The U.S. EPA's Metal Finishing Facility Pollution Prevention Tool (MFFP2T)

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The United States Environmental Protection Agency has developed a pre-release version of a process simulation tool, the Metal Finishing Facility Pollution Prevention Tool (MFFP2T), for the metal finishing industry. This presentation will provide a demonstration of the current version of this tool. The presentation will also provide a brief overview of additional components that can be added to the tool in order to aid metal finishing facilities in evaluating pollution prevention options, identifying and managing the facility's supply chain, aid the facility in documenting regulatory compliance, and support creation of an environmental management system.

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The USEPA's Metal Finishing Facility Pollution Prevention Tool (MFFP2T)

The United States Environmental Protection Agency is currently developing a pollution prevention tool for use in the metal finishing industry, which will be built around a process simulation program. Currently the tool has the ability to create and edit a flowsheet, a database of chemical species that may be present in the simulations, a database of chemical reactions, and basic unit operations of interest in the metal finishing industry. This paper will present the current status of the process simulation software, and provides some information regarding future work to be conducted as part of developing the tool.

User Interface

The primary aspect of any computer program that user must encounter is the user interface. In an effort to develop an interface that is intuitive for the user, and obtain feedback during the development process, this section will present an overview of the current user interface. Upon opening the program, the user will be presented with a blank flowsheet (Figure 1) upon which the process flow diagram

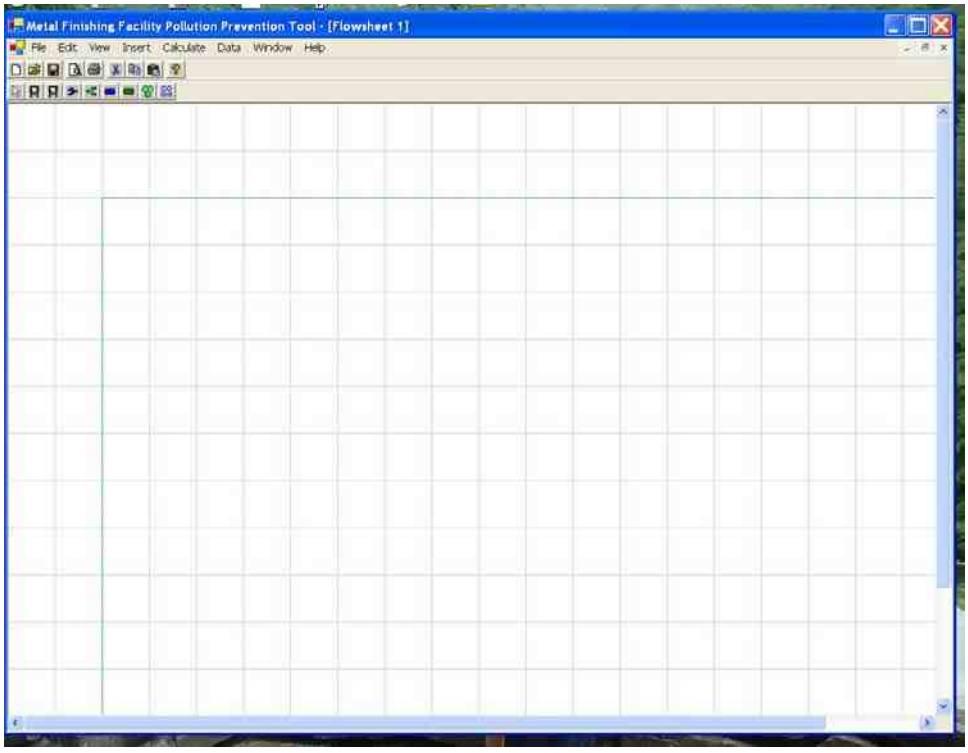
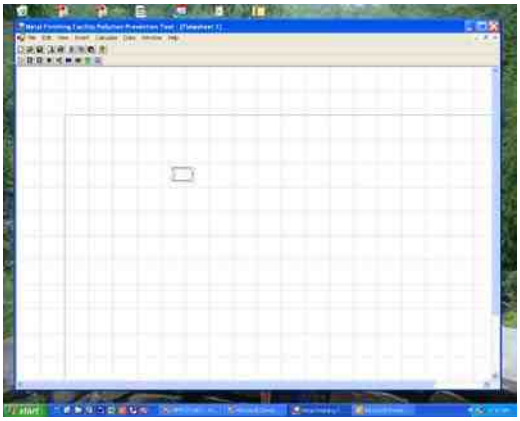


Figure 1. Opening Screen for Metal Finishing Pollution Prevention Tool

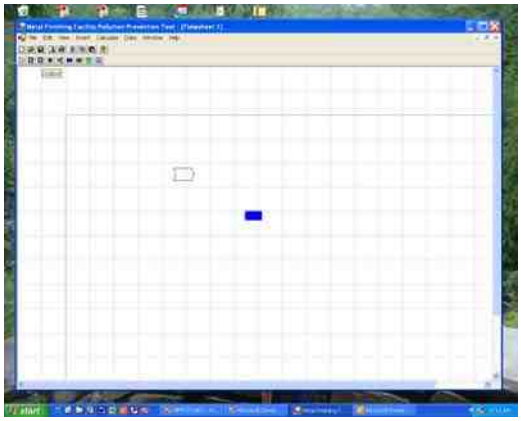
for the simulation can be constructed. The user is presented with two toolbars; the first contains standard Windows functionality (*e.g.*, loading and saving files, printing the

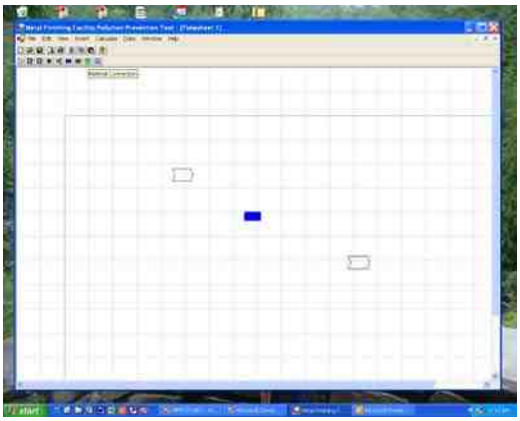
document, etc.) and the second provides for the insertion of unit operations and flow streams. By clicking on the desired unit operation, the user can build the flowsheet, as shown of Figure 2.

Figure 2 demonstrates the process for creating a flowsheet. In this example, the flowsheet is constructed by first selecting the source object, which represents the "storage tank" where chemical feedstocks are kept. The source tanks are the only place where a solutions chemical composition can be set directly; that is, concentrations in other tanks are calculated from models, such as material balances, equilibrium models, plating models, or other appropriate process models. As unit operations are added to the flowsheet, flow streams are used to

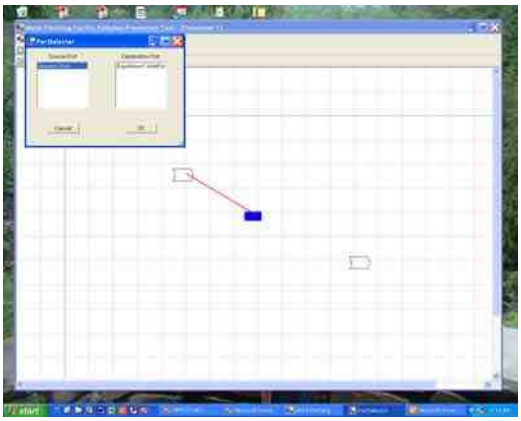


Step 1. Insertion of Source Object.





Step 3. Insertion of Destination Object.



Step 4. Connection of Source Object outlet port to Equilibrium Object inlet port.

Figure 2. Construction of a Flowsheet Using the Metal Finishing Facility Pollution Prevention Tool.

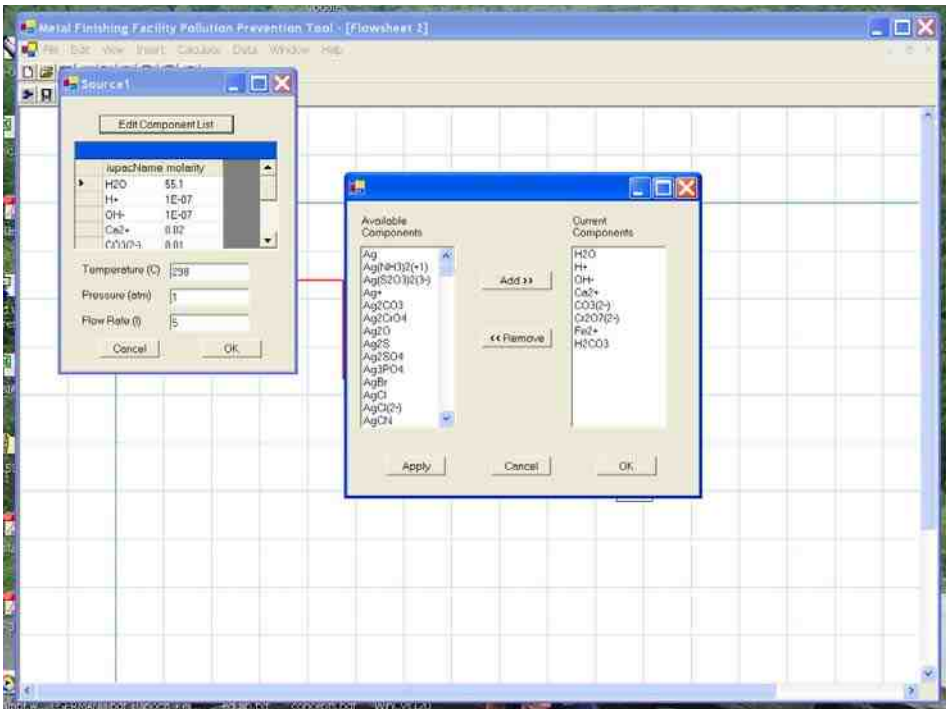


Figure 3. Creation of Editing of Chemicals Using the Editor For the Source Unit Operation.

indicate the material flow from one unit operation to the next. Because unit operations may have multiple connection points, each expecting a particular type of stream, once the user identifies the source and destination unit operations, the program brings up a port selection dialog box that asks the user to select the appropriate source and destination ports. The user then selects the correct ports and the flowsheeting software makes the appropriate connections.

As indicated above, the composition of the material in the feedstock is set using the material editing form, which is shown as Figure 3. This form currently consists of two parts; the first part allows the user to set the concentrations, temperature, pressure, and flow rate of the material stream. The second part is used to add compounds in the property package to the current material object. When a compound is added to the feed stream, its concentration is automatically set to 0. It should be noted that the calculations are all conducted in System International (SI) units, such as molarity (moles/liter). A future modification of the code will be made to allow users to set concentrations in more familiar units, such as milligrams per liter (mg/L), or other traditional units.

The program utilizes two databases; first a chemical database and the second is a reactions database. The chemical database, or property package is a listing of all

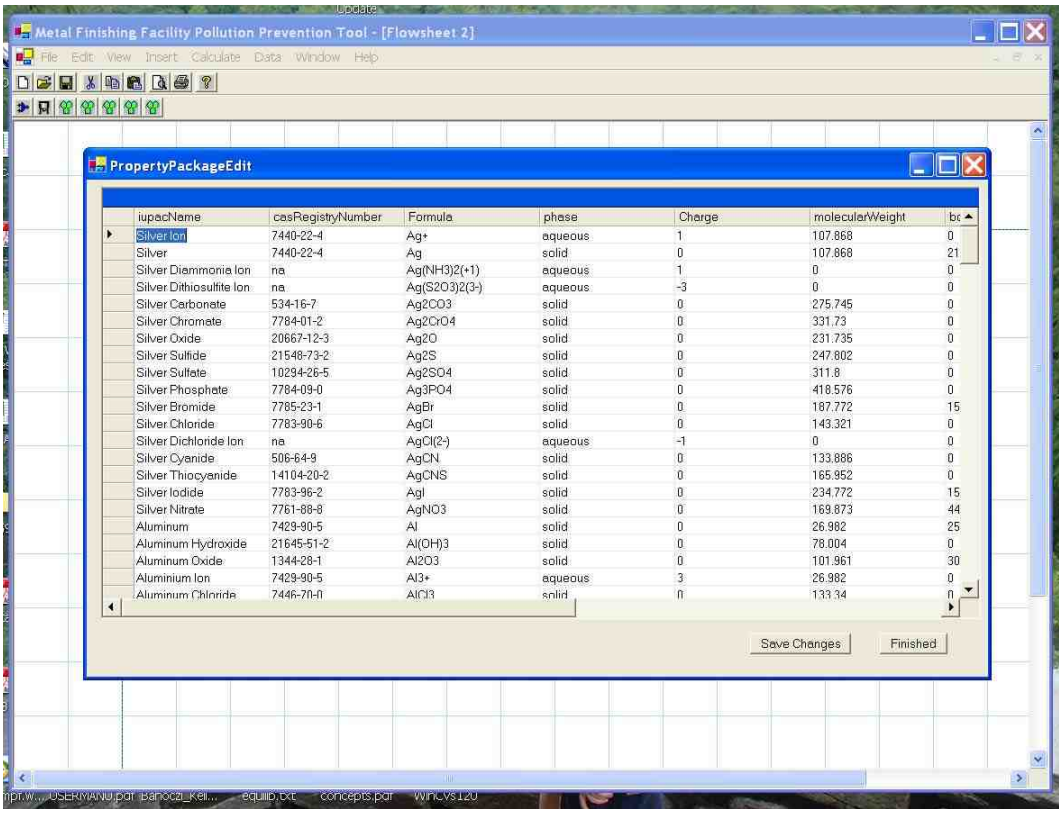


Figure 4. Property Package Edit Form.

chemical species available for use in the program. Currently, a limited test property package has been built, which will be expanded for the release versions. The property package can be accessed and edited using the Property Package Edit Form, shown in Figure 4. This form presents the name, formula, molecular weight, Gibbs Free Energy, and other appropriate information and physical properties of the chemical compound.

The reactions databases actually consists of four separate databases, as follows:

- acid/base reactions,
- solution reactions
- coordination/complexation reactions,
- and Oxidations/Reductions reactions

Creation of separate databases was selected because it separated the different chemical concepts associated with each of the four distinct types of chemical

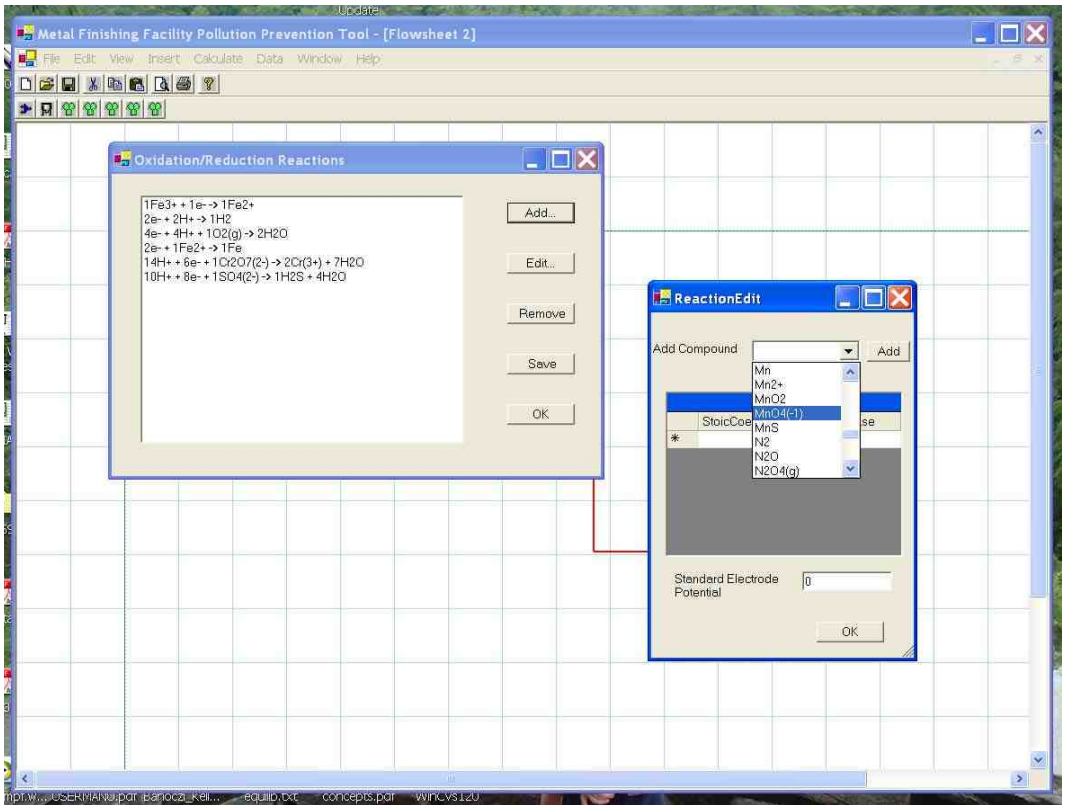


Figure 5. Reaction Database and Reaction Editor.

reactions that commonly occur in water chemistry. Further, the user needs only to consider one type of reaction at a time. The reaction database and reaction editor are shown in Figure 5. The reaction editor also consists of two windows; the first is the list of reactions, and the second lists the chemical species in the reaction. A reaction is created by selected and adding the chemical species involved in the reaction. Once the species have been added, the stoichiometric coefficients are added. The stoichiometric coefficient of a reaction product is positive and the coefficient of a reactant is negative. For example, the coefficients of the oxidation reduction reaction: $Cr_2O_7^{2-} + 14H^{+1} + 6e^{-1} \leftrightarrow 2Cr^{3+} + 7H_2O$ are -1 for the dichromate ion ($Cr_2O_7^{2-}$), -14 for the hydrogen ion (H^{+1}), -6 for the electron (e^{-1}); 2 for Chroimum(III) (Cr^{3+}), and 7 for water (H_2O). The standard electrode potential is also added for use in calculations. The resulting reaction will appear in the reaction database as: 14H+ + 6e- + Cr2O7(-2) -> 2Cr(3+) + 7H2O.

The reactions to be used for a particular unit operation or material flow can be selected using the reaction selection dialog, shown in Figure 6. Each type of

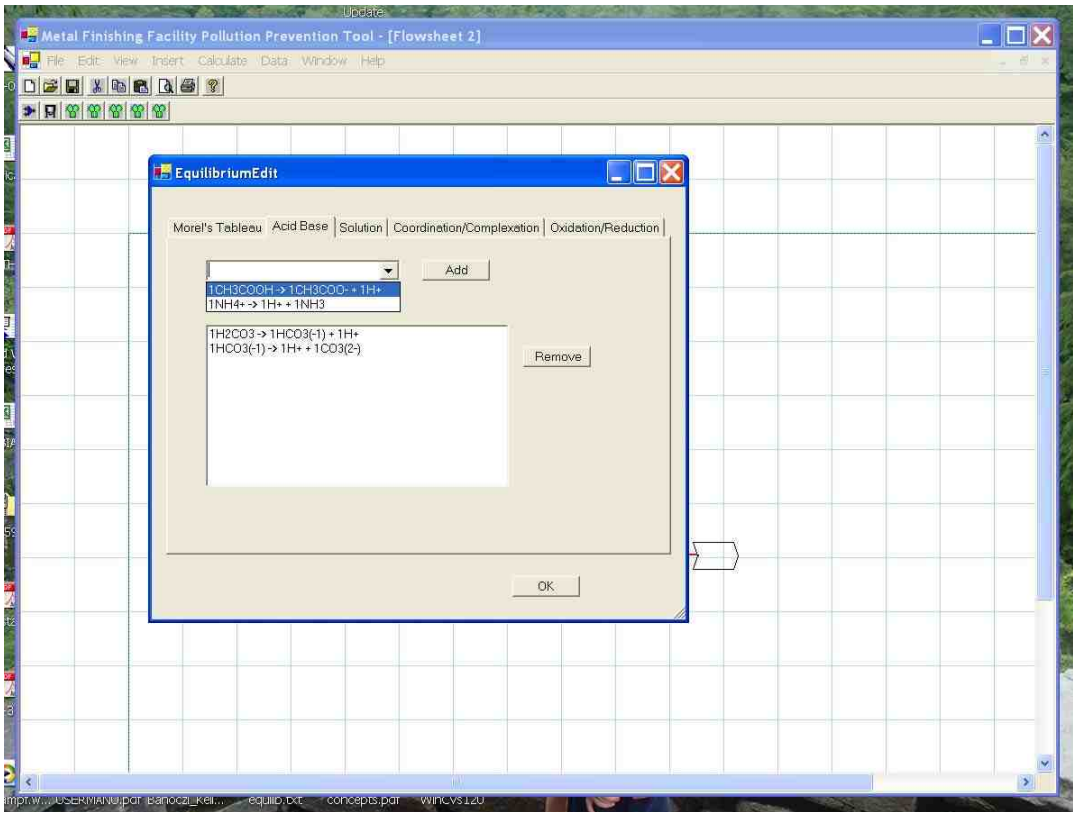


Figure 6. Reaction Selector.

reaction can be selected using the appropriate tab in the selector. Once all desired reactions have been selected, the reaction set is used to construct a tableau as described in Morel and Hering (1993).

Once the flowsheet has been constructed, the finished flowsheet will look like Figure 7. The flowsheet can then be calculated by selecting the calculate command from the calculate menu item. The calculate command goes through each unit operation and requests that it calculates itself.

Status of Process Simulator

Currently, the process simulator is capable of developing a flowsheet and calculating the equilibrium concentrations of chemicals in the flow streams. Additional unit operations must be created that can determine the amount of material plated onto parts, as well as estimate concentrations in rinse tanks based

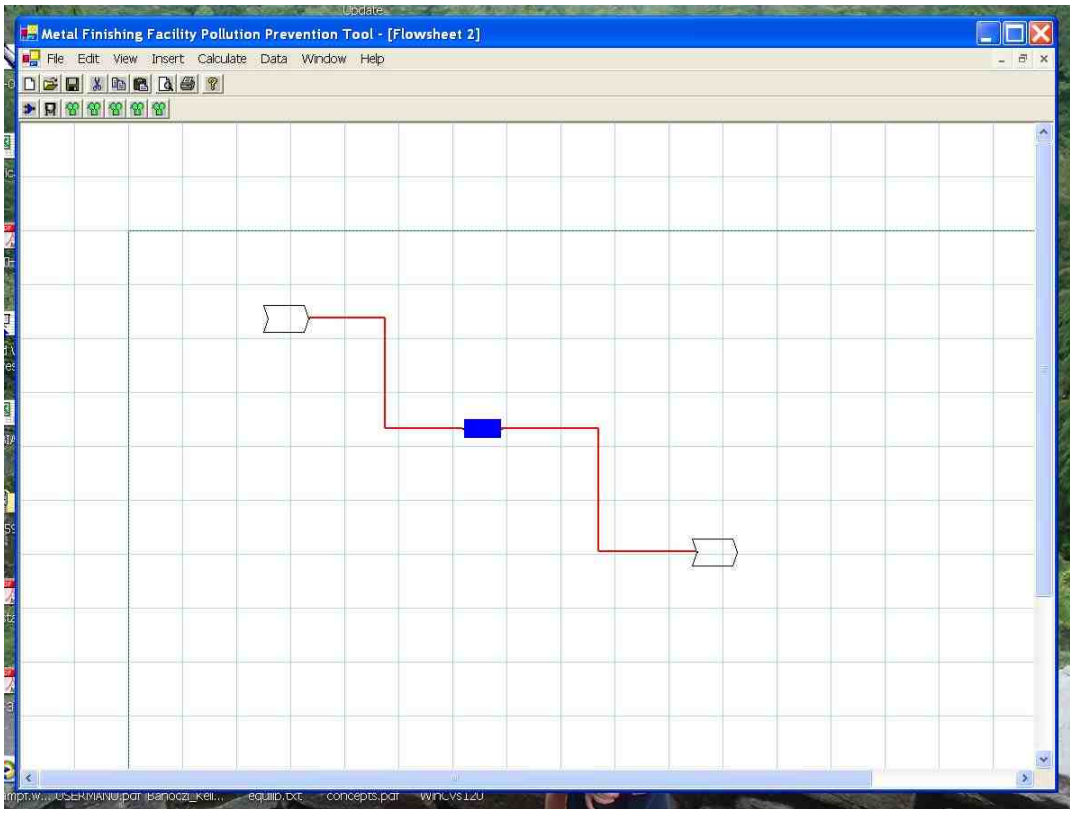


Figure 7. Finished Flowsheet Ready To Be Calculated.

on amount of solutions dragged out from the preceding process tank. In addition, models must be created of typical pollution control unit operations such as ion exchange, hydroxide precipitation, cyanide oxidations, etc.

Once a sufficient number of unit operations have been created, work must be done to verify that the flowsheet calculation converges to the correct value. Flowsheet convergence is not a problem when the flowsheet does not have recycle loops, but once recycle is considered, the input concentrations are dependent on the output concentrations of other unit operations. This cyclical dependence results in the need to tear the recycle streams as described in Westerburg, et al (1979).

Future Work

The process simulator has been created based on the CAPE-OPEN standards developed for chemical process simulation software (CAPE-OPEN Project Team 2000). As previously stated (Barrett and Harten 2003), the intention of using the CAPE-OPEN standards is to utilize process simulation tools developed for the general chemical process industry in the metal finishing pollution prevention tool. Currently, the USEPA has updated the Waste Reduction Algorithm (WAR) (Young and Cabezas 1999) so that it can interact with a

CAPE-OPEN compliant material object and calculate the WAR value for the process stream.

Having the ability to utilize process simulators to evaluate pollution prevention options will provide industry with a powerful tool for waste reduction. The simulator will allow process engineers to estimate the reduction in the quantity of waste generated by a process change without having to take the process offline and modify the process. Additionally, multiple process options can be tested and the results compared in a relatively short period of time, giving the engineer the ability to select the best combination of process modifications.

Future improvements can include the ability to combine the process simulation with a cost analysis program to provide the facility with the ability to conduct an engineering economic analysis of the process modification. In this way, the facility can be proactive in identifying waste reduction opportunities that can reduce waste disposal costs and increase operational efficiency. This would enable the engineer to determine which pollution prevention options are cost effective and communicate the potential cost reductions to management.

Through the ability of the simulator to communicate with other computer programs using either the CAPE-OPEN interfaces, or interfaces developed by others, such as the OLE for Process Control (OPC) interfaces (OPC Foundation, undated), the effect of process conditions on product quality can be evaluated. The process simulation tool and process control packages can then be combined with other applications such as statistical quality control tools, enabling the process engineer to evaluate the effect of process changes on the quality of the finished product. Improvements in product quality will result in less product rework, reducing the mass and/or toxicity of waste production.

Creation of an environmental management system (EMS) enables the facility to evaluate the environmental footprint of the facility. Properly implemented EMS's have the potential to improve corporate image, achieve financial savings through improved efficiency, lead to competitive advantage, and achieve measurable reductions in pollution. Using process simulation tools as part of EMS development can streamline the evaluation of the environmental lifecycle of the process. As EMSs are often initiated or used as part of an environmental compliance program, the process simulation tool, combined with the process control package, can be used to assist in record-keeping functions necessary for regulatory submissions.

Summary

The USEPA has an ongoing effort to create a pollution prevention tool for use by the metal finishing industry. This tool is being constructed around a process simulator. The process simulator will be capable of calculating the quantity of wastes generated by a particular

process flowsheet. Once the amount of wastes generated can be estimated, various options for waste reduction can be investigated and analyzed.

The current status of the project is a basic simulation tool where users can enter unit operations and concentrations of chemical present, and calculate the equilibrium concentrations of the chemicals present. As the tool is developed, additional unit operations will be added to enable the simulation of a metal plating line.

Future work includes the evaluation of the environmental impacts associated with the chemicals present in the generated wastes, as well as methods can that be employed by facilities to reduce the quantity of, or hazards associated with the generated wastes.

References

Barrett, W.M., and Herten, P. (2003), Implementation of the US Environmental Protection Agency's Metal Finishing Facility Pollution Prevention Tool (MFFP2T), AESF / US EPA Conference for Environmental & Process Excellence, Daytona Beach.

CAPE-OPEN Project Team (2000), *Conceptual Design Document (CDD2) for CAPE-OPEN Project*

Morel , F.M.M., and Hering, J.G, (1993) *Principals and Applications of Aquatic Chemistry*, John Wiley and Sons, New York.

OPC Foundation (undated), What is OPC?, webpage at: *http://www.opcfoundation.org/01_about/01_whatis.asp*

Westerburg, A.W., Hutchinson, H.P., Motard, R.L., and Winter, P. (1979) *Process Flowsheeting*, Cambridge University Press, Cambridge.

D. M. Young, and H. Cabezas, (1999) Designing sustainable processes with simulation: the waste reduction (WAR) algorithm, *Computers and Chemical Engineering*, **23(10):**1477.

