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Model for Steam Reforming of Ethanol Using a Catalytic Wall Reactor

J.A. Torres and D. Montané

WOOD BIOPOLYMERS GROUP
Department of Chemical Engineerig · ETSEQ · Rovira i Virgili University

Reactor Modeling

General

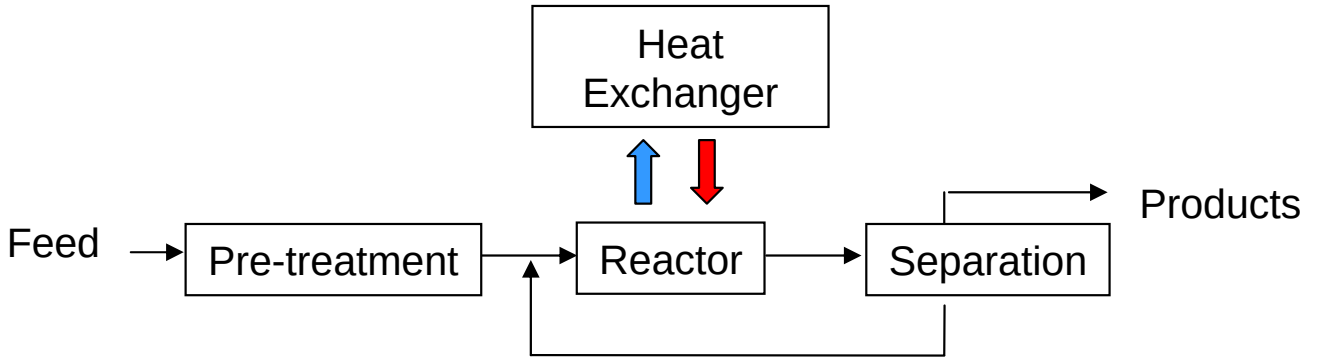
Evaluate the technical feasibility of using a Catalytic Wall Reactor (CWR) to perform Steam Reforming of Ethanol under conditions of high thermal efficiency

Specific Objectives

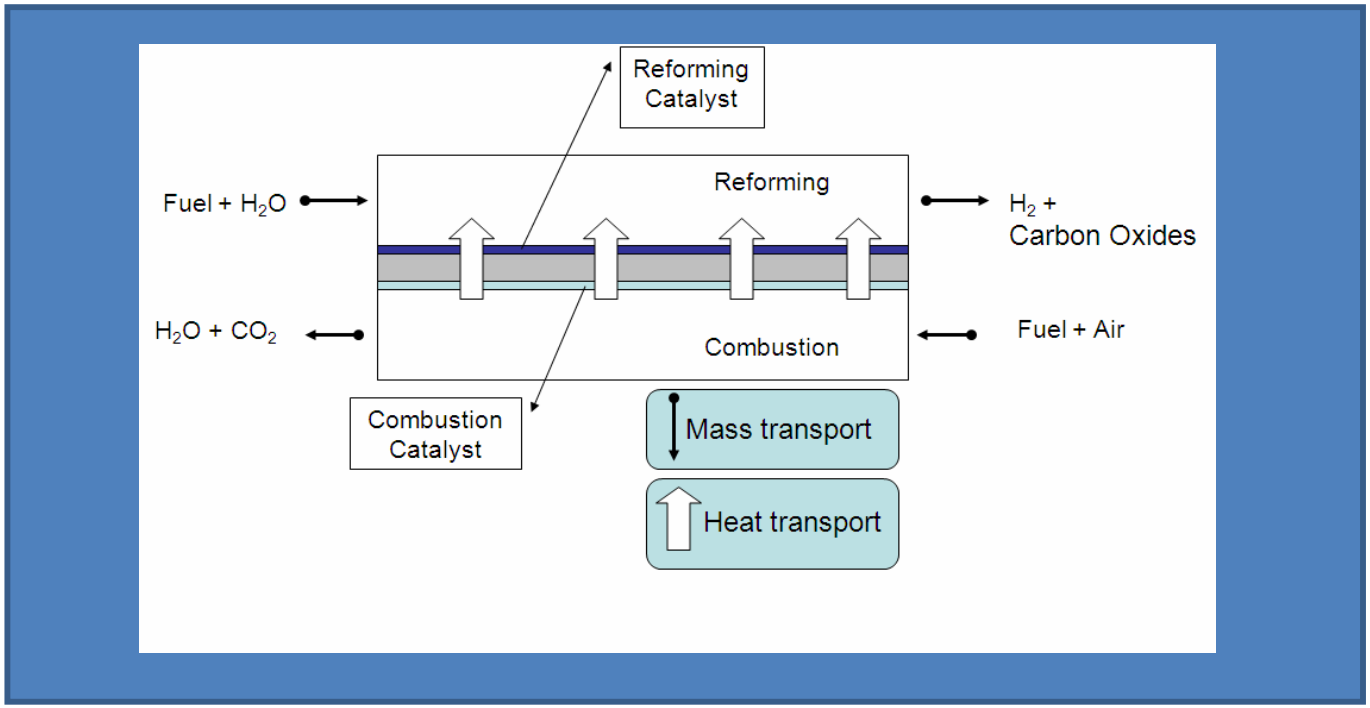
1. Conceptual analysis using multi-physics simulation
2. Anticipate possible operational regime on the CWR before performing the experiments

Some strategies in Reactor Engineering

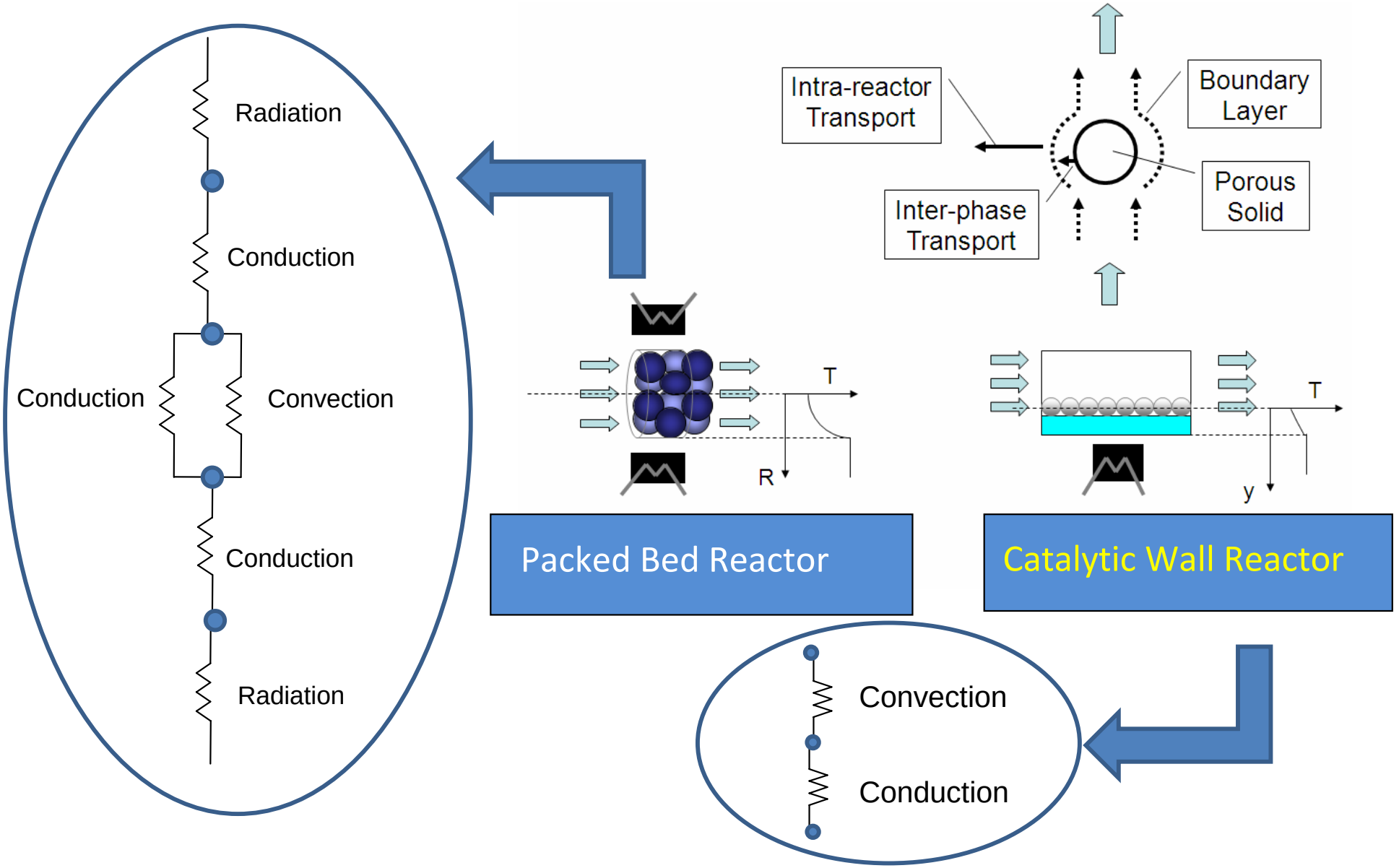
Process Integration



Process Intensification



CWR: a type of Structured Reactor

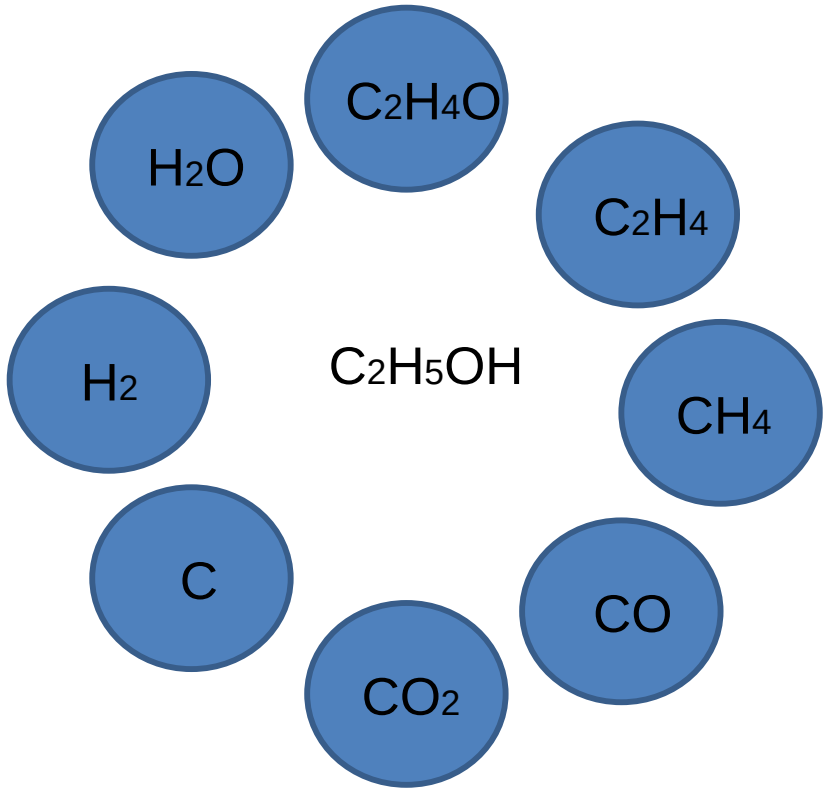


Steam Reforming of Ethanol

Global reaction

$$C_2H_5OH + 3H_2O \rightarrow 2CO_2 + 6H_2$$

Possible products



Catalyst formulations

Active phase	Supports
Ni	La_2O_3
Co	γAl_2O_3
	ZnO
Rh	CeO_2

Main reaction mechanisms

Decomposition reactions

Cracking

Dehydrogenation $C_2H_5OH \rightarrow$ … + C + …

Dehydration

Operational conditions MUST BE carefully controlled to avoid undesired products

Reforming reactions

Ethanol $C_2H_5OH + H_2O \rightarrow 2CO + 4H_2$

Acetaldehyde $C_2H_4O + H_2O \rightarrow 2CO + 3H_2$

Ethylene $C_2H_4 + 2H_2O \rightarrow 2CO + 4H_2$

Water Gas Shift

$CO + H_2O \rightleftharpoons CO_2 + H_2$

Methanation

$CH_4 + H_2O \rightleftharpoons CO + 3H_2$

Mathematical Model

Conservation equations

Continuity $$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho u = 0$$

Mass balance

$$C_0\left(\frac{\partial y_j}{\partial t} + u \cdot \nabla y_j\right) = C_0\left(D_j \nabla^2 y_j\right) + \sum_i \nu_{ij} r_j$$

Energy balance

$$\rho c_p\left(\frac{\partial T}{\partial t} + u \cdot \nabla T\right) = k_e \nabla^2 T + \sum_i \nu_{ij} r_j \Delta H_i$$

Main model parameters

Ideal gas $$\rho_i = \frac{P}{RT}\frac{1}{\sum\left(w_i / MW_i\right)}$$

Mass diffusion coefficient

$$D = D_0\left(\frac{T}{T_0}\right)^{1.75}$$

Linear reaction rate

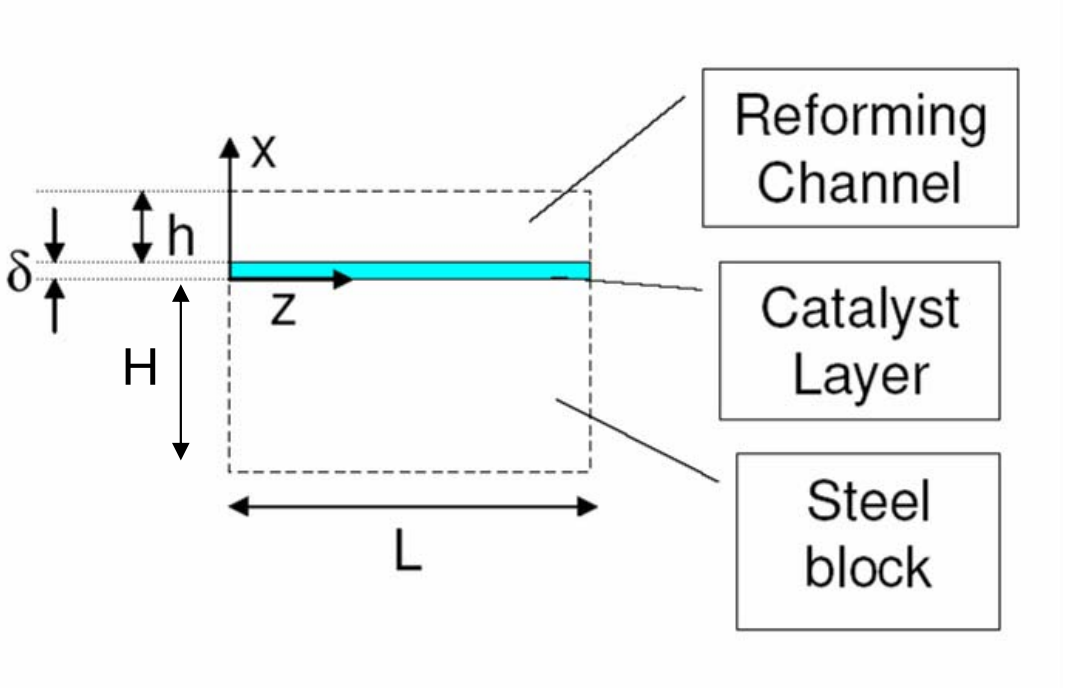
$$-r_j = k_0 \exp\left(\frac{E}{RT}\right) c_j$$

The Chemical Engineering Module facilitated the coupling of transport phenomena and chemical reaction kinetics

Catalytic Wall Reactor model

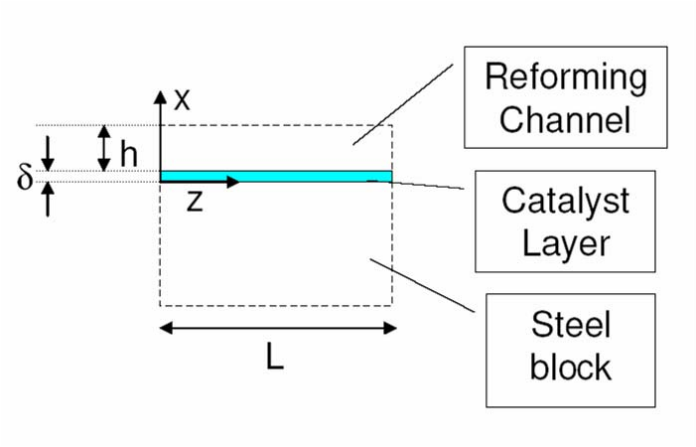
Main assumptions

- Linear expression for the reaction rate
- Balances
  1. Momentum
  2. Mass
  3. Heat
- Heater delivers the energy required by the reaction
- No heat losses

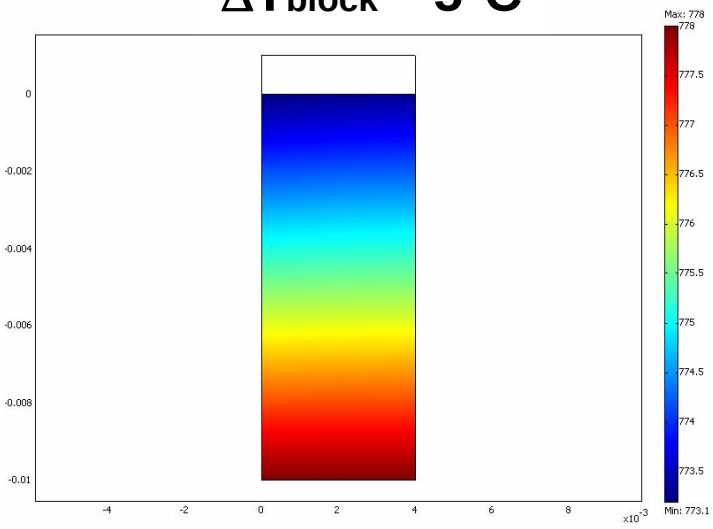


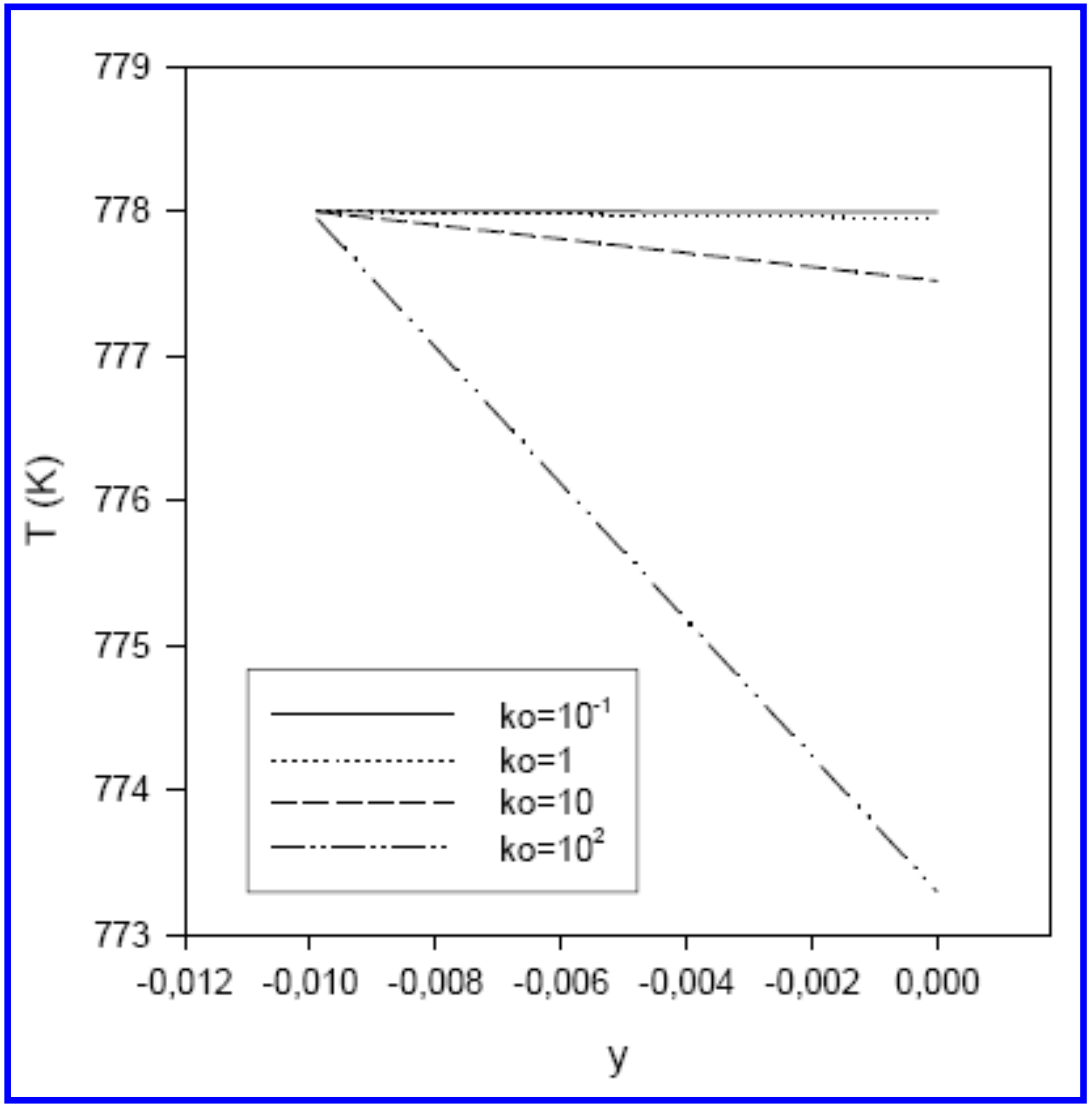
Length scale orders:
$H(10^{-1}m) >> h(10^{-3}m) >> \delta(10^{-5}m)$

Temperature on the block



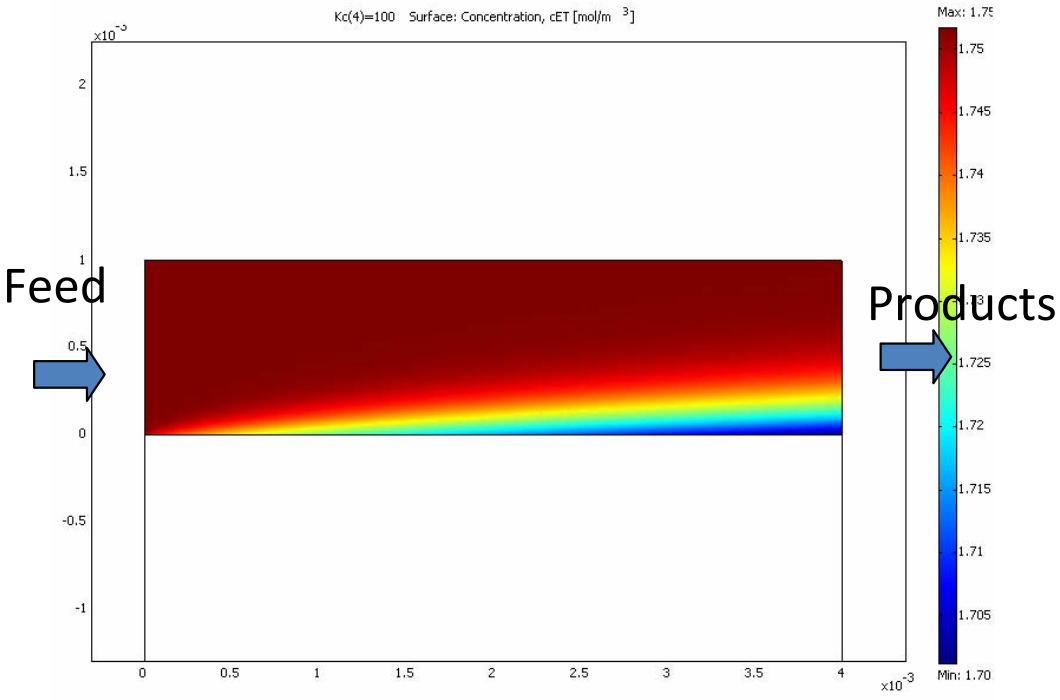
$\Delta T_{block} \sim 5°C$



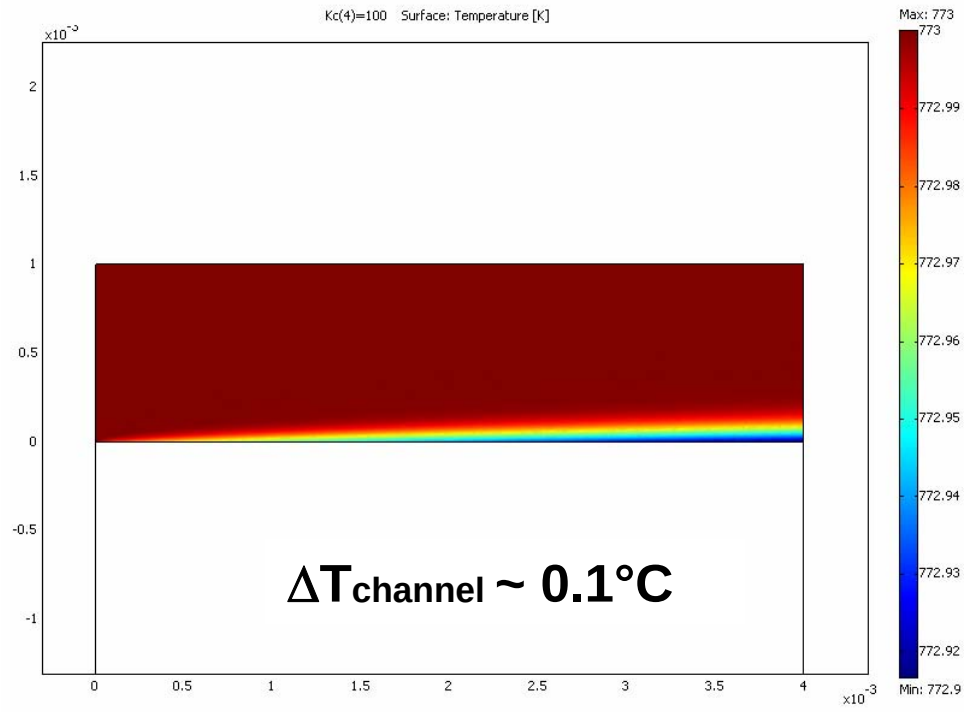


Reforming channel

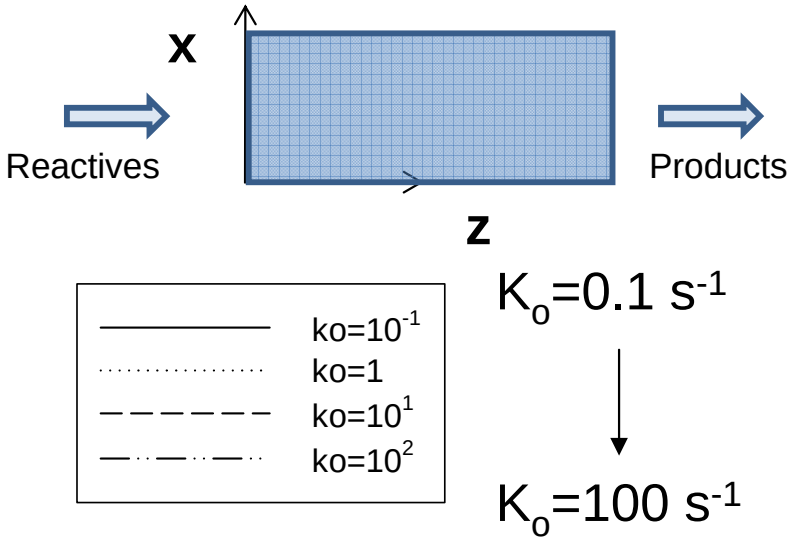
Ethanol concentration



Temperature



Concentration and temperature profiles



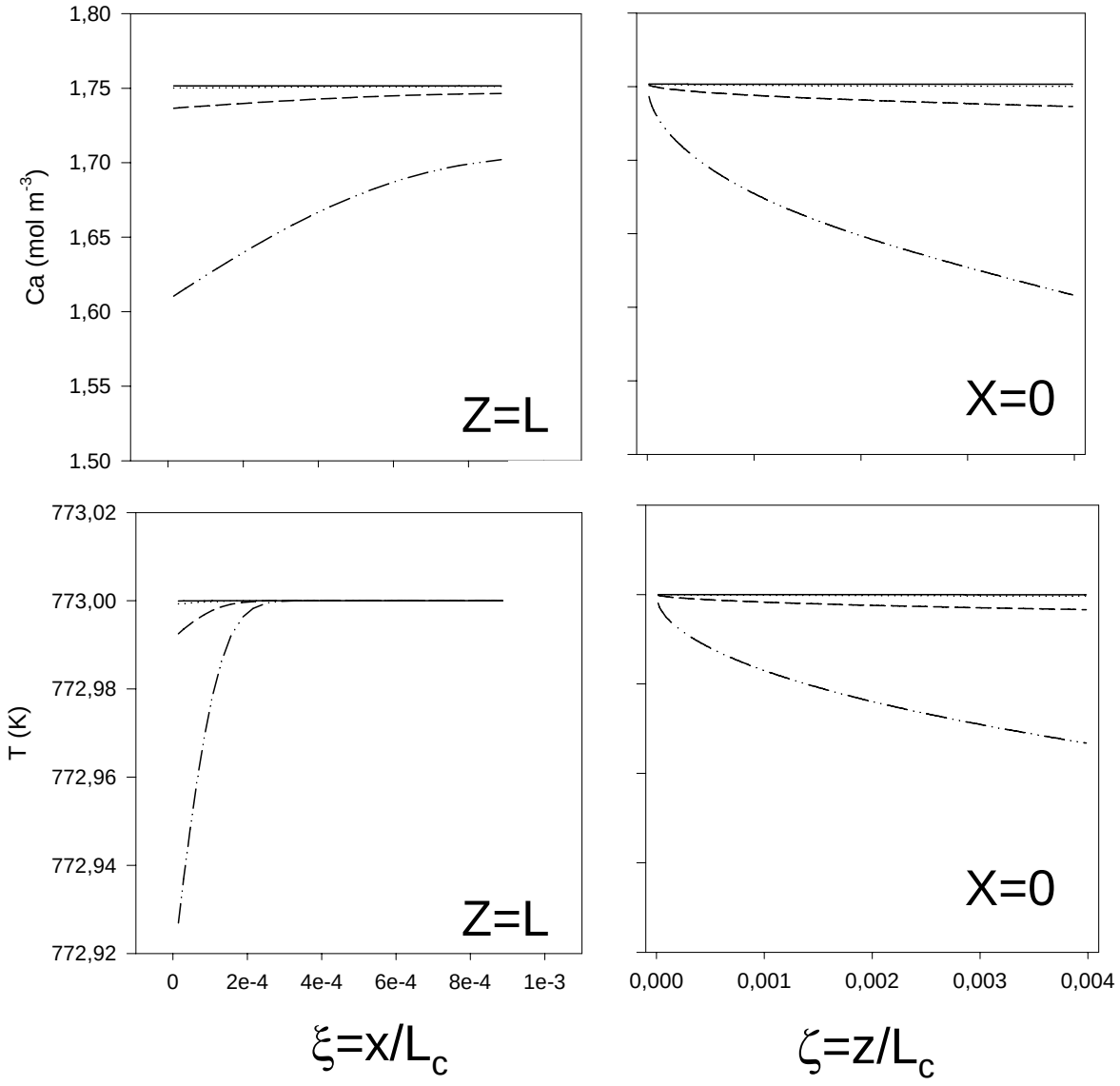
K_o=0.1 s^{-1}

K_o=100 s^{-1}

K_o...frequency factor

ξ...dimensionless length in x-direction

ζ...dimensionless length in z-direction

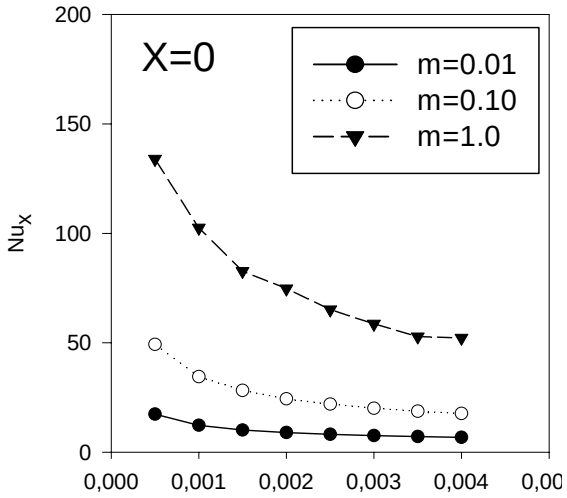


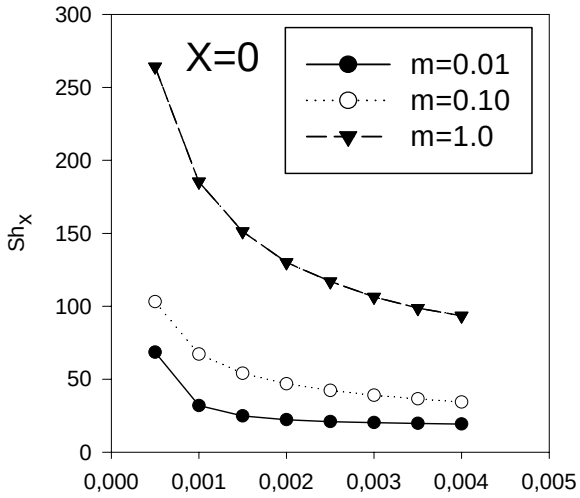
Dimensionless numbers

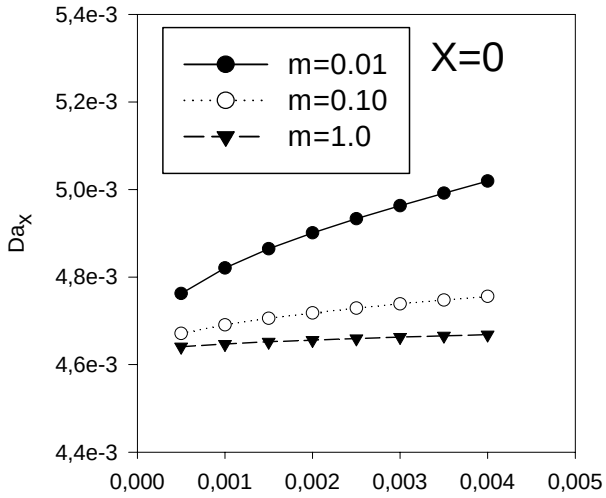
$$Nu = \frac{h \cdot L}{k}$$

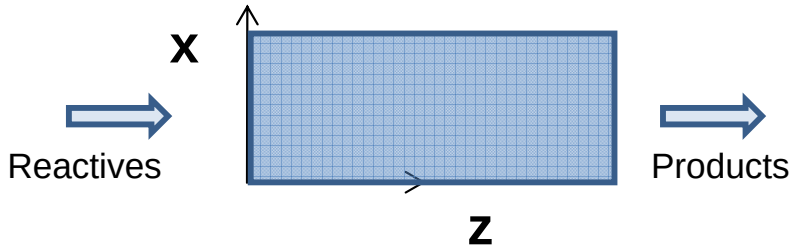
$$Sh = \frac{k \cdot L}{D}$$

$$Da_{ij} = \frac{k_i(T) \cdot C_{j0}^{n-1} \cdot L^2}{D_j}$$









Conclusions

1. The Catalytic Wall Reactor model can be solved using COMSOL Multiphysics
2. CWR maintains a thermal performance adequate for evaluating catalysts under a uniform temperature profile at the studied conditions
3. CWR performance is mainly affected by mass flow rate and reaction kinetic parameters.

Future Work

1. Obtain **a reliable kinetic** for the endothermic SRE reaction **for improving the reactor design**
2. Include **heat losses** in the model → Is it a more realistic model?
3. Modeling of **a 3D geometry** to verify possible influence of end-effects→ Computationally more expensive → Is it a more realistic model?
4. Define **the catalytic plate** as a domain instead of a boundary condition → Computationally more expensive → Is it a more realistic model?

Thanks…

- Audience
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- CHLOE
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