Define product and feed

From processdesign

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Introduction

A key step in the initial phases of chemical process design is the project definition. Along with the customer definition and location of the facility, the definition of the key feeds and products is a key starting step upon which further decisions are built (Towler and Sinnot, 2013). If implementing a new design, key feeds and products should be compared against a similar existing plant or process (Towler and Sinnot, 2013). Both feed and product specifications are found in the Design Basis, a non-exhaustive document containing key information and details of the plant and process.

Although it is a non-exhaustive document, creating the design basis is the most important step in starting a process design. The way in which this is approached involves taking a customer's needs and specifications and translating these into a working design basis. This design basis takes the customer's needs and uses them to make a very specific statement of what problem must be solved. The design basis will generally contain information about the rate of production needed as well as any relevant purity specifications for the primary product. Numerous other pieces of information that impact or constrain the design are included, such as: production units to be used, design codes that are to be followed, raw materials details, plant site information(climate data, infrastructure, land availability, etc), and utilities information(cost, availability, etc). The design basis is created, refined, and shared with and reviewed by the client, before the actual design starts.

Primary Raw Materials

The definition of raw materials on the Design Basis is located in Section 5 (see image). There are 6 main categories: Feedstock name and grade, MSDS form number, Feedstock availability, Feedstock price, Known feedstock impurities, and Additional specifications. It is of vital importance to recognize that, when deciding upon feed specifications, stoichiometry should be considered, along with safety, yield, and environmental hazards (Biegler et al., 1997). It is important to recognize that the raw materials typically contribute the most to the overall cost of production. Therefore, the choice of raw material can represent an area for optimization and monetary saving. An example Raw Material section of the Design Basis is shown below.

Table 1: Example Raw Materials Section (You, 2015).

Feedstock Name Feedstock Grade				
MSDS Form Number				
Feedstock Availability Metric tons/yr Metric tons/day Other				
Feedstock Price($/kg)				
Known feedstock impurities	Name, ppm	Name, ppm	Name, ppm	Name, ppm
Additional Specifications				

Each component of the feed, once decided upon, must be entered in the Design Basis section:

Feedstock name and grade

In this section, the the name of each component of the feed is entered. Along with the generic name of the compound, its formal chemical name, as well as its grade, should be included. No feedstock available in industry will have 100% purity. The most common grade will be "technical" or "industrial". There is also a "laboratory" or "reagent" grade (higher purity), however, it is less common and more expensive.

MSDS form number

The MSDS (material safety data sheet) is an important tool to have when dealing with any material, as it contains key information that can help inform safe decisions regarding the substance. MSDSs contain key physical data about a compound, such as flash point, melting point, boiling point, etc. There is also information on storage and disposal methods. Sources such as Perry's Chemical Engineers' Handbook also contain information about flammability hazards of many chemicals and can be used in conjunction with an MSDS to help decision-making (Seider et al. 2004). In the MSDS form number section, the specific MSDS number of each component must be listed so as to be readily available in case more information is requested.

Feedstock availability

The availability of each feedstock must be recorded. Feedstock availability can be a determining factor when deciding upon a plant capacity. Generally, the availability and price of the necessary feedstock will depend on site location, and as such, feedstock availability is considered when choosing a plant location (Towler and Sinnot, 2013). Whether feedstock availability is recorded on a per year or per day basis depends primarily on the use frequency of each material. This information is dependent on the overall production rate of the facility.

Feedstock price

The price of each material is listed in this sub-section. This information is highly relevant when completing the economic analysis. It is important to note that feedstock price is highly dependent on quantity purchased, with larger purchases having a lower cost per unit. Often, quotations for bulk chemical prices must be obtained directly from suppliers after giving them an approximation of how much would be purchased and for how long.

Known feedstock impurities

Along with the general feedstock grade (recorded in the Feedstock name and grade sub-section), the specific known impurities are recorded in this section. The name of each compound (commonly water, minerals, etc.) is recorded along with their concentrations in ppmw. The impurities are listed with the sale of the feedstock product.

Additional specifications

Any additional pertinent information about the feedstock is listed in this section. Examples include potential alternatives sources or uses.

Primary Products

The Primary Products are defined in Section 4 for the Design Basis (Please see example image below). There are 6 important subsections that must be completed within the design basis when defining the products: product name and grade, MSDS form number, production rate, product purity, product shipment mode, and additional specifications.

Each individual product that will result from the process, including wastes and side products, must be entered in the primary products section of the Design Basis.

Table 2: Example Primary Products Definition Section (You, 2015).

Product Name Product Grade				
MSDS Form Number				
Production Rate Metric tons/yr Metric tons/day Other				
Product Purity(wt%)				
Product Shipment Mode				
Additional Specifications				

Product Name & Grade

In this section of the design basis, the name of each product formed in the process is entered. First will be the primary desired product followed by any major side products or important waste products formed. Additionally, the desired purity (or grade) of each of these products should be specified. For example, if the product is completely pure, it would be 100% grade. However, if the process creates Hydrochloric Acid in a 30% aqueous solution with water as a stabilizer, then the grade would be 30% and so on. Properly defining side products and wastes is important to allow appropriate decisions to be made for waste processing and for choosing how best to deal with any side products. Typically, grades close to 100% are not attainable without excessive processing and added cost of production. Therefore, lower grades are produced to keep cost of production from inhibiting profit while also still meeting specifications.

MSDS Form Number

It is critical that the MSDS form number for any products be included in the design basis. As previously mentioned, the MSDS contains crucial information about about a substance including, but not limited to, safety/hazards information, actions to take in case of a spill/emergency, first aid measures, storage procedures, and basic material properties. This information is important to the health and safety of employees and must be available for reference at any time throughout the design process. In order to have this information readily accessible, the MSDS form numbers must be included for each product in this section.

Production Rate

For any particular chemical process design, the design team is typically given a specified level of production output from which the level of feedstock input is calculated. In other cases, there is a specified level of inputs available for use. If this is the case, then the production rate should be derived from material balances calculated using the stoichiometry of the reaction(s) or levels of inputs available in any given time period (day, week, year, etc.) multiplied by an efficiency factor. As an alternative, the final production rate can be obtained by looking at the output streams in the stream tables after simulating your process in specialized software (Turton et al., 2003).

The rate of product formation should be listed at both a daily and yearly rate, in order to allow for ease of calculations later when computing process economics. The production rate can be listed in other forms as well if they are critical to the design of the plant. For example, if the design problem is given with a desired weekly production rate, then a weekly production rate should be listed here, in addition to a daily and yearly one.

Product Purity

The product purity is the same as the product grade, listed here as a weight percentage (100% is a pure substance), unless additional purity levels are needed, in which case the most pure is listed here (grade then lists the required purity level and each diluted level in addition). The product purity is critical in process formulation in order to define the desired level and efficiency of separation processes needed within the process, which heavily impacts the cost. The product purity will also determine the price at which it can be sold on the market, as well as its potential uses (e.g. high purity laboratory grade chemicals).

Product Shipment Mode

Product shipment mode specifies how the product will be moved from production to distribution centers or customers. This can be largely influenced by the location of the plant. In this section, additional specifications for transport safety as well as handling requirements should be clearly laid out to ensure safe and proper transportation.

Additional Specifications

In this section, any further pertinent information to the process design or information given within the design statement should be listed. The main purpose of this section is to ensure that the main requirements for the process design are all clearly laid out within one easily referenced document. To that end, information that does not fit in any of the other sections can be placed here.

Information Gathering

Gathering the information to complete the primary products and raw materials forms will generally require the use of several sources. One challenge to gathering this data is that some of it isn't well tabulated, such as feedstock impurities and availability. However, there are good places to start when searching for the necessary information.

The MSDS form number for a chemical can be found using the Iowa State University MSDS database. Feedstock availability and price will largely depend on the location of a plant, so information will be location-specific. Furthermore, many companies do not publish a set price for a compound per unit mass. Rather, they give out quotes based on factors such as volume purchased. Some resources to consider for raw material prices are Chemical Week, The Plastics Web, and Ullman's Encyclopedia of Industrial Chemistry. To gather information on feedstock availability, consider contacting distributors, comparing your process to other, similar ones, or using existing data on chemical availability. To find known feedstock impurities, the EPA can be a valuable source of information as well as companies selling the chemical of interest. Product shipment mode can be obtained using common practices information or the safety information on a chemical's MSDS. A simple google search can often yield the necessary information.

Several other sources of information to consider using are: ChemNet, ChemCompass, SigmaAldrich, and the ICIS Chemical Business.

Case Studies

Case Study 1

As a case study, consider a plant which requires 50,000 tonnes/year of 37% formaldehyde in water (containing 8-12 wt% methanol as a stabilizer). Shown below is the primary products and raw materials definition of this process.

4 Primary Products

Product Name Product Grade	Formaldehyde 37%
MSDS Form Number	18508
Production Rate Metric tons per year Metric tons per day Other units	 47,000 129
Product Purity (wt%)	37%
Product shipment mode	
Additional Specifications	8-12% methanol (Stabilizer)

Figure 1: Primary products definition. Taken from Team Born Sinner's (written by Sean Kelton, Michael Gleeson, Thomas Considine and James Xamplas) final report for ChE 351 with J. Cole. Report was submitted on 11/27/13

5 Primary Raw Materials
(Attach additional sheets if needed)

Feedstock name Feedstock grade	Methanol Pure	Oxygen Air	Iron Molybdenum Catalyst Pure	Steam Lab grade
MSDS form number	18510	N/A	12360	N/A
Feedstock availability Metric tons per year Metric tons per day Other units				
Feedstock price ($/kg) (Default: open market price)	$323/MT	N/A	$2.50/kg	TBD

Figure 2: Raw materials definition. Taken from Team Born Sinner's (written by Sean Kelton, Michael Gleeson, Thomas Considine and James Xamplas) final report for ChE 351 with J. Cole. Report was submitted on 11/27/13

Case Study 2

For a second case study, consider a plant producing 100 MMscfds of hydrogen from methane gas using steam methane reforming. The required feedstock for this process is water and methane. The products are carbon dioxide, carbon monoxide, and hydrogen. The balanced equation for steam methane reforming is shown below:

$$CH_4 + H_2O \rightleftharpoons 3H_2 + CO$$

For this case study, the carbon monoxide is converted to other substances (namely, carbon dioxide, methane, and water) using water-gas shift reactors as well as methanation, so it does not appear in the products section. The raw materials and primary products definition are shown below.

Feedstock name Feedstock grade	Methane (CH_4) Industrial		Water (H_2O)	
MSDS form number	1070		W0600	
Feed Stock Availability Metric tons per year Metric tons per day Other Units	24hr/days, 350 days/yr 341,000 975 --		24hr/days, 350 days/yr 383,000 1095 --	
Feedstock Price ($/tons)	240		3	
Known feedstock impurities	Name	ppm (molar)	Name	ppm
	Nitrogen Argon CO_2 C_2H_6	1-5 1-5 1-5 1-5	Barium Fluoride Nitrate	2 4 10
Additional specifications				

Figure 3: Raw materials definition. Taken from team H-bombs(written by John Plaxco, Vincent Kenny, Spencer Saldana, and Erik Zuehlke) Memo 1 for ChE 352 with professor Fengqi You in winter quarter 2015.

Product name Product grade	Hydrogen (H_2) 99.99	Carbon Dioxide (CO_2) Side/Waste Product
MSDS form number	1009	1005
Production Rate Tons per year Tons per day Other Units	24hr/days, 350 days/yr 83,000 237 100 MMSCFD	-- -- -- --
Product Purity (wt%)	99.99	Side/Waste Product
Product shipment code	Compressed, Explosive Gas	N/A
Additional specifications		

Figure 4: Primary products definition. Taken from team H-bombs(written by John Plaxco, Vincent Kenny, Spencer Saldana, and Erik Zuehlke) Memo 1 for ChE 352 with professor Fengqi You in winter quarter 2015.

Conclusion

Within the Design Basis, the definition and description of both the product and feed streams is of utmost importance. Included in these sections are the names of the components, as well as their prices and key characteristics (i.e., chemical purity and grade, MSDS information, etc.). The product and feed definition is essential in both the initial and final stages of plant and process design as it serves as a starting point for facility design. Additionally, it can be used as a reference for all of the key components in the design.

References

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