Catalytic Pellet Reactor Under Uncertainty Design

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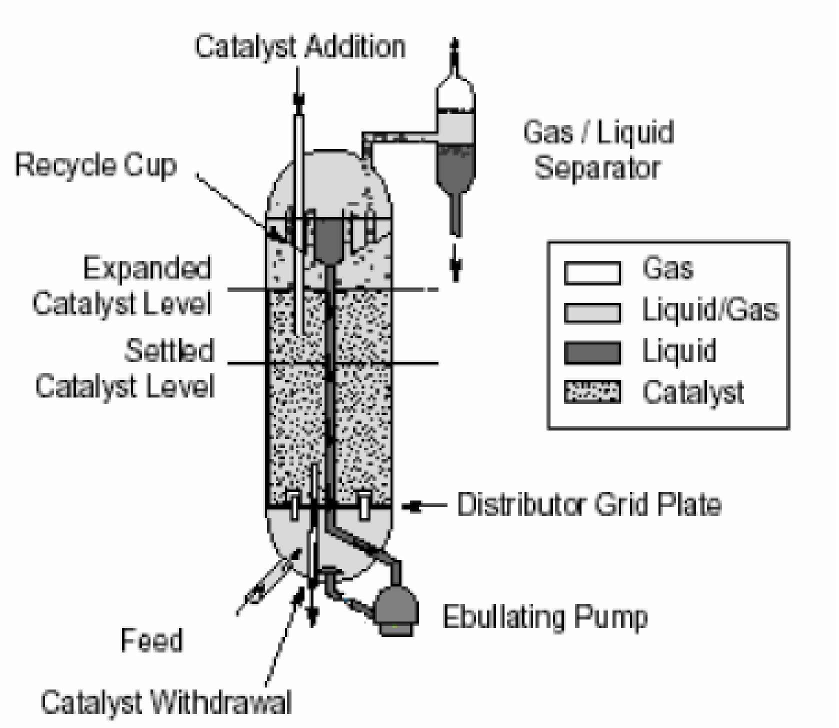
Motivation

- **Catalytic Pellet Reactor**
- **Application:**
  - Catalytic Converters in cars
  - Paraffin Dehydrogenation
  - **Production of Sulfuric Acid**
- **Design Complication**
  - Coupling of Heat and Mass transfer phenomenon
  - **Impact of uncertain parameters**

Fig.1: A Typical Configuration of a Pellet Reactor



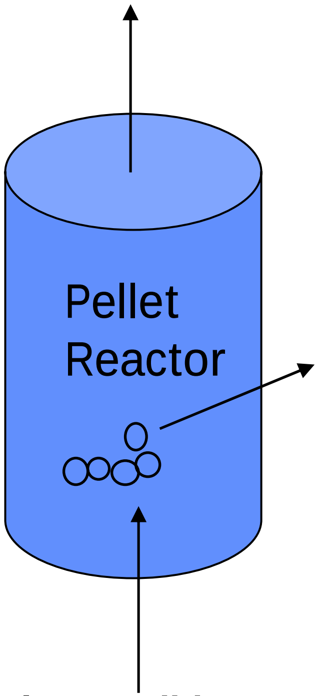
Design Under Uncertainty

- **Uncertain Parameter:**
  - system performance / safety
  - output quality.
- **Lack of understanding lead to:**
  - Loss of Revenue
  - Unsafe Design (Hot Spot, Explosion etc.)
- **Why we want to study it?**
  - Safety Condition
  - Guarantee product quality and maximum profit.
  - Control over design

Product Conversion??

Effectiveness Factor

Diffusion + Reaction



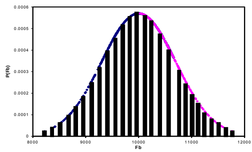
Property Uncertainty

Heat Conductivity: k_e

Mass Diffusivity: D_{ab}

Reaction rate: *a*

???



Inlet Conditions:

C_i and T_i

Operational Uncertainty

Methodology

- **Case Study: Pellet Reactor Design**
  - Develop Models
  - Solve Models in MATLAB
  - Analyze the system response
  - Quantify impact of uncertain parameters: safety, quality
- **Numerical Methods**
  - 1st Order ODE:
    - » R-K Method (ode45)
  - 2nd Order Differential Equation:
    - » Collocation Method
  - Integration:
    - » Adaptive Lobatto Quadrature Integration (quadl)

Case Study: Catalytic Pellet Reactor

- **Catalytic Reaction:**
  - $SO_{2\,(g)} + 1/2\ O_{2(g)} \leftrightarrow SO_{3\,(g)}$
  - 1st Order Heterogeneous reaction: A→B
- **Components of Design**
  - Pellets (T_s, C_s)
    - » Mass
    - » Energy
  - Effectiveness Factor [Fogler]

$$\eta = \frac{actual\ reaction\ rate}{reaction\ rate\ at\ \text{surface}}$$

  - Reactor (T_i, C_i)
    - » Mass
    - » Energy

Fig.2: Expanded View of a Pellet Reactor

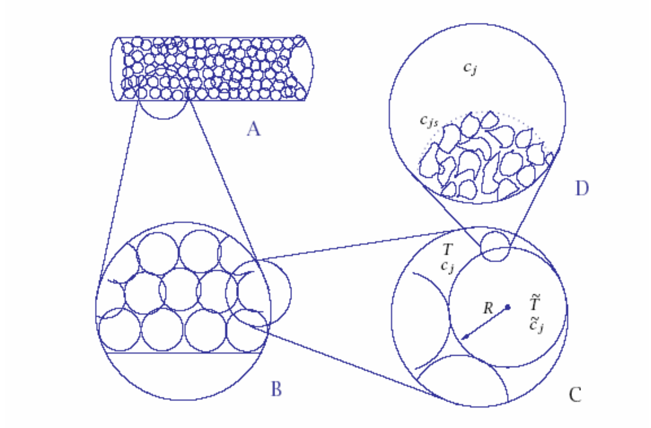


Fig. 3: Pellet Control Volume

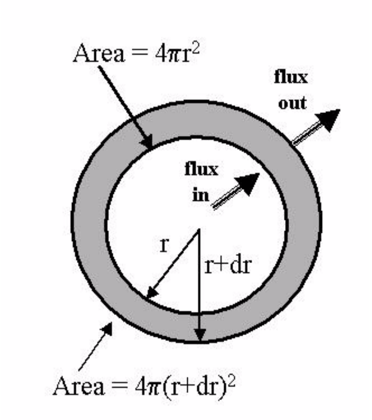
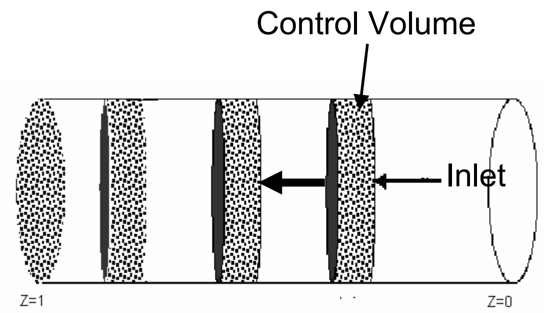


Fig. 4: Reactor Control Volume



Pellet Profiles

- **Steady State**

$$\frac{d^2\varphi}{d\theta^2}+\frac{2}{\theta}\frac{d\varphi}{d\theta}-\Phi^2\exp\left[\gamma\left(1-\frac{1}{\zeta}\right)\right]\varphi=0$$

$$\frac{d^2\zeta}{d\theta^2}+\frac{2}{\theta}\frac{d\zeta}{d\theta}-\beta\exp\left[\gamma\left(1-\frac{1}{\zeta}\right)\right]\varphi=0$$

Boundary Conditions:

r=R: C_s, T_s

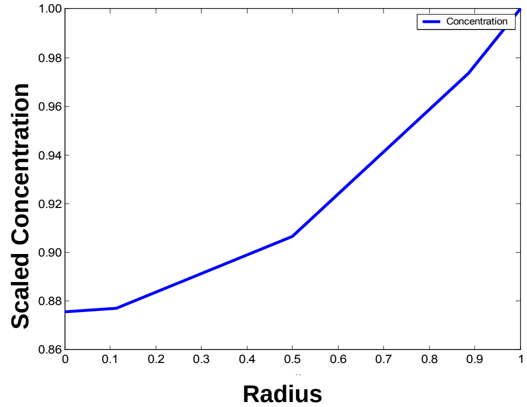
r=0: $dC_s/dz=0$, $dT_s/dz=0$

- **Dynamic State**

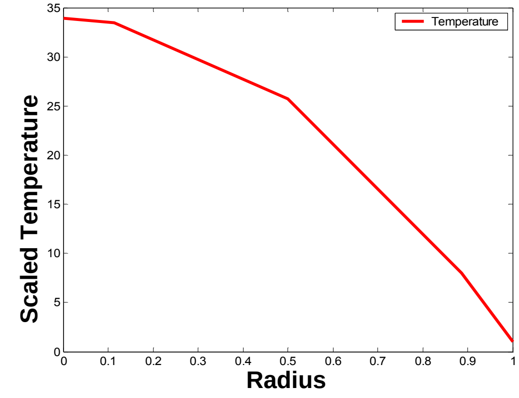
Initial Conditions:

1. t=0: T_o=1
2. t=0: C_o =Steady State result

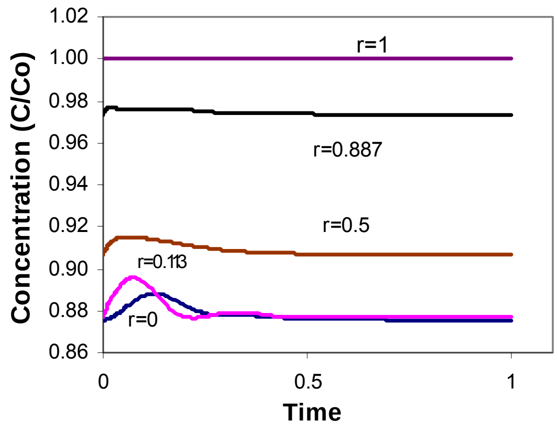
Steady State Pellet Concentration Profile



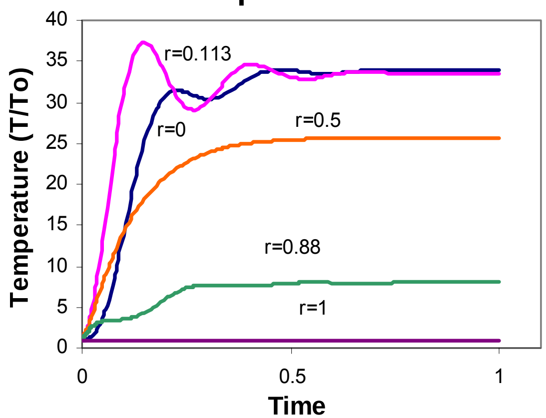
Steady State Pellet Temperature Profile



Dynamic Pellet Concentration Profile



Dynamic Pellet Temperature Profile



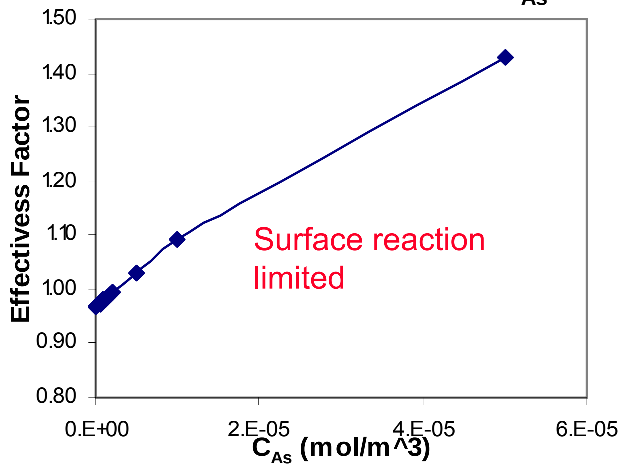
Pellet Sensitivity at Steady State

Nominal Values:

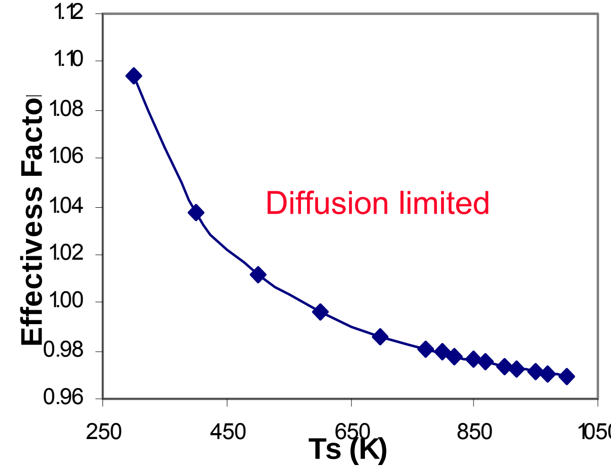
C_{As}=2.46E-6 mol/m^3

T_s= 550K

Effectiveness factor vs. C_{As}



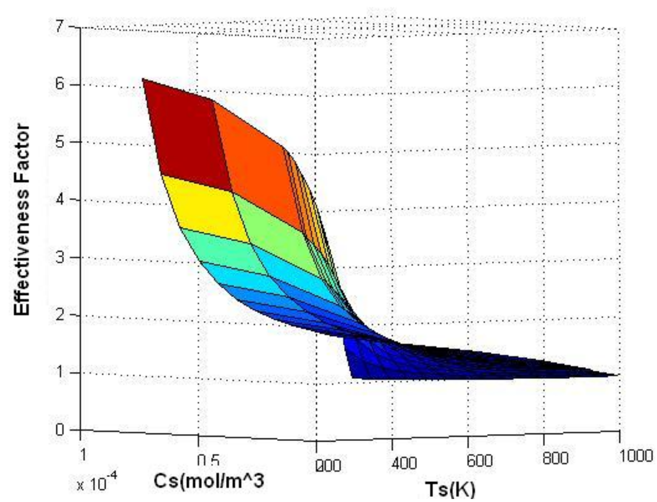
Effectiveness factor vs. T_s



$$\eta = 3\int_0^1 \varphi(\theta)\exp\left[\gamma(1-\frac{1}{\xi})\right]\theta^2 d\theta$$

$$\eta = \frac{actual\ reaction\ rate}{reaction\ rate\ at\ \mathrm{surface}}$$

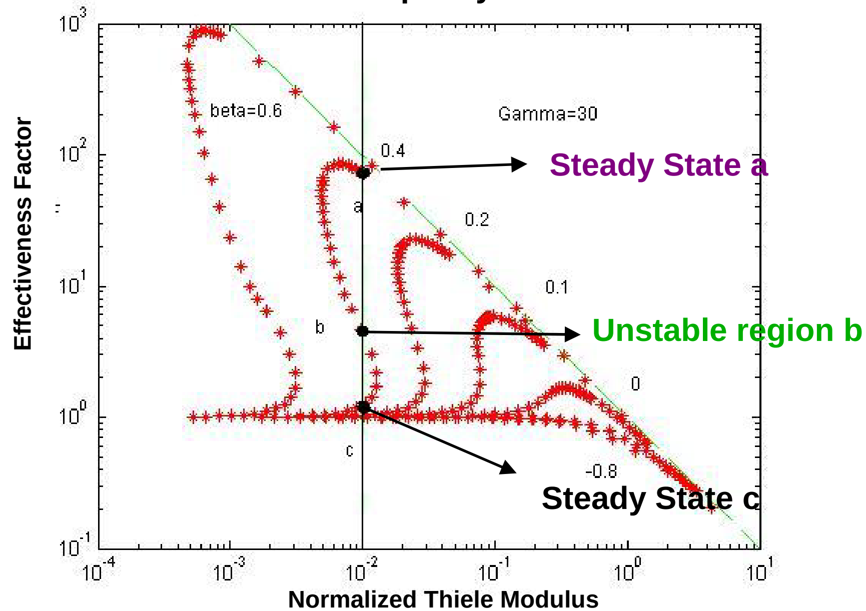
Effectiveness factor vs. Inlet conditions



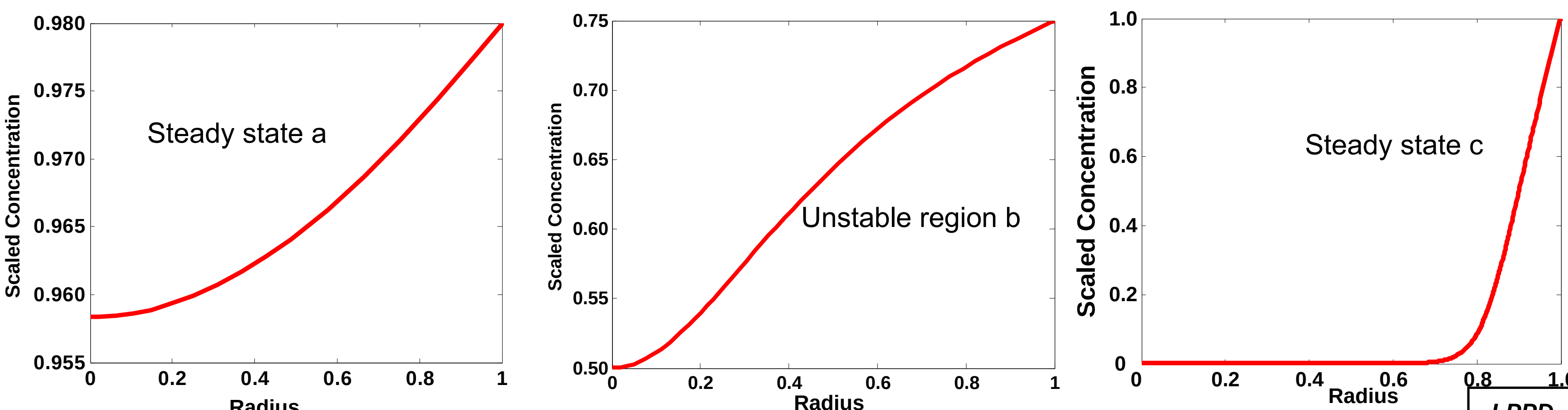
Multiple Steady States for Pellets

Reaction Condition:	Importance:
•**Thiele Modulus** =0.430 $\Phi^2 = \frac{R^2}{D_e}\left[a\exp(-\frac{E_a}{RT_s})\right]$ •**Beta**=0.4 $\beta = \frac{(T_{max} - T_s)}{T_s}$ •**Gamma**=30 $\gamma = \frac{Ea}{RT}$	--**Initial Conditions** --**One steady state may go to another!!**

Multiplicity



Concentration profiles for a single reaction condition



Celia

LPPD

Reactor Profiles

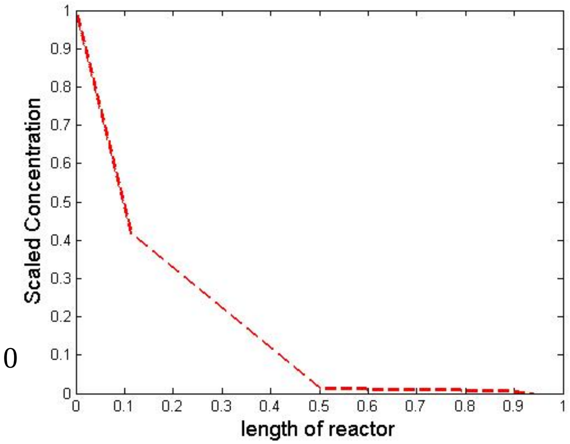
Steady State:

C_i=1.6E-2 mol/m^3
T_i=300K

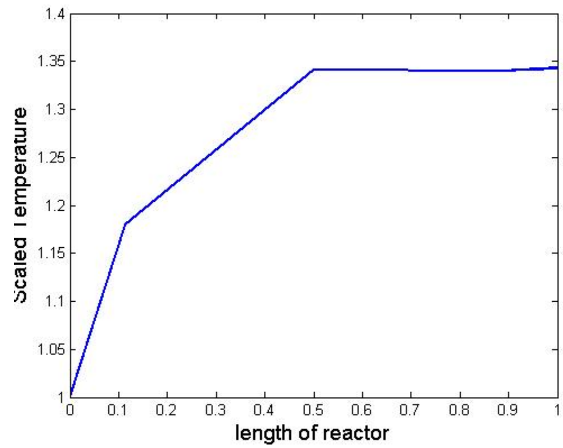
$$\frac{d^2C_r}{dz^2} - \frac{U}{D_{AB}}\frac{dC_r}{dz} - \frac{\eta S_a k_o \rho_b}{D_{AB}} C_r \exp\left[\gamma(1-\frac{1}{T_r})\right] = 0$$

$$\frac{d^2T_r}{dz^2} - \frac{\rho_g C_p U}{k_b} dT_r - \frac{\Delta H \eta S_a C_i \rho_b}{k_b T_i} C_r \exp\left[\gamma(1-\frac{1}{T_r})\right] = 0$$

Steady State Concentration Profile



Steady State Temperature Profile



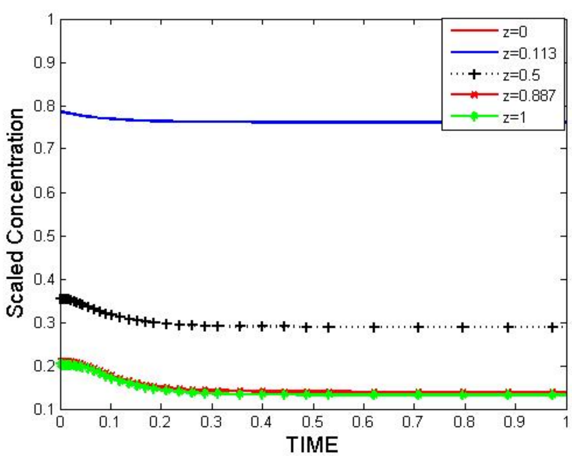
Dynamic State:

Initial Condition: Steady State

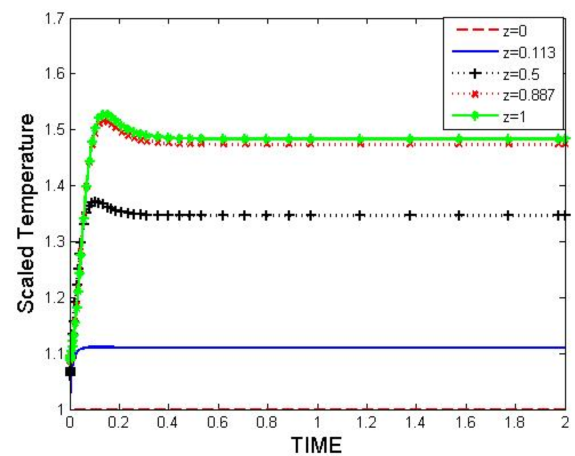
C_i=1.6E-2*5 mol/m^3

T_i=300K

Dynamic Concentration Profile

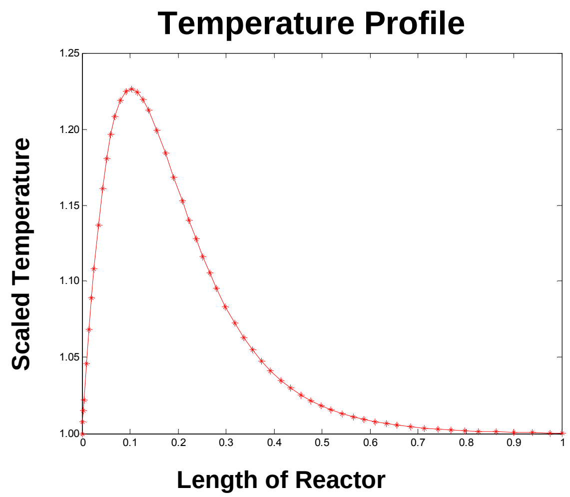


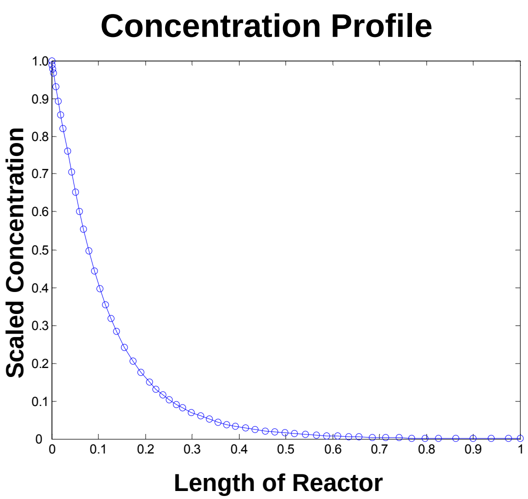
Dynamic Temperature Profile

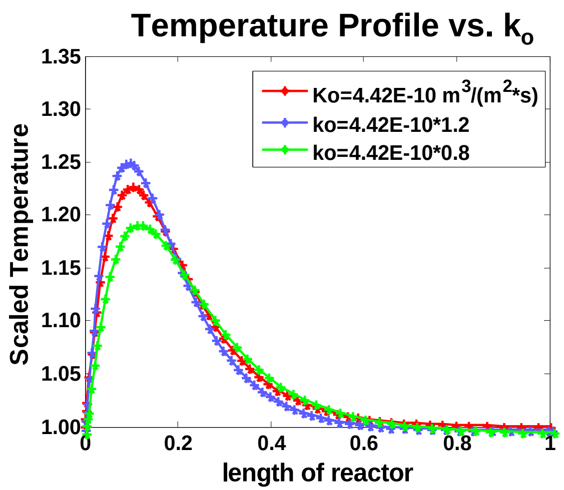


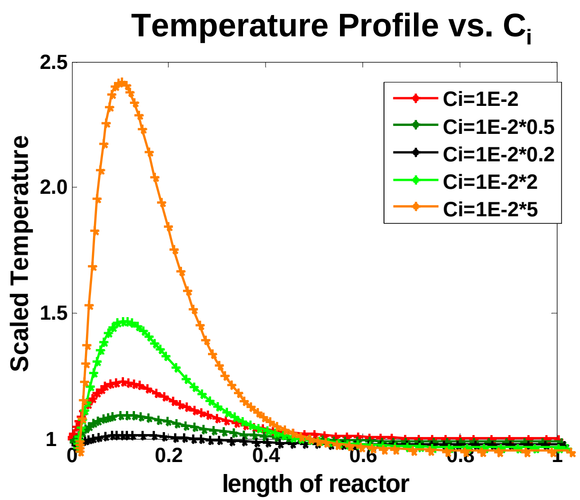
Reactor Safety: Hotspot

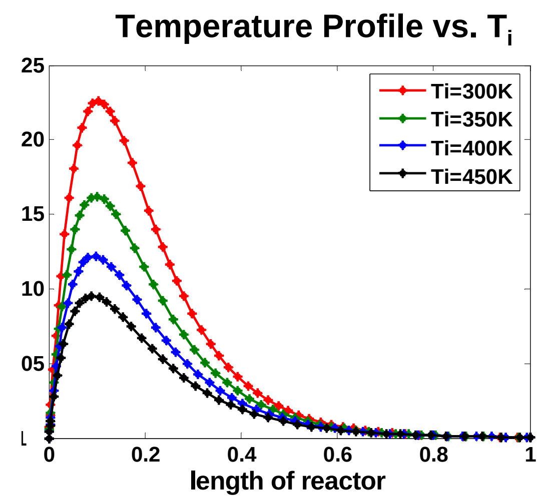
- **"Hotspot"** [Froment.] **:**
  - Temperature Profile reach a maximum
  - Very exothermic reaction
- **Why "hotspot" happens?**
  - Depletion of reactant
  - Cooling





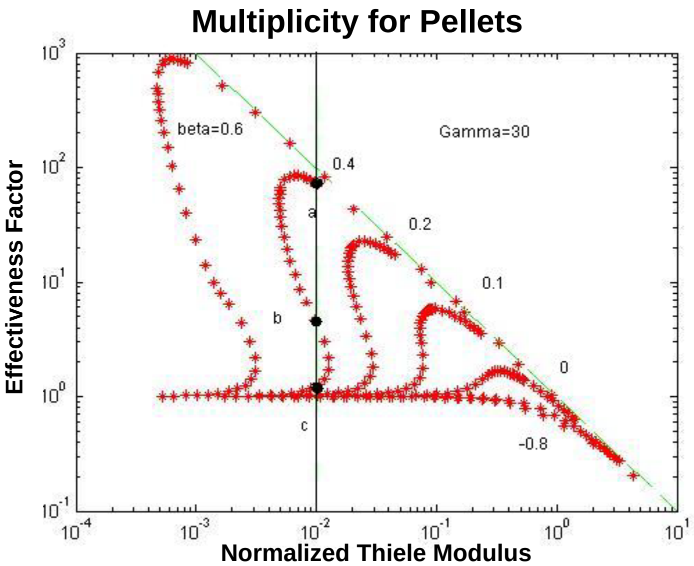


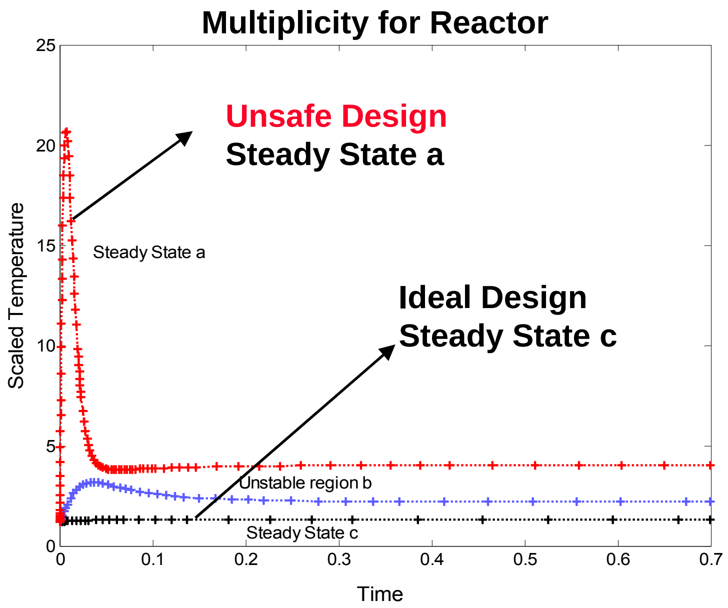




Reactor Safety: Multiplicity

- **How does reactor respond to pellet multiplicity?**
- **By testing uncertainty in inlet conditions, we find unsafe design!**
  - Initial steady state (z=0.5)
    - » T_r=1.2
    - » C_r=0.7
  - Disturbance:
    - » Ti=300K
    - » Ci=1E-2 mol/m^3





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Conclusion

– Pellet steady/dynamic state profiles

– Multiplicity in pellets

– Reactor steady/dynamic state profiles

– Reactor “hotspot”

– **Uncertainty analysis helps to prevent unsafe design!**

References

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