Yield

In chemistry, **yield**, also referred to as **reaction yield**, is the amount of product obtained in a chemical reaction. The **absolute yield** can be given as the weight in grams or in moles (**molar yield**). The **percentage yield** (or **fractional yield** or **relative yield**), which serves to measure the effectiveness of a synthetic procedure, is calculated by dividing the amount of the obtained desired product by the **theoretical yield** (the unit of measure for both must be the same):

Can be simply put as

$$\text{percent yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

The theoretical yield is the amount predicted by a stoichiometric calculation based on the number of moles of all reactants present. This calculation assumes that only one reaction occurs and that the limiting reactant reacts completely. However, the actual yield is always smaller (the percent yield is less than 100%), often very much so, for several reasons:

- Many reactions are incomplete and the reactants are not completely converted to products. If a reverse reaction occurs, the final state contains both reactants and products in a state of chemical equilibrium.
- Two or more reactions may occur simultaneously, so that some reactant is converted to undesired side products.
- Losses occur in the separation and purification of the desired product from the reaction mixture.

- Impurities are present in the starting material which do not react to give desired product

The ideal or *theoretical yield* of a chemical reaction would be 100%, an ideal that is never reached. According to *Vogel's Textbook of Practical Organic Chemistry*, yields close to 100% are called *quantitative*, yields above 90% are called *excellent*, yields above 80% are *very good*, yields above 70% are *good*, yields above 50% are *fair*, and yields below 40% are called *poor*. These names are arbitrary and not universally accepted, and depending on the nature of the reaction in question, these expectations may be unrealistically high. Yields may appear to be 100% or above when products are impure, as the measured weight of the product will include the weight of any impurities.

Purification steps always lower the yield, through losses incurred during the transfer of material between reaction vessels and purification apparatus or imperfect separation of the product from impurities, which may necessitate the discarding of fractions deemed insufficiently pure. The yield of the product measured after purification (typically to >95% spectroscopic purity, or to sufficient purity to pass combustion analysis) is called the *isolated yield* of the reaction. Yields can also be calculated by measuring the amount of product formed (typically in the crude, unpurified reaction mixture) relative to a known amount of an added internal standard, using techniques like gas / liquid chromatography, or NMR spectroscopy. A yield determined using this approach is known as an *internal standard yield*. Yields are typically obtained in this manner to accurately determine the quantity of product produced by a reaction, irrespective of potential isolation problems. Additionally, they can be useful when isolation of the product is challenging or tedious, or when the rapid determination of an approximate yield is desired. Unless otherwise indicated, yields reported in the synthetic organic and inorganic chemistry literature refer to

isolated yields, which better reflect the amount of pure product one is likely to obtain under the reported conditions, upon repeating the experimental procedure.

When more than one reactant participates in a reaction, the yield is usually calculated based on the amount of the limiting reactant, whose amount is less than stoichiometrically equivalent (or just equivalent) to the amounts of all other reactants present. Other reagents present in amounts greater than required to react with all the limiting reagent present are considered excess. As a result, the yield should not be automatically taken as a measure for reaction efficiency.

Conversion (in chemistry)

Conversion and its related terms **yield** and **selectivity** are important terms in chemical reaction engineering. They are described as ratios of how much of a reactant has reacted (X — conversion, normally between zero and one), how much of a desired product was formed (Y — yield, normally also between zero and one) and how much desired product was formed in ratio to the undesired product(s) (S — selectivity).

There are conflicting definitions in the literature for selectivity and yield, so each author's intended definition should be verified.

Conversion can be defined for (semi-)batch and continuous reactors and as instantaneous and overall conversion.

Assumptions

The following assumptions are made:

For multiple parallel reactions, the definitions can also be applied, either per reaction or using the limiting reaction.

- Batch reaction assumes all reactants are added at the beginning.
- Semi-Batch reaction assumes some reactants are added at the beginning; the rest is fed during the batch.
- Continuous reaction assumes reactants are fed and products leave the reactor continuously and in steady state.

Conversion

Conversion can be separated into instantaneous conversion and overall conversion. For continuous processes the two are the same, for batch and semi-batch there are important differences. Furthermore, for multiple reactants, conversion can be defined overall or per reactant.

Instantaneous Conversion

Semi-Batch

In this setting there are different definitions. One definition regards the instantaneous conversion as the ratio of the instantaneously converted amount to the amount fed at any point in time.

Let Me now introduce the next lesson by summarizing a few key points. The topic will be

General Energy Balance Equations

The principle underlying all energy balance calculations is the law of conservation of energy, which states that energy can be neither created nor destroyed. Although this law does not apply

to nuclear reactions, conservation of energy remains a valid principle for bioprocesses because nuclear rearrangements are not involved. In the followings, we will derive the equations used for solution of energy balance problems.

The law of conservation of energy can be written as:

{energy in through system boundaries} − {energy out through system boundaries} = {energy accumulated within the system}

Mass M_1 enters the system while mass M_2 leaves. Both masses have energy associated with them in the form of internal, kinetic, and potential energies; flow work is also being done. Energy leaves the system as heat *h*; shaft work *W* is performed on the system by the surroundings. This is just a general example that we will be assuming in the nest lesson as we dig deeper. We will also assume that the system is homogeneous without charge or surface energy effects.

Energy balance should systematically be realized in order to guarantee the consistency of the proposed system with long-term economic constraints.