Textbook

George Stephanopoulos – Chemical Process Control: An Introduction to Theory and Practice.

Prentice Hall Int. Series in the Physical and Chemical Engineering Sciences (1984)

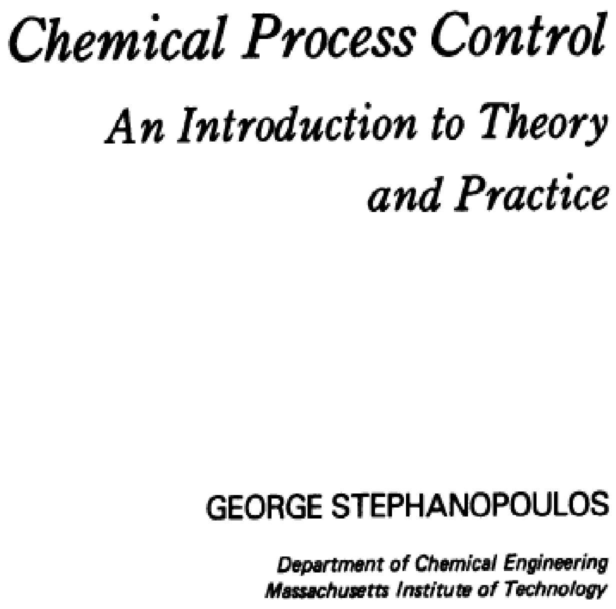
This course is an introduction to theory and practice of **chemical process control** (the control of complete plants is the subject of advanced courses

Aims: A good understanding of physical and chemical phenomena taking place in a chemical process, in particular its dynamics, which are of paramount importance for the design and application of effective control systems.

Part I concerns the development of methods for a theoretical desctiption of chemical processes and understandandig of the chief characteristics of **process dynamics** (described by linear or linearized ODEs of I, II or n-orders)

Part II is an introduction of the concepts of **process control** (identification of control objectives, selection of appropriate measurements and manipulated variables to achieve the preset objectives and to the design and application of control devices)

Contents – 1



Chemical Process Control

An Introduction to Theory and Practice

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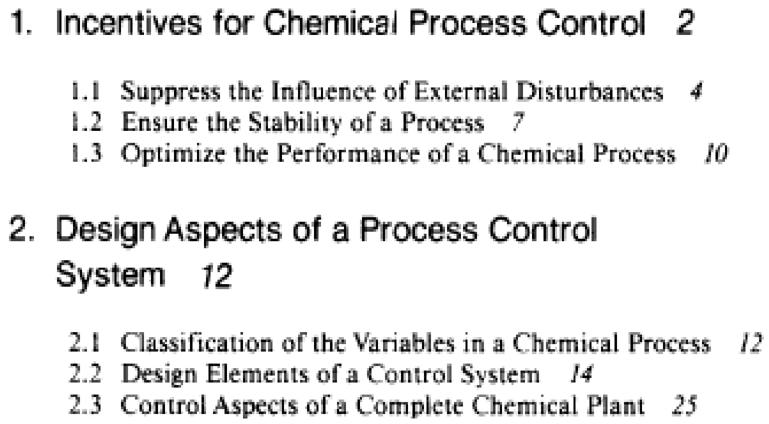

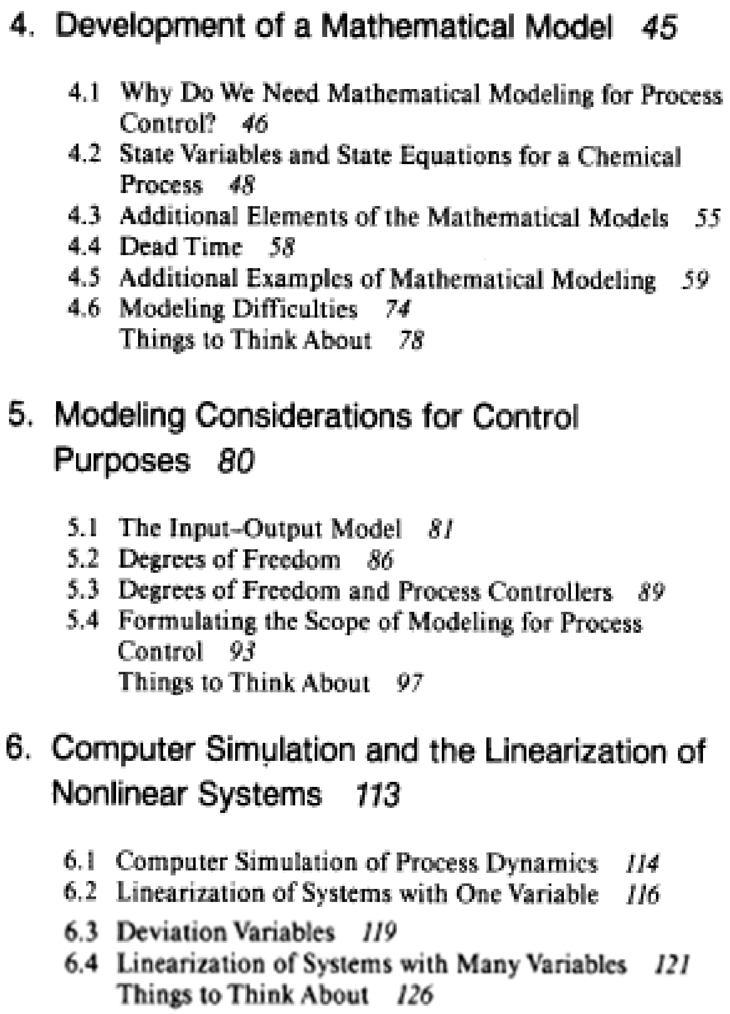

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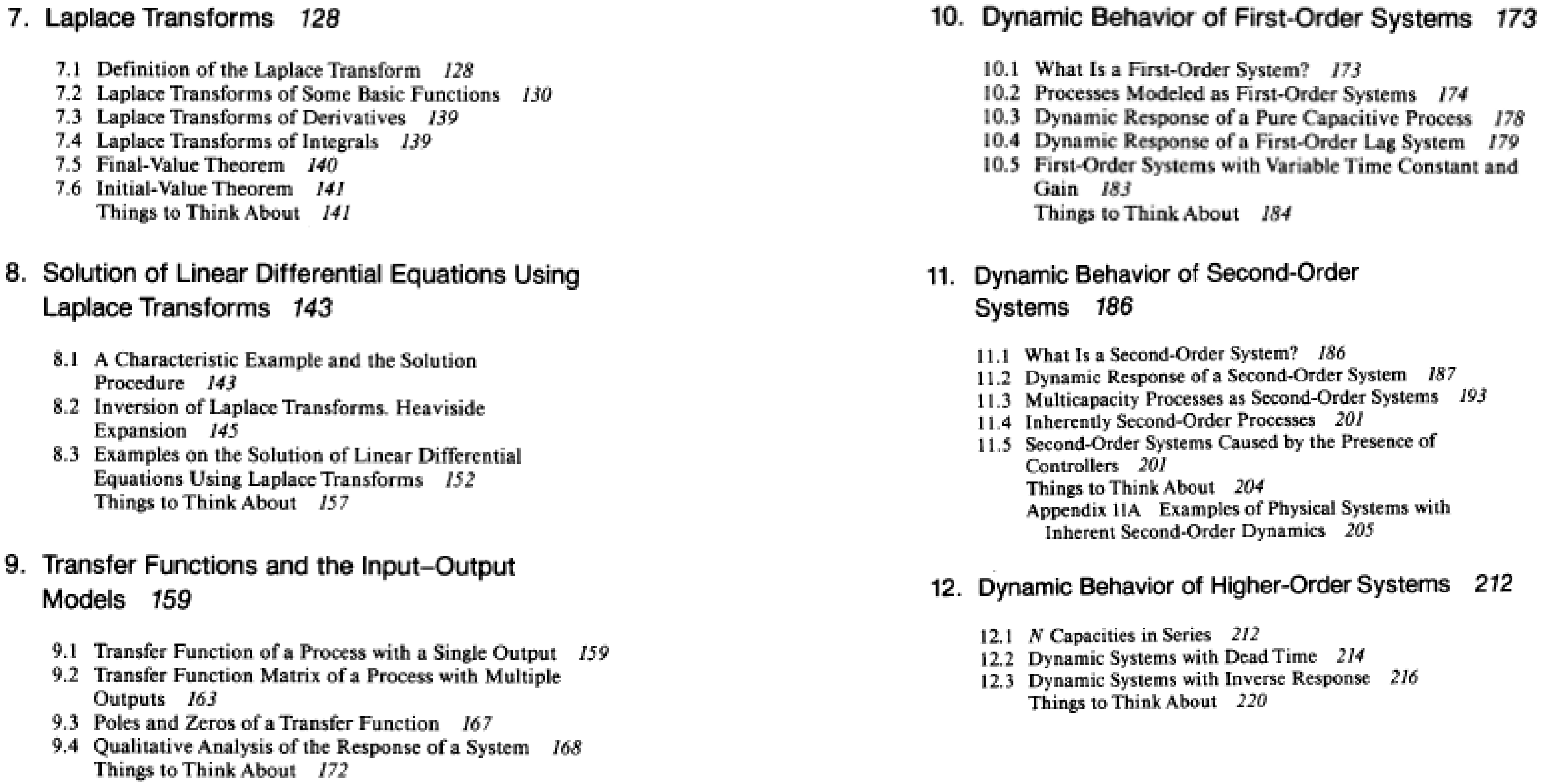

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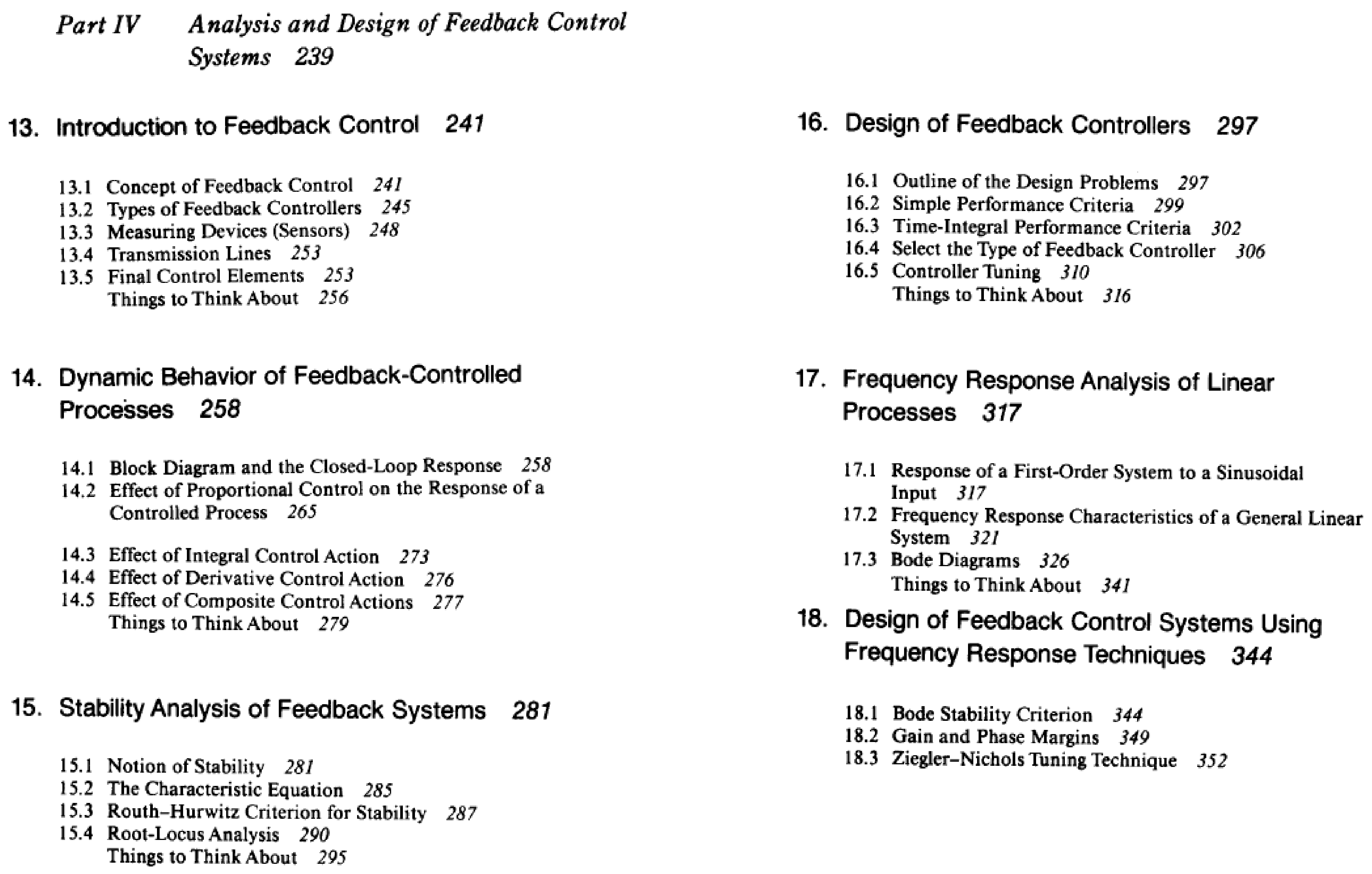

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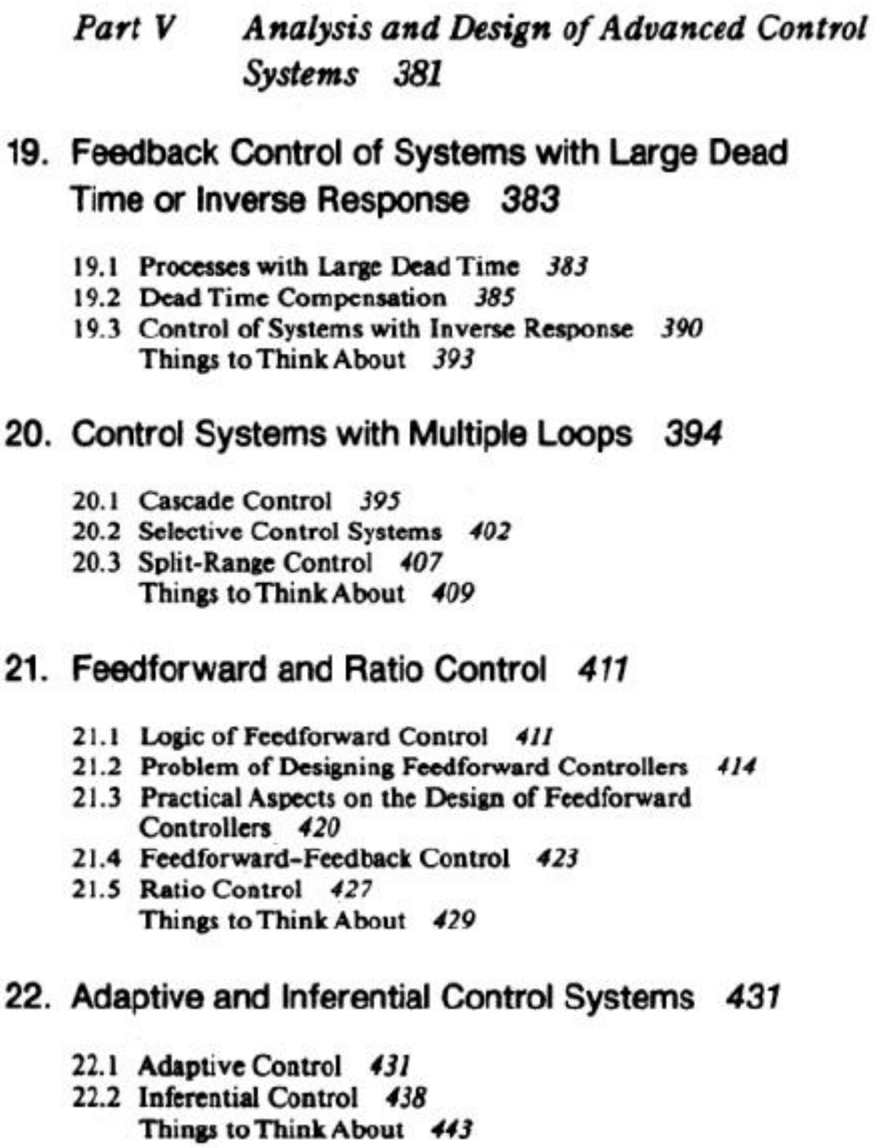


Notes_1 – OUTLINE (chapters 1-2,4-6)

- Characteristics and problems
- Mathematical modeling
- Classification of the variables in a chemical process
- Degrees of freedom
- Requirements of a control system:
    - Suppressing the influences of external disturbances
    - Ensuring the stability of chemical processes
- Input-output model
- Deviation variables
- Linearization

Characteristics and problems - 1

During the operation, a chemical plant must satisfy several requirements:

a) ***Safety*** for the people and the plant (operating variables within allowable limits): pressure, concentration, temperature, ect. should be adequately monitored and controlled, for instance, the pressure in a gas-phase reactor should be limited to the design values; the development of explosive mixtures should be avoided, etc.

b) ***Product specifications*** (production of the desired amounts and quality of final products): production of a certain amount of a product per day (e.g. acetic acid) with an assigned purity level (99%), etc.

c) ***Environmental regulations*** (specifications on the plant effluents and their conditions): regulations establish limits on the concentrations of pollutants that a plant can eject in the atmosphere and/or the quality of the water that can be returned to rivers, etc.

d) ***Operational constraints*** (limits on the elements of the plant when in operation): for instance, tanks should not overflow or go dry, the temperature in a catalytic reactor should not exceed a certain limit in order to preserve the catalyst, etc.

e) **Economics** (control of the operating conditions to maximize the profit): the operating conditions should be controlled at given optimum levels of minimum operating cost and maximum profit.

Characteristics and problems -2

The requirements a)–e) dictate the need for continuous monitoring of the operation of the chemical plant and introduction of control devices/methods to guarantee the pre-set objectives.

A control system should satisfy three general classes of needs:

- *Suppressing the influence of* ***external disturbances***
- *Ensuring the* ***stability*** *of a chemical process*
- ***Optimizing*** *the performance of a chemical process*

Before examining these needs by means of examples, let’s introduce the concept of mathematical modeling

Mathematical modeling - 1

Approaches used to investigate the behaviour of a chemical process:

- ***Experimental approach*** (generally time and effort consuming and quite costly)
- ***Theoretical approach*** (formulation of mathematical equations and subsequent solution) consisting of the conservation equations for mass, energy and momentum combined with the equations of state

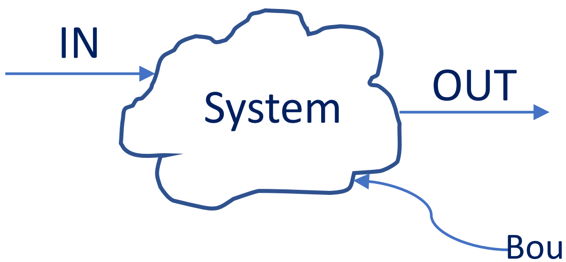
Two chief categories of mathematical models can be introduced:

I) **Concentrated parameter models**, consisting of ordinary differential equations (**ODEs**), applicable for perfectly mixed systems (no spatial gradients)

II) **Distributed parameter models**, consisting of partial differential equations (**PDEs**), applicable for systems with space and time variations

Mathematical modeling - 2

For systems of type I), the principle of conservation of a quantity S states that:



IN

System

OUT

Boudary defining the system

ACCUMULATION=IN-OUT+NET GENERATION

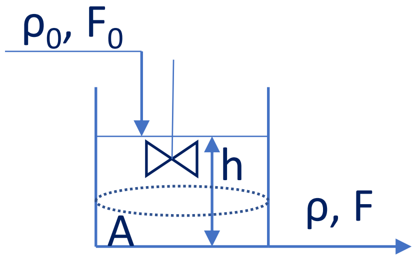
(Over a time period)

The quantity S can be any of the followings:

- Total mass
- Mass of individual components
- Total energy
- Momentum

Mathematical modeling - 3

Total mass conservation in a perfectly mixed tank (stirred tank)



$$(1)\ \underset{\left[\frac{g}{s}\right]}{\underset{\swarrow}{\frac{d}{dt}(\rho \mathrm{V})}} = \underset{\left[\frac{g_{IN}}{s}\right]}{\underset{\swarrow}{\rho_0 F_0}} - \underset{\left[\frac{g_{OUT}}{s}\right]}{\underset{\searrow}{\rho F}}$$

$$F\ (\text{Volumetric flow rate}) \rightarrow \left[\frac{cm}{s}cm^2\right]$$

$$F\rho \rightarrow \left[\frac{cm^3}{s}\frac{g}{cm^3}\right] \rightarrow \left[\frac{g}{s}\right]$$

$$\rho = \rho_0 = const.$$

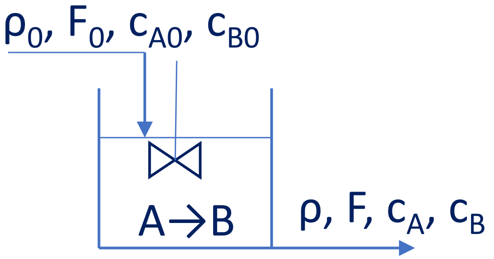
$$(2)\ \frac{d}{dt}(\mathrm{V}) = F_0 - F \qquad +V\left(t=0\right) = V_s$$

Initial condition

$$(2')\ A\frac{d}{dt}(h) = F_0 - F \qquad +h\left(t=0\right) = h_s$$

Mathematical modeling - 4

Mass conservation for components – CSTR under isothermal conditions



$$\rho = \rho_0 = const \qquad r = -kc_A$$

$$(1)\ \rho \frac{d}{dt} V = \rho\left(F_0 - F\right) \ + i.c.$$

$$(2)\ \frac{d}{dt}\left(Vc_A\right) = F_0 c_{A0} - Fc_A - Vkc_A \ + i.c.$$

$$(3)\ \frac{d}{dt}\left(Vc_B\right) = F_0 c_{B0} - Fc_B + Vkc_A + i.c.$$

$$\rho = const = M_A c_A + M_B c_B$$

For a system with *n* components it is possible to write *n* conservation equations for the components, in alternative (*n-1*) conservation equations for the components + the total mass conservation.

For a gas phase system, V is constant and ρ is variable.

Mathematical modeling - 5

Energy conservation equation for an “open” system:

[time rate of change of *internal, kinetic and potential energy* inside the system]=

=[flow of internal, kinetic and potential energy into system]+

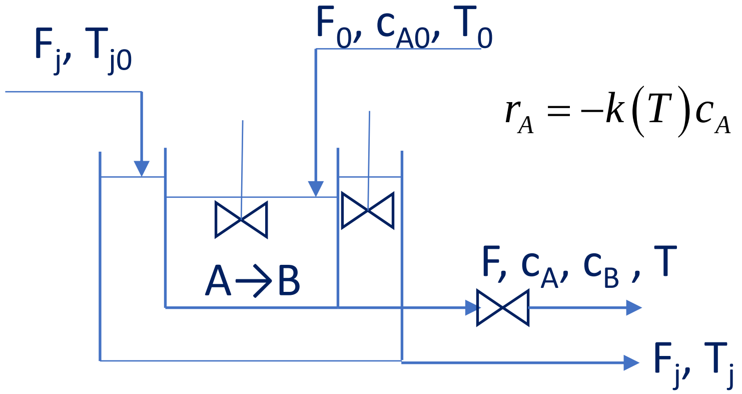
-[flow of internal, kinetic and potential energy out of system]+[heat added]+

-[work done by system on surroundings]

For negligible contributions of kinetic and potential energy and in the case of liquid-phase system, the energy conservation reduces to the **enthalpy conservation equation**

Mathematical modeling - 6

Non-isothermal CSTR (perfect mixing, negligible thermal inertia of the reactor walls, constant densities, constant volumetric flow rate and volume of the coolant)



$$r_A = -k\left(T\right)c_A$$

- Total mass conservation

$$(1)\ \rho\frac{d}{dt}V = \rho\left(F_0 - F\right) \quad +i.c.$$

- Conservation of component A

$$(2)\ \frac{d}{dt}\left(Vc_A\right) = F_0 c_{A0} - Fc_A - Vk\left(T\right)c_A \quad +i.c.$$

$$F = \alpha V$$

$$\rho = M_A c_A + M_B c_B$$

- Enthalpy conservation

$$(3)\ \rho\frac{d}{dt}\left(VH\right) = \rho\left(F_0 H_0 - FH\right) \pm \left|\Delta h\right| Vk\left(T\right)c_A + US\left(T_j - T\right) \quad +i.c. \qquad H = c_p T$$

- (coolant) Enthalpy conservation

$$(4)\ \rho_j V_j \frac{d}{dt}H_j = \rho_j F_j\left(H_{j0} - H_j\right) + US\left(T - T_j\right) \quad +i.c. \qquad H_j = c_{pj}T_j$$

Mathematical modeling- 7

Equation of motion

The basic relationship used for the equations of motion of a system (conservation of momentum) uses the Newton law:

$$\sum_i \overrightarrow{F_i} = m\vec{a} = m\frac{d^2}{dt^2}\vec{s}$$

Equations of state

Equations for the variation of physical properties (ρ, H) with temperature, pressure, composition

Liquid phase densities are usually constant whereas vapor phase densities obey to certain relationship, e. g. the perfect gas law

Classification of the variables in a chemical process

- **Input** variables, which denote the effects of the surroundings on the chemical process
- **Output** variables, which denote the effects of the process on the surroundings

The **input** variables can be further classified in the following categories:

- **manipulated (or adjustable)** variables, if their values can be adjusted freely by the human operator or a control mechanism
- **disturbances**, if their values are not the result of adjustment by an operator or a control system

The **output** variables are classified into the following categories:

- **measured** output variables, if directly measured
- **unmeasured** output variables, if not directly measurable

Degrees of freedom

The **degrees of freedom** of a problem, described by a set of equations, are the indipendent variables that must be specified to provide complete specification. For a problem described by **N** equations with a number **M** of independent variables, we ask two questions:

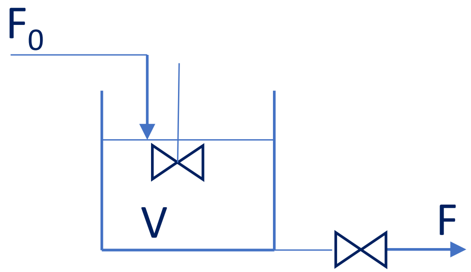
1) is solution of the equations possible?
2) If solution is possible, how many solutions exist?

f (degrees of freedom)=number of variables (**M**) – number of equations (**N**)

- M>N (f>0) → there is at least one solution, more precisely there is an infinite number of solutions because the values of f (M-N) variables can be arbitrarily specified.
- M=N (f=0) → when the number of equations is equal to the number of independent variables (the degrees of freedom are 0) the problem is completely specified and there is only one solution
- M<N (f<0) → there is no solution for the model

Degrees of freedom – Example #1

Stirred tank



Equations

$$1)\ \frac{d}{dt}V = F_0 - F \qquad + i.c.$$

$$2)\ F = \alpha V$$

(linear system)

Indipendent variables

$$\left.\begin{matrix} V \\ F \end{matrix}\right\}\ \textit{Outputs}\ \text{(measurable)}$$

$$F_0 \}\ \textit{Input}\ \text{(disturbance or adjustable variable)}$$

f=M-N=3-2=1. To specify the system another equation is needed: a relation providing how F_0 varies [$F_0(t)$]

Given that F is a function of

the volume (or the liquid level)

$$1^*)\ \frac{d}{dt}V = F_0 - \alpha V \qquad + i.c.$$

Indipendent variables

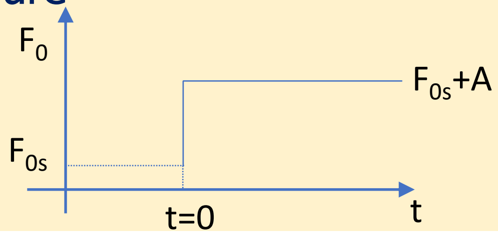
$$V \}\ \textit{Output}$$

$$F_0 \}\ \textit{Input}$$

$$(\alpha \text{ is a parameter})$$

Let's suppose that F_0 is a disturbance that we can measure

$$3)\ F_0 = F_{0s} + A$$

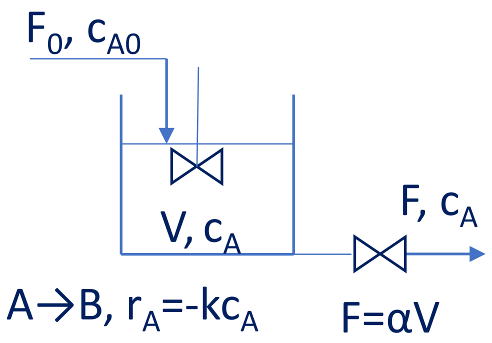


f=M-N=2 (V, F_0) - 2 (eqs. 1* and 3)=0

The system can be defined as a single-input single-output (**SISO**) system

Degrees of freedom – Example #2

Isothermal CSTR



Equations

$$1)\ \frac{d}{dt}V = F_0 - \alpha V \quad + i.c.$$

$$2)\ \frac{d}{dt}(Vc_A) = F_0 c_{A0} - \alpha V c_A - kVc_A \quad + i.c.$$

non linear system (Vc_A, F_0c_{A0})

α and k are parameters

Indipendent variables

$$\left.\begin{matrix} V \\ c_A \end{matrix}\right\} Outputs$$

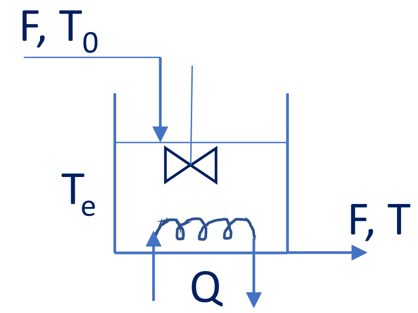
$$\left.\begin{matrix} F_0 \\ c_{A0} \end{matrix}\right\} Inputs$$

f=M-N=4-2=2. To specify the system, two equations are needed: 3) $F_0=f_1(t)$; 4) $c_{A0}=f_2(t)$

The system can be defined as a multiple-input multiple-output (**MIMO**)

Degrees of freedom – Example #3

Stirred tank heater



(F and V const; $H=c_pT$, c_p const)

Equations

$$1)\ V\rho c_p \frac{d}{dt}T = F\rho c_p T_0 - F\rho c_p T + Q + US\left(T_e - T\right)$$

$+i.\mathrm{c}.$

C_p, ρ, U, S, V and F are parameters

Indipendent variables

$$T\Big\}\ Output$$

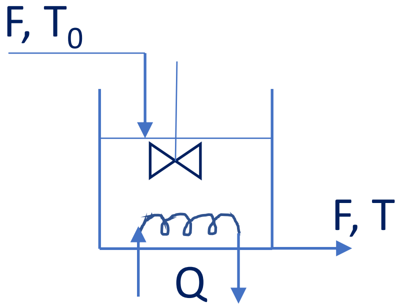
$$\left.\begin{matrix}T_0\\ T_e\\ Q\end{matrix}\right\}\ Inputs$$

f=M-N=4-1=3. To specify the system, three equations are needed: 2) $T_0=f_1(t)$; 3) $T_e=f_2(t)$ and 4) $Q=f_3(t)$

The system can be defined as a multiple-input single-output (**MISO**)

Suppressing the influences of external disturbances – 1

Stirred tank heater



(F, V and other properties at constant values)

It is desired to keep the temperature T at the desired value T_s when the heater is disturbed by a change in the feed temperature T_0

Mathematical model

$$V\rho c_p \frac{d}{dt}T = F\rho c_p T_0 - F\rho c_p T + Q \qquad +i.c.$$

Indipendent variables

$$T\}\ Output$$

$$\left.\begin{matrix} T_0\ (disturbance) \\ Q\ (manipulated\ variable) \end{matrix}\right\}\ Inputs$$

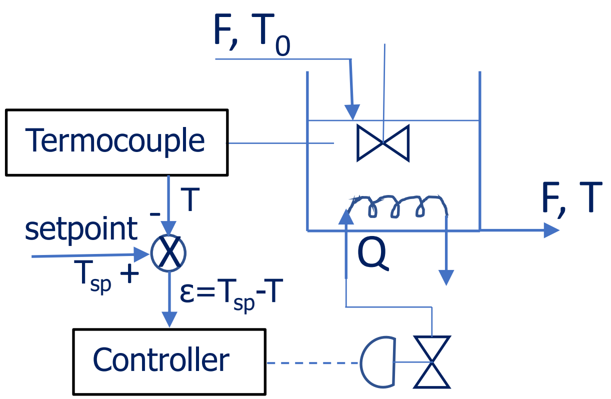
To accomplish the required control, we need at least one manipulated variable (Q), otherwise control cannot be accomplished.

The use of the manipulated variable (Q), in order to eliminate the effects of the disturbance, also introduces another equation and thus the degrees of freedom are reduced by 1

Also the time dpendence of the disturbance is known (T_0(t)) and so, when control is accomplished, f=0.

Suppressing the influences of external disturbances – 2

Feedback temperature control



T_{sp} setpoint, supplied by the operator   ε=T_{sp} –T, deviation

$Q = Q_s + k_c\varepsilon$ When ε=0, the controller does nothing. For ε>0, T<T_{sp}, more heat is supplied, the contrary for ε<0.

This control system, which measures the variable to be controlled (T) after a disturbance has its effect on it, is called **feedback control system**.

The feedback control system consists of:

a) process;
b) measuring instruments or sensors;
c) transducers;
d) transmission lines;
e) controller;
f) the final control element;
g) recording elements.

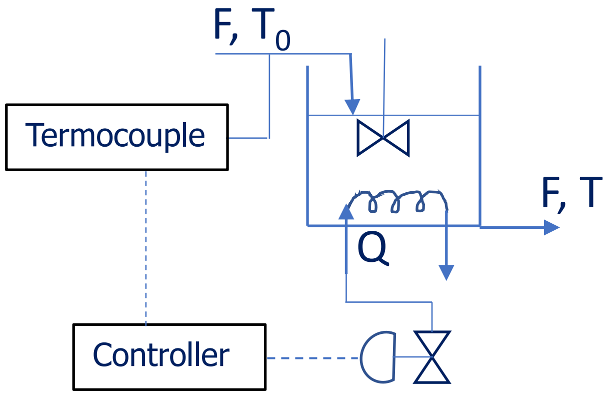
In a feedback control, the control action takes place only after a disturbance has caused a variation on the variable to be controlled.

Suppressing the influences of external disturbances – 3

Feedforward control

Again with reference to the stirred tank heater, a different arrangement can be implemented to keep $T=T_{sp}$ when T_0 (disturbance) changes, by means of adequate change on the manipulated variable Q

Feedforward temperature control



In principle the feedforward control does not wait until the effect of the disturbances has been felt by the system, but acts well before

For steady conditions, the model

$$V\rho c_p \frac{d}{dt}T = F\rho c_p T_0 - F\rho c_p T + Q \quad + i.c.$$

reduces to

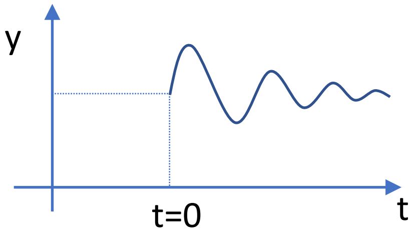
$$Q_s = F\rho c_p \left(T_s - T_{0s}\right)$$

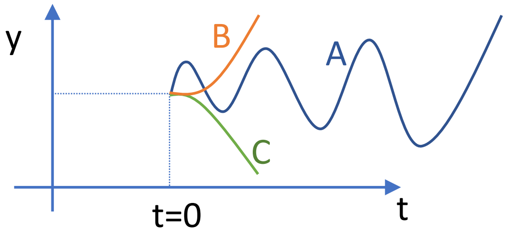
For the requirement $T_s=T_{sp}$

$$Q_s = F\rho c_p \left(T_{sp} - T_{0s}\right)$$

Ensuring the stability of a chemical process – 1

Temporal profile of a variable y (T, c,…) after the action of an external disturbance

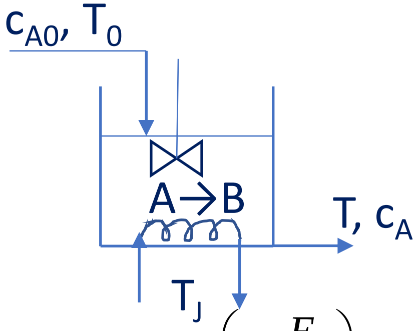




After some time the variable y returns to its initial value. The process is **stable** or **self-regulating** and does not need external intervention for its stabilization.

The variable y, after it is disturbed, does not return to the initial value. Curves A, B and C are representative of an **unstable** behaviour. A control mechanism is needed to force y to return to its initial value

Example: controlling the operation of an unstable CSTR where an irreversible exothermic reaction takes place



$$r_A = -A\exp\left(-\frac{E}{RT}\right)c_A$$

Assumptions of V and F at constant values, T_0 and T_J as input variables, constant properties. The mathematical model, which requires initial conditions, is:

$$\begin{cases} V\dfrac{d}{dt}c_A = F\left(c_{A0}-c_A\right)-kVc_A \\ V\rho cp\dfrac{d}{dt}T = F\rho cp\left(T_0-T\right)+\left|\Delta h\right|kc_AV+US\left(T_J-T\right) \end{cases}$$

Ensuring the stability of a chemical process – 2

For steady conditions

$$\begin{cases} \text{(a)} \quad F\left(c_{A0}-c_A\right)-kVc_A=0 \\ \text{(b)} \quad F\rho cp\left(T_0-T\right)+\left|\Delta h\right|kc_AV+US\left(T_J-T\right)=0 \end{cases}$$

From eqn. (a)

$$c_A=\frac{Fc_{A0}}{F+Vk\left(T\right)} \qquad \begin{cases} c_A \simeq c_{A0} \ low\,T \\ c_A \rightarrow 0 \ \ high\,T \end{cases}$$

From eqn. (b)

$$-US\left(T-T_J\right)-F\rho c_p\left(T-T_0\right)+\left|\Delta h\right|kc_AV=0$$

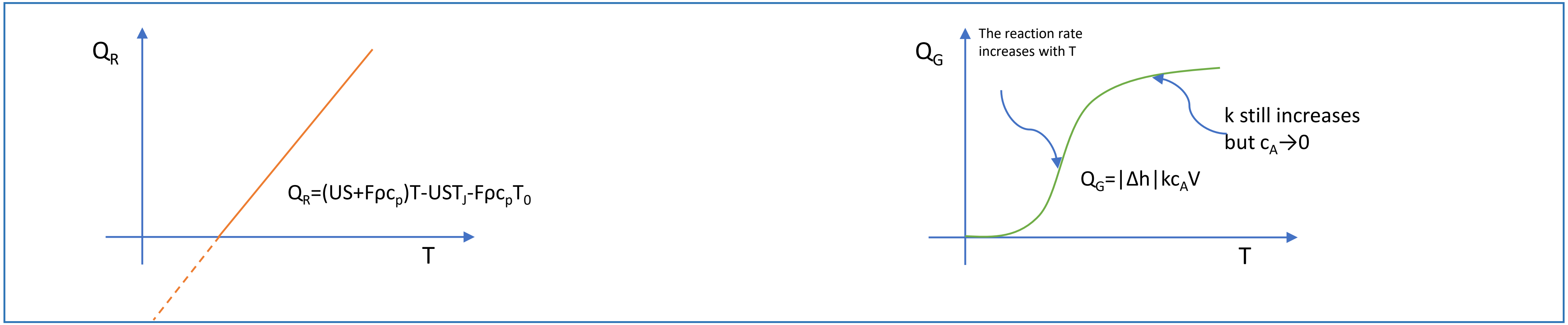
$Q_G=\left|\Delta h\right|kc_AV$ reaction heat

$$Q_R=US\left(T-T_J\right)+F\rho c_p\left(T-T_0\right)$$

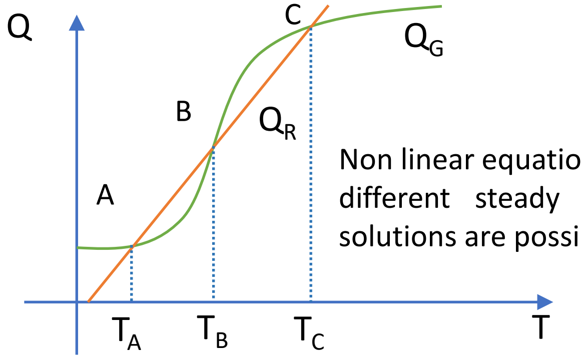
Heat exchanged with the coolant

Heat needed to heat the feed from T_0 to T

For steady conditions the heat generated equals the heat exchanged: $Q_G=Q_R$



Ensuring the stability of a chemical process – 3



Non linear equations → different steady state solutions are possible

There are three steady states A, B, C corresponding to low, medium and high conversions, respectively.

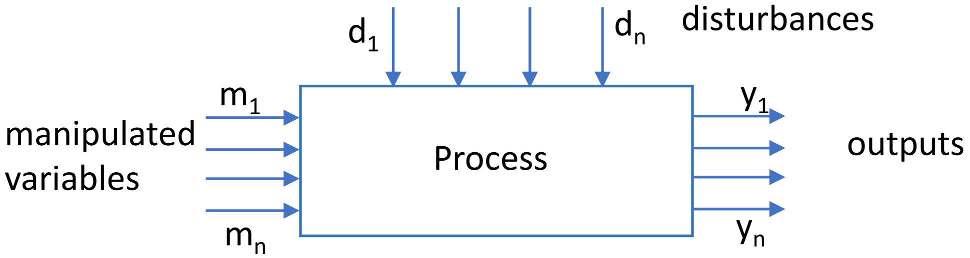
Conditions corresponding to A and C represent equilibrium.

Let’s consider the condition C: when, for an external disturbance, T increases (T_C+ε) Q_R>Q_G and the system goes back to the condition C. For a diminution in the temperature (T_C-ε), Q_G>Q_R and the system again goes back to C. The same considerations apply to condition A.

Instead, for the solution B, given T_B+ε, Q_G>Q_R and the system goes to condition C. For T_B-ε, Q_R>Q_G and the system moves to condition (solution) A. If we plan to work with medium conversions (T_B), we could modify the curve of Q_R by modifications in F, U, etc. or introduce a control.

Input-output model

Every process and related variables can be schematically represented as:



A mathematical model that is convenient and useful to a control system designer should have the following general form: output=f(input variables).

$y_i=f(m_1, m_2,\ldots,m_n,d_1,d_2,\ldots,d_n)$ with reference to the above schematic

This is an **input-output model** and represents directly the cause-and-effect relationship in processing systems. The mathematical models of interest here are not of the direct input-output type, but anyway they are basis for such development. This is straightforward when the variables characterizing the state of the system coincide with the output variables and the equations can be integrated.

In reality analytical solutions can be obtained only for linear odes (ordinary differential equations). In other cases numerical solutions can be computed (not easy for an engineering “practical” approach) or the variables can be transformed so as to obtain linear equations (only in a very few cases).

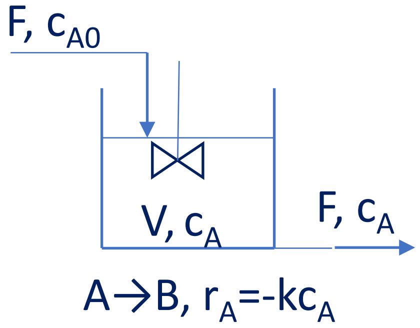
The most applied method consists of the **development of linear models** approximating the dynamic behavior of a non linear system in the neighborhood of specified operating conditions.

Deviation variables – 1

Before discussing the linearization of odes, let’s introduce the deviation variables for a linear system

Deviation variables for a linear system (SISO)

Isothermal CSTR (constant volume V and volumetric flow rate F)



$c_{A0}\}$ *Input*

$c_A\}$ *Output*

$$(1)\ V\frac{d}{dt}c_A = Fc_{A0} - Fc_A - kVc_A \qquad +c_A(t=0)=c_{As}$$

For steady state (1) becomes

$$(2)\ 0 = Fc_{A0s} - Fc_{As} - kVc_{As}$$

Let’s consider (1) - (2)

$$(3)\ V\frac{d}{dt}c_A = V\frac{d}{dt}\left(c_A - c_{As}\right) = F\left(c_{A0} - c_{A0s}\right) - F\left(c_A - c_{As}\right) - kV\left(c_A - c_{As}\right)$$

The deviation variables can be introduced

$$c_A' = c_A - c_{As}$$

$$c_{A0}' = c_{A0} - c_{A0s}$$

$$(3')\ V\frac{d}{dt}c_A' = Fc_{A0}' - Fc_A' - kVc_A'$$

The initial conditions should also be expressed in terms of deviation variables

$$\begin{array}{rl} (*) & c_A(t=0) = c_{As} \\ & \quad\; c_{As} = c_{As} \quad \textcircled{-} \\ \hline (**) & c_A'(t=0) = 0 \end{array}$$

The model in deviation variables consists of (3’)+ (**)

Deviation variables – 2

To specify the problem, $c_{A0}(t)$ should also be assigned and expressed in terms of deviation variables.

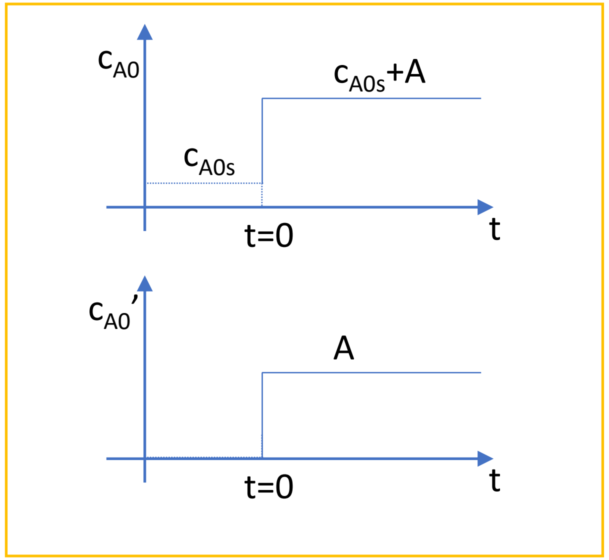
For instance

$$(4)\ c_{A0}(t) = c_{A0s} + A$$

-

$$(4')\ c_{A0s} = c_{A0s}$$

$$c'_{A0}(t) = A$$



A linear ode, expressed in term of deviation variables, preserves the same functional form as the original equation but the initial condition becomes 0.

For the example above F, V, k are parameters (assigned) as well as A (and c_{A0s}).

The steady value of the output c_{As} can be computed from eqn (2)

$$(2)\ 0 = Fc_{A0s} - Fc_{As} - kVc_{As} \Rightarrow c_{As} = \frac{Fc_{A0s}}{F+kV}$$

Linearization of a non-linear equation with one variable – 1

$$(1)\ \frac{d}{dt}x = f(x) \quad with \quad x(0) = x_s; \quad \mathrm{f(x)} \simeq \mathrm{f(x_s)} + \left(\frac{df}{dx}\right)_{x_s}(x - x_s)$$

Linearized equation

$$(2)\ \frac{d}{dt}x = \mathrm{f(x_s)} + \left(\frac{df}{dx}\right)_{x_s}(x - x_s)$$

The steady equation (1) becomes

$$(3)\ 0 = \mathrm{f(x_s)}$$

Let's consider (2)-(3) in order to get the formulation in terms of deviation variables

$$\frac{d}{dt}x = \mathrm{f(x_s)} + \left(\frac{df}{dx}\right)_{x_s}(x - x_s)$$

$$\ominus$$

$$0 = \mathrm{f(x_s)}$$

$$x' = x - x_s$$

$$\frac{d}{dt}(x - x_s) = \left(\frac{df}{dx}\right)_{x_s}(x - x_s) \longrightarrow \boxed{\frac{d}{dt}x' = \left(\frac{df}{dx}\right)_{x_s} x'}$$

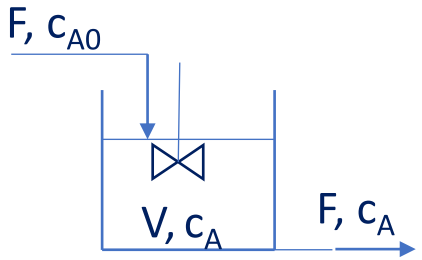
Initial condition

$$\begin{array}{c} x(0) = x_s \\ \ominus \\ x_s = x_s \end{array} \longrightarrow \boxed{x'(0) = 0}$$

Linearized equation expressed in terms of deviation variables

Linearization of a non-linear equation with one variable – 2

Isothermal CSTR (constant V and F)



2A→B, $r_A=-2kc_A^2$

$$(1)\; V\frac{d}{dt}c_A = Fc_{A0} - Fc_A - 2kVc_A^2 \qquad +c_A(t=0)=c_{As}$$

$$c_A^2 = c_{As}^2 + \frac{d}{dc_A}\left(c_A^2\right)\Big|_{c_{As}}\left(c_A - c_{As}\right) = c_{As}^2 + 2c_{As}\left(c_A - c_{As}\right)$$

$$c_A' = c_A - c_{As} \qquad c_{A0}' = c_{A0} - c_{A0s}$$

$$(2)\; V\frac{d}{dt}c_A = Fc_{A0} - Fc_A - 2kV\left(c_{As}^2 + 2c_{As}c_A'\right)$$ Linearized equation

$$\ominus$$

$$0 = Fc_{A0s} - Fc_{As} - 2kVc_{As}^2$$ Steady equation (1)

$$(3)\; V\frac{d}{dt}c_A' = Fc_{A0}' - Fc_A' - 2kV\left(2c_{As}\right)c_A'$$

$$c_A'(0) = 0$$ Initial condition

For a linearized system, the functional form of the equation expressed in terms of deviation variables is different from the original one. The initial condition is again zero.

Linearization of systems with many variables – 1

Dynamic system

$$(a)\ \frac{d}{dt}x_1 = f_1(x_1,x_2) \quad with \quad x_1(t=0)=x_{1s}$$

$$(b)\ \frac{d}{dt}x_2 = f_2(x_1,x_2) \quad with \quad x_2(t=0)=x_{2s}$$

Linearization, neglecting terms of second or superior order

$$f_1(x_1,x_2) \simeq f_1(x_{1s},x_{2s}) + \left.\frac{\partial f_1}{\partial x_1}\right|_{x_{1s},x_{2s}}(x_1-x_{1s}) + \left.\frac{\partial f_1}{\partial x_2}\right|_{x_{1s},x_{2s}}(x_2-x_{2s})$$

$$f_2(x_1,x_2) \simeq f_2(x_{1s},x_{2s}) + \left.\frac{\partial f_2}{\partial x_1}\right|_{x_{1s},x_{2s}}(x_1-x_{1s}) + \left.\frac{\partial f_2}{\partial x_2}\right|_{x_{1s},x_{2s}}(x_2-x_{2s})$$

Linearized system

$$\frac{d}{dt}x_1 = f_1(x_{1s},x_{2s}) + \left.\frac{\partial f_1}{\partial x_1}\right|_{x_{1s},x_{2s}}(x_1-x_{1s}) + \left.\frac{\partial f_1}{\partial x_2}\right|_{x_{1s},x_{2s}}(x_2-x_{2s})$$

$$\frac{d}{dt}x_2 = f_2(x_{1s},x_{2s}) + \left.\frac{\partial f_2}{\partial x_1}\right|_{x_{1s},x_{2s}}(x_1-x_{1s}) + \left.\frac{\partial f_2}{\partial x_2}\right|_{x_{1s},x_{2s}}(x_2-x_{2s})$$

Steady state (a) and (b)

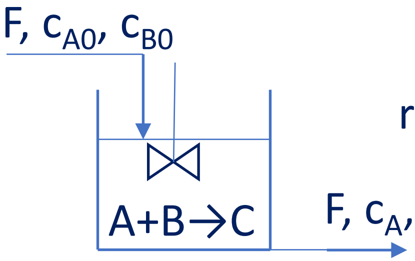
$$0 = f_1(x_{1s},x_{2s}); \quad 0 = f_2(x_{1s},x_{2s})$$

Systems in terms of deviation variables

$$\boxed{\begin{aligned}\frac{d}{dt}x_1' &= \left.\frac{\partial f_1}{\partial x_1}\right|_{x_{1s},x_{2s}}x_1' + \left.\frac{\partial f_1}{\partial x_2}\right|_{x_{1s},x_{2s}}x_2' \\ \frac{d}{dt}x_2' &= \left.\frac{\partial f_2}{\partial x_1}\right|_{x_{1s},x_{2s}}x_1' + \left.\frac{\partial f_2}{\partial x_2}\right|_{x_{1s},x_{2s}}x_2'\end{aligned}} \quad \begin{aligned} x_1'(0)&=0 \\ x_2'(0)&=0\end{aligned}$$

Linearization of systems with many variables – 2

Isothermal CSTR (constant V and F)



$r_A=-kc_Ac_B$

$$\text{(a)}\; V\frac{d}{dt}c_A = Fc_{A0} - Fc_A - \boxed{kVc_Ac_B} \qquad c_A(0)=c_{As}$$

$$\text{(b)}\; V\frac{d}{dt}c_B = Fc_{B0} - Fc_B - \boxed{kVc_Ac_B} \qquad c_B(0)=c_{Bs}$$

Linearization

$$c_Ac_B \simeq c_{As}c_{Bs} + \frac{\partial}{\partial c_A}\left(c_Ac_B\right)\bigg|_s \left(c_A - c_{As}\right) + \frac{\partial}{\partial c_B}\left(c_Ac_B\right)\bigg|_s \left(c_B - c_{Bs}\right) =$$

$$= c_{As}c_{Bs} + c_{Bs}\left(c_A - c_{As}\right) + c_{As}\left(c_B - c_{Bs}\right)$$

$$\begin{cases} c_A' = c_A - c_{AS} \\ c_B' = c_B - c_{BS} \end{cases}$$

Linearized equation in deviation variables

$$V\frac{d}{dt}c_A = Fc_{A0} - Fc_A - kV\left(c_{As}c_{Bs} + c_{Bs}c_A' + c_{As}c_B'\right)$$

$$\boxed{-}$$

$$0 = Fc_{A0s} - Fc_{As} - kVc_{As}c_{Bs}$$

$$(a*)V\frac{d}{dt}c_A' = Fc_{A0}' - Fc_A' - kV\left(c_{Bs}c_A' + c_{As}c_B'\right) \qquad c_A'(0)=0$$

And so on…