# 01622 Advanced Dynamical Systems: Applications in Science and Engineering

## Week 6: Mass and energy balances

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# Learning objectives

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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

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

- $u$ 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

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

the stability is determined by the system matrix, $A$

Characteristic equation

$$P(\lambda) = \det(A - \lambda I) = 0 \tag{3}$$

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

Algebraic multiplicity: $\#$ of identical eigenvalues.
Geometric multiplicity: Dimension of spanned subspace.

# Characteristic functions and equations

Characteristic equation

$$P(\lambda) = \det(A - \lambda I) = 0 \tag{4}$$

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

# Stability – Nonlinear systems

Nonlinear system

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

Steady state

$$0 = f(x_s, u_s, d_s, p) \tag{6}$$

Jacobian matrix

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

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*.

# Lyapunov stability – System and stability

Consider the system

$$\dot{x}(t) = f(x(t)), \tag{8}$$

where $x \in \mathbb{R}^{n_x}$ is the system state and $f : \mathbb{R}^{n_x} \to \mathbb{R}^{n_x}$ is the right-hand side function.

For simplicity, assume that the steady state is $x_s = 0$

Definition 3.3 [1]. The steady state, $x_s = 0$, is stable if for every $R > 0$, there exists an $r > 0$ such that if $\|x(t_0)\| < r$, then $\|x(t)\| < R$ for all $t \geq t_0$. Otherwise, the steady state is unstable.

# Lyapunov stability – Lyapunov functions

Definition 3.7 [1]. A scalar continuous function $V : \mathbb{R}^{n_x} \to \mathbb{R}$ is (globally) positive definite if $V(0) = 0$ and

$$x \neq 0 \qquad \Rightarrow \qquad V(x) > 0. \tag{9}$$

If the result only holds for $\|x\| < R$, then $V$ is locally positive definite.

Definition 3.8 [1]. If i) $V : \mathbb{R}^{n_x} \to \mathbb{R}$ is locally positive definite, ii) has continuous partial derivatives, and iii) its time derivative along any state trajectory is negative semi-definite, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t} V(x(t)) \leq 0, \tag{10}$$

then $V$ is a Lyapunov function for the system (8).

# Lyapunov stability – Lyapunov's theorem for local stability

Theorem 3.2 [1]. Without loss of generality, assume that the steady state of the system (8) is $x_s = 0$. Then, if there exists a Lyapunov function, $V$, the steady state is stable. If, in addition, $\frac{\mathrm{d}}{\mathrm{d}t}V(x(t))$ is negative definite, the steady state is asymptotically stable.

# Open-loop simulation

# Open-loop simulation

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

$$u(t) = u_k, \qquad t \in [t_k, t_{k+1}[, \tag{11a}$$

$$d(t) = d_k, \qquad t \in [t_k, t_{k+1}[ \tag{11b}$$

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

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

$$x_k(t_k) = \begin{cases} x_0 & k = 0, \\ x_{k-1}(t_k), & k = 1, \dots, N-1, \end{cases} \tag{12a}$$

$$\dot{x}_k(t) = f(x_k(t), u_k, d_k, p), \quad t \in [t_k, t_{k+1}], \quad k = 0, \dots, N-1 \tag{12b}$$

# 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

$$\left\{ \text{ Rate of change } \right\} = \left\{ \begin{array}{l} \text{Inlet rate} - \text{Outlet rate} \\ + \text{Production rate} - \text{Consumption rate} \end{array} \right\}$$

Dynamical mass balances

$$\dot{n}(t) = f_{in}(t) - f_{out}(t) + R(t)V \tag{13}$$

# Nuclear reactor models

# Nuclear fission

Chemical symbol

$$^{\text{Mass number}}_{\text{Atomic number}}\text{Chemical element} \tag{14}$$

Fission reaction

$${}^{1}_{0}\text{n} + {}^{235}_{92}\text{U} \xrightarrow{\substack{\text{neutron}\\ \text{absorp.}}} {}^{236}_{92}\text{U} \xrightarrow{\text{fission}} \sum_{i=1}^{N_p} \nu_i \, {}^{a_i}_{z_i}\text{E}_i + \nu_0 \, {}^{1}_{0}\text{n} \tag{15}$$

Negative beta decay followed by neutron emission

$${}^{a_i}_{z_i}\text{E}_i \xrightarrow{\substack{\text{neg. beta}\\ \text{decay}}} {}^{a_i}_{z_i+1}\text{E}_i^* \xrightarrow{\substack{\text{neutron}\\ \text{emission}}} {}^{a_i-1}_{z_i+1}\text{E}_i^* + {}^{1}_{0}\text{n}, \tag{16}$$

# Nuclear reactor model 1

Mass balance

$$\dot{n}(t) = \frac{\rho}{\Lambda} n(t) \tag{17}$$

$\rho$ is the reactivity and $\Lambda$ 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

$$\dot{C}_n(t) = \dot{n}(t)/V = \frac{\rho}{\Lambda} n(t)/V = \frac{\rho}{\Lambda} C_n(t) \tag{18}$$

# Nuclear reactor model 2

Introduce a single neutron precursor group

$$\dot{C}_n(t) = \frac{\rho - \beta}{\Lambda} C_n(t) + \lambda_1 C_1(t), \tag{19a}$$

$$\dot{C}_1(t) = \frac{\beta}{\Lambda} C_n(t) - \lambda_1 C_1(t) \tag{19b}$$

Matrix-vector form

$$\begin{bmatrix} \dot{C}_n(t) \\ \dot{C}_1(t) \end{bmatrix} = \begin{bmatrix} \frac{\rho-\beta}{\Lambda} & \lambda_1 \\ \frac{\beta}{\Lambda} & -\lambda_1 \end{bmatrix} \begin{bmatrix} C_n(t) \\ C_1(t) \end{bmatrix} \tag{20}$$

# Nuclear reactor model 3

Introduce $m$ neutron precursor groups

$$\dot{C}_n(t) = \frac{\rho - \beta}{\Lambda} C_n(t) + \sum_{i=1}^{m} \lambda_i C_i(t), \qquad (21)$$

$$\dot{C}_i(t) = \frac{\beta_i}{\Lambda} C_n(t) - \lambda_i C_i(t), \qquad i = 1, \ldots, m \qquad (22)$$

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

Matrix-vector form

$$\begin{bmatrix} \dot{C}_n(t) \\ \dot{C}_1(t) \\ \vdots \\ \dot{C}_m(t) \end{bmatrix} = \begin{bmatrix} \frac{\rho-\beta}{\Lambda} & \lambda_1 & \cdots & \lambda_m \\ \frac{\beta_1}{\Lambda} & -\lambda_1 & & \\ \vdots & & \ddots & \\ \frac{\beta_m}{\Lambda} & & & -\lambda_m \end{bmatrix} \begin{bmatrix} C_n(t) \\ C_1(t) \\ \vdots \\ C_m(t) \end{bmatrix} \qquad (23)$$

# Nuclear reactor model 4

Introduce thermal reactivity feedback

$$\dot{\rho}(t) \propto C_n(t) \tag{24}$$

Proportionality constants

$$\dot{\rho}(t) = -\kappa H C_n(t) \tag{25}$$

$\kappa$ 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

$$\dot{C}_n(t) = \frac{\rho(t) - \beta}{\Lambda} C_n(t) + \sum_{i=1}^{m} \lambda_i C_i(t), \tag{26a}$$

$$\dot{C}_i(t) = \frac{\beta_i}{\Lambda} C_n(t) - \lambda_i C_i(t), \qquad i = 1, \ldots, m \tag{26b}$$

# General form

General form (continuously-stirred tank reactor) [2]

$$\dot{C}(t) = R(t) \tag{27}$$

Production rate

$$R(t) = S^T(t)r(t) \tag{28}$$

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

$$S(t) = \begin{bmatrix} -1 & & & 1 \\ & \ddots & & \vdots \\ & & -1 & 1 \\ \beta_1 & \dots & \beta_m & \rho(t) - \beta \end{bmatrix}, \quad r(t) = \begin{bmatrix} \lambda_1 C_1(t) \\ \vdots \\ \lambda_m C_m(t) \\ C_n(t)/\Lambda \end{bmatrix} \tag{29}$$

# Energy balances

# Energy balances

Change in internal energy

$$\dot{U}(t) = \underbrace{H(T_{in}(t), P_{in}(t), f_{in}(t))}_{\text{“}H_{in}(t)\text{”}} - \underbrace{H(T_{out}(t), P_{out}(t), f_{out}(t))}_{\text{“}H_{out}(t)\text{”}} + Q_g(t) \tag{30}$$

Enthalpy

$$H(T, P, n) = U(T, P, n) + PV(T, P, n) \tag{31}$$

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 [3].

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

$$H(T, P, n) = nh(T, P) \tag{32}$$

Defining relationship

$$c_P(T, P) = \frac{\partial h}{\partial T}(T, P) \tag{33}$$

Integrate

$$h(T, P) - h(T_0, P_0) = \int_{T_0}^{T} c_P(\tilde{T}, P)\,\mathrm{d}\tilde{T} \tag{34}$$

Special case (constant specific heat capacity)

$$h(T, P) = h(T_0, P_0) + c_P(T - T_0) \tag{35}$$

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

$$U(T,P,n) = H(T,P,n) - PV(T,P,n) \quad (36)$$

Special case (constant mass and specific heat capacity)

$$\dot{U}(t) = nc_P\dot{T}(t) \quad (37)$$

# Enthalpy of inlet and outlet streams

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

$$\begin{aligned} H(T_{in}(t), P, f(t)) - H(T_{out}(t), P, f(t)) \\ = f(t)h(T_{in}(t), P) - f(t)h(T_{out}(t), P) \\ = f(t)\left(h(T_{in}(t), P) - h(T_{out}(t), P)\right) \end{aligned} \tag{38}$$

Write out difference (constant specific heat capacity)

$$\begin{aligned} h(T_{in}(t), P) - h(T_{out}(t), P) &= h(T_0, P_0) + c_P(T_{in}(t) - T_0) \\ &\quad - (h(T_0, P_0) + c_P(T_{out}(t) - T_0)) \\ &= c_P(T_{in}(t) - T_{out}(t)) \end{aligned} \tag{39}$$

Substitute

$$H(T_{in}(t), P, f(t)) - H(T_{out}(t), P, f(t)) = f(t)c_P(T_{in}(t) - T_{out}(t)) \tag{40}$$

# Energy balance

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

$$nc_P\dot{T}(t) = f(t)c_P(T_{in}(t) - T_{out}(t)) + Q_g(t) \tag{41}$$

# Convection heat transfer

Convection

$$Q = -k(T - T_c) \tag{42}$$

# Nuclear reactor models revisited

# Nuclear reactor energy balances

Energy balance equations (reactor core and heat exchanger)

$$n_r c_P \dot{T}_r(t) = f(t) c_P (T_{hx}(t) - T_r(t)) + Q_g(t), \quad (43a)$$

$$n_{hx} c_P \dot{T}_{hx}(t) = f(t) c_P (T_r(t) - T_{hx}(t)) - k_{hx}(T_{hx}(t) - T_c) \quad (43b)$$

Thermal power generation

$$Q_g(t) = Q_{g,0} \frac{C_n(t)}{C_{n,0}} \quad (44)$$

# Nuclear reactor model 5

Reactivity

$$\dot{\rho}(t) = -\kappa \dot{T}_r(t) \tag{45}$$

Mass balance equations

$$\dot{C}_n(t) = \frac{\rho(t) - \beta}{\Lambda} C_n(t) + \sum_{i=1}^{m} \lambda_i C_i(t), \tag{46a}$$

$$\dot{C}_i(t) = \frac{\beta_i}{\Lambda} C_n(t) - \lambda_i C_i(t), \qquad i = 1, \dots, m \tag{46b}$$

Energy balance equations (reactor core and heat exchanger)

$$\dot{T}_r(t) = \frac{f(t)}{n_r}(T_{hx}(t) - T_r(t)) + \frac{Q_g(t)}{n_r c_P}, \tag{47a}$$

$$\dot{T}_{hx}(t) = \frac{f(t)}{n_{hx}}(T_r(t) - T_{hx}(t)) - \frac{k_{hx}}{n_{hx} c_P}(T_{hx}(t) - T_c) \tag{47b}$$

Questions?

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