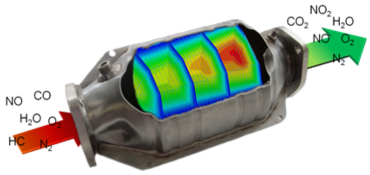

MODEGAT VIII

Bad Herrenalb, Germany
September 21-23, 2025
8th International Symposium on Modeling of Exhaust-Gas After-Treatment

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WORK IN PROGRESS

Influence of inhomogeneities on steady-state conversion in monolithic catalysts – Estimations by an analytical model

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Motivation

- Inhomogeneities in monolithic catalysts
  - Non-uniform sizes of individual channels
  - Velocity profile over front face of the monolith
  - Non-uniform temperature of the monolith
- Goal: estimate impact on steady conversion

Species transport equation

- Single circular channel (radius a, length L)
- Poiseuille velocity profile (mean velocity U)
- 1st order heterogeneous reaction (rate constant k)
- Dimensionless steady axisymmetric concentration equation ($0 \le R = r/a \le 1$, $0 \le Z = z/L \le 1$)

$$\frac{\partial^2 C}{\partial R^2} + \frac{1}{R}\frac{\partial C}{\partial R} - 2\alpha(1-R^2)\frac{\partial C}{\partial Z} = 0, \quad C(R, Z=0) = 1$$

$$\partial C/\partial R\big|_{R=0} = 0, \quad \partial C/\partial R\big|_{R=1} = -Da \cdot C(R=1, Z)$$

- Radial diffusion time / space time $\alpha = a^2 U / LD$
- Damköhler number $Da = k \cdot a / D$, $Da_{NO} = O(1)$
- Standard SCR $4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O$

Eigenvalue problem

- Separation of variables $C = \varphi(R) \cdot \psi(Z)$
- Sturm-Liouville eigenvalue problem (irregular)

$$\alpha \frac{\psi'(Z)}{\psi(Z)} = \frac{\varphi''(R) + \varphi'(R)/R}{2(1-R^2)\cdot\varphi(R)} = \text{const.} = -2\omega$$

- Solution of axial ODE $\psi(Z \mid \alpha, \omega) = \exp(-2\omega Z/\alpha)$
- Radial ODE with boundary conditions

$$\varphi''(R) + \varphi'(R)/R + 4\omega(1-R^2)\cdot\varphi(R) = 0$$

$$\varphi'(R=0) = 0, \quad \varphi'(R=1) = -Da \cdot \varphi(R=1)$$

- Novel combination of approaches for a 1st order homogeneous reaction [1] with an eigenfunction ansatz proposed for a 1st order heterogenous reaction fulfilling the boundary conditions [2]

Novel analytical solution

- Ansatz for eigenfunctions

$$\varphi_{(n)}(R \mid Da, \omega_{(n)}) = \sum_{k=1}^{\infty\,(n)} b_k(Da, \omega_{(n)}) \cdot \left(1 - \frac{Da}{2k+Da} R^{2k}\right)$$

- Insert in ODE and eliminate order $R^{2(k-1)}$ terms

$$\frac{Da}{2+Da} = \omega_{(n)} \sum_{k=1}^{\infty} b_k(Da, \omega_{(n)}), \quad b_1 = 1, \quad b_2 = -\frac{4+Da}{2+Da}\frac{1+\omega_{(n)}}{4}$$

$$b_{k\ge 3}(Da, \omega_{(n)}) = \omega_{(n)} \frac{2k+Da}{k^2}\left(\frac{b_{k-2}}{2(k-2)+Da} - \frac{b_{k-1}}{2(k-1)+Da}\right)$$

Conversion in single channel

- To do: superpose truncated eigenfunctions ($\infty \rightarrow n$) to approximate inlet condition $C(R, Z=0) = 1$
- Here: $C(R, Z \mid \alpha, Da) \approx \dfrac{\varphi_3(R \mid \omega_3(Da))}{\varphi_3(R=0)} \cdot \exp\left(-\dfrac{2\omega_3 Z}{\alpha}\right)$

$$= \left[1 - \omega_3\left(R^2 - \frac{1+\omega_3}{4}\cdot R^4 + \frac{\omega_3(5+\omega_3)}{36}\cdot R^6\right)\right]\cdot\exp\left(-\frac{2\omega_3 Z}{\alpha}\right)$$

$$36Da - (36+27Da)\omega_3 + (6+4Da)\omega_3^2 - (6+Da)\omega_3^3 = 0$$

- Outlet concentration $C_{out} = 4\int_0^1 C(R, Z=1)\cdot(R-R^3)\,\mathrm{d}R$

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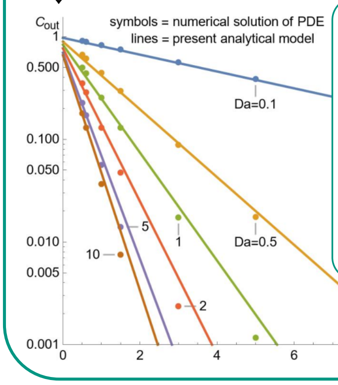

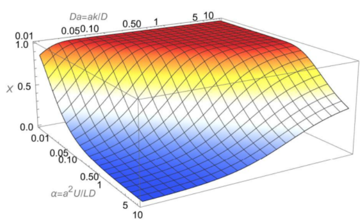

Conversion $X = 1 - C_{out}(\alpha, Da)$

Outlook

- Use single-channel model to study effects of inhomogeneities by statistical/deterministic variation of channel sizes, flow maldistribution and temperature profile in the monolith

[1] H. A. Lauwerier, A diffusion problem with chemical reaction, *Applied Scientific Research Section A* **8** (1959) 366-376
[2] K. M. Nigam, V. K. Srivastava and K. D. P. Nigam, Homogeneous-heterogeneous reactions in a tubular reactor: An analytical solution, *Chem. Eng. J.* **25** (1982) 147-150