

Continuous Stirred Tank Reactor (CSTR): (Follows Middleman p. 301-306 and 340-348)

A stirred tank is the most fundamental of mixers and many common mixers from the Brabender mixer used in lab to a cup of coffee with a spoon can be considered a stirred tank under some set of approximation. Mixing in a stirred tank is complicated and not well described (Middleman p. 340-348) although the use of dimensionless numbers and comparison with literature accounts can lead to some predictive capabilities. Often stirred tanks are used as industrial reactors where a chemical component of a flow stream resides for some time in the tank and then proceeds on to other steps in a chemical process. The residence time distribution becomes a measure of the extent of a chemical reaction in this situation. For mixing one can sometimes assume a constant rate of strain in the stirred tank, Middleman p. 340-348, and the residence time distribution can then be used under this approximation, as a measure of the extent of mixing. Dead zones in a stirred tank for high viscosity fluids should be very familiar to anyone who has worked in a kitchen mixing dough with a hand mixer. Fluid motion in a stirred tank is confined to the immediate region of the mixer blades for high viscosity fluids.

In the simplest approximation that a uniform extent of mixing occurs in the stirred tank, Middleman p. 301-306, this is called the "perfect mixer". Consider a stream of butene in cyclohexane that is converted to butene epoxide by reaction with a peroxide in a CSTR. The flow rate through the tank is Q and the concentration of heptene is C_0 . The tank is at steady state meaning the volumetric in-flow equals the volumetric out-flow. The tank volume is V . The ratio of butene epoxide to butene is governed by the temperature, catalyst concentration, effectiveness of the catalyst and the residence time in the reactor. A master curve in terms of conversion at constant conditions as a function of reaction time can easily be made in the lab. Then a calculation of residence time distribution in the reactor can be directly mapped, using the lab results, to conversion ratio for the desired product. If the butene epoxide is to be used in a second CSTR to produce the final product then this conversion ratio becomes the input concentration for the second CSTR. Typically a synthetic chemical process will involve a number of CSTR's joined in this way. Then we need to determine the residence time distribution (RTD), $f(t)$, for a perfect mixer to approximate the conversion for this CSTR.

In order to determine the RTD, $f(t)$, for the CSTR we consider a simpler situation where a concentration C_0 of a component in a flow stream Q flows into a tank of volume V . At an instant of time all of the concentration C_0 is tagged red so that it can be distinguished from the other reactant in the stirred tank. We then look for the red tagged reactant in the outflow stream to determine the residence time of the reactant in the tank. The amount of tagged material that has left the tank at time " t " is given by the cumulative residence time distribution function, $F(t)$, $F(t)C_0Q$. This is related to the concentration of tagged material in the effluent stream, $QC(t)$,

$$QC(t) = F(t)C_0Q$$

so

$$F(t) = C(t)/C_0$$

Then $F(t)$ is the response, efflux, of the system to a pulse of concentration in the influx.

A material balance for the CSTR under the assumption of perfect mixing yields,

$$V \frac{dC(t)}{dt} = QC_0 - QC(t)$$

with the starting condition that the concentration of the tagged component in the effluent is 0 at $t = 0$, $C(t=0) = 0$. The solution to this differential equation is,

$$F(t) = \frac{C(t)}{C_0} = 1 - e^{-tQ/V}$$

where $V/Q = \bar{t}$ is a kind of time constant for the system. Under the assumption of perfect mixing, this time constant is the mean residence time for the CSTR, $\bar{t} = \frac{V}{Q}$. The

residence time distribution function is the derivative of the cumulative residence time distribution function,

$$f(t) dt = \frac{1}{\bar{t}} e^{-t/\bar{t}} dt$$

The function has a value at $t = 0$ of $1/\bar{t} = Q/V$ which decays exponentially with time. The function has a value at $t = 0$ because mixing is perfect, that is some material is instantaneously in the effluent at the instant material is introduced to the tank. Obviously this is not realistic. Nonetheless, the exponential approximation for a CSTR is a common assumption both in polymer processing and in the chemical process industry as a whole. It is widely used in a wide range of scientific fields as for a first approximation for quantities such as residence time in a lake or ocean or for an approximation of a drug or toxins residence in the human body since it depends only on the system volume and rate of dilution. The function can be modified for dead space using an effective volume rather than the actual volume of the system. Alternatively, tracer studies can be used to measure the mean residence time.