CHEMICAL MANUFACTURING PROCESS & PRODUCT FORMULATION

OVERVIEW: Chemical manufacturing is the process through which a chemical is synthesized from raw materials or other chemical feedstocks. Product formulation is the process by which chemical products, composed of one or more ingredients, are prepared according to the product formula. This module: (1) describes the process for manufacturing the chemicals in the use cluster; and (2) describes the chemical product formulation process, if applicable. In both cases, the descriptions focus on the industrial or laboratory means of synthesis, the necessary starting materials and feedstocks, by-products and co-products, isolated or non-isolated intermediates, and relevant reaction conditions (e.g., temperature, pressure, catalyst, solvents, and other chemicals).

GOALS:

- Describe the processes for manufacturing chemicals in the use cluster.
- Describe the process for formulating chemical products used in the use cluster, if applicable.
- Compile chemical manufacturing and product formulation data to be used by subsequent modules if the impacts of these up-stream processes are being evaluated in a CTSA.

PEOPLE SKILLS: The following lists the types of skills or knowledge that are needed to complete this module.

- Knowledge of chemical feedstocks, synthetic chemical reaction catalysts, and reaction conditions.
- Understanding of chemical manufacturing processes, including both batch and continuous processes, as well as chemical equilibria, kinetics, and heat and mass transfer.

Within a business or DfE project team, the people who might supply these skills include a chemist and a chemical or process engineer. Vendors of the chemicals or chemical formulations may also be a good resource.

DEFINITION OF TERMS:

Catalyst: A substance that accelerates a chemical reaction but which itself is not consumed in the reaction.

Chemical By-product: An unintended chemical compound that is formed by a chemical reaction.

Chemical Intermediate: A chemical substance that is formed during the reaction and then undergoes further reaction to produce a product.

Chemical Product: In a CTSA, refers to products in the use cluster composed of one or more chemicals for which product formulation data must be obtained.

Chemical Reaction: The process that converts a substance into a different substance.

Feedstock: A raw material, pure chemical, or chemical compound that is used to synthesize a chemical.

Unit Operation: A process step that achieves a desired function.

APPROACH/METHODOLOGY: The following presents a summary of the approach or methodology for describing the chemical manufacturing processes and product formulation methods of chemicals or chemical products. Methodology details for Steps 3, 4, and 9 follow this section.

Chemical Manufacturing

Step 1: Obtain chemical information, including CAS RNs, synonyms, melting points, and boiling points from the Chemical Properties module.

Step 2: Determine the primary industrial mode of synthesis for each chemical in the use cluster (refer to data sources in Table 5-5).

Step 3: Develop a chemical manufacturing process flow diagram for the primary mode of synthesis. The diagram should identify the major unit operations and equipment, as well as all input and output streams (see Methodology Details for an example chemical manufacturing process description).

Step 4: Identify any chemical intermediates, catalysts, feedstocks, and chemical products or by-products involved in the synthesis that have the potential for release.

Product Formulation

Step 5: Obtain chemical product formulation data for any chemical products being evaluated in the CTSA from the Performance Assessment module. When proprietary chemical products are being used, only generic formulations may be available.

Step 6: Determine the primary industrial method of formulation for each chemical product being evaluated. Mixing operations, with or without the addition of heat or pressure, are typical manufacturing processes for product formulations.

Step 7: Develop a process flow diagram for the primary industrial method of formulation. The diagram should include the unit operations, material flows, and equipment used in the formulation process. If a chemical reaction occurs in the formulation process, determine if any special reaction conditions are required (e.g., the presence of heat, cooling, a catalyst, etc.). If a product is formulated by mixing only (e.g., does not involve chemical reactions), determine if any special conditions (e.g., heat, pressure, etc.) are required to get ingredients into solution. This information can be used to evaluate the energy impacts of the alternatives.

Step 8: Identify any chemical intermediates, catalysts, feedstocks, and chemical products or by-products involved in the product formulation process that have the potential for release.

Transferring Information

Step 9: Provide the following information to the modules listed below:

- Energy usage resulting from the chemical manufacturing and product formulation processes (e.g., heat, pressure, etc.) to the Energy Impacts module.
- Material streams usage resulting from the chemical manufacturing or product formulation processes (e.g., chemical feedstocks, catalysts, etc.) to the Resource Conservation module.

METHODOLOGY DETAILS: This section presents the methodology details for completing Step 3, 4, and 9 from the Chemical Manufacturing section above.

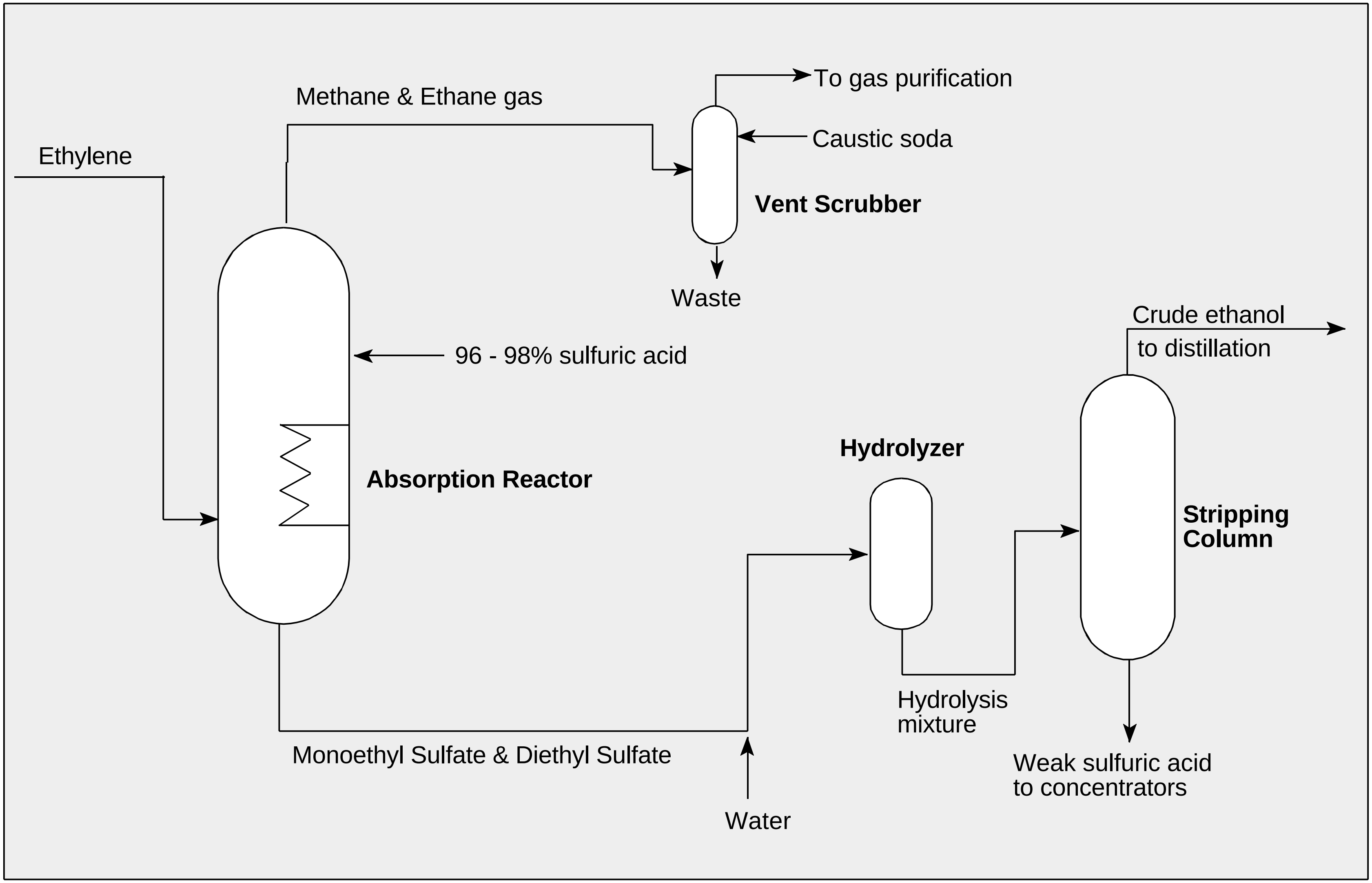
Details: Steps 3 and 4, Example Description of Chemical Manufacturing Process

The following description of the synthetic preparation of ethanol by indirect hydration is an example of the chemical manufacturing process description developed in Steps 3 and 4. The process information was gathered from the data sources listed in the Table 5-5.

<u>Indirect Hydration of Ethanol</u>

The preparation of ethanol from ethylene using sulfuric acid is a three step hydration process as discussed below. A flow diagram for this process is shown in Figure 5-2.

FIGURE 5-2: PROCESS FLOW DIAGRAM FOR THE MANUFACTURE OF ETHANOL BY INDIRECT HYDRATION



Step 1: Formation of monoethyl sulfate and diethyl sulfate by the absorption of ethylene in concentrated sulfuric acid.

$$CH_2 = CH_2 + H_2SO_4 \rightarrow CH_3CH_2OSO_3H$$
(Ethylene) (Sulfuric Acid) (Monoethyl Sulfate)

$$2\ CH_2 = CH_2 + H_2SO_4 \rightarrow (CH_3CH_2O)_2SO_2$$
(Ethylene) (Sulfuric Acid) (Diethyl Sulfate)

Step 2: Formation of ethanol by hydrolysis of ethyl sulfates.

$$CH_3CH_2OSO_3H + H_2O \rightarrow CH_3CH_2OH + H_2SO_4$$
(Monoethyl Sulfate) (Water) (Ethanol) (Sulfuric Acid)

$$(CH_3CH_2O)_2SO_2 + 2\ H_2O \rightarrow 2\ CH_3CH_2OH + H_2SO_4$$
(Diethyl Sulfate) (Water) (Ethanol) (Sulfuric Acid)

$$(CH_3CH_2O)_2SO_2 + CH_3CH_2OH \rightarrow CH_3CH_2OSO_3H + (CH_3CH_2)_2O$$
(Diethyl Sulfate) (Ethanol) (Monoethyl Sulfate) (Diethyl Ether)

Step 3: Reconcentration of the dilute sulfuric acid.

The primary input streams for this process are the hydrocarbon feedstock containing 35-95 percent ethylene, methane, and ethane; 96-98 percent sulfuric acid, and water.

The adsorption is carried out in a column reactor at 80 ^oC and 1.3-1.5 MPa of pressure where the ethylene feedstock is adsorbed in an exothermic reaction with the sulfuric acid. The column is cooled to reduce the reaction temperature and to limit corrosion problems. The hydrolysis of the ethyl sulfates in the second step of the process is done using just enough water to produce a 50-60 percent sulfuric acid solution. The resulting mixture is separated by a stripping column to yield sulfuric acid and a gaseous mixture of alcohol, ether, and water. The gaseous mixture is mixed with water and then distilled until pure. Finally, the sulfuric acid is then reconcentrated using a reboiler and a two stage vacuum evaporation system until the concentration is above 90 percent.

The primary output streams and by-products of this reaction are the following:

- Ethanol (product).
- Dilute 50-60 percent sulfuric acid.
- Scrubber waste containing the unreacted methane and ethane as well as any other gases present.
- Diethyl ether (by-product).

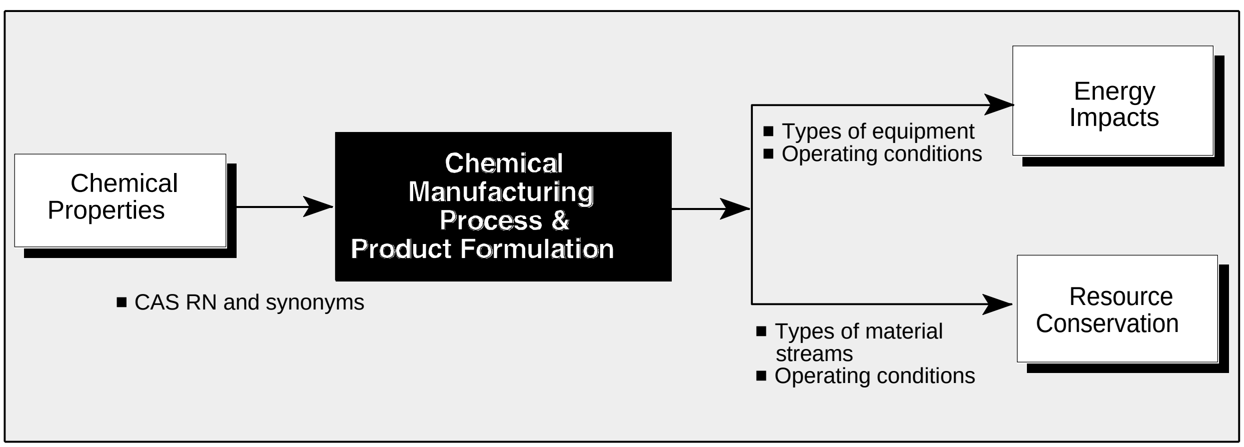
The intermediate compounds of monoethyl sulfate and diethyl sulfate are also present, although they are not waste streams, because they are consumed by the process.

Details: Step 9, Transferring Information

Past CTSAs have not quantitatively evaluated the chemical manufacturing and product formulation processes. Instead, attention has focussed on the relative effects of up-stream processes on energy and other resources consumption. If the effects of up-stream processes on human health and environmental risks are being quantified in a CTSA, the identities of chemical intermediates, catalysts, feedstocks, and chemical products or by-products are transferred to the Chemical Properties module and other modules that ultimately feed into the risk characterization. Process flow diagrams are transferred to the Workplace Practices & Source Release Assessment module.

FLOW OF INFORMATION: In a CTSA, this module receives information from the Chemical Properties module and transfers information, if desired, to the Energy Impacts and Resource Conservation modules. Example information flows are shown in Figure 5-3. This module could also transfer information to other modules if these processes are being fully and quantitatively evaluated. For example, chemical intermediates released during chemical manufacturing process could be evaluated in the hazards summary modules.

FIGURE 5-3: CHEMICAL MANUFACTURING PROCESS & PRODUCT FORMULATION MODULE: EXAMPLE INFORMATION FLOWS



ANALYTICAL MODELS: None cited.

PUBLISHED GUIDANCE: None cited.

DATA SOURCES: Table 5-5 lists data sources for both chemical manufacturing processes and product formulation methods.

TABLE 5-5: SOURCES OF CHEMICAL MANUFACTURING PROCESS AND PRODUCT FORMULATION INFORMATION	
Reference	**Type of Data**
HSDB®. Hazardous Substance Data Bank (HSDB). Updated Periodically.	Contains brief summaries of chemical manufacturing processes.
Kirk-Othmer Encyclopedia of Chemical Technology. Updated Periodically.	Comprehensive source of chemical synthesis processes.
Ullmann, Fritz. 1985. *Ullmann's Encyclopedia of Industrial Chemistry*.	Comprehensive source of chemical synthesis processes.

Note: References are listed in shortened format, with complete references given in the reference list following Chapter 10.