ChemSTEER
Quick Start Guide

Updated May 15, 2015

Overview and Contents

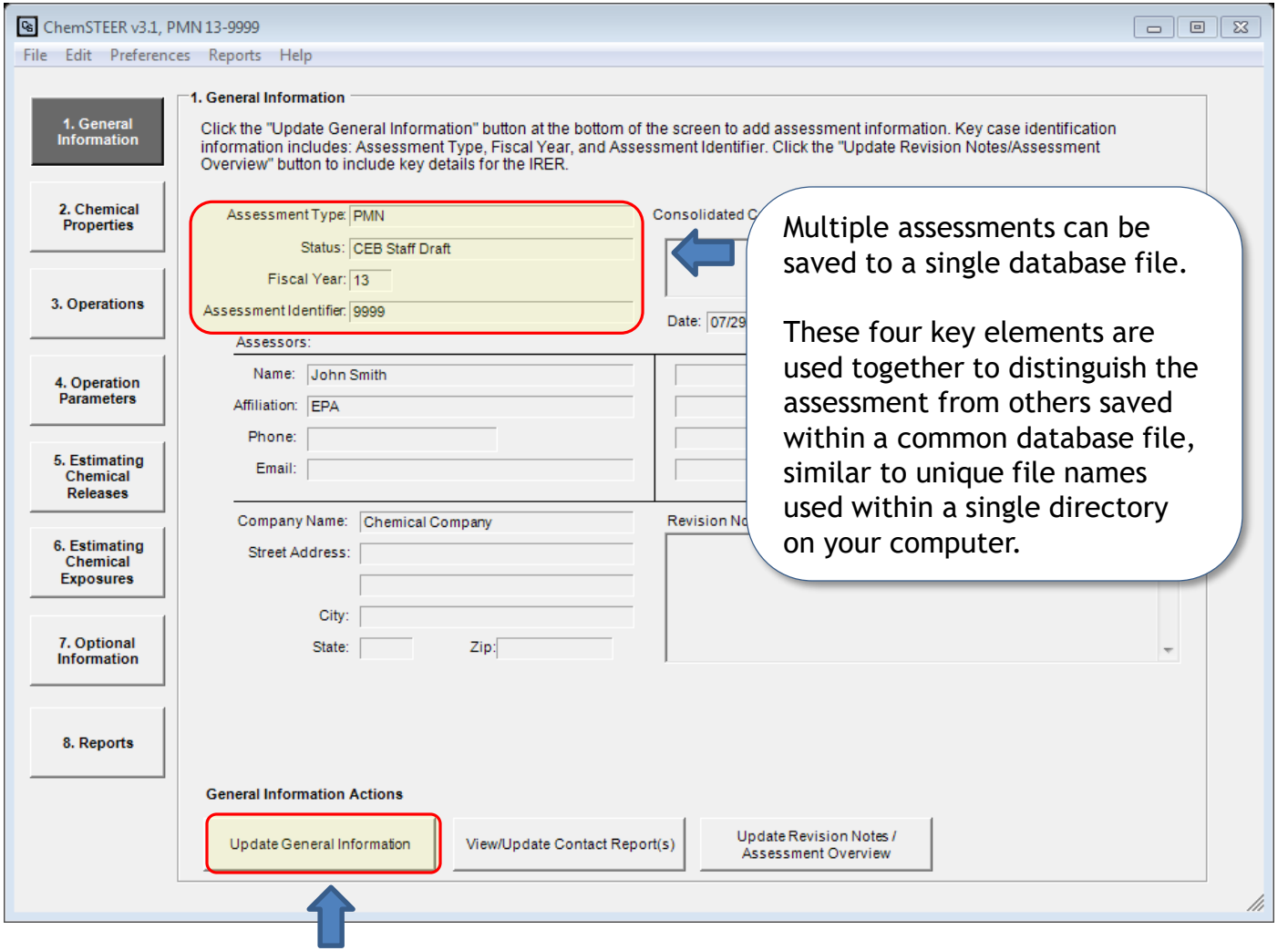
- Welcome to the ChemSTEER Quick Start Guide!
- This guide is intended to provide a new, non-EPA user with an introduction to the ChemSTEER application.
- This guide discusses key information needed to complete a basic assessment, but is not meant to discuss all capabilities and functionalities of ChemSTEER. Please reference the ChemSTEER User Guide for more comprehensive information.
- Contained in this guide are brief overviews of the following main tabs and subtabs available in ChemSTEER:

1. General Information
2. Chemical Properties
3. Operations
   - 3a. Relationships
   - 3b. Description
   - 3c. Physical States
   - 3d. Sources/Activities
   - 3e. Site Information
4. Operation Parameters
   - 4a. Mass Balance Parameters
   - 4b. Container Parameters
   - 4c. Shared Parameters/Factors
5. Estimating Chemical Releases
   - 5a. Release Input Parameters
   - 5b. Estimated Releases
6. Estimating Chemical Exposures
   - 6a. Dermal Model Parameters
   - 6b. Inhalation Model Parameters
   - 6c. Respirator Class & Monitor Review
   - 6d. Activity Exposure Estimates
7. Optional Information
8. Reports

To get started, open ChemSTEER and click "Prepare Assessment" on the splash screen!

1. General Information

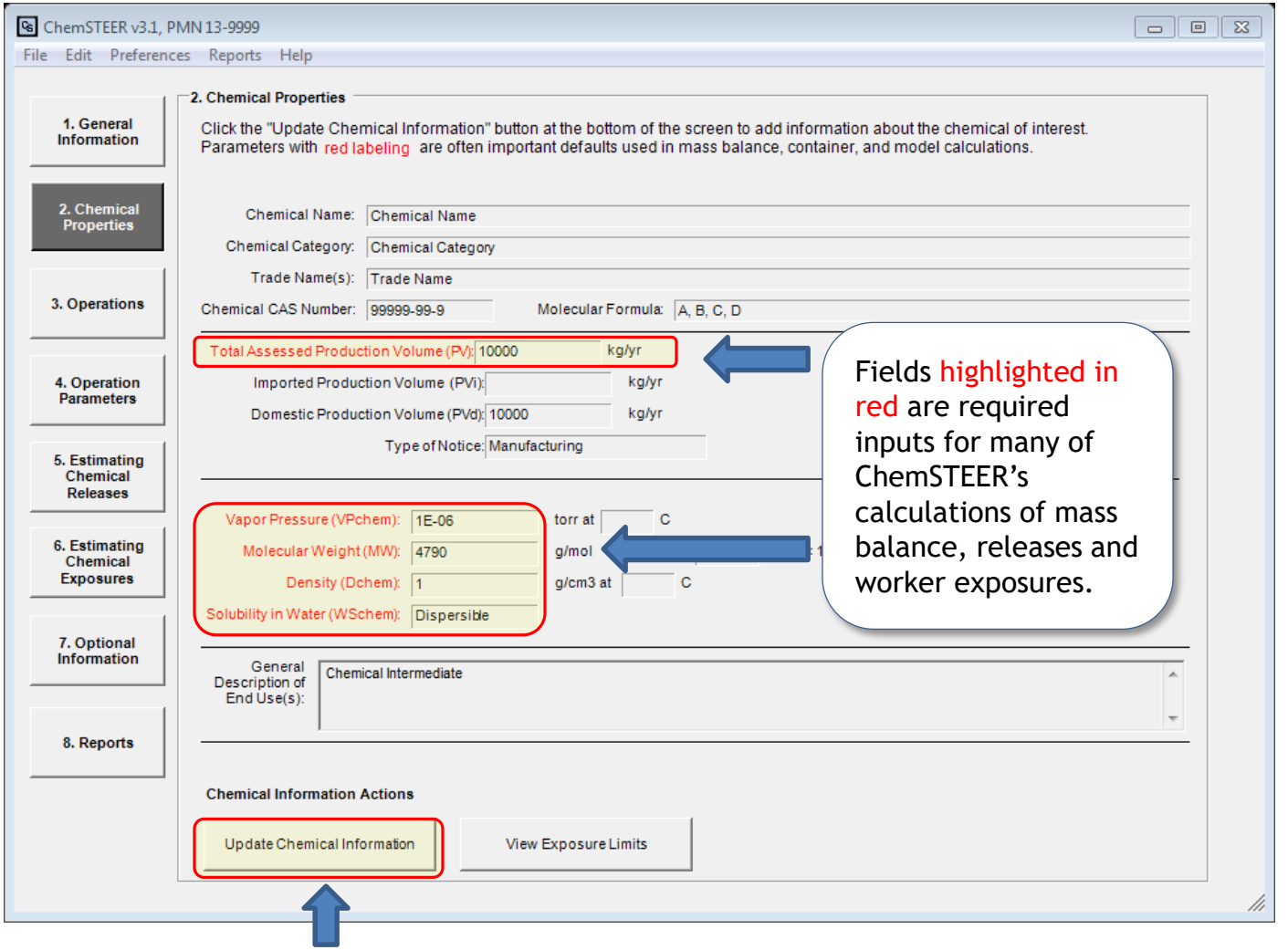
- The *General Information* tab is used to input basic assessment information.
- Key assessment identification fields (which are highlighted in the screenshot) include:
  - Assessment Type;
  - Status;
  - Fiscal Year; and
  - Assessment Identifier
- After the assessment is saved, ChemSTEER displays the case number, i.e., Fiscal Year and Assessment Identifier (ex. P99-9999) in the title bar at the top of the screen.



2. Chemical Properties

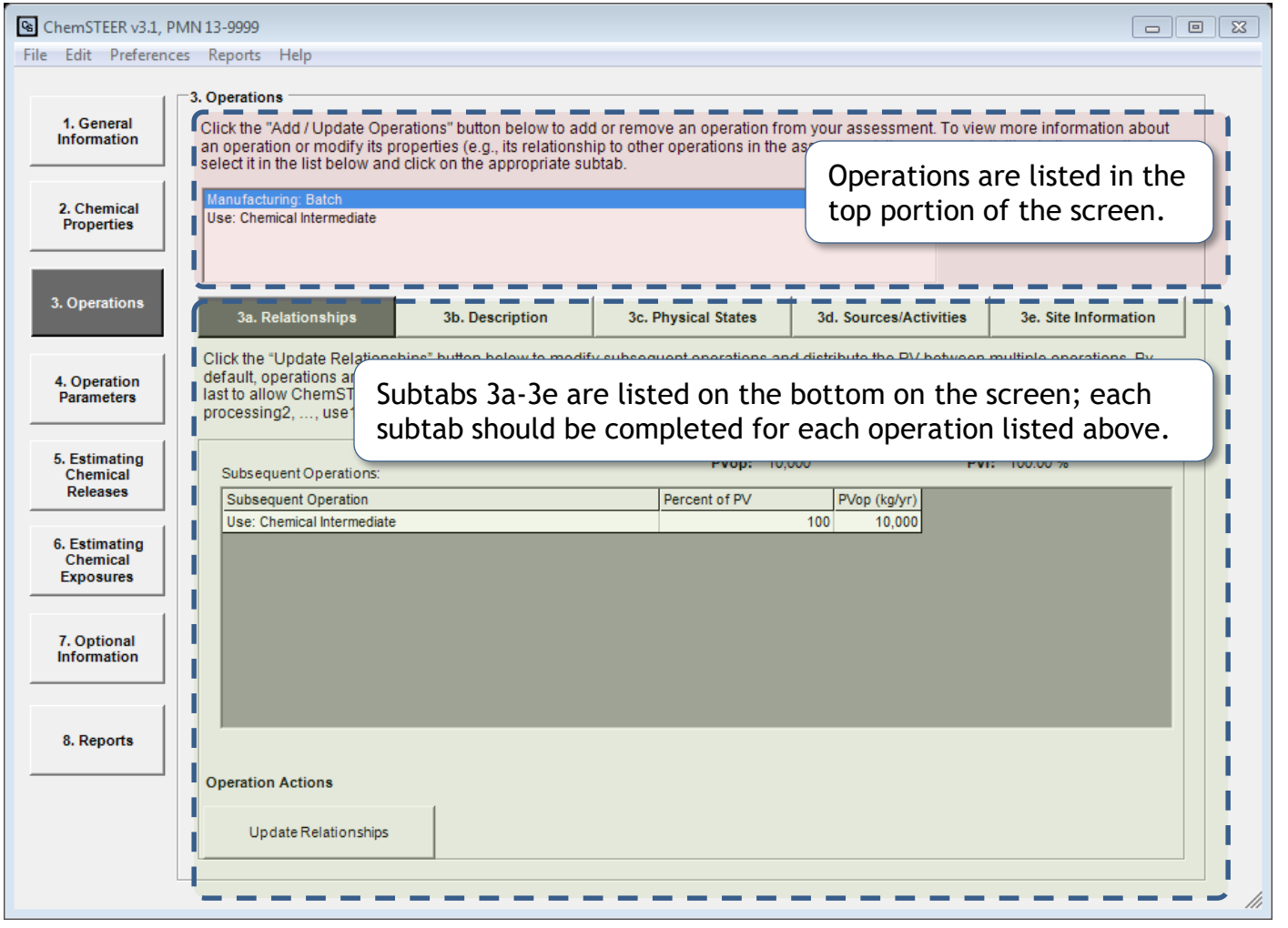
- The *Chemical Properties* tab includes important information on the chemical, production volume (PV), and physical properties.
- Key fields are highlighted in red and include:
  - Total Assessed Production Volume (PV);
  - Vapor Pressure;
  - Molecular Weight;
  - Density; and
  - Solubility in Water

  It is highly recommended that you enter a value for these fields before continuing with the assessment.



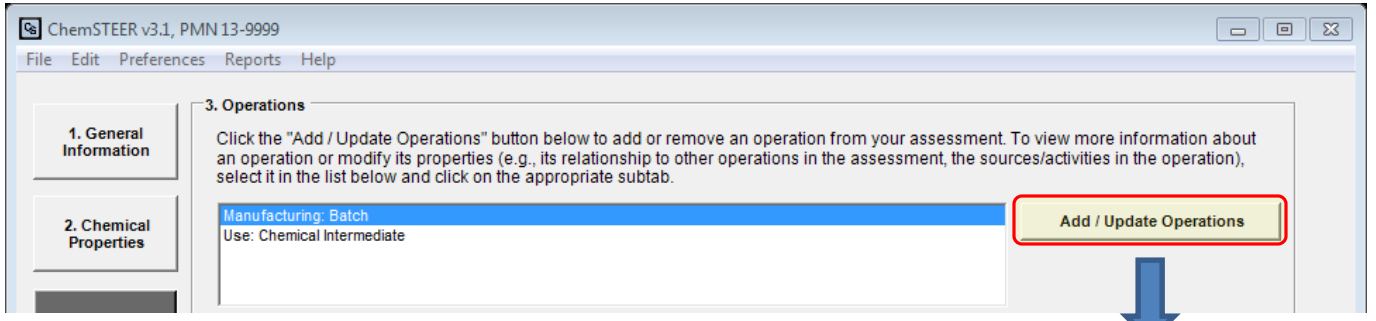
3. Operations - Overview

- Use the *Operations* tab and each of its subtabs to build your scenario and enter necessary information about each operation in your assessment
- An operation is a workplace or set of "homogeneous" workplaces with essentially the same (or similar) processes, equipment, chemical throughputs, procedures, and worker populations, such that the releases and exposures to the chemical being assessed can be assumed similar for all of the workplaces in the set.
- Operations should first be added to the top of the screen; for each operation, you should then complete the five subtabs:
  - 3a) Relationships;
  - 3b) Description;
  - 3c) Physical States;
  - 3d) Sources/Activities; and
  - 3e) Site information.



Note: You must add at least one operation to access the ChemSTEER release and exposure models while preparing an assessment.

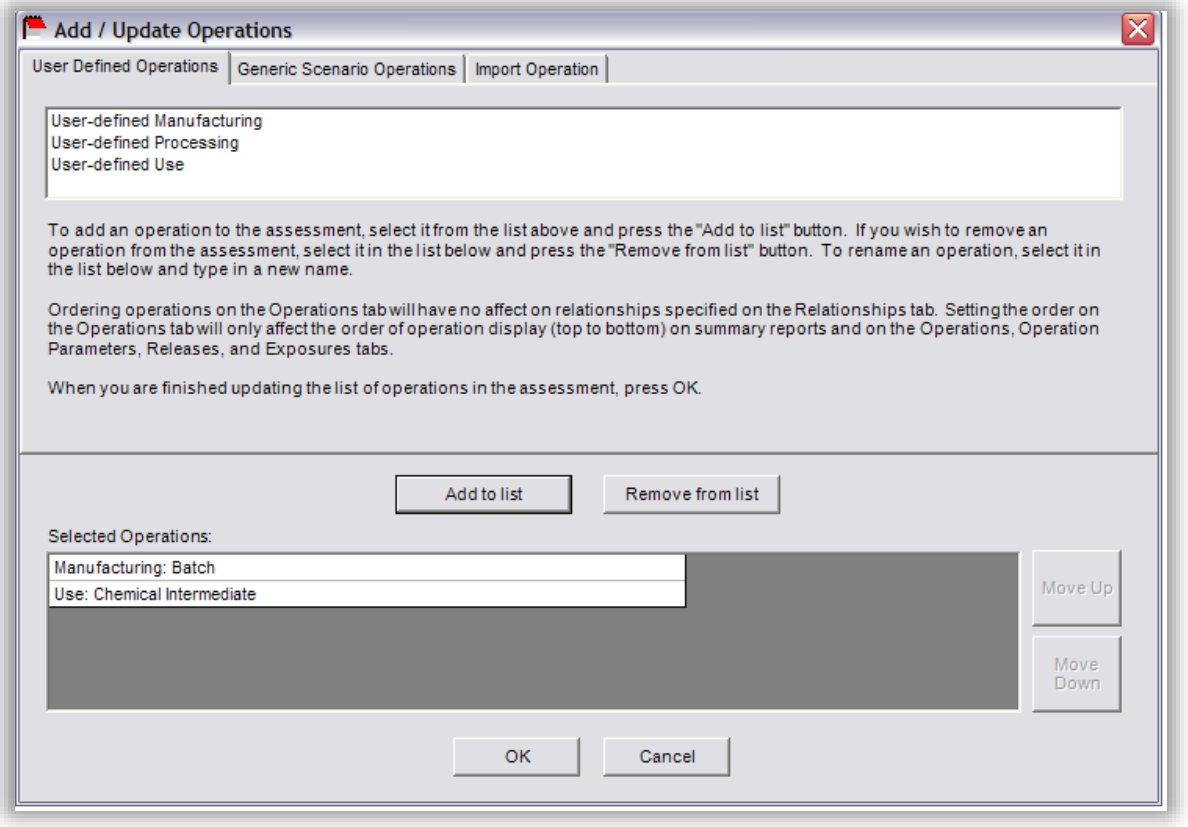
3. Operations --> Add/Update Operations



Begin by clicking the ***Add/Update Operations*** button to choose or define the operation(s) in your assessment.

There are three choices from which to select your operation:

- **User-defined** – These operations have no pre-defined sources/activities, mass balance parameters, or release/exposure models.
- **Generic Scenario** – These operations have been included for specific industry operations and have full or partially defined sources/activities and release and exposure models.
- **Import** - This option allows you to import operations from previously saved assessments.



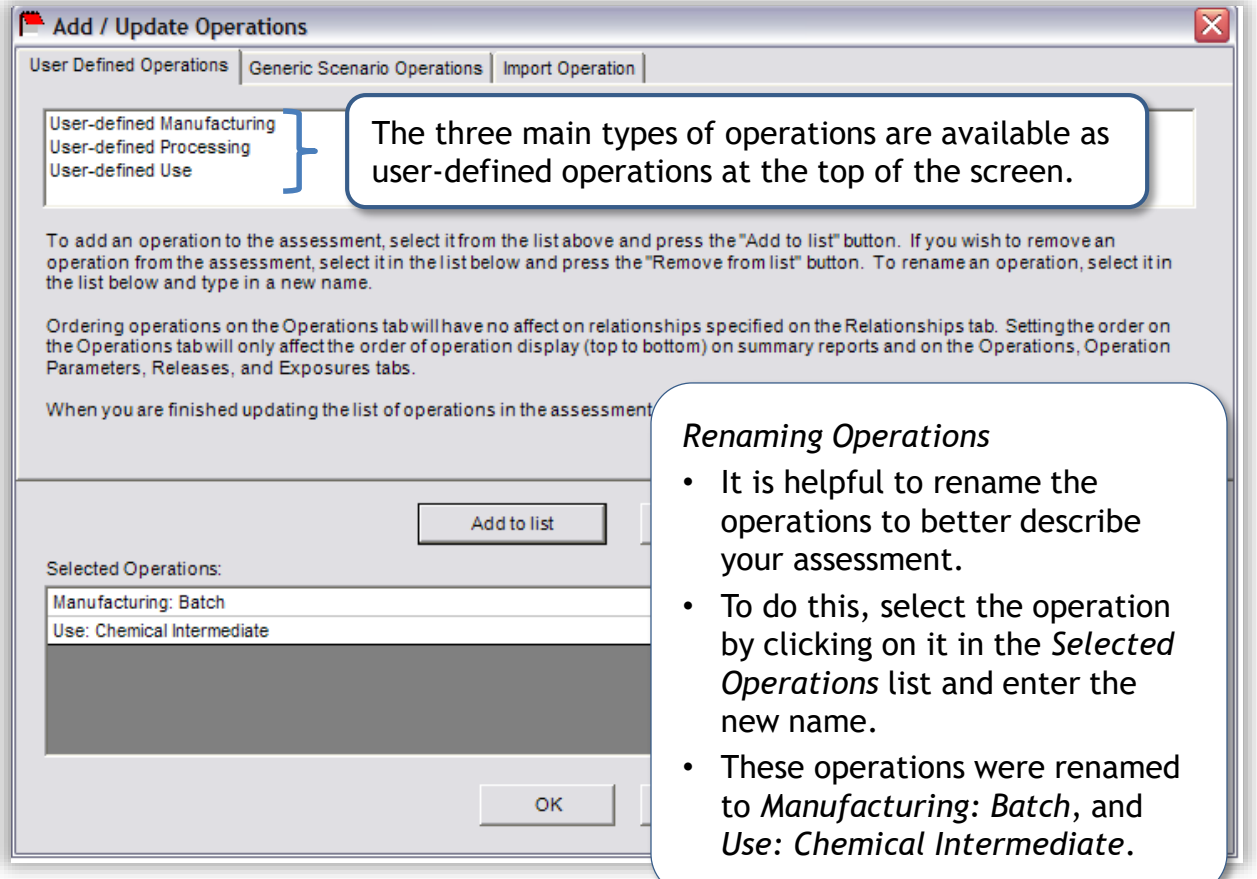
Note: This guide will review user-defined operations. Please refer to the User Guide for Generic Scenario Operations or Import previously saved operations.

3. Operations --> User-defined Operations

Generally, there are three types of operations:

- **Manufacturing** - Chemical is created in this operation and thus, an assessment includes only the chemical exiting from this type of operation.
- **Processing** - Chemical both enters into and exits from this type of operation; example: chemical is received by a formulator and mixed into another product for distribution.
- **Use** - Final use of the chemical and thus, an assessment includes only the chemical entering into this type of operation; the chemical either is converted into another chemical, is incorporated into an article, or is primarily disposed as waste.

To select an operation, you may either double-click on it or click it once and then click the ***Add to list*** button.

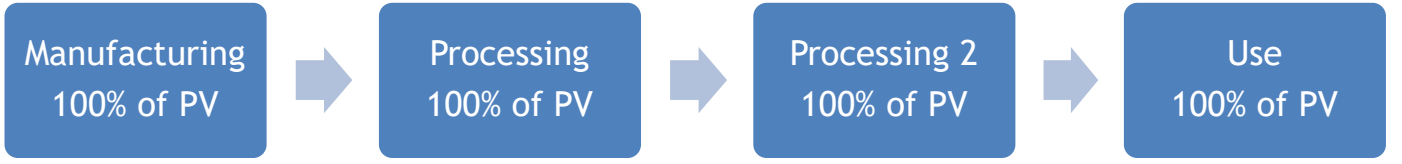


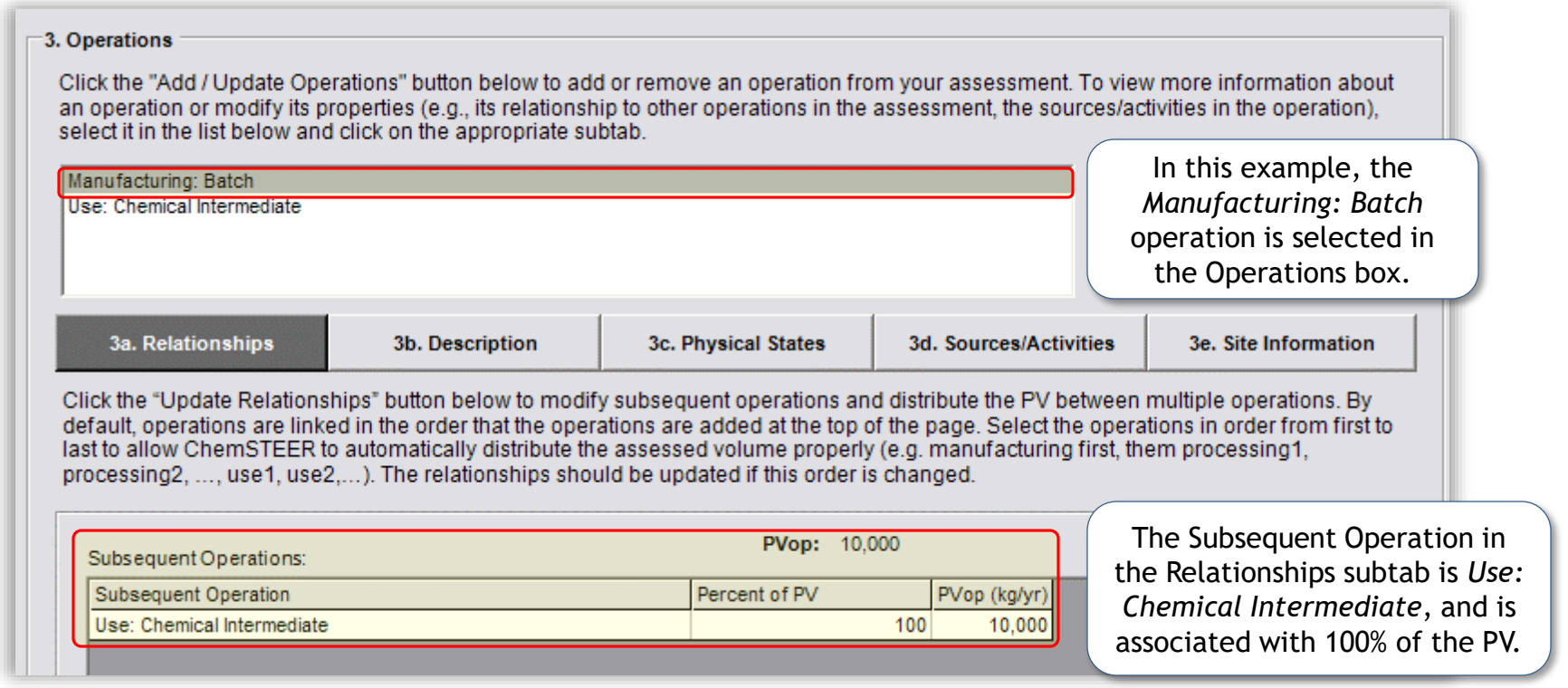
Renaming Operations

- 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.
- These operations were renamed to *Manufacturing: Batch*, and *Use: Chemical Intermediate*.

3a. Operations → 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).
- As a default, ChemSTEER will define the relationships in a straight series relationship as follows (in the order that the operations were added):

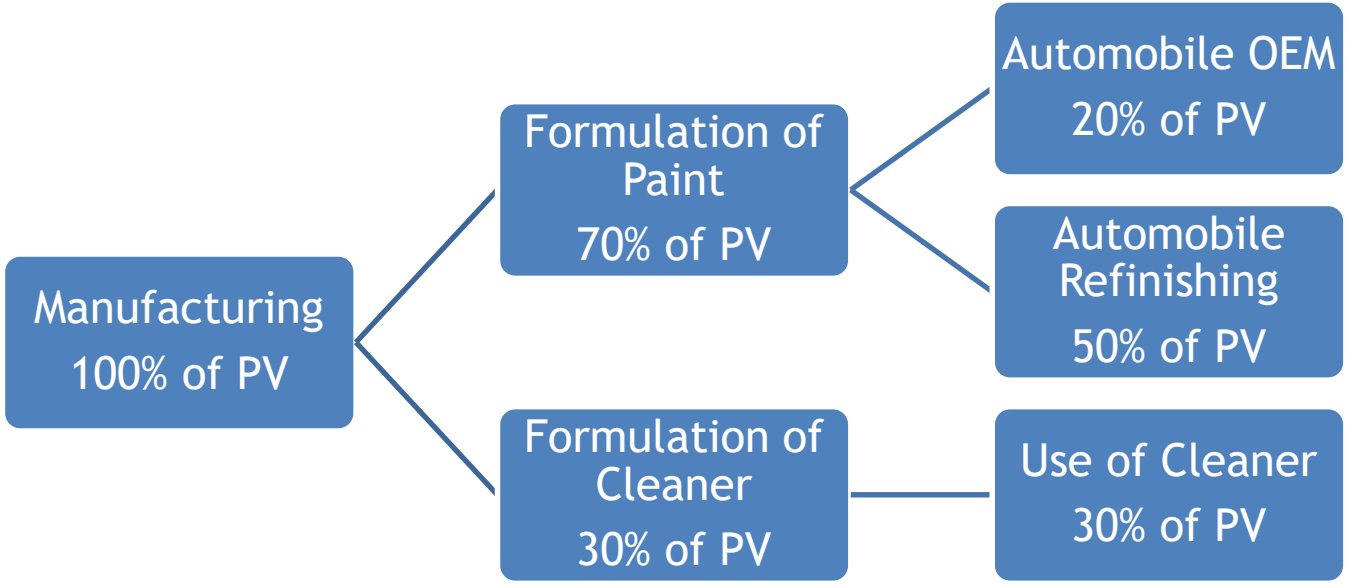




3a. Operations → Relationships (continued)

However, you may also rearrange your operations in ChemSTEER into any desired configuration.

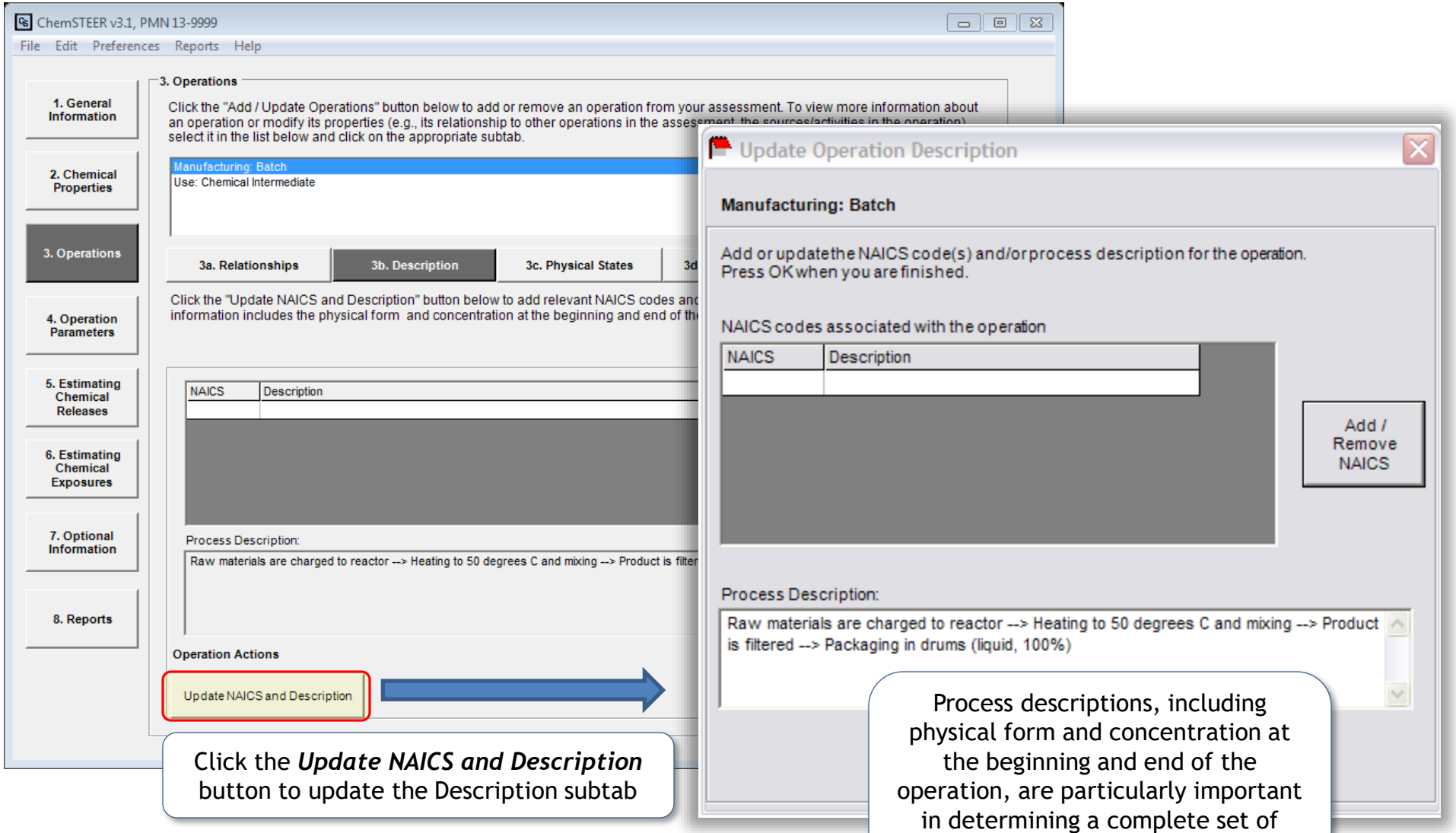
For example:



Please review the User Guide on how to perform more complex relationships.

3b. Operations → Description

The *Description* subtab allows the user to record NAICS Code, related description information, and process description for the operation.

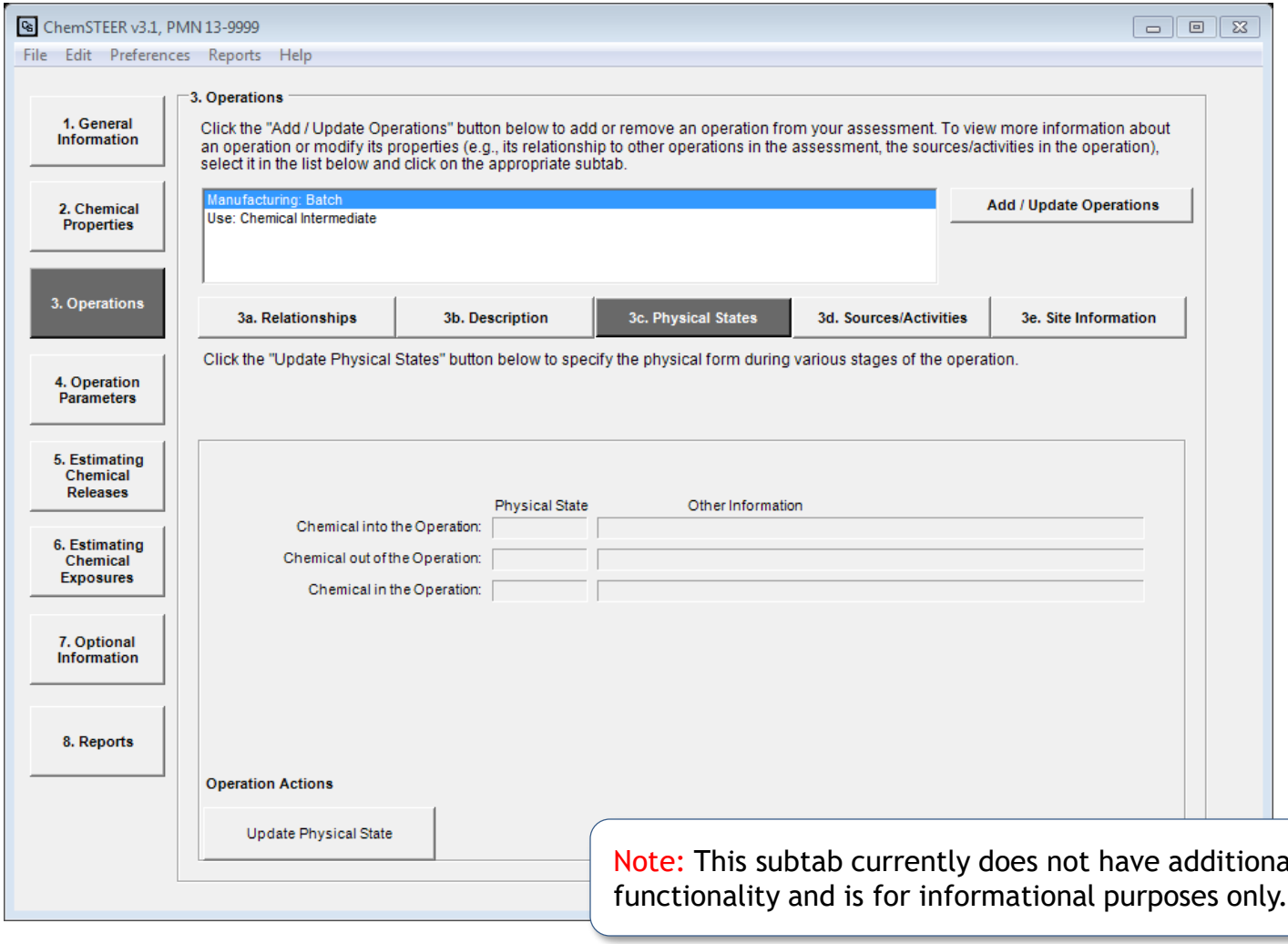


Click the ***Update NAICS and Description*** button to update the Description subtab

Process descriptions, including physical form and concentration at the beginning and end of the operation, are particularly important in determining a complete set of sources/activities to assess.

3c. Operations → Physical States

The *Physical States* subtab allows the user to record physical states for the operation.

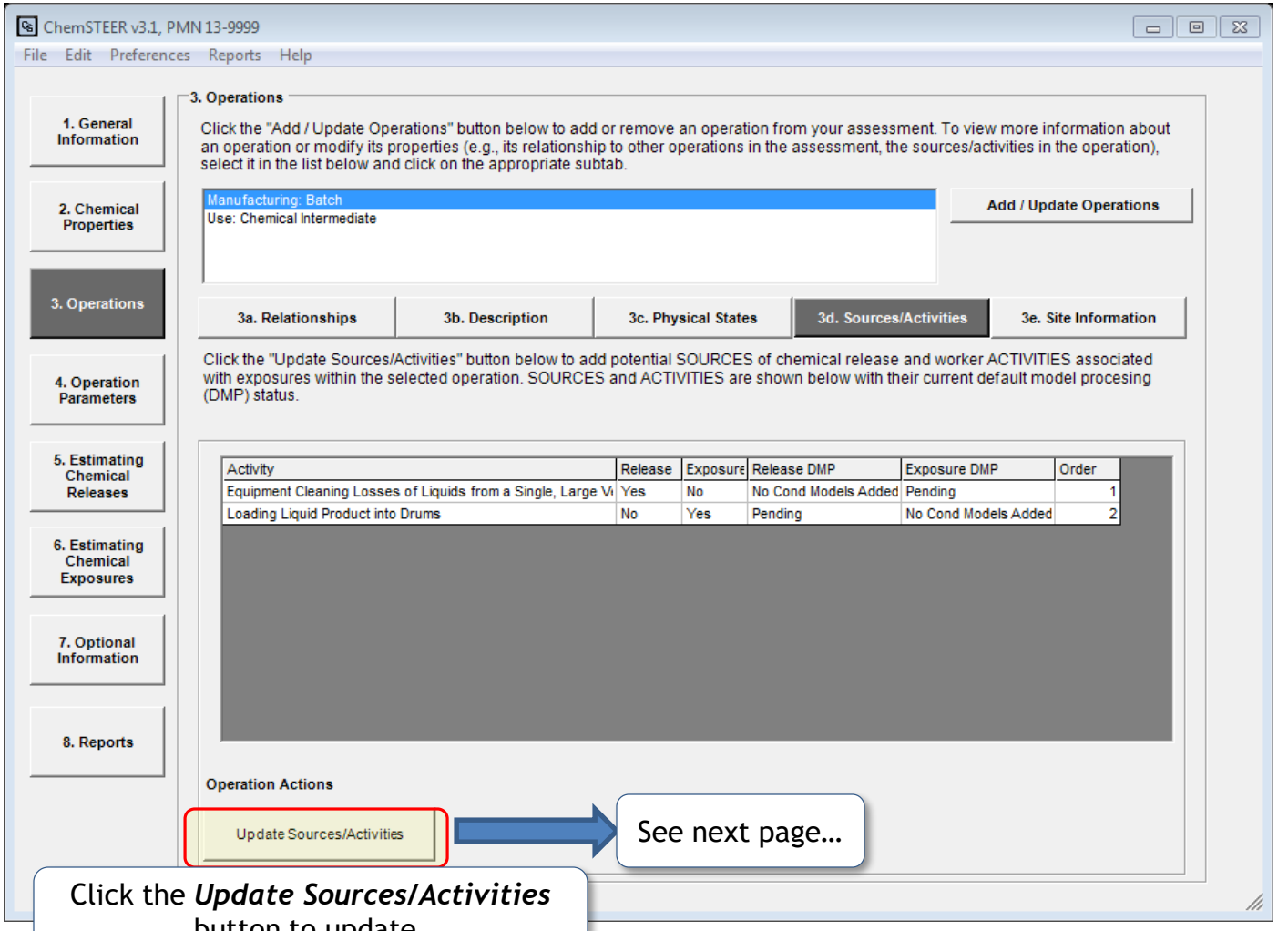


Note: This subtab currently does not have additional functionality and is for informational purposes only.

3d. Operations → Sources/Activities

- In ChemSTEER, the term *Source/Activity* refers to sources and activities in an operation that can/do/will cause releases to the environment and/or worker exposures. Most Sources/Activities have one or more default models that ChemSTEER uses to estimate releases and exposures. Choosing appropriate Sources/Activities allows you to access the models to make these estimates.
- For each operation of the assessment, you must select at least one release source or worker activity for which ChemSTEER will calculate releases and/or exposures.

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

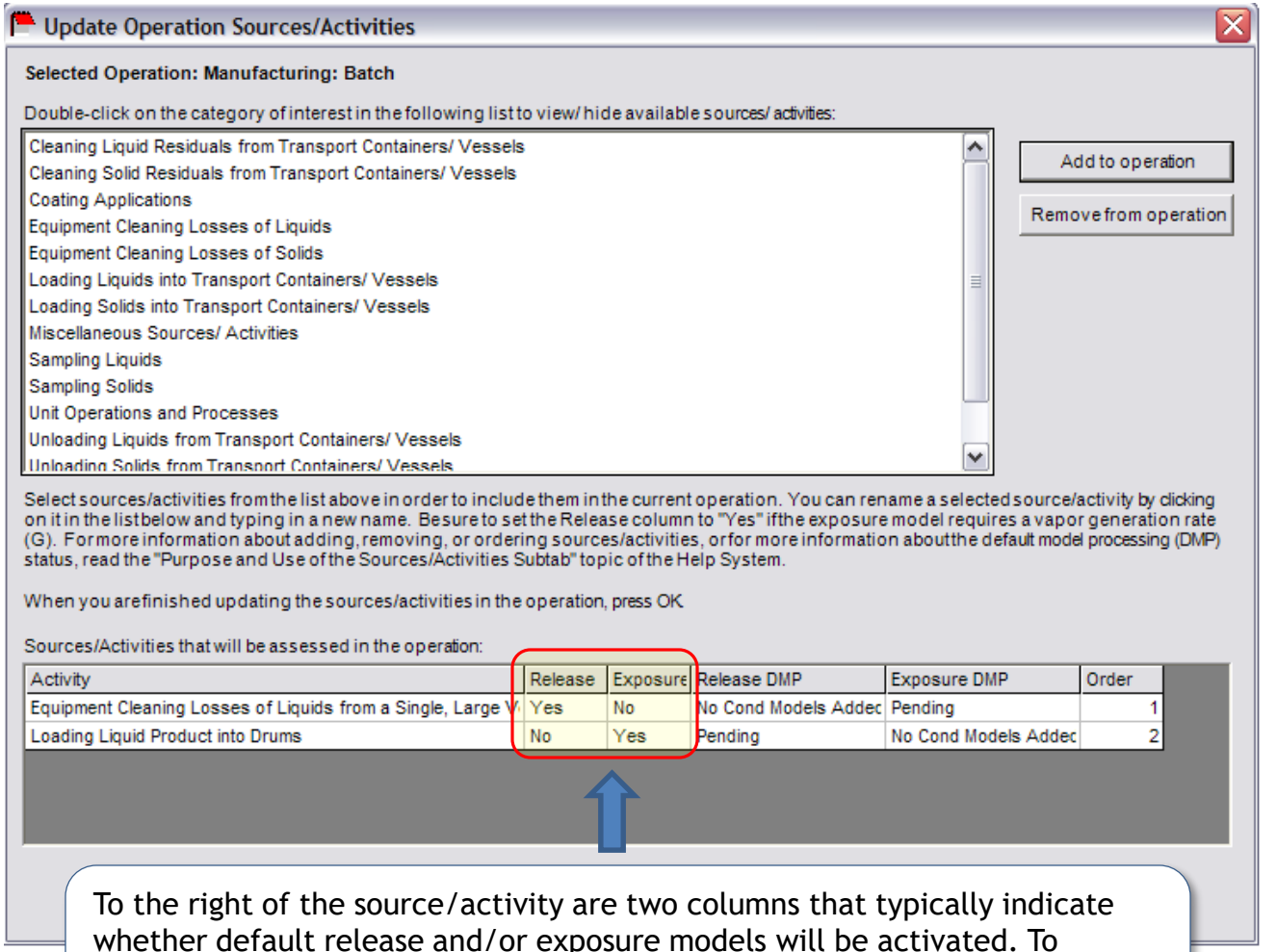


3d. Operations → Sources/Activities (continued)

Clicking on the *Update Source/Activities* button opens the selection screen:

Sources/Activities are listed in categories in the upper list. To show or hide the list of specific sources/ activities, double-click on the category.

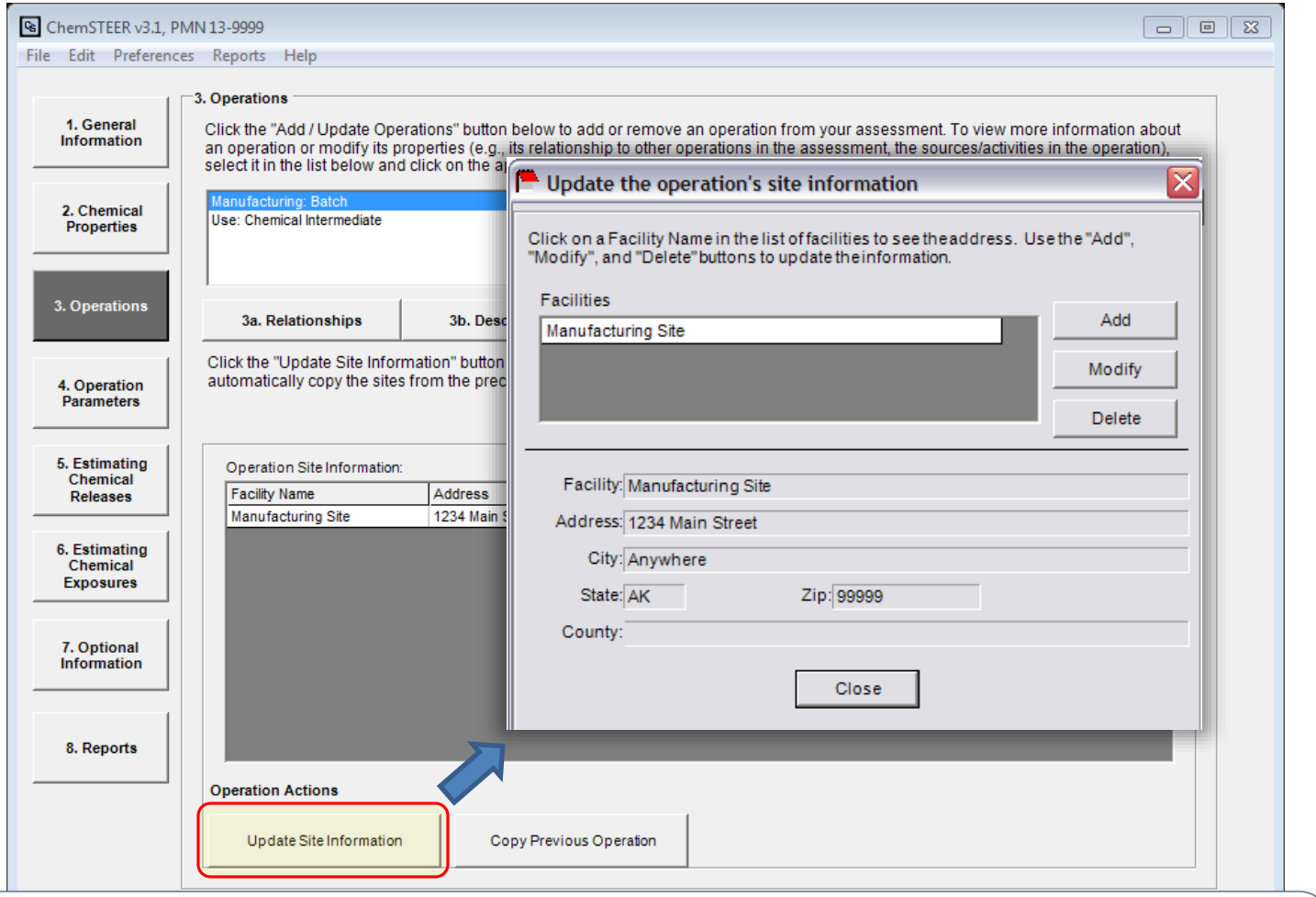
Select the source/activity by either double-clicking it or clicking it once and then clicking the ***Add to operation*** button.



To the right of the source/activity are two columns that typically indicate whether default release and/or exposure models will be activated. To change either of these settings, simply click on the field in the column and type 'Y' (Yes) or 'N' (No).

3e. Operations → Site Information

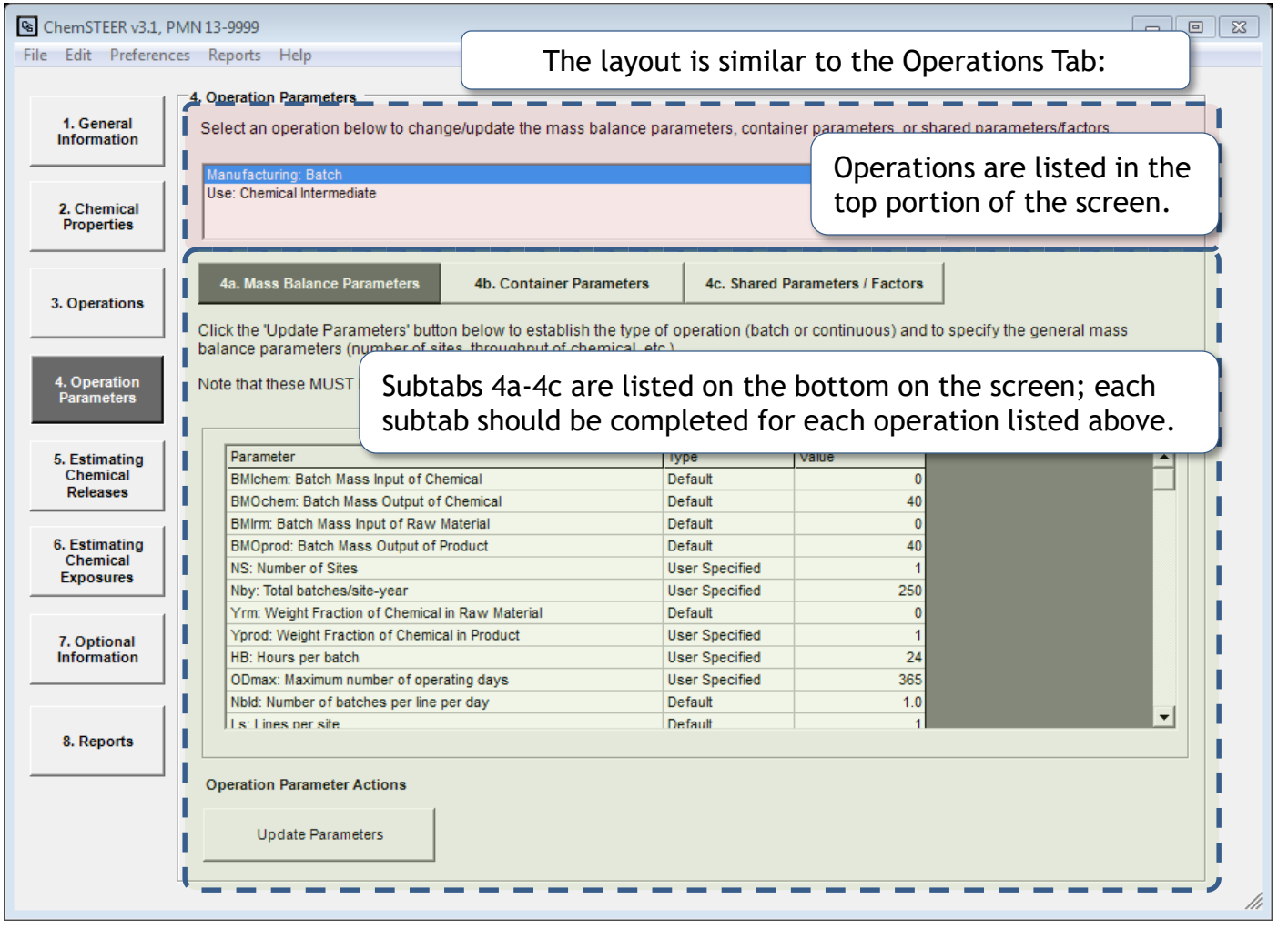
On the *Site Information* subtab, you may enter information regarding the facility or facilities performing the operations of the assessment.



Click the ***Update Site Information*** button to input facility information. If the selected operation is performed at the same facility (or facilities) as the preceding operation, you may wish to copy all of the site information that was entered for the preceding operation. To do this, click the ***Copy Previous Operation*** button.

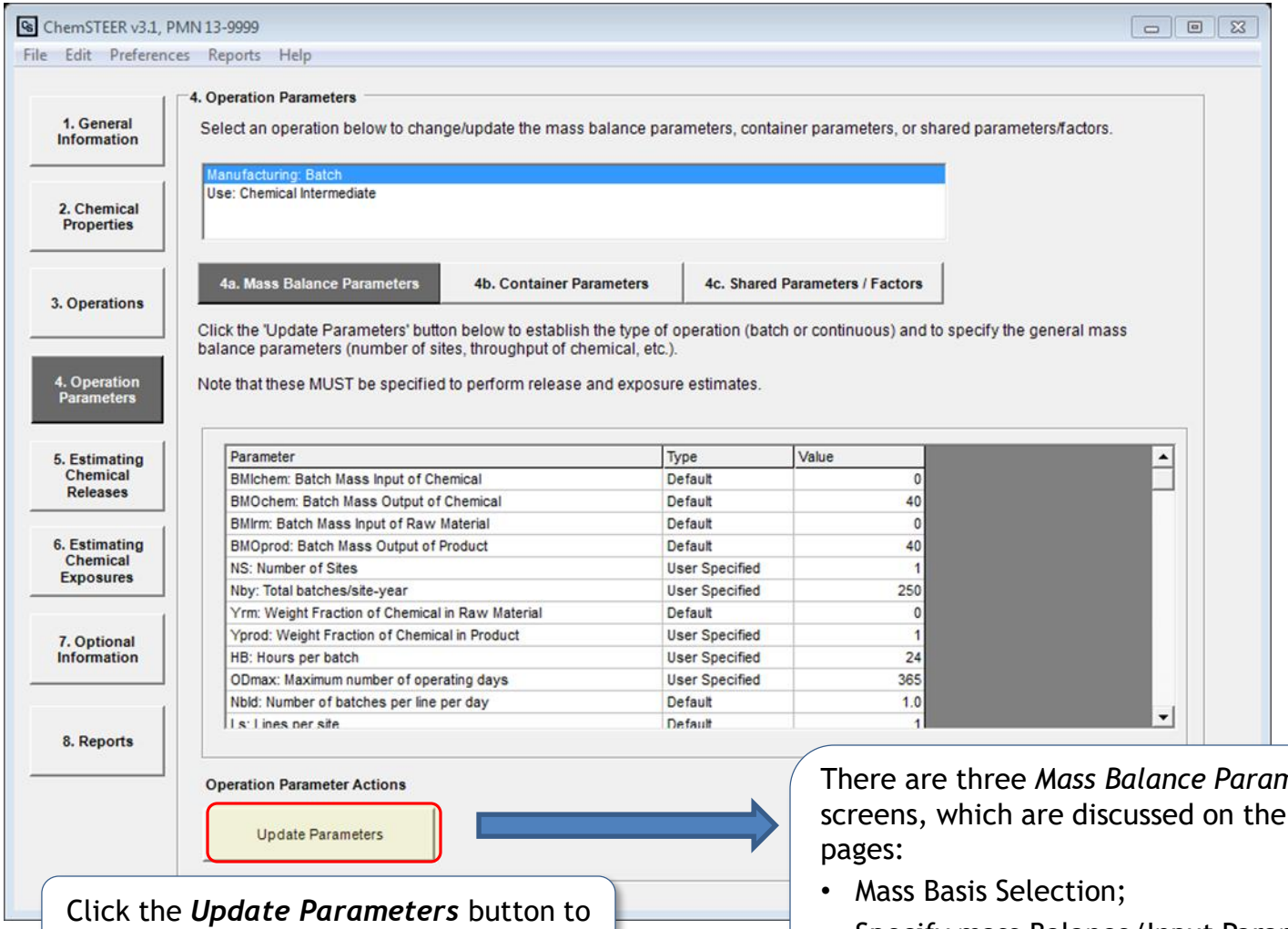
4. Operation Parameters - Overview

- The *Operation Parameters* tab includes key mass balance and container-related parameters for each of the assessed operations.
- These key parameters may be used in generating default values for parameters used in models for release and exposure estimation.
- For each operation, youshould complete the three subtabs:
  - 4a) Mass Balance Parameters;
  - 4b) Container Parameters; and
  - 4c) Shared Parameters / Factors



4a. Operation Parameters → Mass Balance Parameters

You can use the *Mass Balance Parameters* subtab to view and/or update key mass balance parameters for each of the assessed operations. These key mass balance parameters are used frequently in generating default values for parameters used in models for release and exposure estimation.



Click the ***Update Parameters*** button to update the Mass Balance Parameters

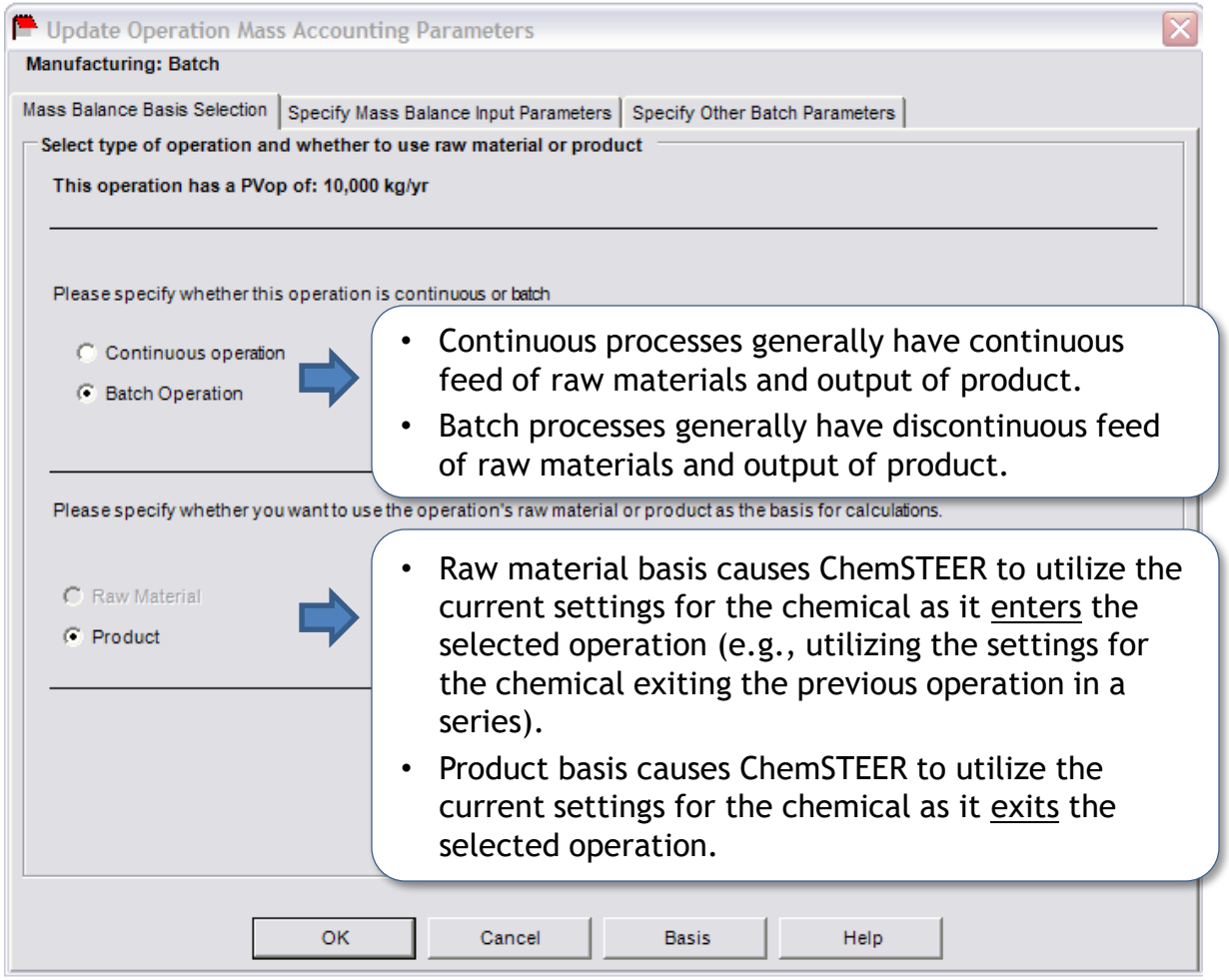
There are three *Mass Balance Parameters* sub-screens, which are discussed on the following pages:

- Mass Basis Selection;
- Specify mass Balance/Input Parameters; and
- Specify Other Batch Parameters

4a. Operation Parameters → Mass Balance Parameters (*Mass Balance Selection*)

On the *Mass Balance Basis Selection* subtab, you must first determine how ChemSTEER will perform calculations:

- Continuous or batch operation; or
- Raw material or product basis.



- Continuous processes generally have continuous feed of raw materials and output of product.
- Batch processes generally have discontinuous feed of raw materials and output of product.

- Raw material 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).
- Product basis causes ChemSTEER to utilize the current settings for the chemical as it exits the selected operation.

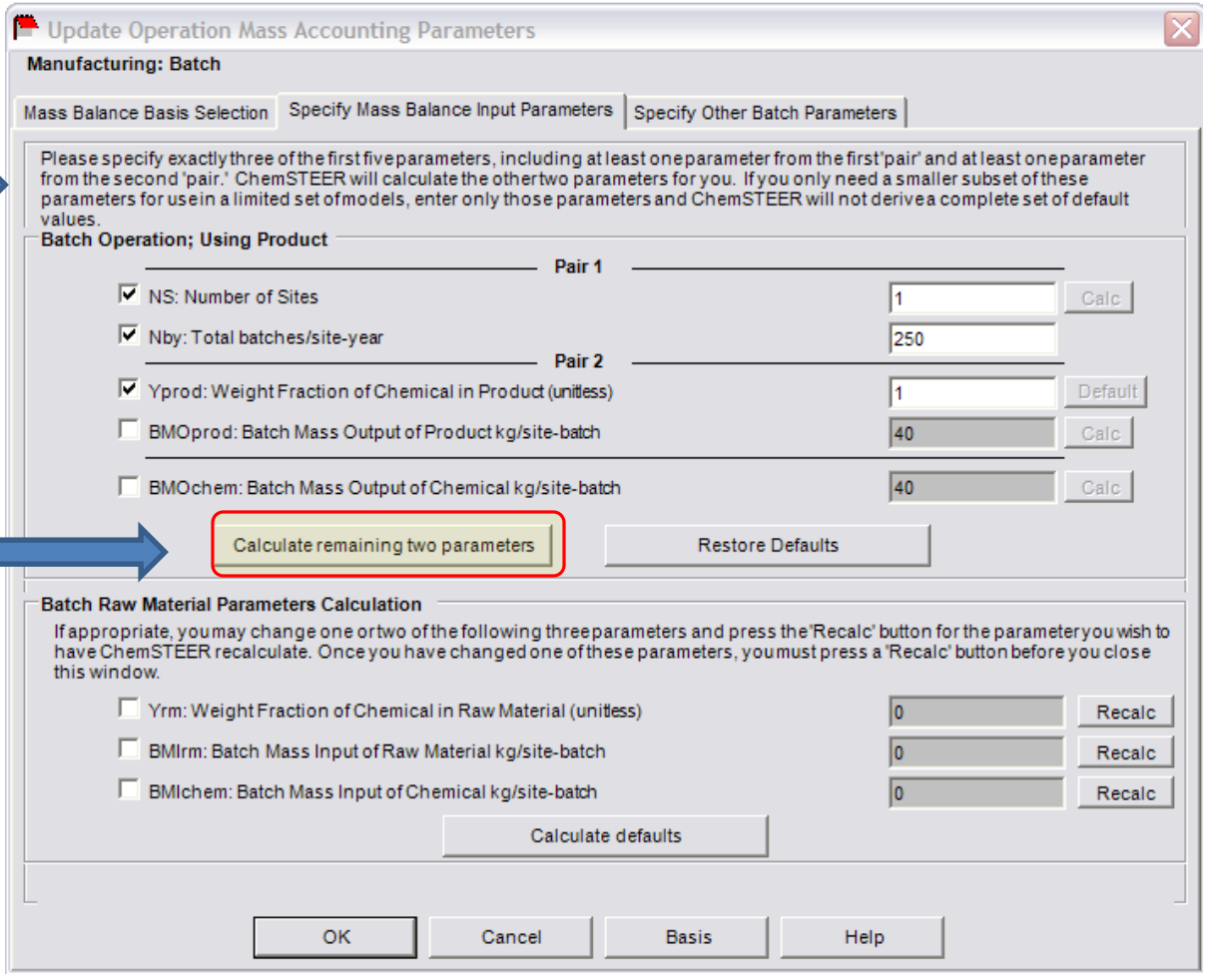
Note: the available options will vary, depending on whether you selected a Manufacturing, Processing, or Use operation on the *Operations* tab.

4a. Operation Parameters → Mass Balance Parameters (*Specify Mass Balance Input Parameters*)

On the *Specify Mass Input Parameters* subtab, you must enter parameters that ChemSTEER uses to calculate the remaining mass balance parameters. These values are required to calculate release and exposure estimates.

Follow the instructions at the top of the screen to choose 3 of the 5 parameters.

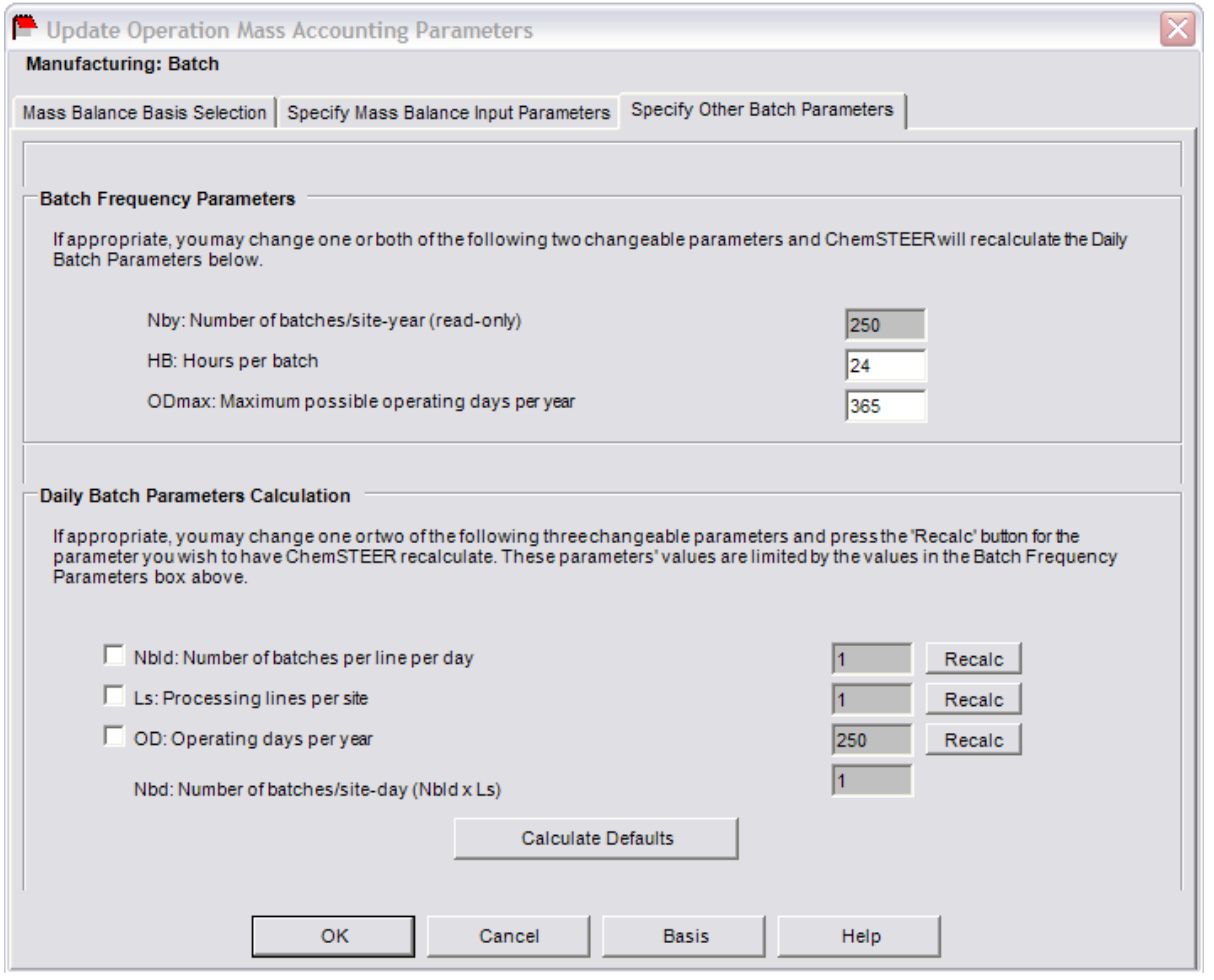
Click the ***Calculating remaining two parameters*** button to have ChemSTEER automatically determine the remaining parameters.



Note: The specific parameters that are displayed on this subtab are determined by which combination of Continuous/ Batch and Raw Material/ Product bases was chosen in the *Mass Balance Basis Selection* subtab.

4a. Operation Parameters → Mass Balance Parameters (*Specify Other Batch Parameters*)

On the *Specify Other Batch Parameters* subtab, you may modify any parameters shown in the screen. This screen is used for *Batch* operations only. You cannot access this tab until a value for at least the Nby parameter (number of batches per site, per year) has been entered or calculated in the Specify Mass Balance Input Parameters subtab for *Batch* operations.

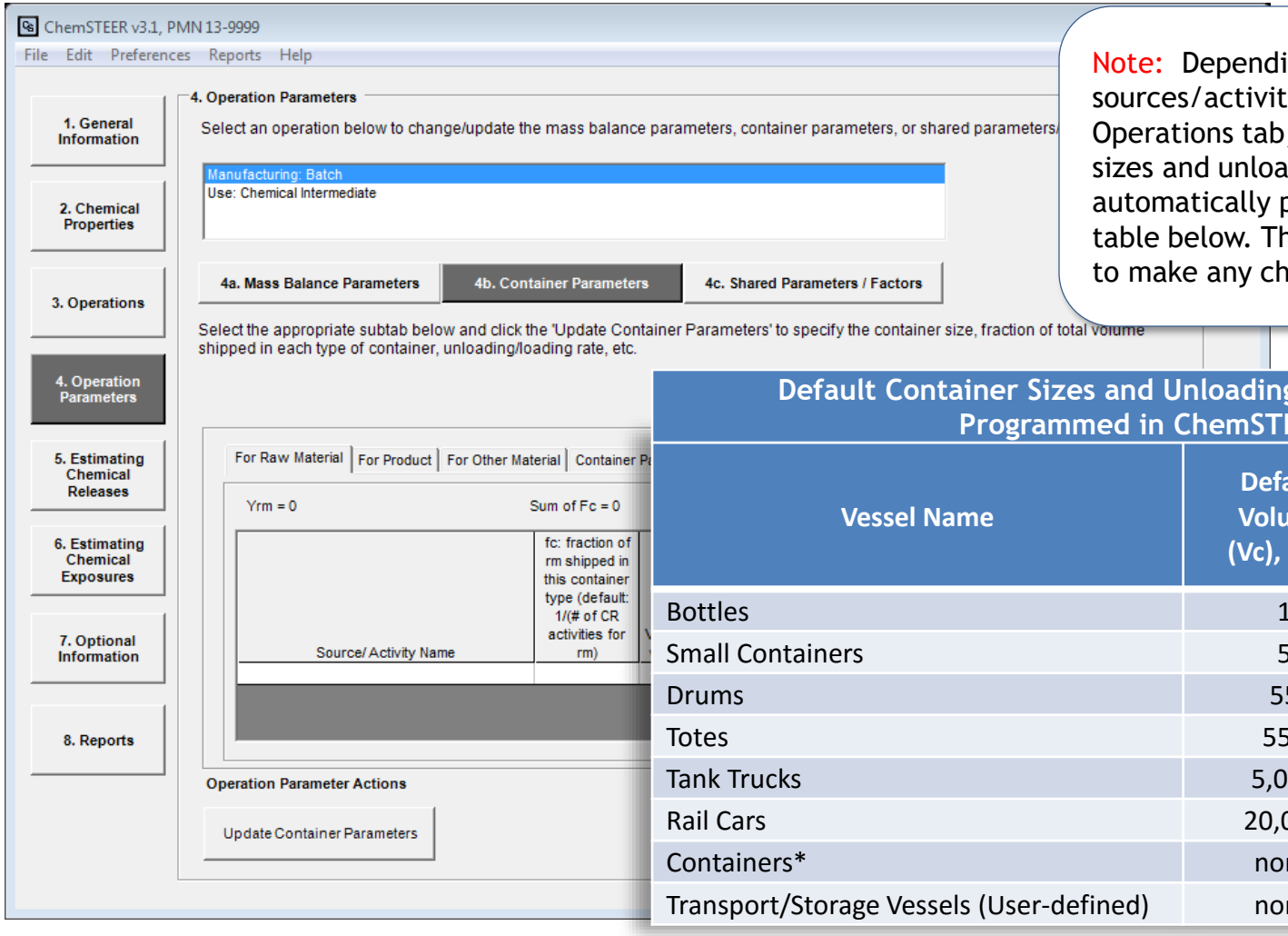


Note: Modifying values on this screen is optional.

ChemSTEER is programmed to automatically calculate values based on the information provided on the "Specify Mass Balance Input Parameters" tab.

4b. Operation Parameters → 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.



Note: Depending on the sources/activities selected on the Operations tab, corresponding container sizes and unloading/loading rates are automatically populated as shown in the table below. Therefore, you will not have to make any changes in most cases.*

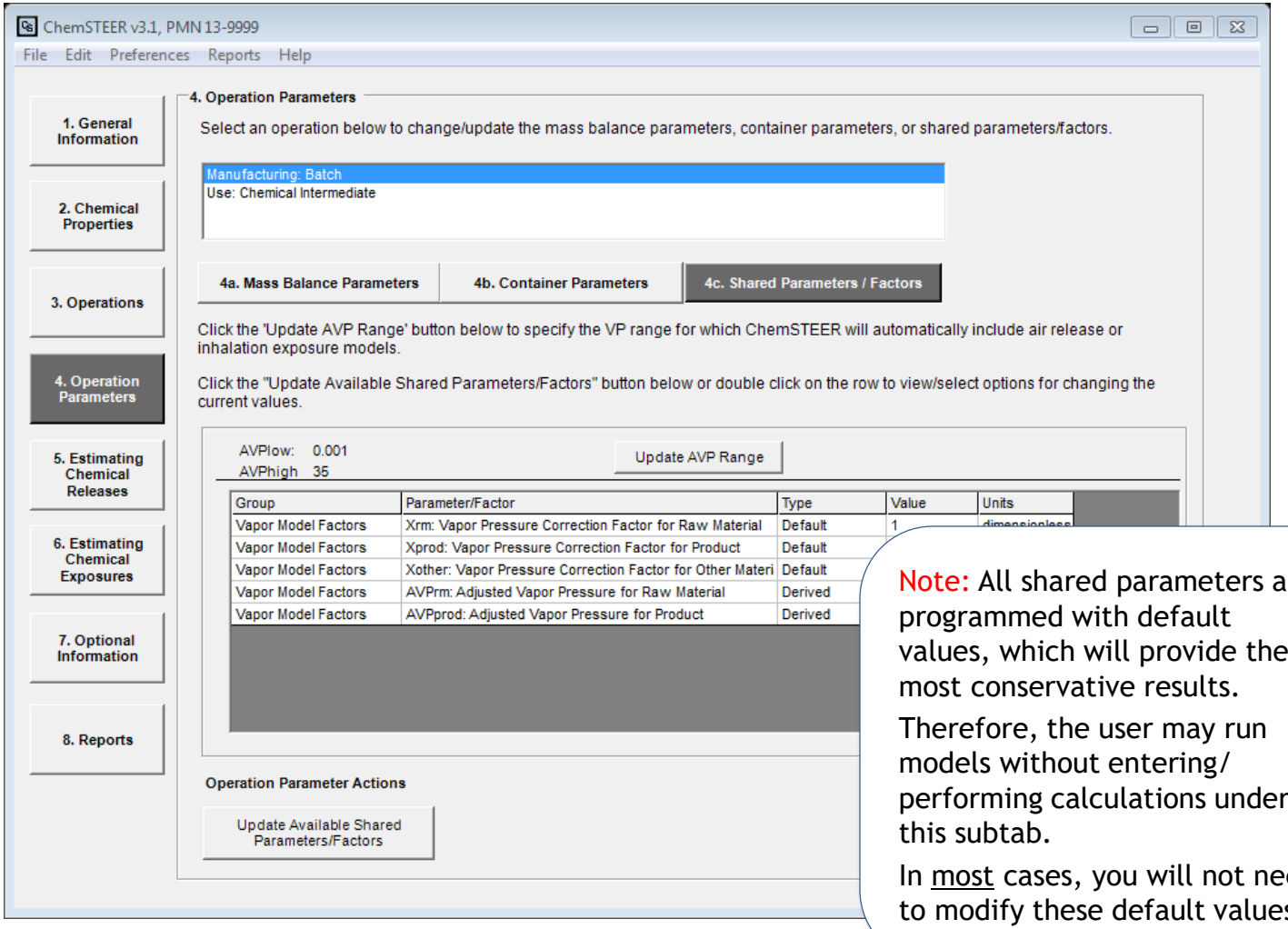
Default Container Sizes and Unloading / Loading Rates Programmed in ChemSTEER

Vessel Name	Default Volume (Vc), [gal]	Default Container Unload/Load Rate (r), [containers/hr]
Bottles	1	60
Small Containers	5	60
Drums	55	20
Totes	550	20
Tank Trucks	5,000	2
Rail Cars	20,000	1
Containers*	none	none
Transport/Storage Vessels (User-defined)	none	none

* Sources/activities related to the Loading or Unloading of Solids into/from Transport Containers/Vessels do not have default container sizes populated; therefore, you must specify a container size on subtab 4b before continuing.

4c. Operation Parameters → Shared Parameters/Factors *(for Advanced Users Only)*

The *Shared Parameters/Factors* subtab contains parameters for a particular operation that are used by more than one model for a particular source/activity (e.g., vapor pressure correction factor used by both the release model and exposure model).



Note: All shared parameters are programmed with default values, which will provide the most conservative results.

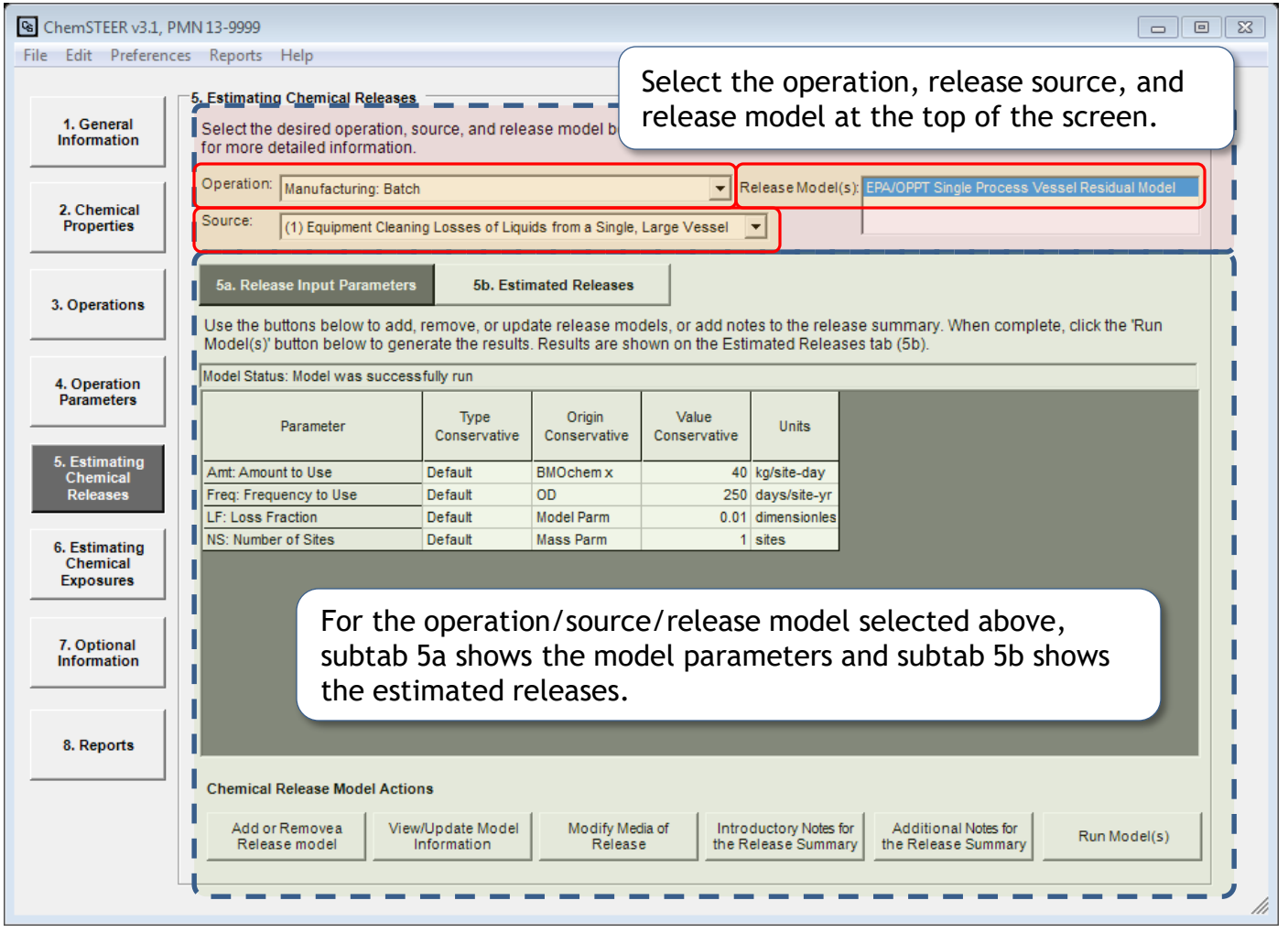
Therefore, the user may run models without entering/ performing calculations under this subtab.

In most cases, you will not need to modify these default values.

5. Estimating Chemical Releases

You can use the *Estimating Chemical Releases* tab to view, update, and run the model(s) used to calculate the releases for each of the operations' sources/activities.
In this tab you may:

- View and/or update which models are used
- View/update the specific model-related parameters
- View the model results (estimated releases)

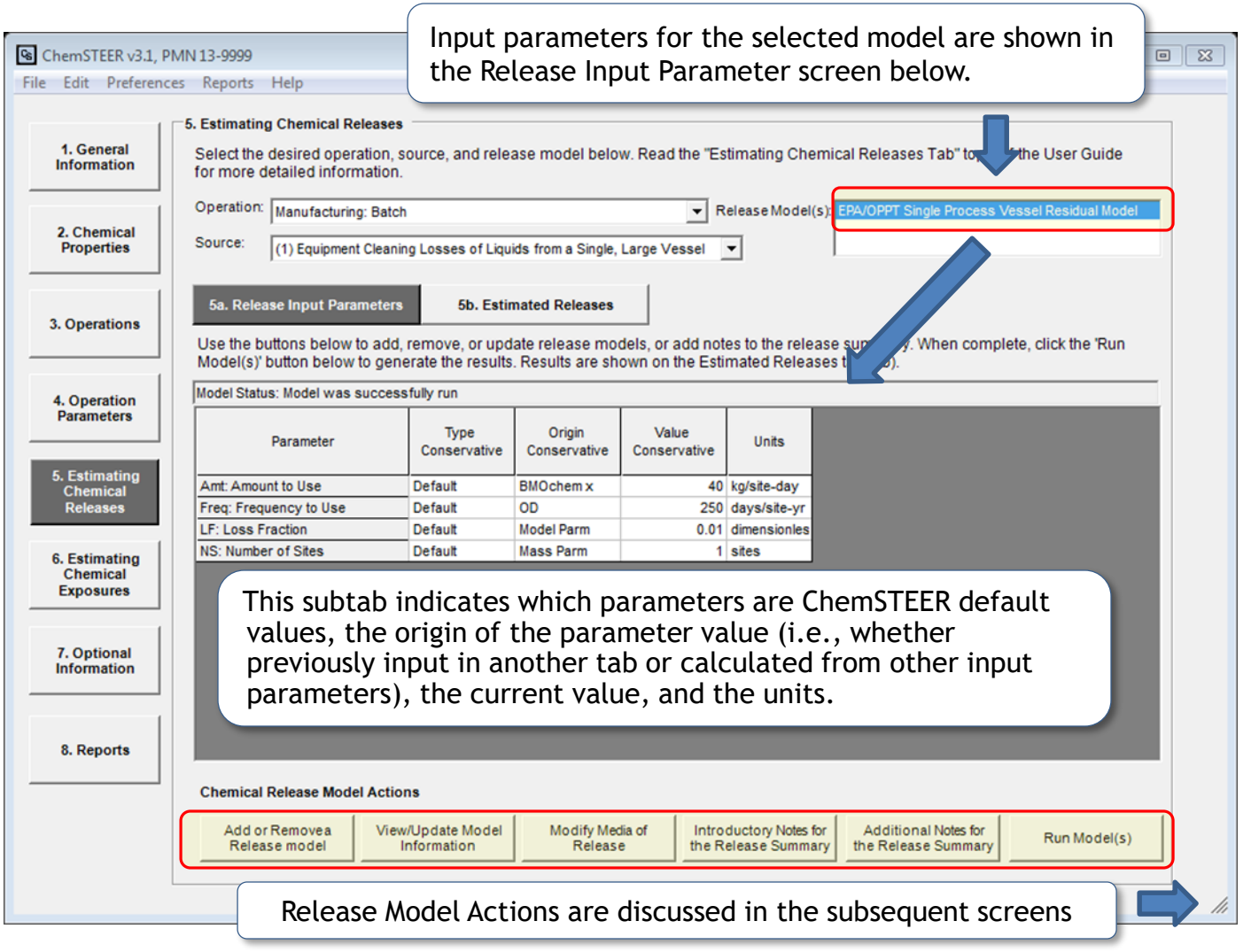


ChemSTEER currently contains 18 different models that can be used to calculate releases, each with their own set of default settings and values.

5a. Releases → Release Input Parameters

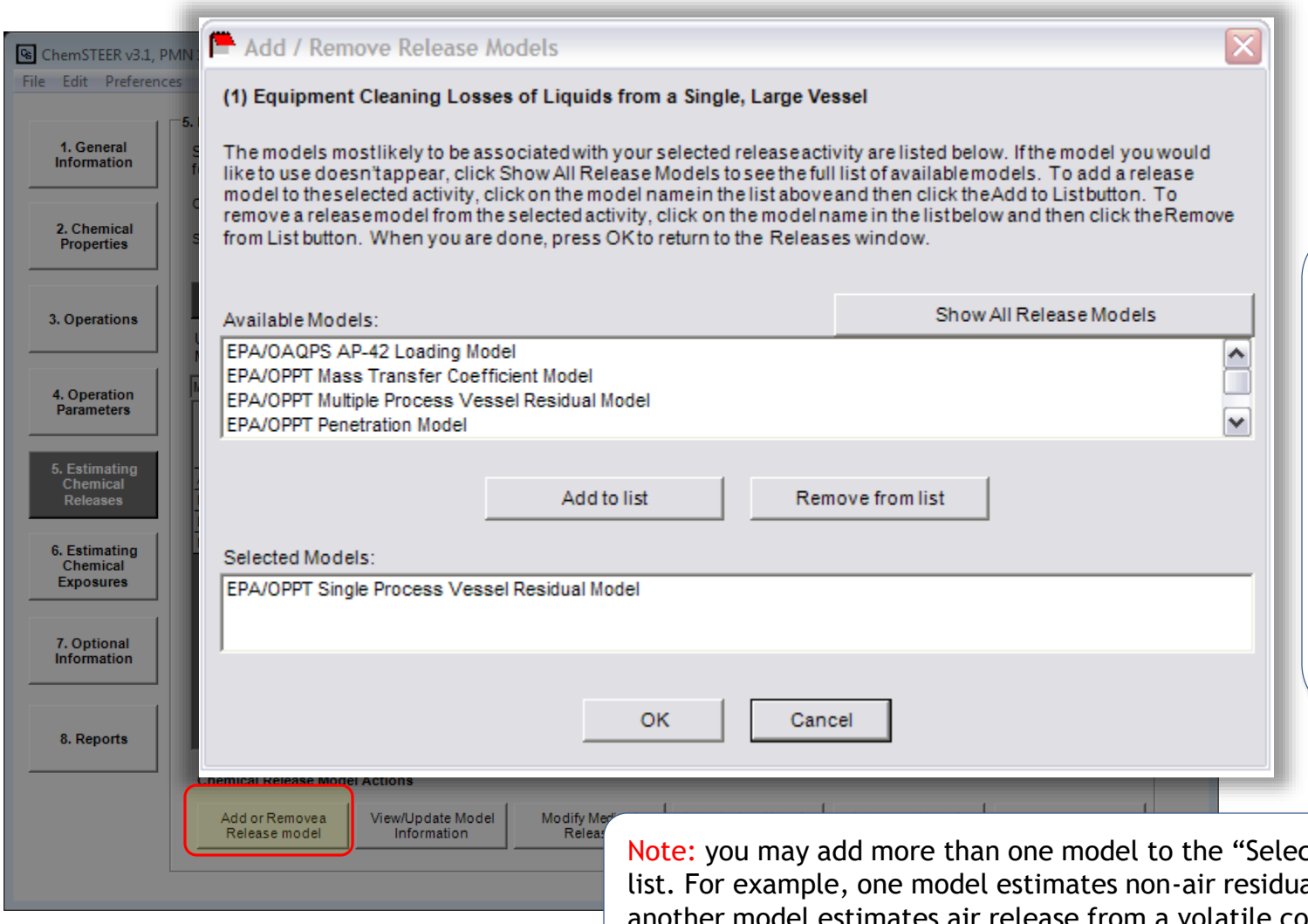
On the Release Input Parameters subtab, there are a number of options for working the release models, which are discussed on the following pages:

- Add/Remove Release Model
- View/Update Model Information
- Modify Media of Release
- Introductory Notes for Release Summary
- Additional Notes for Release Summary
- Run Model(s)



5a. Releases → Release Input Parameters *(Add/Remove Release Model)*

The *Add/Remove Release Model* screen shows the currently selected model(s) and additional available models for the selected Operation/Source.



The upper window shows the most appropriate alternative / additional models for the selected release source.

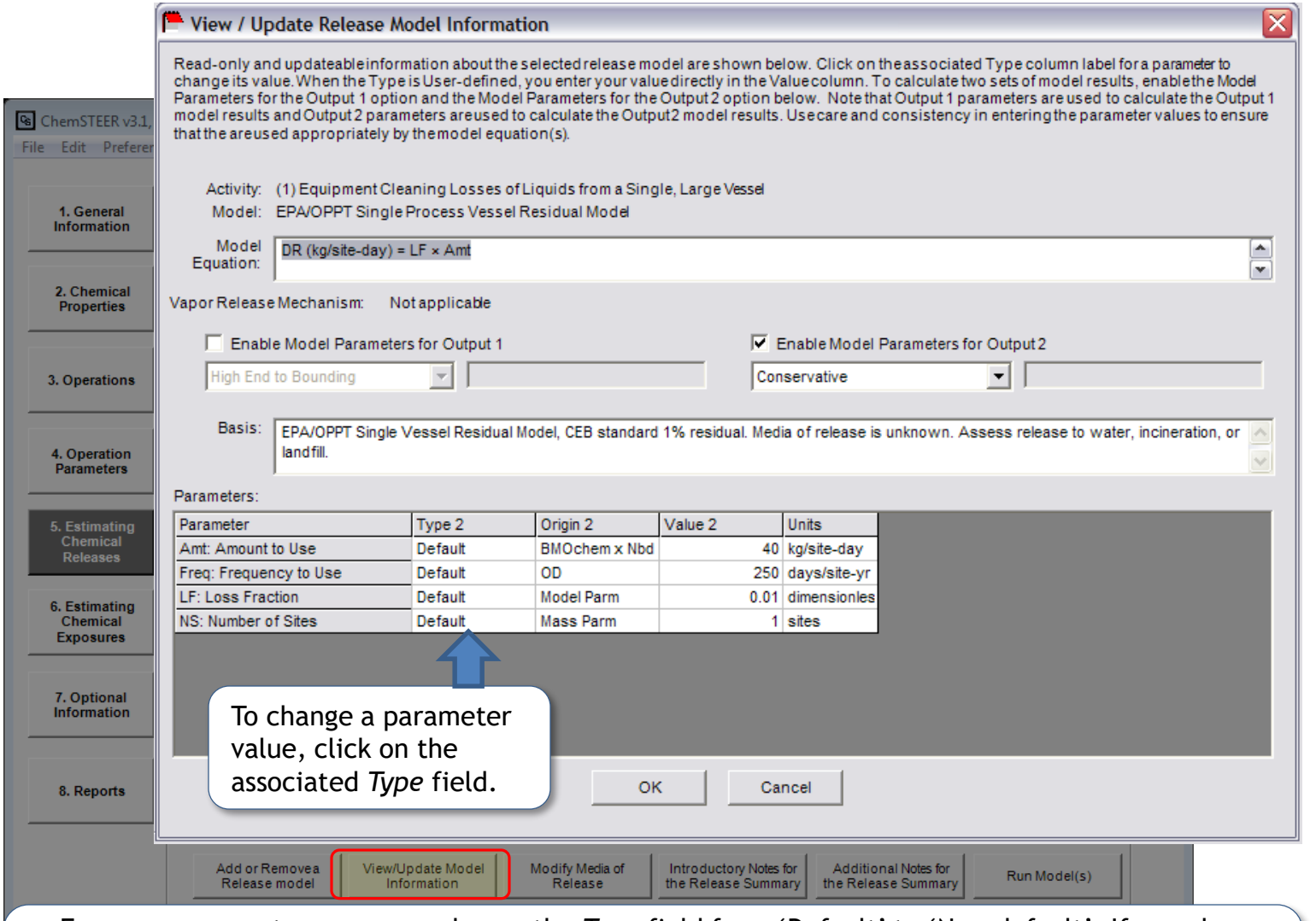
You may select any model listed and add them to the selected models list.

Note: you may add more than one model to the "Selected Models" list. For example, one model estimates non-air residual release, while another model estimates air release from a volatile compound.

5a. Releases → Release Input Parameters *(View/Update Model Information)*

The *View/Update Model Information* screen displays information about the selected model, including:

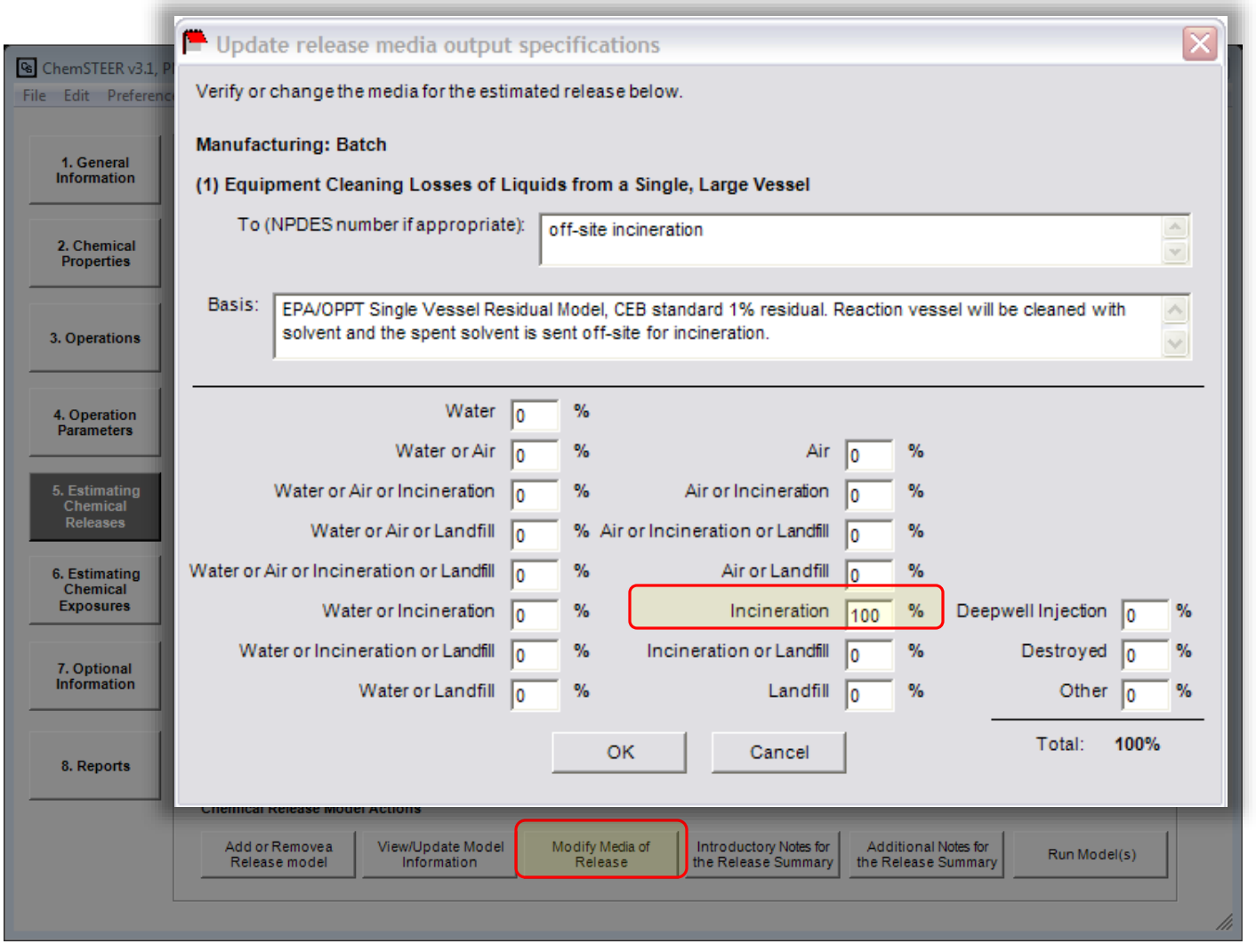
- the equation(s) used in the calculation;
- a description of the basis/source of the model; and
- a list of the parameters used.



- For some parameters, you can 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.

5a. Releases → Release Input Parameters *(Modify Media of Release)*

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



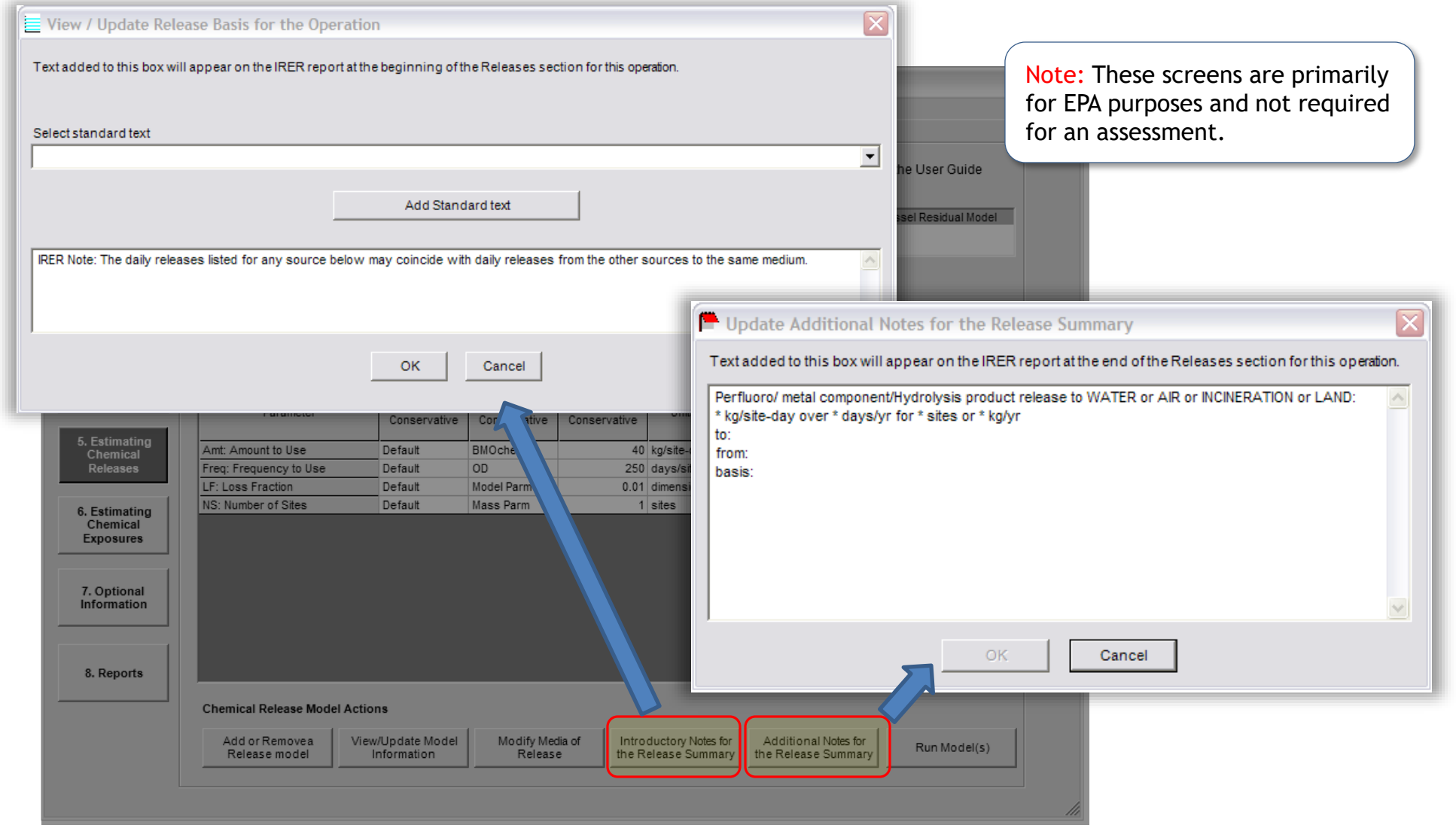
In this screen, the selected operation and release source is listed, as well as the selected release model and description of the model basis/source.

You can apportion the total amount of the calculated release to more than one target. For example, if the residues from the cleaning of the single, large vessel are treated in a WWT system that is 90% efficient in removing the chemical from the final effluent, we would apportion the total release as:

- 90% to sludge (collected and sent to an incinerator); and
- 10% to water.

5a. Releases → Release Input Parameters *(Introductory and Additional Notes for the Release Summary)*

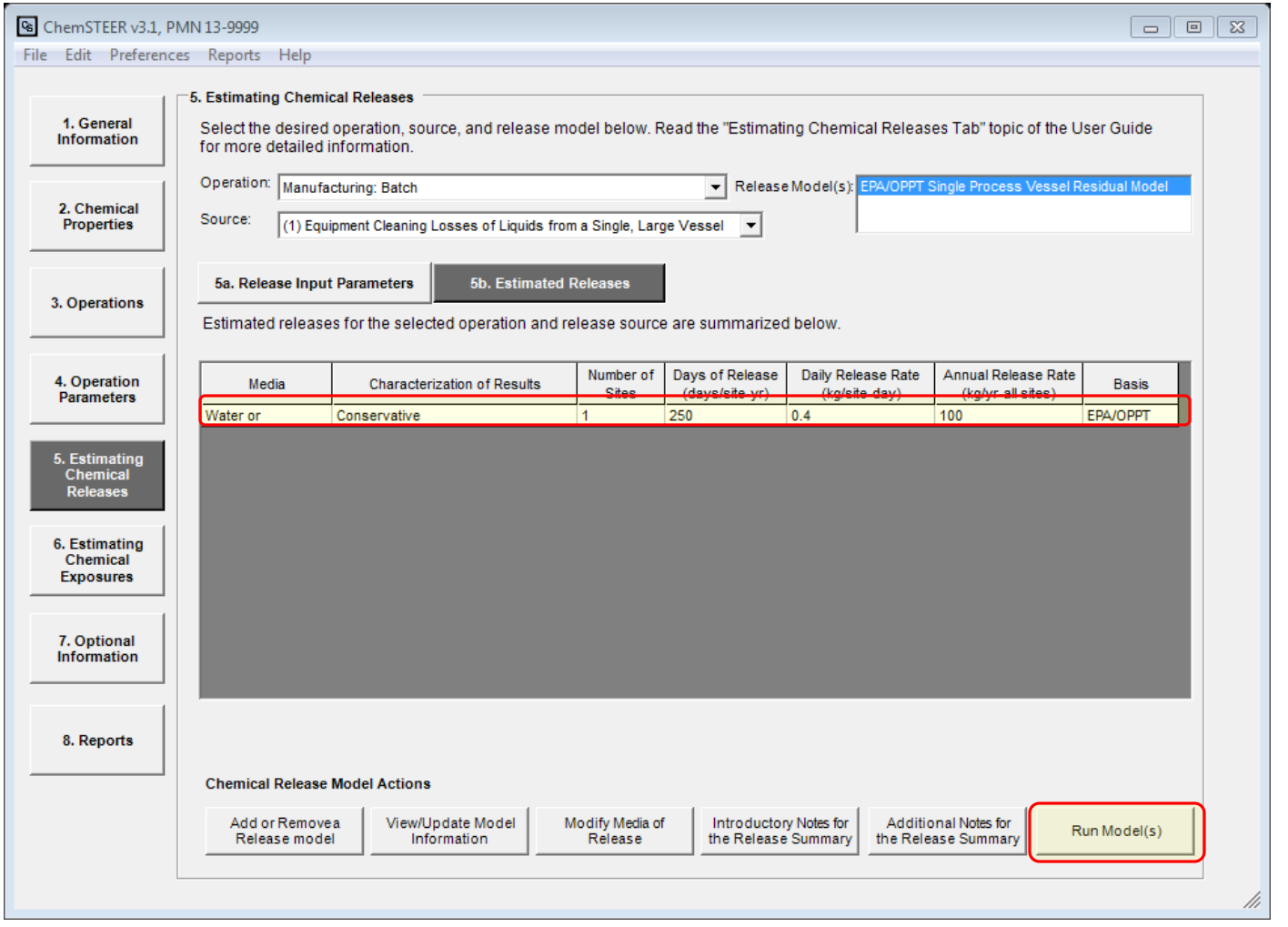
Using the *Introductory Notes for the Release Summary* and/or *Additional Notes for the Release Summary* buttons, you may add additional information related to the release assessments.



5b. Releases → Estimated Releases

Model release estimates are shown on the *Estimated Releases* subtab. This screen displays the:

- Media of release,
- Number of sites releasing the chemical,
- Days of release (days/site-yr),
- Daily release rate (kg/site-day),
- Annual release rate (kg/year; all sites), and
- Basis for the selected release model.



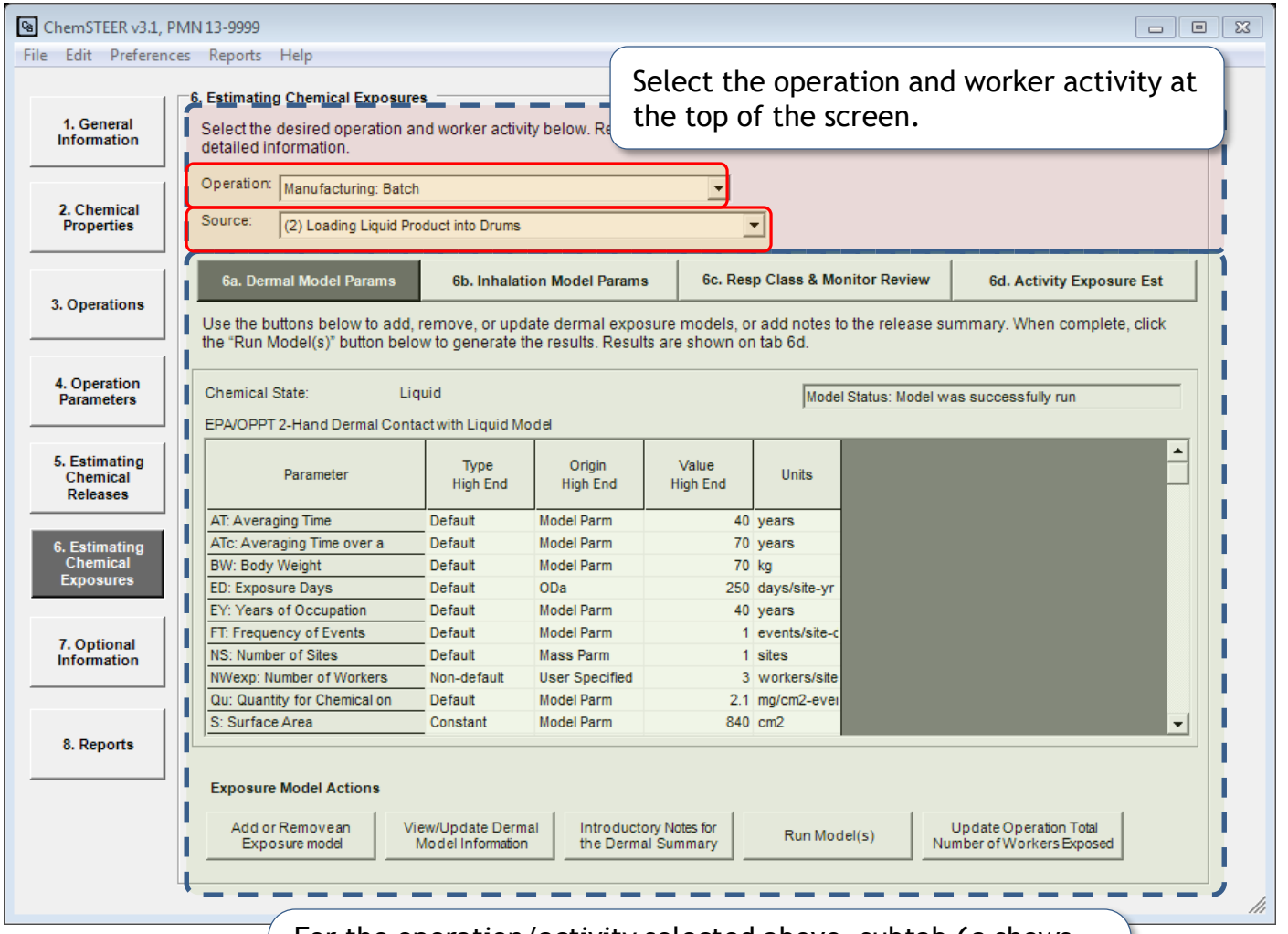
Note: You can click on the ***Run Model(s)*** button at any point while you are on the "*5. Estimating Chemical Releases*" tab to execute the release model calculations.

6. Estimating Chemical Exposures

You can use the *Estimating Chemical Exposures* tab to view, update, and run the model(s) used to calculate the dermal and/or inhalation exposures for each of the operations' activities.

In this tab you may:

- View and/or update which models are used;
- View/update the specific model-related parameters; and
- View the model results (estimated exposures)



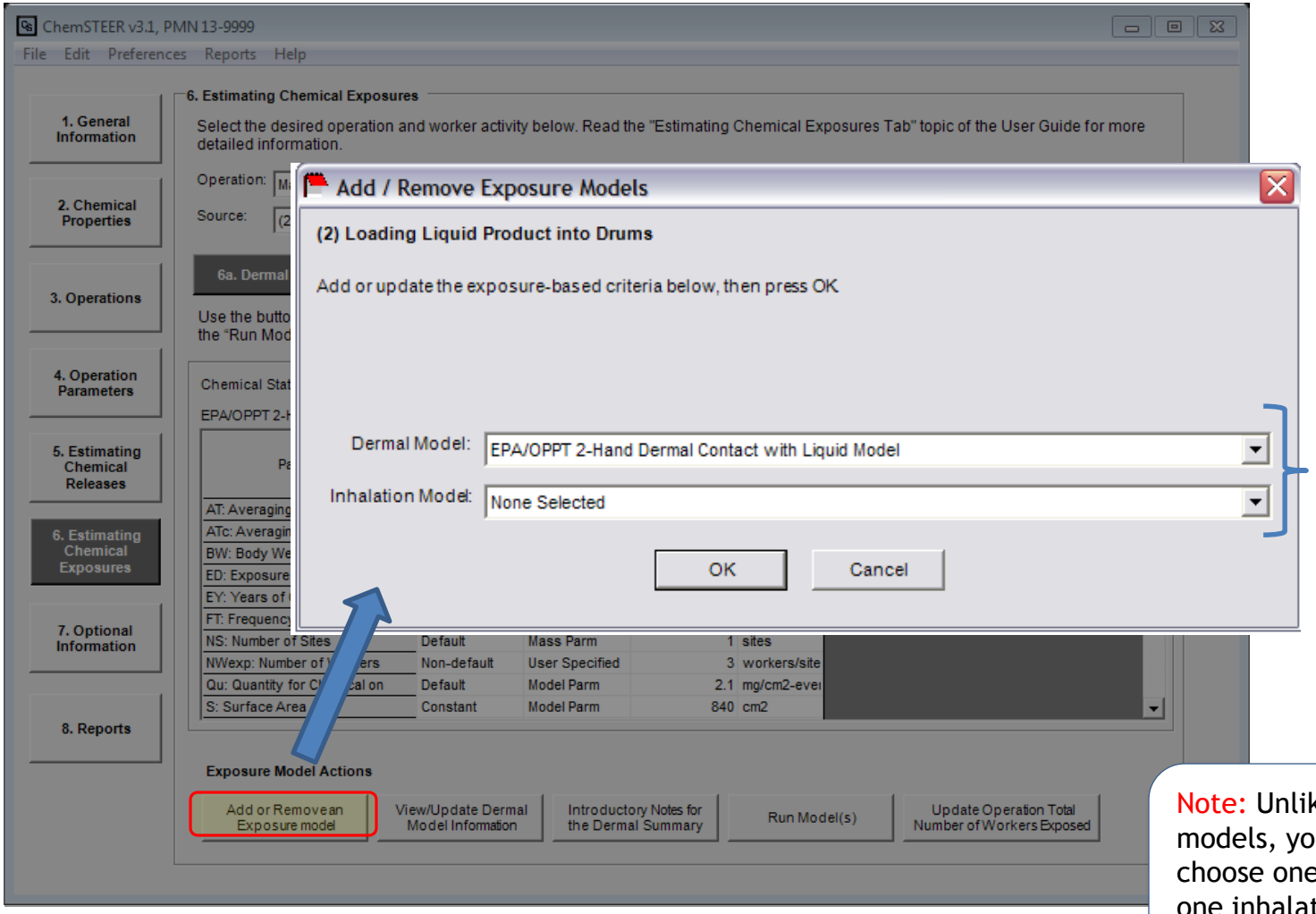
Select the operation and worker activity at the top of the screen.

ChemSTEER currently contains more than 15 different models that can be used to calculate dermal and inhalation exposures, each with their own set of default settings and values.

For the operation/activity selected above, subtab 6a shows the dermal model parameters and subtab 6b shows the inhalation model parameters. Subtab 6d shows the exposure estimates.

6. Exposures →Add or Remove an Exposure Model

The *Add/Remove Exposure Model* screen shows the currently selected models for the selected Operation/Activity. However, you may choose to change the default models that are used for the selected exposure activity.



Use the drop-down menu to select alternative dermal and inhalation models.

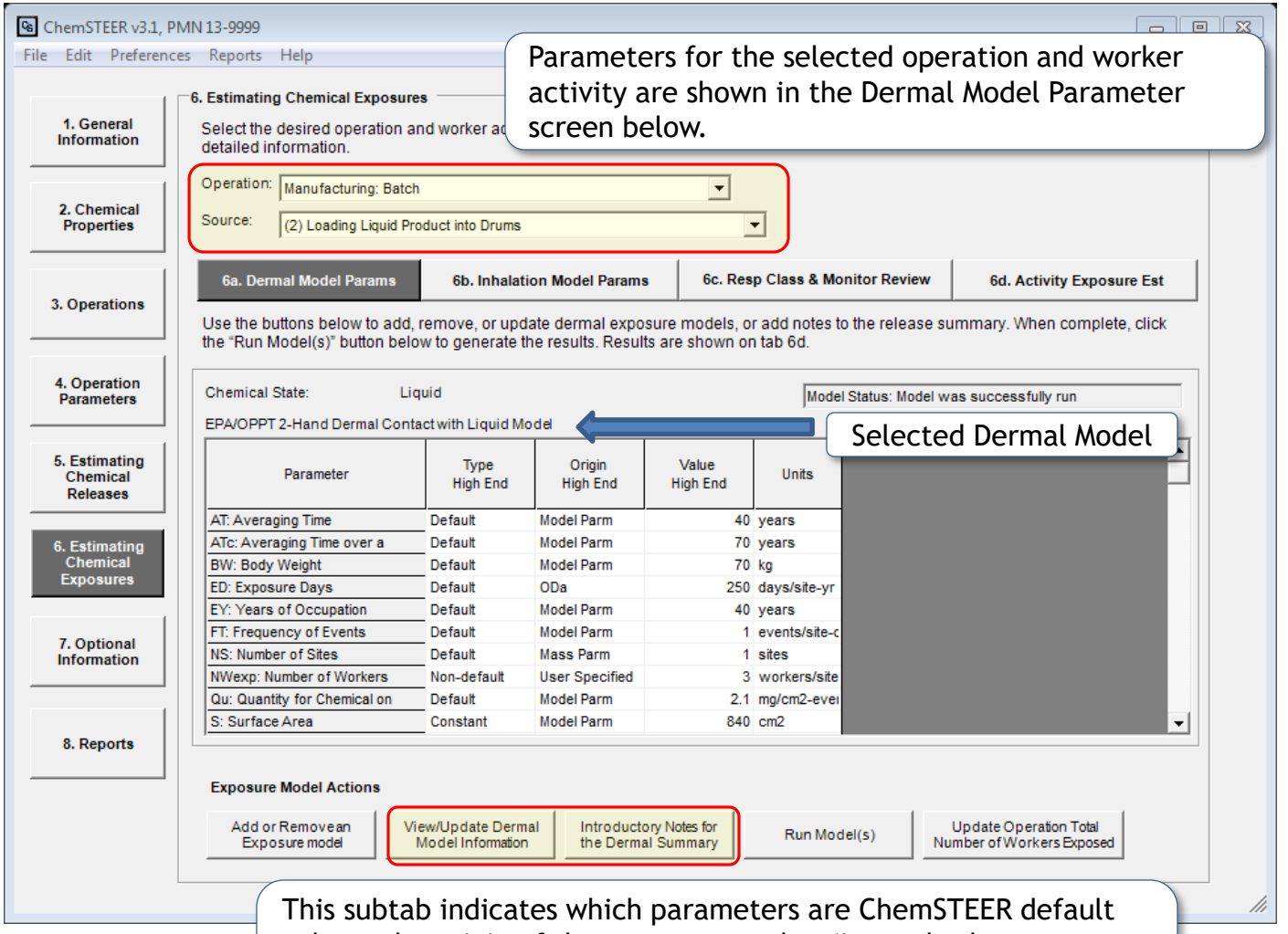
Note: Unlike release models, you can only choose one dermal and one inhalation exposure model per worker activity.

6a. Exposures → Dermal Model Parameters

On the Dermal Model Parameters subtab, there are two Exposure Model Actions that are specific to dermal exposures:

- View/Update Dermal Model Information; and
- Introductory Notes for Release Summary.

Note: Subtab 6b. *Exposures → Inhalation Parameters* contains a corresponding screen for inhalation exposure models.

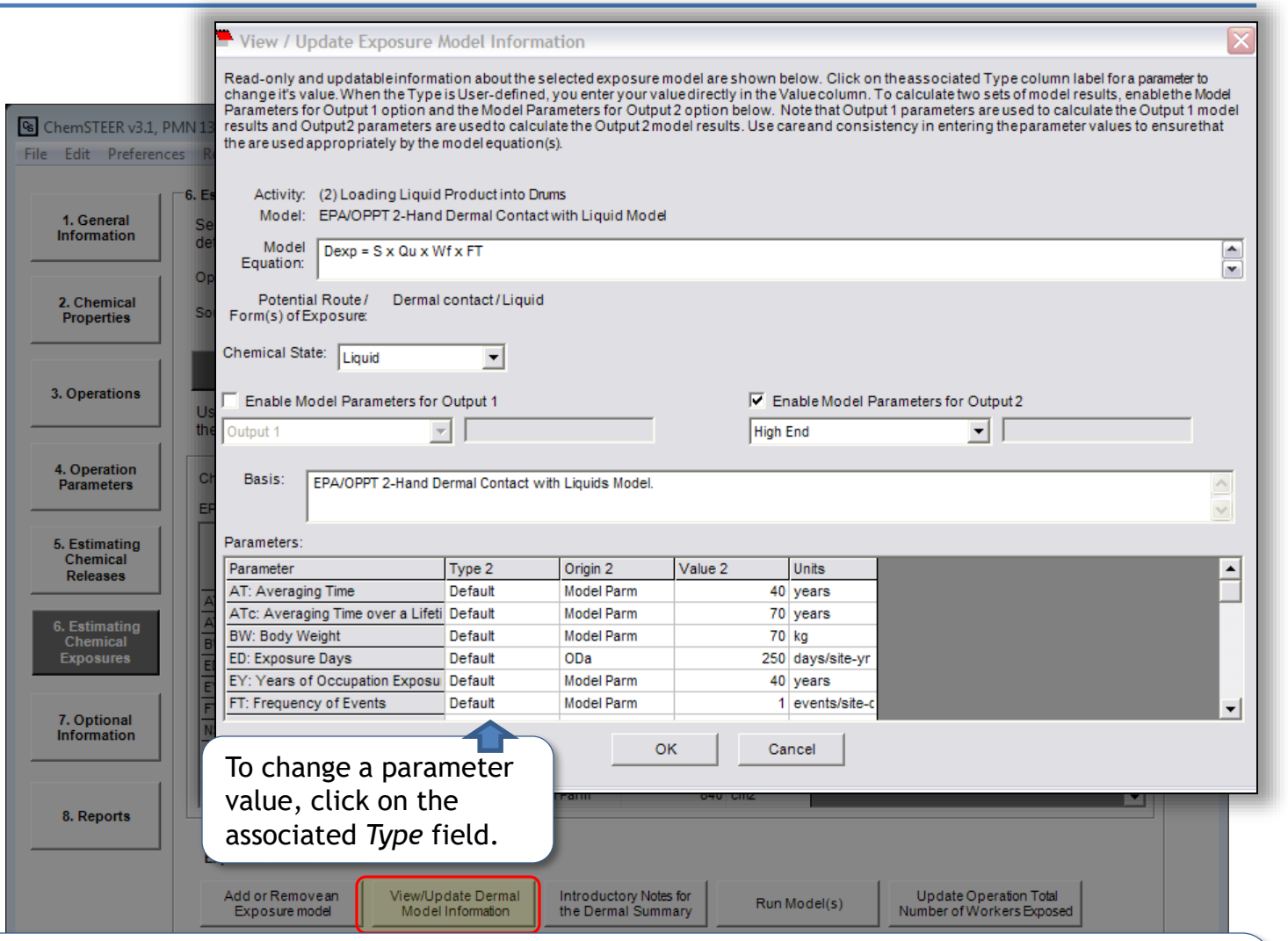


6a. Exposures → Dermal Model Parameters *(View/Update Dermal Model Information)*

The *View/Update Dermal 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.

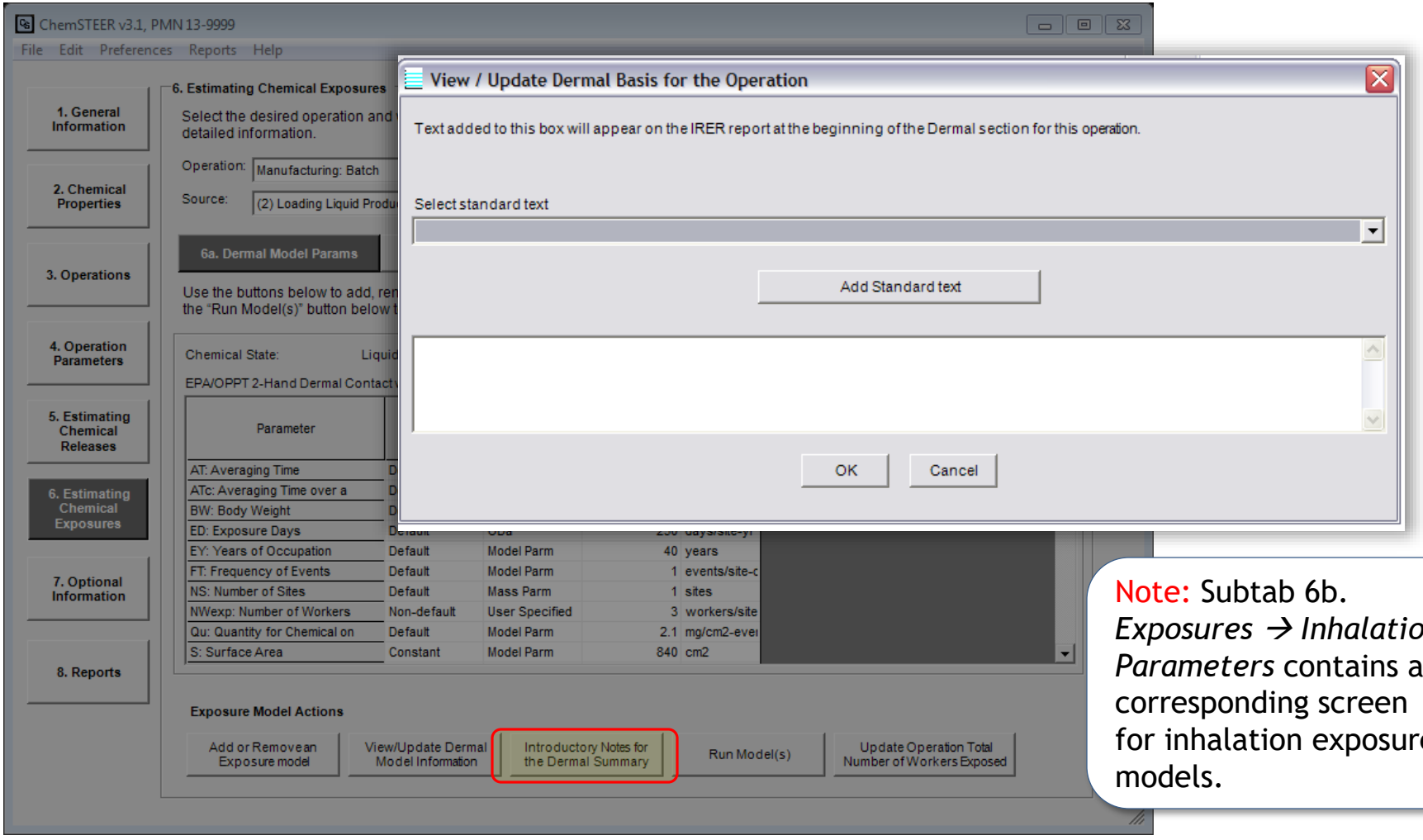
Note: Subtab 6b. *Exposures → Inhalation Parameters* contains a corresponding screen for inhalation exposure models.



- For some parameters, you can 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.

6a. Exposures → Introductory Notes for the Dermal Summary

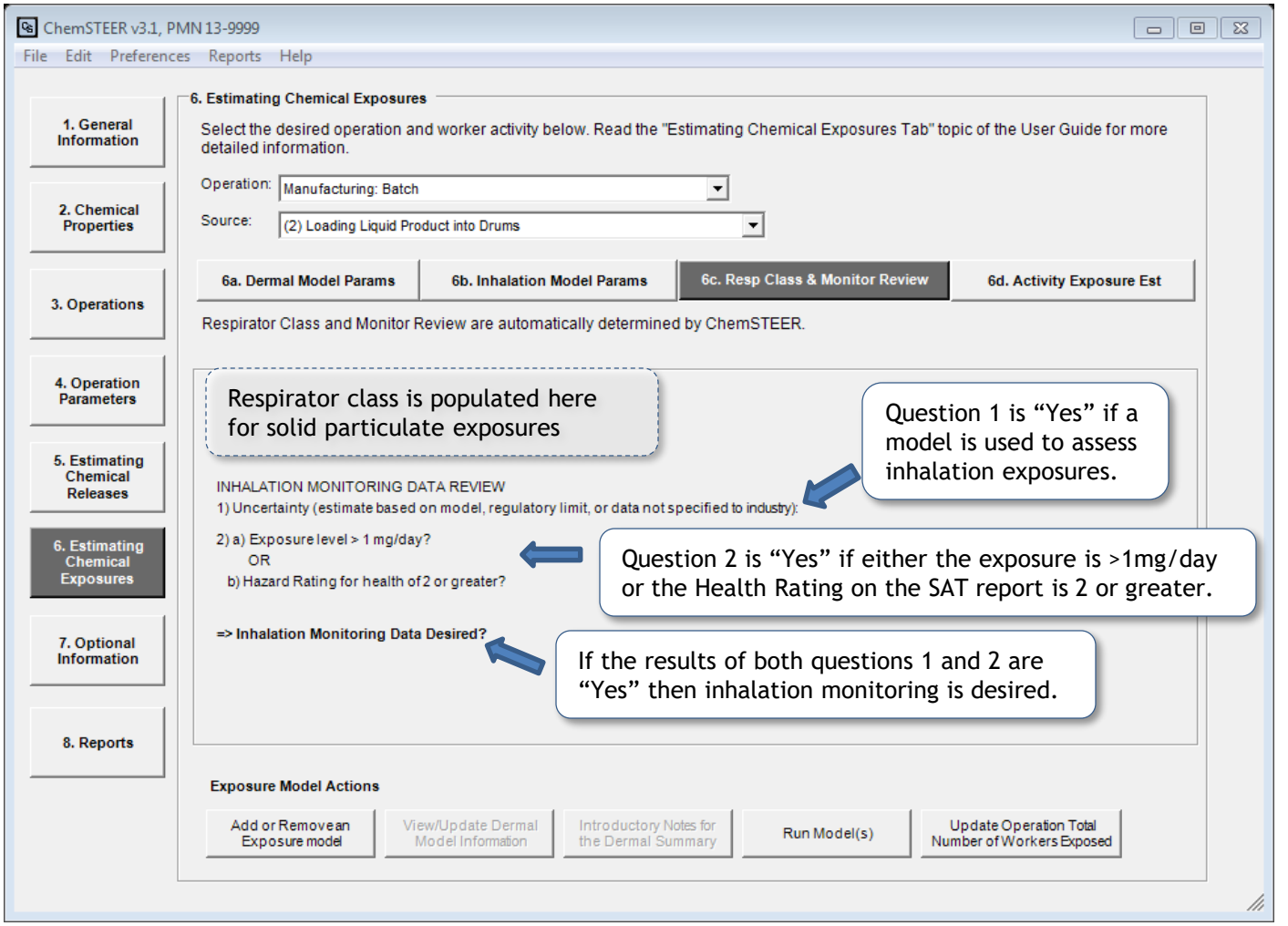
Using ***the Introductory Notes for the Dermal Summary*** and/or ***Introductory Notes for the Inhalation Summary*** buttons, you may add additional information related to the release assessments.



Note: Subtab 6b. *Exposures → Inhalation Parameters* contains a corresponding screen for inhalation exposure models.

6c. Exposures → Respirator Class & Monitor Review *(Read-only)*

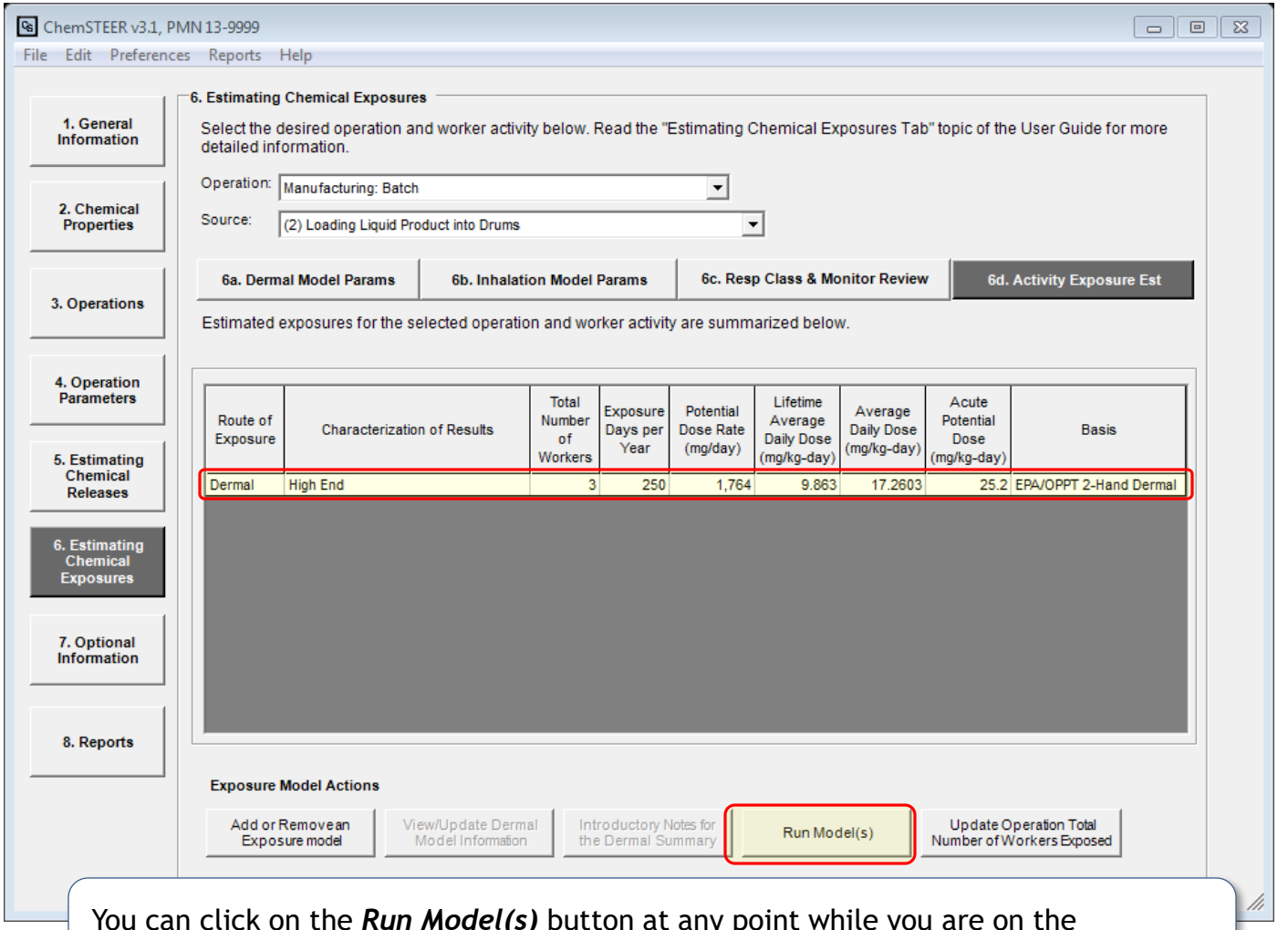
The *Respirator Class and Monitoring Review* subtab is populated automatically and is read-only. This subtab performs a review for all inhalation exposure models.



6d. Exposures → Activity Exposure Estimates

The *Activity Exposure Estimates* subtab shows the results of the exposures calculations. This screen displays the:

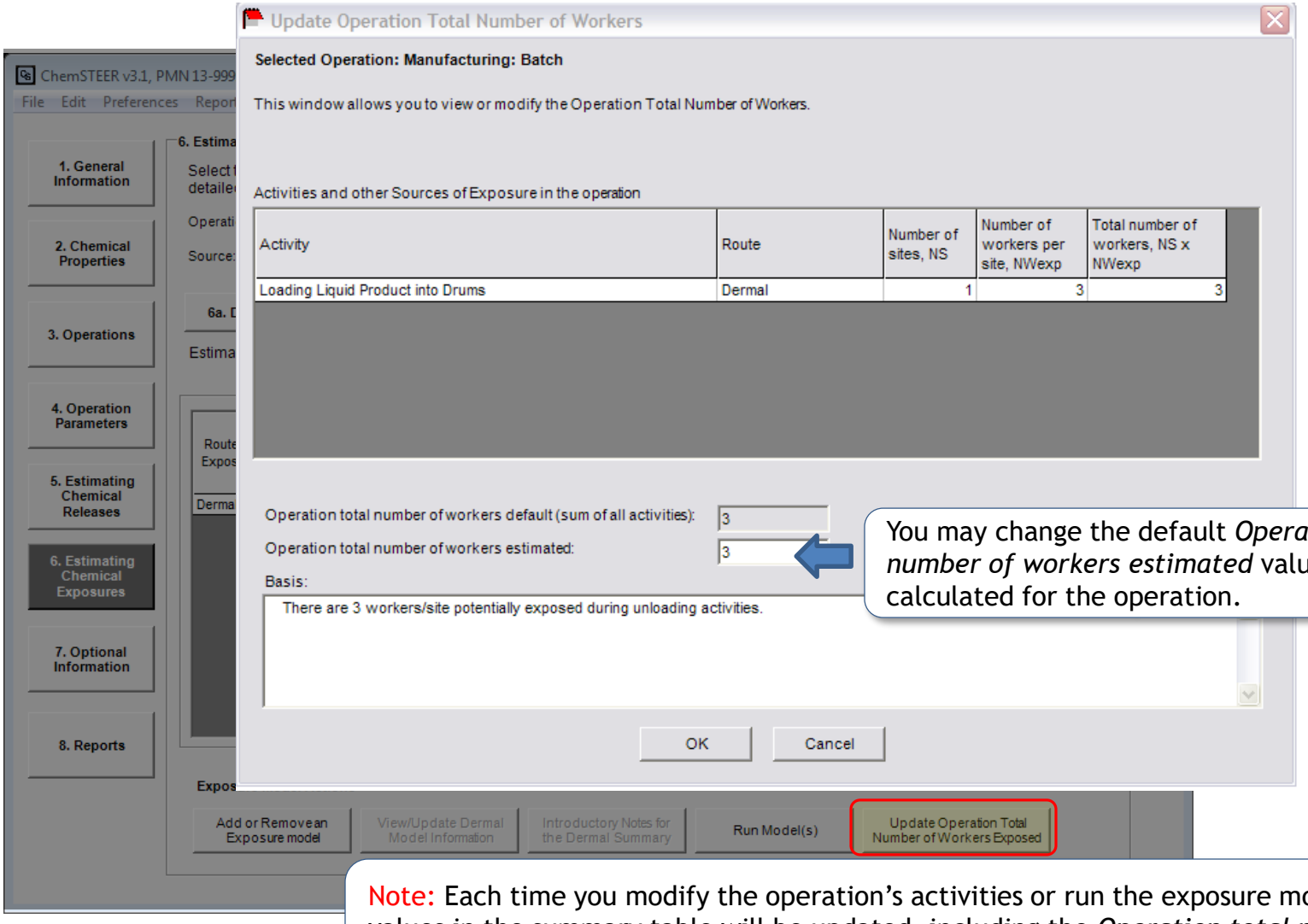
- Route of Exposure (Dermal or Inhalation);
- Number of Workers Exposed;
- Exposure Days per Year;
- Potential Dose Rate (mg/day);
- Lifetime Average Daily Dose (mg/kg-day);
- Acute Potential Dose (mg/kg-day); and
- Basis for each exposure model.



You can click on the ***Run Model(s)*** button at any point while you are on the *Estimating Chemical Exposures* subtab to execute the exposure model calculations.

6. Exposures → Update Operation Total Number of Workers

The *Update Operation Total Number of Workers Exposed* screen shows a summary of the number of workers exposed for each a worker activity in a particular operation.



You may change the default *Operation total number of workers estimated* value that is calculated for the operation.

Note: Each time you modify the operation's activities or run the exposure models, all values in the summary table will be updated, including the *Operation total number of workers estimated* value if you entered an alternate number.

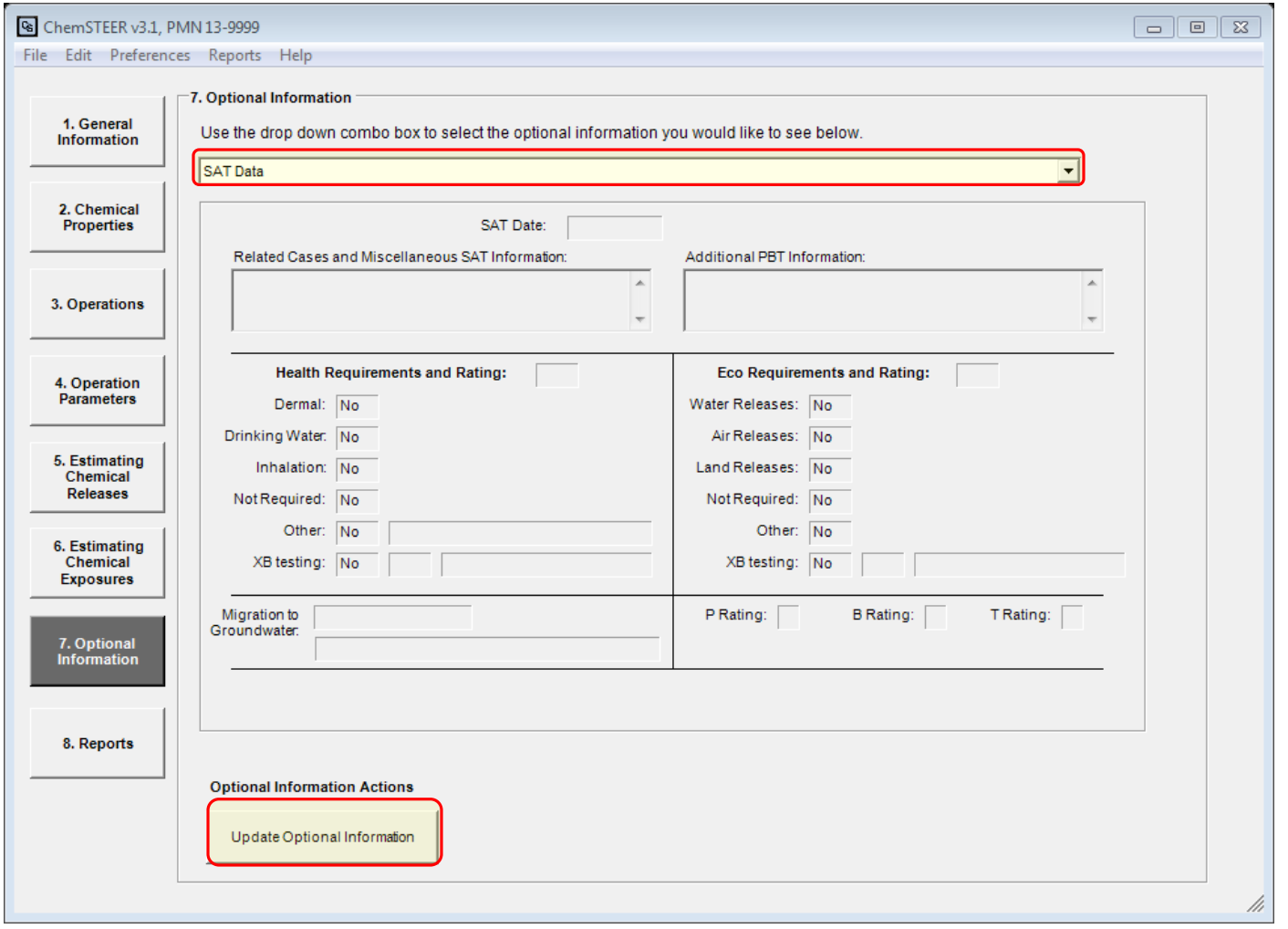
7. Optional Information

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

- MSDS/Label/Exposure Limits;
- Pollution Prevention Considerations
- Notes and Key Assumptions used in the assessment

Some of the input screens are designed to serve EPA's internal assessments, including:

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



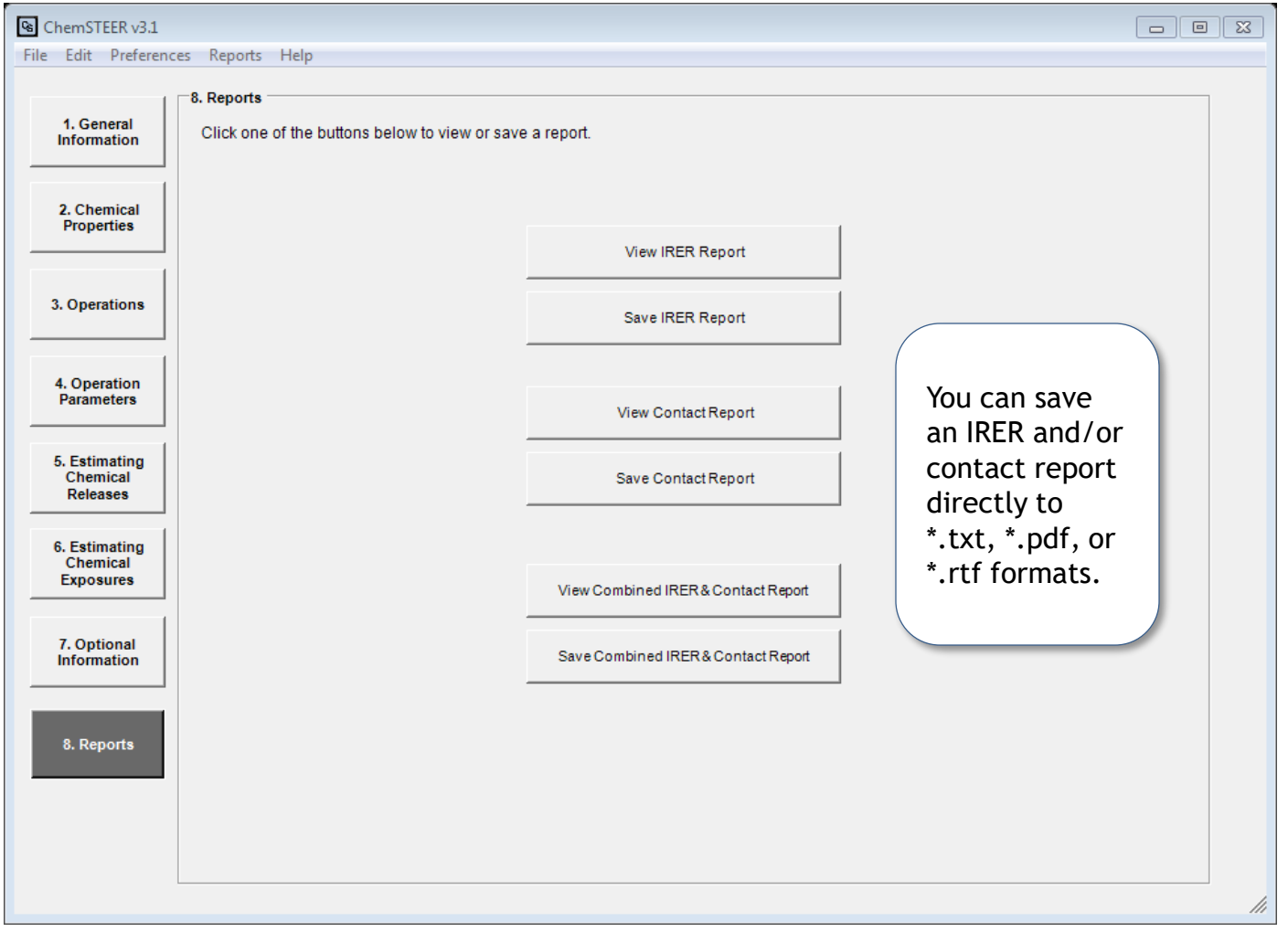
To enter any additional information about your assessment, select the appropriate screen from the dropdown menu and click on the **Update Optional Information** button.

8. Reports

There are two types of reports that are currently programmed into ChemSTEER: the Initial Review Engineering Report (IRER) and the Contact Report. The *Reports* tab can be used to view and save completed IRERs and contact reports.

IRER - EPA currently uses the IRER for its assessments of new chemicals under the Premanufacture Notice program. This report is a summary of the assessment and contains all of the information that is input to or calculated by ChemSTEER.

Contact Report - The Contact Report summarizes information obtained through contact with an individual pertaining to the assessment. This information is input into ChemSTEER in the *General* tab.



Note: Reports can also be generated and saved using the file menu (*Reports* option).

Additional Information

- Contact information and the most recent version of ChemSTEER are available from the following EPA website:

  http://www.epa.gov/oppt/exposure/pubs/chemsteer.htm

- This web site also contains links to other exposure-related information and references available from EPA.