



Control of non-isothermal chemical reaction networks using irreversible port-Hamiltonian systems

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Doctoral course UFC

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Motivations for adopting an **energy-based perspective** in modeling and control

- Physical system can be viewed as a set of **simpler subsystems** that exchange energy through ports,
- Energy is a concept common to all physical domains and is not restricted to linear or non-linear systems: **non-linear** approach,
- Energy can serve as a **lingua franca** to facilitate communication among scientists and engineers from different fields,
- Role of energy and the interconnections between subsystems provide the basis for various control techniques: **Lyapunov based control**.



[Maschke and van der Schaft, 1992, van der Schaft, 2000]

Port-Hamiltonian control systems

$$\dot{x} = J(x) \frac{\partial U}{\partial x}(x) + gu(t),$$

$$y = g(x)^\top \frac{\partial U}{\partial x}(x)$$

$J(x) = -J(x)^\top$ the interconnection matrix

Balance equations expressed by PHS: Conservation of the **Hamiltonian** and of **Casimir's** of the Poisson bracket

$$\frac{dU}{dt} = \frac{\partial U}{\partial x}^\top gu = u^\top y,$$

$$\frac{dC}{dt} = \frac{\partial C}{\partial x}^\top gu = u^\top y_C$$

Poisson bracket: $\{Z, G\}_J = \frac{\partial Z}{\partial x}^\top(x) J(x) \frac{\partial G}{\partial x}(x)$



[Ortega et al., 2001]

Interconnection and damping assignment passivity based control

IDA-PBC objective

Find a static state-feedback control $u(x) = \beta(x)$ such that the closed-loop dynamics is a PH system with interconnection and dissipation of the form

$$\dot{x} = (J_d(x) - M_d(x)) \frac{\partial U_d}{\partial x}(x),$$

$U_d(x)$, has a strict local minimum at x^* ,

$J_d(x, u) = -J_d(x, u)^T$, the *desired* interconnection matrix,

$M_d(x, u) = M_d(x, u)^T \geq 0$, the *desired* dissipation matrix,



The procedure consists in the **matching** of the open and desired closed-loop vector fields

$$J(x) \frac{\partial U}{\partial x}(x) + g(x)\beta(x) = (J_d(x) - M_d(x)) \frac{\partial U_d}{\partial x}(x)$$

with $u = \beta(x)$ a state modulated source. If this **quasi-linear** PDE is satisfied then

$$\dot{x} = (J_d(x) - M_d(x)) \frac{\partial U_d}{\partial x}(x),$$

and

$$\dot{U}_d = -\frac{\partial U_d^T}{\partial x} M_d \frac{\partial U_d}{\partial x} < 0, \forall x \neq x^* \quad , \quad \dot{U}_d(x^*) = 0.$$



First and **second principle** of thermodynamics

Consider a closed system,

$$\frac{dU}{dt} = 0 \quad \text{and} \quad \frac{dS}{dt} = \sigma \left(x, \frac{\partial U}{\partial x} \right) \geq 0$$

$$\text{for PHS} \quad \frac{dS}{dt} = \frac{\partial S}{\partial x}^T J \left(x, \frac{\partial U}{\partial x} \right) \frac{\partial U}{\partial x} = \sigma \geq 0, \quad \text{for any } U(x)$$

This is the reason to consider **quasi Hamiltonian system**: retain much of the PHS structure, but their structure matrices depend explicitly on the gradient of the Hamiltonian (GENERIC, quasi Hamiltonian systems, Brayton-Mooser formulation,..)

[Germela and Öttinger, 1997, Hagos et al., 2001, Otero-Muras et al., 2008, Eberard et al., 2007, Hoang et al., 2011, Favache and Dochain, 2010]

How does IDA-PBC look like?



IDA-PBC design gives a possibly **non-linear PDE**

$$J\left(x, \frac{\partial U}{\partial x}\right) \frac{\partial U}{\partial x}(x) + g(x)\beta(x) = \left(J_d\left(x, \frac{\partial U_d}{\partial x}\right) - M_d(x)\right) \frac{\partial U_d}{\partial x}(x)$$

Hence, there are two big reasons to consider an particular structure for irreversible systems

- **Thermodynamically coherent models**
- **Non-linear control design**

This presentation is based on



- Ramirez, Maschke and Sbarbaro, Irreversible port-Hamiltonian systems: A general formulation of irreversible processes with application to the CSTR, *Chemical Engineering Science*, 2013. → **Modeling**
- Ramirez, Le Gorrec, Maschke and Couenne. On the passivity based control of irreversible processes: a port-Hamiltonian approach. *Automatica*, 2016. → **Control**



$$\dot{x} = R \left(x, \frac{\partial U}{\partial x} \right) J \frac{\partial U}{\partial x} (x) + g \left(x, \frac{\partial U}{\partial x} \right) u,$$
$$y = g^\top \left(x, \frac{\partial U}{\partial x} \right) \frac{\partial U}{\partial x} (x)$$

where $U(x) : \mathbb{R}^n \rightarrow \mathbb{R}$, $S(x) : \mathbb{R}^n \rightarrow \mathbb{R}$ relates to the energy and entropy respectively.

$$R \left(x, \frac{\partial U}{\partial x} \right) = \gamma \left(x, \frac{\partial U}{\partial x} \right) \{S, U\}_J, \quad \gamma \geq 0.$$

$\{S, U\}_J$ defines the **thermodynamic driving force**

First and second principle satisfied by construction

$$\dot{x} = R \left(x, \frac{\partial U}{\partial x} \right) J \frac{\partial U}{\partial x} (x) + g \left(x, \frac{\partial U}{\partial x} \right) u,$$
$$y = g^\top \left(x, \frac{\partial U}{\partial x} \right) \frac{\partial U}{\partial x} (x)$$

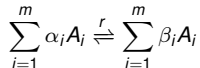
Energy balance

$$\frac{dU}{dt} = \frac{\partial U}{\partial x}^\top g u = y^\top u$$

Entropy balance

$$\begin{aligned} \frac{dS}{dt} &= \frac{\partial S}{\partial x}^\top R J \frac{\partial U}{\partial x} + \frac{\partial S}{\partial x}^\top g u = \gamma \left(x, \frac{\partial U}{\partial x} \right) \{S, U\}_J^\top + y_S^\top u \\ &= \sigma + y_S^\top u \end{aligned}$$

A single chemical reaction



with α_i, β_i the stoichiometric coefficients for species A_i . **The mass balance** is

$$\dot{n}_i = r_i V + F_{ei} - F_{si} \quad i = 1, \dots, m$$

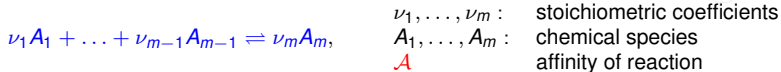
- n_i is the **number of moles** of the species i , $\mathbf{n} = (n_1, \dots, n_m)^\top$,
- $r_i = \bar{\nu}_i r$, where $r(\mathbf{n}, T) = (r_f - r_b)$ is the **reaction rate**
- $\bar{\nu}_i$ is the signed **stoichiometric coefficient**: $\bar{\nu}_i = \alpha_i - \beta_i$,
- F_{ei} and F_{si} are respectively the inlet and outlet **molar flows**, $\mathbf{F}_e = (F_{e1}, \dots, F_{em})^\top$
- The volume V in the reactor is assumed to be **constant** as well as the pressure

The mass balance can be represented as

$$\dot{\mathbf{n}} = C r V + \mathbf{F}_e - \mathbf{F}_i$$

where C is a $m \times 1$ is called the **stoichiometric vector**

A single chemical reaction



together with the definition of the reaction rate:

$$r(\mathcal{A}, T) = r_f(\mathcal{A}, T) - r_r(\mathcal{A}, T)$$

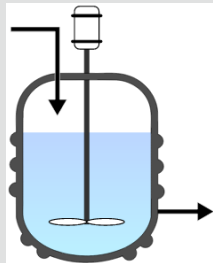
The mathematical model

$$\dot{n}_i = F_{ei} - F_{si} + r_i V$$

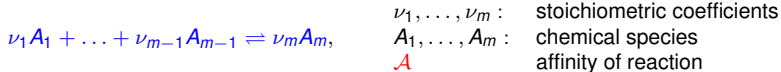
mass balance

$$\dot{S} = \sum_{i=1}^m (F_{ei} s_{ei} - F_{si} s_i) + \frac{Q}{T_e} + \sigma$$

entropy balance



A single chemical reaction



together with the definition of the reaction rate:

$$r(\mathcal{A}, T) = r_f(\mathcal{A}, T) - r_r(\mathcal{A}, T)$$

$U =$ the internal energy

$$J = \begin{bmatrix} 0 & \dots & 0 & \bar{\nu}_1 \\ 0 & \dots & 0 & \vdots \\ 0 & \dots & 0 & \bar{\nu}_m \\ -\bar{\nu}_1 & \dots & -\bar{\nu}_m & 0 \end{bmatrix},$$

stoichiometric matrix

$$g_1 = \underbrace{\begin{bmatrix} \mathbf{n}_e - \mathbf{n} \\ \phi(x, \frac{\partial U}{\partial x}) \end{bmatrix}}_{\text{Mass transfer}},$$

$$g_2 = \underbrace{\begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}}_{\text{Heat transfer}} \frac{1}{T_e},$$

$$\begin{bmatrix} U_1 \\ U_2 \end{bmatrix} = \begin{bmatrix} F \\ Q \end{bmatrix}$$

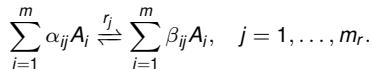
$$\{S, U\}_J = \mathcal{A} = - \sum_{i=1}^m \bar{\nu}_i \mu_i$$

$$\gamma = \frac{rV}{T\mathcal{A}} \geq 0,$$

μ_1, \dots, μ_m : chemical potentials
 rV : molar flow

Chemical reaction network

Consider a chemical reaction network involving m chemical species, among which m_r chemical reactions



The basic structure underlying the dynamics of the vector \mathbf{n} of mole numbers of the chemical species is given by the **mass balance law**:

$$\dot{\mathbf{n}} = \mathbf{C}\mathbf{r}V + \mathbf{F}_e - \mathbf{F}_s,$$

where the $m \times m_r$ matrix \mathbf{C} is called the **stoichiometric matrix** and whose columns are the stoichiometric vectors of each reaction: $\mathbf{C} = [C_1, C_2, \dots, C_{m_r}]$, and $\mathbf{r} = [r_1, r_2, \dots, r_{m_r}]^T$ is the vector whose elements are the reaction rates of each individual reaction.

The **energy and entropy balance** are

$$\dot{U} = U_{in} - U_{out},$$

$$\dot{S} = S_{in} - S_{out} + \sigma$$

IPHS of chemical reaction networks



Consider the chemical reaction network

$$\dot{\mathbf{n}} = \mathbf{C}\mathbf{r}\mathbf{V} + \mathbf{F}_e - \mathbf{F}_s,$$

$$\dot{\mathbf{S}} = \sigma + S_{in} - S_{out},$$

Define a vector containing the non-linear R_j functions of each reaction:

$$\mathbf{R} \in \mathbb{R}^{m_r} = [R_1, \dots, R_m]^\top,$$

then,

$$\dot{\mathbf{x}} = \underbrace{\begin{bmatrix} 0_m & \mathbf{C}\mathbf{R} \\ -\mathbf{R}^\top \mathbf{C}^\top & 0 \end{bmatrix}}_{J_R} \frac{\partial U}{\partial \mathbf{x}} + \begin{bmatrix} \mathbf{F}_e - \mathbf{F}_s \\ S_{in} - S_{out} \end{bmatrix}$$

The entropy balance is

$$\dot{\mathbf{S}} = \frac{\partial \mathbf{S}}{\partial \mathbf{x}} \dot{\mathbf{x}} = \frac{\partial \mathbf{S}}{\partial \mathbf{x}} J_R \frac{\partial U}{\partial \mathbf{x}} = -\mathbf{R}^\top \mathbf{C}^\top \boldsymbol{\mu} = \sum_{i=1}^{m_r} \sigma_i$$

where σ_i is the entropy production due to the i -th chemical reaction.



Alternatively,

The dynamic of the complete reaction is

$$\dot{x} = \sum_{i=1}^{m_k} X_i + g(x, u) = \underbrace{\left(\sum_{i=1}^{m_r} R_i J_i \right)}_{J_R} \frac{\partial U}{\partial x} + g(x, u).$$

Notice that

$$J_i = \begin{bmatrix} 0_m & C_i \\ -C_i^T & 0 \end{bmatrix},$$

with C_i the $m \times 1$ stoichiometric vector.



The idea

look for the conditions to derive a stabilizing state feedback which renders the closed-loop system in the form

$$\dot{x} = -\mathcal{M}\left(x, \frac{\partial U}{\partial x}, \frac{\partial A}{\partial x}\right) \frac{\partial A}{\partial x}(x),$$

with $\mathcal{M}\left(x, \frac{\partial U}{\partial x}, \frac{\partial A}{\partial x}\right) > 0$.

The time variation of A is in this case

$$\dot{A} = -\frac{\partial A^\top}{\partial x}(x) \mathcal{M}\left(x, \frac{\partial U}{\partial x}, \frac{\partial A}{\partial x}\right) \frac{\partial A}{\partial x}(x) \leq 0$$

and under some additional properness conditions the closed-loop system becomes asymptotically stable.

A class of Lyapunov function



The availability function

Use the negative of the total entropy as a convex extension to construct the availability function using thermodynamic considerations [Ydstie and Alonso, 1997, Alonso and Ydstie, 2001].

Consider Gibb's relation

$$dU = TdS - PdV + \sum_{i=1}^{N-2} \mu_i dn_i = w(z)^\top dz.$$

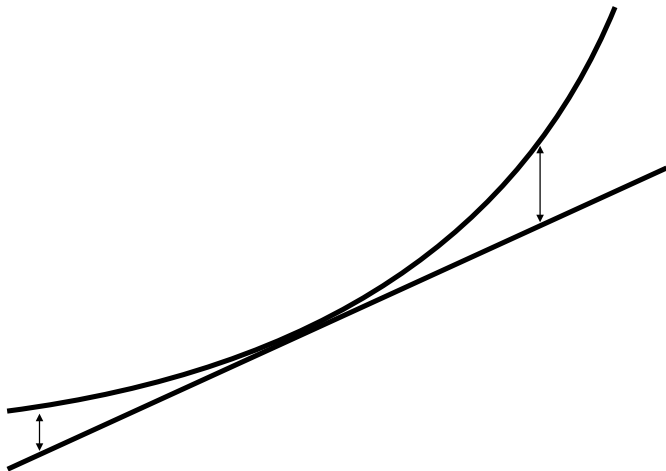
With $z = [S, V, n_1, \dots, n_{N-2}]^\top$ and $w(z) = [T(z), -P(z), \mu_1(z), \dots, \mu_{N-2}(z)]$. Since U is a homogeneous function of degree 1, from Euler's Theorem

$$U = w(z)^\top z, \quad w(z) = \frac{\partial U}{\partial z}(z)$$

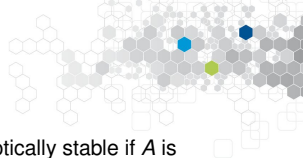
So we define an **energy based** availability function

$$A(x, x^*) = U(x) - \left[U(x^*) + \frac{\partial U}{\partial x}(x^*)^\top (x - x^*) \right] \geq 0$$

The energy based availability function



Stabilization condition



The closed-loop equilibrium x^* of a controlled IPHS is asymptotically stable if A is strictly convex and x^* satisfies:

$$\gamma \{S, U\}_J \{A, U\}_J + \tilde{y}^\top u = -s, \quad \tilde{y} = g^\top \frac{\partial A}{\partial x}.$$

where $s > 0$, with strict equality only at x^* , u^* , where u^* is the steady state value of the control-input at the desired equilibrium. Proof (sketch):

$$\begin{aligned} \frac{dA}{dt} &= \frac{\partial A^\top}{\partial x}(x) \frac{dx}{dt}, \\ &= \left(\frac{\partial U}{\partial x}(x) - \frac{\partial U}{\partial x}(x^*) \right)^\top R J \frac{\partial U}{\partial x}(x) + \left(\frac{\partial U}{\partial x}(x) - \frac{\partial U}{\partial x}(x^*) \right)^\top g u, \\ &= R \left(-\frac{\partial U}{\partial x}(x^*)^\top J \frac{\partial U}{\partial x}(x) \right) + \left(\frac{\partial U}{\partial x}(x) - \frac{\partial U}{\partial x}(x^*) \right)^\top g u, \quad \text{Def. IPHS} \\ &= \gamma \{S, U\}_J \{A, U\}_J + \tilde{y}^\top u, \quad \text{Def. Poisson Br} \end{aligned}$$

A globally stabilizing solution



Consider the following solution

$$\tilde{y}^\top u = -R\{A, U\}_J - \sigma_d[A, A]_M + R_d\{A, A\}_{J_d}$$

with $R_d = \gamma_d \{S, A\}_{J_d}$ and $\sigma_d = \gamma_d \{S, A\}_{J_d}^2$ with $\gamma_d > 0$.

where σ_d is a **closed-loop entropy rate**.

The condition is equivalently written in terms of the control $u = \beta(x)$

$$\beta(x) = g^\dagger(x) \left(R_d J_d - \sigma_d M \right) \left(\frac{\partial U}{\partial x}(x) - \frac{\partial U}{\partial x}(x^*) \right) - g^\dagger(x) R J \frac{\partial U}{\partial x}(x)$$

and the matching condition

$$g^\perp(x) \left(R_d J_d - \sigma_d M \right) \left(\frac{\partial U}{\partial x}(x) - \frac{\partial U}{\partial x}(x^*) \right) - g^\perp(x) R J \frac{\partial U}{\partial x}(x) = 0$$

Proposition



Assume A is strictly convex and that there exist matrices $M(x) \geq 0$ and $J_d(x) = -J_d^T(x)$, scalar functions $\gamma_d > 0$ such that $\sigma_d = \gamma_d \{S, A\}_{J_d}^2$ and $R_d = \gamma_d \{S, A\}_{J_d}$, and a full-rank left annihilator $g^\perp(x)$ of $g(x)$ that verify the matching equation. Then the control $u = \beta(x)$ globally asymptotically stabilizes the closed-loop equilibrium x^* . Furthermore, the closed-loop system is

$$\dot{x} = \left(-\sigma_d M + R_d J_d \right) \frac{\partial A}{\partial x}.$$

The closed-loop system is IPHS with dissipation $s = \sigma_d \frac{\partial A}{\partial x}^T M \frac{\partial A}{\partial x}$.

A useful corollary



Corollary

x^* is asymptotically stable with $u = \beta(x)$ if

$$g^\perp J = 0, \quad g^\perp J_d = 0, \quad g^\perp M = 0.$$

Remark

Using IDA-PBC is not obvious when dealing with irreversible processes. The present result can be interpreted as a thermodynamic equivalent, with structure and dissipation matrices $R_d J_d$ and $\sigma_d M$ (**interconnection** and **entropy assignment**), and energy function A (**energy shaping**)



Assumptions

- The reactor operates in liquid phase,
- The molar volumes of each species are identical and the total **volume is constant**,
- The **initial number of moles is equal to the number of moles of the inlet** of the same species,
- For a given temperature T there is only one possible steady state for the mass.

The last assumption doesn't imply that the chemical reaction network doesn't admit multiple stable or unstable equilibrium points.

Remark

The assumption on **constant volume** assures that the availability function **A is strictly convex**.

Recall the IPHS formulation of the CRN



$$\dot{x} = \underbrace{\begin{bmatrix} 0_m & \mathbf{CR} \\ -\mathbf{R}^T \mathbf{C}^T & 0 \end{bmatrix}}_{J_R} \frac{\partial U}{\partial x} + \begin{bmatrix} \mathbf{n}_e - \mathbf{n} & \mathbf{0} \\ \phi(x, \frac{\partial U}{\partial x}) & \frac{1}{T_e} \end{bmatrix} \begin{bmatrix} \frac{F}{V} \\ Q \end{bmatrix} = \underbrace{\left(\sum_{i=1}^{m_r} R_i J_i \right)}_{J_R} \frac{\partial U}{\partial x} + g u$$

One possible annihilator: $g^\perp(x) = \begin{bmatrix} \tilde{n}_2 & -\tilde{n}_1 & 0 & \dots & 0 & 0 & 0 \\ 0 & \tilde{n}_3 & -\tilde{n}_2 & \dots & 0 & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 & 0 \\ 0 & 0 & \dots & 0 & \tilde{n}_m & -\tilde{n}_{m-1} & 0 \end{bmatrix}$

The matching equation (using the Corollary with $J_d = J_R$)

$$g^\perp J_R = g^\perp \mathbf{CR}$$

where g^\perp denotes the matrix obtained by removing the last column of g^\perp . Hence the Corollary is satisfied if

$$g^\perp \mathbf{C} = g^\perp C_1 = g^\perp C_2 = \dots = g^\perp C_{m_r} = 0$$

Solving the matching equation



it suffices to check that for each individual reaction

$$g_{-}^{\perp} C_i = \begin{bmatrix} 0 & \dots & 0 & \bar{\nu}_{i1}\tilde{n}_2 - \bar{\nu}_{i2}\tilde{n}_1 \\ 0 & \dots & 0 & \bar{\nu}_{i2}\tilde{n}_3 - \bar{\nu}_{i3}\tilde{n}_2 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & \bar{\nu}_{im-1}\tilde{n}_m - \bar{\nu}_{im}\tilde{n}_{m-1} \end{bmatrix} = 0.$$

which is true if

$$\frac{\tilde{n}_1}{\bar{\nu}_{i1}} = \frac{\tilde{n}_2}{\bar{\nu}_{i2}} = \dots = \frac{\tilde{n}_{m-1}}{\bar{\nu}_{im-1}} = \frac{\tilde{n}_m}{\bar{\nu}_{im}}.$$

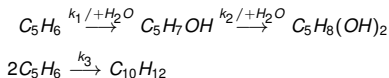
Since by assumption the initial numbers of moles of each species equals the numbers of moles at the inlet, i.e., $\mathbf{n}(t = 0) = \mathbf{n}_0 = \mathbf{n}_e$ we have

$$\frac{n_{0i} - n_i}{\bar{\nu}_{ij}} = \xi, \quad \text{De Donder's extent of reaction} \rightarrow \text{(always holds)}$$

The second condition in the Corollary is solved by any matrix $M(x) = M^T(x) \geq 0$ for which the first m rows and columns forms a null submatrix. This comes from the fact that the last column of g_{-}^{\perp} is zero.

A classical benchmark: the van der Vusse reactor

A non-isothermal CSTR with series/parallel reactions,



The reactor model is

$$\begin{aligned}\dot{c}_1 &= -k_1(T)c_1 - k_3(T)c_1^2 + (c_{10} - c_1)u_1 \\ \dot{c}_2 &= k_1(T)c_1 - k_2(T)c_2 - c_2u_1 \\ \dot{T} &= \vartheta(\mathbf{c}, T) + \frac{u_2}{\rho C_p} + (T_0 - T)u_1,\end{aligned}$$

with a thermodynamic “linearized” energy balance

$$\vartheta(\mathbf{c}, T) = -\frac{\Delta H_1 k_1(T)c_1 + \Delta H_2 k_2(T)c_2 + \Delta H_3 k_3(T)c_1^2}{\rho C_p}.$$

The rate coefficients k_i are dependent on the reactor temperature via the Arrhenius equation

$$k_i(T) = k_{i0} \exp \frac{E_i}{RT}, \quad i = 1, 2, 3.$$

The IPHS model



We complete the model with the balance equations of $C_5H_8(OH)_2$ and $C_{10}H_{12}$,

$$\dot{c}_3 = k_2(T)c_2$$

$$\dot{c}_4 = \frac{1}{2}k_3(T)c_1^2$$

The stoichiometric matrices are

$$J_1 = \begin{bmatrix} 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 \end{bmatrix}, J_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \end{bmatrix}, J_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/2 \\ 1 & 0 & 0 & -1/2 & 0 \end{bmatrix}.$$

Assumption

The approximated internal energy and energy availability function satisfy

$$\frac{\partial U}{\partial \mathbf{c}} = \begin{bmatrix} \mu_{V1} \\ \mu_{V2} \\ \mu_{V3} \\ \mu_{V4} \end{bmatrix}, \quad \frac{\partial A}{\partial \mathbf{c}} = \begin{bmatrix} \kappa_1(c_1 - c_1^*) \\ \kappa_2(c_2 - c_2^*) \\ \kappa_3(c_3 - c_3^*) \\ \kappa_4(c_4 - c_4^*) \end{bmatrix}$$

The IPHS model



The CRN can then be written as

$$\dot{x} = (R_1 J_1 + R_2 J_2 + R_3 J_3) \begin{bmatrix} \mu_{V1} \\ \mu_{V2} \\ \mu_{V3} \\ \mu_{V4} \\ T \end{bmatrix} + \begin{bmatrix} (c_{10} - c_1) & 0 \\ -c_2 & 0 \\ 0 & 0 \\ 0 & 0 \\ \frac{\rho C_p}{T} (T_0 - T) & \frac{1}{T} \end{bmatrix} u$$

where $x = [c_1, c_2, c_3, c_4, S]^T$, $u = [u_1, u_2]^T$, $R_1 = \frac{k_1(T)}{T} c_1$, $R_2 = \frac{k_2(T)}{T} c_2$, $R_3 = \frac{k_3(T)}{T} c_1^2$ and such that $-\Delta H_1 = \mu_{V1} - \mu_{V2}$, $-\Delta H_2 = \mu_{V2} - \mu_{V3}$ and $-\Delta H_3 = \mu_{V1} - \frac{1}{2} \mu_{V4}$. Notice that c_3 and c_4 don't affect the computation of the controller.

C_{A0}	5.0 mol/l	k_{10}	$1.287 \times 10^1 2 \text{ h}$
T_0	403.15 K	k_{20}	$1.287 \times 10^1 2 \text{ h}$
C_p	3.01 kJ/(kg K)	k_{30}	$9.403 \times 10^9 \text{ l} / (\text{mol h})$
ρ	0.94342 kg/l	E_1 / R	-9758.3 K
ΔH_1	4.20 kJ/mol	E_2 / R	-9758.3 K
ΔH_2	-11.00 kJ/mol	E_3 / R	-8560.0 K
ΔH_3	-41.85 kJ/mol		

Numerical simulations

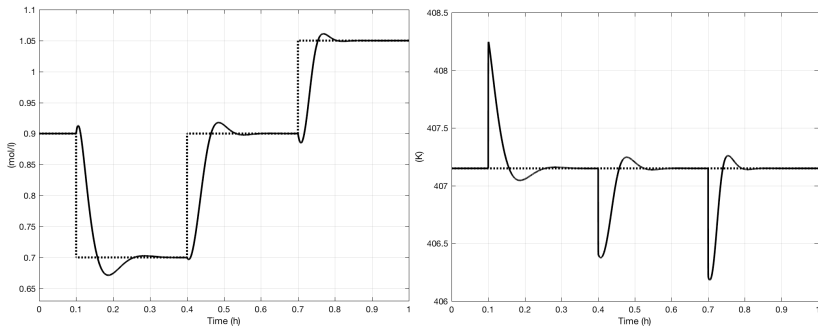


Figure: Molar concentration c_2 and temperature









Some final remarks



- IPHS are thermodynamically coherent models which retain passivity features of PHS and satisfy the **second principle**.
- Thermodynamically coherent systems cannot be in PHS form, hence **standard PBC** techniques such as IDA-PBC **cannot** be applied directly.
- In this work the closed-loop system is interpreted as a thermodynamic system, hence the **control parameters are related with thermodynamic quantities**, such as the reaction rates in the case of chemical reactions.
- For a general non-linear non-isothermal chemical reaction network the solution of the matching equation follows directly from the IPHS model.

Future work

Deal with the distributed case (the tubular reactor).

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