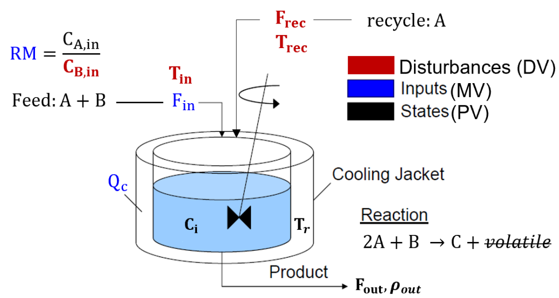

Figure 1: Schematic diagram of the CSTR and the surrounding cooling jacket.

1 Continuous Stirred Tank Reactor

Figure1 illustrates a schematic diagram of the vessel and the surrounding cooling jacket. A nonlinear exothermic and irreversible reaction, $2A+B \rightarrow C+volatiles$, takes place in the vessel, which is assumed to be always perfectly mixed.

The feed stream of mixture of reagents A and B enters the tank at the mole ratio of $RM = \frac{concentration(A)}{concentration(B)}$ and volumetric rate F_{in}. The product stream C exits continuously at the volumetric rate F_{out}, which may include some impurities of not reacted components A and B. Perfect removal of volatile components are assumed resulting in a variable outlet density (ρ_{out}). Outlet volumetric rate is calculated under assumption of constant volume of the reacting liquid. There is also a recycled line of component A from a downstream unit in the process, which is considered an external bounded disturbance.

The concentration of all components C_A, C_B, C_C together with the reactor temperature T_r are assumed as the four state variables of the system. Alternatively, the process variables (PVs) within the system consist of the four state variables, as well as the product flow rate F_{out} and density ρ_{out}, which are either directly measurable or can be estimated with high accuracy.

The feed mole ratio RM, feed flow rate F_{in}, and set point of reactor temperature $T_{r,SP}$, are considered as process manipulated variables (MVs). There is an inner PID controller on the cooling jacket loop, which receives the desired reactor temperature $T_{r,SP}$ and manipulates the cooling power Q_c.

The process is also subject to various external disturbances (DVs), which are outlined below:

- feed B concentration $C_{B,in}$ (measurable)
- feed fluid temperature T_{in} (measurable)
- recycled fluid temperature T_{rec} (unmeasurable)
- recycled fluid flow rate F_{rec} (unmeasurable)

Detailed formulation of the state transition, control input and output functions are provided below:

$$
\begin{aligned}
\frac{dC_A}{dt} &= \frac{1}{V_r}\left(F_{in}C_{A,in} + F_{out}C_A + F_{rec}C_{A,rec}\right) + G_A \\
\frac{dC_B}{dt} &= \frac{1}{V_r}\left(F_{in}C_{B,in} + F_{out}C_B + F_{rec}C_{B,rec}\right) + G_B \\
\frac{dC_C}{dt} &= \frac{1}{V_r}\left(F_{in}C_{C,in} + F_{out}C_C + F_{rec}C_{C,rec}\right) + G_C \\
\frac{dT_r}{dt} &= \frac{1}{\rho_{out}C_P V_r}\big(\rho_{in}C_{P,in}F_{in}T_{in} - \rho_{out}C_P F_{out}T_r \\
&\quad + \rho_{rec}C_{P,rec}F_{rec}T_{rec} + R_r \Delta H_r V_r + Q_c\big)
\end{aligned}
$$

where

$$
\begin{aligned}
\rho_{in} &= \frac{1}{\frac{x_{A,in}}{\rho_A} + \frac{x_{B,in}}{\rho_B}} \\
\rho_{out} &= \frac{1}{\frac{x_A}{\rho_A} + \frac{x_B}{\rho_B} + \frac{x_C}{\rho_C}} \\
C_{P,in} &= \frac{F_{in}C_{A,in}M_A}{F_{in}\rho_{in}} C_{P,A} + \frac{F_{in}C_{B,in}M_B}{F_{in}\rho_{in}} C_{P,B} \\
C_P &= x_A C_{P,A} + x_B C_{P,B} + x_C C_{P,C} \\
Fout &= \frac{\rho_{in}F_{in} + \rho_{rec}F_{rec}}{\rho_{out}}
\end{aligned}
$$

and

$$
\begin{aligned}
x_{B,in} &= \frac{1}{1 + RM\frac{M_A}{M_B}} \\
x_{A,in} &= 1 - x_{B,in} \\
x_A &= \frac{V_r C_A M_A}{V_r C_A M_A + V_r C_B M_B + V_r C_C M_C} \\
x_B &= \frac{V_r C_B M_B}{V_r C_A M_A + V_r C_B M_B + V_r C_C M_C} \\
x_C &= \frac{V_r C_C M_C}{V_r C_A M_A + V_r C_B M_B + V_r C_C M_C}
\end{aligned}
$$

and

$$
\begin{aligned}
k_r &= k_0 \; exp(-\frac{E_r}{R_g T_r}) \\
R_r &= k_r C_A C_B \\
G_A &= -2R_r \\
G_B &= -R_r \\
G_C &= +R_r
\end{aligned}
$$

and Q_c is the cooling jacket power.

Table1 summarizes all variables and parameters used in the above equations:

Var	**Description**	**Unit**	**Value**
V_r	Tank liquid volume	m^3	21.7
$C_{A,in}$	Inlet concentration of A	mol/m^3	
$C_{B,in}$	Inlet concentration of B	mol/m^3	
G_A	Generation/Consumption rate of A	mol/hr	
G_B	Generation/Consumption rate of B	mol/hr	
G_C	Generation/Consumption rate of C	mol/hr	
$C_{P,in}$	Heat Capacity of inlet fluid	$J/kg.K$	
C_P	Heat Capacity of product	$J/kg.K$	
ρ_{in}	Inlet fluid density	kg/m^3	
$x_{A,in}$	mass fraction of inlet component A	-	
$x_{B,in}$	mass fraction of inlet component B	-	
x_A	mass fraction of outlet A	-	
x_B	mass fraction of outlet B	-	
x_C	mass fraction of outlet C	-	
M_A	Molar mass of component A	g/mol	62.07
M_B	Molar mass of component B	g/mol	166.13
M_C	Molar mass of component C	g/mol	254
E_r	Activation energy		0.7×10^5
R_g	gas constant	$J/kg.K$	8.314
K_0	Reaction rate constant		
R_r	Reaction rate		
ΔH_r	Reaction heat	J/mol	32.4×10^5
ρ_A	Density of component A	kg/m^3	1110
ρ_B	Density of component B	kg/m^3	1520
ρ_C	Density of component C	kg/m^3	1160
$C_{P,A}$	Heat capacity of component A	$J/kg.K$	2386
$C_{P,B}$	Heat capacity of component B	$J/kg.K$	1197
$C_{P,C}$	Heat capacity of component C	$J/kg.K$	2306.4