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Process Intensification for Autothermal Reaction

Manal Moftah Saleh

University of Wollongong

November, 2015

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The world is currently facing critical challenges:

- Future energy requirements.
- Greenhouse emissions.
- Rising oil prices and "peak" oil resources

Possible solutions:

- natural gas $\rightarrow$ syngas $\rightarrow$ liquid fuels/H_2.

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- Future energy requirements.
- Greenhouse emissions.
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Possible solutions:

- natural gas $\rightarrow$ syngas $\rightarrow$ liquid fuels/H_2.

Aim: develop mathematical models for autothermal processes to maximize product concentration.

Models based on **CSTR**. Advantages are:

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Models based on **CSTR**. Advantages are:

- Operated continuously.

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Models based on **CSTR**. Advantages are:

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Models based on **CSTR**. Advantages are:

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- Relatively easy to maintain temperature control.
- Control of the equipment and grade of final product is simplified.
- Single or cascade.

Autothermal reactor

What is an autothermal reactor?

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- Investigate the chemical mechanism

$$\mathrm{A} \xrightarrow[k_1]{Q_1<0} \mathrm{B} \xrightarrow[k_2]{Q_2>0} \mathrm{C}\cdot$$

where $k_i = a_i \exp\left[\frac{-E_i}{RT_i}\right] \qquad i = 1, 2.$

- Maximize the product concentration (C).

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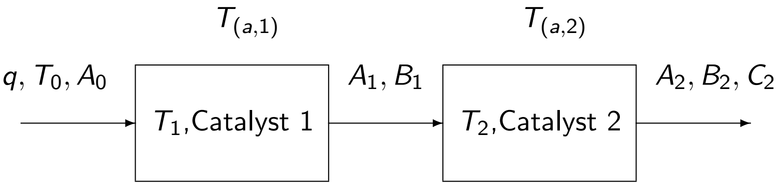
Diabatic **CSTR**

A diabatic process is a process that occurs with the transfer of heat between a system and its surroundings.



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Characteristic Temperature T_c

Normally reaction terms written as

$$a \exp\left[\frac{E}{RT}\right].$$

The pre-exponential factor in the studied model is written as

$$a = \frac{E\alpha}{RT_c^2} \exp\left[\frac{E}{RT_c}\right].$$

Dimensional model equations: Reactor one

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Concentration of reactant A

$$V_1 \frac{dA_1}{dt} = q(A_0 - A_1) - V_1 a_1 \exp\left[\frac{-E_1}{RT_1}\right] A_1. \quad (1)$$

Concentration of intermediate B

$$V_1 \frac{dB_1}{dt} = q(B_0 - B_1) + V_1 a_1 \exp\left[\frac{-E_1}{RT_1}\right] A_1. \quad (2)$$

Concentration of product C

$$V_1 \frac{dC_1}{dt} = q(C_0 - C_1) + 0. \quad (3)$$

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Temperature inside the reactor

$$c_{pg}\rho_g V_1 \frac{dT_1}{dt} = qc_{pg}\rho_g(T_0 - T_1) - Q_1 V_1 a_1 \exp\left[\frac{-E_1}{RT_1}\right] A_1 - J_1\chi_1 S_1(T_1 - T_{a,1}). \quad (4)$$

The pre-exponential factor

$$a_1 = \frac{E_1\alpha}{RT_{c1}^2} \exp\left[\frac{E_1}{RT_{c1}}\right]. \quad (5)$$

Reactor two:

Concentration of reactant A

$$V_2 \frac{dA_2}{dt} = q(A_1 - A_2) + 0. \quad (6)$$

Concentration of reactant B

$$V_2 \frac{dB_2}{dt} = q(B_1 - B_2) - V_2 a_2 \exp\left[\frac{-E_2}{RT_2}\right] B_2. \quad (7)$$

Concentration of reactant C

$$V_2 \frac{dC_2}{dt} = q(C_1 - C_2) + V_2 a_2 \exp\left[\frac{-E_2}{RT_2}\right] B_2. \quad (8)$$

Temperature inside the reactor

$$c_{pg}\rho_g V_2 \frac{dT_2}{dt} = q c_{pg}\rho_g (T_1 - T_2) + Q_2 V_2 a_2 \exp\left[\frac{-E_2}{RT_2}\right] B_2 - J_2\chi_2 S_2 (T_2 - T_{a,2}). \quad (9)$$

The pre-exponential factor

$$a_2 = \frac{E_2\alpha}{RT_{c2}^2}\exp\left[\frac{E_2}{RT_{c2}}\right]. \quad (10)$$

$A_1^* = 0.1$

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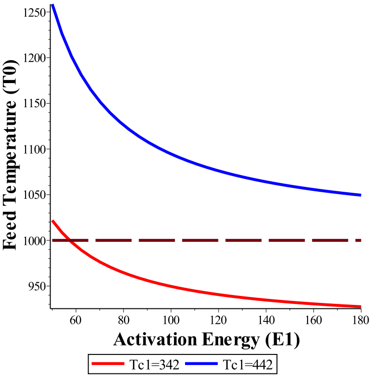
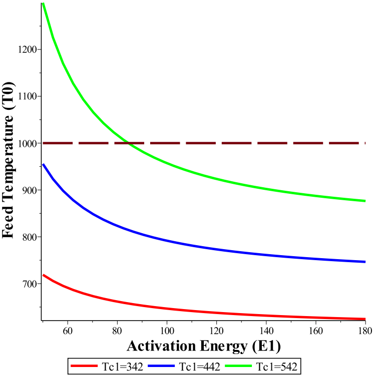
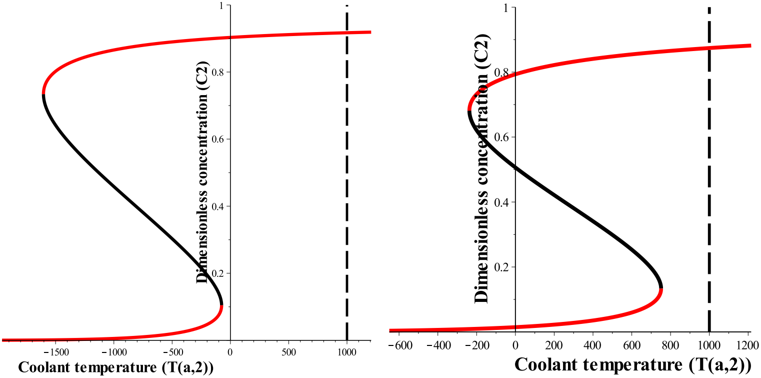


(a) $Q_1 = 205.8(\mathrm{KJ\,mol}^{-1})$



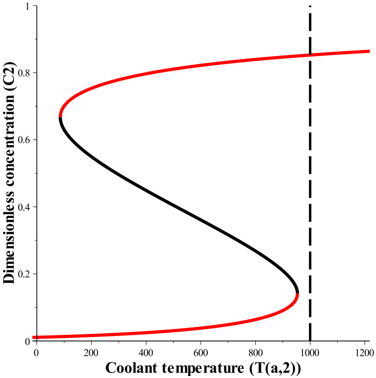
(b) $Q_1 = 100(\mathrm{KJ\,mol}^{-1})$

Steady-state diagrams ($A_1^* = 0.1$)

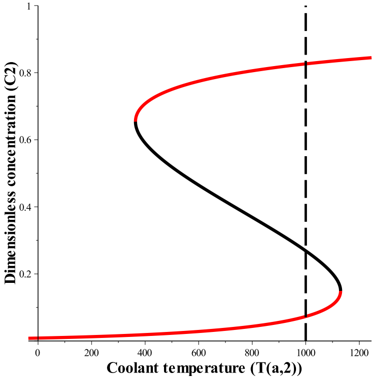


(c) $T_{c2} = 405(\mathrm{K})$.

(d) $T_{c2} = 435(\mathrm{K})$.



(e) $T_{c2} = 442(\mathrm{K})$.



(f) $T_{c2} = 448(\mathrm{K})$.

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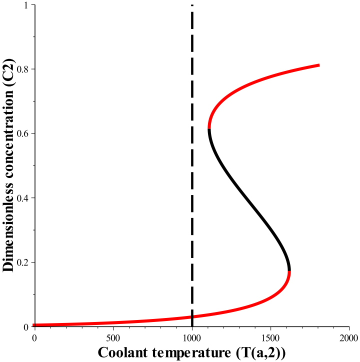
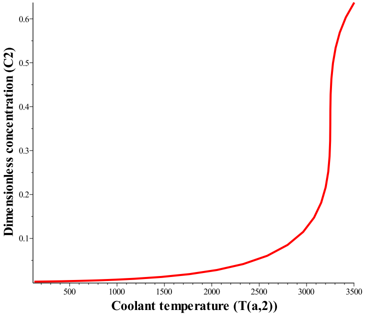


(g) $T_{c2} = 464(\mathrm{K})$.



(h) $T_{c2} = 511(\mathrm{K})$.

LP unfolding diagram

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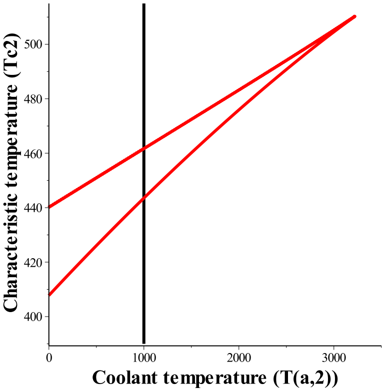

LP unfolding diagram

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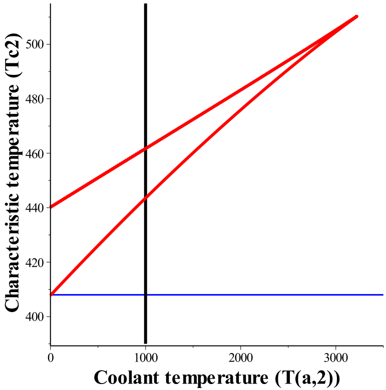
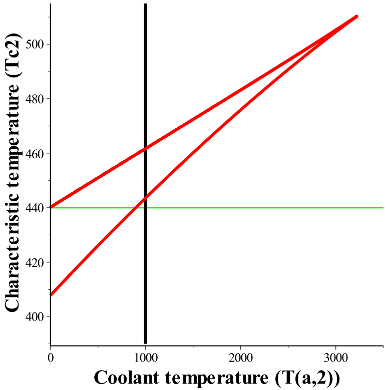


LP unfolding diagram



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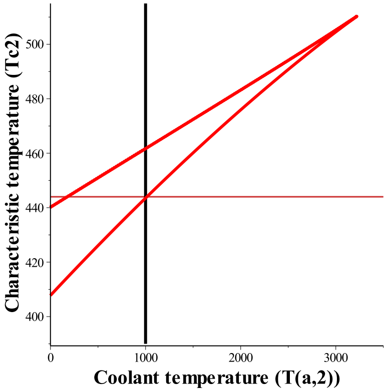

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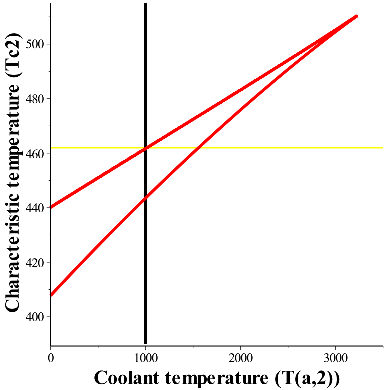

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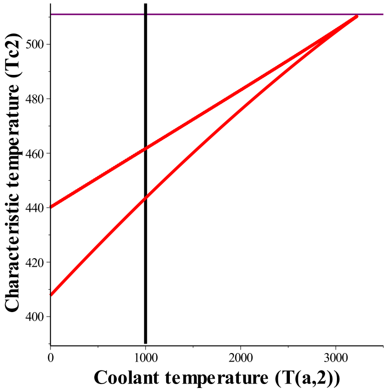

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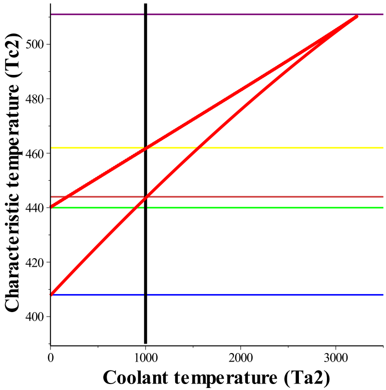

The key idea

- 90 % conversion ($C_2^* = 0.9$).
- $A_1^* < 0.1$.
- Six steady-state diagrams.
- $LP_{ig} < 298(K)$
- LP unfolding diagram.

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- Reaction occurring in two reactors: endothermic in **R1** and exothermic in **R2**.

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- Reaction occurring in two reactors: endothermic in **R1** and exothermic in **R2**.
- high conversion in **R1** (low endothermicity).

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- Reaction occurring in two reactors: endothermic in **R1** and exothermic in **R2**.
- high conversion in **R1** (low endothermicity).
- Steady-state solutions.
- Interesting results.

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- Assoc Prof. Mark I Nelson and co-supervisors.
- My family (husband) for preceding help and suitable environment.
- The organiser of NSW ANZIAM meeting.