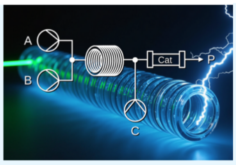
Karlsruhe Institute of Technology

GeCatS Infoday "From Flow Chemistry to Continuous Processes: New Alternatives for Chemical Production on Laboratory and Ton Scale"



P 08

9 December 2025
DECHEMA-Haus, Frankfurt am Main

A-priori estimation of axial dispersion and residence time distribution in laminar flow through helically coiled tubes

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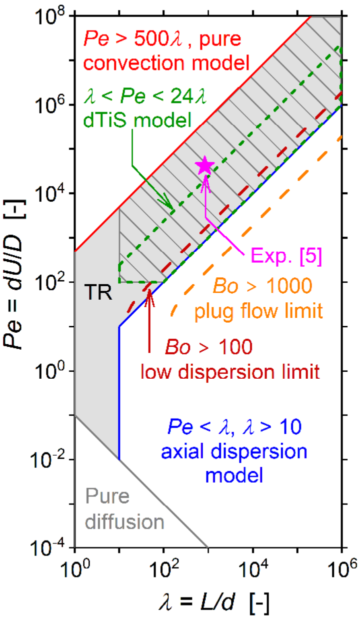
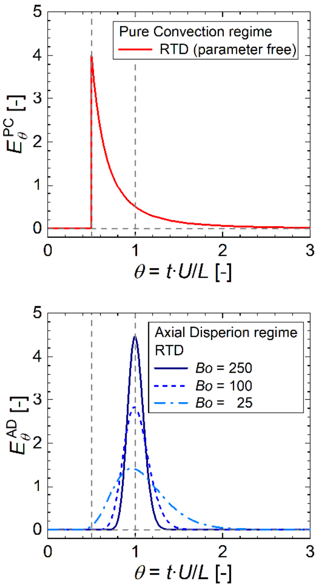
Motivation

- Flow chemistry and continuous processes offer the advantage of controlled residence times
- Often a helically coiled capillary serves as residence time providing unit (see event logo in poster header)
- Here, a predictive model for the residence time distribution (RTD) of solutes in laminar solvent flow through helically coiled tubes is proposed

Dispersion map straight tubes

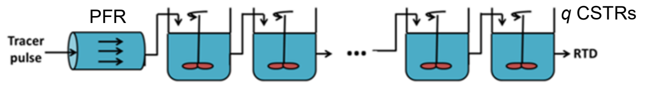
- Circular pipe (diameter $d = 2a$, length L), laminar solvent flow (mean velocity U), passive solute (molecular diffusivity D), $Bo = LU/D_{ax} \approx 192\lambda/Pe$
- Dispersion regime map[1] adapted from Levenspiel[2]



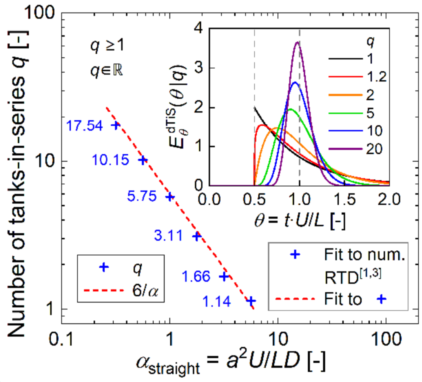


- Mechanistic model for hatched part of transition regime (TR) and delayed-Tank-in-Series model for dashed region as function of $\alpha = Pe/4\lambda = a^2U/LD$ (see ref[1])

RTD model for straight tubes



$$E_\theta^{\mathrm{dTiS}}(\theta \geq 0.5 \mid q) = \frac{2q^q}{\Gamma(q)}(2\theta - 1)^{q-1}\exp\left[-q(2\theta - 1)\right]$$



$$q = \frac{6}{\alpha_{\mathrm{straight}}} = \frac{6LD}{a^2U}$$

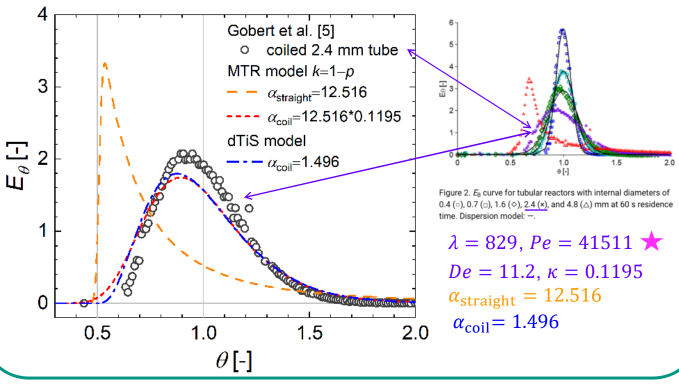
$$0.25 \leq \alpha_{\mathrm{straight}} \leq 6$$

RTD model for coiled tubes

- CFD based correlation for dispersion reduction factor[4]

$$\kappa = \frac{D_{\mathrm{ax,coil}}}{D_{\mathrm{ax,straight}}} = \left\{1 + 0.9415\left[\log_{10}(520De^2) - 2\right]^{1.983}\right\}^{-1} \leq 1$$

$$De = Re\sqrt{d/2R_{\mathrm{coil}}} \qquad \alpha_{\mathrm{coil}} = \kappa \cdot \alpha_{\mathrm{straight}}, \; E_\theta^{\mathrm{coil}} = E_\theta^{\mathrm{dTiS}}(\theta \mid \alpha_{\mathrm{coil}})$$



Since $\alpha_{\mathrm{straight}}$ and the dispersion reduction factor κ depend on prior known parameters, the dTiS model can be used to estimate or predict the solute RTD in a solvent flowing laminar through a helically coiled tube. The model is particularly suited for the transition regime often encountered in continuous flow chemistry where the axial dispersion model fails.

[1] M. Wörner, Dispersion and residence time distribution of laminar tubular flow in the transition regime – models for flow chemistry and beyond, *Chem. Eng. Sci.* **318** (2025) 122116
[2] O. Levenspiel, Chemical Reaction Engineering, 3rd ed. 1999, John Wiley & Sons, Hoboken, NJ, Fig. 15.2
[3] J. A. T. A. Dantas, P.R. Pegoraro, J.A.W. Gut, Determination of the effective radial mass diffusivity in tubular reactors … , *Int. J. Heat Mass Transfer* **71** (2014) 18-25
[4] F. Florit, R. Rota, R., K.F. Jensen, Dispersion in coiled tubular reactors: a CFD and experimental analysis on the effect of pitch, *Chem. Eng. Sci.* **233** (2021) 116393
[5] S.R.L. Gobert, S. Kuhn et al., Characterization of milli and microflow reactors: mixing efficiency and residence time distribution, *Org. Process Res. Dev.* **21** (2017) 531–542