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/cm^3

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	l estimate hpd and dpy
Cleaning reactor	< 80%	4	1.5	25

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	l 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**.

Blank Spreadsheet of Model Inputs

OPERATION(S): Workplace / workpla such that estimates can be assumed to	aces with same/similar operations s of releases and exposures be the same.	<u>Media of Rel</u> Water Air Landfill Incineration	ease <u>Exposure Routes</u> Inhalation Dermal Drinking water
	Manufacturing		1
	(PMN chemical is created or	r formed)	
VP			Example Release(s)
MW	Need 3 variables for chemS	TEER entry:	* equipment cleaning
Density	Production Volume?		* sampling
Sol	# of sites?		
	Batch size?		too water and
	Batches/Year?		Exposure Activities(s)
	Wt fraction?		 loading into transport
SAT/Model	# of workers?		containers
ECO (EpiSuite)			* sampling
Health (SARs)	Site(s) typically controlled by the s	submitter	
	minimal in number (1 - 3), lower #	of workers	
	larger, single point releases]
	SUBSEQUENT OPERATIO	N:	
	transport of product / chemic	cal:	
	% and type of container.		-
	Processing	ted or destroyed	l
enu matadala	(PMN chemical heither creat	ted or destroyed	I) IEurometa Balanas(a)
raw materials	Mand 2 unighter for share?	TEED aster	Example Release(s)
(product/chemical)	Need 3 variables for chems	TEER entry.	 equipment cleaning container residue
import DMM	# OF SILES F	a days?	container residue
Volume Imported?	Wit fraction chemical in prod	ig days r	
volume imported?	# of workers?	uctr	
	# Of WORKERS?		* unloading & loading containers * vapor release from unloading
	Sites controlled by the submitter a	and others	& loading operations
	SUBSEQUENT OPERATIO	N:	
	transport of product / chemic	cal:	
	lise		7
	/DMN is transformed or dest	(hewort	Example Release(s)
	(Finite is transformed or dest		*equipment cleaning
raw materials	Need 3 variables for chemS	TEER entry	*container residue
	# of sites?	and anot	* End use releases
%PMN in Product	Use Rate?		Ling use releases
	Wt fraction chem in product?	2	Exposure Activities(s)
	Operating days/year?	5.11	unloading transport containers
	operating days years		end use activities
	Sites typically controlled by others		* coating applications
	Can have 1000's use sites large	# of workers	* unit operations and processing
	smaller releases over a number of	f sites	* Miscellaneous activities

Completed Spreadsheet of Model Inputs



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.



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General		
Assessment Type:	PMN	Consolidated Case: No Last Saved: 7/13/04 3:18:52 PM
Status:	CEB Staff Draft	
Fiscal Year:		
Assessment Identifier:	0000	Date: 07/13/2004 CBI: No Number of Contact Reports: 0
Assessors:		· · · · · · · · · · · · · · · · · · ·
Name: Scott	Prothero	L Crawford
Affiliation: USE	PA	ERG, Inc (Contractor)
Phone: 202-5	55-1234	404-555-0987
Email: proth	ero.scott@epa.gov	leslie.crawford@erg.com
		-
Company Name	XYZ Chemical Co.	Revision Notes / Assessment Overview:
Street Address	1313 mockingbird Lane	
City	Anywhere	
State	AK Zip: 99999	
		<u>.</u>

The ChemSTEER General Tab - Entering General Information

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.

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.
- <u>Total assessed production volume</u> (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.

ChemSTEER 05/27/2004 Ver	ision - 0000
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Chemical Name: Case Study	/ Chemical
Chemical Category:	
Trade Name(s):	
Chemical CAS Number: 999-99-9	Molecular Formula:
Total Assessed Production Volume (I	PV): [100000 kg/yr
Imported Production Volume	e (PVi): kg/yr
Domestic Production Volume	s (FVd): 100000 kg/yr
Type of	Notice: Manufacturing
Vapor Pressure (VPchem):	torrat 20 C
Molecular Weight (MW):	50 g/mol % < 500: % < 1000:
Density (Dchem):	1.815 g/cm3 at C
Solubility in Water (WSchem):	g/Lat C
General Chemical interme	ediate for off site reactions
End Use(s):	
	Update Chemical Information View Exposure Limits
Parameters with red labeling are	often important defaulte used in mass balance, container, and model calculations
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*<u>Note</u>: 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.

The ChemSTEER Chemical Tab - Entering Chemical Information (continued)

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

- <u>Vapor pressure</u> (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.
- <u>Density</u> (Dchem, g/cm3) the density of the pure chemical to be assessed; you may also enter the reference temperature (oC) for this value
- <u>Solubility in water</u> (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)

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Chemical Category:			
Trade Name(s):			
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Imported Production	Volume (PVi):		
Demostic Production	Volume (FVd)	rgryn	
Domestic Production			
	Type of Notice: Mar	ufacturing	
Vapor Pressure (VPc)	hem): 1	torrat 20 C	
Molecular Weight (I	MW): [150	g/mol % < 500: % < 1000:	
Density (Dcl	hem): 0.815	g/cm3 at C	
Solubility in Water (WScl	hem):	g/Lat C	
General Chemica Description of End Use(s):	al intermediate for off s	te reactions	
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*<u>Note</u>: 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.

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.

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lick the "Update Operations" button below to add or remove an operation from your assessment. To view more information about an	operation or
odify its properties (e.g., its relationship to other operations in the assessment, the sources/activities in the operation), select it in the li	ist below and
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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*).

User-defined Processing	
User-defined Use Adhesives Formulation Operatii Automobile OEM Spray Coating Automobile Refinish Spray Coa Recirculating Water Cooling To	20 2 In Additive Use Operation
To add an operation to the asse from the assessment, select it in and type in a new name.	ssment, select it from the list above and press the "ådd to list" button. If you wish to remove an operation the list below and press the "Bemove from list" button. To rename an operation, select it in the list below
When you are finished updating	the fat of operations in the assessment, press DK.
Selected Operations:	Add to list Bemove from list
Manufacture of Chemical Use of Intermediate Formulat	ion .

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.

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eratione		
lick the "Undate	Operations" button below to add or remove an operation from your assessment. To view more information about an operation or	
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The ChemSTEER Operations Tab – Entering Information on the Relationships Between Operations

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Edit Preferences Reports Help		
ral Chemical Operations Operation Parameters 1	Releases Exposures Optional Information	
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elect the operations in the list at the top of this page in	n order from first to last to allow ChemSTEER to automatically distribute the assessed volume	
elect the operations in the list at the top of this page in operly (e.g., manufacturing first, then processing1, pro	n order from first to last to allow ChemSTEER to automatically distribute the assessed volume ocessing2,, use1, use2,).	

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:



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.

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neral Chemical Operations Operation Par	eters Releases Exposures Optional Information	
perations		
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odify its properties (e.g., its relationship to oth	operations in the assessment, the sources/activities in the oper-	ation), select it in the list below and
lick on the appropriate subtab.	M	
Manufacture of Chemical		
Use of Intermediate Formulation		
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La La La Divisional Chaines	n en las estas a l	
elationships Description Privateal States	ources/Activities Site Information	
	nysical State Other Information	
Chemical into the Operation:	NA - chemical is manufactured	
Chemical out of the Operation:	Formulation 80% chemical in reaction mixture	
Chemical in the Operation:		
	Liedata Physical State	
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The ChemSTEER Operations Tab – Entering Information on the Sources / Activities

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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.

Add to operation
Add to operation
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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.

It Preferences Reports Help Chemical Operations Opera tions the "Update Operations" button b y its properties (e.g., its relationshi on the appropriate subtab. If acture of Chemical of Intermediate Formulation ionships Description Physical S peration Site Information: actify Name Ar YZ Chemical Co. 13	o tion Parameters Release below to add or remove an p to other operations in the p to other operations in the States Sources/Activitie	es Exposures Opti operation from your a e assessment, the sou Update <u>Operation</u> s Site Information	nal Information ssessment. To rces/activities i	n	formation about an on), select it in the li	i operation or list below and
I Chemical Operations Opera tions the "Update Operations" button b y its properties (e.g., its relationshi on the appropriate subtab. Identical of Intermediate Formulation ionships Description Physical S peration Site Information: acility Name Ar YZ Chemical Co. 13	tion Parameters Release below to add or remove an p to other operations in the States Sources/Activitie	es Exposures Opti operation from your a e assessment, the sou Update <u>Operation</u> s Site Information City	nal Information ssessment. To rces/activities i	n o view more in in the operation	formation about an on), select it in the li	i operation or list below and
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the "Update Operations" button b y its properties (e.g., its relationshi on the appropriate subtab. ufacture of Chemical of Intermediate Formulation ionships Description Physical S peration Site Information: acility Name Ar YZ Chemical Co. 13	velow to add or remove an p to other operations in the States Sources/Activitie	operation from your a e assessment, the sou Update <u>O</u> perations Site Information	ns	o view more in in the operation	formation about an on), select it in the li	operation or list below and
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The ChemSTEER Operation Parameters Tab

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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.
- Mass Accounting Basis Selection Continuous or Batch processes: <u>Continuous</u> processes run 24 hours per day over a number of days per year; <u>Batch</u> processes occur over less than 24 hours, thus an operation may perform one or more batches per day.
- Mass Accounting Basis Selection Influent or Effluent basis: Influent basis causes ChemSTEER to utilize the current settings for the chemical as it <u>enters</u> the selected operation (e.g., utilizing the settings for the chemical exiting the previous operation in a series). <u>Effluent</u> basis causes ChemSTEER to utilize the current settings for the chemical as it <u>exits</u> the selected operation.

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

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

Strategy: If you know more about the <u>product</u> 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 <u>raw material</u> 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 <u>125</u> <u>batches per year (Nby)</u> in order to process the amount of chemical being assessed (PV = 100,000 kg/yr) and that <u>800 kg of chemical is manufactured in each batch (BMOchem)</u>.

Since the chemical is	Update Operation Mass Accounting Parameters	×
<u>created</u> in this	Manufacture of Chemical	
operation, the input	Mass Ralance Pasis Celection Specify Mass Ralance Input Parameters Coacity Other Patch Parameters	
parameters listed in	mass balance basis deletion opeony more balance injent administra [specify onler balant-administers]	1
the lower half of the	Please specify exactly three of the first five parameters, including at least one parameter from the first 'pair' and at least one parameters for you. If you only need a smaller subset of these parameters	eter from the
screen are not	limited set of models, enter only those parameters and ChemSTEER will not derive a complete set of default values.	
applicable in this	Batch Operation; Using Product	
case. In addition, by	Pair 1	
clicking the Specify	V NS: Number of Sites	Galculate
Other Batch	Nby: Total batches per year 125	
Parameters subtab	Yorod: Weight Eraction of Chemical in Product (unitiess)	Defaulte
additional parameters	F DVO v 4 Dvist V v 0 4 v 4 (Dvist V v 2 4 v 4 (Dvist V v 2 4 v 4 v 2 4 v 4 v 2 4 v 4 v 2 4 v 4 v	Densuita
may be specified		Faichtare
(e.g., hours per	BMDchem: Batch Mass Output of Chemical kg/site-batch 800	Calculate
batch).		
	Calculate remaining two parameters Restore Defaults	
*Note: You are highly	Ratch Raw Material Parameters Calculation	
encouraged to review	If appropriate, you may change one or two of the following three parameters and press the 'Recalc' button for the parameter you	wish to have
this topic in the	ChemSTEER recalculate. Once you have changed one of these parameters, you must press a 'Recalc' button before you close	e this window.
ChemSTEER Help	Yrm: Weight Fraction of Chemical in Raw Material (unitless)	<u>R</u> ecalc
System for a more	BMIm: Batch Mass Input of Raw Material kg/site-batch	<u>R</u> ecalc
complete description	BMIchem: Batch Mass Input of Chemical kg/site-batch	<u>R</u> ecalc
(refer to Guide to		
Using ChemSTEER	<u>Calculate defaults</u>	
Tabs – Operation	No mass balance discrepancy exists	
Parameters Tab –		
Mass Balance	OK Cancel <u>B</u> asis <u>H</u> elp	
Parameters Subtab).		

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	Ele Edit Preferences Reports Help General Chemical Operation Parameters Releases Exposures Optional Information	×
the list of	Operation Parameters	
container-	Manufacture of Chemical Use of Intermediate Formulation	
related		
s that were		
chosen for the	Mass Balance Parameters Container Parameters Shared Parameters / Factors	
selected	The container-related sources/activities for the selected operation and the associated container-related parameters are shown in the	
operation (e.g.,	appropriate subtabs below. To view/update these parameters, double-click on the desired source/activity.	
product into	For Raw Material For Product For Other Material Container Parameters by Activity	
drums) along	0D = 125	
with the current		
values for the	Ncy (containers / r (containers / OHa (hours / source/ Activity Name / steurar) ODa (daus/ur) steudau) houri dau)	
parameters (for	Loading Liquid Product into Drums 1,013.04 125 8.1043 20 0.4052	
new		
assessments		
these are		
default values)		

es Ralance Parameters	Container Paramet	ters Shared Parame	ters / Factors				
a and a second second		1 strated i didina	201010				
0D = 125							ſ
Source/ A	ctivitu Name	Ncy (container	DD.a (daus/ur)	Ncd (containers / site-dau)	r (containers /	OHa (hours /	
Loading Liquid Produ	ict into Drums	1,013.04	125	8.1043	20	0.4052	

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.

 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 (Vc) is 55 gallons. By changing Vc 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.

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

Verify/Select	Container Parameters	
Container Parameters	Verify/Select Container Parameters for Product Verify/Select Container Parameter	ters by Source/Activity
Verify/Select	Loading Liquid Product into Drums	
Container Parameters by	Verify or change the container information below, the press OK to return to the	main window.
Source/Activity subtab	Please note that you may only select up to two of the parameters in the 1st an up to two parameters in the 2nd and 3rd groups. When taken together, you c parameters on the window.	d 2nd groups and you can only selec an only change up to three
 Approximately 1,013 drums of 	OD: Number of Operating Days	125
our cnemical	Mar Museker of containers are also per user (containers (also user)	L 010.04
filled over the	No. Number of containers per site per year (containers/site-year) ODa (days/yr): days/year for the activity	125
125-batch	Second Group	
campaign and		8.1043
drums will be	Third Group	
filled per day.	r (containers/hour): unloading/loading rate	20
 The default drum 	🔽 OHa (hours/day):	0.4052
unloading rate is	Calculate reproject the extended	1
20 drums per		J
determines the		
total number of		1
hours (OHa)	OK <u>B</u> asis <u>R</u> estore Defaults	Cancel
spent filling the	1	
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

Container Parameters		
enly/Select Container Parameters for Product	nity/Select Container Parameters	by Source/Activity
Loading Liquid Product into Drums		
Verify or change the container information below	, the press OK to return to the ma	in window.
Please note that you may only select up to two or up to two parameters in the 2nd and 3rd groups parameters on the window.	If the parameters in the 1st and 2r When taken together, you can be	nd groups and you can only select only change up to three
OD: Number of Operating Days		125
	- First Group	
Ncy: Number of containers per site per year I	(containers/site-year)	1,013.04
OD a (days/yr): days/year for the activity		125
	- Second Group	
Vcd (containers/site-day)		8.1043
	- Third Group	
I (containers/hour): unloading/loading rate		4
T OHa (hours/day):		2.0261
Calculat	e remaining two parameters	
OK Basis	Bestove Delavite	Carcel
gan	Liowae Deradara	Carta

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.

The ChemSTEER Releases Tab

neral Chemical Operations	Operation Paramete	ers Releases E	xposures Option	al Information]		
timating Chemical Relea	ses					
or the operation selected in the ource is selected, all of the as elect the model and click "Vie iformation.	ne "Operation" box bel sociated release mode w/Update Model Info	ow, all sources tha els will be shown in rmation''. Read th	at have an associ the "Release Mo e "Purpose and U	ated chemical re odel(s)'' box. To Ise of the Relea	lease are listed in the "Source" box. view or modify the release model eq ses Tab" topic of the Help System fo	When a release uation parameters or more detailed
eration: Lu con con	191		R	elease Model(s)		
Manufacture of Che	emical		I	PA/OPPT Sing	e Process Vessel Residual Model	
ource: Equipment Cleaning	Loosoo of Liquido from	n a Single 1 area)	land T	PA/OPPT Mas	s Transfer Coefficient Model	
JE quipment Cleaning	Losses of Liquids from	n a single, Large V	Vessei 🔳			
elease Input Parameters	vimated Releases					
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dodel Status: Model never rur	n					
8	Tune	Origin	Value	Linite		
Parameter	Conservative	Conservative	Conservative	CT ING		
Parameter Amit: Amount to Use	Conservative	Conservative BMOchem x	Conservative 800	kg/site-day		
Parameter Amt: Amount to Use Freq: Frequency to Use	Conservative Default Default	Conservative BMOchem x OD	800 125	kg/site-day days/site-yr		
Parameter Amt: Amount to Use Freq: Frequency to Use LF: Loss Fraction	Default Default Default	BMOchem x OD Model Parm	800 125 0.01	kg/site-day days/site-yr dimensionles		
Parameter Amt: Amount to Use Freq: Frequency to Use IF: Loss Fraction NS: Number of Sites	Default Default Default Default Default	Conservative BMOchem x OD Model Parm Mass Parm	2005ervative 800 125 0.01 1	kg/site-day days/site-yr dimensionles sites		
Parameter Amit Amount to Use Freq: Frequency to Use Fr: Loss Fraction NS: Number of Sites	Default Default Default Default Default	Conservative BMOchem x OD Model Parm Mass Parm	800 125 0.01	kg/site-day days/site-yr dimensionles sites		
Parameter Amt: Amount to Use Freq: Frequency to Use LF: Loss Fraction NS: Number of Sites	Default Default Default Default Default	Conservative BMOchem x OD Model Parm Mass Parm	Conservative 800 125 0.01 1	kg/site-day days/site-yr dimensionles sites		
Parameter Amt: Amount to Use Freq: Frequency to Use LF: Loss Fraction NS: Number of Sites	Default Default Default Default Default	Conservative BMOchem x OD Model Parm Mass Parm	Conservative 800 125 0.01 1	kg/site-day days/site-yr dimensionles sites		
Parameter Amt: Amount to Use Freq: Frequency to Use LF: Loss Fraction NS: Number of Sites	Default Default Default Default Default	Conservative BMOchem x OD Model Parm Mass Parm	Conservative 800 125 0.01 1	kg/site-day days/site-yr dimensionles sites		
Parameter Amt: Amount to Use Freq: Frequency to Use LF: Loss Fraction NS: Number of Sites	Default Default Default Default Default	Conservative BMOchem x OD Model Parm Mass Parm	Conservative 800 125 0.01 1	kg/site-day days/site-yr dimensionles sites		
Parameter Amt: Amount to Use Freq: Frequency to Use LF: Loss Fraction NS: Number of Sites	Default Default Default Default Default	Conservative BMOchem x OD Model Parm Mass Parm	Conservative 800 125 0.01 1	kg/site-day days/site-yr dimensionles sites		

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.

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.

	2 18 26 19 March 1				
tead-only and updateable inf alue. When the Type is User Updu 1 option and the Mode 2 parameters are used to calc y the model equation(s). Activity: Equipment Cle Model: EPA/DPPT Si	ormation about the sel defined, you enter you al Parameters for the 0 ulate the Output 2 mo aning Losses of Liquic ngle Process Vessel F	lected release model ur value directly in th lutput 2 option below del results. Use care ds from a Single, Larg tesidual Model	are shown below. e Value column. To . Note that Output and consistency in e Vessel	lick on the associated Type column label calculate two sets of model results, enable parameters are used to calculate the Out ntering the parameter values to ensure th	for a parameter to change its the Model Parameters for the put 1 model results and Outpu at the are used appropriately
Model DR (kg/site-d Equation: DR occurs ov	ay) = LF × Amt /er [Freq] days/year				<u>×</u>
Mechanism: Residual remo	ved from and/or dispo	sed from a single pro	cess vessel		
Enable Model Param	eters for Output 1			able Model Parameters for Output 2	
High End to Bounding			Juor	ervative	
arameters:					<u>.</u>
and motor of		Origin 2	Value 2	Inits	
Parameter	Type 2	Ungin 2	the second se		
Parameter Amt: Amount to Use	Type 2 Default	BMOchem x Nbd	800	.g/site-day	
Parameter Amt: Amount to Use Freq: Frequency to Use	Type 2 Default Non-default	BMOchem x Nbd User-defined	800	.g/site-day lays/site-yr	
Parameter Ami: Amount to Use Freq: Frequency to Use LF: Loss Fraction	Type 2 Default Non-default Default	BMOchem x Nbd User-defined Model Parm	800 25 0.01	.g/site-day lays/site-yr limensionles	
Parameter Amt: Amount to Use Freq: Frequency to Use LF: Loss Fraction VS: Number of Sites	Type 2 Default Non-default Default Default	BMOchem x Nbd User-defined Model Parm Mass Parm	800 25 0.01 1	g/site-day lays/site-yr imensionles ites	
Parameter Am: Amount to Use Freq: Frequency to Use LF: Loss Fraction NS: Number of Sites	Type 2 Default Default Default Default	BMOchem x Nbd User-defined Model Parm Mass Parm	800 23 0.01 1	g/site-day lays/site-yr imensionles ites	

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.

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.

							-
enty or change the media for the estimated) releas	e below.					
Manufacture of Chemical							
quipment Cleaning Losses of Liqui	ls fror	n a Single, Large Vessel					
To (NPDES number if appropriate);				-			-
	<u> </u>						¥.
Basis: EPA/OPPT Single Vessel Residu	ual Mov	del CER standard 1% residual				_	1
EFAUOFFT Single vessel nesidi	AGI MUU	Jei, CED stanuaru 1% lesiuuai.				1	
1							2
Water 0	- %						
Water or Air 0	~ %	Air	0	*			
Water or Air or Incineration 0	- %	Air or Incineration	0	*			
Water or Air or Landfill 0	- %	Air or Incineration or Landfill	0	%			
Vater or Air or Incineration or Landfill	- %	Air or Landfill	0	2			
	- %	Incineration	0	2	Deepwell Injection	0	%
Water or Incineration 100	and the second second	Incineration or Landfill	0	2	Destroyed	0	%
Water or Incineration 100 Water or Incineration or Landfill	%	Them to reactor to the manual				1. C. L.	
Water or Incineration 100 Water or Incineration or Landfill 0 Water or Landfill 0	- %	Landfill	0	2	Other	0	%
Water or Incineration 100 Water or Incineration or Landfill 0 Water or Landfill 0	*	Landfill		2	Other 	0	%

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 operation sel arce is selected, a ect the model and	ected in the "Operation" box below, all so II of the associated release models will be click "View/Update Model Information".	urces that have shown in the "R Read the "Purp	an associated chem elease Model(s)" bo ose and Use of the I	iical release are listed in x. To view or modify the Releases Tab'' topic of	the "Source" box. Whe e release model equation the Help System for more	n a release parameter detailed
ormation. ration: Manufact urce: Equipmen	ure of Chemical	Larne Vessel	Release Mo	odel(s): <mark>T Single Process Vessel</mark> T Mass Transfer Coeffic	Residual Model ent Model	
lease Input Param	eters Estimated Releases		,			
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
/ater or Incineratio	n Conservative	1	25	8	200	EPA/OPP

The ChemSTEER Releases Tab (continued)

Edit	Preferences	Beports Help					_
neral (Chemical 0	perations Operation Parameters R	eleases Exposure	s Optional Informa	ation		
stimatir	ng Chemica	l Releases		• •			
or the o ource is elect the	peration sele selected, all e model and on.	cted in the "Operation" box below, all of the associated release models will click "View/Update Model Information	sources that have be shown in the "R ". Read the "Purp	an associated cherr elease Model(s)" bo ose and Use of the	nical release are listed in x. To view or modify the Releases Tab'' topic of	the "Source" box. When a release model equation the Help System for more	n a release parameter: detailed
eration:	Manufach	re of Chemical		Release Mo	odel(s):		
	Imanulacio	are or crientical		EPA/OPP	T Single Process Vessel T Mass Transfer Coeffic	Residual Model	
ource:	Equipment	Cleaning Losses of Liquids from a Sin	gle, Large Vessel		r mass fransfer coeffic	en moder	
		inc					
elease	Input Parame	eters Estimated Heleases					
	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
Air		Output 2	1	25	0.1139	2.8466	EPA/OPP
4							

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.,

		itput 2 option beio el results. Use car	the Value column. To w. Note that Output e and consistency in	a calculate two sets 1 parameters are us entering the parame	of model results, enable the red to calculate the Output ster values to ensure that	he Model Parameters for the #1 model results and Output the are used appropriately
Activity: Equipment Cleaning Model: EPA/OPPT Mass Tr	Losses of Liquids ansfer Coefficien	: from a Single, La t Model	rge Vessel			
Model DR (kg/site-day) = (Equation: DR occurs over [Fre	(G × 3600 × 0Ha) eq] days/year	/ 1000				2
Mechanism: Volatilization of chem	nical from "static"	pool				
Example Model Decomplete i	for Outrad 1			anhla Madal Param	where for Outruit 2	
I Enable Model Parameters i	or output 1			nable model matan	eters for output 2	
Output 1	<u> </u>		JOut	put 2	-	
Basis: EPA/OPPT Mass T	ransfer Coefficien	t Model.				<u> </u>
Basis: EPA/OPPT Mass T.	ransfer Coefficien	v Model				×
Basis: EPA/OPPT Mass Tr arameters: Parameter	ransfer Coefficier	t Model.	Value 2	Units		-
Basis: EPA/OPPT Mass Tr srameters: Parameter K Area	ransfer Coefficier Type 2 Model Output	t Model. Origin 2 Model Parm	Value 2 6647.61	Units cm2		
Basis: EPA/OPPT Mass T srameters: Varea t: Diameter of Opening / Pool Ler	Type 2 Model Output Default	Model Origin 2 Model Parm Model Parm	Value 2 6647.61 92	Units cm2 cm	_	2 2 2
Basis: EPA/OPPT Mass T arameters: Parameter k Area Diameter of Opening / Pool Ler reg: Frequency to Use	Type 2 Model Output Default Non-default	Model Drigin 2 Model Parm Model Parm User-defined	Value 2 6647.61 92 255	Units cm2 cm days/site-yr		-
Basis: EPA/OPPT Mass T arameters: Area Diameter of Opening / Pool Ler rece Frequency to Use 2: Vapor Generation Rate	Type 2 Model Output Default Non-default Model Output	Model Drigin 2 Model Parm Model Parm User-defined Model Parm	Value 2 6647.61 92 25 0.0316291	Units cm2 cm days/site-yr g/s		-
Basis: EPA/DPPT Mass T arameter: Araneter L Diameter of Opening / Pool Ler iero, Frequency to Use Vagor Generation Rate AV: Molecular Weight E. Namber of Steel	Type 2 Model Output Default Non-default Model Output Default Default	t Model. Drigin 2: Model Parm Model Parm User-defined Model Parm Chem Parm	Value 2 6647.61 92 25 0.0316291 150	Units cm2 cm days/site-yr g/s g/mol cites		2
Basis: EPA/OPPT Mass T araneters: Aneas Diameters: Canadian Copening / Pool Ler- ring: Frequency to Use : Vapor Generation Rate : Vapor Generation Rate : Vapor Generation Rate : Nanote of Stest	Type 2 Model Output Default Non-default Model Output Default Default Default	Model Origin 2: Model Parm Model Parm User-defined Model Parm Chem Parm Mass Parm Core Parm	Value 2 6647.61 92 0.0316291 150 1	Units cm2 cm days/site.yr g/mol sites boues/dau		
Basis: EPA/OPPT Mass T arameter: Aranee Diameter of Opening / Pool Ler reg. Frequency to Use 3: Vapor Generation Rate MV: Molecular Weight 35: Number of Stee Dis. Openating Hours for the Activ. - Tennenature	Type 2 Model Output Default Non-default Model Output Default Default Default	Model	Value 2 6647.61 32 2.55 0.0316291 150 1 1 299	Units cm2 cm days/site.yr g/s g/mol sites hous/day K		
Basis: EPA/OPPT Mass T arameters: "Parameter Diameter of Opening / Pool Ler rice; Frequency to Use 3: Vapor Generation Rate 4: Windiscutar Weight S: Number of Sites This: Opening Hours for the Activ Temperature P-Vapor Pressure	Type 2 Model Output Default Nor-default Model Output Default Default Default Default	Model.	Value 2 6647.61 92 25 0.0316291 150 1 1 1 288	Units cm2 cm g/s g/md sites hours/day K ter		

the EPA/OPPT Single Vessel Residual model).

The second model shown (the *EPA/OPPT Mass Transfer Coefficient* model) calculates the amount of chemical <u>vapor</u> 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).

The ChemSTEER Exposures Tab

e Edit Preferences Reports	Help	1	- 1-		
eneral Chemical Operations (Operation Paramet	ers Releases	Exposures Option	al Information	
stimating Chemical Exposure	es				
For the operation selected in the " exposure activity is selected, the a model equation parameters, click the Help System for more detailed	'Operation'' box be associated inhalati on the desired sub information.	elow, all activities t on or dermal mode tab and click "Vie	hat have an associ el and its parameters w/Update Model Ir	ated worker exp s will be shown nformation''. Re	posure are listed in the "Activity" box. When a worker in the respective subtab below. To view or modify the ad the "Purpose and Use of the Exposures Tab" topic
peration:		Source:			
Annufacture of Chemical	2	 Loading Ligu 	id Product into Dru	ms	
Chemical State: Liquid EPA/0PPT 2-Hand Dermal Conta	act with Liquid Mod	fel		Model	Status: Model was successfully run
Chemical State: Liquid EPA/0PPT 2-Hand Dermal Conta Parameter	act with Liquid Moo	del Origin	Value	Model	Status: Model was successfully run
Chemical State: Liquid EPA/DPPT 2-Hand Dermal Conta Parameter	act with Liquid Moo Type High End	del Origin High End	Value High End	Model	Status: Model was successfully run
Chemical State: Liquid EPA/OPPT 2-Hand Dermal Conta Parameter AT: Averaging Time	act with Liquid Moo Type High End Default	del Origin High End Model Parm	Value High End 40	Model Units years	Status: Model was successfully run
Chemical State: Liquid EPA/OPPT 2-Hand Dermal Conta Parameter AT: Averaging Time ATc: Averaging Time over a	Type High End Default Default	del Origin High End Model Parm Model Parm	Value High End 40 70	Model Units years years	Status: Model was successfully run
Chemical State: Liquid EPA/OPPT 2-Hand Dermal Conta Parameter AT: Averaging Time ATc: Averaging Time over a BW: Body Weight	Type High End Default Default Default	del Drigin High End Model Parm Model Parm	Value High End 40 70 70	Model Units years years kg	Status: Model was successfully run
Chemical State: Liquid EPA/OPPT 2-Hand Dermal Conta Parameter AT: Averaging Time ATc: Averaging Time over a BW: Body Weight ED: Exposure Days	Type High End Default Default Default Default	del Origin High End Model Parm Model Parm ODa	Value High End 40 70 70 125	Model Units years kg days/site-yr	Status: Model was successfully run
Chemical State: Liquid EPA/OPPT 2-Hand Dermal Conta Parameter AT: Averaging Time ATc: Averaging Time over a BW: Body Weight ED: Exposure Days EY: Years of Occupation	Type High End Default Default Default Default Default Default	del High End Model Parm Model Parm ODa Model Parm ODa	Value High End 40 70 70 125 40	Model Units years kg days/site-yr years	Status: Model was successfully run
Chemical State: Liquid EPA/OPPT 2-Hand Dermal Conta Parameter AT: Averaging Time ATc: Averaging Time over a BW: Body Weight ED: Exposure Days EY: Years of Occupation FT: Frequency of Events	Type High End Default Default Default Default Default Default Default	del Drigin High End Model Parm Model Parm OD a Model Parm Model Parm	Value High End 40 70 70 125 40 1	Model Units years kg days/site-yr years events/site-c	Status: Model was successfully run

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)

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 M	odel Informatio	n				
Read-only and updatable informatii value. When the Type is User-defin Output 1 option and the Model Par parameters are used to calculate th the model equation(s). Activity: Loading Liquid Proc	on about the select ned, you enter you ameters for Dutput ie Dutput 2 model duct into Drums	cted exposure mode ar value directly in t t 2 option below. N results. Use care a	el are shown below, he Value column. To lote that Dutput 1 p and consistency in e	Click on the ass calculate two se arameters are use ntering the param	sciated Type column label for a param ets of model results, enable the Model I ed to calculate the Dutput 1 model resu leter values to ensure that the are used	eter to change it's Parameters for ults and Output 2 d appropriately by
Model: EPA/OPPT Mass B	alance Model					
Model I = Cm x b x h Equation: LADD = (I x ED x Y	′)/(BW/xATcx3	165 days/yr)				<u>×</u>
Mechanism: Inhalation of chemic	cal vanors					_
Enable Model Parameters for D Typical Basis: EPA/OPPT Mass Ba	lutput 1		Er Wors	able Model Parar t Case	neters for Dutput 2	×
Parameters:						
Parameter	Type 2	Origin 2	Value 2	Units		<u>^</u>
EY: Years of Occupation Exposur	E 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		1
k: Mixing Factor	Default	Model Parm	0.1	dimensionles		
MW: Molecular Weight	Default	Chem Parm	150	g/mol		
NS: Number of Sites	Default	Mass Parm	1	sites		-1
I NWexn: Number of Workers Fxnr	ni Default	Hser Snecified	1	workers/site		
NWexn: Number of Workers Exn	ii Default	User Snecified	1 IKCa	workers/site		

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 <u>2.0261 hours/day</u>.

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).

e Help System for more detailed info eration:	ormation.	Source	¢					
enufacture of Chemical	1	Loadir	ng Liquid Prod	luct into Drum	\$			
Characterization of Results	Total Number of	Exposure Days per Year	Potential Dose Rate (mg/day)	Lifetime Average Daily Dose	Average Daily Dose (mg/kg-dau)	Acute Potential Dose	Basis	
Vorst Case	Workers 1	125	142.53	(mg/kg-day) 0.3985	0.6973	(mg/kg·day)	FPA/OPPT Mass Balance	
ligh End	1	125	1,411.2	3.9452	6.9041	20.16	EPA/OPPT 2-Hand	

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 <u>EPA-related assessments</u> 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

Use the drop down combo box I MSDS / Label / Exposure Limi	to select the optional information you would like to see below.	
MSDS Requirements Expo	isure Limits	
	MSDS Included: No	
General Equipment:	gloves/goggles/glasses/local exhaust ventilation/general mechanical ventilation	
Respirator:	air purifying/organic vapor/supplied air	
Health Effects:	flammable initiant to skin/eyes/lungs/mucous membrane	-
	Update Optional Information	

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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.