Process Networks with Chemical Engineering Applications

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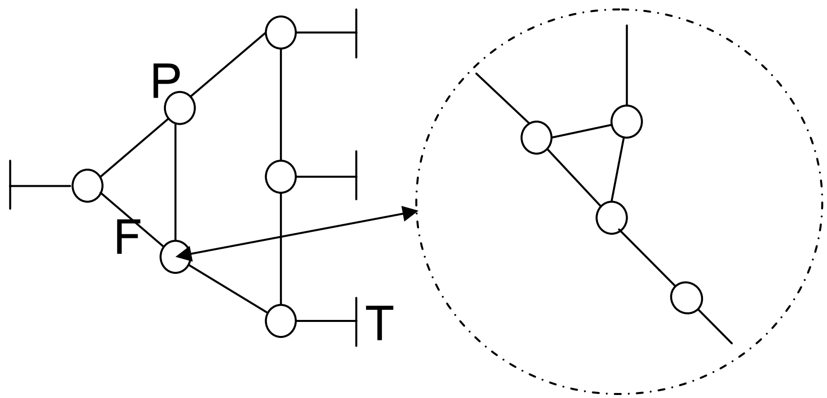
Objectives

- Describe a systematic framework for modeling process networks
- Develop passivity based methods for stability analysis and control of process networks
- Establish a variational principle for process networks
- Develop a reactor-diffusion network and a plant-wide control case study

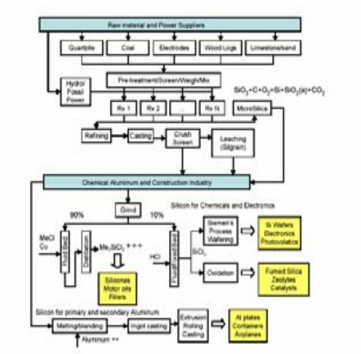
Process Networks

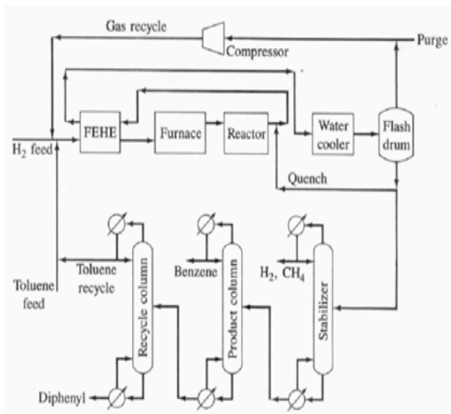


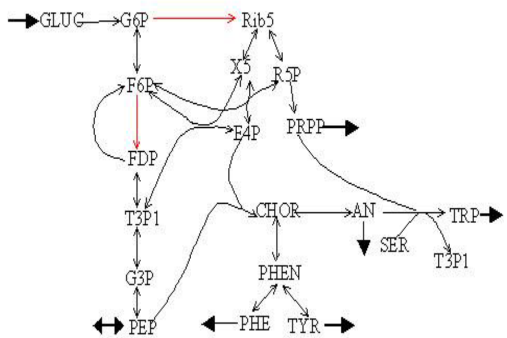
- Define
  - Graph, G = (P,T,F)
    - Process (node)
    - Terminal
    - Flow
  - Inventory of each node, v_j
    - Extensive quantities, conserved at each node $$\frac{dv}{dt} = p + \sum_i f_i$$
    - e.g. $v = [U, V, M_1, ..., M_n, ...]^T$
  - Potential of each node, w_j
    - Intensive quantities, continuous around any loop
    - e.g. $w = [\frac{1}{T}, \frac{P}{T}, \frac{\mu_1}{T}, ... \frac{\mu_n}{T} ...]^T = \frac{\partial S}{\partial v}$
    - Potential differences (W) act as driving forces for flow through constitutive relationships

Examples of Process Networks

- Supply Chain Networks
- Process Flowsheets
- Biological Systems
- Chemical Reaction Pathways







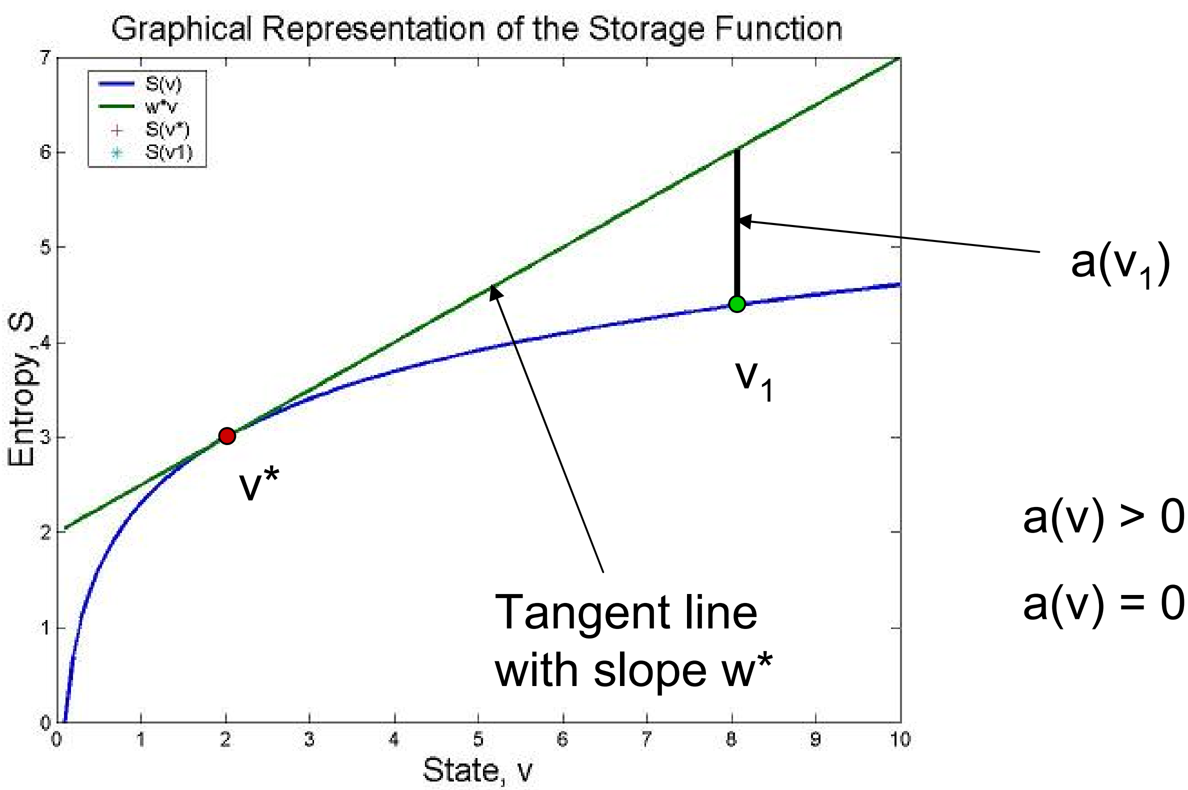
Passivity Background

- Passivity theory is used to show network stability
  - Originated from electrical circuit theory
  - A feedback or parallel connected system of passive subsystems is also passive
- Passivity inequality

$$\frac{dV(x)}{dt} \leq u^T y - \epsilon_0 x^T x$$

  - With *x,u,y* the states, inputs, and outputs to the network
  - $V(x) \geq 0, x \neq 0; V(0) = 0$
  - Network is strictly passive if $\epsilon_0 > 0$
- Problem: To find a practical storage function

Exploitation of Entropy to Develop a Storage Function



$a(v) > 0, w \neq w^*$

$a(v) = 0, w = w^*$

Storage Function Defined

- At each node:

$$a(v) = w^{*T}(v - v^*) - (S(v) - S(v^*)) \geq 0$$

- For the whole network

$$A(t) = \sum_{i=1}^{n_p} a_i(v_i) \geq 0$$

- Differentiation and using deviation variables gives

$$\frac{dA}{dt} = \sum_{j=1}^{n_p} -\bar{w}_j \frac{d\bar{v}_j}{dt}$$

- Use a result similar to Tellegen's Theorem (Proof shown in Jillson,Ydstie 2005)

$$\sum_{j=1}^{n_p} w_j^T \frac{dv_j}{dt} = \sum_{j=1}^{n_p} w_j^T p_j + \sum_{k=1}^{n_f} W_k^T f_k + \sum_{j=1}^{n_t} w_j^T f_j$$

  - Based only on topology of network

- Substituting into the previous equation

$$\frac{dA}{dt} = -\sum_{k=1}^{n_f} \bar{W}_k^T \bar{f}_k - \sum_{j=1}^{n_p} \bar{w}_j^T \bar{p}_j - \sum_{j=1}^{n_t} \bar{w}_j^T \bar{f}_j$$

Flow between nodes

Production within nodes

Boundary conditions

Passivity of Process Networks

- If

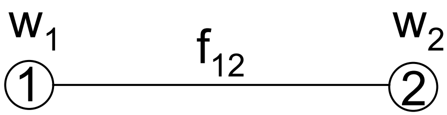
$$\sum_{k=1}^{n_f} \bar{W}_k^T \bar{f} + \sum_{j=1}^{n_p} \bar{w}_j^T \bar{p}_j \geq \epsilon_0 \sum_{j=1}^{n_p} \bar{w}_j^T \bar{w}_j$$

Then

$$\frac{dA}{dt} \leq -\underbrace{\sum_{j=1}^{n_t} \bar{w}_j^T \bar{f}_j}_{u^T y} - \epsilon_0 \underbrace{\sum_{j=1}^{n_p} \bar{w}_j^T \bar{w}_j}_{x^T x} \longrightarrow \text{Network is Strictly Passive!}$$

  - True for positive constitutive flow and production rates

Multi-component Flow



- Inventories and Potentials

$$v = [U, V, M_1, \ldots, M_n] \qquad w = [\frac{1}{T}, \frac{P}{T}, -\frac{\mu_1}{T}, \ldots, -\frac{\mu_n}{T}]$$

- Convective and Diffusive Flow

$$f = -k\hat{z}\frac{\partial P}{\partial x} - \Lambda\frac{\partial w}{\partial x} \qquad k > 0 \qquad \Lambda > 0$$

$$\hat{z} = [\widehat{H}, z_1, \ldots, z_n]$$

$$\widehat{H} = \hat{U} + P\hat{V}$$

- Using the Gibbs-Duhem equation

$$0 = \frac{\widehat{V}}{T}dP + \widehat{H}d(\frac{1}{T}) + \underline{z}^T d(-\frac{\underline{\mu}}{T}) \quad \Rightarrow \quad -\frac{dP}{dx} = \frac{T}{\widehat{V}}(\underline{z}^T\frac{d(-\frac{\underline{\mu}}{T})}{dx} + \widehat{H}\frac{d(\frac{1}{T})}{dx})$$

  - Plugging in this expression into the flow equation and integrating over a length, *L*, gives:

$$f = (< \frac{k}{\widehat{V}}T\widehat{z}\widehat{z}^T > + < \Lambda >)W = \underline{\Lambda}W$$

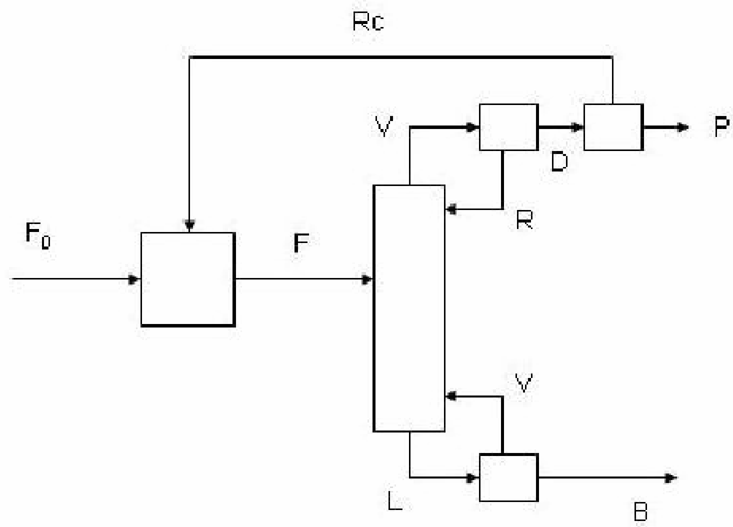
  - Potential Flow relationship is positive

Reactor-Distillation Model

(similar to Kumar and Daoutidis, 2002)

- Reactor Model: CSTR:

  A → B → C with 1st order kinetics
- Distillation Model:
  - CMO
  - 15 trays
  - Saturated Liquid Feed on 4th tray
  - Constant Relative volatilities {4,2,1}
- Fixed Feed rate and purge ratio
- 10 flows, 5 units (not counting flows within the distillation column)



Pressure driven flows

- Mass of each species in each unit → inventory
- Introduce the pressure of each unit as a function of the total mass → potential
  - Bulk flow between units would be a linear function of the differences in pressure $f_{ij} = k_{ij}(P_i - P_j)$
  - Control laws could be written to derive the *k* values, e.g:

$$k_f = \frac{F_0 + R_c + K_f(N_r - N_r^{sp})}{P_r - P_{dc}}$$

  - Problems arise with recycle loops, due to non-passive pump units

Inventory Controllers

- For total mass in four units

$$F = F_0 + R_c + K_f(N_r - N_r^{sp})$$
$$B = L - V + K_b(N_b - N_b^{sp})$$
$$D = V - R + K_d(N_d - N_d^{sp})$$
$$Rc + P = D + K_p(N_p - N_p^{sp})$$

  - At steady state, these become units' mass balances
  - Account for 4 degrees of freedom, leaving 6 remaining

Remaining Degrees of Freedom

- Inventory control on single component (*A*) in reboiler

$$V = \frac{1}{y_b^A}(Lx_{15}^A - Bx_b^A + K_v(N_b^A - N_b^{Asp}))$$

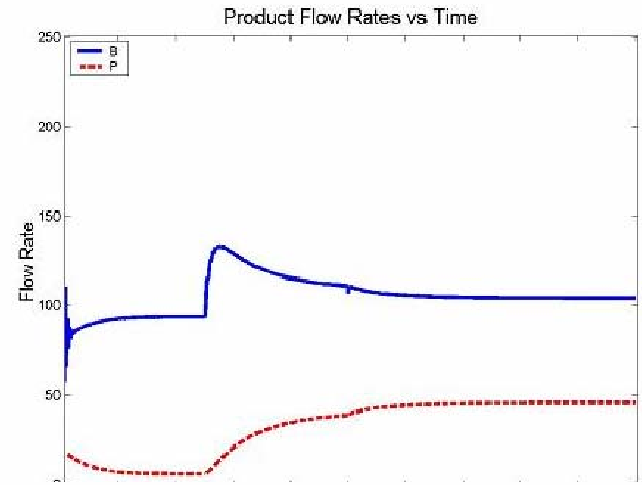
- Fixed Feed rate
- Fixed Purge Ratio
- Fixed Reflux
- Mass Balance Constraints on Distillation Column

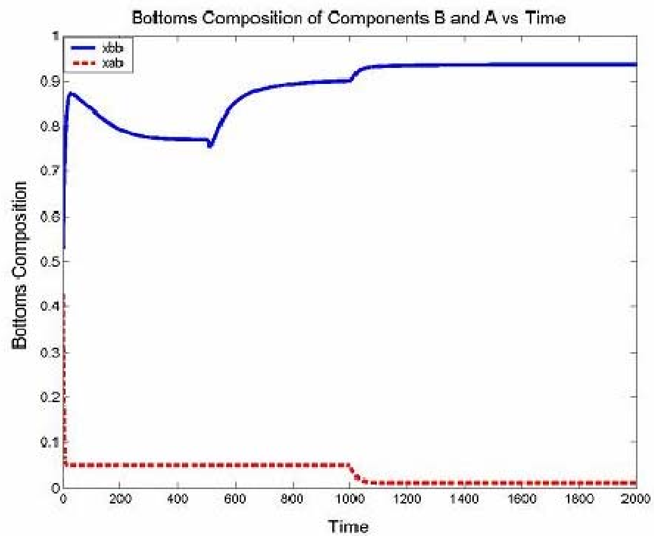
$$V_{bottom} = V_{top}$$

$$L = F + R$$

Simulation Results

- For a step change in the fixed feed rate (at t=500 from F_0 = 100 to 150) and a change in the set point of the number of moles of A in the reboiler (at t = 1000 from $N^{A}_{b}{}^{sp}$ = 9 to 2 (in effect changing x^A from 0.050 to 0.011):





Variational Principle for Process Networks

- Define the entropy production

$$\sigma_s(f) = \int_0^{f_k} W(\hat{f})d\hat{f} \longrightarrow$$ Contribution due to flow

$$\sigma_s(p) = \int_0^{p_k} w(\hat{p})d\hat{p} \longrightarrow$$ Contribution due to production

- For the complete network

$$\sigma_s(f,p) = \sum_{k=1}^{n_f} \sigma_s(f_k) + \sum_{i=1}^{n_p} \sigma_s(p_i) \geq 0$$

Optimality

- Theorem: The total entropy production is minimized along all system trajectories

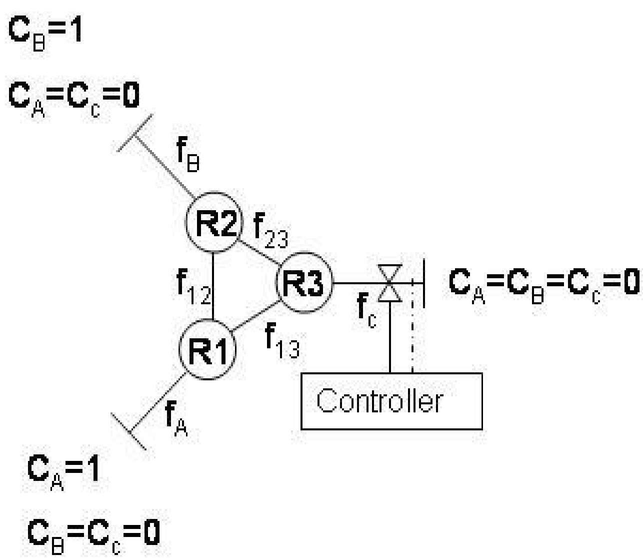
$$\int_0^t \sum_{k=1}^{n_f} \sigma_s(f_k)+\sum_{i=1}^{n_p} \sigma_s p_i dt \geq \int_0^t \sum_{k=1}^{n_f} \sigma_s(f_k^*)+\sum_{i=1}^{n_p} \sigma_s(p_i^*) dt$$

for fixed node and terminal potentials, and positive monotonic constitutive expressions

(Proof in Jillson, Ydstie 2005)

Reactor Network Example

- Three reactor nodes, and three terminals
  - Reaction: A+B → C
  - Transport governed by diffusion



9 ODE's

$$\frac{dv_i}{dt} = \sum f_{ij} + p_i$$

27 Algebraic constitutive

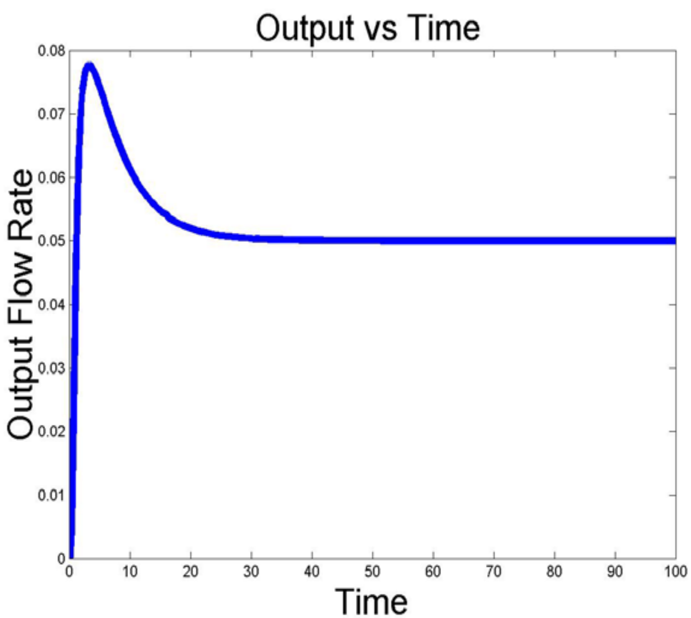
$$f_{ij} = L_{ij}(C_i - C_j)$$

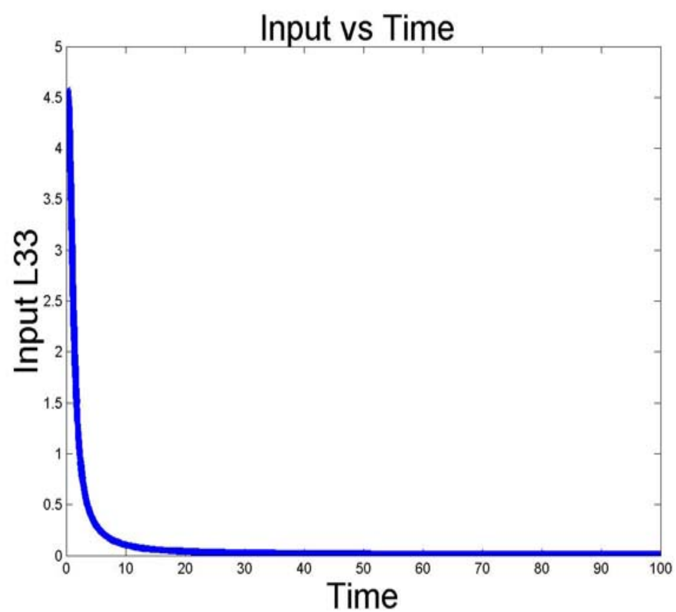
$$p_{ik} = \nu_k k_r^T C_i$$

Control of Example

- Objective: Control flow rate of C at T3
- Stabilized by a PI flow controller (K = 50, 1/τ = 10) to a set-point, fc(3) = 0.05

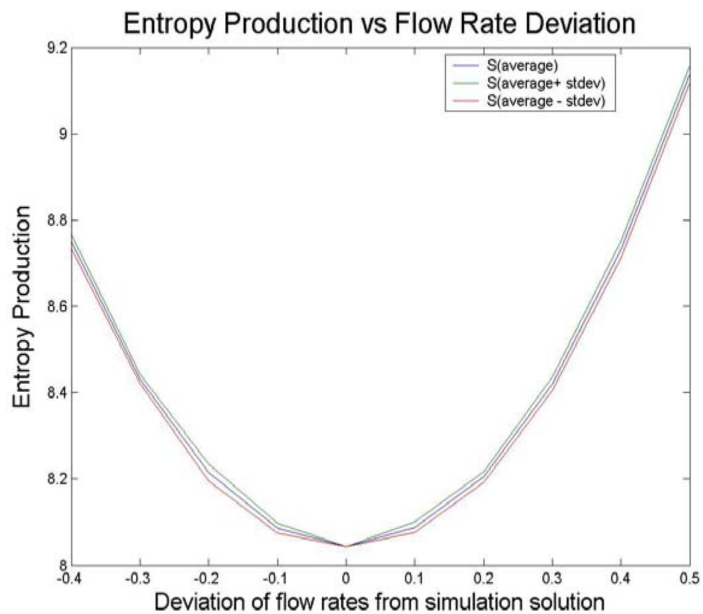
  fC(3) → y L3,3 of fC → u





Optimality Result

- Minimal entropy production in unperturbed solution, compared to a randomly perturbed network



Conclusions

- Process Networks modeled as a graph with state *v* and potential *w* at each node
- Storage function, *A*, used to show passivity provided flow and production rates are monotonic and positive
- Simulation examples presented to demonstrate theory

Acknowledgments

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