

01622 Advanced Dynamical Systems: Applications in Science and Engineering

Week 3: Mass and energy balances

Tobias K. S. Ritschel,
Asst. Prof. in Stochastic Adaptive Control

Department of Applied Mathematics and Computer Science,
Technical University of Denmark

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Learning objectives

Learning objectives

1. Derive models using mass and energy balances
2. Use time delays to describe transport phenomena
 - ▶ Describe pitfalls of time-varying time delays
3. Analyze the stability of steady states
4. Analyze the effect of feedback control laws
5. Perform numerical simulation studies
6. Perform closed-loop simulations

Stability theory

System

General form

$$\dot{x}(t) = f(x(t), u(t), d(t), p) \quad (1)$$

- ▶ u are manipulated inputs, i.e., we can use them to control the process
- ▶ d are process inputs that we do not have control over
- ▶ p are model parameters

Stability – Linear systems

For linear systems, e.g., in the form

$$\dot{x}(t) = A(p)x(t) + B(p)u(t) + E(p)d(t), \quad (2)$$

the stability is determined by the system matrix, A

Characteristic equation

$$P(\lambda) = \det(A - \lambda I) = 0 \quad (3)$$

- ▶ Unstable: Largest real part positive, $\max_{i \in \{1, \dots, n\}} \operatorname{Re} \lambda_i > 0$
- ▶ Marginally stable: Largest real part zero, $\max_{i \in \{1, \dots, n\}} \operatorname{Re} \lambda_i = 0$,
and algebraic multiplicity equal to geometric multiplicity
- ▶ Asympt. stable: Largest real part negative, $\max_{i \in \{1, \dots, n\}} \operatorname{Re} \lambda_i < 0$

Algebraic multiplicity: # of identical eigenvalues.

Geometric multiplicity: # of identical eigenvectors.

Characteristic functions and equations

Characteristic equation

$$P(\lambda) = \det(A - \lambda I) = 0 \quad (4)$$

Note: Since λ can be complex, the characteristic polynomial, $P(\lambda)$, can also be complex for arbitrary λ . Consequently, the condition is that both the real and imaginary parts are zero, i.e., the eigenvalues, λ , must satisfy two algebraic equations simultaneously.

Stability – Nonlinear systems

Nonlinear system

$$\dot{x}(t) = f(x(t), u(t), d(t), p) \quad (5)$$

Steady state

$$0 = f(x_s, u_s, d_s, p) \quad (6)$$

Jacobian matrix

$$A = \frac{\partial f}{\partial x} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix} \quad (7)$$

The stability analysis can be carried out based on the Jacobian matrix, A , evaluated in the steady state, x_s , u_s , and d_s . However, the results are only *local*.

Open-loop simulation

Open-loop simulation

Zero-order hold parametrization: Assume that manipulated inputs and disturbance variables are piecewise constant

$$u(t) = u_k, \quad t \in [t_k, t_{k+1}[, \quad (8a)$$

$$d(t) = d_k, \quad t \in [t_k, t_{k+1}[\quad (8b)$$

The intervals $[t_k, t_{k+1}]$ are called *control intervals*

Open-loop simulation ($\{u_k, d_k\}_{k=0}^{N-1}$ are given)

$$x_k(t_k) = \begin{cases} x_0 & k = 0, \\ x_{k-1}(t_k), & k = 1, \dots, N-1, \end{cases} \quad (9a)$$

$$\dot{x}_k(t) = f(x_k(t), u_k, d_k, p), \quad t \in [t_k, t_{k+1}], \quad k = 0, \dots, N-1 \quad (9b)$$

Balance equations

Balance equations

Mass and energy balances

$$\left\{ \text{Change} \right\} = \left\{ \text{In} - \text{Out} + \text{Produced} - \text{Consumed} \right\}$$

Dynamical mass and energy balances

$$\left\{ \text{Rate of change} \right\} = \left\{ \text{Inlet rate} - \text{Outlet rate} \right. \\ \left. + \text{Production rate} - \text{Consumption rate} \right\}$$

Dynamical mass balances

$$\dot{n}(t) = f_{in}(t) - f_{out}(t) + R(t)V \quad (10)$$

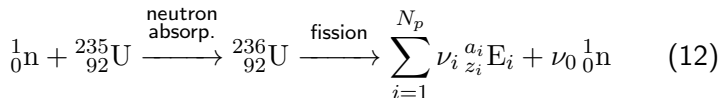
Nuclear reactor models

Nuclear fission

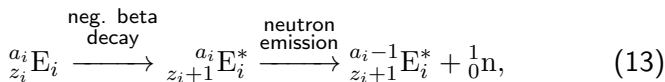
Chemical symbol

$$\begin{array}{c} \text{Mass number} \\ \text{Atomic number} \end{array} \text{Chemical element} \quad (11)$$

Fission reaction



Negative beta decay followed by neutron emission



Nuclear reactor model 1

Mass balance

$$\dot{n}(t) = \frac{\rho}{\Lambda} n(t) \quad (14)$$

ρ is the reactivity and Λ is the mean neutron generation time

Question: Is it stable?

We often express the mass balances in terms of concentrations, $C_n(t) = n(t)/V$. If the volume V is constant

$$\dot{C}_n(t) = \dot{n}(t)/V = \frac{\rho}{\Lambda} n(t)/V = \frac{\rho}{\Lambda} C_n(t) \quad (15)$$

Nuclear reactor model 2

Introduce a single neutron precursor group

$$\dot{C}_n(t) = \frac{\rho - \beta}{\Lambda} C_n(t) + \lambda_1 C_1(t), \quad (16a)$$

$$\dot{C}_1(t) = \frac{\beta}{\Lambda} C_n(t) - \lambda_1 C_1(t) \quad (16b)$$

Matrix-vector form

$$\begin{bmatrix} \dot{C}_n(t) \\ \dot{C}_1(t) \end{bmatrix} = \begin{bmatrix} \frac{\rho - \beta}{\Lambda} & \lambda_1 \\ \frac{\beta}{\Lambda} & -\lambda_1 \end{bmatrix} \begin{bmatrix} C_n(t) \\ C_1(t) \end{bmatrix} \quad (17)$$

Nuclear reactor model 3

Introduce m neutron precursor groups

$$\dot{C}_n(t) = \frac{\rho - \beta}{\Lambda} C_n(t) + \sum_{i=1}^m \lambda_i C_i(t), \quad (18)$$

$$\dot{C}_i(t) = \frac{\beta_i}{\Lambda} C_n(t) - \lambda_i C_i(t), \quad i = 1, \dots, m \quad (19)$$

where $\beta = \sum_{i=1}^m \beta_i$

Matrix-vector form

$$\begin{bmatrix} \dot{C}_n(t) \\ \dot{C}_1(t) \\ \vdots \\ \dot{C}_m(t) \end{bmatrix} = \begin{bmatrix} \frac{\rho - \beta}{\Lambda} & \lambda_1 & \cdots & \lambda_m \\ \frac{\beta_1}{\Lambda} & -\lambda_1 & & \\ \vdots & & \ddots & \\ \frac{\beta_m}{\Lambda} & & & -\lambda_m \end{bmatrix} \begin{bmatrix} C_n(t) \\ C_1(t) \\ \vdots \\ C_m(t) \end{bmatrix} \quad (20)$$

Nuclear reactor model 4

Introduce thermal reactivity feedback

$$\dot{\rho}(t) \propto C_n(t) \quad (21)$$

Proportionality constants

$$\dot{\rho}(t) = -\kappa H C_n(t) \quad (22)$$

κ is the reactivity proportionality constant and H is the ratio between the power production proportionality constant and the heat capacity of the reactor core

Mass balance equations

$$\dot{C}_n(t) = \frac{\rho(t) - \beta}{\Lambda} C_n(t) + \sum_{i=1}^m \lambda_i C_i(t), \quad (23a)$$

$$\dot{C}_i(t) = \frac{\beta_i}{\Lambda} C_n(t) - \lambda_i C_i(t), \quad i = 1, \dots, m \quad (23b)$$

General form

General form (continuously-stirred tank reactor)

$$\dot{C}(t) = R(t) \quad (24)$$

Production rate

$$R(t) = S^T(t)r(t) \quad (25)$$

Stoichiometric matrix and reaction rates ($n = m + 1$)

$$S(t) = \begin{bmatrix} -1 & & & 1 \\ & \ddots & & \vdots \\ & & -1 & 1 \\ \beta_1 & \dots & \beta_m & \rho(t) - \beta \end{bmatrix}, \quad r(t) = \begin{bmatrix} \lambda_1 C_1(t) \\ \vdots \\ \lambda_m C_m(t) \\ C_n(t)/\Lambda \end{bmatrix} \quad (26)$$

Energy balances

Energy balances

Change in internal energy

$$\dot{U}(t) = \underbrace{H(T_{in}(t), P_{in}(t), f_{in}(t))}_{\text{"}H_{in}(t)\text{"}} - \underbrace{H(T_{out}(t), P_{out}(t), f_{out}(t))}_{\text{"}H_{out}(t)\text{"}} + Q_g(t) \quad (27)$$

Enthalpy

$$H(T, P, n) = U(T, P, n) + PV(T, P, n) \quad (28)$$

The right-hand side of the energy balance involves enthalpies because it accounts for both 1) the internal energy of the inlet and outlet streams and 2) the work associated with the streams [1].

Other aspects that may affect the energy balance

- ▶ Kinetic energy
- ▶ Potential energy
- ▶ Shaft work (work done without adding or removing mass)

Enthalpy

Enthalpy of mixture

$$H(T, P, n) = nh(T, P) \quad (29)$$

Defining relationship

$$c_P(T, P) = \frac{\partial h}{\partial T}(T, P) \quad (30)$$

Integrate

$$h(T, P) - h(T_0, P_0) = \int_{T_0}^T c_P(\tilde{T}, P) d\tilde{T} \quad (31)$$

Special case (constant specific heat capacity)

$$h(T, P) = h(T_0, P_0) + c_P(T - T_0) \quad (32)$$

Note: The specific heat capacity may either be given per kilogram (or similar) or per moles

Internal energy

Relation between enthalpy, volume, and internal energy

$$U(T, P, n) = H(T, P, n) - PV(T, P, n) \quad (33)$$

Special case (constant mass and specific heat capacity)

$$\dot{U}(t) = f(t)c_P\dot{T}(t) \quad (34)$$

Enthalpy of inlet and outlet streams

Difference in inlet and outlet enthalpy (constant pressure and same mass flow rate)

$$\begin{aligned} H(T_{in}(t), P, f(t)) - H(T_{out}(t), P, f(t)) \\ = f(t)h(T_{in}(t), P) - f(t)h(T_{out}(t), P) \\ = f(t)(h(T_{in}(t), P) - h(T_{out}(t), P)) \end{aligned} \quad (35)$$

Write out difference (constant specific heat capacity)

$$\begin{aligned} h(T_{in}(t), P) - h(T_{out}(t), P) &= h(T_0, P_0) + c_P(T_{in}(t) - T_0) \\ &\quad - (h(T_0, P_0) + c_P(T_{out}(t) - T_0)) \\ &= c_P(T_{in}(t) - T_{out}(t)) \end{aligned} \quad (36)$$

Substitute

$$H(T_{in}(t), P, f(t)) - H(T_{out}(t), P, f(t)) = f(t)c_P(T_{in}(t) - T_{out}(t)) \quad (37)$$

Energy balance

Energy balance (constant pressure and heat capacity and same flow rates)

$$nC_P\dot{T}(t) = f(t)c_P(T_{in}(t) - T_{out}(t)) + Q_g(t) \quad (38)$$

Convection heat transfer

Convection

$$Q = -k(T - T_c) \quad (39)$$

Nuclear reactor models revisited

Nuclear reactor energy balances

Energy balance equations (reactor core and heat exchanger)

$$n_r c_P \dot{T}_r(t) = f(t) c_P (T_{hx}(t) - T_r(t)) + Q_g(t), \quad (40a)$$

$$n_{hx} c_P \dot{T}_{hx}(t) = f(t) c_P (T_r(t) - T_{hx}(t)) - k_{hx} (T_{hx}(t) - T_c) \quad (40b)$$

Thermal power generation

$$Q_g(t) = Q_{g,0} \frac{C_n(t)}{C_{n,0}} \quad (41)$$

Nuclear reactor model 5

Reactivity

$$\dot{\rho}(t) = -\kappa \dot{T}_r(t) \quad (42)$$

Mass balance equations

$$\dot{C}_n(t) = \frac{\rho(t) - \beta}{\Lambda} C_n(t) + \sum_{i=1}^m \lambda_i C_i(t), \quad (43a)$$

$$\dot{C}_i(t) = \frac{\beta_i}{\Lambda} C_n(t) - \lambda_i C_i(t), \quad i = 1, \dots, m \quad (43b)$$

Energy balance equations (reactor core and heat exchanger)

$$\dot{T}_r(t) = \frac{f(t)}{n_r} (T_{hx}(t) - T_r(t)) + \frac{Q_g(t)}{n_r c_P}, \quad (44a)$$

$$\dot{T}_{hx}(t) = \frac{f(t)}{n_{hx}} (T_r(t) - T_{hx}(t)) - \frac{k_{hx}}{n_{hx} c_P} (T_{hx}(t) - T_c) \quad (44b)$$

Questions?

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