For a recycle reactor the relationship between the volume and other parameters is given by $V = (R+1)F_{A-in} \int_{Rx_o/(R+1)}^{x_0} \frac{dx_A}{-r_A}$

For 'simple' kinetics such as first order reaction (under isothermal conditions), for a given volume, PFR will have higher conversion and CSTR will have a lower conversion. At low recycle ratio, the recycle reactor will behave like a PFR and at high recycle ratio, it will behave like a CSTR. At intermediate recycle ratio, the conversion in a recycle reactor will be between that of a PFR and CSTR.

However, for a few type of 'unusual' kinetics, (again, under isothermal conditions), for a given volume, a recycle reactor may not go monotonically from a PFR or a CSTR when recycle ratio is increased. We will illustrate this with an example.

Consider a liquid phase reaction A→ B, where the reaction rate is given by $-r_A = \frac{k_1 C_A}{1+k_2 C_A^2}$. The reaction is conducted at isothermal conditions and the inlet concentration of A is 1 mol/lit. The rate constants are $k_1 = 0.01\ \text{s}^{-1}$ and $k_2 = 30\ \text{lit}^2\ \text{mol}^{-2}$. The volumetric flow rate is 10 lit s^{-1}. We want to convert 95% of A. Determine the volume of the reactor, if the reaction is to be conducted in a (i) PFR (ii) CSTR (iii) Recycle reactor. For the last case, determine if there is an optimal recycle ratio, which will minimize the volume of the reactor.

Ans: For a PFR, $V = F_{A-in} \int_0^{x_0} \frac{dx_A}{-r_A}$

Q = 10 lit/s, C_{A-in} = 1 mol/lit. F_{A-in} = 10 mol/s. x_0 = 0.95.

$$-r_A = \frac{k_1 C_A}{1+k_2 C_A^2} = \frac{k_1 C_{A-in}(1-x)}{1+k_2 C_{A-in}^2 (1-x)^2} = \frac{0.01\times 1(1-x)}{1+30\times 1^2 (1-x)^2} = \frac{0.01(1-x)}{1+30(1-x)^2}$$

$$\text{Hence } \frac{1}{-r_A} = \frac{1+k_2 C_A^2}{k_1 C_A} = \frac{1+30(1-x)^2}{0.01(1-x)} = \frac{100}{(1-x)} + 3000(1-x)$$

$$\text{Volume} = F_{A-in} \int_0^{x_0} \frac{dx_A}{-r_A} = 10 \int_0^{0.95} \left(\frac{100}{(1-x)} + 3000(1-x) \right) dx$$

$$= 10\left[-100\times\ln(1-x) + 3000\times x - 1500\times x^2\right]_0^{0.95}$$

$$= 10\left[299.5732 + 2850 - 1353.8\right] = 17958 \text{ lit}$$

For CSTR,

$F_{A\text{-}in} + V(r_A)_{out} = F_{A\text{-}out}$.

CA-out = CA-in (1-0.95)=0.05 mol/lit

$$r_{A-out} = \frac{-k_1 C_{A-out}}{1+k_2 C_{A-out}^2} = \frac{-0.01\times 0.05}{1+30\times 0.05^2} = -4.6512\times 10^{-4}$$

$F_{A\text{-}out} = Q\ C_{A\text{-}out} = 10 * 0.05 = 0.5$ mol/s

$V = (F_{A\text{-}in} - F_{A\text{-}out})/(-r_{A\text{-}out})$

=20425 lit

For recycle reactor, we know the result when R = 0 and R = infinity. Let us get the answer when R = 1.

$$V = (R+1)F_{A-in} \int_{Rx_o/(R+1)}^{x_0} \frac{dx_A}{-r_A}$$

When R = 1,

$$V = (2)10\int_{0.475}^{0.95}\left(\frac{100}{(1-x)} + 3000(1-x)\right)dx = 20\left[-100\times \ln(1-x) + 3000\times x - 1500\times x^2\right]_{0.475}^{0.95}$$

$$= 20\left[1795.8 + 100\times \ln(1-0.475) - 3000\times 0.475 + 1500\times 0.475^2\right]$$

=12896 lit

When R = 2

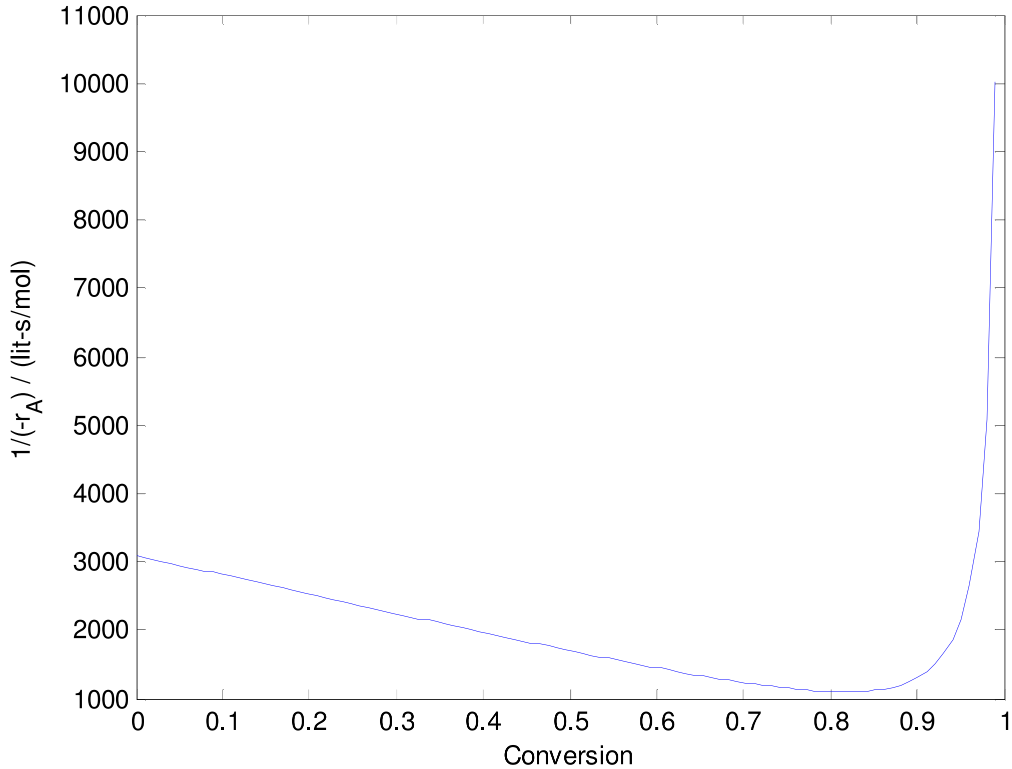
$$V = (3)10\int_{0.633}^{0.95}\left(\frac{100}{(1-x)} + 3000(1-x)\right)dx = 30\left[-100\times \ln(1-x) + 3000\times x - 1500\times x^2\right]_{0.633}^{0.95}$$

$$= 30\left[1795.8 + 100\times \ln(1-0.633) - 3000\times 0.633 + 1500\times 0.633^2\right]$$

=11915 lit

Thus, for this reaction, when the recycle ratio is changed from 0 to infinity, the volume vs recycle ratio goes is not monotonic, and it goes through a minimum.

The plot of $\frac{1}{-r_A}$ vs x is given below



A table of x vs $\frac{1}{-r_A}$ is given here (Note: Values are approximate)

X (no units)	$\frac{1}{-r_A}$ (lit-s/mol)
0	3100
0.19	2553.5
0.3990	1969.4
0.5985	1453.6
0.8075	1097
0.95	2150
1	Infinity

Thus, the minimum is between 0.8 and 0.9.

There is an optimal recycle ratio which will minimize the volume of the reactor. It can be derived analytically.

$$V = (R+1) F_{A-in} \int_{Rx_o/(R+1)}^{x_0} \frac{dx_A}{-r_A} = G(R) = \int_{Rx_o/(R+1)}^{x_0} \frac{(R+1) F_{A-in}}{-r_A} dx_A$$

To minimize the volume, set $\frac{dV}{dR} = G'(R) = 0$

To differentiate inside integral, note that if $G(R) = \int_{a(R)}^{b(R)} f(R,x)\,dx$, then

$$G'(R) = \int_{a(R)}^{b(R)} \frac{\partial f}{\partial R} dx + f(R,b)\frac{\partial b}{\partial R} - f(R,a)\frac{\partial a}{\partial R}$$

Here, b(R) = x0, a constant
a(R) = R x0 / (R+1), obviously a function of R, and

$$f(R,x) = \frac{(R+1)F_{A-in}}{-r_A}$$

Hence, $\frac{\partial f}{\partial R} = \frac{F_{A-in}}{-r_A}$, $\frac{\partial b}{\partial R} = 0$ and $\frac{\partial a}{\partial R} = \frac{x_0}{(R+1)^2}$

$$f(R,a) = \frac{(R+1)F_{A-in}}{-r_A\big|_{x=\frac{Rx_0}{R+1}}} \text{ and } f(R,b) = \frac{(R+1)F_{A-in}}{-r_A\big|_{x=x_0}}$$

Hence, for minimization of volume, G'(R) = 0, we get

$$0 = \int_{Rx_o/(R+1)}^{x_0} \frac{F_{A-in}}{-r_A} dx_A + 0 - \frac{(R+1)F_{A-in}}{-r_A\big|_{x=\frac{Rx_0}{R+1}}} \frac{x_0}{(R+1)^2}$$

We can cancel $F_{A\text{-in}}$, and one (R+1), and then re-arranging, we get

$$\frac{1}{-r_A\big|_{x=\frac{Rx_0}{R+1}}} = \frac{\int_{Rx_o/(R+1)}^{x_0} \frac{1}{-r_A} dx_A}{x_0}(R+1).$$

This can be re-written as $\frac{1}{-r_A\big|_{x=\frac{Rx_0}{R+1}}} = \frac{\int_{Rx_o/(R+1)}^{x_0} \frac{1}{-r_A} dx_A}{x_0 - \frac{Rx_0}{(R+1)}}$. i.e. The $x_{A,1}$ must chosen such that it is the average value of the integral.

Of course, if separation of the product stream is easy and economical, then optimal conditions would change. Similarly, if two reactors are acceptable, then a CSTR + PFR is better.

In our particular example, if only one reactor is acceptable, then recycle reactor is the best. Now, what is the optimal value of recycle ratio, which will minimize the volume? It depends on the final conversion desired.

Example: If the final conversion is less than 0.8, then ($1/-r_A$) vs x is a continuously decreasing function, and CSTR is the best choice. If x = 0.95, we know that a recycle reactor is the best, and we need to find the optimal R. One can obtain the values of volume vs R and if it is done with enough granularity (i.e. small steps of R) we can identify the best R. Once the R is finalized, the volume can be found.

Otherwise, the entire function can be written in terms of R, including the integration and optimization can be done.

$$V=(R+1)F_{A-in}\int_{Rx_o/(R+1)}^{x_0}\frac{dx_A}{-r_A}$$

$$V=(R+1)\times 10\times\int_{R0.95/(R+1)}^{0.95}\frac{1+k_2C_{A-in}^2(1-x)^2}{k_1C_{A-in}(1-x)}dx$$

$$=(R+1)\times 10\times\int_{R0.95/(R+1)}^{0.95}\left(\frac{1}{k_1C_{A-in}(1-x)}+\frac{k_2C_{A-in}(1-x)}{k_1}\right)dx$$

$$V=(R+1)\times 10\times\left[\frac{-1}{k_1C_{A-in}}\ln(1-x)+\frac{k_2C_{A-in}}{k_1}x-\frac{k_2C_{A-in}}{k_1}\frac{x^2}{2}\right]_{R0.95/(R+1)}^{0.95}$$

$$V=(R+1)\times 10\times\left[\begin{array}{l}\frac{-1}{k_1C_{A-in}}\ln(1-0.95)+\frac{k_2C_{A-in}}{k_1}0.95-\frac{k_2C_{A-in}}{k_1}\frac{0.95^2}{2}\\ +\ln\left(1-R0.95/(R+1)\right)-\frac{k_2C_{A-in}}{k_1}R0.95/(R+1)+\frac{k_2C_{A-in}}{k_1}\frac{\left(R0.95/(R+1)\right)^2}{2}\end{array}\right]$$

Differentiate this w.r.t. 'R' and set it to zero, and solve for R. This will be lengthy, but is doable (or use a software like Mathematica to get analytical solution, or an implementation of numerical method such as *fminsearch* in Matlab). That recycle ratio is the optimal one.
For this problem, the function *fminsearch*, gives R-best = 2.7350. The corresponding volume is 11,795 lit.