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The Segregation Number in Polymer Reactor Engineering

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Nauman defined in his review paper [1] that "the segregation number is . . . a ratio of characteristic times; a characteristic time for micromixing divided by a characteristic time for macromixing:"

$$N_{seg} = \tau_{micro}/\tau_{macro}$$

and has also selected as "a logical characteristic time for the macromixing is the mean residence time $\bar{t}$." The final result of his derivation for a spherical droplet is

$$N_{seg} = 0.55r^2/\pi^2 D\bar{t}$$

for a continuously stirred tank reactor (CSTR), where D is the diffusion coefficient and micromixing results from molecular diffusion between droplets (of packets or eddies) and the bulk of reactor fluid, and r is the radius of these droplets or eddies. It is supposed that an agitator dispersed the fluid down to the characteristic radius of r.

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The segregation number is a valuable tool and its introduction is a major advance in polymer reactor engineering. The proposed form is correct and practical to show the effect of changing mean residence time on segregation at otherwise constant conditions, most importantly for constant temperature.

If one wants to show the effect of temperature on segregation for one particular reaction, or wants to compare widely different polymerizations for segregation effects, the natural time unit seems to be the reciprocal of the first-order kinetic constant $\tau_{macro} = 1/k$. Namely, the monomer is in the polymerization reactor for the selected residence time to undergo polymerization to the desired degree. The rate of this conversion and consequently the residence time, i.e., the time available for macromixing, is governed by the specific rate of polymerization and this is customarily characterized by the kinetic constant. For reactions of higher order or of unknown mechanism, a pseudofirst-order rate "constant" can be expressed as

$$k = \frac{\text{average reaction rate in moles per unit volume and unit time}}{\text{average concentration in moles per unit volume}}$$

where the concentration, the reaction rate, and the diffusion coefficient all have to be expressed for the same component in the system. For a CSTR the average reaction rate is the steady-state rate and the average concentration is the steady-state discharge concentration.

This simplification was first suggested by Wagner [2] for cases of unknown mechanism in pore diffusion influenced heterogeneous catalytic kinetics. The pseudofirst-order rate "constant" is defined in general as

$$\text{"k"} = \left(-\frac{dC}{dt}\right)\frac{1}{C}$$

For power kinetics this is equivalent to

$$\text{"k"} = k_n C^{n-1}$$

In CSTR this leads to

$$\frac{C_{in} - C_{out}}{\bar{t} C_{out}} = k_n C_{out}^{n-1}$$

where $\bar{t}$ is the average residence time.

For real first-order reactions in a CSTR at 50% conversion, i.e., when

$C_{out} = 0.5C_{in}$, $1/\bar{t} = k$. When conversion is higher than 50%, $1/\bar{t} < k$, and if conversion is less than 50%, $1/\bar{t} > k$, but within a useful conversion range they will be in the same order of magnitude. This can also be shown for tubular reactors.

Now if we use for $\tau_{macro} = 1/k$

$$N_{seg} = \frac{\tau_{micro}}{\tau_{macro}} = \frac{0.55r^2}{\pi^2 D \frac{1}{k}} = \frac{0.55}{2} r^2 \frac{k}{D}$$

where

$$r^2 \frac{k}{D} = DaII = \phi^2$$

then the segregation number, except for the numerical constant, is the same as the second Damköhler number that was first introduced in 1936 for characterizing diffusion influenced reaction rates [3]. This, in turn, is the same as the square of the Thiele modulus used in heterogeneous catalysis since 1936 [4]. The general usefulness of the so-called "effectiveness factor" that follows from the work of Damköhler and Thiele for other than heterogeneous catalytic systems was shown by Weisz [5].

The introduction of the segregation number by Naumann becomes more significant by being a special case of the Damköhler-II number, which is a more fundamental dimensionless number. In this way a greater unity of basic chemical engineering principles becomes apparent.

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