



# **Plantwide process control**

**Davide Manca** 

Lecture 8 of "Dynamics and Control of Chemical Processes" – Master Degree in Chemical Engineering



# Introduction

Plant-wide process control includes systems and methodologies necessary to control a whole chemical plant comprising several interconnected unit operations.

The main problem to solve is: how to design the control loops and the systems needed to operate the plant?

Given a complex and integrated process, involving several interacting units, we have to identify and design the control logics, the instrumentation, the control loops, and the operative strategies to operate the plant safely while satisfying some targets (i.e. process constraints, operative limits, law specifications).

First, it is worth identifying the key variables that influence the process.

It is also needed to investigate and determine the dynamic behavior of the plant as a function of the interconnected units.

The process control problem must consider the complexity of the plant equipment. The design of the control system based on the single units is necessary but neither satisfactory nor enough.



# Introduction

It is possible to identify **nine** points for the design of a plant-wide control system:

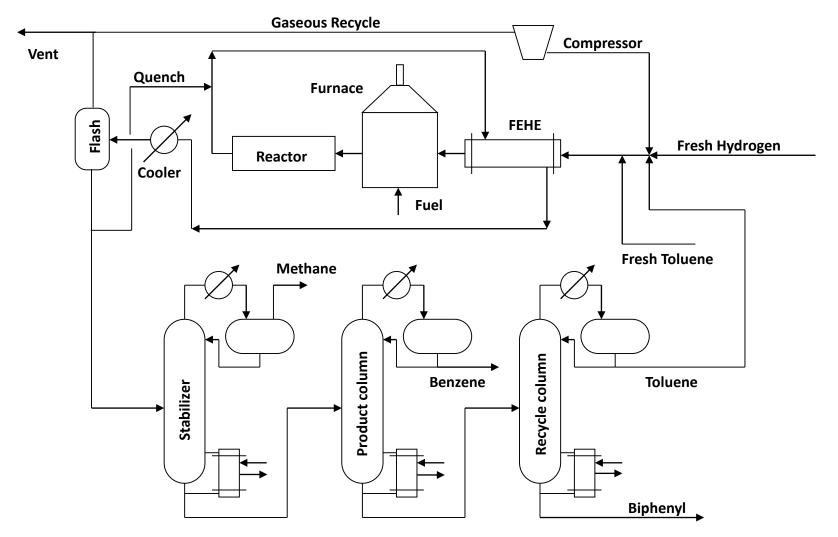
- 1. Energy management
- 2. Product quantity
- 3. Product quality
- 4. Operational, environmental, safety constraints
- 5. Liquids levels and process pressures (inventories)
- 6. Fresh feeds of the reactants (make-up)
- 7. Material balances on the various components
- 8. Economic optimization
- 9. Process optimization



### **Example: HDA process**

Toluene + Hydrogen → Benzene + Methane

#### 2 Benzene → Biphenyl + Hydrogen





© Davide Manca – Dynamics and Control of Chemical Processes – Master Degree in ChemEng – Politecnico di Milano

# **Example: HDA process**

Some questions:

- How to control the reactor temperature in order to prevent *runaway* reactions?
- How to increase/decrease the benzene production according to the market demand?
- How to keep the product (benzene) purity high enough to sell it?
- How to determine the optimal purge flow-rate?
- How to improve the process selectivity in order to minimize the biphenyl production?
- How to avoid the tanks overfilling or the gas pressure going beyond the safety threshold?
- How to manage the interconnected units from the energetic viewpoint?
- How to test a control strategy within the design stage?



## **Further considerations**

As a first step, the number of possible control solutions is extremely high and it grows in a combinatorial way with the number of available plant degrees of freedom.

Following a hierarchical procedure to approach the problem, it is possible to restrict considerably the number of alternatives to be evaluated. At the same time, it does **NOT** exist only one solution, only one optimal point.



# **Historical evolution**

#### Causes

- Significant changes of mentality in the 70s of last century (energetic crisis, austerity)
- Higher energetic integration
- Gradual removal of intermediate tanks capable of absorbing the flow disturbances and decouple both massively and energetically the process units
- Increase of the recycle streams
- Increase of the product purity specifications and yields/selectivities
- Processes optimized only in steady-state conditions

#### Consequences

More "stiff" and "nervous" processes  $\rightarrow$  processes more difficult to be controlled dynamically.



### **Historical evolution**

We believe that chemical process control must move beyond the sphere of unit operations into the realm of <u>viewing the plant as a whole system</u>. The time is ripe in the chemical and petroleum industry for the <u>development of a plantwide control design procedure</u>.

...we strongly believe that the final evaluation of any plantwide control structure requires <u>rigorous nonlinear dynamic simulations, not linear transfer function analysis</u>.

Luyben, Tyréus & Luyben, 1998



#### **Process design**

Respect to the classical hierarchical approach to process design, introduced by Douglas in the book "Conceptual Design" (1988), it is worth coupling, from the very beginning, the basic system approach to "Dynamic controllability".

It is wrong referring to the control system as something that comes after the process design stage. It is wrong introducing control remedies to the crystallized structure of the process layout. The process and control engineers should interact when the plant structure is still fluid. Design compromises should be reached by mediating the assigned specifications in steady state with the control ones, which are obviously dynamic.

According to Luyben, Tyréus & Luyben (1998), process design has an impact on controllability which is considerably higher than the impact of any control algorithm (see classical or advanced control).



#### **Integrated processes**

Three fundamental aspects, related to the chemical processes integration, induce the call for a plantwide approach to control systems.

The call for a plant-wide control system derives from three key issues of chemical processes integration:

- Effects produced by material recycles
- Effects produced by energy integration
- The need to take in account the **accumulation** of chemical compounds



# **Material recycles**

Material recycle is adopted mainly for **six** different reasons:

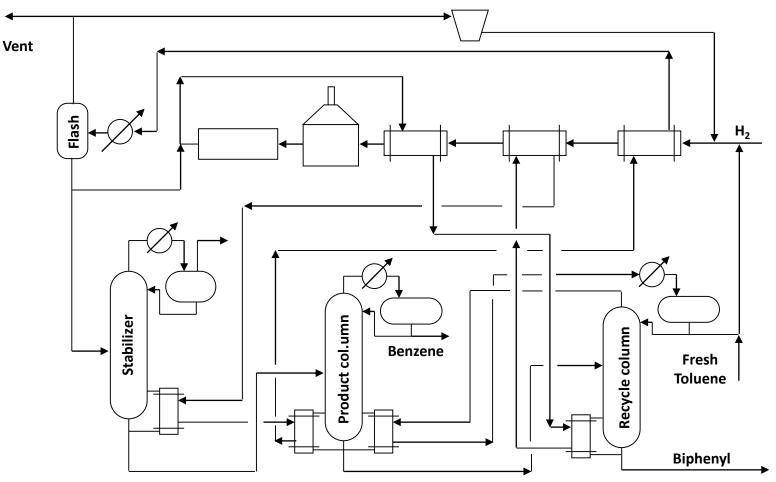
- 1. Increase the conversion: mainly when there are reversible reactions in the process
- 2. Improve the economic return: the introduction of a recycle allows reducing the reactor size or the number of reactors in series. A reactor with a stripping column is cheaper than a big reactor (with complete conversion) or than three reactors in series.
- 3. Improve the yield: in case of series reactions  $A \rightarrow B \rightarrow C$  with the intermediate B being the main product, it is necessary to limit the production of C. Low conversion of B and a high recycle of A should be carried out.
- 4. Provide thermal inertia: for strongly exothermic reactions usually a big excess of a reactant is used in order to limit the  $\Delta T$ .
- 5. Avoid secondary reactions: often a big excess of a reactant is used in order to avoid the limiting reactant to give by-products.
- 6. Control the product properties: the conversion is limited in order to obtain certain properties (*e.g.*, polymerization processes). Consequently, a high recycle of the reactants (monomers) is necessary.



# **Energy integration**

The energetic integration among the units is adopted to improve the thermodynamic efficiency of the process. The introduction of P/P heat exchangers (*e.g.*, FEHE), makes the process much more interconnected and sensitive to instabilities, due to the interaction and feedback among the units.

A typical example is represented by the HDA process (alternative 6, Douglas, 1988)





#### **Components accumulation**

The compounds present in the process can be: reactants, products or inert substances.

It is necessary to solve a material balance for each compound. The accumulation problem should not be underestimated.

It is necessary to solve the following problems:

- Quantification of the vents
- Quantification of the fresh feed
- Separation of the product streams



#### **Series units**

In the uncommon processes where the units are simply connected in series, without any material and/or thermal recycles, the plant-wide control can be split into a single control problem for each unit of the process.

In facts there is lack of: recycles, coupling, and feedback effects connecting the downstream with the upstream units. The disturbances propagate linearly along the process.



#### **Consequences of the recycle**

The presence of recycle streams deeply modifies the plant behavior either in steady state or in dynamics.

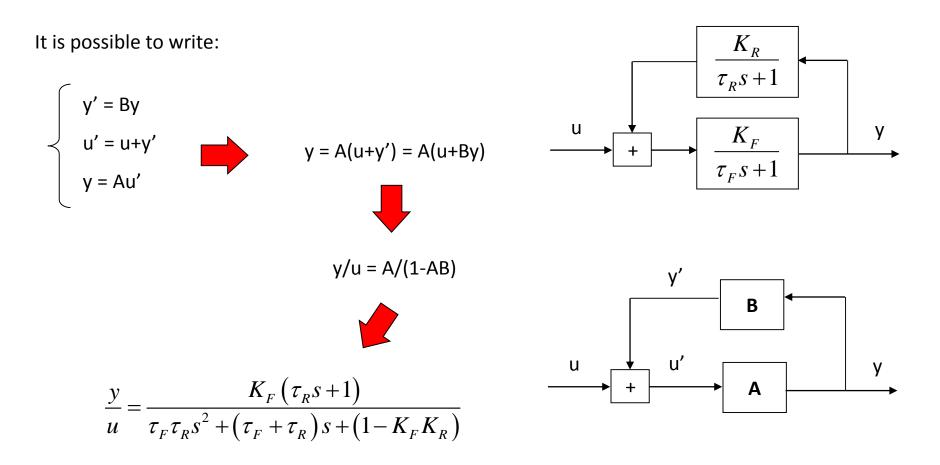
The presence of a recycle leads to two fundamental effects:

- 1. Impact on the process dynamics. The **overall time constant** can be quite different from the sum of the time constants of the single units.
- 2. The recycle causes the so-called *snowball* effect. This is observed in both the steady state and dynamic responses of the system.



### Time constants in systems with recycle

Let us consider the simple representation of a system with a recycle by means of two <u>first-order</u> transfer functions:





#### Time constants in systems with recycle

Starting from two <u>first-order systems</u>, a global <u>second order</u> transfer function is obtained. The characteristic equation of the system is:

$$\frac{\tau_F \tau_R}{(1 - K_F K_R)} s^2 + \frac{\tau_F + \tau_R}{(1 - K_F K_R)} s + 1 = 0$$

The time constants of the whole system is:

$$\tau_{S} = \sqrt{\frac{\tau_{F}\tau_{R}}{1 - K_{F}K_{R}}}$$

If:  $K_F K_R \rightarrow 1 \implies \tau_S \rightarrow \infty$ 

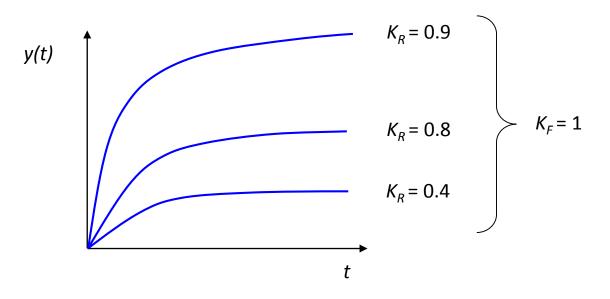
This suggests that the time constant of a process with a material recycle can be much higher than the single time constants of the units belonging to that recycle.



#### Time constants in systems with recycle

The gain of the global system may vary considerably depending on the the gain of the recycle. The steady state gain of the system is:  $K_E$ 

$$K_{S} = \frac{K_{F}}{1 - K_{F}K_{R}}$$



This means that any change within the recycle takes to a quite long response of the system and a slower return to the steady state.

The control loop, due to the intrinsically slow system response, could need some time before exerting an effective action. The actuation time could be extremely long.



Systems with recycle(s) are prone to exhibit large variations in the flow-rates amplitude of the recycle streams. Such systems are extremely sensitive to small disturbances regarding the recycle flow-rates. This is called *snowball* effect.

- The snowball effect is NOT a dynamic feature but it is intrinsically stationary.
- Nevertheless this produces consequences on the system dynamics.
- It has nothing to do with the stability of the system at the closed loop.
- It is <u>influenced</u> instead by the control system structure.
- The <u>amplitude</u> of the snowball effect is highly influenced by the <u>adopted control system</u>.

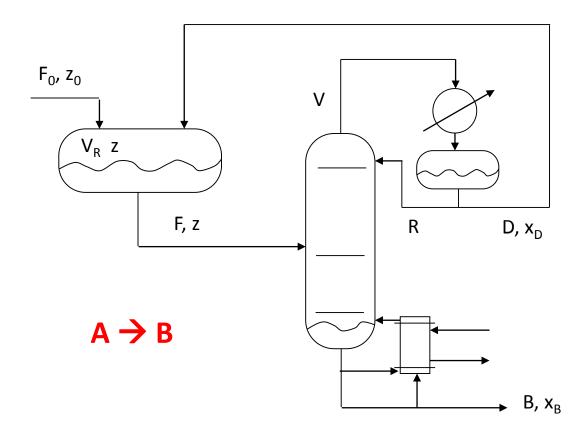
The wide oscillations of the recycle streams, introduced by the snowball effect, produce a negative influence on the separation section that can be even not able to manage so wide operative intervals (*e.g.*, flooding, weeping).



A rule of thumb is:

At least one stream belonging to the recycle structure should be controlled in terms of flowrate: FC.

Let us now consider a simple process (reactor + column) with recycle:

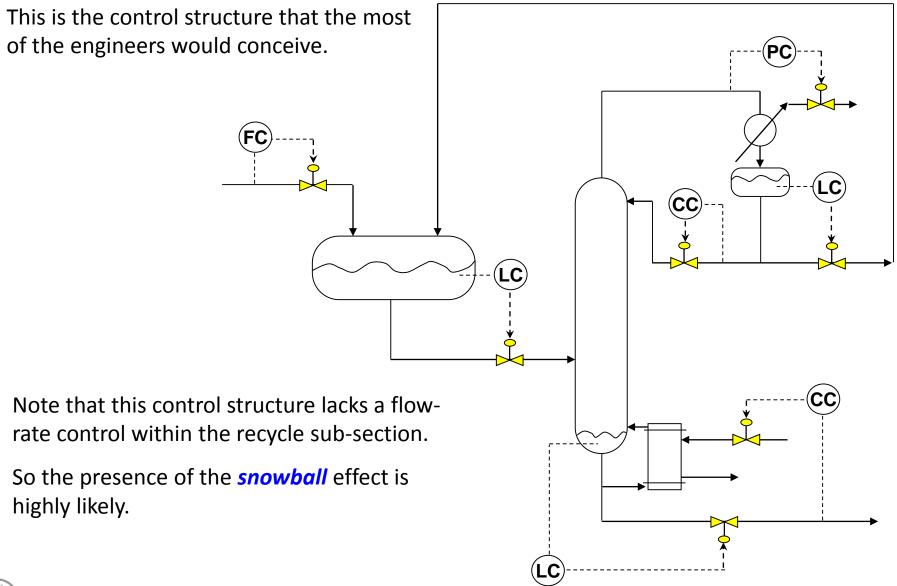




Proceeding to the implementation of the control structure and working in the conventional way, the choice of the control loop is the following:

- 1. The fresh feed is flow-rate controlled by means of the flow-rate: **FC**
- 2. The reactor level is controlled by manipulating the outlet flow: LC
- 3. The distillate purity is controlled by manipulating the reflux flow-rate: **CC**
- 4. The bottom product purity is controlled by manipulating the heat provided by the reboiler: **CC**
- 5. The level of the reflux drum is controlled by means of the distillate flow-rate (which is also the recycle stream): **LC**
- 6. The level in the bottom of the column is controlled by manipulating the bottom product flow-rate: LC
- 7. The column pressure is controlled by manipulating the coolant stream in the condenser: **PC**





To get an idea of what might happen in case of snowball effect, it is worth writing the material balances and evaluating the recycle stream in normal conditions or after some disturbances to the feed composition:

Base case $x_A^{feed} = 0.9 \rightarrow$  $F_{recycle} = 260.5$  kmol/h $x_A^{feed} = 0.8 \rightarrow$  $F_{recycle} = 205$  kmol/h $x_A^{feed} = 1.0 \rightarrow$  $F_{recycle} = 330$  kmol/h

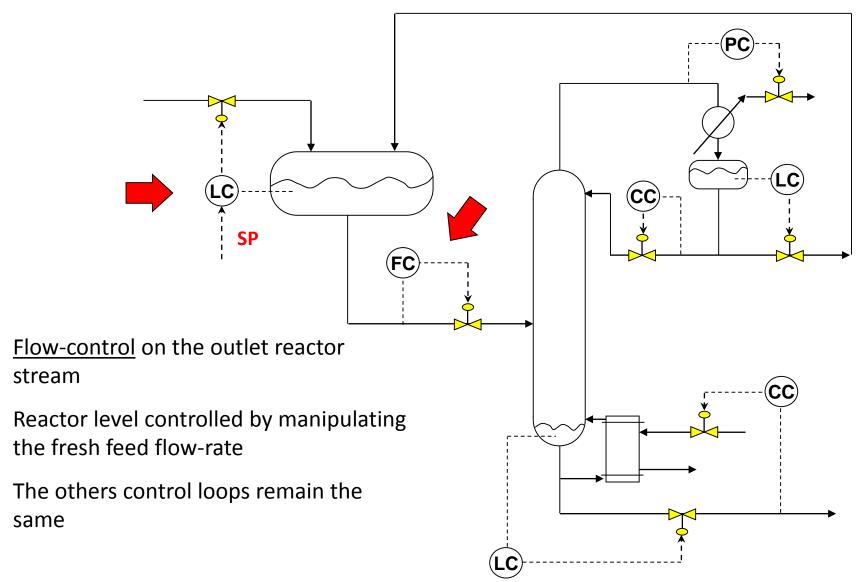
A **25%** of disturbance on  $x_A$  produces a **60%** of variation on  $F_{recycle}$ .

Base case	$F_{fresh}$ = 239.5 $\rightarrow$	F <sub>recycle</sub> = 260.5 kmol/h	
	$F_{\text{fresh}}$ = 215 $\rightarrow$	F <sub>recycle</sub> = 187	kmol/h
	$F_{fresh}$ = 265 $\rightarrow$	F <sub>recycle</sub> = 362	kmol/h

A **23%** of disturbance on  $F_{\text{fresh}}$  produces a **94%** of variation on  $F_{\text{recycle}}$ .

#### We have a *snowball* effect

An alternative, to the classical control structure already proposed, exists:





1.

2.

3.

A flow control has been introduced within the recycle section. This allows to considerably reduce the oscillation of the recycle flow-rate produced by the disturbances to the system.

It worth observing that the production cannot be modified by regulating directly the fresh feed because it is necessary to control the reactor level.

Actually, the regulation of the plant production is done by assigning the level set-point.

By doing so, if  $x_A^{feed}$  or  $F_{fresh}$  are disturbed,  $F_{recycle}$  remains constant (0% variation).

In order to modify the production from 215 kmol/h to 265 kmol/h (+23%) the reactor hold-up should be changed from 1030 to 1520 kmol (+48%). At the same time the recycle flow-rate goes from 285 to 235 kmol/h (-18%). The variation is now much more limited.

This is due to the presence of the control loop on the reactor outlet flow-rate, belonging to the recycle system.



# Interaction between the reactor and the separation sections

In the adopted control structure, it is possible to act on the production rate only by modifying the reactor operative conditions.

In case of liquid phase reaction, it is necessary to modify the level, in case of gas phase reaction it is necessary to modify the pressure.

Similarly it is possible to act on the concentrations of the reactants (and products, in case of reversible reactions), on the catalyst activity, or on the quantity of initiator.

Some variables have a large influence on the operation of the unit, and they are called **DOMINANT** variables. A system controlling the dominant variables is called: **PARTIAL CONTROL**.

This is called <u>partial control</u> because often the manipulated variables are less then the controlled variables. In these cases, the set-points of the dominant variables are manipulated in order to reach the fixed economic and/or process targets.



# **Plant-wide process control**

The nine points briefly presented at the beginning of this section will be now outlined and their main features will be described. These nine points should guide the process/control engineer to an optimal and rational synthesis.

- 1. Define the control objectives
- 2. Determine the control Degrees of Freedom
- 3. Define the energy management system
- 4. Set production rate
- 5. Control product quality and ensure safety, environmental, and operational constraints
- 6. Fix a flow in every recycle loop and control inventories (Pressures and Liquid Levels)
- 7. Check the component balances
- 8. Control the single Unit Operations
- 9. Optimize the process economics and improve the dynamic controllability



#### **1. Define the control objectives**

Assess the steady-state design and dynamic control objectives for the process.

The "best" control structure for a plant depends upon the design and control criteria established.

These objectives include reactor and separation yields, product quality specifications, product grades and demand determination, environmental restrictions, and the range of safe operating conditions.



#### **2. Determine the control Degrees of Freedom**

Count the number of control valves available.

Most of these valves will be used to achieve basic regulatory control of the process: set production rate, maintain gas and liquid inventories, control product qualities, and avoid safety and environmental constraints.

Any valves that remain after these vital tasks have been accomplished can be utilized to enhance steady-state economic objectives or dynamic controllability.

During the course of the subsequent steps, we may find that we lack suitable manipulators to achieve the desired economic control objectives. Then we must change the process design to obtain additional handles. For example, we may need to add bypass lines around heat exchangers and include auxiliary heat exchangers.



### 3. Define the energy management system

Make sure that energy disturbances do not propagate throughout the process by transferring the variability to the plant utility system.

The high grade of thermal coupling between different units must be avoided, in the example: reactor/FEHE or: reactor/distillation column by means of reboilers and condensers.

The risk is to have a positive feedback and process instability.

The extreme energy integration (see pinch technology) leads to a highly optimized process economics and simultaneously to poor the process controllability. In these cases it is necessary to introduce bypass lines or auxiliary heat exchangers in order to ensure a correct dynamic behavior of the process.



#### 4. Set the production rate

Identify the variables that dominate the productivity of the reactor and determine the most appropriate manipulated variable(s) to control the production rate.

To obtain higher production rates, we must increase overall reaction rates. This can be accomplished by raising temperature (higher specific reaction rate), increasing reactant concentrations, increasing reactor holdup (in liquid-phase reactors), or increasing reactor pressure (in gas-phase reactors).

Temperature is often the dominant variable in the reactor.

If this is not true, we must find another dominant variable, such as the concentration of the limiting reactant, flow-rate of initiator or catalyst to the reactor, reactor residence time, reactor pressure, or agitation rate.



#### **5. Control the product quality**

Select the "best" valves to control each of the product-quality, safety, and environmental variables.

We should select manipulated variables such that the dynamic relationships between the controlled and manipulated variables feature small time constants and dead-times and large steady-state gains.

It should be noted that we are establishing the product-quality loops first, before the material balance control structure (Buckley, 1964).



# 6. Control a flowrate in every recycle loop and control pressures and liquid levels

Set a flow control in every recycle loop (in order to avoid the snowball effect).

Gas recycle loops are normally set at maximum circulation rate, as limited by compressor capacity, to achieve maximum yields (Douglas, 1988).

Once we have fixed a flow in each recycle loop, we then determine which valve should be used to control each inventory variable of the different units (reactors, columns, drums, tanks, ...).



#### 7. Check component balances

*Identify how chemical components enter, leave, and are generated or consumed in the process.* 

Product and inert components must have an exit/purge path from the system. It is also worth taking in mind the unreacted components.

Remind the **integral** effect exerted by the recycle streams.

Need of liquid and gaseous purge.

The purge flow-rate is adjusted in order to reach the right compromise between capital and operative expenses (Douglas, 1988).



#### 8. Control individual unit operations

Establish the control loops necessary to operate each of the individual unit operations.

Several effective control schemes have been established over the years for individual chemical units.



# 9. Optimize the economics and improve the dynamic controllability

Establish the best way to use the remaining control degrees of freedom.

After satisfying all of the basic regulatory requirements, we usually have additional degrees of freedom involving control valves that have not been used and set-points in some controllers that can be adjusted.

It is also possible to introduce new degrees of freedom by means of bypass streams or auxiliary heat exchangers.



# **Bibliography**

- Buckley, P. "Techniques of Process Control", New York, Wiley, (1964)
- Douglas, J. "Conceptual Design of Chemical Processes", New York, McGraw-Hill, (1988)
- Luyben, W., Tyréus B. & Luyben, M. "Analysis of Control Structures for Reaction/Separation/Recycle Processes with Second-Order Reactions", *Ind. Eng. Chem. Res.*, **35**, 758-771, (1996)
- Luyben, W., Tyréus B. & Luyben, M. "Plantwide Control Design Procedure", AIChE J., 43, 3161-3174, (1997)
- Luyben W.L., B.D. Tyreus, M.L. Luyben, "Plantwide Process Control", McGraw-Hill, (1998)
- Morud, J & Skogestad, S. "Dynamic Behavior of Integrated Plants", J. Proc. Cont., 6, 145-156, (1996)
- Shinskey, F. "Process Control Systems", New York, McGraw-Hill, (1988)
- Tyréus B. & Luyben, W. "Dynamics and Control of Recycle Systems: 4. Ternary Systems with One or Two Recycle Streams", *Ind. Eng. Chem. Res.*, **32**, 1154-1162, (1993)

