Scale-Up in Plug-Flow Reactors: Laminar Feed

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Similarity parameters are derived to correlate the selectivity of mixing controlled parallel reactions within plug-flow reactors with two types of static mixing elements for both aqueous and viscous solutions. For the case of laminar reactor feed, the Kolmogoroff time is shown to correlate selectivity in turbulent reactors provided the reactor Reynolds number $Re < Re_C$. The upper limit Re_C for the reactor Reynolds number is constrained by the ratio of reactant feed-to-total volumetric flow rate. Moreover, for larger reactor Reynolds number $Re > Re_C$, the inertial time scale defined in terms of a reactor feed length correlates selectivity. Scaling laws are derived for both reactor diameter and length, and suggestions are made for predicting selectivity with larger turbulent feed rates.

Introduction

When the Reynolds number (Re) of a reactor is sufficiently large, scale-up of macroscopic properties such as the friction factor, velocity distribution, and blending time is essentially independent of Re. This is also true on a smaller scale for some turbulent phenomena, such as mixing on a time scale defined by the eddy dissipation or breakup time $t_d \propto l_e/u'$, where the latter represents the ratio of the energy containing eddy size l_e to the root-mean-square (rms) turbulent velocity u' (Davies, 1972).

Micromixing, however, over length scales on the order of the Kolmogoroff length l_k does depend on the reactor Re. For example, on the scale of the Kolmogoroff length, one can define a viscous or Kolmogoroff time $t_k = (\nu^3/\epsilon)^{1/4}$, where $t_k \ll t_d$ the inertial time.

These mixing times represent the combined effects of either inertia and convection (t_d) or viscosity and convection (t_k), and the choice of these scales is important in the determination of the selectivity of fast multiple chemical reactions and thus the scale-up of such reactors (Baldyga et al., 1997; Forney and Nafia, 1998). The choice, as demonstrated below, depends on whether reactant feed rates are either laminar or turbulent. Moreover, for laminar feed rates, the choice is strongly influenced by the magnitude of the reactant flow rate. These processes are useful, in particular, for the production of fine specialty chemicals (Paul, 1988).

Mixing and chemical reaction in fully turbulent liquids occur within laminar shear layers of thickness l_k, the Kolmogoroff length, between contacting eddies. For example, the data of Bolzern et al. (1985) plotted in Figure 1 represent the selectivity of mixing sensitive parallel reactions in a coaxial fully developed, turbulent tube and reactant feed flows. The universal curve of selectivity plotted vs. the tube, Kolmogoroff time t_k demonstrates that scale-up is independent of both the inertial and molecular diffusion times (the latter implies independence of the Schmidt number, as shown by Li and Toor, 1986).

For the case of laminar feed tubes, however, the choice of mixing times is either the viscous (Kolmogoroff) time scale or an inertial scale (proportional to the eddy dissipation time) for small or large feed rates, respectively (Baldyga et al., 1997; Forney and Nafia, 1998). Comparison of these time scales requires the computation of the maximum mixing time representing the rate-limiting step. Unfortunately, accurate calculation of each time scale is difficult and requires an estimate of a universal constant whose magnitude may be disputed in the literature.

In the present article, which considers laminar feed rates, a simple physical interpretation is provided for the choice of

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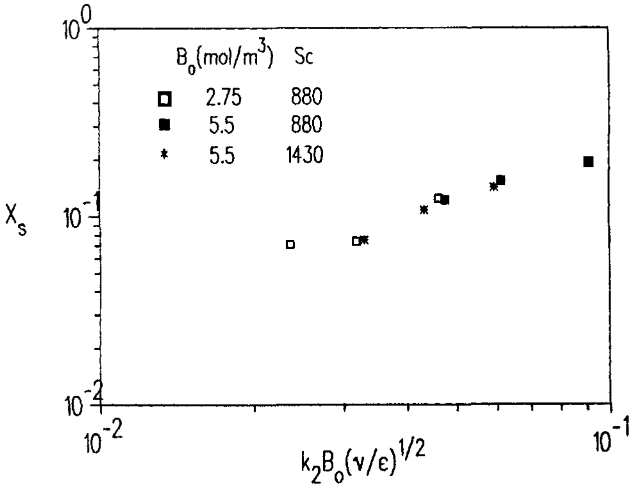

Figure 1. Selectivity of mixing sensitive parallel reactions in fully developed turbulent tube flow.

time scale. Moreover, for a given plug-flow reactor design and volume ratio of reactants, the form of the time scale is shown to depend only on the magnitude of the reactor Reynolds number. Additional descriptions of competing reactor designs and the problem of eddy decay are given in the Appendix.

Similarity

Turbulence

Nearly isotropic turbulence occurs in a variety of large Reynolds number flows. Locally isotropic turbulence, defined as turbulence in equilibrium over a range of smaller eddy size, occurs downstream from a grid, in fully developed pipe flow and in jets and wakes. For example, local isotropy may often be found in the decay of free turbulence, that is, not dominated by shear at a solid wall. Thus, the large eddies formed by fluid motion near the nozzle of a free jet are not isotropic, but as the eddies decay transferring energy to smaller fluid fragments, the smaller eddies formed become independent of the nozzle geometry and eventually become nearly isotropic. In the latter case, the eddy spectrum in the equilibrium range depends only on the local eddy dissipation rate and the kinematic viscosity. Further discussion of local isotropy is provided by Brodkey (1967, p. 304) and Kresta (1998).

In the present section, the reactor Reynolds number is assumed to be sufficiently large such that the fine scale structure of the turbulence is locally isotropic. It is recognized that the latter assumption may not be appropriate for certain static mixer designs, but the definition of κ and ϵ given below are useful provided the velocity and length scales are interpreted in terms of the pressure drop and friction factor, as described in the next section.

The turbulent kinetic energy κ can thus be written in the form:

$$\kappa \propto (u')^2, \tag{1}$$

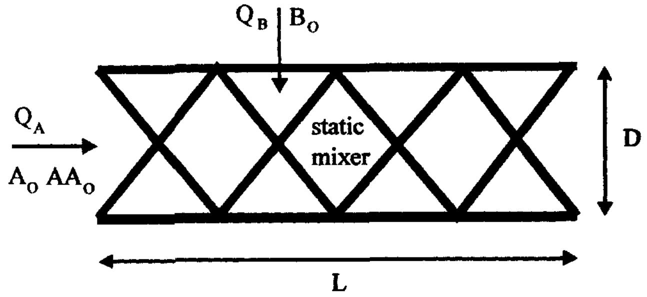

Figure 2. Plug-flow reactor.

and the dissipation rate (power input per unit mass) is

$$\epsilon \propto (u')^3/l_e, \tag{2}$$

where l_e is the average size of the energy containing eddies and u' is the rms turbulent velocity. It is now convenient to write the eddy dissipation time ($\propto \kappa/\epsilon$) in terms of local turbulent properties, or

$$t_d \propto l_e/u' \propto (l_e^2/\epsilon)^{1/3}, \tag{3}$$

and the Kolmogoroff time

$$t_k \propto (\nu/\epsilon)^{1/2}. \tag{4}$$

Thus, the ratio

$$\frac{t_d}{t_k} \propto \sqrt{Re_l}, \tag{5}$$

where $Re_l = u'l_e/\nu$ is the eddy Reynolds number.

Plug-flow reactors

Consider a turbulent fluid flowing through a circular tube of diameter D as shown in Figure 2. For steady flow the stress of the fluid on the mixing elements is balanced by the pressure drop along the tube of length L. It is common practice to express the ratio of shear stress to the form drag ρu^2 in the form of the Fanning friction factor

$$f = \frac{\Delta P}{2\rho u^2}\left(\frac{D}{L}\right), \tag{6}$$

where for smooth surfaces f depends on the tube Reynolds number Re. However, if Re is large and the tube walls are rough (or the tube contains static mixing elements) and the flow is turbulent, then f is a constant and independent of Re. Here, we assume that $Re > 3000$, which is the lower limit for the Blasius equation for roughness elements larger than 5% of the tube diameter (Davies, 1972, p. 32). In this case, form drag is important and the eddies caused by the impact of the fluid with the mixing elements dissipate most of the kinetic energy.

Limiting the discussion to plug-flow reactors containing static mixing elements such that the tube void fraction is α, the dissipation rate per unit mass is

$$\epsilon = \frac{\Delta P Q}{\alpha \rho (\pi D^2/4)}, \tag{7}$$

where $Q = \pi(D^2/4)u$ is the total reactor volume flow rate. Substituting for ΔP from Eq. 6 into Eq. 7, one obtains

$$\epsilon = 2\frac{f}{\alpha}\frac{u^3}{D}. \tag{8}$$

Definition of the Fanning friction factor gives $u'/u = f^{1/2}$ (Davies, 1972). Thus, from Eq. 2 and Eq. 8 one would expect $l_e \propto (\alpha f^{1/2} D)$, or the eddy dissipation time in Eq. 3 applied to plug-flow reactors becomes

$$t_d \propto (\alpha/f)(D/u). \tag{9}$$

Finally, writing the ratio of eddy dissipation-to-Kolmogoroff time, as is done in Eq. 5, the latter becomes

$$t_k \propto \sqrt{\alpha/f}\,(D/u)/\sqrt{Re}, \tag{10}$$

where $Re = uD/\nu$ is the reactor Reynolds number.

In order to correlate selectivity data within plug-flow reactors containing different static mixing elements, it is convenient to define

$$t_{ki} = t_{k0}\left(\frac{\alpha_i}{f_i}\right)^{1/2}, \tag{11}$$

where the reference value is

$$t_{ko} = (D/u)/\sqrt{Re}. \tag{12}$$

Combining Eqs. 11 and 12, one obtains a value proportional to the Kolmogoroff time in the form

$$t_{ki} = \frac{\nu^{1/2} D^{1/2}}{u^{3/2}}\left(\frac{\alpha_i}{f_i}\right)^{1/2}, \tag{13}$$

where the index i refers to static mixing elements of specified geometry.

Scale-Up

When the reactant feed is laminar, the selectivity of a parallel reaction scheme is correlated with either a viscous or an inertial time scale. The limitations on the use of either scale are described in terms of both the reactor and the feed-tube Reynolds numbers. Expressions are also developed for the scale-up of both the reactor diameter and length in terms of reactor flow rate. A number of useful expressions are developed below.

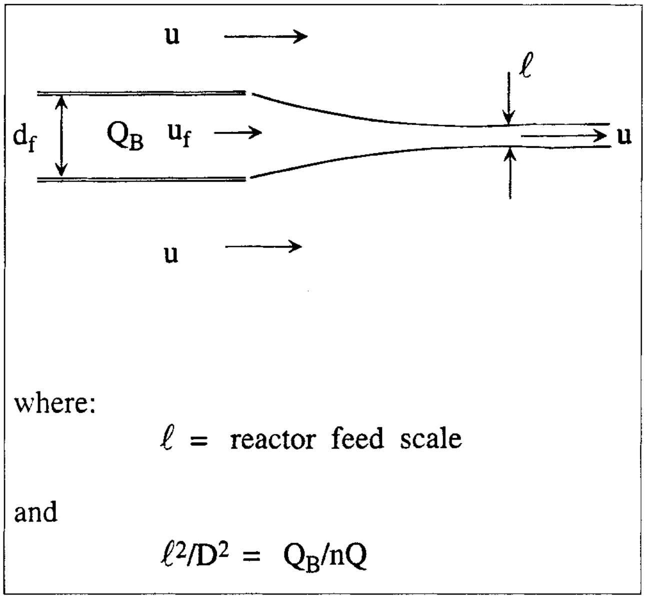

Figure 3. Laminar feed tube and length scale.

The small feed-tube Reynolds number in Figure 3 is assumed to be laminar in the present study or $Re_f < 2{,}500$ (Davies, 1972), where

$$Re_f = \frac{4Q_B}{\pi n d_f \nu}. \tag{14}$$

Here, n is the number of feed tubes and d_f is the diameter of each feed tube. Thus, it is possible to define a reactor feed scale $l = (Q_B/\pi n u)^{1/2}$, as was done earlier (Baldyga et al., 1997) from conservation of mass at the feed nozzle where l represents the diameter of a thread of fluid traveling at the ambient velocity u of the reactor stream. It is convenient, here to define the reactor feed scale l in terms of the flow ratio of reactants and reactor diameter D, or

$$(\ell/D)^2 = Q_B/nQ, \tag{15}$$

as demonstrated in Figure 3.

When the reactor feed length is smaller than the Kolmogoroff length defined by

$$\ell_k = (\nu^3/\epsilon)^{1/4}, \tag{16}$$

or $l < l_k$, we assume that the appropriate time scale for mixing is the viscous or Kolmogoroff time. In this case, the reactor feed stream is entrained between ambient turbulent eddies. If, $l > l_k$, however, we assume the time scale for mixing to be an inertial scale proportional (but not equal) to the ambient eddy dissipation time. The choice of the mixing time is therefore determined by the magnitude of the ratio l/l_k, as described by Forney and Nafia (1998) and Forney and Chang-Mateu (1998).

Substituting ϵ defined by Eq. 8 into Eq. 16 and noting that the mean reactor velocity $u \propto Q/D^2$ and reactant flow rate $Q_B = Q(Q_B/Q)$, one obtains a ratio of the feed-to-

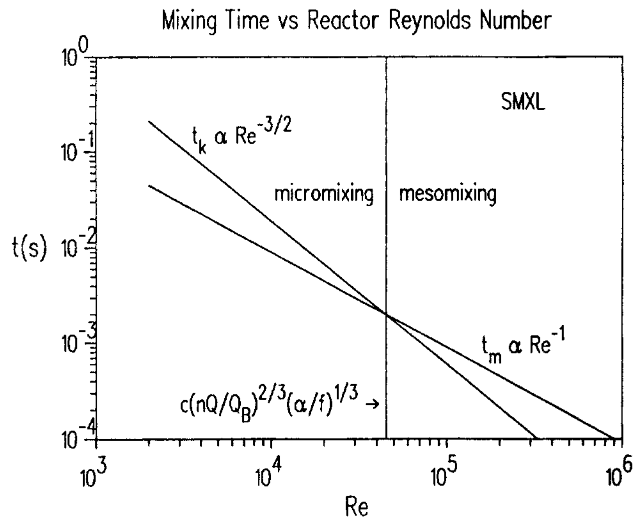

Figure 4. Mixing time vs. tube Reynolds number in static mixer.

$D = 3.3$ cm, $\nu = 0.89 \times 10^{-6} \mathrm{m^2 \cdot s^{-1}}$; $nQ/Q_B = 6 \times 10^3$.

Kolmogoroff length of the form

$$\frac{\ell}{\ell_k} \alpha \left(\frac{Q}{D\nu}\right)^{3/4} \left(\frac{f}{\alpha}\right)^{1/4} \left(\frac{Q_B}{nQ}\right)^{1/2}. \tag{17}$$

Since the reactor Reynolds number $Re \, \alpha \, Q/D\nu$, setting $l/l_k = 1$ in Eq. 17 provides a transition reactor Reynolds number that is constrained by the flow ratio of reactants in the form

$$Re_c = c\left(\frac{\alpha}{f}\right)^{1/3} \left(\frac{nQ}{Q_B}\right)^{2/3}, \tag{18}$$

where the universal constant c must be established from experimental data. The choice of time scale is therefore determined by the magnitude of the reactor Reynolds number. For $Re < Re_c$, the scale is the viscous or Kolmogoroff time defined by Eq. 13, while for $Re > Re_c$, the mixing time is the inertial value defined below the subsection on mesomixing.

A comparison of both scales is demonstrated in Figure 4 for a tubular reactor containing a SMXL static mixer. The values of the flow ratio of reactants and static-mixer properties indicate that an increase in volume flow rate shifts the mixing scale from the Kolmogoroff (micromixing) to the inertial (mesomixing) value at the transition Reynolds number $Re_c = 45{,}000$. One therefore wishes to remain on either the left or right of the transition value Re_c for accurate scale-up, since the physics of mixing changes at Re_c.

Micromixing ($\ell/\ell_k \leq 1$)

Comparison of two data points with equal selectivity but $Re < Re_c$ from the work of Baldyga et al. (1997) in Table 1, indicates that the Damköhler number defined by the viscous time scale in Eq. 13 is sufficient to scale the selectivity X_Q. Scale-up is therefore possible for equal kinetics and stoichiometry with constant Damköhler number $Da \, \alpha \, B_o t_k$ for the feed tubes in Figure 2, where B_o is the rate-limiting reactant concentration.

Table 1. Micromixing, Example Parameters for SMXL Mixer (Data from Baldyga, Bourne and Hearn, 1997)

Data Point	X_Q	Re	Sc	Da	Re_f	ℓ/ℓ_K	Q/Q_B
aqueous	.225	22,000	~ 900	1.2	120	~ 1.4	3,000
viscous	.225	4,400	~ 9,000	1.3	24	~ 0.4	3,000

Transition $Re_c = 45{,}000$.

Substitution for $u \, \alpha \, Q/D^2$ in Eq. 13, one obtains a reactor diameter of the form

$$D \, \alpha \left(\frac{f}{\alpha}\right)^{1/7} \left(\frac{Q^{3/7}}{B_o^{2/7} \nu^{1/7}}\right). \tag{19}$$

Since the ratio of reaction length-to-reactor diameter $L/D \, \alpha \, ut_k/ut_d$, one obtains

$$\frac{L}{D} \, \alpha \, \frac{\sqrt{\alpha/f}}{\sqrt{Re}},$$

or

$$\frac{L}{D} \, \alpha \left(\frac{\alpha}{f}\right)^{3/7} \left(\frac{\nu^{3/7}}{B_o^{1/7} Q^{2/7}}\right). \tag{20}$$

The exponents on the flow rate Q are identical to the values determined recently by Hearne (1995).

Mesomixing ($l/l_k > 1$)

Comparison of two data points in Table 2 with roughly equal selectivity but $Re > Re_c$ from the work or Bourne et al (1992) indicates that the Damköhler number based on an inertial time scale (defined below) is sufficient to scale the selectivity X_Q. The inertial time scale is defined as $t_m \, \alpha \, (l^2/\epsilon)^{1/3}$, with the reactant feed length l substituted for the integral scale l_e in Eq. 3 (see Baldyga et al., 1995). Substituting ϵ from Eq. 8 and the feed length l from Eq. 15, the inertial time scale becomes

$$t_m \, \alpha \left(\frac{Q_B}{nQ}\right)^{1/3} \left(\frac{\alpha}{f}\right)^{1/3} \left(\frac{D}{u}\right). \tag{21}$$

Table 2. Mesomixing, Example Parameters for SMXL Mixer (Data from Bourne, Lenzner and Petrozzi, 1992)

Data Point	X_Q	Re	Sc	micro Da	meso Da	ℓ/ℓ_K	Q/Q_B
aqueous	.151	45,000	~ 900	.09	2.8	~ 13	464
aqueous	.162	45,000	~ 900	.09	3.4	~ 17	278

Transition $Re_c = 6{,}700$.

This expression indicates that for a constant flow ratio of reactants, the mixing time scale is proportional to the resident time.

Scale-up is now possible for equal kinetics and stoichiometry with constant Damköhler number $Da \propto B_o t_m$. Substituting $u \propto Q/D^2$ in Eq. 21, one obtains the reactor diameter

$$D \propto \left(\frac{nQ}{Q_B}\right)^{1/9} \left(\frac{f}{\alpha}\right)^{1/9} \left(\frac{Q^{1/3}}{B_o^{1/3}}\right). \tag{22}$$

Since the ratio of reaction length-to-reaction diameter $L/D \propto ut_m/ut_d$, one obtains

$$\frac{L}{D} \propto \left(\frac{Q_B}{nQ}\right)^{1/3} \left(\frac{\alpha}{f}\right)^{1/3}. \tag{23}$$

The exponent for the flow rate Q in Eq. 23 is identical to the value determined by Hearn (1995) and the reactor length-to-diameter ratio is a constant for a fixed, flow ratio of reactants.

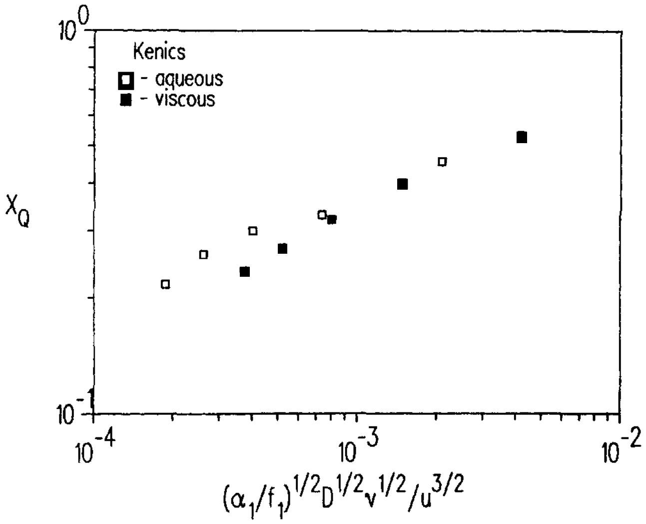

Figure 5. Selectivity vs. viscous or Kolmogoroff time in Kenics mixer for $Re < Re_C$.

$D = 0.04$ m; $\alpha = 0.9$; $L = 0.72$ m; $f_1 = 1.9$; $Re_C = 45{,}000$ (data from Baldyga et al., 1997).

Correlation of Data

Micromixing

The data correlated were taken from the work of Baldyga et al. (1997). In these experiments the selectivity of competing reactions (azocoupled) was measured in two types of static mixers, each operating at one of two fluid viscosities. In the reaction scheme below

$$A + B \rightarrow R$$
$$R + B \rightarrow S$$
$$AA + B \rightarrow Q,$$

the yield of Q or the selectivity X_Q was measured as a function of total volume flow rate, $Q = Q_A + Q_B$, through the static mixer of diameter, D, as illustrated in Figure 2. In this case, B was introduced slowly from two radial feed tubes. In all of the experiments the initial concentration of components A_o and AA_o were 0.02 and 0.08 mol/m^3, respectively, and the limiting reactant was B (sulfanilic acid). The indicated viscosities were changed by the addition of hydroxyethyl cellulose (HEC) (Gholap et al., 1994). Moreover, for both static mixers it was determined that the selectivity X_Q was dependent on the viscosity if the reactor-tube Reynolds number $Re < Re_C$, where Re_C was estimated to be 45,000 as described below. The latter data are considered to be micromixing controlled and are independent of the total feed-tube flow rate Q_B.

The transition Reynolds number $Re_C = 45{,}000$ was determined from the data of Baldyga et al. (1997, Fig. 5). In this case the viscous and aqueous data representing selectivity coalesce at a volume flow rate of $Q \sim 1.3$ dm^3/s, where the reactor Reynolds number $Re = Re_C$. Similar results were determined from the same publication (Baldyga, et al., 1997, Fig. 6). Substitution of the static mixer characteristics into Eq. 18 yields a universal constant $c = 1.9 \times 10^2$.

Data for the Kenics mixer, where $B_o = 50$ mol/m^3, are shown in Figure 5, where X_Q has been plotted vs. the Kolmogoroff time as defined in Eq. 13. As indicated, the data appear to be correlated with t_{k1} (Kenics mixer) for both the viscosities of 0.89 mPa s (aqueous) and 3.6 mPa s (viscous) for a reactor Reynolds number $Re < 45{,}000$.

Data for the Sulzer SMXL mixer, where $B_o = 30$ mol/m^3, are shown in Figure 6, where X_Q has been plotted vs. the Kolmogoroff time as defined in Eq. 13. The data appear to be correlated with t_{k2} (SMXL mixer) for both the viscosities of 0.89 mPa s and 8.9 mPa s for reactor Reynolds number $Re < 45{,}000$.

If the stoichiometry of regents A, AA, and the volumetric ratio of $Q_A/Q_B = 3{,}000$ are fixed in all of the experiments,

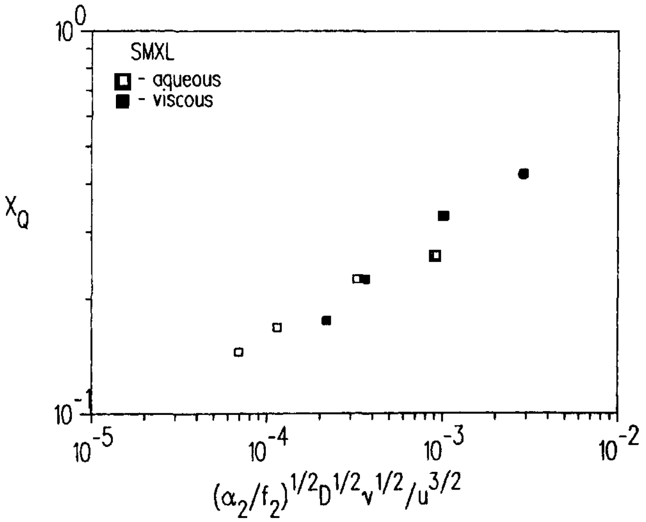

Figure 6. Selectivity vs. viscous or Kolmogoroff time in Sulzer SMXL mixer for $Re < Re_C$.

$D = 0.033$ m; $\alpha = 0.9$; $f_2 = 2.56$; $Re_C = 45{,}000$ (data from Baldyga et al., (1997).

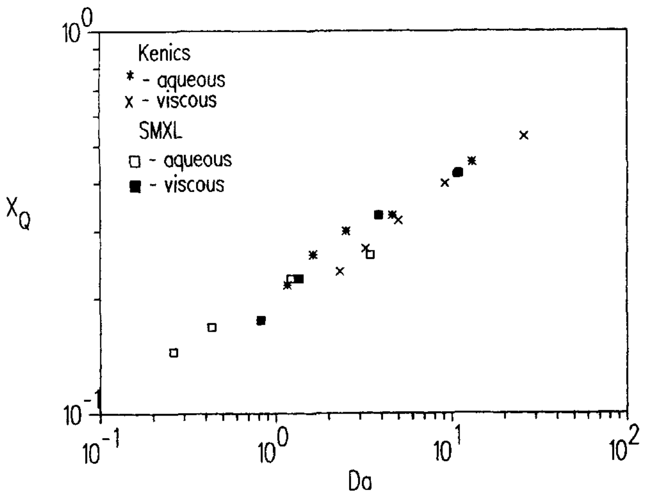

Figure 7. Selectivity vs. Damköhler number defined with the Kolmogoroff time scale.
Same data as in Figures 5 and 6.

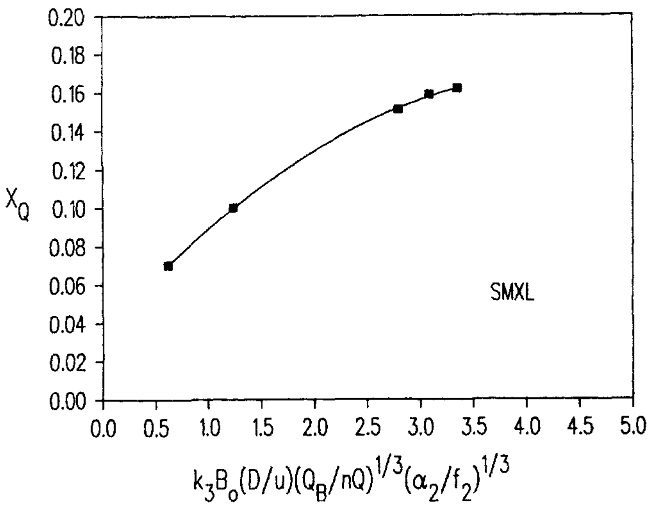

Figure 8. Selectivity vs. Damköhler number defined with the inertial or mesomixing time scale for $Re > Re_c$.
Data from Bourne et al., 1992, for $Re > Re_C$; $Re_C = 6{,}700$.

the selectivity X_Q should depend on the Damköhler number defined as the ratio of micromixing-to-reaction time. Thus, substituting Eq. 13 for the mixing time, one has the similarity parameter.

$$Da = \frac{k_3 B_o \nu^{1/2} D^{1/2}}{u^{3/2}} \left(\frac{\alpha_i}{f_i} \right)^{1/2}, \tag{24}$$

where $i = 1{,}2$ refers to the static mixer design of Kenics or SMXL, respectively and f_i is the constant Fanning friction factor for each design.

Figure 7 plots values of the selectivity X_Q vs. Damköhler number as defined by Eq. 24 with $k_3 = 125$ m^3/mols. As shown, this dimensionless group appears to properly correlate the data for both static mixer designs for various values of the fluid viscosity, flow rates, pipe diameter, and limiting reactant concentrations, provided the reactor Reynolds number $Re < 45{,}000$.

Mesomixing

In this section, data (averaged for repeat runs) were chosen for equal stoichiometry ($\xi = 1$) from the work of Bourne et al. (1992, Fig. 3 and table VII). The reaction was the same as that described in the preceding subsection, but, in contrast, the transition $Re_C = 6{,}700$ is much smaller than the reactor Reynolds number or $Re > Re_C$. Thus, the Damköhler number based on the inertial time scale defined by Eq. 21 was used to correlate the selectivity data for an SMXL static mixer, as shown in Figure 8. The form of the Damköhler number is

$$Da = k_3 B_o \left(\frac{D}{u} \right) \left(\frac{Q_B}{nQ} \right)^{1/3} \left(\frac{\alpha_2}{f_2} \right)^{1/3}. \tag{25}$$

Recent selectivity data from the work of Taylor (1998) and Taylor et al. (1998) are also correlated with the Damköhler number defined by Eq. 25. The parallel reaction system is the acid (HCL), base (NaOH) reaction in parallel with the slow decomposition of dimethoxypropane (DMP), where the rate constant for the latter is $k_2 = 700$ m^3/kmol-s. The main feed contained 0.2 kmol/m^3 of DMP (C) and 0.21 kmol/m^3 of NaOH (A), which was combined with a side stream of 2.0 kmol/m^3 of HCL (B). The total volumetric flow ratio of $Q_A/Q_B = 10$ was fixed for all data where the side stream consisted of two ($n = 2$) feed tubes of diameter $d_f = 0.051$ cm.

The laminar feed data ($Re_f < 2{,}500$) of Taylor et al. (1998) are plotted in Figure 9. A kinematic viscosity $\nu = 2.58 \times 10^{-6}$ m^2/s for a Kenics static mixer ($f_1 = 1.9$) and an average void fraction ($\alpha_1 = 0.73$) were assumed. The reactor transition Reynolds number for these conditions is $Re_C = 850$, while the range of reactor Reynolds numbers is $Re \geq Re_C$. As indicated in Figure 9, the inertial or mesomixing time is the correct

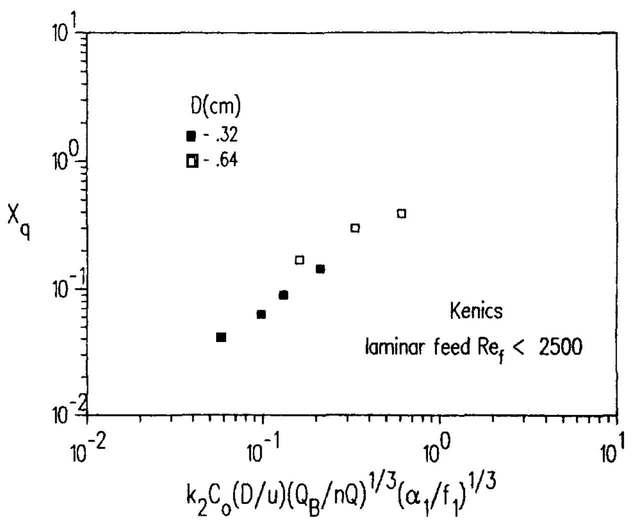

Figure 9. Selectivity vs. Damköhler number defined with the inertial or mesomixing time scale for $Re > Re_c$.
$Re > Re_C$, where $Re_C = 850$ (data from Taylor et al., 1998).

scale for these conditions. Additional data from the work of Taylor et al. (1998) for turbulent feed tubes ($Re_f > 2{,}500$) are discussed in the Appendix.

Conclusion

Mixing controlled parallel reactions in turbulent plug-flow reactors with laminar feed streams are shown to be correlated with either a viscous or an inertial time scale. The choice between time scales is shown to depend on the magnitude of a transition reactor Reynolds number Re_C that is constrained by the reactant volumetric flow ratio.

For a reactor Reynolds number $Re < Re_C$, the Damköhler number defined in terms of the viscous scale (Kolmogoroff) is sufficient to scale selectivity. In contrast if $Re > Re_C$, the inertial scale (mesomixing) is the appropriate scale. The selectivity is shown to be insensitive to the Reynolds number, provided Re does not cross the transition value during scale-up. Scale-up relations to predict the reactor diameter and length are provided for both cases, that is, Re either greater or less than Re_C.

Notation

c = universal constant
D = molecular diffusivity, $m^2 \cdot s^{-1}$; pipe dia., m
Da = Damköhler number
d_f = feed-tube dia. m
f = Fanning friction factor
k = rate constant, $m^3 \cdot mol^{-1} \cdot s^{-1}$
L = tube or reaction length, m
ℓ = reactant feed length scale, m
ℓ_e = integral length scale, m
ℓ_k = Kolmogoroff length, m
n = number of feed tubes
P = pressure, $N \cdot m^{-2}$
Q = total volume flow rate, $m^3 \cdot s^{-1}$
Q_A = flow rate of reactant A, $m^3 \cdot s^{-1}$
Q_B = total flow rate of reactant B, $m^3 \cdot s^{-1}$
Re = reactor Reynolds number
Re_f = feed-tube Reynolds number
Re_ℓ = eddy Reynolds number
Sc = Schmidt number
t_k = Kolmogoroff time, s
t_d = eddy dissipation time, s
t_m = inertial time scale, s
u = superficial fluid viscosity, $m \cdot s^{-1}$
u' = root-mean-square turbulent velocity fluctuation, $m \cdot s^{-1}$
X_Q = selectivity or product distribution

Greek letters

ϵ = turbulent energy dissipation, $m^2 \cdot s^{-3}$
κ = turbulent kinetic energy, $m^2 \cdot s^{-2}$
ν = kinematic viscosity, $m^2 \cdot s^{-1}$
ρ = fluid density, $kg \cdot m^{-3}$
α = static mixer tube void fraction
ξ = stoichiometric ratio

Subscripts

i = static mixer geometry
1,2 = Kenics or SMXL, respectively

Literature Cited

Baldyga, J., J. R. Bourne, B. Dubuis, A. W. Etchells, R. V. Gholop, and B. Zimmermann, "Jet Reactor Scale-Up for Mixing Controlled Reactions, *Trans. Inst. Chem.*, 73(A5), 497 (1995).

Baldyga, J., J. R. Bourne, and S. J. Hearn, "Interaction Between Chemical Reactions and Mixing on Various Scales," *Chem. Eng. Sci.*, **52**, 457 (1997).

Bolzern, O., J. R. Bourne, and G. Tovstiga, "Micromixing and Fast Reactions in the Core of Turbulent Pipe Flow," *Chem. Eng. Commun.*, **38**, 1 (1985).

Bourne, J. R., J. Lenzner, and S. Petrozzi, "Micromixing in Static Mixers: An Experimental Study," *Ind. Eng. Chem. Res.*, **31**, 1216 (1992).

Brodkey, R. S., *The Phenomena of Fluid Motions*, Dover, New York (1995).

Davies, J. T., *Turbulent Phenomena*, Academic Press, New York, 49 (1972).

Forney, L. J., and N. Nafia, "Turbulent Jet Reactors: Mixing Time Scales," *Trans. Inst. Chem. Eng.*, **76**, 728 (1998).

Forney, L. J., and M. Chang-Mateu, "Scale-Up for Micromixing in Plug Flow Reactors," AIChE Meeting, Miami, FL (1998).

Gholap, R. V., S. Petrozzi, and J. R. Bourne, "Influence of Viscosity on Product Distribution of Fast Competitive Chemical Reactions," *Chem. Eng. Technol.*, **17**, 102 (1994).

Hearn, S., "Turbulent Mixing Mechanisms in Motionless Mixers," *PhD Diss.*, Univ. of Birmingham, Birmingham, England (1995).

Kresta, S., "Turbulence in Stirred Tanks: Anisotropy, Approximate and Applied," *Can. J. Chem. Eng.*, **76**, 563 (1998).

Li, K. T., and H. L. Toor, "Turbulent Reactive Mixing with a Series-Parallel Reaction: Effect of Mixing on Yield," *AIChE J.*, **32**, 1312 (1986).

Paul, E. L., "Design of Reaction Systems for Specialty Organic Chemicals," *Chem. Eng. Sci.*, **43**, 1773 (1988).

Taylor, R. A., W. R. Penney, and H. X. Vo, "Scale-Up Methods for Fast Competitive Chemical Reactions in Pipeline Mixers," AIChE Meeting, Miami (1998).

Taylor, R. A., "Scale-Up Methods for Fast Chemical Reactions in Pipeline Mixers," MS Thesis, Univ. of Arkansas, Fayetteville, AR (1998).

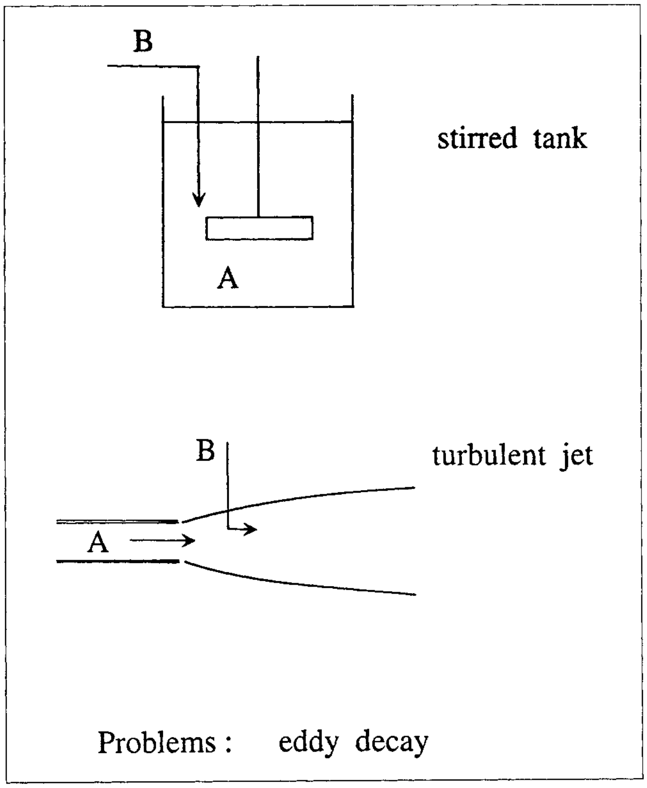

Figure A1. Stirred tank and turbulent jet reactor.

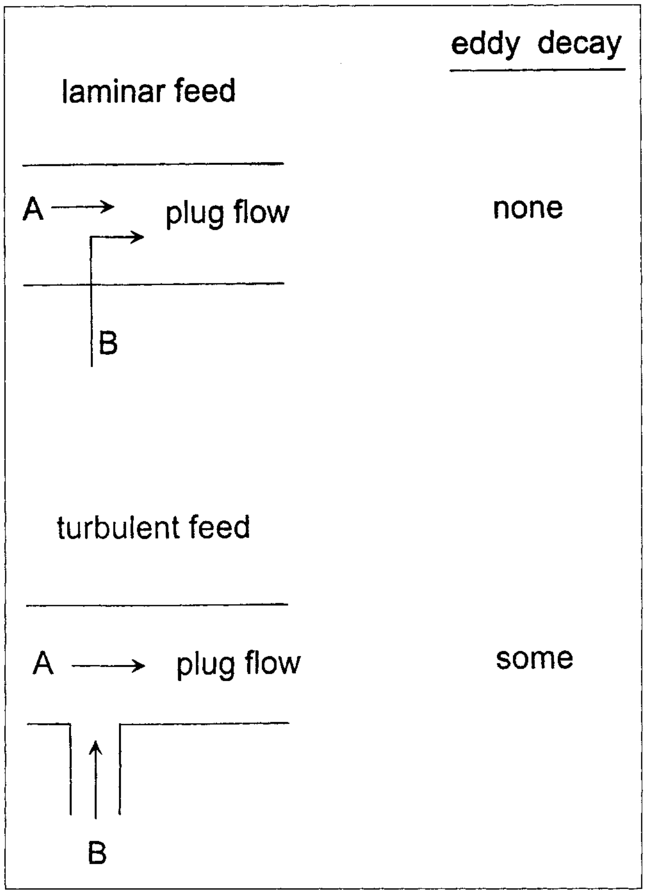

Figure A2. Laminar and turbulent feed in a plug-flow reactor.

Appendix

Eddy decay

For the reactor designs shown in Figure A1, the mixing times within the ambient fluid near the injection point of B are subject to eddy decay. That is, the turbulent length and time scales change with position as B is convected away from the injection point, thus complicating scale-up. A useful alternative is a plug-flow reactor as shown in Figure A2, which may contain static mixing elements. The plug-flow design reduces eddy decay depending on the nature of the reactor feed. In particular, if B is introduced in a laminar feed, eddy decay is minimized and scale-up problems are reduced.

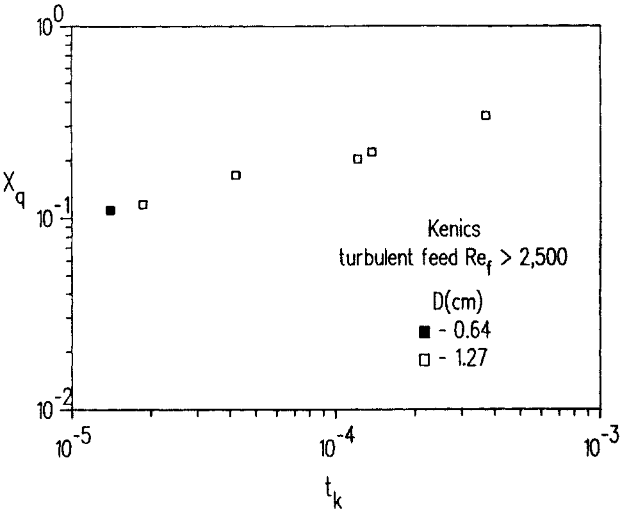

Figure A3. Selectivity vs. Damköhler number defined with the viscous or Kolmogoroff time scale.

Data are for turbulent feed (data from Taylor et al., 1998).

Turbulent feed

The turbulent feed, selectivity data ($Re_f > 2{,}500$) vs. the Kolmogoroff time from the recent work of Taylor (1998) and Taylor et al. (1998) are plotted in Figure A3. These data correspond to several points for the large reactor diameter ($D = 1.27$ cm) and with a turbulent feed Reynolds number covering the range $2{,}800 < Re_f < 21{,}000$. The remaining data point for the intermediate reactor size ($D = 0.64$ cm) has a feed Reynolds number $Re_f = 4{,}960$.

Because both the feed and ambient streams are turbulent, an unsuccessful attempt was made to correlate these limited data with a Kolmogoroff time based on the more intense turbulence at the feed-tube nozzle. In the latter case, the viscous or Kolmogoroff time defined by Eq. 13 is reduced for the feed-tube nozzle conditions, since $d_f \ll D$ and $u_f \gg u$. Thus, the larger ambient value for t_k within the tube (rate limiting) is the correct mixing scale for the turbulent feed case.

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