Reactor Design I: 2. Isothermal Reactor Design

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To design a reactor, we must solve the general mole balance given by: $\frac{dN_A}{dt} = F_{A0} - F_A + \int^V r_A dV$

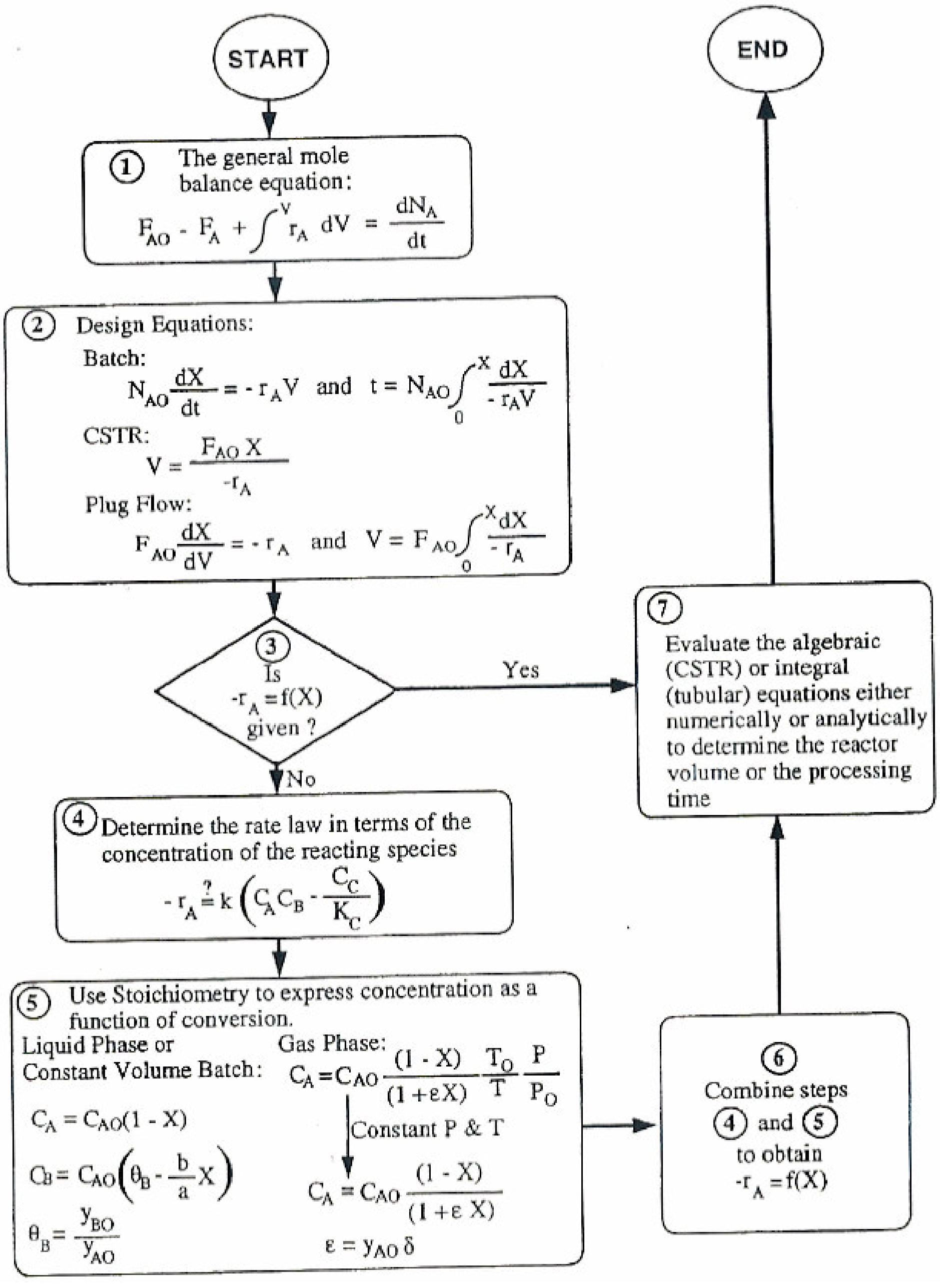
This balance is general in that it can be applied to ALL the reactor types (CSTR, PFR, Batch), and is valid for both steady and unsteady state situations.

[Exercise 1: simplify the general balance to the three specific forms for the three basic reactor types using physical justification.]

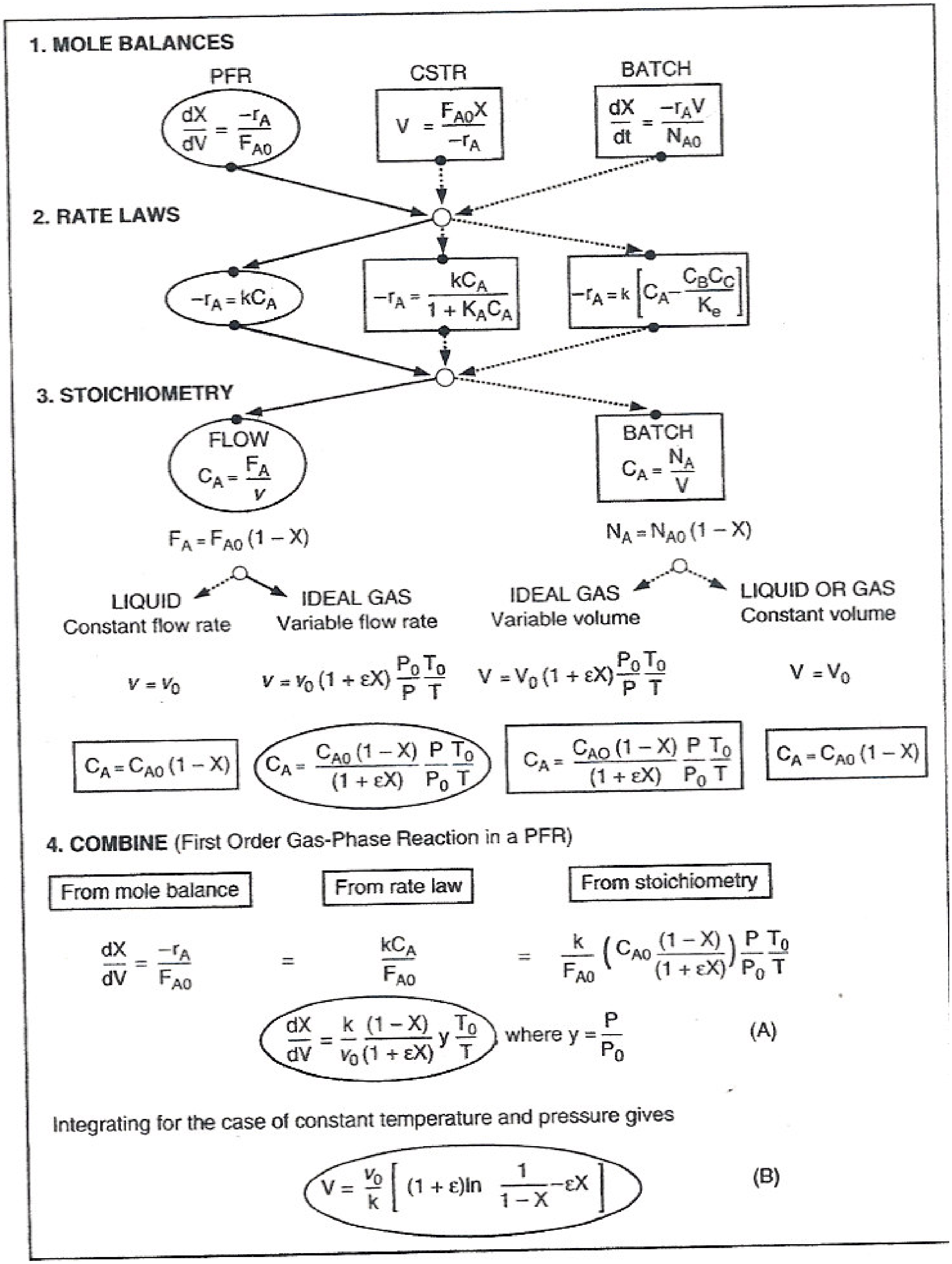
Designing the reactor means using this equation to determine the required size of the reactor (the balance contains the variable *V*) and the exit concentrations of the various chemical species.

Solving this equation is complicated by the presence of the reaction rate r_A function.

If this function is given in a convenient form, then the balance becomes easy to solve. If this function is not presented conveniently, we must formulate the rate such that the balance still becomes easy to solve. Fogler (1999) presents one such algorithm (see below). But don't get lost in the details; always understand that designing the reactor is essentially solving this general balance.



Fogler also presents the same algorithm in a more specific form as follows:



It is important to bear in mind that these are idiot's tools; if you properly understand your intention in reactor design, and if you remember that, by the end of the day, you are just solving a material balance, there is no need to stick to such prescriptive recipes. For your particular problem, you might indeed find a better way to do it.

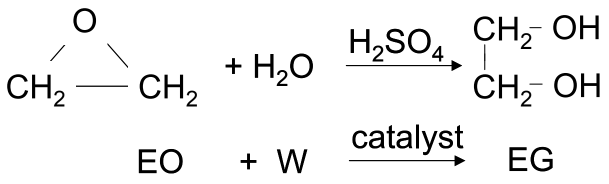
DESIGN OF A CHEMICAL PLANT

Produce 90 000 metric tons ethylene glycol (EG) per annum from ethane

C_2H_6 dehydrogenation: $C_2H_6 \rightarrow C_2H_4 + H_2$

C_2H_4 oxidation: $C_2H_4 + \frac{1}{2} O_2 \rightarrow C_2H_4O$

Ethylene oxide (EO) hydrolysis:

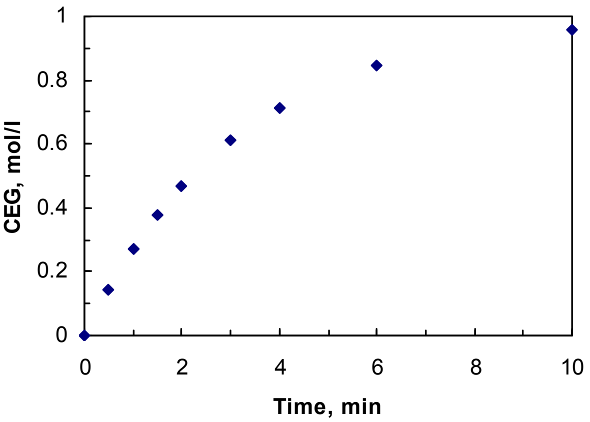


(These are the same reaction; latter is simpler expression.)

Determination of the rate law

The rate law and specific reaction rate constant k were determined experimentally in a batch reactor. 500ml of a 2M-solution of ethylene oxide (EO) in water was mixed with 500ml of water containing 0.9 wt.-% sulphuric acid. The temperature was maintained at 55°C. The concentration of ethylene glycol (EG) was recorded as a function of time:

Time, min	0.0	0.5	1.0	1.5	2.0	3.0	4.0	6.0	10.0
C_{EG}, mol/l	0.000	0.145	0.270	0.376	0.467	0.610	0.715	0.848	0.957



1. Stoichiometric table

(liquid phase reaction V=constant)

Species	Initial	Change	Remaining	Concentration
EO	$N_{EO,0}$	$-N_{EO,0} X_{EO}$	$N_{EO,0} - N_{EO,0} X_{EO}$	$(N_{EO,0} - N_{EO,0} X_{EO})/V$
W	$N_{W,0}$	$-N_{EO,0} X_{EO}$	$N_{W,0} - N_{EO,0} X_{EO}$	$(N_{W,0} - N_{EO,0} X_{EO})/V$
EG	0	$N_{EO,0} X_{EO}$	$N_{EO,0} X_{EO}$	$N_{EO,0} X_{EO}/V$
Total	$N_{T,0}=N_{EO,0} + N_{W,0}$		$N_T=N_{EO,0} + N_{W,0} - N_{EO,0} X_{EO}$	

Thus, the concentration of

Ethylene oxide (EO) $C_{EO} = C_{EO,0} \cdot (1 - X)$

Water (W) $C_W = C_{W,0} - C_{EO,0} \cdot X$

Ethylene glycol (EG) $C_{EG} = C_{EO,0} \cdot X$

With
$$C_{EO,0} = \frac{2\frac{\text{mol}}{\text{l}} \cdot 0.5\,\text{l}}{0.5\,\text{l} + 0.5\,\text{l}} = 1\frac{\text{mol}}{\text{l}}$$

$$C_{W,0} = \frac{1000\frac{\text{g}}{\text{l}} \cdot (0.5\,\text{l} + 0.5\,\text{l})}{18\frac{\text{g}}{\text{mol}}} = 55.5\frac{\text{mol}}{\text{l}}$$

Thus:

- Large excess of water is present!
- Concentration of water remains almost constant
  $\Rightarrow$ volume remains constant

2. Mole balances for batch reactor

For ethylene oxide (EO): $r_{EO} \cdot V = \frac{dN_{EO}}{dt}$

For water (W): $r_W \cdot V = \frac{dN_W}{dt}$

For ethylene glycol (EG): $r_{EG} \cdot V = \frac{dN_{EG}}{dt}$

According to stoichiometric equation:

$$\frac{-dN_{EO}}{dt} = \frac{-dN_W}{dt} = \frac{dN_{EG}}{dt}$$

Thus, $-r_{EO} = -r_W = r_{EG}$

Thus, one equation left:

$$r_{EG} \cdot V = \frac{dN_{EG}}{dt}$$

$$r_{EG} = \frac{d(N_{EG}/V)}{dt} \qquad r_{EG} = \frac{d(C_{EG})}{dt}$$

$$-r_{EO} = \frac{d(C_{EG})}{dt}$$

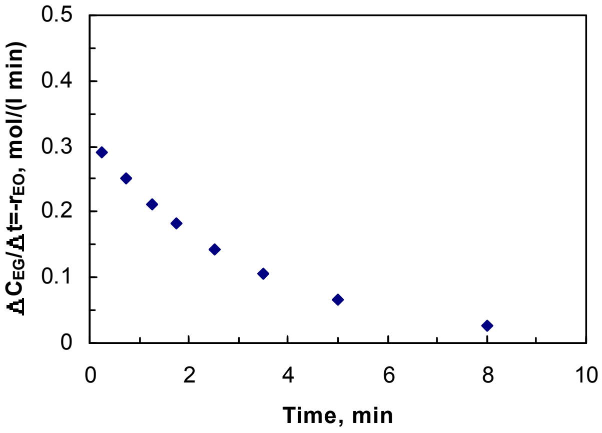
Methods to determine the rate law

Water is in large excess and its concentration can be considered to be constant. Hence, it is not possible with these measurements to determine the effect of the concentration of water on the rate of reaction.

The reaction is far from equilibrium. Hence, it might be assumed that the product, ethylene glycol, does not affect the rate of reaction.

Differential method:

Assume a power-law rate dependency for the rate of ethylene oxide (EO) consumption: $-r_{EO} = k \cdot C_{EO}^{n}$



From the mole balance, $r_{EO} = \frac{d(C_{EO})}{dt}$ or $-r_{EO} = \frac{d(C_{EG})}{dt}$ the tangent of the concentration-time plot equals the rate of consumption of ethylene oxide (EO):

From the measured concentration of ethylene glycol (EG) the concentration of ethylene oxide can be determined:

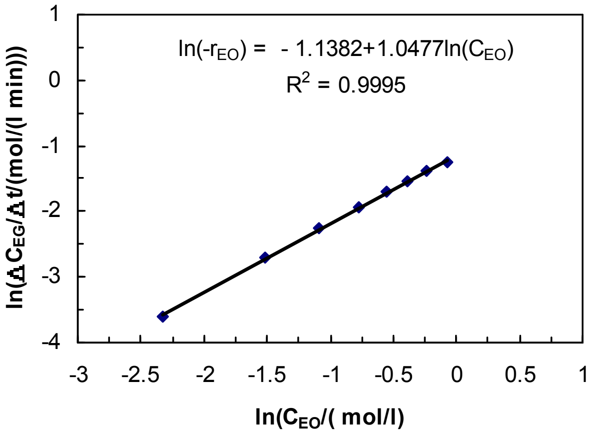
$C_{EO} = C_{EO,0} - C_{EG}$

Plot ln(-r$_{EO}$) vs. ln(C$_{EO}$).

$-r_{EO} = k \cdot C_{EO}^{n}$

$$\ln(-r_{EO}) = \ln(k) + n \cdot \ln(C_{EO})$$

The slope of this line will be the reaction order with respect to ethylene oxide and the intercept will be equal to ln(k).



Thus, $-r_{EO} = 0.32 \cdot C_{EO}^{1.05}$ mol/(l·min)

The reaction order is almost 1 with respect to ethylene oxide.

Alternative: Integral method

For this method a certain reaction order has to be assumed.

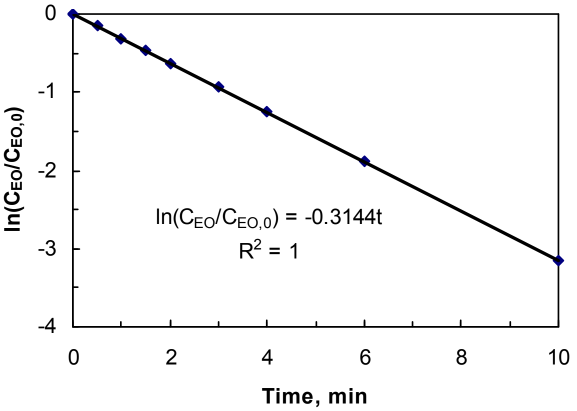
a) Assume 1st order dependency $-r_{EO} = k \cdot C_{EO}$

and $r_{EO} = \frac{d(C_{EO})}{dt}$

Combine $r_{EO} = -k \cdot C_{EO} = \frac{d(C_{EO})}{dt}$

$$-k \cdot \int_{t=0}^{t=t} dt = \int_{C_{EO,0}}^{C_{EO}} \frac{d(C_{EO})}{C_{EO}}$$

$$-k \cdot t = \ln\left(\frac{C_{EO}}{C_{EO,0}}\right)$$



Plot ln(C$_{EO}$/C$_{EO,0}$) vs. time. If the reaction is 1st order with respect to ethylene oxide, the plot will be a straight line going through the origin, with a slope equalling –k.

Thus, $-r_{EO} = 0.3144 \cdot C_{EO}$ mol/(l·min)

a. Assume 2nd order dependency