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Mixing Considerations in Chemical Reactor Scale-Up

Andrew Fiore, Ph.D.

Andrew Spann, Ph.D.

Nagi Elabbasi, Ph.D.

contact@veryst.com
www.veryst.com

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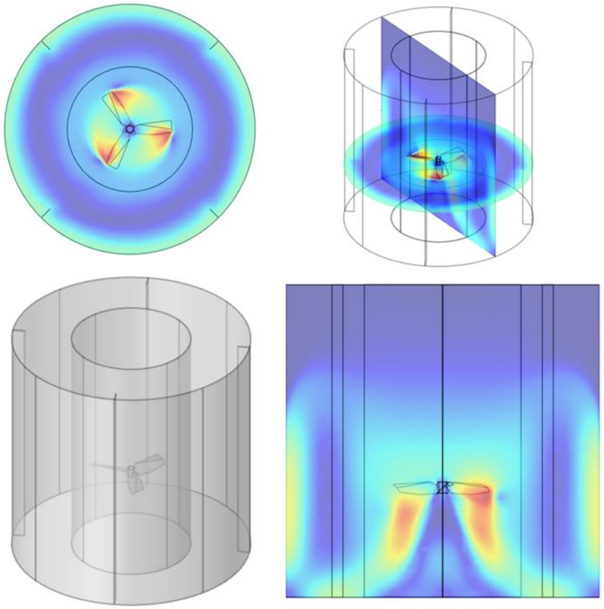
Scale-up In Chemical Reactors

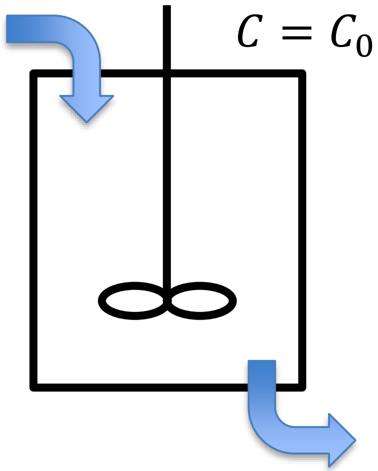
- Scaling chemical reactors from lab scale to pilot scale to production scale requires a detailed understanding of the physical system
  - Coupled heat transfer, mass transfer, reaction kinetics, fluid flow
- Chemical reactor scale-up considerations
  - Geometric similarity
  - Ratio of surface area to volume
  - Energy input, generation, and removal rates
  - Rate-limiting transport processes
  - Mixing efficiency



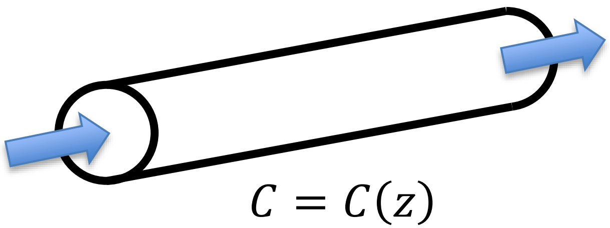
Mixing in Chemical Reactions

- Two ideal reactor models are often used to illustrate the importance of mixing on reaction yield and selectivity

Continuously Stirred Tank Reactor (CSTR) – complete mixing (uniform concentration everywhere)



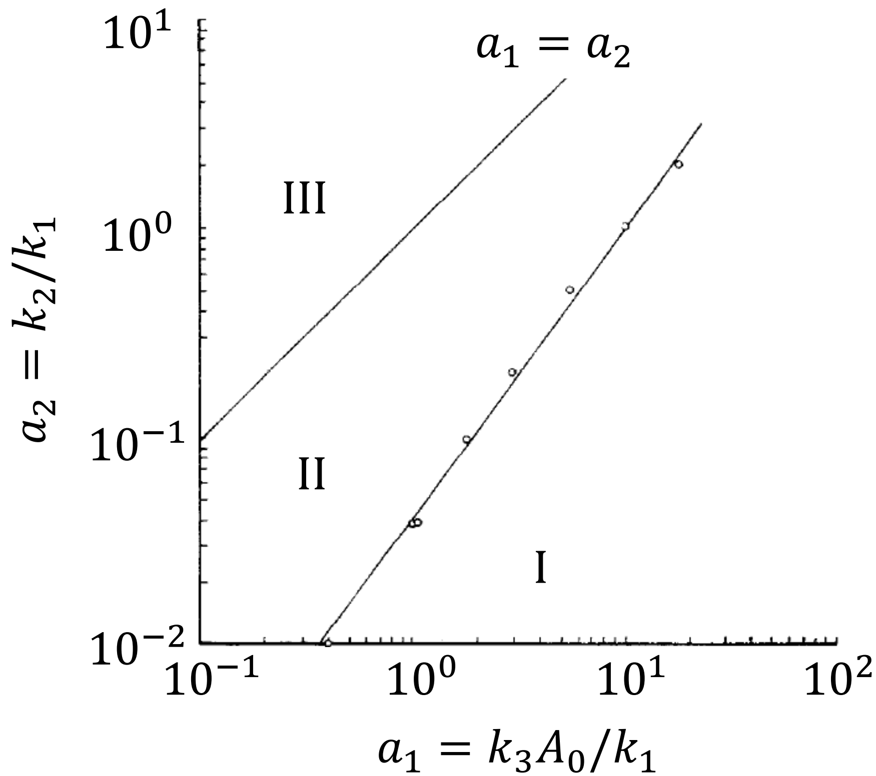
Plug Flow Reactor (PFR) – zero axial mixing (spatially varying concentration)



- More complicated mixing models can be developed from combinations of these simple models

Mixing in Chemical Reactions

- The Van de Vusse reaction system demonstrates the reactor design tradeoffs inherent in the simple PFR and CSTR models



$$\begin{cases} A \xrightarrow{k_1} B \xrightarrow{k_2} C \\ A + A \xrightarrow{k_3} D \end{cases}$$

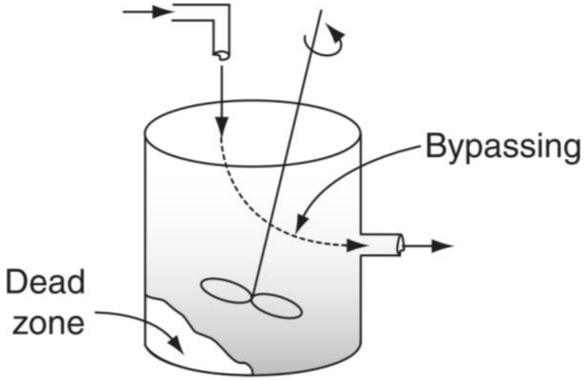
B is the desired product
C and D are undesired byproducts

Region	Highest Yield of B	Highest Selectivity
I	CSTR	CSTR
II	PFR	CSTR
III	PFR	Either

Van de Vusse, Chem. Eng. Sci., 1964

Non-Ideal Mixing – Turbulence

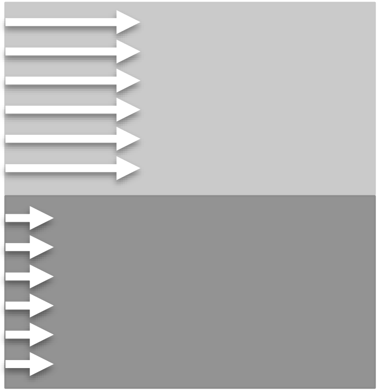
- Ideal mixing models (PFR, CSTR) may not be valid at larger scales, and are unlikely to be useful approximations for complicated reactor schemes
- Non-ideal mixing is controlled by fluid mechanics within the reactor and is often quantified using a residence time distribution
  - Dead zones
  - Short-circuits
  - Recirculation regions
- Turbulence changes the flow pattern within the reactor
- Turbulence can affect mixing without significantly modifying the residence time distribution

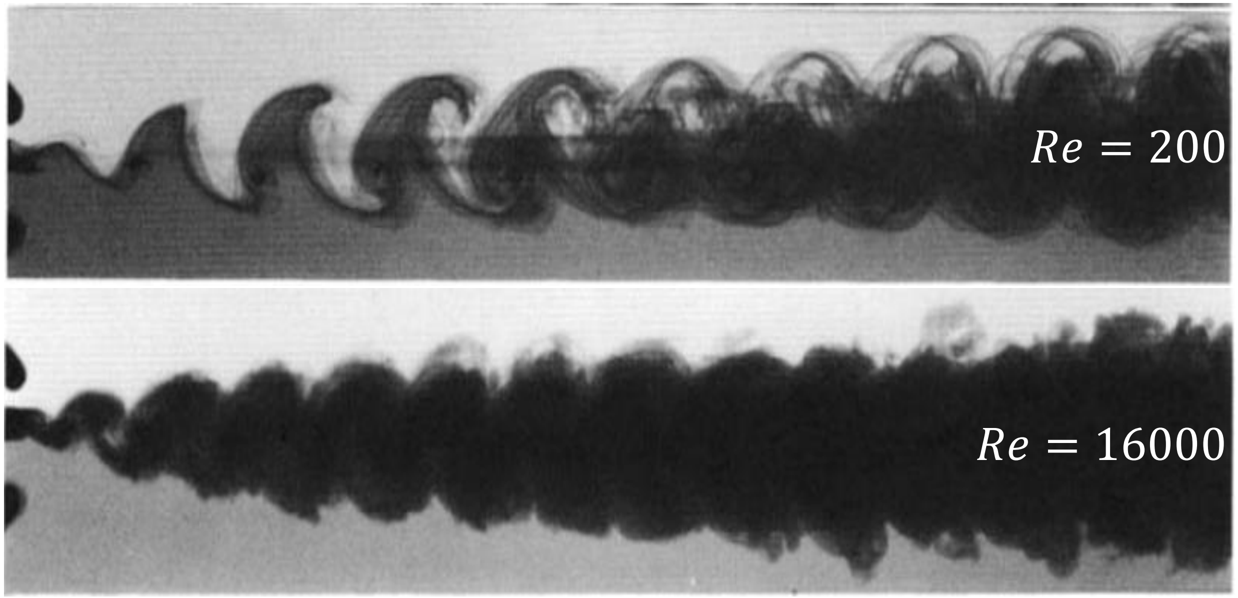


Adapted from Figure 13.3 (Fogler, 2010)

How Turbulence Affects Mixing

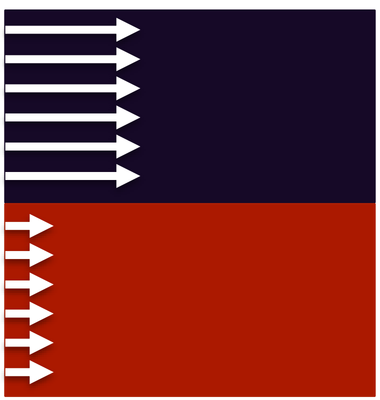
- Turbulence increases mixing through eddies and vortices – the chaotic motion in turbulent flows causes dissolved species to effectively diffuse far more quickly than by molecular diffusion alone
- Example: Reaction in a shear flow (Breidenthal, *J. Fluid Mech.*, 1981)
  - Fast fluid is light grey; slow fluid is medium grey; reaction product is dark grey

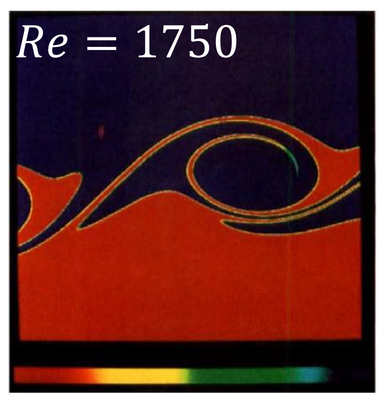


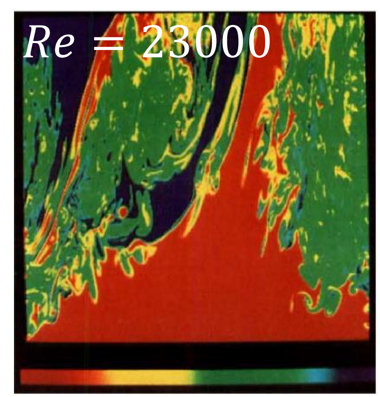


How Turbulence Affects Mixing

- Turbulence increases mixing through eddies and vortices – the chaotic motion in turbulent flows causes dissolved species to effectively diffuse far more quickly than by molecular diffusion alone
- Example: Reaction in a shear flow (Koochesfahani and Dimotakis, *J. Fluid Mech.*, 1986)
  - Fast fluid is dark blue; slow fluid is red; intermediate colors indicate reactant products

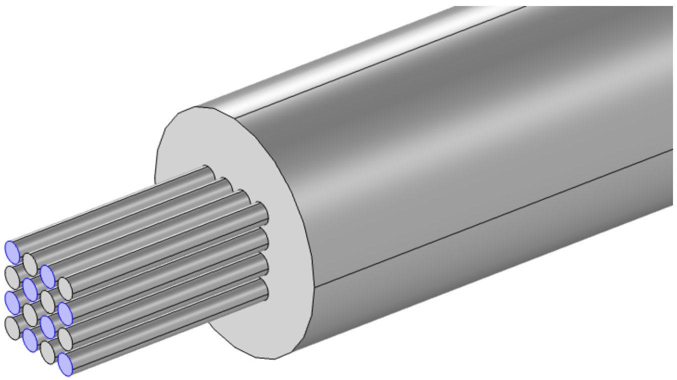


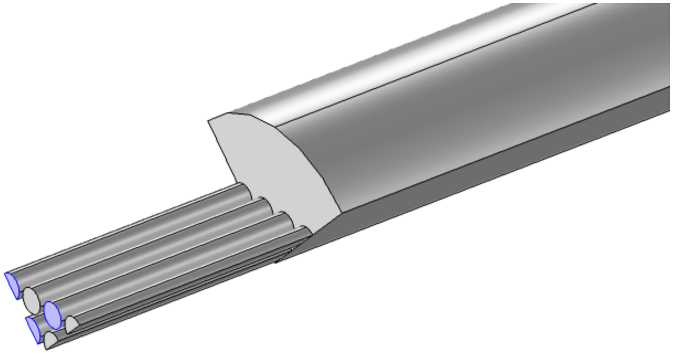




A Model Reactor Setup for Mixing Studies

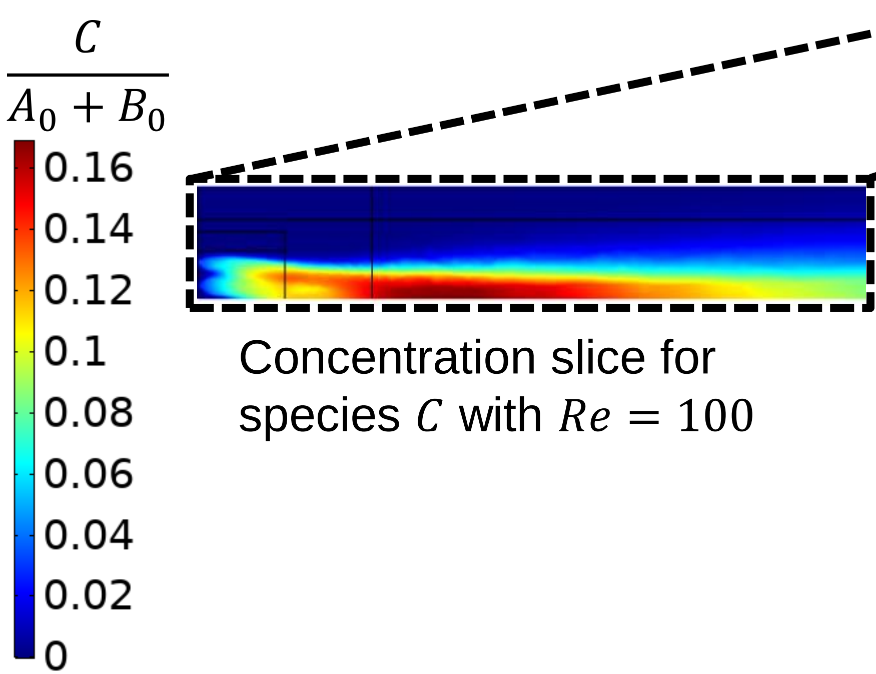
- To model the effect of turbulent mixing on the chemical reaction, we use a multi-inlet tubular reactor, shown at right (top)
  - Different reactants enter the reactor through alternating inlets, indicated by the surfaces highlighted in blue
- The reactor has two planes of symmetry, so we model only one-quarter of the reactor, shown at right (bottom)



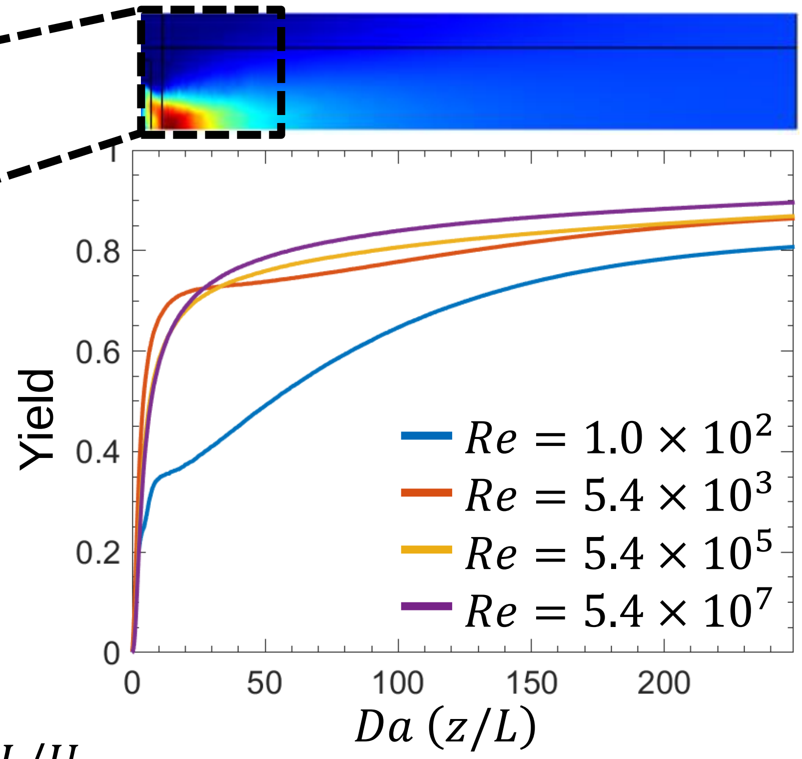


Yield in Bimolecular Reactions

- We start by considering a simple bimolecular reaction: $A + B \xrightarrow{k_1} C$
- The yield of species C is shown below as a function of dimensionless distance along the reactor



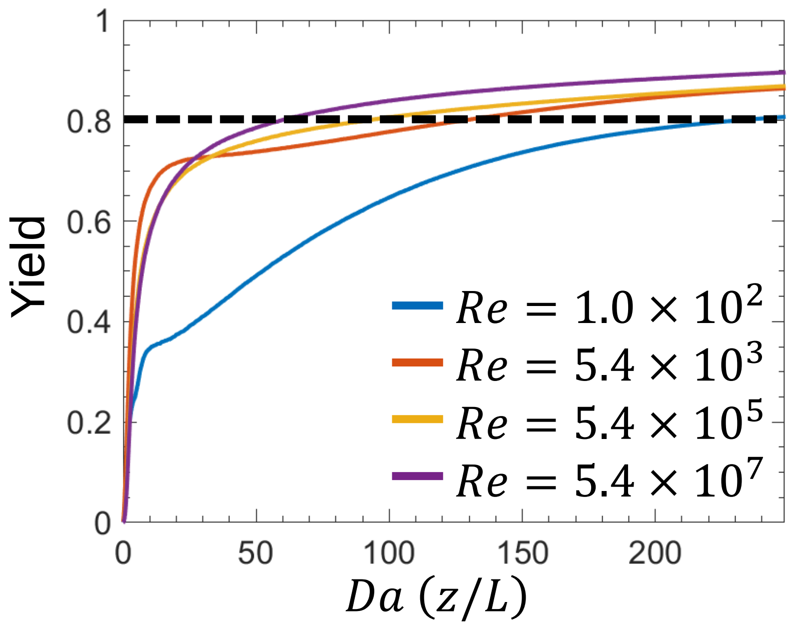
Concentration slice for species C with $Re = 100$



Damkohler number, $Da = k_1 A_0 L / U$

Implications in Reactor Design and Scale-up

- The residence time required to achieve 80% conversion of the product decreases with increasing Reynolds number, and is much lower for turbulent flows than laminar ones, as highlighted in the table below



$Re = \frac{UL}{\nu}$	$Da = k_1 A_0 \left(\frac{L}{U}\right)$
1.0×10^2	230.2
5.4×10^3	127.3
5.4×10^5	90.6
5.4×10^7	59.0

In the table above, the Damkohler number, Da, provides the desired reactor size

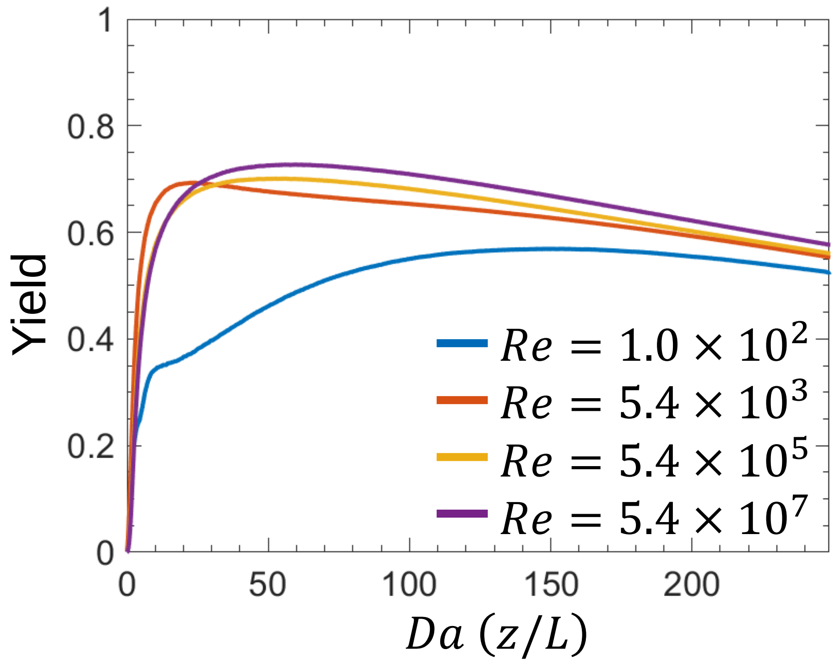
Yield in Bimolecular Reactions with Product Decomposition

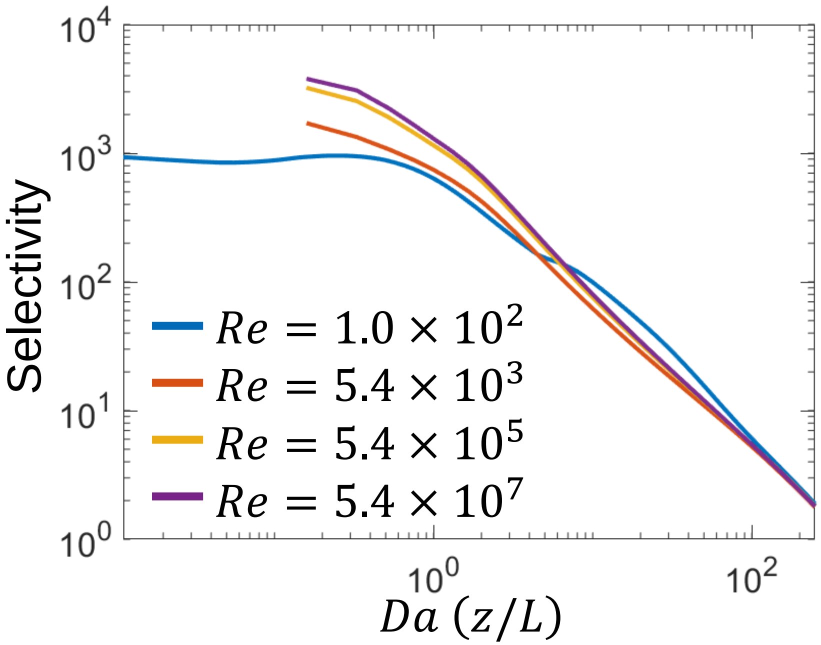
- Suppose that the original bimolecular reaction is accompanied by decomposition of the product to an undesired byproduct

$$A + B \xrightarrow{k_1} C$$

$$C \xrightarrow{k_2} D$$

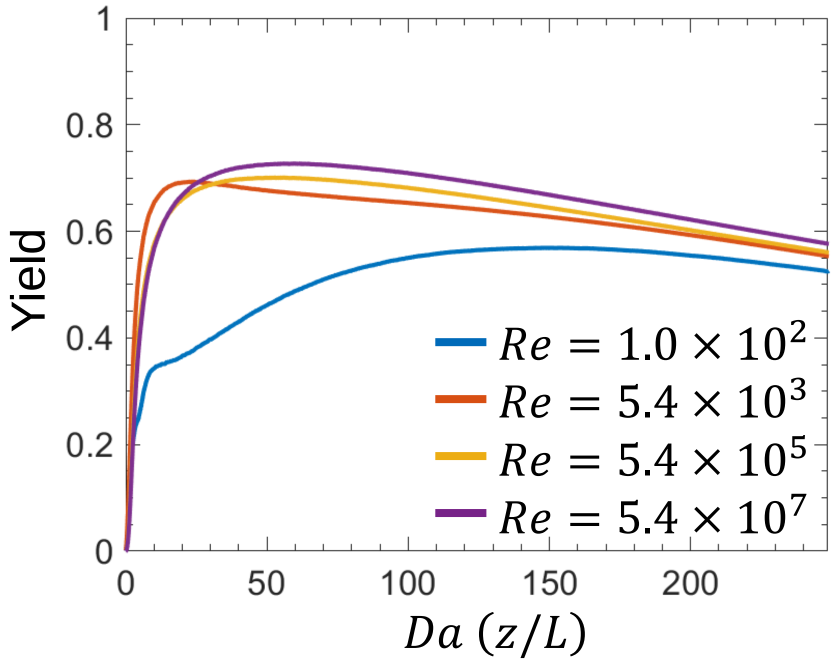
- The yield (left) and selectivity (right) of species C is shown below as a function of dimensionless distance along the reactor





Implications in Reactor Design and Scale-up

- The reactor size for optimal yield at each Reynolds number is summarized in the table below

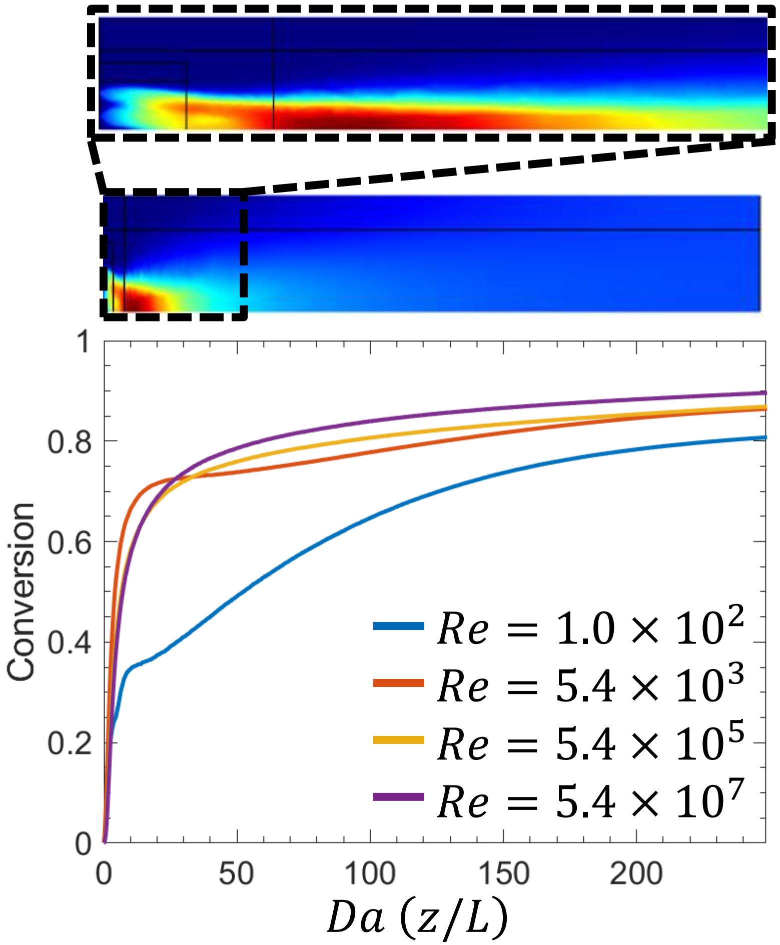


$Re = \frac{UL}{\nu}$	Da	Optimal Yield
1.0×10^2	150.1	57%
5.4×10^3	23.5	69%
5.4×10^5	56.1	70%
5.4×10^7	59.3	73%

$$Da = k_1 A_0 \left(\frac{L}{U}\right)$$

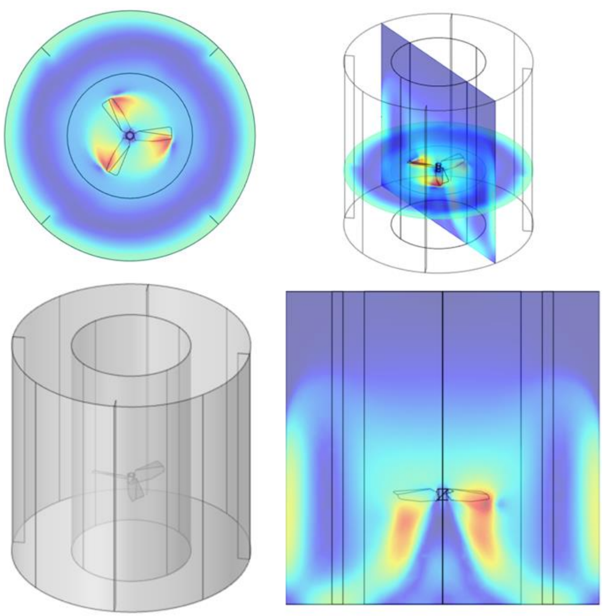
Summary

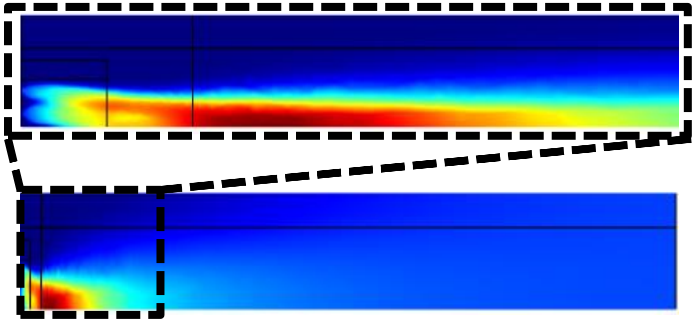
- Chemical reactor scale-up is a complex problem involving detailed understanding of fundamental physics
- Simulations are a useful tool to understand how physics change with scale
- Mixing and turbulence affect the yield of chemical reactions, even in geometrically similar reactors
- Multiphysics simulations using COMSOL can be used to optimize reactor designs at scale



Summary

- At Veryst, we combine insight into fundamental physics of chemical reactors with computational models to help our clients solve reactor scale-up problems, including
  - Stirred tank reactors
  - Packed bed reactors
  - Flow reactors (laminar flow, plug flow)
  - Microreactors





References

- Broadwell, J.E. and Breidenthal, R.E., 1981. Structure in turbulent mixing layers and wakes using a chemical reaction. *Journal of Fluid Mechanics*, *109*, pp.1-24.
- Koochesfahani, M.M. and Dimotakis, P.E., 1986. Mixing and chemical reactions in a turbulent liquid mixing layer. *Journal of Fluid Mechanics*, *170*, pp.83-112.
- Fogler, H.S., 2010. *Essentials of Chemical Reaction Engineering*. Pearson Education.
- Van de Vusse, J.G., 1964. Plug-flow type reactor versus tank reactor. *Chemical Engineering Science*, *19*(12), pp.994-996.