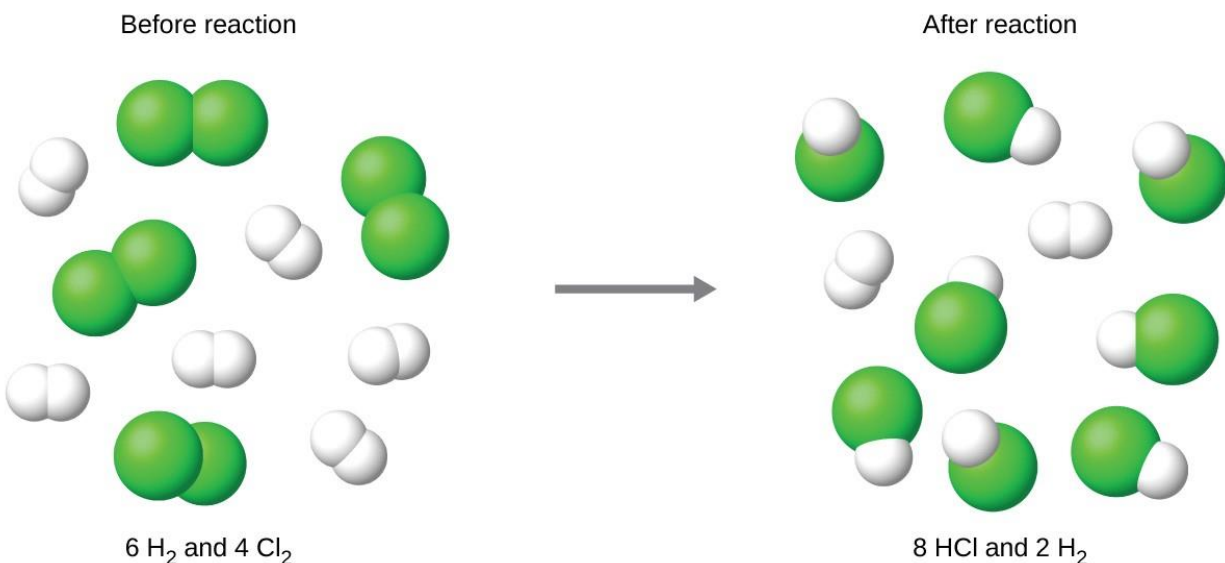


Conversion Efficiency, Selectivity, and Yield in the Chemical Industry

In the chemical industry, the economic viability of a process is paramount. It is insufficient to merely demonstrate that a reaction can proceed; one must quantify its efficiency in transforming valuable raw materials into desired products. This requires a precise set of metrics that describe the consumption of reactants and the formation of products. This chapter defines and interrelates the three fundamental performance measures for any chemical process: **Conversion**, **Selectivity**, and **Yield**. A thorough understanding of these concepts is essential for the design, optimization, and economic analysis of chemical reactors.



1. Conversion (X_a)

Conversion quantifies the extent to which a reactant is consumed in a chemical reaction.

Definition: The conversion of a reactant A is the fraction (or percentage) of that reactant fed to the reactor that is consumed by the reaction.

The general expression for the conversion of species A is given by:

$$X_A = \frac{\text{Moles of A consumed}}{\text{Moles of A fed}}$$

This can also be written in terms of molar flow rates (F_j) for continuous-flow systems:

$$X_A = \frac{F_{A,\text{in}} - F_{A,\text{out}}}{F_{A,\text{in}}}$$

where:

- $F_{A,\text{in}}$ is the molar flow rate of A into the reactor.
- $F_{A,\text{out}}$ is the molar flow rate of A leaving the reactor.

Conversion is a measure of reactor performance and reaction extent. It ranges from 0 (no reaction) to 1 (or 100%, complete consumption). The choice of which reactant's conversion to report is often based on its economic importance or its status as the limiting reactant.

Ex: A reactor feeds 1000 mol of A. After reaction, 300 mol of A remain unreacted. Calculate the conversion of A.

Sol:

Feed = 1000 mol A; unreacted = 300 mol.

Reacted = 1000 – 300 = **700 mol**.

Conversion = 700/1000 = 0.70 = 70.0%

2. Selectivity ($S_{\{B/A\}}$)

In complex reaction networks, a consumed reactant can follow multiple pathways to form different products. **Selectivity** is the measure that quantifies the distribution of products from the consumed reactant.

Definition: Selectivity toward a desired product B with respect to a reactant A is the ratio of the amount of B formed to the amount of A that was consumed to produce B .

A more practical and universally applicable definition accounts for the stoichiometric coefficients of the desired reaction:

$$\text{Selectivity (\%)} = \frac{\text{moles of desired product}}{\text{moles of all products from the reacted reactant}} \times 100$$

Ex: In the oxidation of ethylene, 30 mol of ethylene react. 24 mol of ethylene oxide (desired) and 6 mol of CO_2 (undesired) are produced. Determine selectivity to ethylene oxide.

Sol:

30 mol reacted \rightarrow 24 mol ethylene oxide (desired), 6 mol CO_2 (undesired).

Total products = 24 + 6 = 30.

Selectivity = 24 / 30 = 0.8 = 80.0%.

3. Yield

While selectivity measures the efficiency *after* reaction has occurred, **Yield** measures the overall success of the process from the initial feed.

Definition: The yield of a desired product B with respect to a reactant A is the ratio of the amount of B actually formed to the maximum theoretical amount of B that could be formed if *all* of the fed reactant A were converted exclusively to B according to the desired reaction.

The yield is given by:

$$\text{Formula: } Y_D = \frac{\text{moles of desired product D formed}}{\text{maximum possible moles of D}}$$

Yield represents the overall effectiveness of the process in utilizing the feedstock. It is the metric most directly linked to raw material costs and is often the key performance indicator (KPI) reported to management.

Ex: A factory uses 1000 kg of a feedstock containing reactant A. After processing, they recover 750 kg of the desired product B. The maximum theoretical amount of product B that could be made from the 1000 kg of feedstock is 900 kg. What is the overall yield of the process?

Solution

1. Identify the values:

1. Actual amount of product B formed = 750 kg
2. Maximum theoretical amount of product B = 900 kg

2. Use the formula for overall yield

$$\text{Overall Yield} = \frac{\text{Actual amount of B}}{\text{Maximum theoretical amount of B}} \times 100\%$$

3. Calculate the yield:

$$\text{Overall Yield} = \left(\frac{750 \text{ kg}}{900 \text{ kg}} \right) \times 100\% = 83.3\%$$

This means that the process was 83.3% successful in converting the final desired product.

This means that the process was 83.3% successful in converting the initial feedstock into the final desired product.

4. The Fundamental Relationship: Yield, Conversion, and Selectivity

Yield is directly dependent on both conversion and selectivity. A simple formula can show how they are connected:

Yield = Conversion x Selectivity

This formula highlights a crucial trade off in chemical processes:

- You can have a high conversion but a low yield if selectivity is poor, meaning many undesired byproducts were formed.
- You can have high selectivity, but a low yield if the conversion is low, meaning not enough reactant was consumed.

Example of the relationship

Consider a reaction with 100 moles of reactant A.

- **Conversion (X):** 90% of A is consumed. (90 moles reacted)
- **Selectivity (S):** Of the 90 moles that reacted, 80% formed the desired product B, and 20% formed an undesired byproduct C.
- **Yield (Y):**
 - **Moles of B formed:** 90 moles * 80% = 72 moles
 - **Maximum possible moles of B:** If 100 moles of A reacted completely, 100 moles of B would have been formed (assuming a 1:1 ratio).

$$\text{Yield of B: } \frac{72 \text{ moles B}}{100 \text{ moles max B}} = 0.72, \text{ or } 72\%$$

Notice that the final yield (72%) is the product of the conversion (90%) and the selectivity (80%)

Optimizing a reaction

The interplay between these three factors is the basis for reaction optimization. A chemical engineer must consider the following to maximize profit and efficiency:

- **Maximize desired product:** This requires finding a balance between pushing conversion as high as possible without sacrificing selectivity.
- **Control reaction conditions:** Temperature, pressure, catalysts, and residence time all affect the rate of competing reactions, influencing both conversion and selectivity.
- **Analyze economic factors:** The cost of separating byproducts versus the value of the desired product determines the most profitable operating conditions. In some cases, a lower conversion might be more profitable if it leads to significantly higher selectivity, reducing downstream separation costs.

Importance in Industry

In large-scale production, such as the manufacturing of fertilizers, plastics, fuels, and pharmaceuticals, even small improvements in yield or conversion can result in significant cost savings and reductions in waste. Understanding and optimizing these parameters helps in:

- Minimizing raw material costs.
- Improving process safety and control.
- Reducing environmental emissions and waste.
- Enhancing profitability and competitiveness.

This document explores these concepts in depth, including their definitions, calculations, industrial relevance, and practical applications.

For example, in methanol production from CO and H₂, the reaction does not go to completion. The unreacted gases are separated and sent back to the reactor, increasing overall conversion and reducing waste.