

# Continuously Stirred Tank Reactor, part 1 of 3

The continuously stirred tank reactor project involves the development, simplification, and analysis of a model for a physical setting that includes chemical mixing with the added complication of a chemical reaction with a temperature-dependent reaction rate. The reaction generates heat, so there is a positive feedback loop: the heat increases the reaction rate, which generates more heat, further increasing the rate. In extreme cases, this could lead to an explosive acceleration of the reaction, but here we look at a scenario where the heat generation is controlled and the result is some desired chemical end product.

The task of part 1 is to develop the model from a set of physical assumptions. In a later part of the project, the model will be nondimensionalized, which will involve replacing the original variables with dimensionless counterparts. It is helpful to use a naming convention of making all of the symbols for original dimensional quantities be capital letters and then using their lower case counterparts for the dimensionless versions. For this reason, we'll use  $T$  for time, rather than  $t$ . Since  $T$  will then be taken, we'll use  $U$  for the temperature. The temperature has to be given using an absolute temperature scale; that is, Kelvin instead of Celsius.

A mixing problem has a dependent variable that represents the amount of the solute in the mixing container. With a chemical reaction occurring, there are multiple chemicals present, including one product and at least one reactant. For now, we'll assume that we need only keep track of one of the reactants. We'll use the concentration  $C$  in moles per  $\text{m}^3$  rather than the total mass or total number of moles as the measure of how much chemical is present.

## Step 1 – Identify conserved quantities and link them to the variables $C$ and $U$

Differential equations in chemical engineering are obtained from conservation laws, with equations of the form “Rate of change of conserved quantity equals the sum of the rates of processes that increase the quantity minus the sum of the rates of processes that decrease the quantity.” Neither concentration nor temperature are conserved quantities. Instead, the conserved quantities are the amount of reactant and the heat energy. Formulas are needed to link these two quantities to the concentration and temperature. Three parameters are needed:

1. The (constant) volume  $V$ , in  $\text{m}^3$ ;
2. The density of the fluid  $\rho$ , in  $\text{kg}/\text{m}^3$ ;
3. The specific heat of the fluid  $c_p$ , in  $\text{J}/(\text{kg K})$ .

Dimensional analysis is very helpful in determining the correct way to combine parameters and variables to calculate a quantity. Dimensions can be multiplied along with the variables; for example,  $\rho c_p$  is in  $\text{J}/(\text{m}^3\text{K})$ .

## Step 2 – Construct the Model Equations

The changes in the total amount of reactant and the total amount of heat energy are determined by several physical processes:

1. Fluid flows into the reactor with flow rate  $q$  in  $\text{m}^3/\text{sec}$ . This fluid has concentration  $C_0$  and temperature  $U_0$ . The well-stirred mixture flows out of the reactor with the same flow rate  $q$ . These two flows carry their reactant amount and heat energy into and out of the reactor along with the fluid.

2. The chemical reaction proceeds at a rate proportional to the amount of reactant, with rate constant  $k$  in  $\text{sec}^{-1}$ . This reaction reduces the concentration of the reactant.
3. The chemical reaction also increases the heat energy at a rate proportional to the rate of the reaction, with proportionality constant  $Q$  in J/mole.
4. The reactor loses heat energy to the environment because its temperature  $U$  is higher than that of the environment, which we assume to be the same as the inlet temperature  $U_0$ . This cooling process occurs at a rate proportional to the difference between the reactor temperature and the environment temperature, with rate constant  $h$  in J/(K sec).

One more equation is needed to augment the two differential equations. The rate constant  $k$  is temperature dependent and is assumed to be given by the Arrhenius formula  $k = k_0 e^{-E/RU}$ , where  $E$  is the activation energy in J/mole,  $R$  is the universal gas constant in J/(mole K), and  $k_0$  represents the limiting value of the rate constant as the temperature becomes infinite. [Since the temperature is not actually infinite, the value of  $k$  at any given temperature is quite a bit smaller than  $k_0$ .] Rather than substituting this messy formula into the differential equations, it is better just to leave  $k$  in the differential equations and include the Arrhenius formula as a separate algebraic equation.

## Part 1 report

Eventually, the work of part 1 will comprise one short section of the project paper. For now, just determine the model equations and postpone the writing until these have been confirmed.