SKF 3143

Process Control and Dynamics: Development of Mathematical Model

Mohd. Kamaruddin Abd. Hamid, PhD

kamaruddin@cheme.utm.my

www.cheme.utm.my/staff/kamaruddin

Learning Objectives

When I complete this chapter, I want to be able to do the following:

1. Model process control using mathematical approach

Mathematical Modelling for Process Control?

- To improve understanding of the process
  - Process models can be analysed to investigate process behaviour without the unexpected hazard of operating the real process
  - Necessary when it is not feasible to perform dynamics experiments in the plant or before the plant is actually constructed
- To train operating personnel
  - Plant operators can be trained to operate a complex process and deal with emergency situations
  - Training for operators without exposure to dangerous conditions in the real plant situation
- To design the control strategy for a new process
  - A process model allows alternative control strategies to be evaluated
  - This is suitable for new processes that we have little operating experience

Mathematical Modelling for Process Control?

- To select controller settings
  - A dynamic model of the process may be used to develop appropriate controller settings
- To design the control law
  - Modern control techniques often incorporate a process model into the control law
  - This techniques are called model-predictive or model-based control
- To optimise process operating conditions
  - Incentive in most processing plants to adjust operating conditions periodically so that the plant maximises profits or minimises costs
  - A steady-state model of the process and appropriate economic information can be used to determine the most profitable process conditions

Model Classification

Models can be considered in three different classifications, depending on how they are derived:

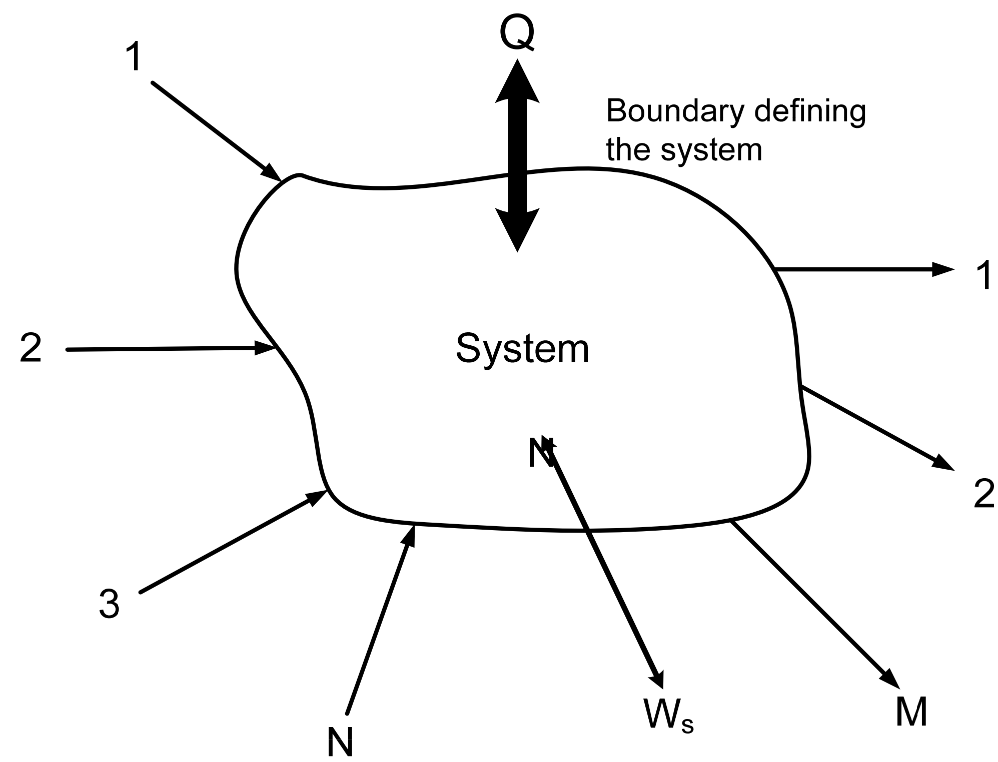
1. Theoretical models developed using the principles of chemistry and physics
2. Empirical models obtained from a mathematical (statistical) analysis of process operating data
3. Semiemperical models that are a compromise between (1) and (2), with one or more parameters to be evaluated from plant data.

- Advantages of semiemperical models:
  1. Can be extrapolated over a wider range of operating conditions
  2. Provide the capability to infer how unmeasured or unmeasurable process variables vary as the process operating conditions change

Principle of Conservation

Accumulation S = Inlet S - Outlet S + Generation S - Consumption S

- The quantity of S can be any of the following fundamental quantities:
  - Total mass
  - Mass of individual components
  - Total energy
  - Momentum
- Total mass and energy cannot be generated, neither do they disappear



Principle of Conservation

- Total Mass Balance

$$\frac{d(\rho V)}{dt} = \sum_{i:inlet} \rho_i F_i - \sum_{j:outlet} \rho_j F_j$$

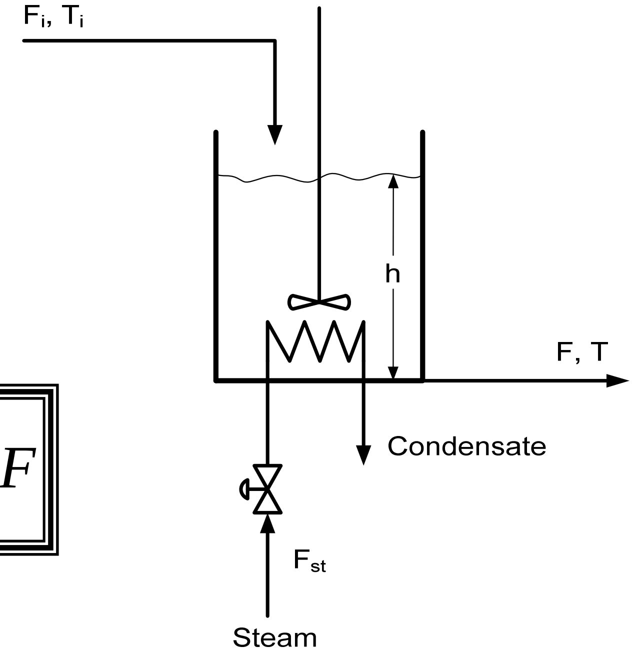
- Mass balance on Component A

$$\frac{d(n_A)}{dt} = \frac{d(c_A V)}{dt} = \sum_{i:inlet} c_{Ai} F_i - \sum_{j:outlet} c_{Aj} F_j \pm rV$$

- Total energy balance

$$\frac{dE}{dt} = \frac{d(U + K + P)}{dt} = \sum_{i:inlet} \rho_i F_i h_i - \sum_{j:outlet} \rho_j F_j h_j \pm Q \pm W_s$$

Modelling of Stirred Heating Tank



- State variables: Level (*h*) and Temperature (*T*)
- Parameters: ρ, A, c_p and T_{ref}
- Overall balance on the tank

$$\frac{d(\rho A h)}{dt} = \rho F_i - \rho F \quad \Rightarrow \quad \boxed{A\frac{dh}{dt} = F_i - F}$$

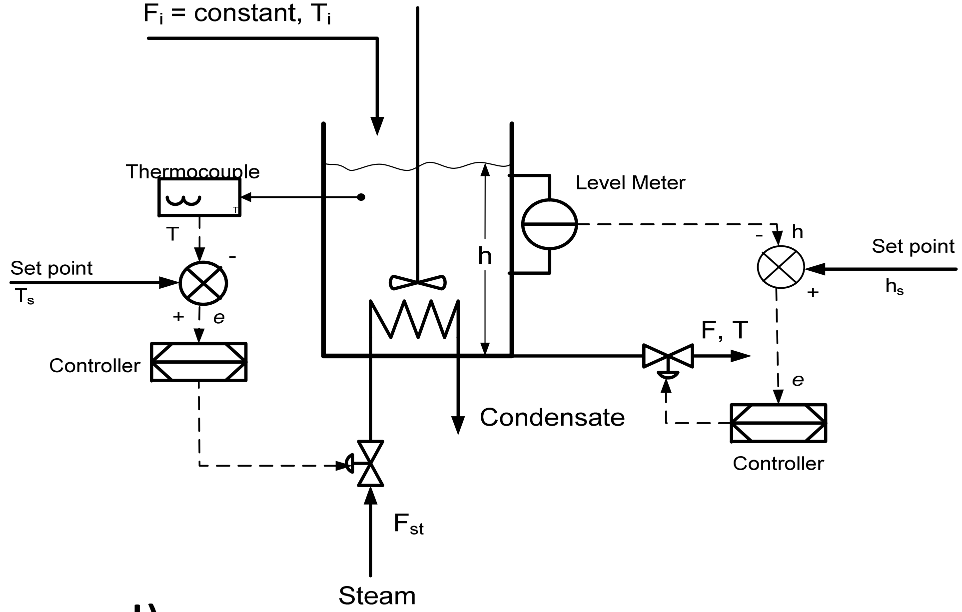
- Total energy balance

$$\frac{d\left[\rho A h c_p (T - T_{ref})\right]}{dt} = \rho F c_p (T_i - T_{ref}) - \rho F c_p (T - T_{ref}) + Q$$

- If T_{ref}=0 $\Rightarrow$ $A\dfrac{d(hT)}{dt} = F_i T_i - FT + \dfrac{Q}{\rho c_p}$

$$A\frac{d(hT)}{dt} = Ah\frac{dT}{dt} + AT\frac{dh}{dt} = Ah\frac{dT}{dt} + T(F_i - F) = F_i T_i - FT + \frac{Q}{\rho c_p}$$

Modelling of Stirred Heated Tank



- State Equations

$$A\frac{dh}{dt} = F_i - F$$

$$A\frac{d(hT)}{dt} = F_iT_i - FT + \frac{Q}{\rho c_p}$$

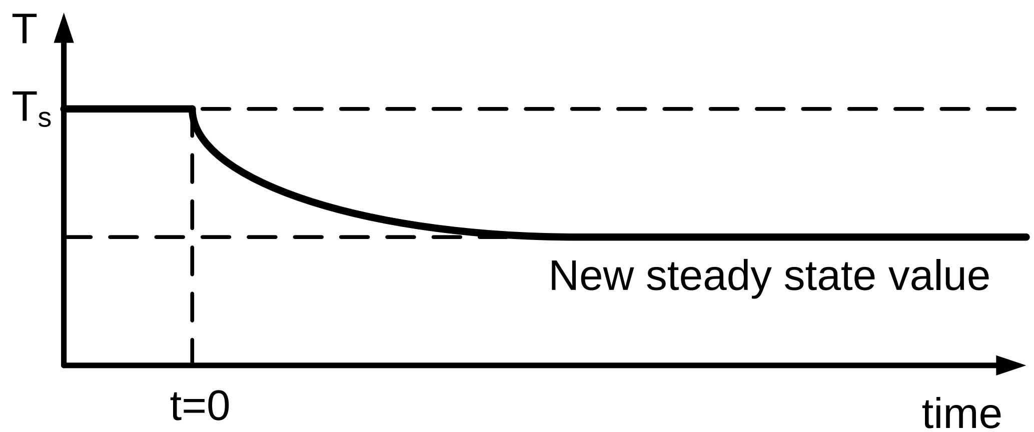
- State variables: h and T
- Output variables: h and T (measured)
- Input variables
  - Disturbances: T_i and F_i
  - Manipulated: Q and F (feedback)
- Parameters: A, ρ, c_p

Stirred Heated Tank Dynamic

- At initial state, the rate of accumulation is set to zero:

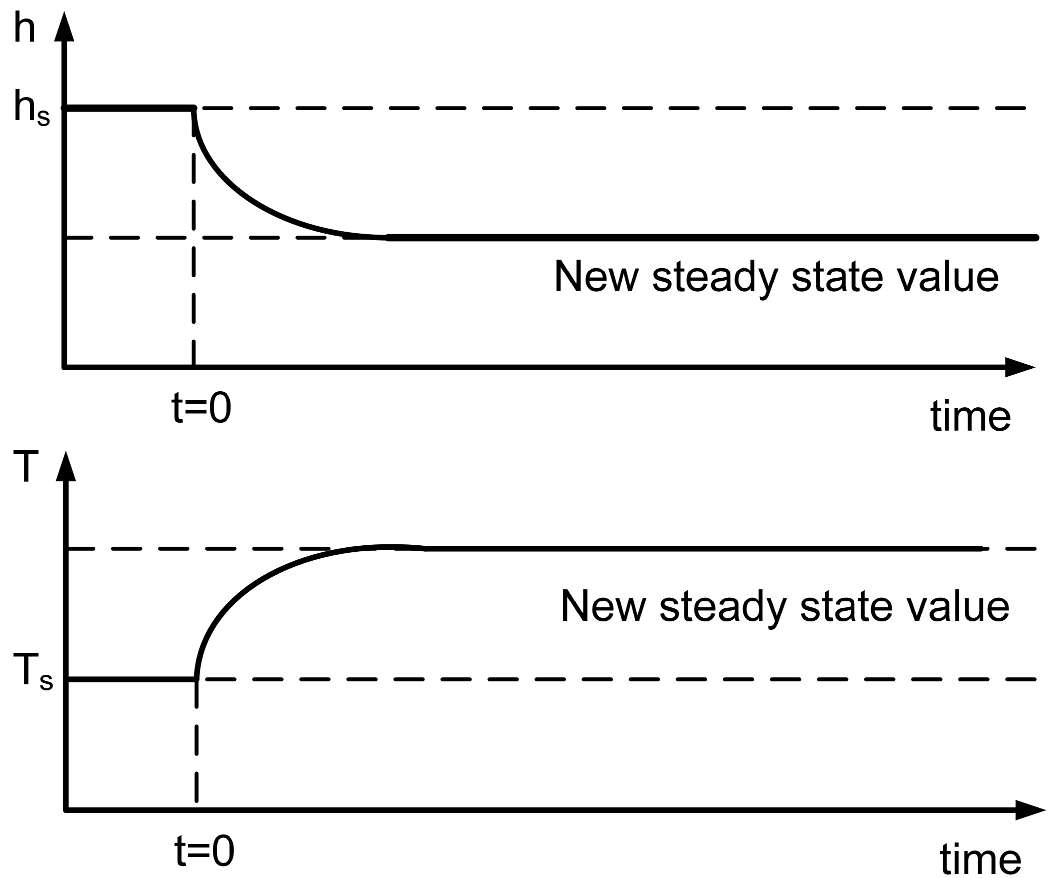
$$0 = F_{i,s} - F_s \quad \text{and} \quad 0 = F_{i,s}\left(T_{i,s} - T_s\right) + \frac{Q_s}{\rho c_p}$$

- Consider the inlet temperature T_i decreases by 10%
  - The liquid level remain the same since T_i does not influence h_s
  - Temperature T will start decreasing as T_i change
  - It will start from $T(t = 0)=T_s$



Stirred Heated Tank Dynamic

- At t = 0 the inlet flow rate F_i decreases by 10%
  - Values of h and T will change due to this phenomenon
  - Using the initial conditions h(t = 0) = hs and T(t = 0) = T_s



Additional Elements of the Mathematical Models

- Transport Rate Equations

  The amount of heat (Q) supplied by steam to the liquid tank heater

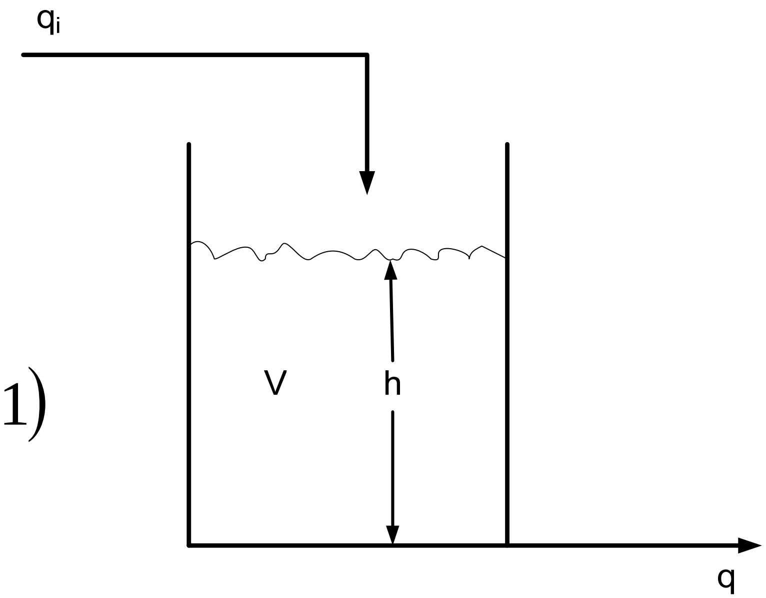
$$Q = UA_t\left(T_{st} - T\right)$$

- Kinetic Rate Equations
  - The reaction rate of a first-order reaction taking place in CSTR
  - Depend on the order of the reaction

$$r = k_o e^{-E/RT} C_A$$

- Reaction and phase equilibria relationship
  - Liquid phase temperature = Vapour phase temperature
  - Liquid phase pressure = Vapour phase pressure
  - Chemical potential of component *i* in the liquid phase = chemical potential of component *i* in the vapour phase

Liquid Storage Systems



- q_i and q are volumetric flow rates
- A mass balance yields

$$\frac{d(V\rho)}{dt} = q_i\rho - q\rho \qquad (3.1)$$

- Since V = Ah, and ρ = constant

$$A\frac{dh}{dt} = q_i - q \qquad (3.2)$$

- There are three important variations of the liquid storage process:

1. The inlet or outlet flow rates might be constant

   Outflow q might be maintained by a constant-speed, fixed-volume (metering) pump.

   $q = \bar{q}$ (the overbar denotes a steady-state value of flow)

Liquid Storage Systems

2. The tank exit line may function as a resistance to flow from the tank or may contain a valve that provides significant resistance to flow at a single point

Flow may be assumed to be linearly related to the driving force, the liquid head (analogy Ohm's law E = IR)

$$h = qR_v \qquad (3.3)$$

Rv is the resistance of the line. Rearranging equation above gives

$$q = \frac{1}{R_v} h \qquad (3.4)$$

Substitute (3.4) into (3.2) yields a first-order linear differential equation:

$$A\frac{dh}{dt} = q_i - \frac{1}{R_v} h \qquad (3.5)$$

Liquid Storage Systems

3. When a valve has been placed in the exit line and turbulent flow can be assumed, a more realistic expression for q can be obtained

The pressure difference driving flow through the valve is

$$\Delta P = P - P_a \qquad (3.6)$$

Because ΔP is proportional to q^2 from the Bernoulli relation,

$$q = C_v \sqrt{P - P_a} \qquad (3.7)$$

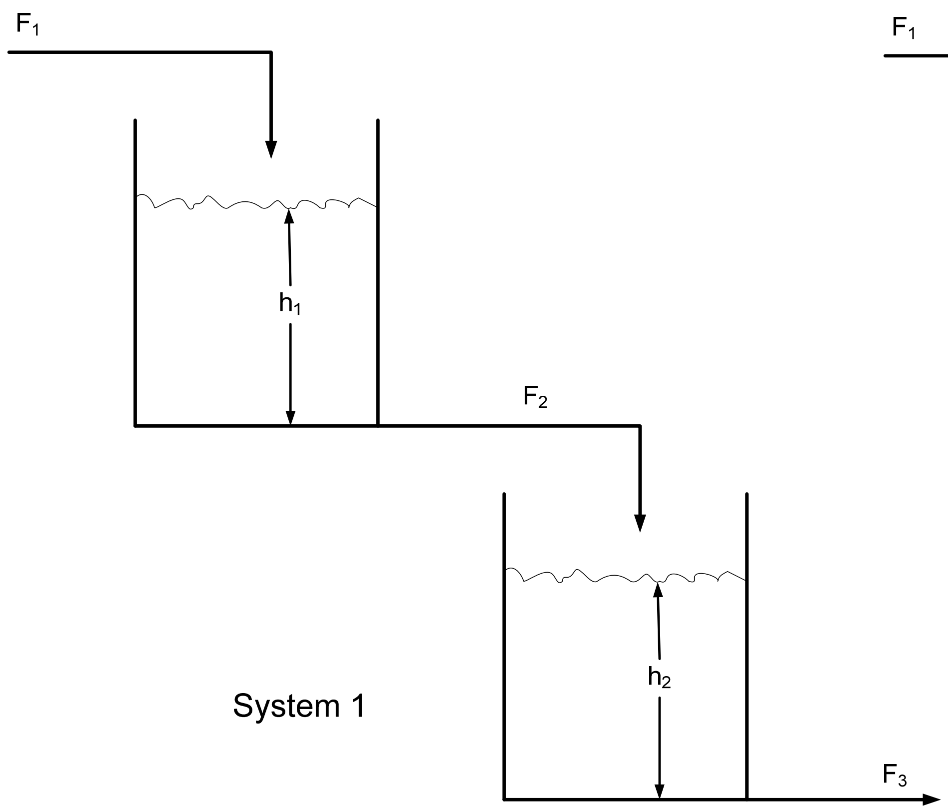
where, C_v, called the valve coefficient. Assume the flow discharges at ambient pressure P_a and that the upstream pressure P is the pressure at the bottom of the tank

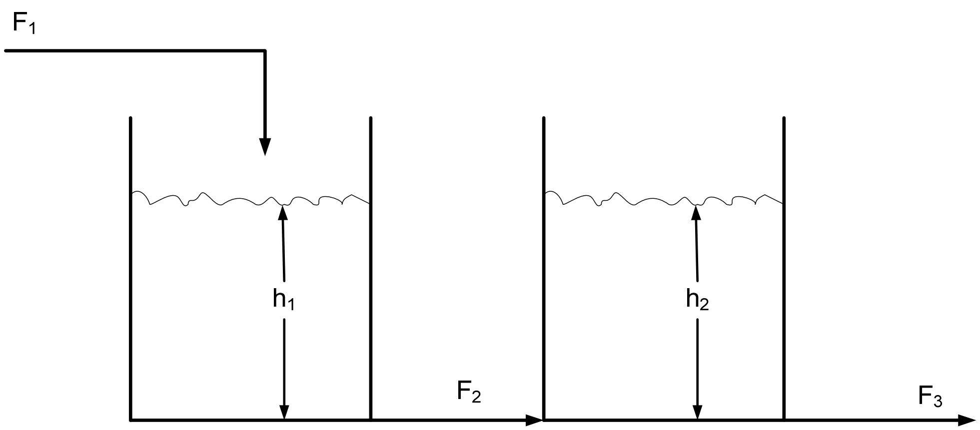
$$P = P_a + \frac{\rho g}{g_c} h \qquad (3.8)$$

$$A\frac{dh}{dt} = q_i - C_v \sqrt{\rho \frac{g}{g_c} h} \qquad (3.9)$$

Example

- Develop the mathematical model for each of the two systems

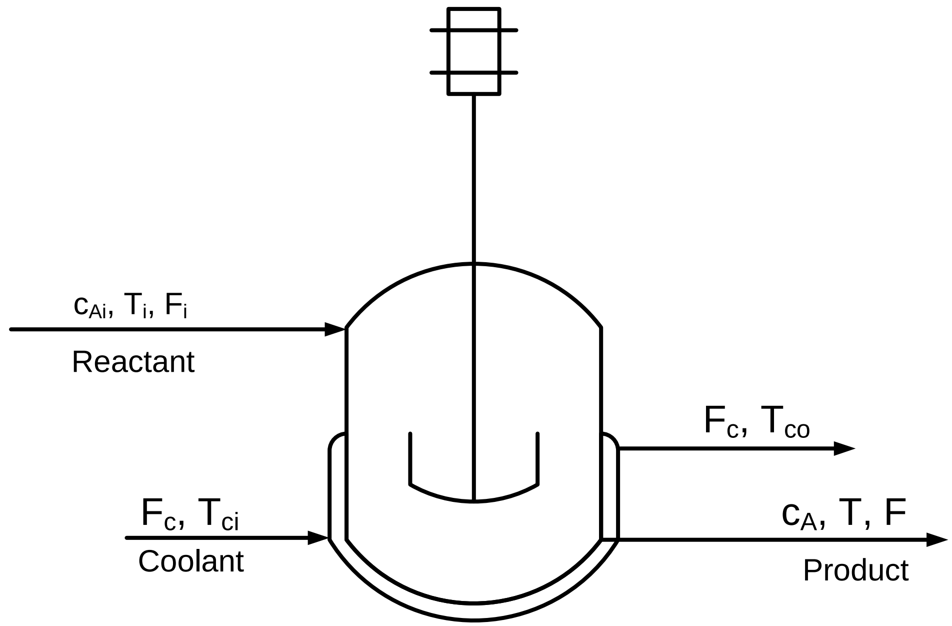




System 2

Example

Using the given diagram, give the state variables and develop the state equations. A simple exothermic reaction A→B takes place in the reactor



The fundamental dependent quantities:

- Total mass of the reacting mixture
- Mass of chemical A in the reacting mixture
- Total energy of the reacting mixture in the tank

References:

- Seborg, D. E., Edgar, T. F., Mellinchamp, D. A. (2003). *Process Dynamics and Control*, 2nd. Edition. John Wiley, ISBN: 978-04-71000-77-8.
- Marlin, T. E. (2000). *Process Control: Designing Processes and Control System for Dynamic Performance*, 2nd. Edition. McGraw Hill, ISBN: 978-00-70393-62-2.
- Stephanopoulos, G. (1984). *Chemical Process Control. An Introduction to Theory and Practice*. Prentice Hall, ISBN: 978-01-31286-29-0