

# Chemical Reaction Engineering - Part 1

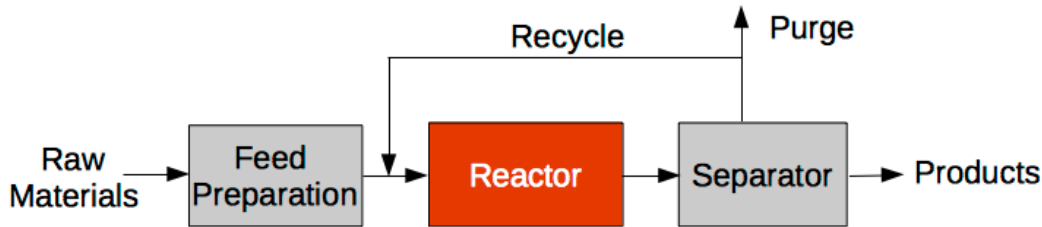
Richard K. Herz, rherz@ucsd.edu, www.ReactorLab.net

## Intro to Chemical Reaction Engineering or CRE

What is CRE? (1) Designing new chemical reactors to make products that you can sell. (2) Analyzing the performance of existing reactors so you can improve their performance. (3) Doing experiments and analyzing data in order to determine reaction rate equations. (4) Developing new catalysts to speed up desired reactions. (5) Developing new reaction pathways that minimize risk and environmental impact.

What is a chemical reactor? Not just tanks in chemical plants but also any space in which a chemical reaction takes place. In size from a single living cell to the ozone hole.

Reactors are the "heart" of a chemical process. They are where raw materials get converted into valuable products.



## Why learn CRE?

Why would you want to learn how to do Chemical Reaction Engineering?

There are lots of possible motivations, e.g.,

- get a job
- start a company that makes a product... and a lot of money
- invent a new "green" process that is sustainable and reduces waste products
- make a renewable fuel and contribute to energy independence for US

What is your motivation?

Let's go through a little scenario that might occur to you. Let's say you are shopping in the store and balking at paying the price for an expensive shampoo. You look at the bottle and wonder how much it cost to make the stuff in the bottle.

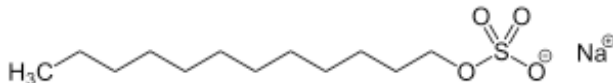
Hmmm. It's basically soap with some color and perfume. Retail for \$22 (in 2012). Can't cost more than a few cents to make. There must be a big profit margin!

You are nearing graduation and need to figure out how to pay your rent, buy food, etc. Maybe you and some friends can start a company and make a great shampoo for a better price and still make a lot of money. You have a couple engineer friends to help, an artistic friend to design the packaging, someone who can make a web store, and a friend who can sell anything to anyone. You can do this!



Wikipedia tells us that a major component of shampoo is sodium lauryl sulfate. The formula is  $\text{CH}_3(\text{CH}_2)_{11}\text{OSO}_3\text{Na}$ .

The molecule has a long carbon tail that is hydrophobic (hates water but loves oil) and a sulfate head that is hydrophilic (loves water). Such a molecule is a "surfactant."



In a mixture of oil (the oily dirt on your hair) and water (your shower) a surfactant molecule will segregate to the oil-water interface (or surface), sticking its tail in the oil and its head in the water. This reduces the energy between the oil and water phases and allows the oily dirt to be broken up into small droplets, floated off your hair, and flushed down the shower drain.

Can we make sodium lauryl sulfate? Sodium lauryl sulfate is made by sulfonation of lauryl alcohol using either oleum (concentrated sulfuric acid), chlorosulfuric acid, or sulfur trioxide gas. Lauryl alcohol is made by hydrogenation of the methyl ester of lauryl alcohol using high pressure hydrogen gas and a solid catalyst such as copper chromite.

The methyl ester of lauryl alcohol is made by transesterification of the triglyceride of lauryl alcohol by reaction with methyl alcohol (methanol) with sodium hydroxide as a catalyst. The triglyceride of lauryl alcohol is a major component of coconut oil and palm kernel oil.

Transesterification of triglycerides is also used to make biodiesel.

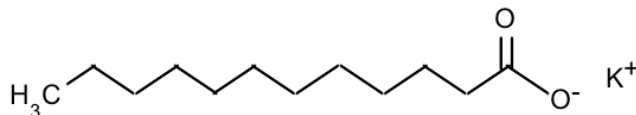
This sounds a little too ambitious for the kitchen in our apartment!

Let's make coconut oil soap for our first shampoo sample. We will buy lauryl alcohol and "saponify" it, or make it into liquid soap, by reacting it with potassium hydroxide, then finally neutralizing the soap with a mild organic acid such as citric acid.

The saponification reaction was used by our ancestors to make the first soap by reacting animal tallow (fat) and ashes from fire that contained lye (sodium hydroxide).

This process of research and evaluating and selecting options is a key characteristic of engineering, in this case chemical reaction engineering. Eventually we want to come up with a new ingredient, method of manufacture, or product that we can patent!

We will end up with the potassium salt of the carboxylic acid of lauryl alcohol (salt of lauric acid, dodecanoic acid).



Now we have a reaction to work with. The next question: where will we conduct the reaction?

That is, what type of container - what type of reactor - will we use to perform the reaction?

Since we are just getting started, it makes sense that we want to start out by making small batches of our shampoo.

We can experiment with the process, test our product on our hair, and start making some sales.

So we might consider using a stirred cooking pot for the first reactor.

**Warning:** Before deciding to carry out any process you need to check the safety of the chemicals and the process! Then double-check! A pot over an open flame is probably not a good idea.

A stirred pot is a type of reactor - a batch reactor.



We will want to see how the rate of our reaction varies with temperature and concentration of sodium hydroxide. We can design experiments, record data, analyze the results and improve our process.

Later, as our sales pick up and we settle on a good process, we will want to make larger quantities of our shampoo.

Our batch-by-batch production has many steps and is labor-intensive. We will want to see if we can develop a continuous process that uses a continuous flow reactor rather than a batch reactor.

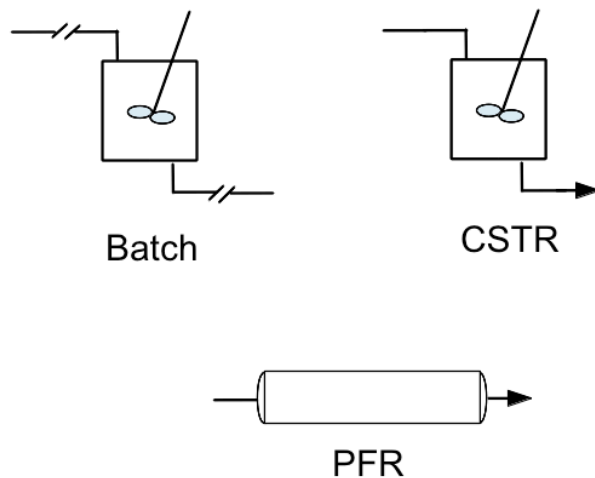
There are three basic types of chemical reactors:

- Batch reactor
- Continuous Stirred Tank Reactor or CSTR
- Plug Flow Reactor or PFR

There are also variations on each of these basic types, as we will see later. They can also be used in combinations with themselves or each other.

*Continued next page...*

We will get very familiar with these three types of reactors.



What similarities do you see between the three reactor types?

What differences do you see?

Think and come up with some ideas before you go to the next page.

*Continued next page...*

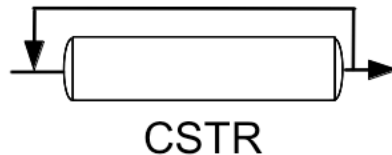
The Batch and CSTR are similar in that they are well-mixed tanks (or other containers). In contrast, fluid flows through the PFR in a plug-like manner (no radial variation in flow rate) with no mixing up- or down-stream.

The CSTR and the PFR are similar in that fluid flows continuously through them.

Batch reactors are often used for production of relatively small amounts of expensive chemicals such as pharmaceuticals.

Batch reactors that are not completely sealed that but have some components flowing either into or out of the reactor are called semi-batch reactors. Batch fermentors that use yeast to ferment sugars to ethanol give off carbon dioxide gas that flows out of the reactor.

CSTR can be approximated by a PFR with a large recycle flow. This configuration is used to get CSTR behavior when using solid catalysts. We could also stop the inlet and outlet flow and approximate a batch reactor this way with solid catalysts.



A PFR can be approximated in a couple ways:

- fluid flowing down a pipe in turbulent flow
- fluid flowing through a bed of packing, either inert packing or catalyst pellets

The later case is called a "packed bed reactor" and is usually modeled as a PFR.

The catalytic converter on an automobile can be modeled as a PFR. It is composed of many, small, parallel flow channels whose walls are coated with a porous solid catalyst.

A pipe with laminar flow is much more complicated to model than a PFR. We may do that later in the course.

Note the word "approximated" above. We never get perfect behavior or perfect solutions. Trying to do so would take an infinite amount of time and money. We want approximate solutions that are good enough for the design stage we are at (conceptual design, scale up, construction drawings, etc.)

In a batch reactor, the fluid composition changes with time. The contents are well-mixed so there are negligible spatial variations. The balance equation will be an ordinary differential equation (ODE) with time as the independent variable.

CSTRs and PFRs can be operated under steady-state conditions after they start up.

In a CSTR operating at steady-state, there are negligible variations in time and space. The balance equation will be an algebraic equation.

In a PFR operating at steady-state, there are negligible temporal variations. However, conditions vary down the reactor (e.g., reactant concentration decreases), so there are spatial variations. The balance equation will be an ODE with position down the reactor as the independent variable.

When we get to writing the equations, we will see that the balances for the batch and the PFR are similar. Can you think of an explanation for that? Hint: think of the stream flowing into the PFR as a series of batches of fluid.

The three types of reactors have their own advantages and disadvantages. Which one we pick depends on our application.

Batch reactors are good for small production runs. They are often found in pharmaceutical manufacturing plants or in biological reaction processes. They require many operating steps (fill, mix, heat, react, cool, empty, clean) for each batch and may require hiring more workers.

CSTRs and PFRs are commonly used when you want to make a large amount of product every day during a year. They are found in petroleum refineries that make gasoline and diesel fuel.

A mixer can circulate the fluid in a Batch or CSTR over heat transfer surfaces and provide good temperature uniformity. A PFR has no moving internal parts and may be cheaper to construct than would be an equivalent CSTR.

How many other advantages and disadvantages can you think of?