

## Turbulent Systems with Instantaneous Reaction and No Reaction: Development of Key Relationships

Consider a system in turbulent flow with known flow pattern and consider:

- A) Mixing of two nonreacting species of same diffusivity.
- B) Instantaneous reaction between A & B when species A is maintained at  $C_{Ai}$  at surface I and B at  $C_{Bo}$  at surface B.

(Instantaneous concentration) = (time averaged value) + (fluctuations)

$$C^o = \tilde{C}^o + c^o$$

$$C_t = \tilde{C}_t + c_t$$

Recall

$$C_t = bC_A - aC_B$$

Assume that boundary conditions are steady and independent of time. Then

$$\frac{\tilde{C}^o - C_o^o}{C_i^o - C_o^o} = f_T(z_1, z_2 \dots z_n) \quad (1)$$

$$\frac{\tilde{C}_t - C_{to}}{C_{ti} - C_{to}} = \frac{b\tilde{C}_A - a\tilde{C}_B + aC_{Bo}}{bC_{Ai} + aC_{Bo}} = f_T(z_1, z_2 \dots z_n) \quad (2)$$

While formally the same function  $f_T$  (in the same turbulent field with fixed equivalent boundary conditions, BC) describe the mixing and mixing + instantaneous reaction case one cannot obtain the time average behavior of the reaction system considering only the time average behavior of the non-reacting one.

At any instant of time  $C_t = 0$  defines the instantaneous reaction surface while  $\tilde{C}_t = 0$  clearly does not since

$$C_t = \tilde{C}_t + c_t = 0 \Rightarrow \tilde{C}_t = -c_t$$

Thus  $\tilde{C}_t = 0$  describes a surface at which time averaged stoichiometric ratio of concentrations is seen. Reaction occurs at moving surfaces in a zone surrounding the surface  $\tilde{C}_t = 0$ . The width of that zone depends on the magnitude and distribution of concentration fluctuations  $c_t$  i.e., depends on the turbulent field.

In some problems it is useful to spatially average eq (2) and bars (e.g.  $\bar{C}_i$ ) indicate such a spatial average:

$$\frac{\bar{C}_i - C_{i0}}{C_{ti} - C_{i0}} = \frac{b\bar{C} - a\bar{C}_B}{bC_{Ai} + aC_{Bo}} = aC_{Bo} = \bar{f}_T(z_1) \quad (3)$$

Then solution for  $z_{1f}$  can be obtained from  $\bar{C}_i = 0 \Rightarrow \frac{\beta}{\beta+1} = \bar{f}(z_{1f})$  to provide an estimate for the minimum distance (time) necessary for completion of reaction.

Intuition tells us that reaction rate (instantaneous reaction), reactant time average concentration profiles and reactant conversion must be a function of the turbulent field.

Let us relax now the assumption that the rate is infinite. Consider it merely very fast. Then we would be interested in time averaged concentration at every point i.e.

$$\begin{aligned} R &= kC_A C_B = k(\tilde{C}_A + c_A)(\tilde{C}_B + c_B) \\ &= k[\tilde{C}_A \tilde{C}_B + c_A \tilde{C}_B + c_B \tilde{C}_A + c_A c_B] \\ R &= k[\tilde{C}_A \tilde{C}_B + \langle c_A c_B \rangle] \end{aligned}$$

where  $\langle c_A c_B \rangle$  is the cross correlation of concentration fluctuations.

Even the dominant term  $\tilde{C}_A \tilde{C}_B$  depends on the turbulent field.

Let us assume that in our turbulent field we can characterize the concentration fluctuations with a Gaussian (normal) p.d.f. i.e.

$$\phi(c_t)dc_t = \text{fraction of fluid elements with concentration fluctuation in the range}$$

$c_t$  to  $c_t + dc_t$  or number of fluctuations between  $c_t+dc_t$

Then the following criteria must be satisfied:

$$\begin{aligned} \int_{-\infty}^{\infty} \phi(c_t)dc_t &= 1 \\ \int_{-\infty}^{\infty} c_t \phi(c_t)dc_t &= 0 \end{aligned}$$

A Gaussian p.d.f with zero mean is:  $\phi(c_t) = \frac{1}{\sigma\sqrt{2\pi}} e^{-c_t^2/2\sigma^2}$

It follows that the ensemble averaged concentration is given by:

$$\tilde{C}_i = \int_{-\infty}^{\infty} (\tilde{C}_i + c_i) \phi(c_i) dc_i$$

The variance of concentration fluctuations is denoted by many symbols in the literature and we show here three ( $\tilde{c}_i^2, \Gamma_i^2, \sigma^2$ )

$$\tilde{c}_i^2 = \Gamma_i^2 = \int_{-\infty}^{\infty} c_i^2 \phi(c_i) \phi(c_i) dc_i = \sigma^2$$

In our instantaneous reaction system

$$C_i = bC_A - aC_B = \tilde{C}_i + c_i > 0 \text{ when A is present}$$

$$\tilde{C}_i + c_i < 0 \text{ when B is present}$$

$$C_A = \frac{C_i}{b} = \frac{\tilde{C}_i + c_i}{b} \text{ when } \tilde{C}_i + c_i > 0 \text{ for } c_i > -\tilde{C}_i$$

$$\tilde{C}_A = \int_{-\infty}^{\infty} (C_A + c_A) \phi(c_A) dc_A = \frac{1}{b} \int_{-\tilde{C}_i}^{\infty} (\tilde{C}_i + c_i) \phi(c_i) dc_i \quad (4)$$

$$\tilde{C}_A = \frac{1}{b} \left[ \tilde{C}_i \frac{1}{\sigma\sqrt{2\pi}} \int_{-\tilde{C}_i}^{\infty} e^{-x^2/2\sigma^2} dx + \frac{1}{\sigma\sqrt{2\pi}} \int_{-\tilde{C}_i}^{\infty} x e^{-x^2/2\sigma^2} dx \right]$$

by changing the variable

$$\frac{x}{\sigma\sqrt{2}} = t \quad dx = \sigma\sqrt{2} dt$$

$$\tilde{C}_A = \frac{1}{b} \left[ \tilde{C}_i \frac{1}{\sqrt{\pi}} \int_{-\frac{\tilde{C}_i}{\sigma\sqrt{2}}}^{\infty} e^{-t^2} dt + \sigma\sqrt{\frac{2}{\pi}} \int_{-\frac{\tilde{C}_i}{\sigma\sqrt{2}}}^{\infty} t e^{-t^2} dt \right]$$

and recalling that

$$\operatorname{erfc} z = \frac{2}{\sqrt{\pi}} \int_z^{\infty} e^{-t^2} dt = 1 - \operatorname{erf}(z) \quad ; \quad \operatorname{erf}(-z) = -\operatorname{erf}(z) \quad ; \quad \operatorname{erf}(-z) = 1 + \operatorname{erf}(z)$$

we get:

$$\begin{aligned} \tilde{C}_A &= \frac{1}{b} \left[ \tilde{C}_i \cdot \frac{1}{2} \operatorname{erfc} \left( \frac{-\tilde{C}_i}{\sqrt{2}} \right) - \frac{\sigma}{\sqrt{2\pi}} e^{-t^2} \Big|_{\frac{-\tilde{C}_i}{\sigma\sqrt{2}}} \right] \\ &= \frac{1}{b} \left[ \tilde{C}_i \frac{1}{2} \operatorname{erfc} \left( \frac{-\tilde{C}_i}{\sigma\sqrt{2}} \right) + \frac{\sigma}{\sqrt{2\pi}} e^{-\tilde{C}_i^2/2\sigma^2} \right] \end{aligned}$$

But  $\sigma_d = \sigma / \tilde{C}_t$  so that

$$\begin{aligned}
 \frac{b\tilde{C}_A}{\tilde{C}_t} &= \frac{1}{2} \operatorname{erfc}\left(-\frac{\tilde{C}_t}{\sigma\sqrt{2}}\right) + \frac{\sigma}{\tilde{C}_t\sqrt{2\pi}} e^{-\tilde{C}_t^2/2\sigma^2} \\
 &= \frac{1}{2} \left[ 1 - \operatorname{erf}\left(-\frac{1}{\sigma_d\sqrt{2}}\right) \right] + \frac{\sigma_d}{\sqrt{2\pi}} e^{-\frac{1}{2\sigma_d^2}} \\
 &= \frac{1}{2} \left[ 1 + \operatorname{erf}\left(\frac{1}{\sigma_d\sqrt{2}}\right) + \frac{\sigma_d}{\sqrt{2\pi}} e^{-\frac{1}{2\sigma_d^2}} \right] \\
 &= \frac{1}{2} \left[ 1 + 1 - \operatorname{erfc}\left(\frac{1}{\sigma_d\sqrt{2}}\right) + \frac{\sigma_d}{\sqrt{2\pi}} e^{-\frac{1}{2\sigma_d^2}} \right]
 \end{aligned}$$

Finally we can write:

$$\begin{aligned}
 \operatorname{ierfc}(z) &= -z \operatorname{erfc} z + \frac{1}{\sqrt{\pi}} e^{-z^2} = \int_z^\infty \operatorname{erfc}(z) dz \\
 \frac{b\tilde{C}_A}{\tilde{C}_t} &= 1 - \frac{1}{2} \operatorname{erfc}\left(\frac{1}{\sigma_d\sqrt{2}}\right) + \frac{\sigma_d}{\sqrt{2\pi}} e^{-\frac{1}{2\sigma_d^2}} \\
 &= 1 + \frac{\sigma_d}{\sqrt{2}} \left[ -\frac{1}{\sigma_d\sqrt{2}} \operatorname{erfc}\left(\frac{1}{\sigma_d\sqrt{2}}\right) + \frac{1}{\sqrt{\pi}} e^{-\frac{1}{2\sigma_d^2}} \right] \\
 \frac{b\tilde{C}_A}{\tilde{C}_t} &= 1 + \underbrace{\frac{\sigma_d}{\sqrt{2}} \operatorname{ierfc}\left(\frac{1}{\sigma_d\sqrt{2}}\right)}_{g(\sigma_d)} = 1 + g(\sigma_d) \tag{4a}
 \end{aligned}$$

Similarly one can show

$$\frac{a\tilde{C}_B}{\tilde{C}_t} = g(\sigma_d) \tag{4b}$$

This happens for  $\tilde{C}_t + c_t < 0$        $c_t < -\tilde{C}_t$

$$\begin{aligned} C_t &= bC_A - aC_B \\ C_B &= -\frac{C_t}{a} = -\frac{\tilde{C}_t + c_t}{a} \\ \tilde{C}_B &= \int_{-\infty}^{\infty} (\tilde{C}_B + c_B) \phi(c_B) dc_B = \frac{1}{2} \int_{-\infty}^{-\tilde{C}_t} (\tilde{C}_t + c_t) \phi(c_t) dc_t \\ &= -\frac{1}{a} \left[ \tilde{C}_t \int_{-\infty}^{-\tilde{C}_t} \phi(c_t) dc_t + \int_{-\infty}^{-\tilde{C}_t} c_t \phi(c_t) dc_t \right] \\ &= -\frac{1}{a} \left[ \tilde{C}_t \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{-\tilde{C}_t} e^{-x^2/2\sigma^2} dx + \frac{1}{\sigma\sqrt{\pi}} \int_{-\infty}^{-\tilde{C}_t} x e^{-x^2/2\sigma^2} dx \right] \end{aligned}$$

with the change in variable:

$$-\frac{x}{\sigma\sqrt{2}} = t \quad dx = -\sigma\sqrt{2} dt$$

we get:

$$\begin{aligned} &= \frac{1}{a} \left[ \tilde{C}_t \frac{1}{\sqrt{\pi}} \int_{\infty}^{\frac{\tilde{C}_t}{\sigma\sqrt{2}}} e^{-t^2} dt - \sigma \sqrt{\frac{2}{\pi}} \int_{\infty}^{\frac{\tilde{C}_t}{\sigma\sqrt{2}}} t e^{-t^2} dt \right] \\ &= \frac{1}{a} \left[ \tilde{C}_t \left(-\frac{1}{2}\right) \operatorname{erfc}\left(\frac{1}{\sigma_d\sqrt{2}}\right) + \frac{\sigma_d \tilde{C}_t}{\sqrt{2\pi}} e^{-\frac{1}{2\sigma_d^2}} \right] \\ \frac{a\tilde{C}_B}{\tilde{C}_t} &= \frac{\sigma_d}{\sqrt{2}} \left[ -\frac{1}{\sigma_d\sqrt{2}} \operatorname{erfc}\left(\frac{1}{\sigma_d\sqrt{2}}\right) + \frac{1}{\sqrt{\pi}} e^{-\frac{1}{2\sigma_d^2}} \right] \\ \frac{a\tilde{C}_B}{\tilde{C}_t} &= \frac{\sigma_d}{\sqrt{2}} \operatorname{erfc}\left(\frac{1}{\sigma_d\sqrt{2}}\right) = g(\sigma_d) \end{aligned} \tag{4b}$$

Equations (4a) and (4b) establish that the time averaged concentration profiles of individual species and, therefore, the average rate of reaction, depend upon both  $\tilde{C}_t$  (which can be determined from the analogous mixing problem  $\tilde{C}^o$ ) and  $\sigma_d$  i.e on the turbulence field.

Note that when  $\tilde{C}_t = 0$  eqs (4a) and (4b) cannot be used. One must go back to their derivation: i.e eq (4).

$$\begin{aligned}
\tilde{C}_t &= 0 \\
\tilde{C}_A &= \frac{1}{b} \int_0^\infty c_t \phi(c_t) dc_t = \frac{1}{b} \frac{1}{\sigma \sqrt{2\pi}} \int_0^\infty x e^{-x^2/2\sigma^2} dx \\
&= \frac{\sigma}{b} \sqrt{\frac{2}{\pi}} \int_0^\infty t e^{-t^2} dt = -\frac{\sigma}{b\sqrt{2\pi}} e^{-t^2} \Big|_0^\infty = \frac{\sigma}{b\sqrt{2\pi}} \\
\tilde{C}_A &= \frac{\sigma}{b\sqrt{2\pi}} \tag{4a'}
\end{aligned}$$

Similarly

$$\begin{aligned}
\tilde{C}_B &= \frac{\sigma}{a\sqrt{2\pi}} \tag{4b} \\
\sigma &= \Gamma_t
\end{aligned}$$

An alternative approach is to go back to eqs (1) and (2) and rewrite them for instantaneous concentrations:

$$\frac{\tilde{C}^o + c^o - C_o^o}{C_i^o - C_o^o} = f_1(z_1, z_2, \dots, z_n) \tag{5}$$

$$\tilde{f}_1 = f_T \tag{6}$$

$$c^o = (C_i^o - C_o^o) f_1 - (\tilde{C}^o - C_o^o)$$

$$\frac{c^o}{(C_i^o - C_o^o)} = f_1 - \frac{\tilde{C}^o - C_o^o}{C_i^o - C_o^o} = f_1 - f_T$$

Square the relative concentration deviation and time average

$$\frac{\langle c^{o2} \rangle}{(C_i^o - C_o^o)^2} \Rightarrow \langle (f_1 - f_T)^2 \rangle = \tilde{f}_1^2 - 2\tilde{f}_1 f_T^2 + f_T^2 = \langle f_1^2 \rangle - f_T^2 = \langle f_1^2 \rangle - f_T^2(z_1, z_2, \dots, z_n) \tag{7}$$

Where  $\langle \rangle$  and  $\sim$  are both used to indicate ensemble averaging.

Similarly

$$\frac{\langle c_t^2 \rangle}{(C_t^o - C_o^o)^2} = \langle (f_1 - f_T)^2 \rangle = f_2^2(z_1, \dots, z_n) \tag{8}$$

Now we want to characterize the concentration fluctuation RMS value in a system with reaction (instantaneous) in terms of system with no reaction but with the same turbulent field.

Let  $\Gamma^o = \sqrt{\langle c^{o2} \rangle}$  and  $\Gamma_t = \sqrt{\langle c_t^2 \rangle}$ . These are the Root Mean Square Concentration Fluctuations (RMSCF).

Then from eq (7) and (8):

$$\frac{\Gamma_t}{\Gamma^o} = \left( \frac{C_{t_i} - C_{t_o}}{C_i^o - C_o^o} \right) \quad (9)$$

Concentration fluctuations in the same turbulent field in the system with instantaneous reaction and no reaction (dilute) are the same if the boundary conditions (BC) can be reproduced.

Let  $C_o^o = 0$  ,  $C_i^o = C_{A_i}$

Then  $C_{t_i} = b C_{A_i}$        $C_{t_o} = -a C_{B_o}$

$$\frac{\Gamma_t}{\Gamma^o} = \frac{b C_{A_i} + a C_{B_o}}{C_{A_i}} = b(1 + \beta) \quad (10)$$

$\Gamma^o$  now is the RMS fluctuation that would exist at the point of interest if no B was present in the feed but all else was the same as in the reaction system.

The relative fluctuations can be defined as:

$$\gamma_t = \frac{\Gamma_t}{\tilde{C}_t} \quad , \quad \gamma_o = \frac{\Gamma_o}{\tilde{C}_o} \quad (11)$$

Using eq (1) and (2) one can show that

$$\begin{aligned} \tilde{C}_t &= C_{t_o} + (C_{t_i} - C_{t_o}) f_T \\ \Gamma_t &= \Gamma^o (C_{t_i} - C_{t_o}) / (C_i^o - C_o^o) \\ \gamma_t &= \frac{\Gamma_t}{\tilde{C}_t} = \frac{\Gamma^o (C_{t_i} - C_{t_o}) / (C_i^o - C_o^o)}{C_{t_o} + (C_{t_i} - C_{t_o}) f_T} = \gamma^o \frac{\tilde{C}_o (C_{t_i} - C_{t_o}) / (C_i^o - C_o^o)}{C_{t_o} + (C_{t_i} - C_{t_o}) f_T} \\ \tilde{C}_o &= C_o^o + (C_i^o - C_o^o) f_T \\ \gamma_t &= \gamma^o \frac{\frac{C_o^o (C_{t_i} - C_{t_o})}{(C_i^o - C_o^o)} + (C_{t_i} - C_{t_o}) f_T}{C_{t_o} + (C_{t_i} - C_{t_o}) f_T} \end{aligned}$$

Therefore in general we get:

$$\gamma_t = \gamma^o \frac{\frac{C_o^o}{C_i^o - C_o^o} + f_T}{\frac{C_{t_o}}{C_{t_i} - C_{t_o}} + f_T} \quad (12)$$

But when  $C_o^o \equiv 0$  and  $C_{t_i} = bC_A$  and  $C_{t_o} = -aC_{B_o}$

Then

$$\begin{aligned} \gamma_t &= \gamma^o \frac{f_T}{-\frac{aC_{B_o}}{bC_A + aC_{B_o}} + f_T} = \gamma^o \frac{f_T}{-\frac{\beta}{1+\beta} + f_T} \\ \gamma_t &= \gamma^o \frac{f_T}{f_T - \frac{\beta}{1+\beta}} \\ \gamma_t &= \gamma^o \frac{f_T(z_1, z_2)}{f_T(z_1, z_2) - \beta/(1+\beta)} \end{aligned} \quad (12a)$$

One can show that  $\gamma_t = \sigma_d$  (13)

The time average concentration profiles are now completely determinable.

Equations (4a) (4b) define  $\tilde{C}_A, \tilde{C}_B$  (or eqs (4a'), (4b')).

Equation (2) defines  $\tilde{C}_i$ .

Equations (12) and (13) define  $\gamma_t(\sigma_d)$  in terms of measured turbulent fluctuations in the system with no reaction ( $\gamma^o$ ); and Eq (1) or (2) define  $f_T(z_1, z_2)$  for the system of interest.

Consider now mixing two dilute fluid streams (solute A in solvent + solute B in solvent with  $D_A=D_B$ ) when reaction between A and B is instantaneous. Consider a tubular reactor. Let  $z_1$  be the reduced distance measured downstream from the point of contact of two streams and  $z_2$  reduced radial distance. Eq (5) would give the instantaneous concentration profile with  $f_1$  depending on mixer geometry and flow parameters. Given RMS concentration fluctuations in the nonreacting problem, the time average concentration profiles and conversion can be computed. The key is to get a mixture uniform on a coarse scale so that the ensemble averaged concentration at certain location  $z_1$ ,  $\tilde{C}^o$ , is the same as the cross-sectional average concentration,  $\langle C^o \rangle$  at the same location, which for a nonreacting system by mass balance must be equal to the inlet concentration.

$$\tilde{C}^o = \bar{C}^o = \bar{C}_o^o$$

This can be done by evenly dispersing one fluid into the other.



In a homogeneous turbulence field  $\Gamma^o$  depends only on  $z_1$ . If uniformity on a coarse scale is reached at position  $z_{10}$  where RMS concentration fluctuation is  $\Gamma_o^o$  then

$$\frac{\Gamma^o}{\Gamma_o^o} = \frac{f_2(z_1)}{f_2(z_{10})} \quad (14)$$

This implies

$$\frac{\Gamma_t}{\Gamma_{t_o}} = \frac{\Gamma^o}{\Gamma_o^o} = \frac{f_2(z_1)}{f_2(z_{10})} \quad (15)$$

Due to continuity and non-permeability of the walls we also have:

$$\tilde{C}_t = \bar{C}_t = \bar{C}_{t_o} \quad (16a)$$

$$\tilde{C}_A(z_1) = \bar{C}_A(z_1) \quad (16b)$$

$$\tilde{C}_B(z_1) = \bar{C}_B(z_1) \quad (16c)$$

where bar - denotes the mixing cup averaging.

If we use two streams at stoichiometric ratio, then  $\bar{C}_{t_o} = 0$  and for  $z_1 > z_{10}$   $\tilde{C}_t = 0$

Then from eq (4a;)

$$\tilde{C}_A = \frac{\sigma}{b\sqrt{2\pi}} = \frac{\Gamma_t}{b\sqrt{2\pi}} \quad (4a')$$

and from eq (10)

$$\Gamma_t = (1 + \beta/b)\Gamma^o \quad (10)$$

It follows that

$$\tilde{C}_A = \frac{(1 + \beta)\Gamma^o}{\sqrt{2\pi}} = \bar{C}_A \quad (17)$$

Then at  $z_{10}$

$$\bar{C}_A(z_{10}) = \frac{(1 + \beta)\Gamma_o^o}{\sqrt{2\pi}}$$

So that we ultimately get:

$$\frac{\bar{C}_A(z_1)}{\bar{C}_A(z_{10})} = \frac{\Gamma^o(z_1)}{\Gamma_o^o(z_{10})} \quad (18)$$

If one measures isotropic turbulence properties along  $z_1$ , one can from eq (19) predict conversion along  $z_1$  when the reactants are fed in stoichiometric ratio by:

$$x_A = x_B = 1 - \frac{\Gamma^o}{\Gamma_o^o} \quad (19)$$

This was confirmed by Beek et al., Chem. Engr. Progr. Symp. Ser. No. 25, Vol. 55, 23 (1959).

In case of a nonstoichiometric mixture, eq (4a) must be used

$$\frac{b\tilde{C}_A}{\tilde{C}_t} = \frac{b\bar{C}_A}{\bar{C}_{t_o}} = 1 + g(\gamma_t) \quad (4a)$$

where

$$\begin{aligned} \bar{C}_{t_o} &= bC_{A_o} - aC_{B_o} = bC_{A_o}(1 - \beta) \\ \beta &= \frac{a\bar{C}_{B_o}}{bC_{A_o}} = \frac{a\bar{C}_{B_o}}{b\bar{C}_{A_o}} \text{ at } z_{10} \end{aligned}$$

For  $\beta > 1$ , A is the limiting reactant and

$$x_A = 1 + (\beta - 1)(1 + g(\gamma_t)) \quad (20)$$

For  $\beta < 1$ , B is the limiting reactant and

$$x_B = 1 + \frac{\beta - 1}{\beta} g(\gamma_t) \quad (21)$$

Stoichiometric requirement is:

$$x_A = \beta x_B = \beta + (\beta - 1)g(\gamma_t) = 1 + (\beta - 1) + (\beta - 1)g(\gamma_t) = 1 + (\beta - 1)(1 + g(\gamma_t))$$

At  $z_{10}$   $x_A = 0$

$$\frac{\beta}{1 - \beta} = g(\gamma_{t_o}) \quad (22)$$

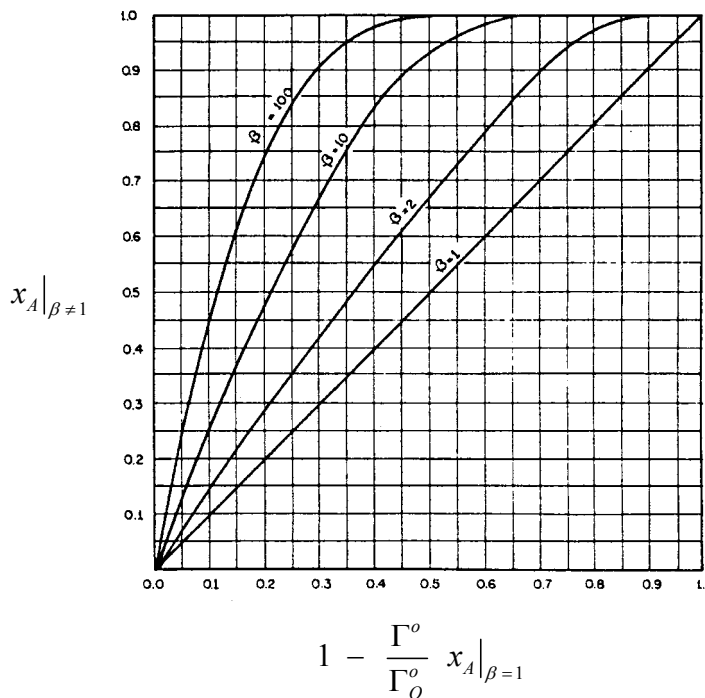
$$\gamma_{t_o} = \frac{\Gamma_{t_o}}{\bar{C}_{t_o}} = \frac{\Gamma_{t_o}}{\bar{C}_t} \quad \bar{C}_t = \Gamma_{t_o} / \gamma_{t_o} \quad (23)$$

$$x_A = 1 + (\beta - 1) \left[ 1 + g \left( \gamma_{t_o} \frac{\Gamma_o^o}{\Gamma_o^o} \right) \right] \quad (24)$$

Knowing reactant feed ratio and stoichiometry of reaction i.e  $\beta$  , and having measured  $\gamma_{i_0}, \Gamma_0^o$  and  $\Gamma^o$  as a function of position  $z_1$  conversion can be predicted by eq (24).

Degree of accomplished mixing is  $x_A$  when  $\beta = 1$ .

**FIGURE 1:** Fractional conversion as a function of accomplished mixing.  
(Tran Tour, AIChE J., 8, 70 (1962))



For  $x_{A_{stoich}} = 99$  degree of accomplished mixing  $\Rightarrow 0.99$  at  $\beta = 1$ . But  $x_A = 0.99$  at  $\beta = 2$  at degree of mixing of only 0.83. The fractional decrease in length by increasing  $\beta$  is significant.

Increasing  $\beta$  from 1 to 2 approximately halves the required length for reaction and mixing.

Figure A is a function of mixer geometry and  $Re, Sc$ . For a given system at  $Sc, Re = \text{const}$  lines of constant  $1 - \frac{\Gamma^o}{\Gamma_0^o}$  are lines of constant position.

At the position that corresponds to 20% accomplished mixing a change of  $\beta$  from 1 to 10 increases  $x_A$  from 0.2 to 0.48.

At 60% mixing  $\beta$  increase from 1 to 10 increases  $x_A$  from 0.4 to 0.8.

At 90% mixing  $\beta$  increase from 1 to 1.4 changes  $x_A$  from 0.9 to 0.99.

Working at nonstoichiometric ratio is very effective in getting high conversion of limiting reactant in turbulent systems.

**FIGURE 2:** Bulk composition vs.  $\beta$  for fixed values of accomplished mixing.  
(Fran Tour, AIChE J., 8, 70 (1962))

