Production Volume? 100,000
of sites? 1
Batch size? 1000
Batches/Year?
Wt fraction? 80%
of workers?

Site(s) typically controlled by the submitter
minimal in number (1 - 3), lower # of workers
larger, single point releases

Example Release(s) →
* equipment cleaning → **lg vessel*
* sampling x
**rinsed w/ watre every 5 batches*

Exposure Activities(s) →
* loading into transport containers *
* sampling x
**loaded into 40 gal drums*

SUBSEQUENT OPERATION:

transport of product / chemical:
% and type of container:

raw materials
(product/chemical)
OR
import PMN
Volume Imported?

Processing
(PMN chemical neither created or destroyed)
Need 3 variables for chemSTEER entry:
of sites?
batches per year / operating days?
Wt fraction chem in product?
of workers?

Sites controlled by the submitter and others

Example Release(s) →
* equipment cleaning
* container residue

Exposure Activities(s) →
* unloading & loading containers
* vapor release from unloading & loading operations

SUBSEQUENT OPERATION:

transport of product / chemical:
% and type of container:

raw materials →

%PMN in Product
80% in formulation
40 gal drums

Use
(PMN is transformed or destroyed)
Need 3 variables for chemSTEER entry:
of sites?
Use Rate? 10 kg formulation / site / day
Wt fraction chem in product 80%
Operating days/year? 250

Sites typically controlled by others
Can have 1000's use sites, large # of workers
smaller releases over a number of sites

Example Release(s) →
*equipment cleaning
*container residue
* End use releases *incinerated destroyed*

Exposure Activities(s) →
unloading transport containers x
end use activities:
* coating applications
* unit operations and processing
* Miscellaneous activities

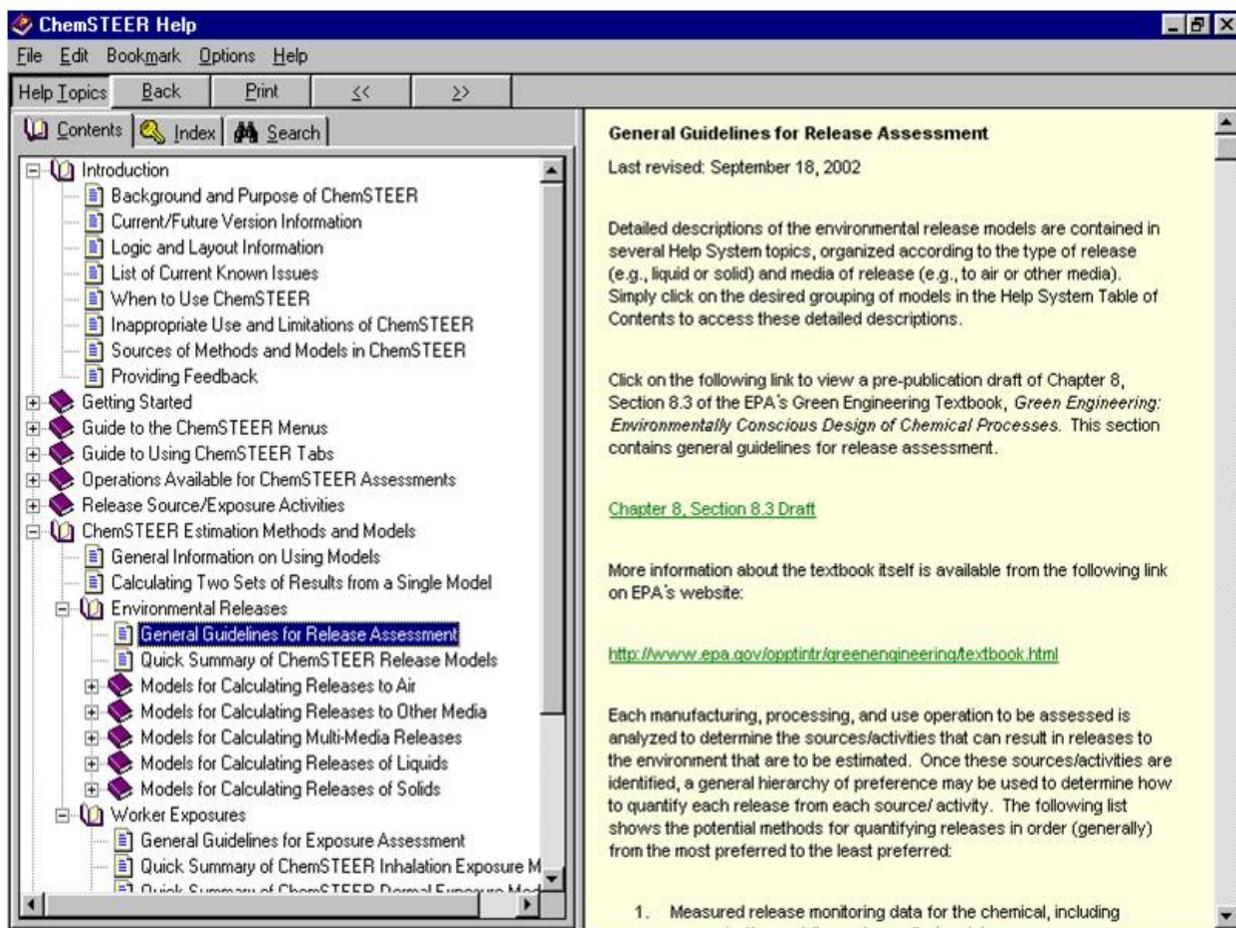
Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001 Appendix G. ChemSTEER Case Study

The ChemSTEER Help System

The ChemSTEER **Help System** provides extensive descriptions of how ChemSTEER is organized, and how the release and worker exposure estimates are made in an assessment. Full documentation is included on each of the methods and models that are used to perform the calculations (e.g., input parameters, default settings and values, equations that are used, and associated logic algorithms).

All users are strongly encouraged to review this Help System prior to creating their first assessment and use it regularly as a resource to assist in future assessments. Taking the time to learn and understand the complex functions of this tool will enable you to perform screening-level assessments of environmental releases and worker exposures with greater ease and flexibility.

To access the ChemSTEER Help System, click on the **Help** menu item and select **Index**. Then, simply select a topic from the menu on the left and view the content in the screen on the right.



Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001 Appendix G. ChemSTEER Case Study

The ChemSTEER General Tab - Entering General Information

The screenshot shows the ChemSTEER software interface with the 'General' tab selected. The window title is 'ChemSTEER 05/27/2004 Version - 0000'. The menu bar includes 'File', 'Edit', 'Preferences', 'Reports', and 'Help'. The main menu includes 'General', 'Chemical', 'Operations', 'Operation Parameters', 'Releases', 'Exposures', and 'Optional Information'. The 'General' tab contains the following fields and controls:

- Assessment Type: PMN
- Status: CEB Staff Draft
- Fiscal Year: [empty]
- Assessment Identifier: 0000
- Consolidated Case: No
- Last Saved: 7/13/04 3:18:52 PM
- Date: 07/13/2004
- CBI: No
- Number of Contact Reports: 0
- Assessors:
 - Assessor 1: Name: Scott Prothero, Affiliation: US EPA, Phone: 202-555-1234, Email: prothero.scott@epa.gov
 - Assessor 2: Name: L Crawford, Affiliation: ERG, Inc (Contractor), Phone: 404-555-0987, Email: leslie.crawford@erg.com
- Company Name: XYZ Chemical Co.
- Street Address: 1313 mockingbird Lane
- City: Anywhere
- State: AK, Zip: 99999
- Revision Notes / Assessment Overview: [empty text area]

At the bottom of the form are three buttons: 'Update General Information', 'View/Update Contact Report(s)', and 'Update Revision Notes / Assessment Overview'.

When you click the **General** tab (above) a screen displaying general information about the assessment is shown. To add or modify the General information, click the **Update General Information** button.

1. Select the Assessment Type – choose from this list of various EPA labels to describe assessment types that EPA uses ChemSTEER to perform.
2. Enter an assessment Identifier – Enter a descriptive unique title in this field. This field will be the saved “name” of your assessment and is the primary means of identifying this assessment among a list of assessments in a single ChemSTEER database file.
3. Verify/modify the Date of the assessment – this field is automatically populated with the current date for a new assessment. You should enter a new date to reflect when the assessment was completed.
4. Enter Assessor information: you may enter the name, affiliation, phone number, and email address for one or two assessors (i.e., persons preparing the assessment).
5. Enter the Company information: you may enter the company name, address, city, state, zip code, and contact information for the assessment.

Note: Status and Revision options are used for internal EPA reports and may be left incomplete. When you click the **View/ Update Comments** tab, a screen displaying a text field is shown. You may enter key information about the assessment here.

Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001
Appendix G. ChemSTEER Case Study

The ChemSTEER Chemical Tab - Entering Chemical Information (continued)

When you click the **Chemical** tab (below), a screen displaying information about the chemical being assessed is shown. To add or modify information about the chemical, click the **Update Chemical Information** button. Enter the following information about the chemical being assessed in the appropriate fields:

- *Chemical name*
- *Chemical category*
- *Trade name(s)*
- *CAS number (if known)*
- *Molecular formula*
- *Domestic production volume (PVd, kg/yr)* – the annual amount of the chemical to be assessed that is manufactured domestically
- *Imported production volume (PVi, kg/yr)* – the annual amount of the chemical to be assessed that is imported to the U.S.
- *Total assessed production volume (PV, kg/yr)* – the total annual amount of the chemical to be assessed (PV = PVd + PVi); ChemSTEER automatically sums your entries for PVd and PVi, and displays PV.

***Note:** PV is the most often used parameter throughout most assessments. VP, MW, Dchem, and Wschem may be needed depending upon which release or exposure models are used in the assessment.

Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001
Appendix G. ChemSTEER Case Study

The ChemSTEER Chemical Tab - Entering Chemical Information (continued)

Enter the following information about the chemical being assessed in the appropriate fields:

- Vapor pressure (VPchem, torr) – the vapor pressure of the pure chemical to be assessed; you may also enter the reference temperature (oC) for this value
- Molecular weight (MW, g/mol) – the molecular weight of the chemical to be assessed
- % < 500 g/mol and % < 1000 g/mol – for use with high molecular weight polymers; indication of the distribution of molecular weight of the chemical to be assessed.
- Density (Dchem, g/cm³) – the density of the pure chemical to be assessed; you may also enter the reference temperature (oC) for this value
- Solubility in water (WSchem, g/L) – the solubility of the pure chemical in water; you may also enter the reference temperature (oC) for this value or simply check the box indicating the chemical is 'dispersible'
- General description of end use(s)

ChemSTEER 05/27/2004 Version - 0000

File Edit Preferences Reports Help

General Chemical Operations Operation Parameters Releases Exposures Optional Information

Chemical

Chemical Name: Case Study Chemical

Chemical Category:

Trade Name(s):

Chemical CAS Number: 999-99-9 Molecular Formula:

Total Assessed Production Volume (PV): 100000 kg/yr

Imported Production Volume (PVi): kg/yr

Domestic Production Volume (PVd): 100000 kg/yr

Type of Notice: Manufacturing

Vapor Pressure (VPchem): 1 torr at 20 C

Molecular Weight (MW): 150 g/mol % < 500: % < 1000:

Density (Dchem): 0.815 g/cm³ at C

Solubility in Water (WSchem): g/L at C

General Description of End Use(s): chemical intermediate for off site reactions

Update Chemical Information View Exposure Limits

Parameters with red labeling are often important defaults used in mass balance, container, and model calculations.

***Note:** PV is the most often used parameter throughout most assessments. VP, MW, Dchem, and Wschem may be needed depending upon which release or exposure models are used in the assessment.

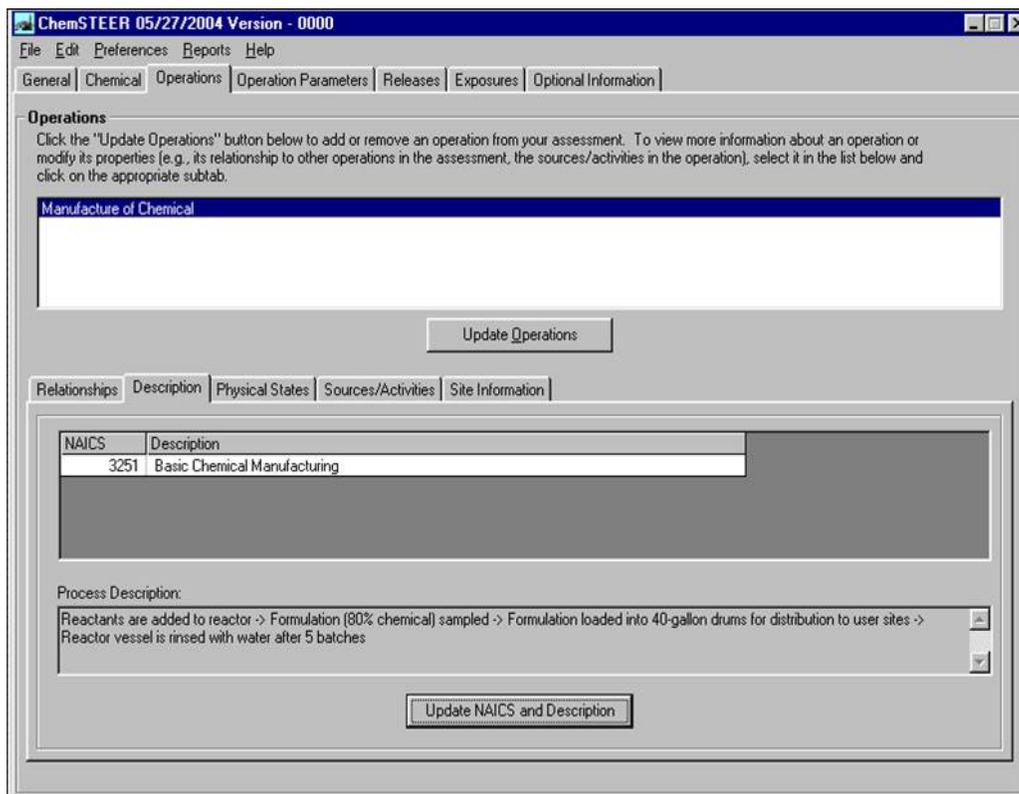
Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001 Appendix G. ChemSTEER Case Study

The ChemSTEER Operations Tab – Entering Scenario Information

Click on the **Operations** tab and each of its subtabs to build your scenario and enter necessary information about each operation in your assessment.

Choosing Operations for the Scenario

The first step in building a scenario to be assessed is to choose the operations. Begin by clicking the **Update Operations** button to choose the operations in your scenario.

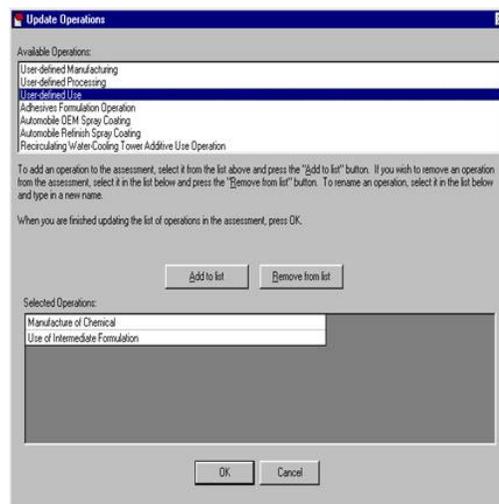


At the top of the **Update Operations** screen is a list of *Available Operations* that you may choose (shown on the right). To select an operation, you may either double-click on it or click it once and then click the **Add to list** button.

The selected operation then appears in the *Selected Operations* list at the bottom of the **Update Operations** screen. Continue this process for each operation you wish to include in your assessment.

Renaming Operations

It is helpful to rename the operations to better describe your assessment. To do this, select the operation by clicking on it in the *Selected Operations* list and enter the new name (e.g., *Manufacture of Chemical*).



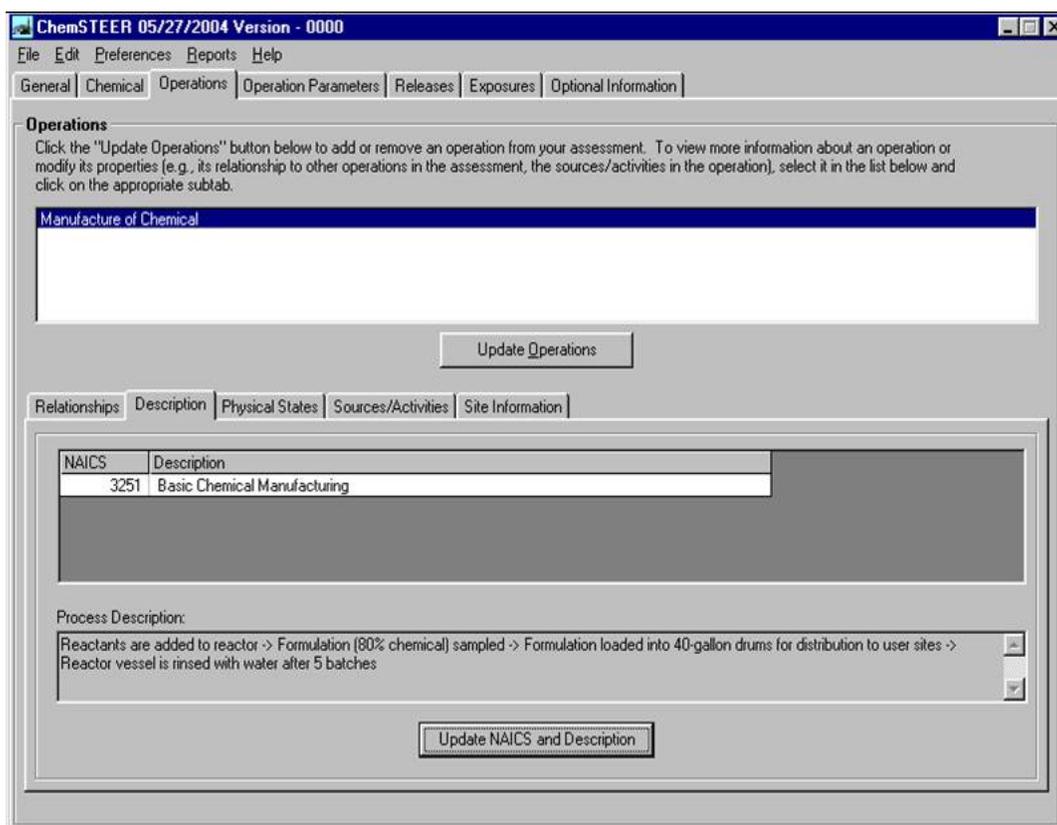
Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001
Appendix G. ChemSTEER Case Study

Entering Operation Descriptions

You may enter North American Industrial Classification System (NAICS) codes and other descriptions associated with each operation of the assessment by clicking on the **Description** subtab within the **Operations** screen.

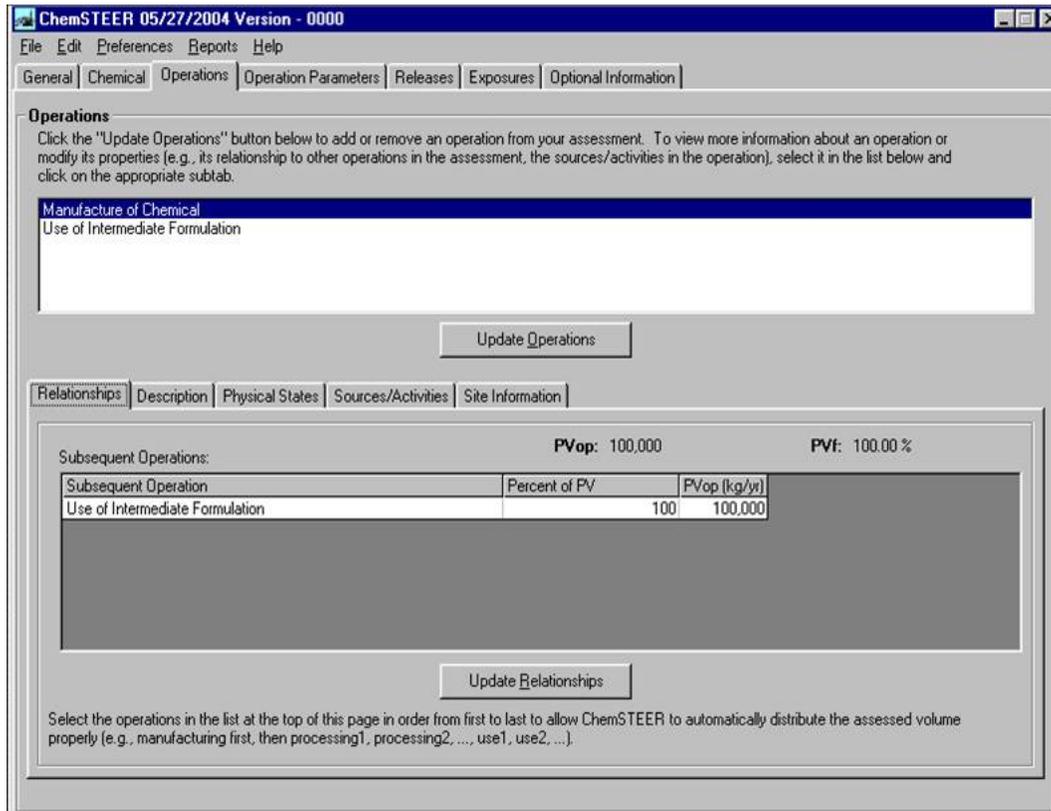
Select the desired operation at the top of the **Operations** screen and click the **Update NAICS and Description** button to view the **Update Operation Description** screen.

1. To add an associated NAICS code, click the **Add/Remove NAICS** button and select a NAICS code from the list of codes.
2. You may also enter further details about the selected operation by typing them within the **Process Description** box in the **Update Operation Description** screen.



**Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001
Appendix G. ChemSTEER Case Study**

The ChemSTEER Operations Tab – Entering Information on the Relationships Between Operations

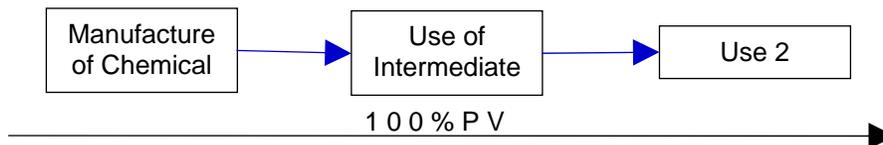


Defining Operation Relationships

The next step in building your assessment scenario is to indicate the relationships of your chosen operations (i.e., the order in which they are performed). Click on the **Relationships** subtab in the **Operations** screen.

Select the desired operation at the top of the **Operations** screen to view the current settings: subsequent operation(s), fraction of PV, and PV in each subsequent operation. Click the **Update Relationships** button to modify any of these relationship settings.

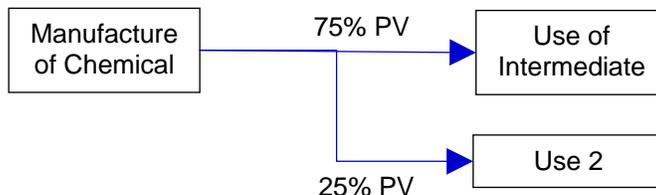
For example, if we had chosen a second use operation for the manufactured chemical formulation, ChemSTEER defaults to a simple, straight series relationship:



Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001
Appendix G. ChemSTEER Case Study

The ChemSTEER Operations Tab – Entering Information on the Relationships Between Operations
(continued)

The *Relationships* subtab can be used to modify the relationship to:

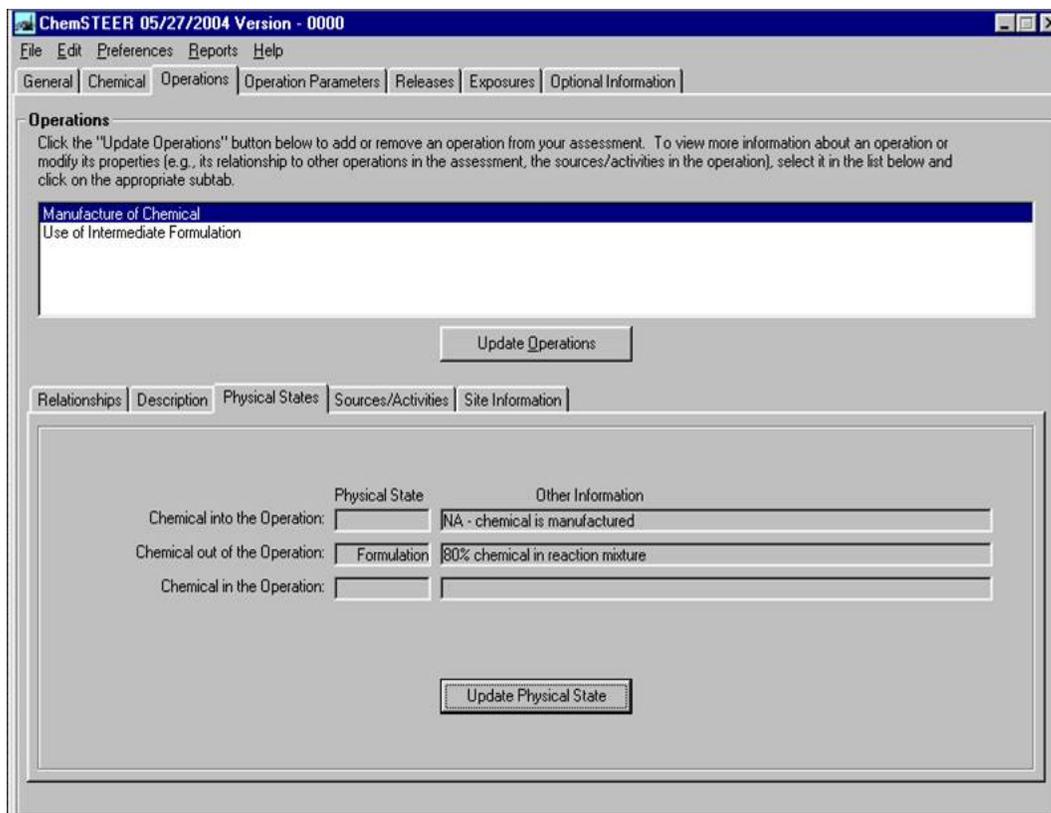


Defining Physical State(s) of the Chemical

You should enter information pertaining to the physical state of the chemical being assessed within each operation by clicking on the *Physical States* subtab within the *Operations* screen.

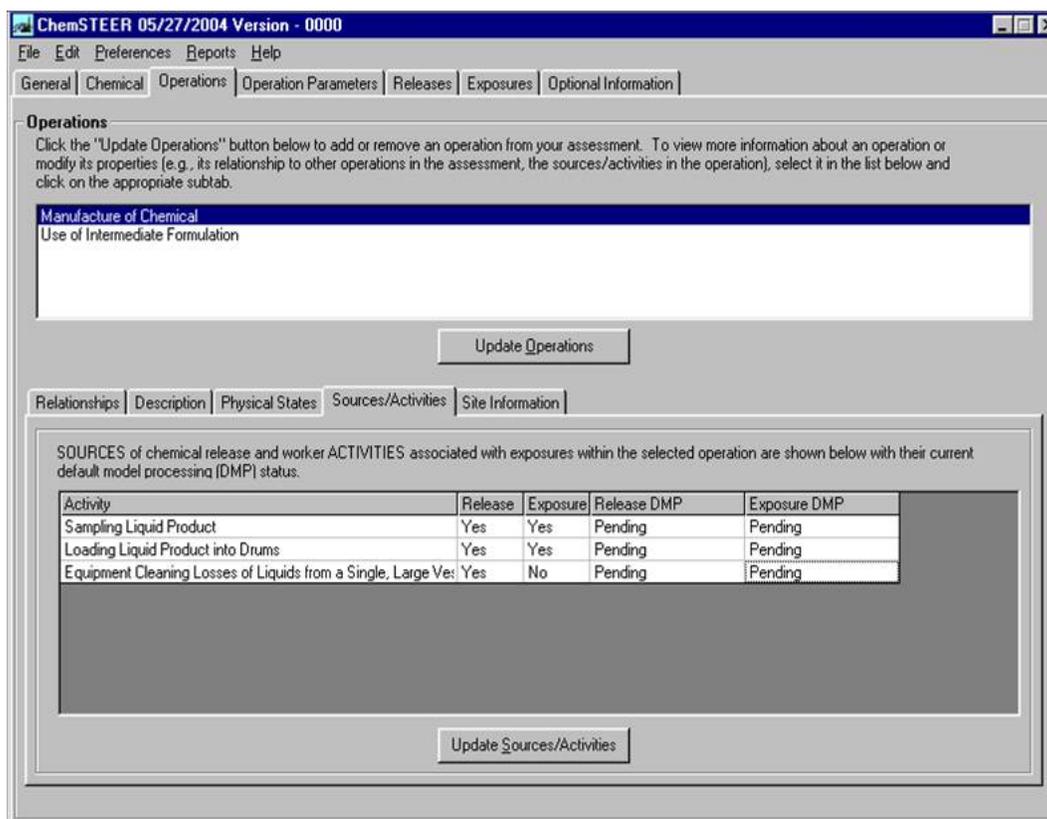
Appropriate terms include liquid, solid, vapor, gas with additional modifiers if needed (e.g., molten liquid, etc.). Formulation (as shown above) should not be used as it does not adequately describe physical state.

Select the desired operation at the top of the *Operations* screen and click the *Update Physical State* button.



Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001 Appendix G. ChemSTEER Case Study

The ChemSTEER Operations Tab – Entering Information on the Sources / Activities



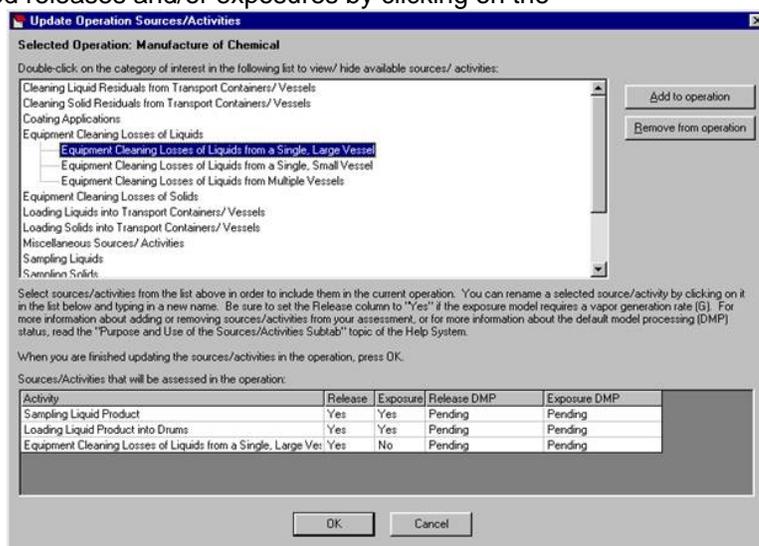
Identifying Operation Sources/Activities

For each operation of the assessment, you must identify at least one release source or worker activity for which ChemSTEER will calculate estimated releases and/or exposures by clicking on the **Sources/Activities** subtab within the **Operations** screen.

This selection is critical, as it will determine which default release/exposure models are used for the calculations.

Select the desired operation at the top of the **Operations** screen and click the **Update Sources/Activities** button. Sources/Activities are listed under categories shown in the *available sources/activities* list. To view or hide the list of specific sources/ activities, double-click on the category of interest. Select the source/activity by either double-clicking on it or clicking it once and then clicking the **Add to list** button.

The ChemSTEER Operations Tab (continued)



Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001
Appendix G. ChemSTEER Case Study

Entering Operation Facility Information

You may enter information regarding the facility or facilities that are performing the operations of the assessment by clicking the **Site Information** subtab within the **Operations** screen.

Select the desired operation at the top of the **Operations** screen and click the **Site Information** button.

If you have no information about the facility or facilities for the operation, type “unknown” in the Facility Name field.

NOTE: Providing sufficient information about the facility location(s) will usually avoid the use of the most conservative assumptions (e.g., lowest stream flow) for the environmental exposure portion of the EPA exposure assessment.

ChemSTEER 05/27/2004 Version - 0000

File Edit Preferences Reports Help

General Chemical Operations Operation Parameters Releases Exposures Optional Information

Operations

Click the "Update Operations" button below to add or remove an operation from your assessment. To view more information about an operation or modify its properties (e.g., its relationship to other operations in the assessment, the sources/activities in the operation), select it in the list below and click on the appropriate subtab.

Manufacture of Chemical
Use of Intermediate Formulation

Update Operations

Relationships Description Physical States Sources/Activities Site Information

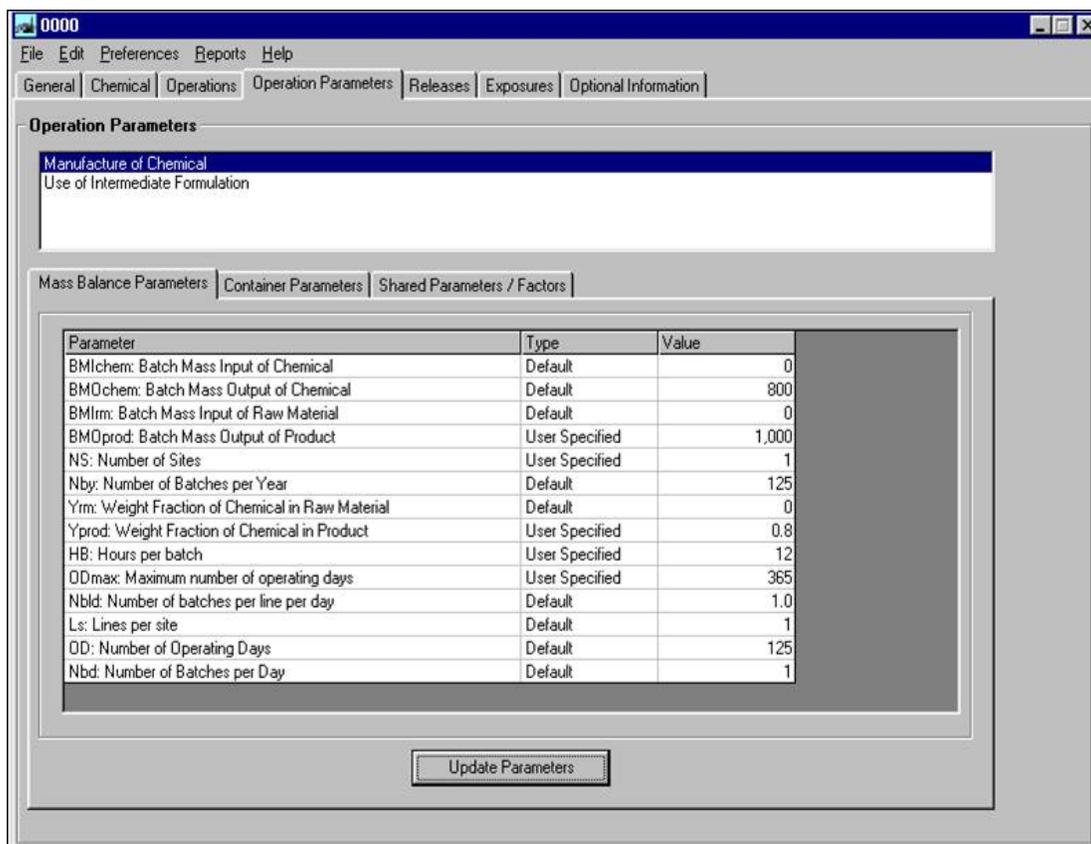
Operation Site Information:

Facility Name	Address	City	State	Zip	County
XYZ Chemical Co.	1313 Mockingbird Lane	Anywhere	AK	99999	

Update Site Information Copy Previous Operation

Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001 Appendix G. ChemSTEER Case Study

The ChemSTEER Operation Parameters Tab



Click on the **Operation Parameters** tab and each of the subtabs to verify or edit the default values for key operation parameters (e.g., mass balance of chemical into and out of the operation, calculation of the number of containers filled and/or emptied during the operation).

Entering Mass Balance Parameters

ChemSTEER allows a great amount of flexibility in which input parameters can be entered for each assessment.

We will set the mass balance parameters for the *Manufacture of Chemical* operation:

1. Click the **Update Parameters** button to enter the mass balance parameters for the selected operation.
2. **Mass Accounting Basis Selection - Continuous or Batch processes:** Continuous processes run 24 hours per day over a number of days per year; Batch processes occur over less than 24 hours, thus an operation may perform one or more batches per day.
3. **Mass Accounting Basis Selection - Influent or Effluent basis:** Influent basis causes ChemSTEER to utilize the current settings for the chemical as it enters the selected operation (e.g., utilizing the settings for the chemical exiting the previous operation in a series). Effluent basis causes ChemSTEER to utilize the current settings for the chemical as it exits the selected operation.

For the *Manufacture of Chemical* operation, we will select a *Batch* process with an *Effluent* basis.

Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001 Appendix G. ChemSTEER Case Study

The ChemSTEER Operation Parameters Tab -- Entering Mass Balance Parameters (continued)

Strategy: If you know more about the product of an operation (i.e., typical production rates and composition of the chemical within the product), selecting *Effluent* as the basis is often the most practical strategy. Similarly, if more is known about the use of the chemical as a raw material for the selected operation, selecting *Influent* is often the best approach.

Continue entering the mass balance parameters for the *Manufacture of Chemical* operation:

4. *Specify Mass Balance Input Parameters* - The second subtab contains the input parameters that ChemSTEER utilizes to calculate the remaining mass balance parameters. You must specify exactly three of the five parameters listed in upper portion of this subtab.
5. For the *Manufacture of Chemical* operation, it is known that the manufacturers: a) operate one site (NS); b) that the product formulation contains 0.8 kg chemical/kg formulation (Yprod) (i.e., 80% chemical; and c) that 1,000 kg of formulation is produced in each batch (BMOprod).
6. When you have completed entering the three known parameters, click on the **Calculate remaining two parameters** button.

After entering the three known values, ChemSTEER determines that the site must perform 125 batches per year (Nby) in order to process the amount of chemical being assessed (PV = 100,000 kg/yr) and that 800 kg of chemical is manufactured in each batch (BMOchem).

Since the chemical is created in this operation, the input parameters listed in the lower half of the screen are not applicable in this case. In addition, by clicking the **Specify Other Batch Parameters** subtab additional parameters may be specified (e.g., hours per batch).

***Note:** You are highly encouraged to review this topic in the **ChemSTEER Help System** for a more complete description (refer to *Guide to Using ChemSTEER Tabs – Operation Parameters Tab – Mass Balance Parameters Subtab*).

The screenshot shows a dialog box titled "Update Operation Mass Accounting Parameters" with a sub-tab "Manufacture of Chemical". It has three sub-tabs: "Mass Balance Basis Selection", "Specify Mass Balance Input Parameters" (which is active), and "Specify Other Batch Parameters".

Below the sub-tabs is a text box: "Please specify exactly three of the first five parameters, including at least one parameter from the first 'pair' and at least one parameter from the second 'pair.' ChemSTEER will calculate the other two parameters for you. If you only need a smaller subset of these parameters for use in a limited set of models, enter only those parameters and ChemSTEER will not derive a complete set of default values."

The "Specify Mass Balance Input Parameters" sub-tab contains two sections:

- Batch Operation; Using Product:** This section has two pairs of parameters. Pair 1 includes "NS: Number of Sites" (checked, value 1) and "Nby: Total batches per year" (value 125). Pair 2 includes "Yprod: Weight Fraction of Chemical in Product (unitless)" (checked, value 0.8) and "BMOprod: Batch Mass Output of Product kg/site-batch" (checked, value 1000). There is also an unchecked option "BMOchem: Batch Mass Output of Chemical kg/site-batch" with a value of 800. Buttons for "Calculate" are next to each input field. At the bottom of this section are "Calculate remaining two parameters" and "Restore Defaults" buttons.
- Batch Raw Material Parameters Calculation:** This section has three unchecked options: "Yrm: Weight Fraction of Chemical in Raw Material (unitless)" (value 0), "BMIrm: Batch Mass Input of Raw Material kg/site-batch" (value 0), and "BMlchem: Batch Mass Input of Chemical kg/site-batch" (value 0). Each has a "Recalc" button. A "Calculate defaults" button is at the bottom.

At the bottom of the dialog box, it says "No mass balance discrepancy exists" and has "OK", "Cancel", "Basis", and "Help" buttons.

Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001 Appendix G. ChemSTEER Case Study

The ChemSTEER Operation Parameters Tab -- Entering Container Parameters

The **Container Parameters** subtab allows you to verify and/or edit the default settings for how the mass balance around loading and unloading containers with materials containing the chemical. We will set the container parameters for the *Manufacture of Chemical* operation.

The **Container Parameters** subtab displays the list of container-related sources/activities that were chosen for the selected operation (e.g., loading liquid product into drums) along with the current values for the key container parameters (for new assessments these are ChemSTEER default values).

The screenshot shows the 'Container Parameters' subtab in the ChemSTEER software. The 'Container Parameters by Activity' subtab is selected, displaying a table of parameters for the activity 'Loading Liquid Product into Drums'. The table includes columns for Source/Activity Name, Ncy (containers / site-year), ODa (days/yr), Ncd (containers / site-day), r (containers / hour), and OHa (hours / day). The values for 'Loading Liquid Product into Drums' are: Ncy = 1,013.04, ODa = 125, Ncd = 8,1043, r = 20, and OHa = 0.4052.

Source/ Activity Name	Ncy (containers / site-year)	ODa (days/yr)	Ncd (containers / site-day)	r (containers / hour)	OHa (hours / day)
Loading Liquid Product into Drums	1,013.04	125	8,1043	20	0.4052

This screenshot is identical to the one above, showing the 'Container Parameters by Activity' subtab with the same table of parameters for 'Loading Liquid Product into Drums'.

These sources/activities can be viewed according to what type of material is handled by clicking on each of the subtabs, **Raw Material**, **Product**, or **Other Material**. Additional parameters are summarized in the **Container Parameters By Activity** subtab.

1. **Verify/Select Container Parameters** - Double-click on a container-related source/activity to view the **Verify/Select Container Parameters for Product** subtab. As a default, ChemSTEER assumes the volume of each drum (V_c) is 55 gallons. By changing V_c from 55 to 40 gallons, the number of drums filled per year is adjusted using this new volume, as well as the chemical density and total PV.

**Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001
Appendix G. ChemSTEER Case Study**

The ChemSTEER Operation Parameters Tab -- Entering Container Parameters (continued)

2. *Verify/Select Container Parameters*
– Click the **Verify/Select Container Parameters by Source/Activity** subtab

- Approximately 1,013 drums of our chemical formulation will be filled over the 125-batch campaign and approximately 8 drums will be filled per day.
- The default drum unloading rate is 20 drums per hour, which determines the total number of hours (OHa) spent filling the drums each day

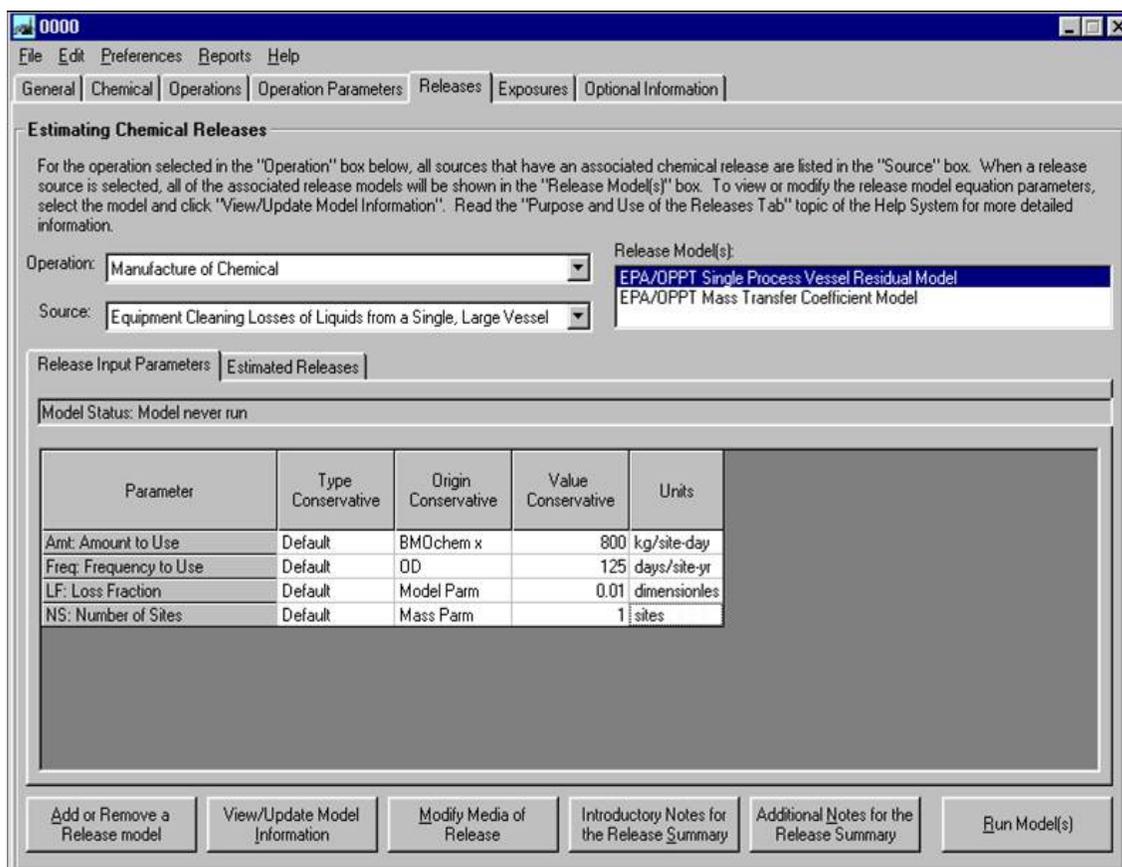
3. You may choose three parameters in this screen to specify and ChemSTEER will adjust the remaining two parameters accordingly. Let's assume that in our scenario, the loading rate is 4

drums per hour. We will specify: a) the total days per year (ODa) is kept at 125 days/year; b) the number of drums filled per day (Ncd) is kept at 8.1043 drums/site-day; and 3) the drum fill rate (r) is changed from 20 to 4 drums/hr.

- After clicking the **Calculate remaining two parameters** button, ChemSTEER determines that: the number of containers filled per year (Ncy) is approximately 1,013 drums/year; and it will take slightly longer than 2 hours/day to fill them (OHa). OHa is used later to calculate fugitive releases and inhalation exposures.

**Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001
Appendix G. ChemSTEER Case Study**

The ChemSTEER Releases Tab



Click on the **Releases** tab to view or modify the models (i.e., algorithms) and associated input parameters used to calculate the releases to water, air, incineration, and/or landfill from each of the chosen sources within each of the operations of your assessment. Then click Run Model(s) to generate release estimate results from the model(s).

1. Select an operation from the *Operation* drop down list.
2. Select a source for which releases are calculated from the *Release Activity* drop down list.
 - The models that are used to calculate the releases from the selected source within the selected operation appear in the *Release Model(s) for Selected Activity* box.
 - The parameters used by the selected release model appear in the **Release Input Parameters** subtab. This subtab also indicates which parameters are ChemSTEER default values, the source of the parameter value (i.e., whether previously input in another tab or calculated from other input parameters), the current value, and the units.

***Note:** ChemSTEER currently contains over a dozen different models that can be used to calculate releases, each with their own set of default settings and values. You are highly encouraged to review the *ChemSTEER Estimation Methods and Models – Environmental Releases* in the **ChemSTEER Help System** for a more complete description of the models and their bases before selecting alternative models to the ChemSTEER defaults and/or modifying default input values.

Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001 Appendix G. ChemSTEER Case Study

The ChemSTEER Releases Tab (continued)

Adding or Removing Release Models

Click on the **Add or Remove a Release Model** button in the **Releases** screen to change the default models that are used for the selected release source.

The **Add/Remove Release Models** screen will appear with a list of the most appropriate alternative models for the selected release source.

Read-only and updateable information about the selected release model are shown below. Click on the associated Type column label for a parameter to change its value. When the Type is User-defined, you enter your value directly in the Value column. To calculate two sets of model results, enable the Model Parameters for the Output 1 option and the Model Parameters for the Output 2 option below. Note that Output 1 parameters are used to calculate the Output 1 model results and Output 2 parameters are used to calculate the Output 2 model results. Use care and consistency in entering the parameter values to ensure that they are used appropriately by the model equation(s).

Activity: Equipment Cleaning Losses of Liquids from a Single, Large Vessel
Model: EPA/OPPT Single Process Vessel Residual Model

Model Equation: DR (kg/site-day) = LF × Amt
DR occurs over [Freq] days/year

Mechanism: Residual removed from and/or disposed from a single process vessel

Enable Model Parameters for Output 1 Enable Model Parameters for Output 2

High End to Bounding Conservative

Basis: EPA/OPPT Single Vessel Residual Model, CEB standard 1% residual.

Parameters:

Parameter	Type 2	Origin 2	Value 2	Units
Amt: Amount to Use	Default	BMDchem x Nbd	800	kg/site-day
Freq: Frequency to Use	Non-default	User-defined	25	days/site-yr
LF: Loss Fraction	Default	Model Parm	0.01	dimensionless
NS: Number of Sites	Default	Mass Parm	1	sites

OK Cancel

View/Update Model Information

Click on the **View/Update Model Information** button in the **Releases** screen to modify the default model parameter values to be used in the calculations.

The **View/Update Release Model Information** screen displays information about the selected model, including: the equation(s) used in the calculation, a description of the basis/source of the model, and a list of the parameters used by the model.

1. To change a parameter value, click on the associated *Type* field.
2. For some parameters, you will change the *Type* field from 'Default' to 'Non-default'. If you choose 'Non-default', you may then click on the associated *Value* field and enter the new value for the parameter (other parameters will prompt you to select from a specified list of alternative values).
 - In our scenario, the reaction tank is rinsed once every 5 batches, which is 125 batches/5 = 25 times per year. Therefore, we will change the default frequency of release (Freq) from 125 to 25 days/year.

Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001
Appendix G. ChemSTEER Case Study

The ChemSTEER Releases Tab (continued)

Modifying the Target Media of Release

Click on the **Modify Media of Release** button in the **Releases** screen to change the default media (i.e., water, air, incineration, landfill) to which the selected source releases will be emitted.

The *Update release media output specifications screen* will appear. In this screen, the selected operation and release source is listed, as well as the selected release model and description of the model basis/source.

In this screen, you can apportion the total amount of the calculated release to more than one target media. Another modification that you may enter in this screen is establishing alternative target media designations.

For example, if the wash water from the reactor vessel rinse (containing residual chemical) may alternatively be incinerated or released to water, the value 100% should be typed in the box next to 'Water or Incineration'.

Run the Models

Click the **Run Model(s)** button in the **Releases** tab to execute the release model calculations.

Update release media output specifications

Verify or change the media for the estimated release below.

Manufacture of Chemical

Equipment Cleaning Losses of Liquids from a Single, Large Vessel

To (NPDES number if appropriate):

Basis:

Water	<input type="text" value="0"/>	%	Air	<input type="text" value="0"/>	%			
Water or Air	<input type="text" value="0"/>	%	Air or Incineration	<input type="text" value="0"/>	%			
Water or Air or Incineration	<input type="text" value="0"/>	%	Air or Incineration or Landfill	<input type="text" value="0"/>	%			
Water or Air or Landfill	<input type="text" value="0"/>	%	Air or Landfill	<input type="text" value="0"/>	%			
Water or Air or Incineration or Landfill	<input type="text" value="0"/>	%	Incineration	<input type="text" value="0"/>	%	Deepwell Injection	<input type="text" value="0"/>	%
Water or Incineration	<input type="text" value="100"/>	%	Incineration or Landfill	<input type="text" value="0"/>	%	Destroyed	<input type="text" value="0"/>	%
Water or Incineration or Landfill	<input type="text" value="0"/>	%	Landfill	<input type="text" value="0"/>	%	Other	<input type="text" value="0"/>	%
Water or Landfill	<input type="text" value="0"/>	%						

Total: **100%**

**Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001
Appendix G. ChemSTEER Case Study**

The ChemSTEER Releases Tab (continued)

View Release Estimates

Click on the **Estimated Releases** subtab in the **Releases** tab to view the results of the calculations. This screen displays the media of release, the number of sites releasing the chemical, the daily release rate (kg/site-day), the annual release rate (kg/year; all sites), the days of release (days/site-yr), and the basis for the selected release model.

The results for our case study show that 8 kg of chemical per day is released from the manufacturing site over 25 days per year (this is equivalent to 200 kg chemical released per year). The releases are emitted to either water or incineration.

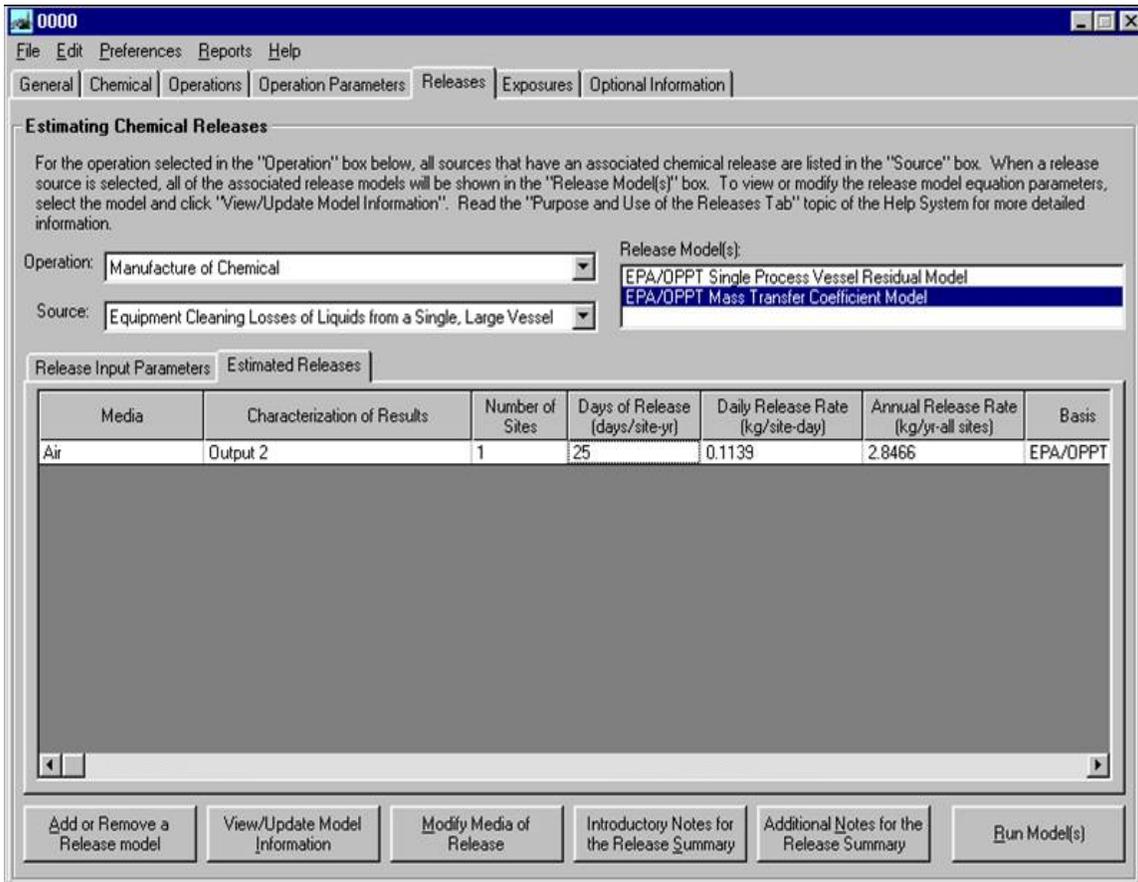
The screenshot shows the 'Releases' tab in the ChemSTEER software. The 'Estimated Releases' subtab is active, displaying a table with the following data:

Media	Characterization of Results	Number of Sites	Days of Release (days/site-yr)	Daily Release Rate (kg/site-day)	Annual Release Rate (kg/yr-all sites)	Basis
Water or Incineration	Conservative	1	25	8	200	EPA/OPPT

Below the table, there are several buttons: 'Add or Remove a Release model', 'View/Update Model Information', 'Modify Media of Release', 'Introductory Notes for the Release Summary', 'Additional Notes for the Release Summary', and 'Run Model(s)'.

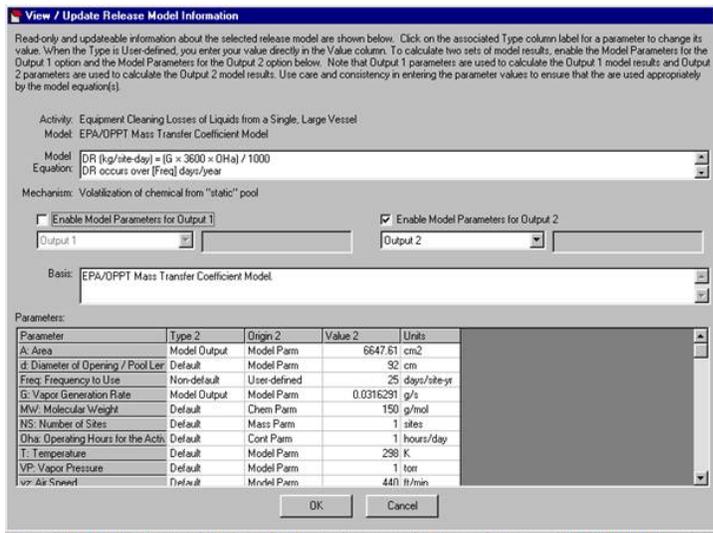
**Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001
Appendix G. ChemSTEER Case Study**

The ChemSTEER Releases Tab (continued)



A Source Can Have More Than One Release

In some cases, a source can have associated with it more than one release, and thus more than one release model. In our example, the *Equipment Cleaning Losses of Liquids from a Single, Large Vessel* source used a model that calculated the amount of residual chemical released with the rinse water (i.e., the *EPA/OPPT Single Vessel Residual* model).



The second model shown (the *EPA/OPPT Mass Transfer Coefficient* model) calculates the amount of chemical vapor released to air during the cleaning activity. As previously discussed, this model can also be modified or removed from the assessment.

The amount of fugitive chemical released to air during the reactor vessel cleaning is estimated to be 0.1139 kg chemical per day over 25 days per year (equivalent to 2.8466 kg chemical per year).

Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001 Appendix G. ChemSTEER Case Study

The ChemSTEER Exposures Tab

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File Edit Preferences Reports Help

General Chemical Operations Operation Parameters Releases Exposures Optional Information

Estimating Chemical Exposures

For the operation selected in the "Operation" box below, all activities that have an associated worker exposure are listed in the "Activity" box. When a worker exposure activity is selected, the associated inhalation or dermal model and its parameters will be shown in the respective subtab below. To view or modify the model equation parameters, click on the desired subtab and click "View/Update Model Information". Read the "Purpose and Use of the Exposures Tab" topic of the Help System for more detailed information.

Operation: Source:

Dermal Model Input Parameters | Inhalation Model Input Parameters | Activity Exposure Estimates

Chemical State: Model Status: Model was successfully run

EPA/OPPT 2-Hand Dermal Contact with Liquid Model

Parameter	Type High End	Origin High End	Value High End	Units
AT: Averaging Time	Default	Model Parm	40	years
ATc: Averaging Time over a	Default	Model Parm	70	years
BW: Body Weight	Default	Model Parm	70	kg
ED: Exposure Days	Default	ODa	125	days/site-yr
EY: Years of Occupation	Default	Model Parm	40	years
FT: Frequency of Events	Default	Model Parm	1	events/site-c
NS: Number of Sites	Default	Mass Parm	1	sites

Add or Remove an Exposure model | View/Update Dermal Model Information | Introductory Notes for the Inhalation Summary | Run Model(s)

The Exposures Tab

Click on the **Exposures** tab to view or modify the models (i.e., algorithms) and associated input parameters used to calculate the inhalation and dermal exposures to workers while performing each of the chosen activities within each of the operations of your assessment. Then click Run Model(s) to generate release estimate results from the model(s).

1. Select an operation from the *Operation* drop down list.
2. Select a source for which exposures are calculated from the *Exposure Activity* drop down list.
 - The models that are used to calculate the dermal and inhalation exposures from the selected activity within the selected operation appear with the associated form of the chemical.

The parameters used by the dermal and inhalation exposure models appear in the **Dermal Model Input Parameters** subtab and the **Inhalation Model Input Parameters** subtab, respectively. These subtabs also indicate which parameters are ChemSTEER default values, the source of the parameter value (i.e., whether previously input in another tab or calculated from other input parameters), the current value, and the units.

***Note:** ChemSTEER currently contains more than 15 different models that can be used to calculate exposures, each with their own set of default settings and values. You are highly encouraged to review the *ChemSTEER Estimation Methods and Models – Worker Exposures* topic in the **ChemSTEER Help System** for a more complete description of the models and their bases before selecting alternative models to the ChemSTEER defaults and/or modifying default input values.

The ChemSTEER Exposures Tab (continued)

Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001 Appendix G. ChemSTEER Case Study

Adding or Removing Exposure Models

Click on the **Add or Remove an Exposure Model** button in the **Exposures** screen to change the default models that are used for the selected exposure activity.

The **Add/Remove Exposure Models** screen will appear with drop down lists of alternative dermal and inhalation models that you may choose to use in the assessment.

View / Update Exposure Model Information

Read-only and updatable information about the selected exposure model are shown below. Click on the associated Type column label for a parameter to change it's value. When the Type is User-defined, you enter your value directly in the Value column. To calculate two sets of model results, enable the Model Parameters for Output 1 option and the Model Parameters for Output 2 option below. Note that Output 1 parameters are used to calculate the Output 1 model results and Output 2 parameters are used to calculate the Output 2 model results. Use care and consistency in entering the parameter values to ensure that they are used appropriately by the model equation(s).

Activity: Loading Liquid Product into Drums
Model: EPA/OPPT Mass Balance Model

Model: $I = Cm \times b \times h$
Equation: $LADD = (I \times ED \times Y) / (BW \times ATc \times 365 \text{ days/yr})$

Mechanism: Inhalation of chemical vapors

Chemical State: Vapor Uncertainty (estimate based on model, regulatory limit, or data not specific to industry?)

Enable Model Parameters for Output 1 Enable Model Parameters for Output 2

Typical Worst Case

Basis: EPA/OPPT Mass Balance Model

Parameters:

Parameter	Type 2	Origin 2	Value 2	Units
EY: Years of Occupation Exposure	Default	Model Parm	40	years
G: Vapor Generation Rate	Model Output	Model Parm	6.790192E-03	g/s
h: Exposure Duration	Non-default	User Specified	2	hrs/day
k: Mixing Factor	Default	Model Parm	0.1	dimensionless
MW: Molecular Weight	Default	Chem Parm	150	g/mol
NS: Number of Sites	Default	Mass Parm	1	sites
NW/exm: Number of Workers Exposed	Default	User Specified	1	workers/site

OK Cancel

View/Update Model Information

Click on either the **Dermal Model Input Parameters** or the **Inhalation Model Input Parameters** subtab and click the **View/Update Model Information** button in the **Exposures** screen to modify the default model parameter values to be used in the calculations.

The **View/Update Exposure Model Information** screen displays information about the selected model, including: the equation(s) used in the calculation, a description of the mechanism of exposure, the chemical state, the basis/source of the model, and a list of the parameters used by the model.

1. To change a parameter value, click on the associated *Type* field.
2. For some parameters, you will change the *Type* field from 'Default' to 'Non-default'. If you choose 'Non-default', you may then click on the associated *Value* field and enter the new value for the parameter (other parameters will prompt you to select from a specified list of alternative values).
 - In our scenario, we previously found that drums are filled for approximately 2 hours per day (see *Entering Container Parameters*). Therefore, we may change the default exposure duration (h) from the default of the ChemSTEER estimate of 2.0261 hours/day.

**Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001
Appendix G. ChemSTEER Case Study**

The ChemSTEER Exposures Tab (continued)

Run the Models

Click the **Run Model(s)** button in the **Exposures** tab to execute the exposure model calculations.

View Exposure Estimates

Click on the **Activity Exposure Estimates** subtab to view the results of the calculations. This screen displays the type of exposure, the estimated value, and the associated units.

The results for our case study show that the workers may inhale approximately 141 mg of chemical vapors per day during drum filling activities. In addition, they come into contact with 1,411 mg of the liquid chemical on their hands daily during the filling activity. These values are potential dose rates.

The inhalation and exposure models also calculate several other types of dose rates: lifetime average daily dose, average daily dose, and acute potential dose (all in units of mg/kg-day).

Estimating Chemical Exposures

For the operation selected in the "Operation" box below, all activities that have an associated worker exposure are listed in the "Activity" box. When a worker exposure activity is selected, the associated inhalation or dermal model and its parameters will be shown in the respective subtab below. To view or modify the model equation parameters, click on the desired subtab and click "View/Update Model Information". Read the "Purpose and Use of the Exposures Tab" topic of the Help System for more detailed information.

Operation: Source:

Characterization of Results	Total Number of Workers	Exposure Days per Year	Potential Dose Rate (mg/day)	Lifetime Average Daily Dose (mg/kg-day)	Average Daily Dose (mg/kg-day)	Acute Potential Dose (mg/kg-day)	Basis
Worst Case	1	125	142.53	0.3985	0.6973	2.0361	EPA/OPPT Mass Balance
High End	1	125	1,411.2	3.9452	6.9041	20.16	EPA/OPPT 2-Hand

Sustainable Futures / P2 Framework Manual 2012 EPA-748-B12-001 Appendix G. ChemSTEER Case Study

The ChemSTEER Optional Information Tab

The *Optional Information* Tab

To enter additional information about your assessment, click on the *Optional Information* tab.

This tab contains several input screens that you may select from the drop down list, including:

- MSDS/Label/Exposure Limits
- Pollution Prevention Considerations
- General assumptions used in the assessment

Some of the input screens are designed to serve EPA-related assessments and may be left incomplete, including:

- SAT Data
- Exposure-based Criteria
- Other Uses, Occupational Exposure Rating, and Consumer Use.

Saving and Opening Your Assessments

You can save assessments as individual records in a database file containing multiple records or as their own individual database files using File/ Save or /Save As options on the Menu Bar.

If you open an Assessment (record) from an existing database file, you may view and/or edit the assessment on the ChemSTEER interfaces (screen views).

You may choose File/ Save Assessment to

overwrite the Assessment that is in the existing database file with the working assessment that is displayed on the ChemSTEER interfaces.

If the existing database file contains more than one Assessment record, a table of Assessment records will appear that includes four fields in the record: Type, Identifier, Status, and Date. These fields must be completed on the General screen (the first screen that appears after running ChemSTEER).

You should review the ChemSTEER Help topics under the Guide to ChemSTEER Menus (File) to learn more about saving and opening assessments.

The screenshot shows the 'Optional Information' tab in the ChemSTEER software. The window title is 'Case Study - Mock PMN'. The menu bar includes 'File', 'Edit', 'Reports', and 'Help'. The 'Optional Information' tab is selected, and a dropdown menu shows 'MSDS / Label / Exposure Limits'. Below this, there are sections for 'MSDS Requirements' and 'Exposure Limits'. The 'MSDS Included' checkbox is checked (Yes), and the 'Label Included' checkbox is unchecked (No). The 'General Equipment' dropdown is set to 'gloves/goggles/glasses/local exhaust ventilation/general mechanical ventilation'. The 'Respirator' dropdown is set to 'air purifying/organic vapor/supplied air'. The 'Health Effects' dropdown is set to 'flammable irritant to skin/eyes/lungs/mucous membrane'. An 'Update Optional Information' button is at the bottom.

