First-principles («theoretical») dynamic models of chemical processes

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MolBNL
MOLECULAR BIOLOGY AND NANOTECHNOLOGY LABORATORY
UNIVERSITY OF TRIESTE

ANDREA MIO, PhD
MolBNL @ DIA-UniTS; www.molbnl.it
amio@units.it - 0405583440

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WHAT'S THE PURPOSE OF DYNAMIC MODEL?

- To improve process understanding and for operator training
  - Dynamic simulators can be used as «virtual processes» to train the operators to face both normal and abnormal (emergency) situations
  - They can be used as Operator Training Systems (OTSs)
    - The real control system is interfaced to the dynamic simulator
- To develop a control strategy for a new process, or to improve an existing control strategy
  - Different control alternatives can be evaluated on the model
    - E.g., different pairings between controlled variables and manipulated variables
  - The model can be used for controller tuning (i.e., to assign appropriate values to the control law parameters)
  - The model itself could be incorporated within the control law
- To optimize the process operating conditions
  - Usually, a steady-state model is sufficient

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WHICH KIND OF DYNAMIC MODEL?

- First-principles (theoretical) models
  - They use the **principles** of chemical engineering, and of chemistry, physics, biology, physiology, pharmacology, …
    - They represent the physical knowledge of the system
    - They can be used in a wide range of operating conditions (model extrapolation)
    - Their parameters have physical meaning
    - Often, they are difficult to derive, and can be «slow» from a calculation viewpoint
- Empirical models (data-driven models; black-box models)
  - They are obtained by **fitting** experimental data
    - They can be used in a limited range of operating conditions (no extrapolation)
    - Their parameters rarely have physical meaning
    - They are relatively easy to derive and fast to calculate
- Semi-empirical models (hybrid models; grey-box models)
  - They are a combination of first-principles and empirical models
    - A compromise of their pros and cons

«Essentially, all models are wrong, but some are useful»

Box, G.E.P., and Draper, N.R. (1987). Empirical Model Building and Response Surfaces, John Wiley & Sons, Hoboken, NJ

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FIRST-PRINCIPLES MODELS

- Basically, they can be derived by using two kinds of equations
  1. Conservation laws (mass; energy; momentum)
     - Ordinary differential equations (ODEs) -> concentrated parameter models
     - Partial differential equations (PDEs) -> distributed parameter models
  2. Constitutive equations
     - Algebraic equations (AEs): thermodynamic equilibrium, mass/energy transport, physical properties, kinetic equations, …
  - The set of ODEs and Aes results in a system of differential and algebraic equations (DAEs)
- First-principles models represent an abstraction of reality
  - They can incorporate macroscopic and/or microscopic characteristics of the real system
  - The level of details to be included in the model depends on the required use of the model
  - A compromise between accuracy and complexity is needed
    - The more the model is accurate, the more is complex
    - The more the model is complex, the more it costs to develop, the more difficult it is to use
  - Some simplifications usually need to be considered

The model must not be more complex than required for the particular application it is developed for.
Fit-all-purpose models do not exist!

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DEGREES OF FREEDOM OF A DYNAMIC MODEL

- Number N_F of degrees of freedom (d.o.f.) of a set of equations

$$\boxed{N_F = N_V - N_E}$$

  N_V = number of model variables
  N_E = number of independent equations

- $N_F = 0$: the model is exactly specified
  - The set of equations has a solution
- $N_F > 0$: the model is underspecified
  - There are more variables than equations
  - The N_E equations have an infinite number of solutions, because N_F variables can be assigned arbitrarily
- $N_F < 0$: the model is overspecified
  - There are more equations than variables
  - The set of equations has no solution

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HOW TO FIND THE NUMBER OF DEGREES OF FREEDOM

1. List all quantities in the model that are known constants (or parameters whose values can be determined)
   - E.g., from equipment size, physical properties
2. Determine the number N_E of independent equations and the number N_V of process variables
   - Time t is not a process variable: it is neither an input nor an output
3. Calculate the number of d.o.f.: $N_F = N_V - N_E$
4. Identify the N_E output variables that will be calculated using the process model
5. Identify the N_F input variables that must be assigned in order to saturate the N_F d.o.f.
   - They may be either manipulated variables or disturbances

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EXAMPLES: writing the dynamic models of some systems

- Stirred and heated tank, constant volume (SEMD, p.21)
- Stirred and heated tank, variable volume (SEMD, p. 22)
- Stirred tank, constant volume, with electrical resistance having non-neglibible thermal capacitance (SEMD, p.23)

- Suggestion for independent study
  - Models for other systems (SEMD, p. 24-30)
  - Numerical integration of sets of differential equations (Matlab; SEMD Appendix C, p.480-482)

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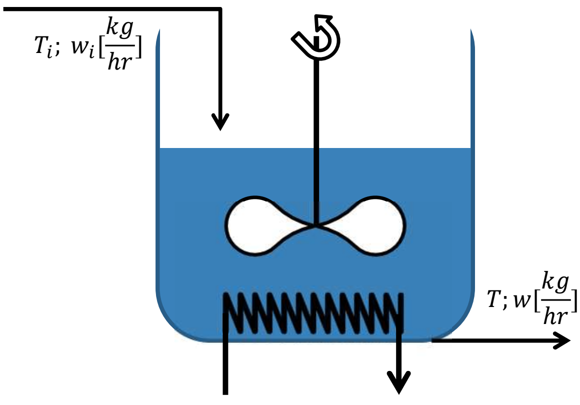
Stirred and heated tank, constant volume

- Assumptions:
  1. Perfect mixing → $T_{out}(t) = T = T_{internal}(t)$
  2. $w_i = w$ → no accumulation
  3. Constant Cp → independent on T
  4. Constant ρ → independent on T
  5. No heat losses with surroundings
  6. $\dot{Q}_{el}(t) = \dot{Q}_{liq}(t)$ → Electrical power dissipated is transferred continuously to the system



- Dynamic model? → $T(t)$? $V(t)$?

$$\frac{dT}{dt} = \frac{\dot{Q}_{liq}}{\rho V c_P} + \frac{w_i(T_i - T)}{\rho V}$$

- Parameters: $N_P = \rho, c_P, V = 3$
- Variables: $N_V = w_i, T_i, \dot{Q}_{el}, T = 4$
- Equations: $N_E = 1$
- D.o.f.: $N_F = N_V - N_E = 3$

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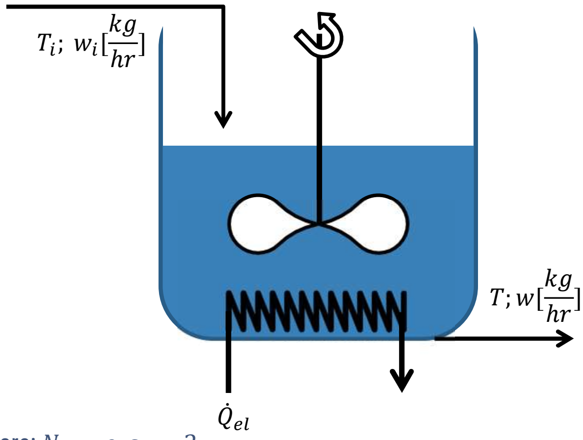
Stirred and heated tank, variable volume

- Assumptions:
  1. Perfect mixing → $T_{out}(t) = T = T_{internal}(t)$
  2. $w_i \neq w$ → accumulation!!!!
  3. Constant Cp → independent on T
  4. Constant ρ → independent on T
  5. No heat losses with surroundings
  6. $\dot{Q}_{el}(t) = \dot{Q}_{liq}(t)$ → Electrical power dissipated is transferred continuously to the system



- Dynamic model? → $T(t)?$ $V(t)?$

$$\frac{dT}{dt} = \frac{\dot{Q}_{liq}}{\rho V c_P} + \frac{w_i(T_i - T)}{\rho V}$$

$$\frac{dV}{dt} = \frac{w_i - w}{\rho}$$

- Parameters: $N_P = \rho, c_P = 2$
- Variables: $N_V = w_i, w, T_i, \dot{Q}_{el}, T, V = 6$
- Equations: $N_E = 2$
- D.o.f.: $N_F = N_V - N_E = 4$

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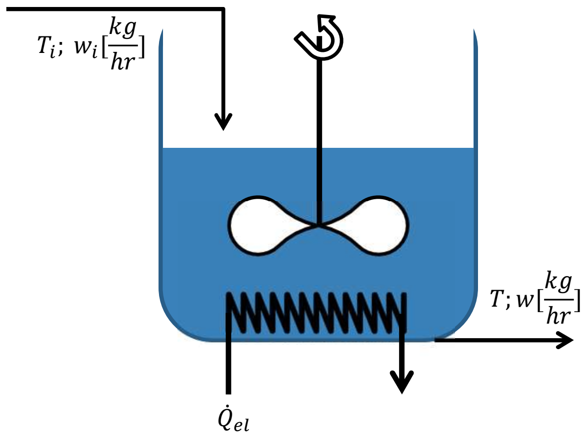
Stirred and heated tank, constant volume, resistance thermal capacitance

- Assumptions:
  1. Perfect mixing → $T_{out}(t) = T = T_{internal}(t)$
  2. $w_i = w$ → no accumulation
  3. Constant Cp → independent on T
  4. Constant ρ → independent on T
  5. No heat losses with surroundings
  6. $\dot{Q}_{el}(t) \neq \dot{Q}_{liq}(t)$ → Electrical power dissipated is NOT transferred continuously to the system



- Dynamic model? → $T(t)?$ $V(t)?$

$$\frac{dT}{dt} = \frac{h_e S_e (T_e - T)}{\rho V c_P} + \frac{w\,(T_i - T)}{\rho V}$$

$$\frac{dT_e}{dt} = \frac{\dot{Q}_{el}}{c_{p,e} M_e} - \frac{h_e S_e (T_e - T)}{c_{p,e} M_e}$$

- Parameters: $N_P = \rho, c_P, V, c_{P,e}, M_e, S_e, h_e = 7$
- Variables: $N_V = w_i, T_i, \dot{Q}_{el}, T, T_e = 5$
- Equations: $N_E = 2$
- D.o.f.: $N_F = N_V - N_E = 3$

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