Emission ProFiler©2005 SPRI Calculation and Reporting Software Targets NJDEP Pilot Plant, R&D General Permit Compliance

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ABSTRACT

Emission ProFiler (EP) was designed for pharmaceutical batch processing applications. Emission ProFiler incorporates an innovative and customized approach to air quality and permit compliance management. EP provides a platform that facilitates rapid modeling of sequential unit operations enabling a faster turn-around time for environmental approval of new / modified research and development processes.

Emission ProFiler was developed to address the requirements of both the Pilot Plant Permit and the new General Permit for Research & Development issued by the New Jersey Department of Environmental Protection (NJDEP).

Emission ProFiler is a Windows-based system that calculates, tracks and reports emissions in the kilo to pilot plant-scale batch production of pharmaceutical products. EP is based on US EPA Office of Quality Planning and Standards (OAQPS) calculation methods. EP maintains all individual unit operations by experiment for each product in the system. Control devices are also tracked in the system to calculate pre- and post-control emissions. To verify the calculations, a detailed step-by-step printout of each unit operation's calculations is available with references in the calculations to the appropriate US EPA equation. The reports in the system are used to meet state, federal and internal reporting requirements.

Although primarily an air permit compliance tool, EP has the additional ability to simultaneously track information on wastewaster and hazardous waste production from pharmaceutical processes for use in other regulatory systems.

INTRODUCTION

Research & Development (R&D) pharmaceutical batch processing of active pharmaceutical ingredients (API) in New Jersey provides a compliance challenge to engineers, who are often held accountable for short-term health effect (SHE) impacts. On one hand, regulatory requirements of NJDEP Air Permits need to be met with professional competence and thoroughly documented as part of an overall environmental management plan. On the other hand, an expanding, diverse and rapidly evolving pipeline necessitates a speedy and highly-focused environmental assessment of batch processes heading for plant scale-up. The key to meeting both goals lies in the engineering toolbox. Unlike off-the-shelf software, Emission ProFiler does not attempt to meet every environmental need, confuse the user with a multitude

of overlapping windows, or require lengthy set-up better meant for manufacturing facilities. Its simplicity lends itself to modeling of sequential unit operations within a smart and logical framework. With a batch recipe in one hand and Emission ProFiler in the other, an engineer can weed out troublesome operations, apply control device removals, determine emission rate compliance, and keep a tab on HAP and other targeted pollutants. Reports can be customized by the user for both regulatory purposes and internal tracking.

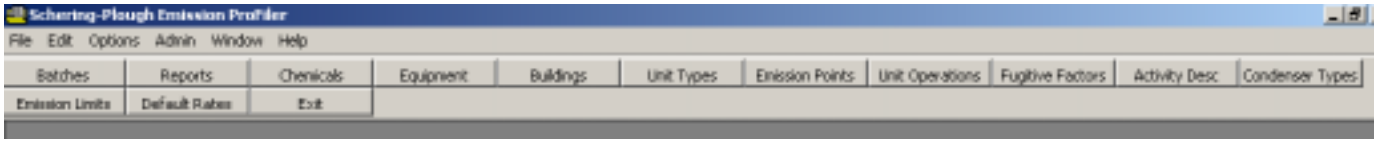
Emission ProFiler SYSTEM

The Emission ProFiler system is a Windows-based program developed in Microsoft's Visual Basic to calculate, track and report VOC and HAP emissions in the batch production of pharmaceutical products. Emission ProFiler is based on US EPA Office of Quality Planning and Standards (OAQPS) calculation methods. [1,2,3] EP maintains all individual unit operations for each experiment in the system. Control devices are also tracked in the system to calculate pre- and post-control emissions. To verify the calculations, a detailed step-by-step printout of each unit operation's calculations is available with references in the calculations to the appropriate US EPA equation. The reports in the system are used to meet state, federal and internal reporting requirements.

Figure 1. Emission ProFiler Start-up Screen.

Figure 2 shows the main toolbar in Emission ProFiler.

Figure 2. Emission ProFiler Main Toolbar.

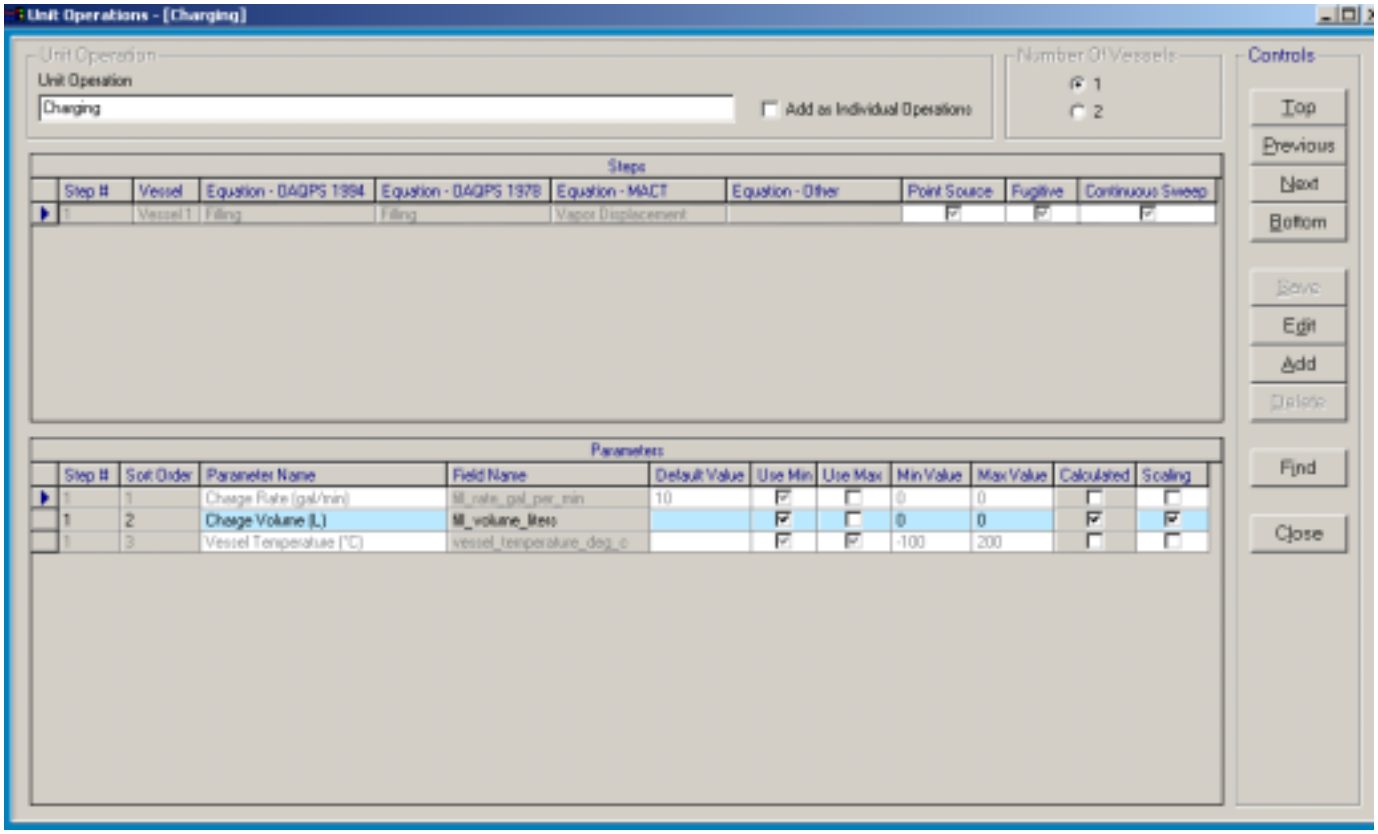


In Emission ProFiler users enter batch product information, produce reports or maintain support databases. The support databases contain information that is used throughout the system. Emission ProFiler's support databases are as follows:

- Chemicals
- Equipment
- Buildings
- Unit Types
- Emission Points
- Unit Operations
- Fugitive Factors
- Activity Description
- Condenser Types
- Emission Units
- Default Rates

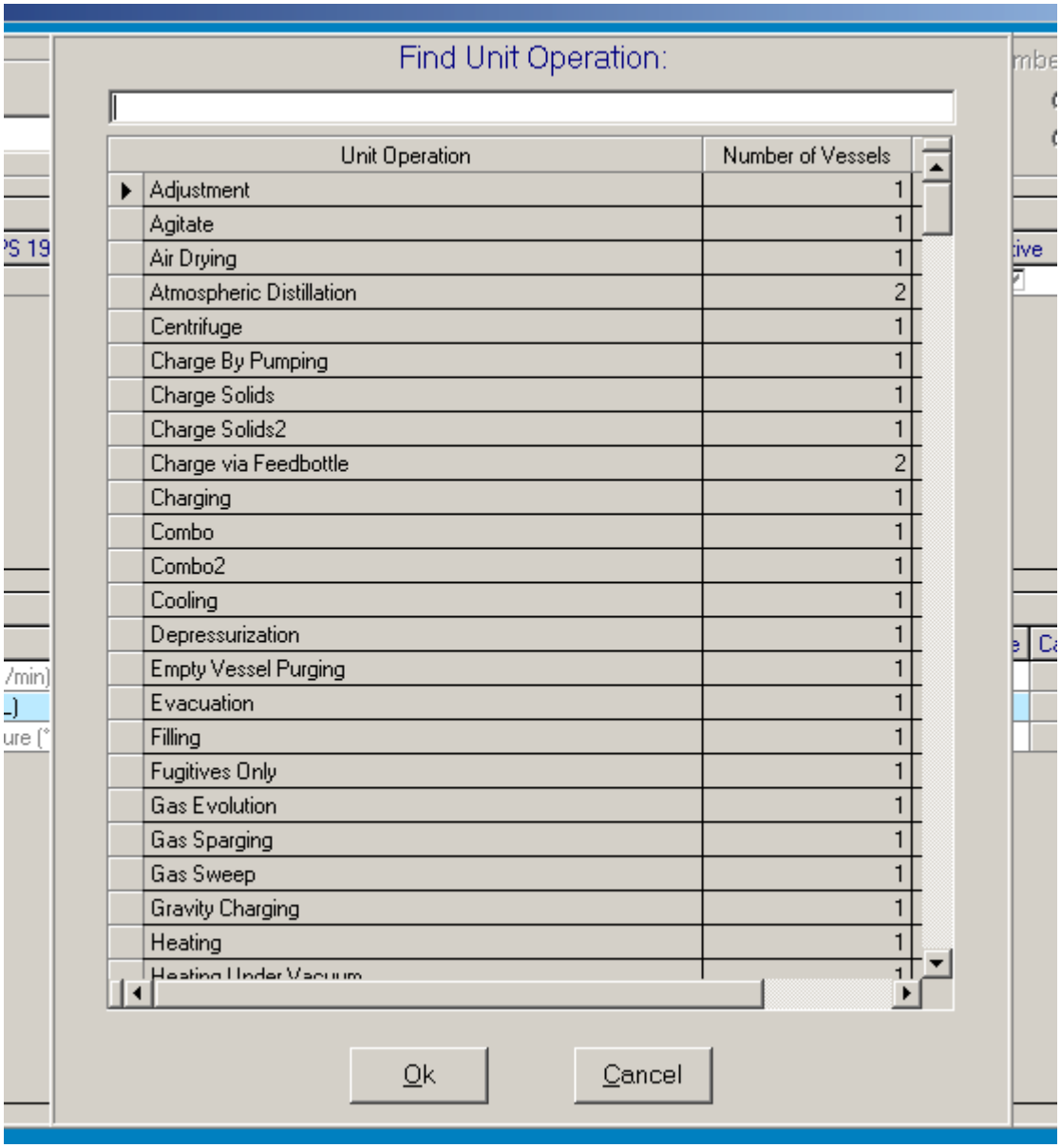
Each support databases is a separate button in the Emission ProFiler toolbar. An example of the support databases for Unit Operations is shown in Figure 3. The Unit Operations table includes information on the operation type, OAQPS equation type, required input parameters and default input parameters.

Figure 3. Support Table – Unit Operations



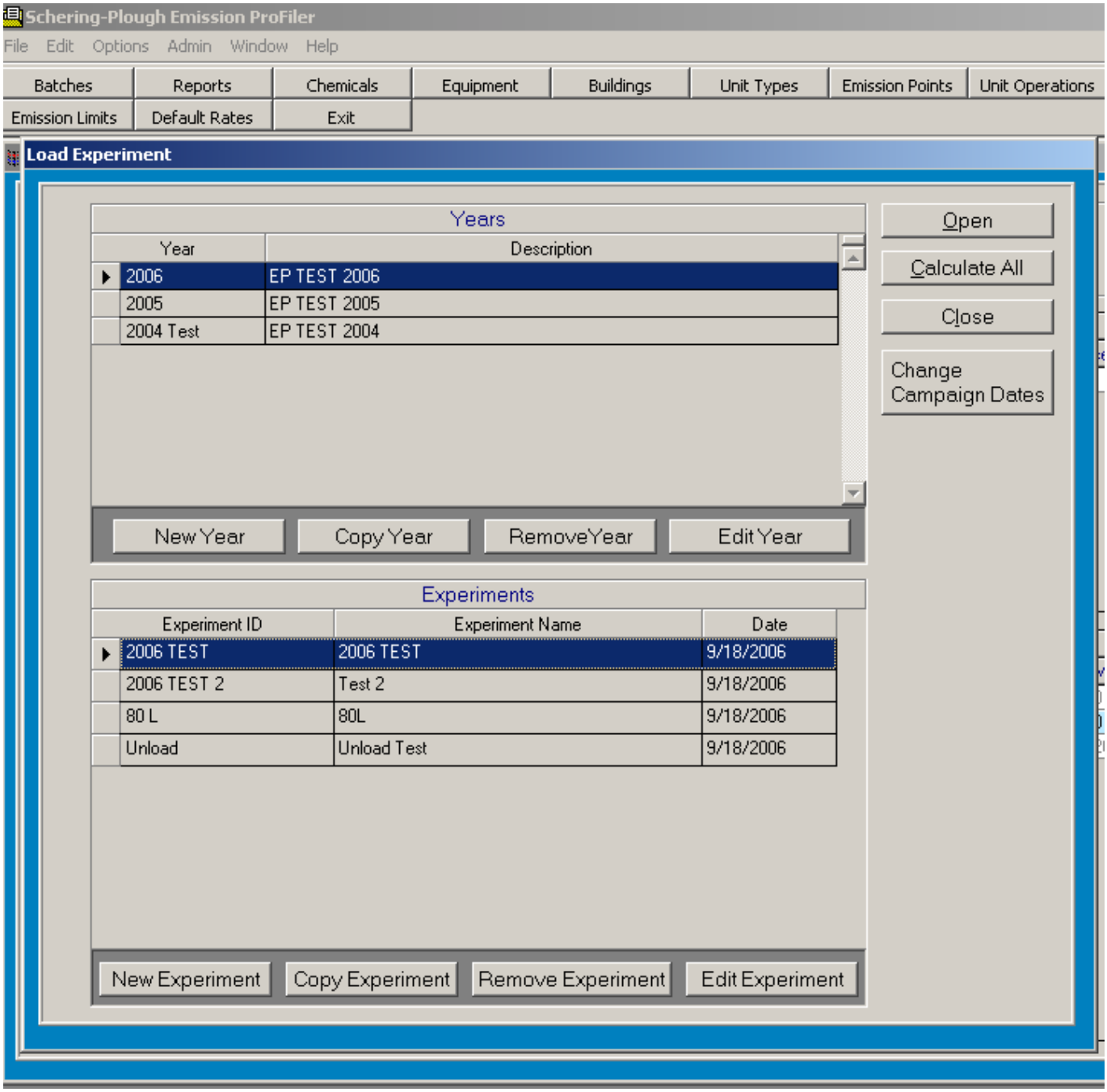
The maneuvering controls in Figure 3 are similar to those used throughout EP. The user can move through the records in the database with the Top, Previous, Next or Bottom button or use the Find button to display a list of all records in the database (Figure 4). To modify existing data the user selects the Edit button. The Add button allows the user to enter a new unit operation type. After editing or adding new information, the user presses the Save button to save all of the new information. The Delete button allows the user to remove records.

Figure 4. Unit Operations Find Screen.



The entry of batch experiment information is in the Batches module. Pressing the Batches button displays the Load Experiment screen shown in Figure 5. This screen allows the user to select a year to work with. When a year is selected (highlighted), all of the existing experiments in the selected year are displayed in the bottom grid. In the experiments grid, the user can select an experiment to work with or add/remove experiments.

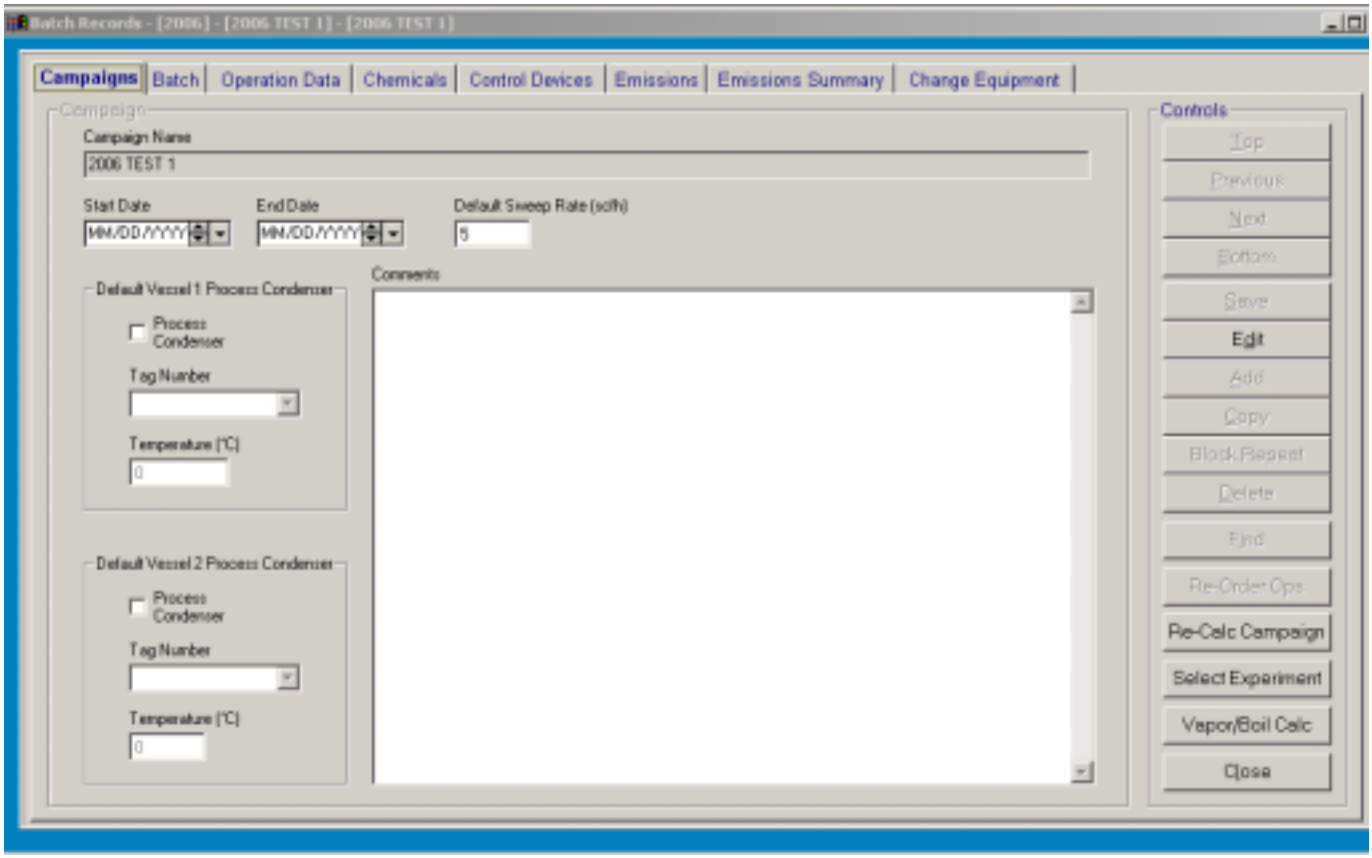
Figure 5. Batch Records Year / Experiment Selection Screen.



After selecting an experiment to work with, the user presses the Open button. Opening an experiment (Figure 6) displays the campaigns screen. The experiment information consists of a flip card that supplies detailed information on the campaign, individual batch unit operations, chemicals used in the process, control devices and emissions information at the batch record level. Figure 6 shows the campaigns flip card. On the campaigns flip card the experiment start and stop time is recorded along with default

information for any process condensers present and a data field for adding specific comments about the experiment campaign.

Figure 6. Campaigns Screen for a Selected Experiment.

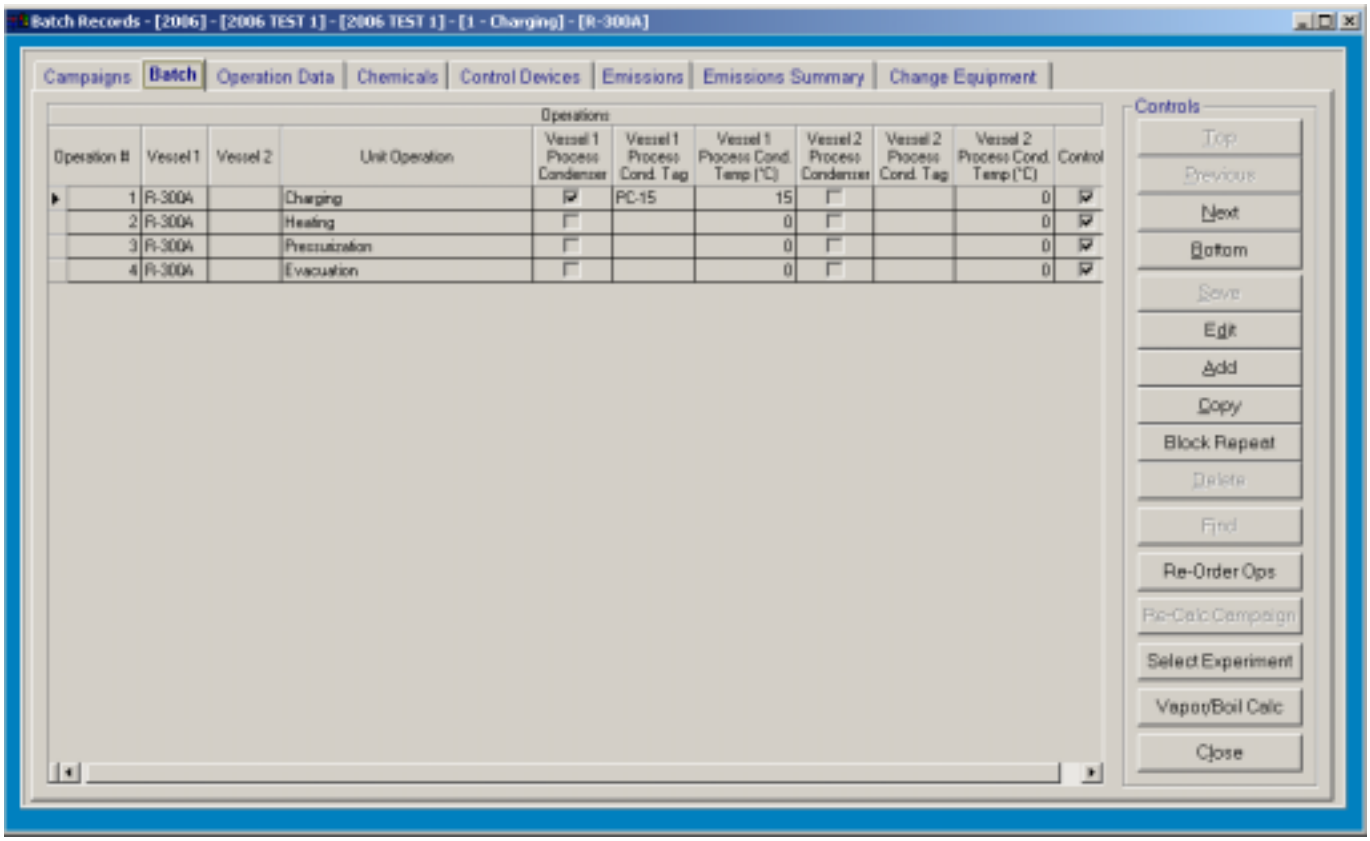


The Copy button at the campaign level allows the user to a make a complete copy of the selected campaign including all batch record steps, chemicals and control devices.

Selecting the Batch flip card (Figure 7) displays a list of the individual unit operations that make up the entire batch record cycle. To add a new step to this batch record, the user presses the Add button. The Copy button will copy an existing batch record with all of its information and add it as a new record at the end of the batch record cycle. There is also a block repeat function that allows selecting one or more unit operations and copying them as many times as necessary. If the order of the unit operations in the batch record needs to be changed, the operations can be rearranged using the Re-Order Ops button.

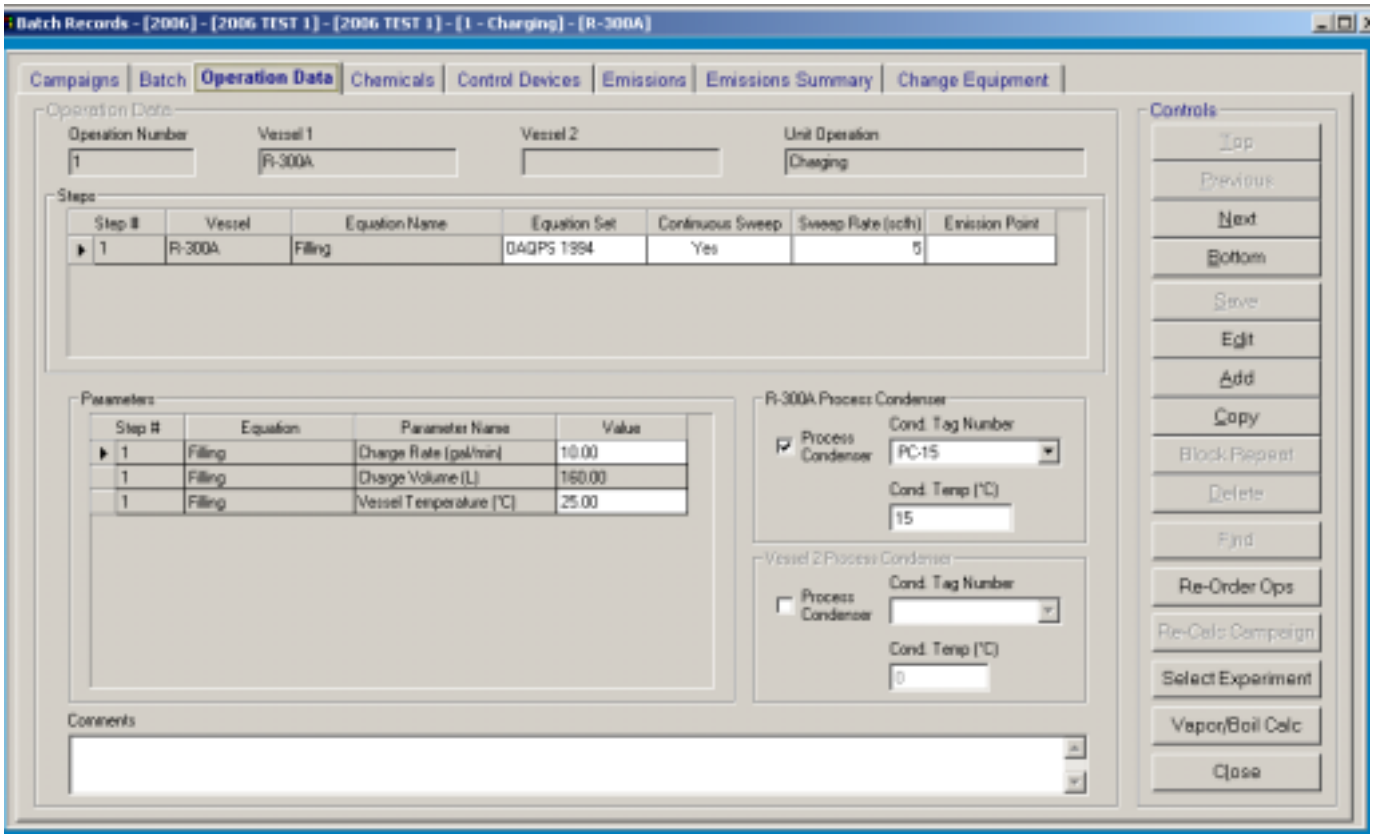
To look at the detailed information about an individual unit operation in the batch record, the user clicks on a record in the grid. The selected record then becomes highlighted. Once a record is highlighted, the user can look at detailed input and emissions information for that unit operation on the following flip cards.

Figure 7. Batch Record Grid



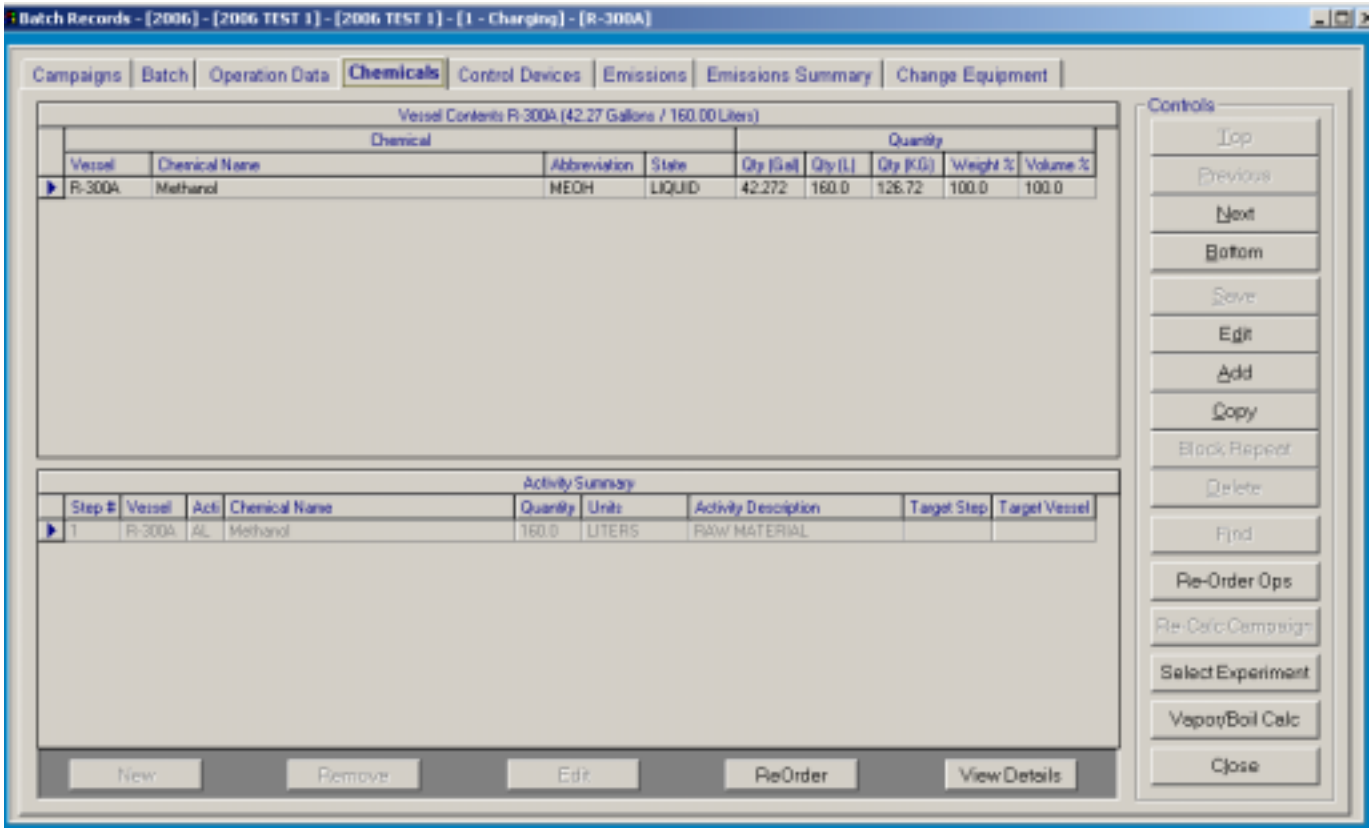
Selecting the Operation Data flip card (Figure 8) displays the input data for the individual unit operation. The unit operation input data fields will vary depending on the required information for a unit operation. Figure 8 displays an example for a vessel Charging operation. The required input fields are vessel charge rate and the exit temperature from the vessel. The amount of material charged to the vessel is determined on the Chemicals flip card. On the Operation Data screen the user is also able to indicate if a process condenser is present and if a continuous gas sweep takes place during this unit operation. The Steps grid at the top part of the screen, shows unit operations that composed this step. Some unit operations can have more than one step. In the case of a Charging operation, there is only one step. In this grid the OAQPS equation set used is documented along with information about a continuous gas sweep on the operation step.

Figure 8. Unit Operation Op Data Input Screen.



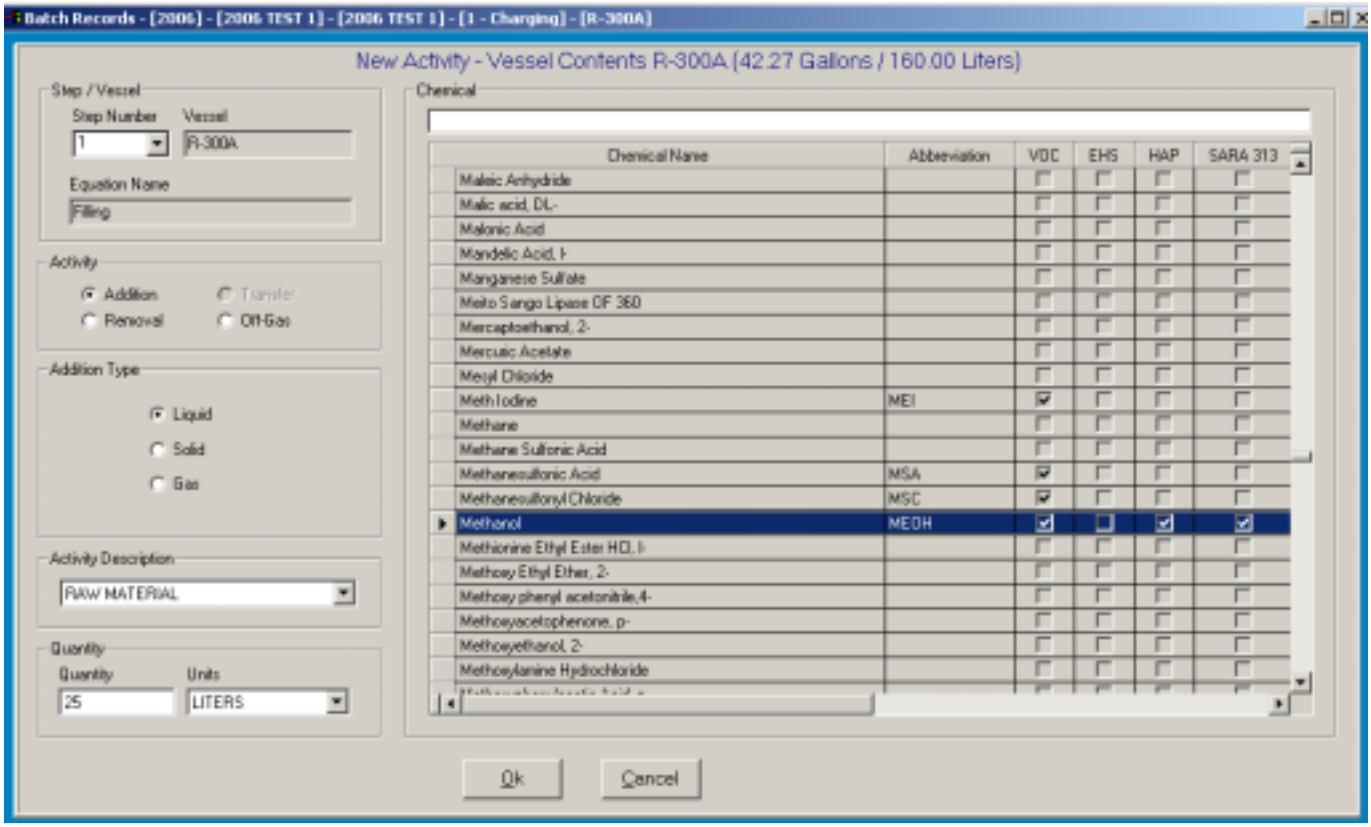
Selecting the Chemicals flip card (Figure 9) displays the screen that shows the chemicals used in the selected unit operation. The top grid on this screen shows the contents of the vessel that is the results of any previous unit operation along with the activity in this unit operation. The Activity Summary grid at the bottom of the page, shows the chemical transactions for this specific unit operation.

Figure 9. Unit Operation Chemical Usage Screen.



To add or remove a chemical in the Activity Summary section the buttons on the lower half of the screen are used. Selecting New, Remove or Edit displays the chemical activity screen (Figure 10).

Figure 10. Chemical Activity Screen.



On this screen, the user can add or remove chemicals from the unit operation and set the quantity of the material selected. The Addition activity allows the user to select the following:

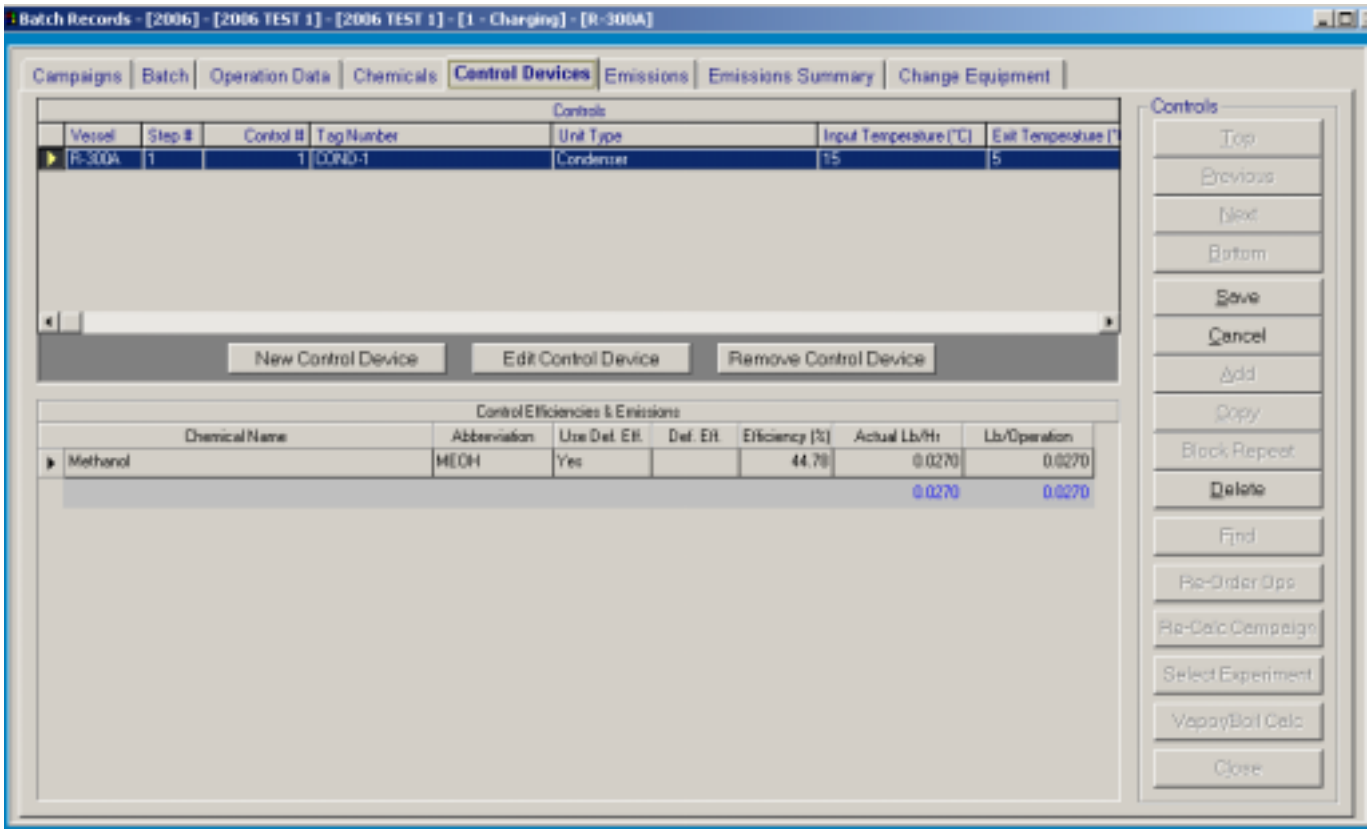
- Raw Material
- Adjustment (addition)
- Transfer To

The Removal activity is where the user documents what is removed in this batch step and the fate of the removed material. The removal selections are as follows:

- Adjustment (removal)
- Dissolved Solid
- Drums
- Hazardous Waste
- Off-Gas
- Product
- Reclaim
- Transfer From

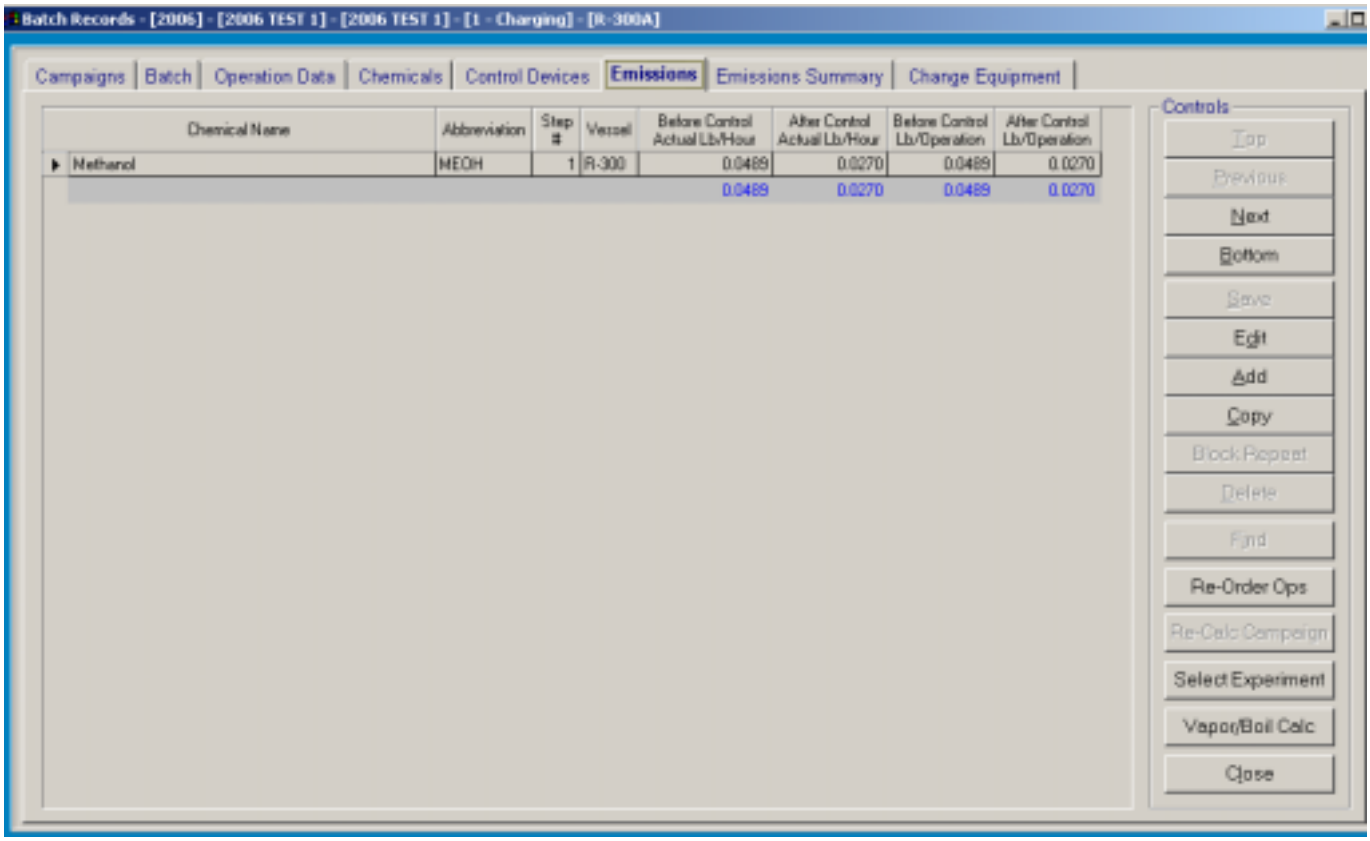
Selecting the Control Devices tab (Figure 11) displays the control devices that may be attached to the vessel in this unit operation. The user can add as many control devices as required. Clicking on a control device (highlighted) in the top grid will display the control efficiency of the device and the after control emissions for each chemical in the unit operation in the grid on the bottom half of the screen.

Figure 11. Unit Operation Control Devices screen.



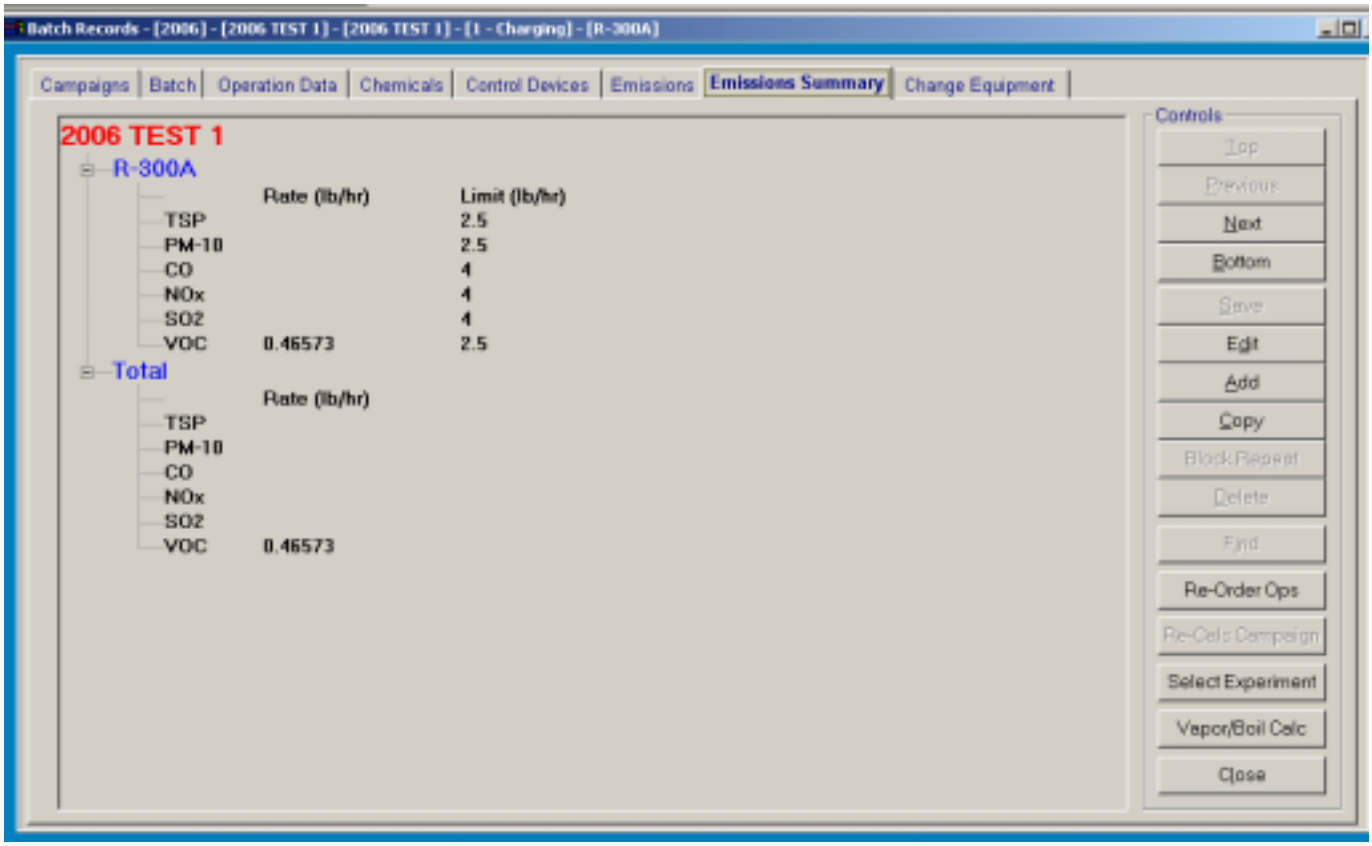
Selecting the Emissions tab (Figure 12) displays the pre- and post-controlled emission for each chemical in the unit operation in pounds per hour and for pounds per operation.

Figure 12. Unit Operation Emissions screen.



The Emission Summary screen (Figure 13) shows a roll-up of the emissions by species for each vessel in the experiment and also displays the vessel's emission limits by species.

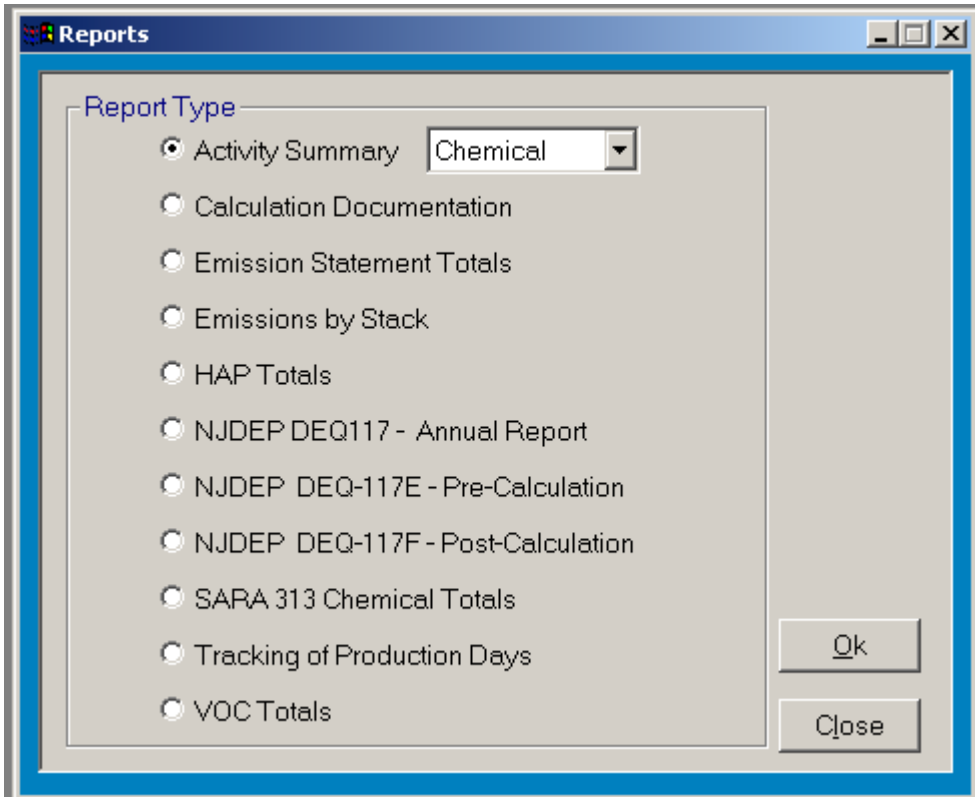
Figure 13. Unit Operation Emissions Summary Screen.



REPORTS

The reports in the Emission ProFiler system are used to provide compliance information for federal, state and internal reporting needs. The various reports in the EP system are listed in Figure 14. The reports in EP were developed using Business Objects' Crystal Reports.

Figure 14. Emission ProFiler Report Types.



Figures 15 and 16 shows an example of the New Jersey Post Experiment Review Form. This report displays the emissions from each vessel used in the experiment and compares the emissions by regulated species to the required emission limits. This report is required after every experiment is run to document the experiment compliance status.

Figure 15. New Jersey Post Experiment Review Form – Page 1.

DEQ-117F Page 1

PILOT PLANT IN-HOUSE
POST EXPERIMENT REVIEW FORM

1. **Test Date:** 1/1/1900 **Experiment Identification #:** 2006 TEST 1
   Pre-Experiment Identification #:
2. **Experiment Title:** 2006 TEST 1
3. **Emissions:** _____ **Recalculation of emissions (see page 2)**
   _____ **Emissions are adequately represented by the Pre-Experiment Review Form. Experiment ran within the expected parameters of the emission calculations.**
4. **Describe any upsets or equipment malfunctions which may have affected emissions:**
   _____
   _____
5. **Continuous Emission Monitors used (if applicable):**
   _____
6. _____ **Check here if permit limit was exceeded.**

   Any exceedance of operating or emission requirements specified by the Department must be reported to the Regional Office within one working day by telephone and within three working days in writing after knowledge of the exceedance. However, any opertion of the equipiment which may cause off-property effects, including odors, shall be reported immediately by calling the HOT LINE 609-292-7172, in accordance with the Air Polution Control Act, 26:2C-19 (e).
7. **Signature:**

Figure 16. New Jersey Post Experiment Review Form – Page 2.

DEQ-117F Page 2

Experiment Identification #: 2006 TEST 1

Experiment Title: 2006 TEST 1

Date: Thursday January 25, 2007 at 10:25:41PM

Source Designation:

R-300A

Category Subcategory	LBS/HR Actual Maximum	Permit Allowable
CO		4.000
NOx		4.000
SO2		4.000
TSP		2.500
PM2.5		N/A
PM10		2.500
HAP	0.466	N/A
Total VOC	0.466	2.500
TXS		0.000
MeCl2		2.500
Greenhouse		N/A

☒ **Batch has met NJDEP guidelines for summary emissions limits.**

☐ **Batch has failed to meet NJDEP guidelines for summary emissions limits:**

Figure 17 shows an example of one page of a Calculation Documentation report. This report is for an evacuation unit operation in the batch record, pages of this report detail the calculation methodologies and provides the specific EPA reference for the equations used.

Figure 17. Example of the Calculation Documentation Report Detailing Unit Operation Calculations.

Department: 2006
Campaign #: 2006 TEST 1
Unit Type: Reactor
Tag #: R-300A
Process Condenser: None
Continuous Sweep: No Sweep Rate: 5.00

Product: 2006 TEST 1
Operation #: 4.00
Unit Operation: Evacuation
Step #: 1
Equation Name: Evacuation
Equation Set: OAQPS 1994

Step 11. Calculate the uncontrolled emission rate of each constituent **OAQPS 1978 EQ. # 2**

$$SE = \frac{(760)\,(X)\,(VRS)\,(MW)}{(R)\,(T)}$$

Where,
- X = mole fraction of constituent
- VRS = volume of total VOC vapor discharged, in ft^3/hr
- MW = molecular weight
- T = temperature (°K)
- R = ideal gas law constant - 999 mmHg cubic ft/lb-mole °K

Chemical Name	Abbreviation	P (mmHg)	X	VRS	MW	T (°K)	SE (lb/hr)
Methanol	MEOH	0.00	1.00	37.37	32.00	298.15	3.9028

Step 12. Calculate the uncontrolled emission rate per operation over multiple purges.

SE (lb/hr) = SE (lb/hr) * Number of Purges

SUMMARY

Emission ProFiler is a valuable program that provides succinct environmental assessment of R&D API processes. This tool is invaluable in the lab to kilo/ pilot scale-up phase of development and is of necessity before tech transfer to a manufacturing facility is considered. Simplicity, flexibility and speed give Emission ProFiler an advantage over mass-marketed alternatives that tend to create bottlenecks. Based upon sound, pre-loaded equations (OAQPS [1], CTG [2] and MACT [3]), engineers can model R&D processes and gain immediate feedback regarding environmental compliance with NJDEP-issued Air Permits.

REFERENCES

1. Control of Volatile Organic Emission from Manufacture of Synthesized Pharmaceutical Products; U.S. Environmental Protection Agency; Research Triangle Park, 1978; EPA-450/2-78-029.

2. Control of Volatile Organic Compound Emissions from Batch Processes – Alternative Control Techniques Information Document; U.S. Environmental Protection Agency; Research Triangle Park, 1994; EPA-450/R-94-020.

3. National Emission Standards for Hazardous Air Pollutants for Pharmaceuticals Production – Proposed Rule; Federal Register: April 10, 2000; 65 FR 19152.

KEY WORDS

Batch Emission Calculation, Emission Inventory, Environmental Data Management