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Steady-state and Dynamic Flowsheet Simulations of Solids Processes: Part I

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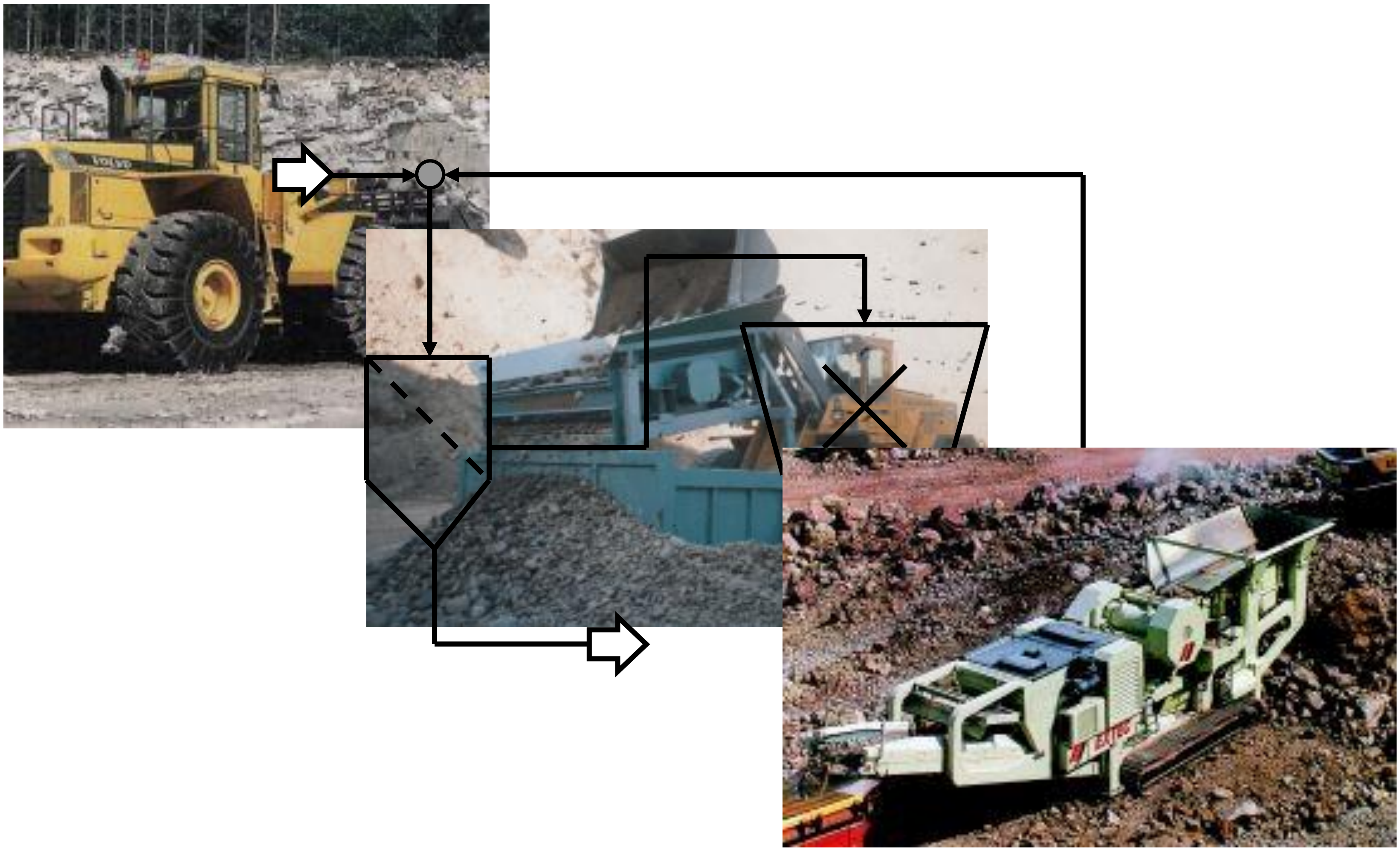
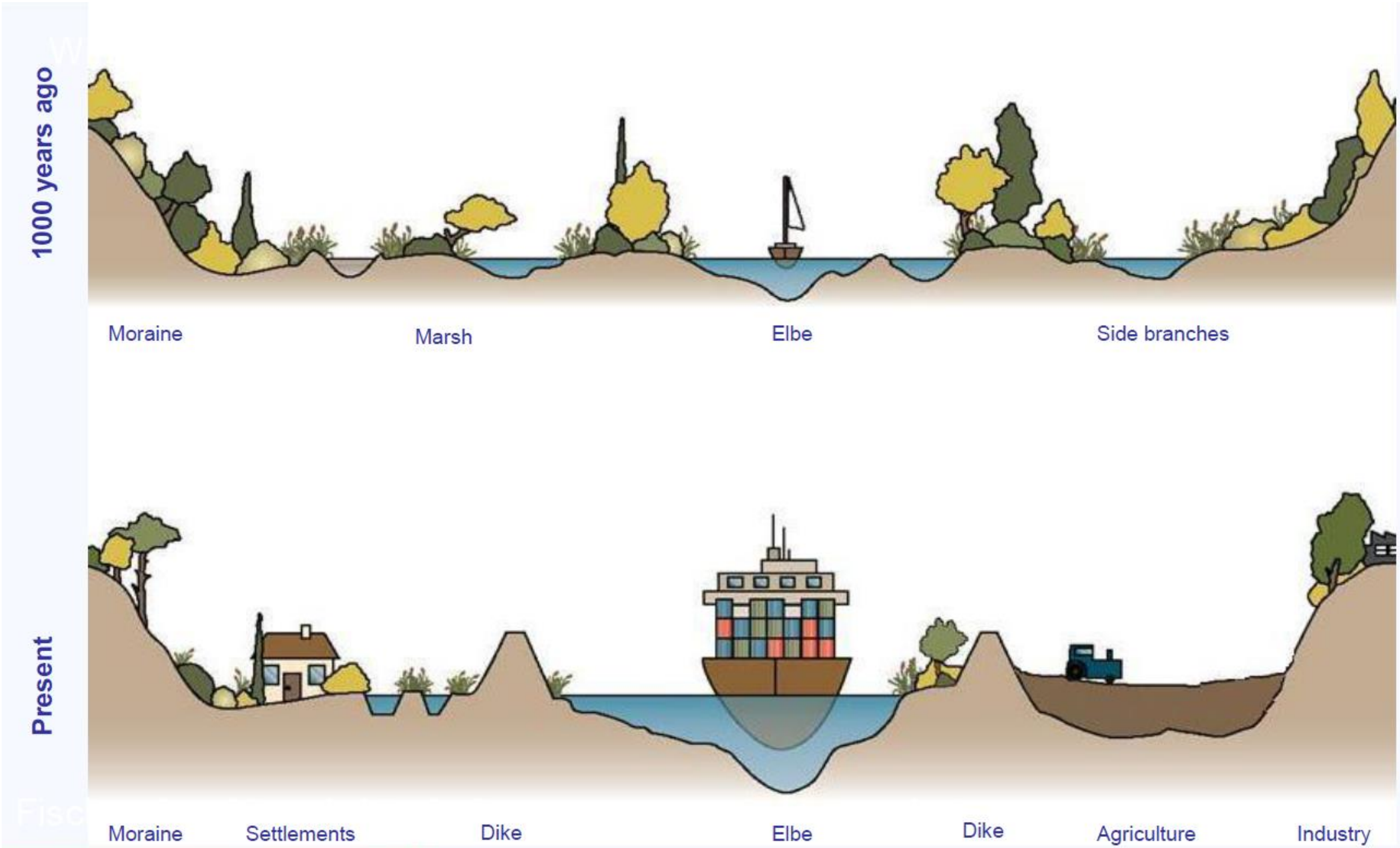
- Most industrial processes consist of complex interconnection of different apparatuses and production steps

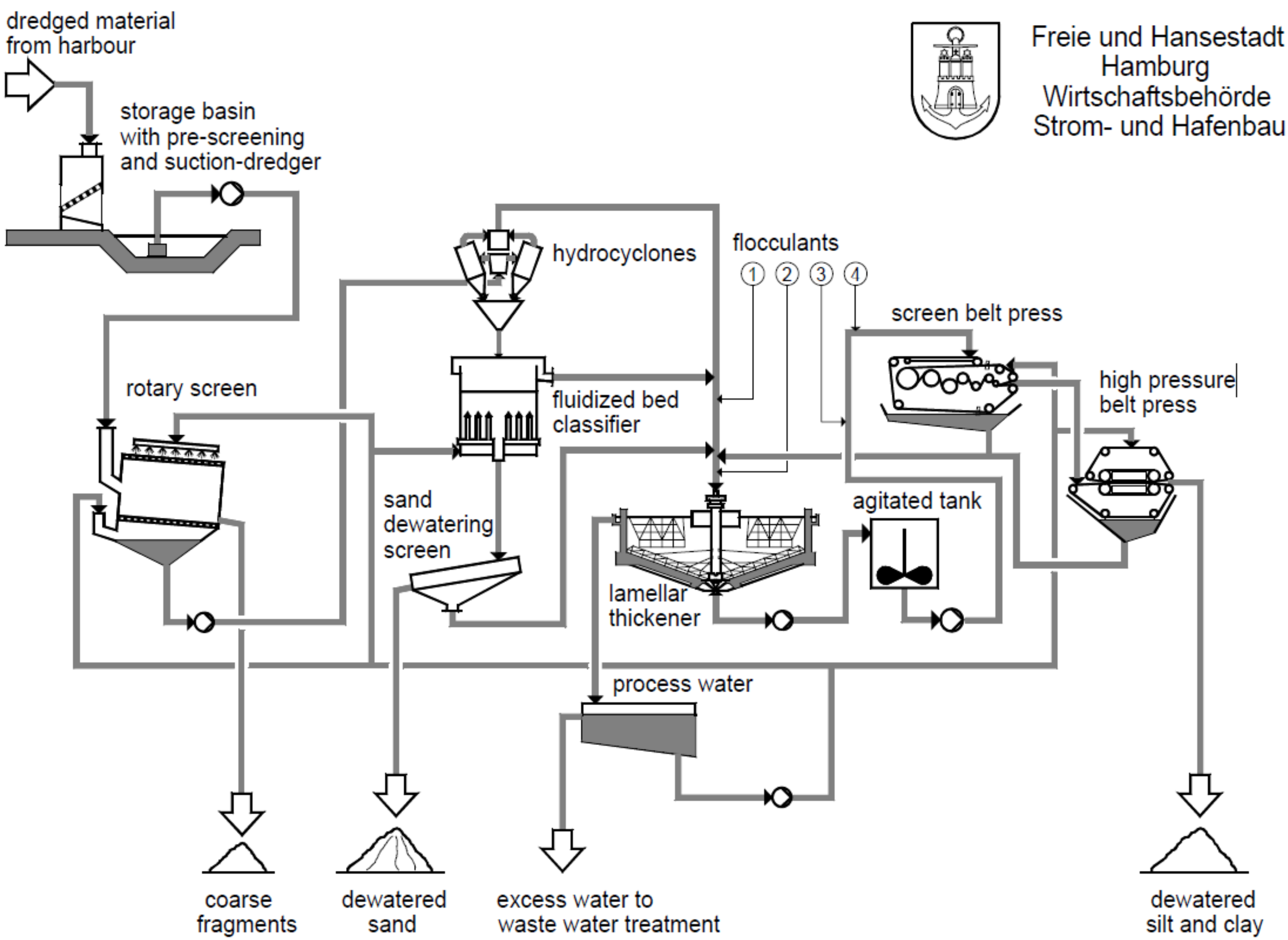


- Dredging in port Hamburg has a long tradition (first steam dredger was bought in the mid. 19th century)



A. Netzband. Sediment management concept of the port Hamburg, Hamburg Port Authority.

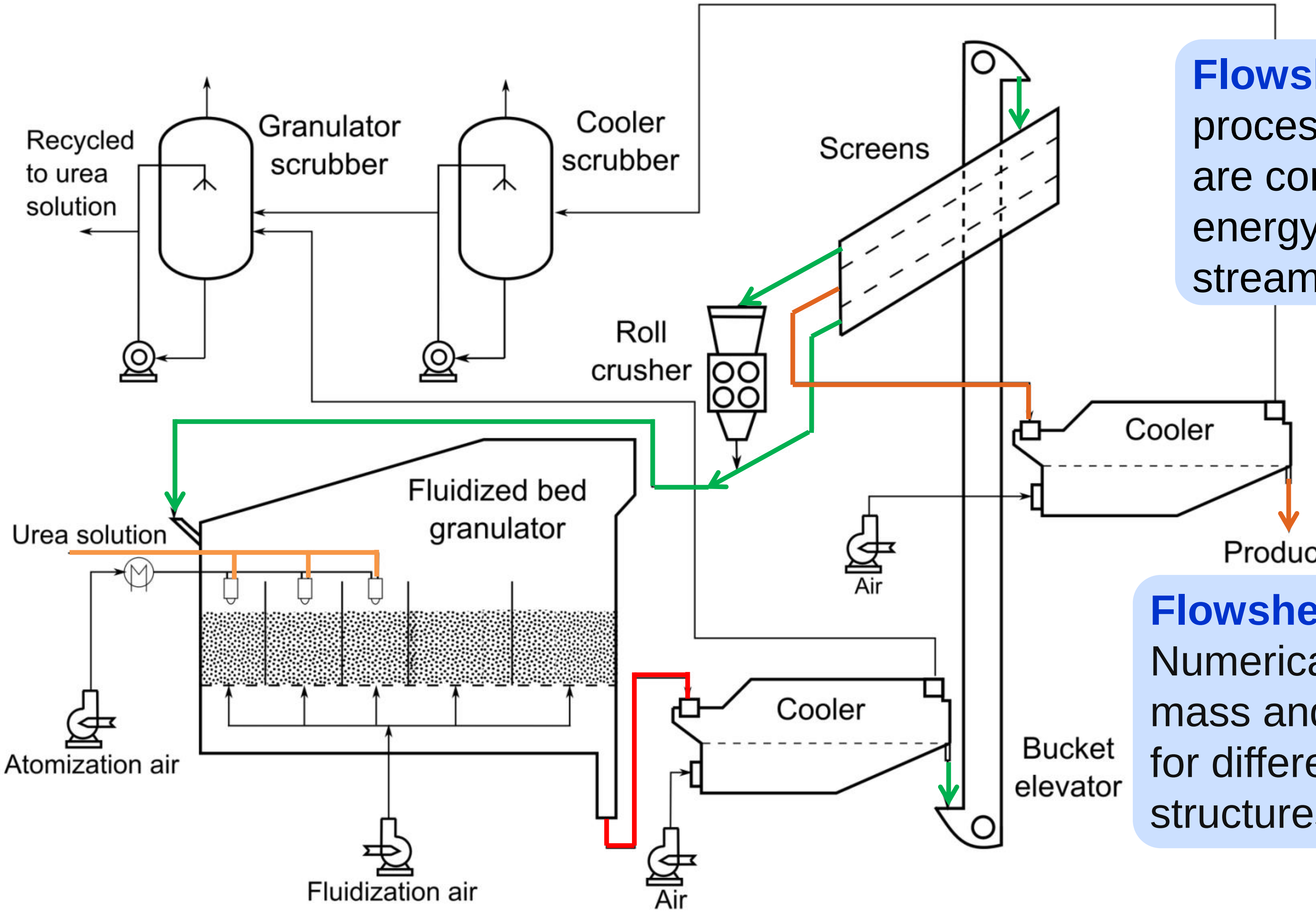
Examples of industrial processes
METHA process



H.-D. Detzner. The Hamburg Project METHA: large scale separation dewatering and reuse of polluted sediments, Europ. Water Poll. Contr. 5.

Examples of industrial processes
METHA process

Example: Urea granulation



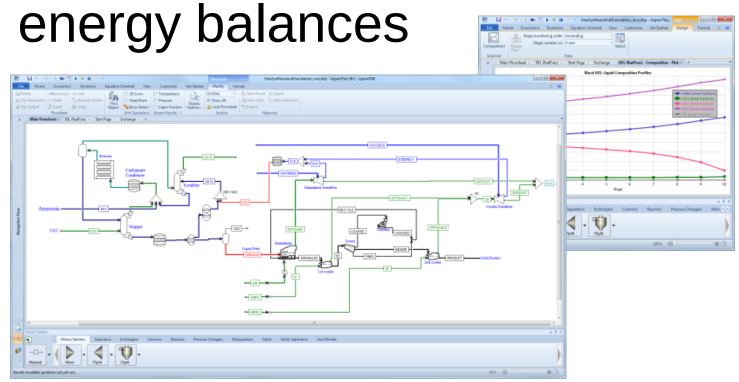
Flowsheet: Network of process units, which are connected by energy and material streams

Flowsheet simulation: Numerical calculation of mass and energy balances for different process structures

Brochure Uhde UFT fluid bed granulation – superior technology

Flowsheet simulation
What is Flowsheeting?

- Flowsheeting is:
  - the use of a computer program to model a production process
  - used to obtain mass and energy balances



- Flowsheeting is used for:
  - planning purposes, e.g. rough sizing and costing of equipment
  - testing hypotheses, e.g. process behavior, process alternatives
  - process optimization, e.g. operating conditions, process alternatives

- What does flowsheet simulation not address:
  - detailed apparatus layout (e.g. influence of the change of the nozzle position in a granulator)

Benefits of flowsheet simulation

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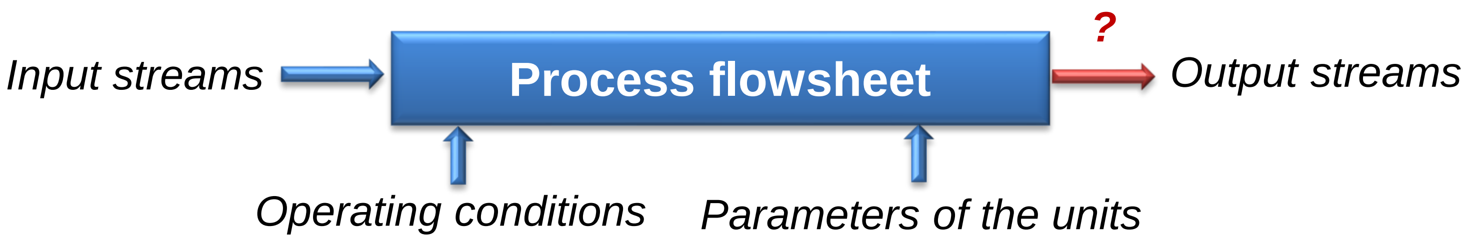
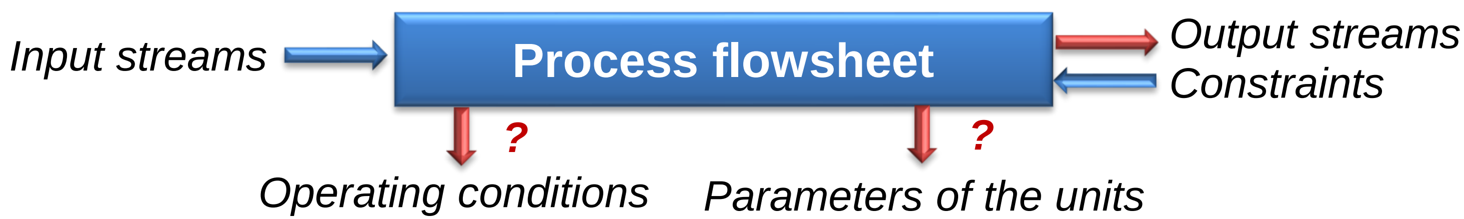
- flowsheet simulation is more efficient compared to the manual subsequent calculation of models for different apparatuses
- shows effects of changes of one processes unit on the entire process
- reduces the measurement efforts required to obtain the material and population balance for all streams of a process
- allows for holistic optimization of complex processes with regard to energy, quality, yield, ..
- structured library of process models allows easy access to up-to-date modeling knowledge
- operator training – the simulator gives an answer to:
  ‚What happens when I change this parameter?'

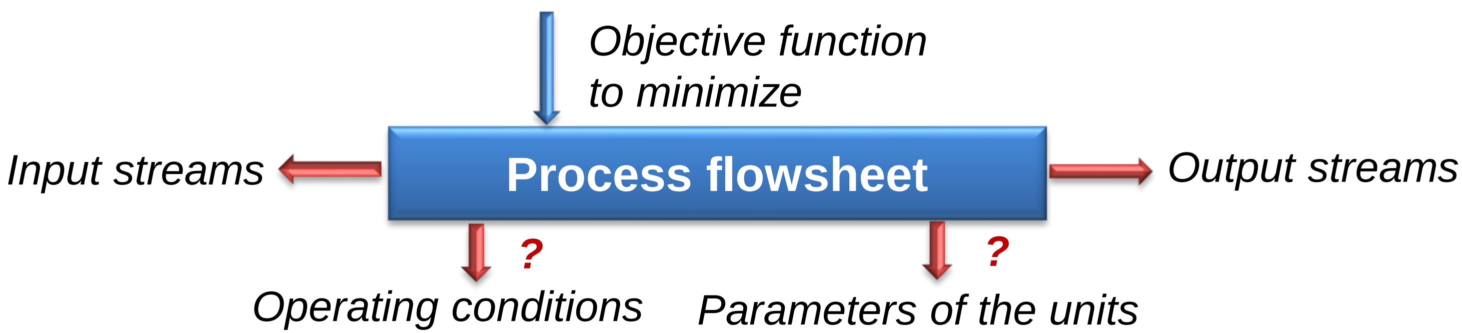
- With help of process simulator, three main types of problems can be solved:
  - **Simulation**



  - **Design**



  - **Optimization**



Use of flowsheet simulation systems in industry

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- flowsheet simulation is well established in industry
  - for modeling, simulation, design and optimization of fluid processes
  - common tools are Aspen Plus, Aspen Hysis, Pro/II, UniSim, …
- in contrast, solids processes are mostly designed unit by unit
  - numerical models exist for unit operations, but in different tools (Excel, Matlab, C/C++ or FORTRAN code etc.)
  - the entire process is normally not simulated at once
- Why? Because in the past most simulation packages were…
  - not well suited to describe solids processes
    - lack of unit operation models
    - insufficient data structure to describe a disperse phase
  - mostly limited to quite narrow industrial sectors (e.g. mining, gravel and sand etc.)

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Fluid processes

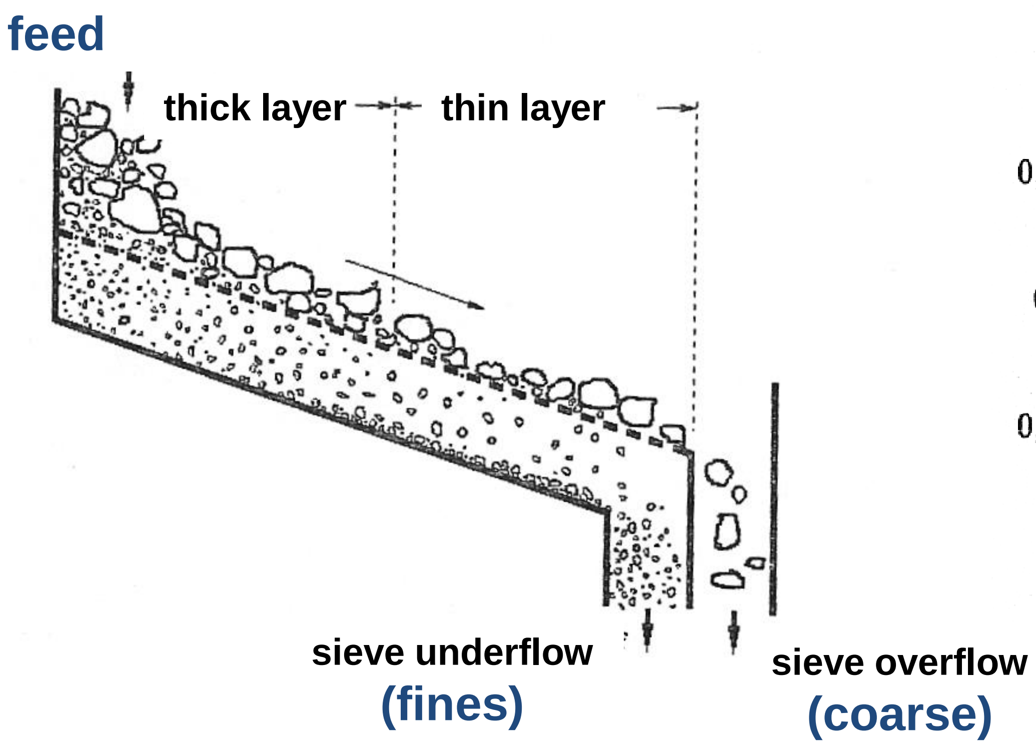
- concentrated parameters
  (pressure, temperature,...)
- completely characterized by
  chemical composition
  - phase equilibrium
  - mixture properties

Solids processes

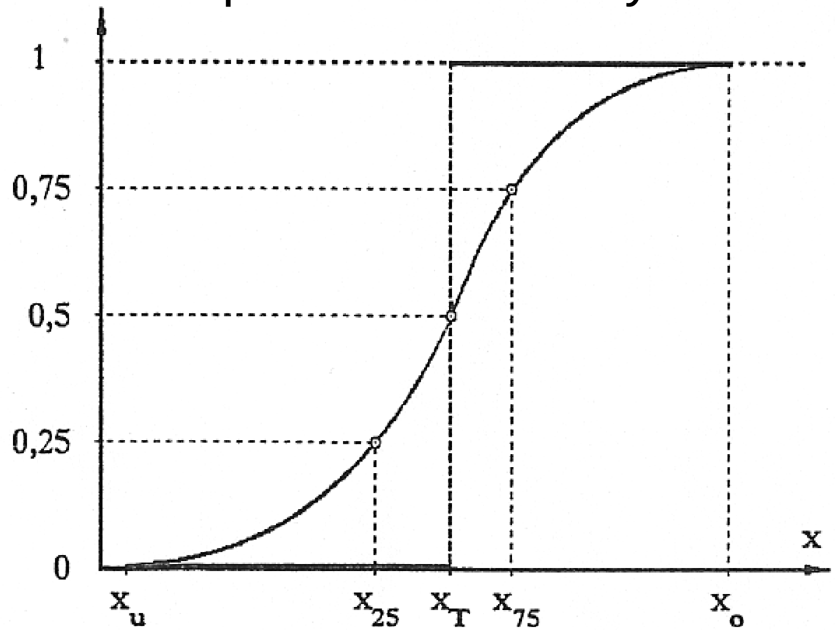
- distributed parameters
  (particle size distribution,…)
- characterization requires
  more information
  - particle size distribution
    for each particle type
  - moisture content
    for each particle type
  - …
- bulk properties cannot be calculated
  from single particles properties

⇨ **Complex structure for material streams is needed**

- Continuous sieving



- Separation efficiency

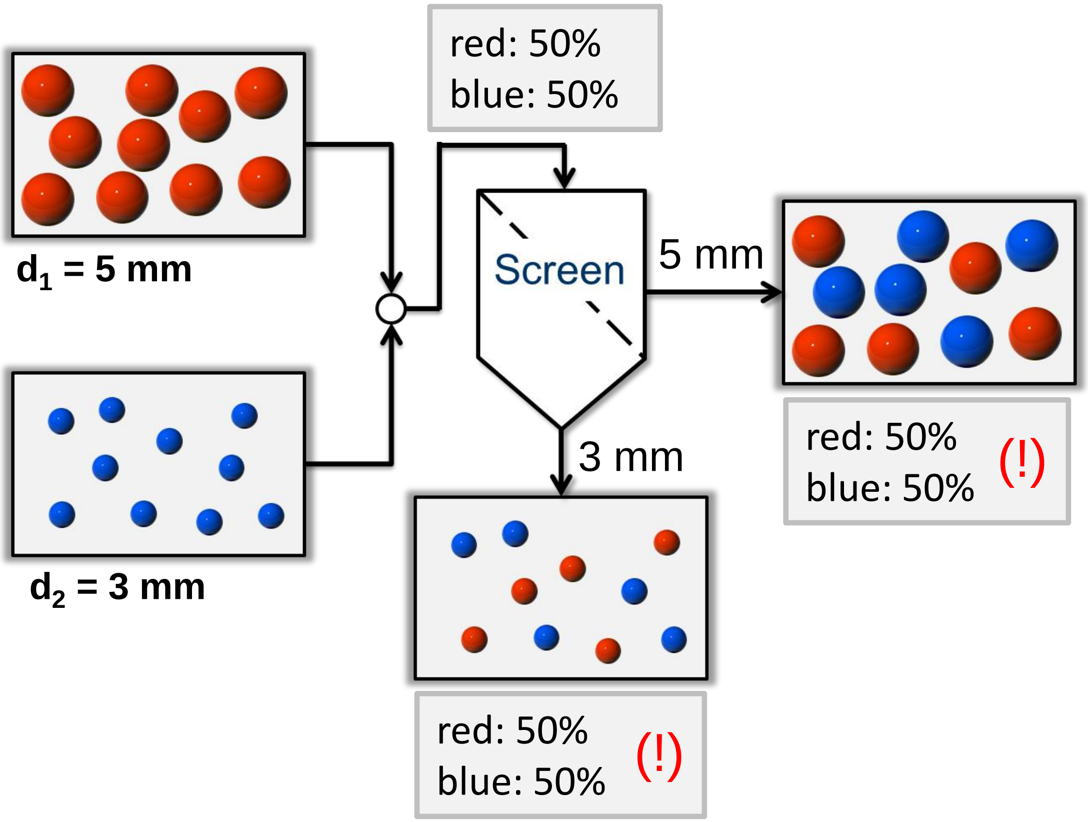


- Separation efficiency

$$T(x) = g \cdot \frac{q_{coarse}(x)}{q_{input}(x)}$$

g – coarse mass fraction

- Distributed properties (particle size distribution, porosity distribution…) are used for description of solids materials
- Characterization of solids can require more information: shape factors, particle strength…
- Size-dependent secondary attributes can be used: residual moisture, density…



Treatment of solids without consideration of dependent distributed properties may lead to their mixing and incorrect handling

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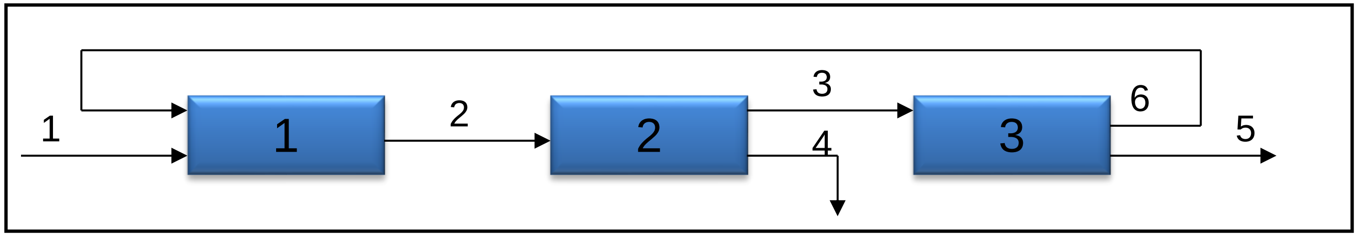
- Mathematical model of specific process consists of:

  - ## Functional model

    Functional model describes mathematical dependencies between Input and Output variables of each process element

  - ## Structural model

    Structural model describes coupling between elements according to the structure of investigated process



Flowsheet simulation
Functional and structural model

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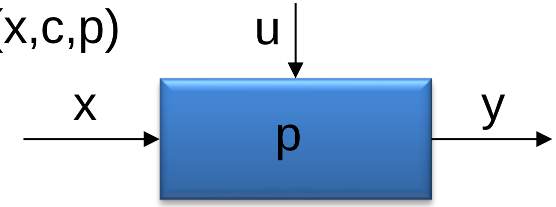
- Functional model can consist of:
  - Balance equations (mass and/or energy)
  - State equations (i.e. ideal gas law)
  - Equations of process kinetics (i.e. reaction kinetics)

- Model M transforms vector of input variables x into vector of output variables y

$y = M(x,c,p)$



x Input variables

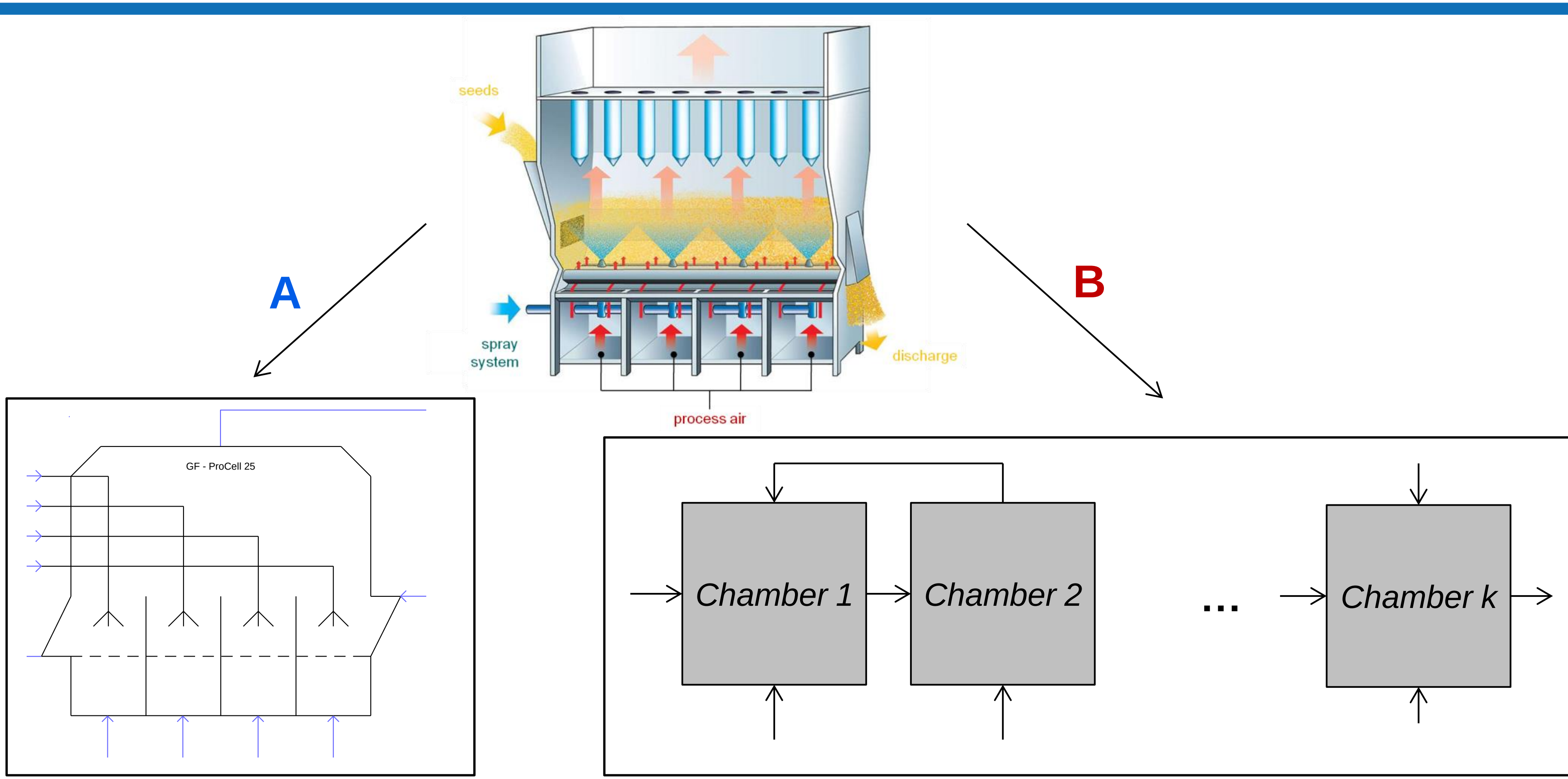
y Output variables

u Operating conditions

p Model parameters

- Functional model can describe:
  - Single apparatus, for example screen
  - Group of apparatuses or process substeps, for example circulated fluidized bed

Flowsheet simulation
Model representation



- A: smaller computational effort (unnecessary initialization and copy operations can be avoided)
- B: higher flexibility of process configuration

Flowsheet simulation

Functional and structural model

- Structural model describes coupling between units

  → represents process structure

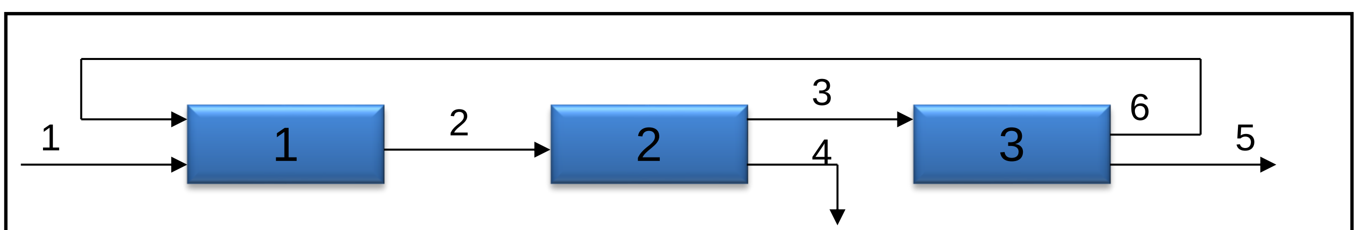
- Example Incidence Matrix:

  Each row is related to one column, each row is related to unit

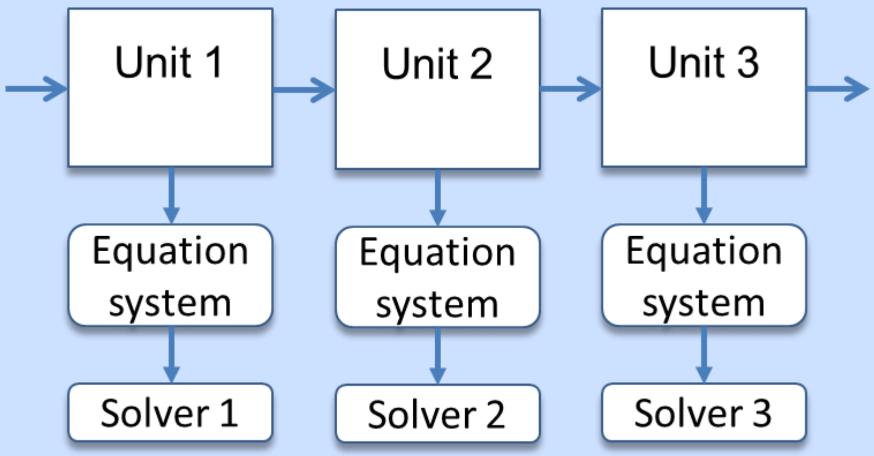
$$s_{ij} = \begin{cases} -1, \text{ if stream } u_j \text{ is output of unit } x_i \\ 1, \text{ if stream } u_j \text{ is the input of unit } x_i \\ 0, \text{ otherwise} \end{cases}$$

$$\begin{array}{c|c} i \rightarrow \;\; 1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 & j \downarrow \\ S = \begin{pmatrix} -1 & 0 & 0 & 1 & 1 & 0 \\ 1 & -1 & 0 & 0 & 0 & 1 \\ 0 & 1 & -1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 & -1 \end{pmatrix} & \begin{matrix} 0 \\ 1 \\ 2 \\ 3 \end{matrix} \end{array}$$

Element 0: Environment



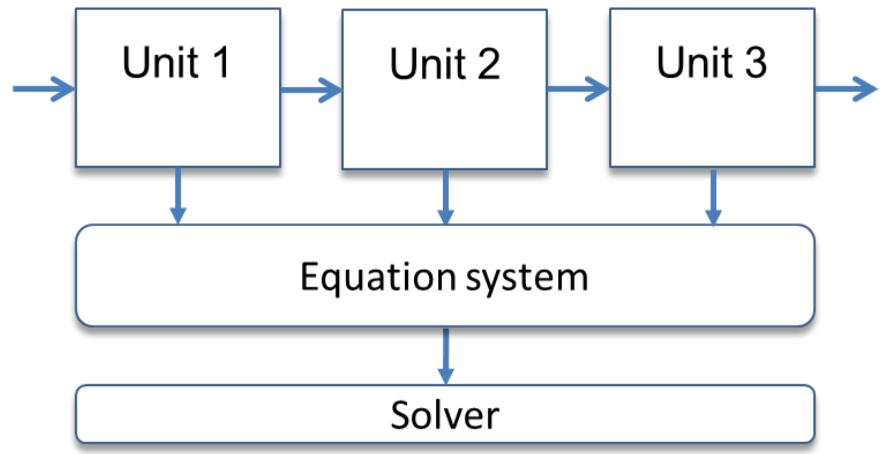
Flowsheet simulation
Modular vs. simultaneous approach



Sequential-modular (modular)

- Conceptual simplicity
- Correspondence to the physical structure of processes
- Higher flexibility
- Possibility to use different numerical methods to calculate models
- Difficulties in processing flowsheets with recycle streams

Examples: ASPEN Plus, ChemCad, HySim



Equation-oriented (simultaneous)

- Equations are homogenized and calculated by one solver
- Better convergence rate, especially for complex flowsheets with recycles
- Difficulties with simultaneous simulation of fast and slow changed components
- Usage with heterogeneous models is complicated

Examples: SpeedUp, gProms, DIVA, Diana

Flowsheet simulation
Modular approach

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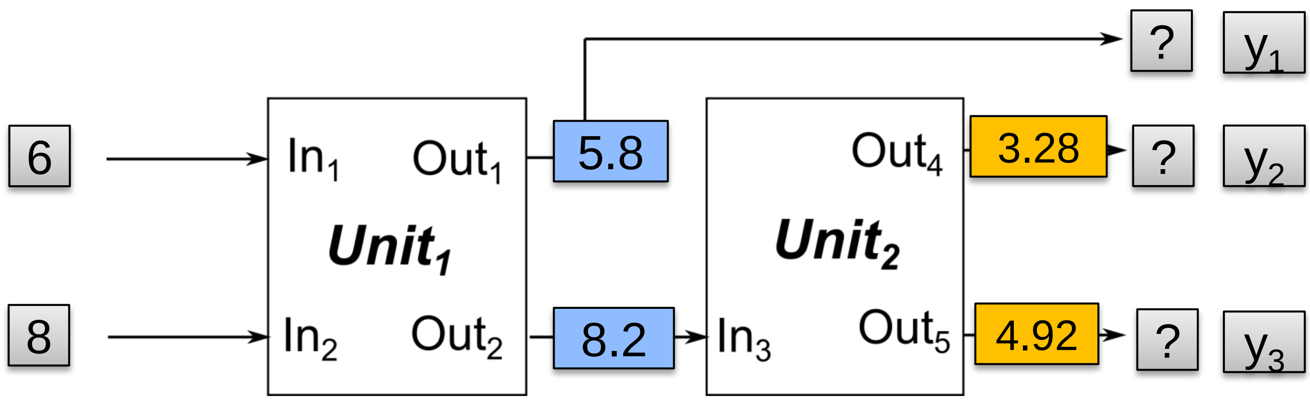
Unit 1

$$Out_1 = 0.3 \cdot In_1 + 0.5 \cdot In_2$$
$$Out_2 = 0.7 \cdot In_1 + 0.5 \cdot In_2$$

Unit 2

$$Out_4 = 0.4 \cdot In_3$$
$$Out_5 = 0.6 \cdot In_3$$



Equation-oriented approach

$$\begin{cases} Out_1 = 0.3 \cdot In_1 + 0.5 \cdot In_2 \\ Out_2 = 0.7 \cdot In_1 + 0.5 \cdot In_2 \\ Out_4 = 0.4 \cdot In_3 \\ Out_5 = 0.6 \cdot In_3 \end{cases}$$

Modular approach

1. Calculation of $Unit_1$
2. Calculation of $Unit_2$

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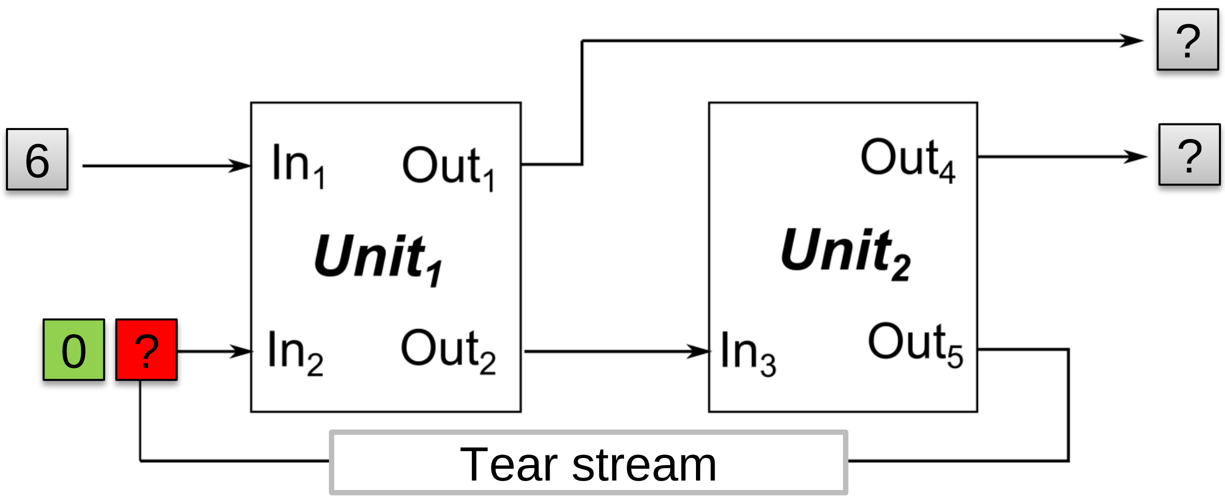
Unit 1

$$Out_1 = 0.3 \cdot In_1 + 0.5 \cdot In_2$$
$$Out_2 = 0.7 \cdot In_1 + 0.5 \cdot In_2$$

Unit 2

$$Out_4 = 0.4 \cdot In_3$$
$$Out_5 = 0.6 \cdot In_3$$



Iteration 1

$Unit_1$: $Out_1 = 1.8$
$Out_2 = 4.2$

$Unit_2$: $Out_4 = 1.68$
$Out_5 = 2.52$

Tear stream

Iteration 0: 0

Iteration 1: 2.52

Difference: 2.52

Iteration 2

$Unit_1$: $Out_1 = 3.06$
$Out_2 = 5.46$

$Unit_2$: $Out_4 = 2.184$
$Out_5 = 3.276$

Tear stream

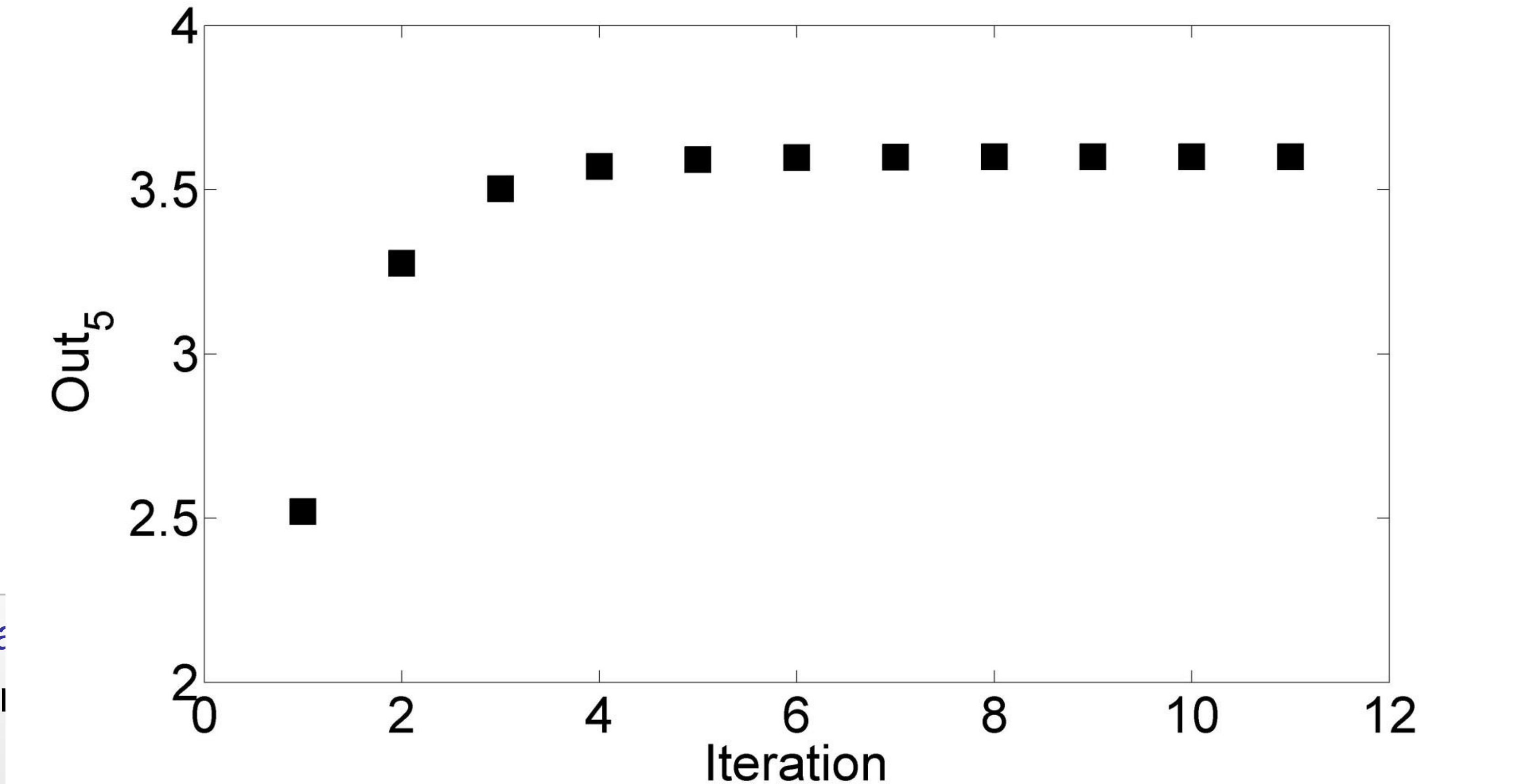
Iteration 1: 2.52

Iteration 2: 3.276

Difference: 0.756

Unit 1

Unit 2



Itera

Ur

Unit$_2$: Out$_4$ =1.68
Out$_5$ =2.52

Iteration 1: 2.52

Difference: 2.52

Unit$_2$: Out$_4$ =2.184
Out$_5$ =3.276

52

Iteration 2: 3.276

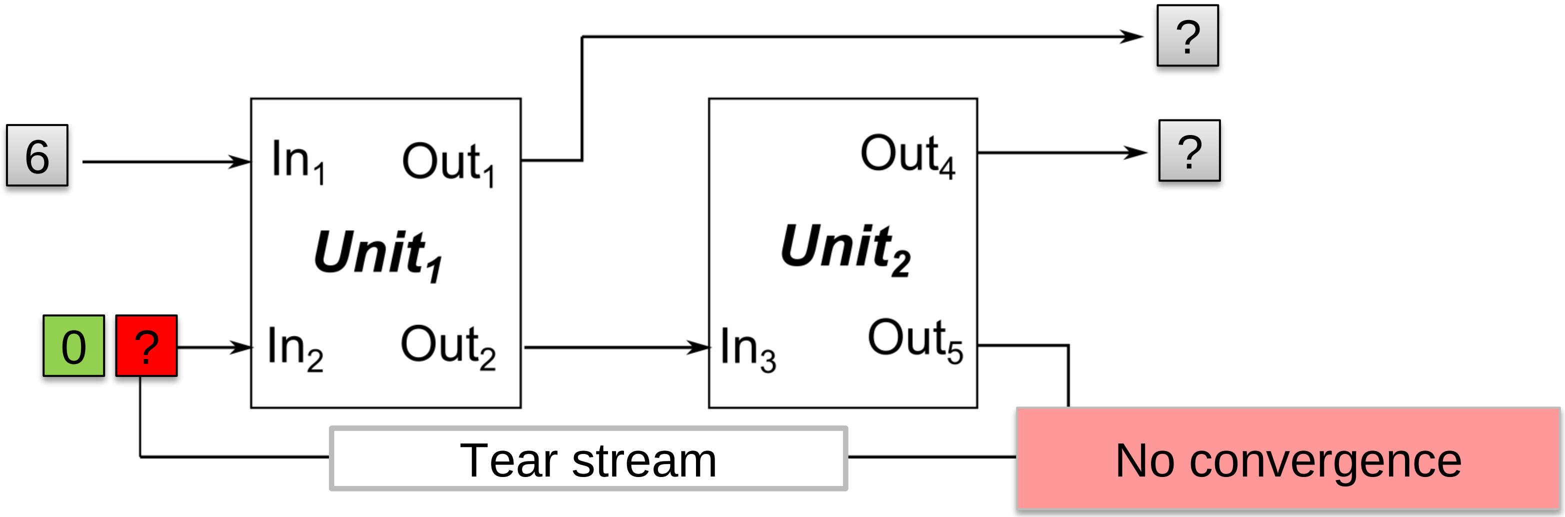
Difference: 0.756

Unit 1

$$Out_1 = 0.3 \cdot In_1 + 0.5 \cdot In_2$$
$$Out_2 = 0.7 \cdot In_1 + 2 \cdot In_2$$

Unit 2

$$Out_4 = 0.4 \cdot In_3$$
$$Out_5 = 0.6 \cdot In_3$$



Iteration 1

Unit$_1$: Out$_1$ =1.8
Out$_2$ =4.2

Unit$_2$: Out$_4$ =1.68
Out$_5$ =2.52

Tear stream

Iteration 0: 0

Iteration 1: 2.52

Difference: 2.52

Iteration 2

Unit$_1$: Out$_1$ =3.06
Out$_2$ =9.24

Unit$_2$: Out$_4$ =3.696
Out$_5$ =5.544

Tear stream

Iteration 1: 2.52

Iteration 2: 5.544

Difference: 3.024

- To improve calculation performance the convergence methods can be applied

  x – represents guessed tear variable

  $F(x)$ – calculated value after new unit calculation

- Direct substitution: $$x_k = F(x_k)$$

- Relaxation-acceleration: $$x_{k+1} = \lambda \cdot F(x_k) + (1-\lambda)x_k$$

- Wegstein's method – implements parabolic extrapolation using results of two previous iterations

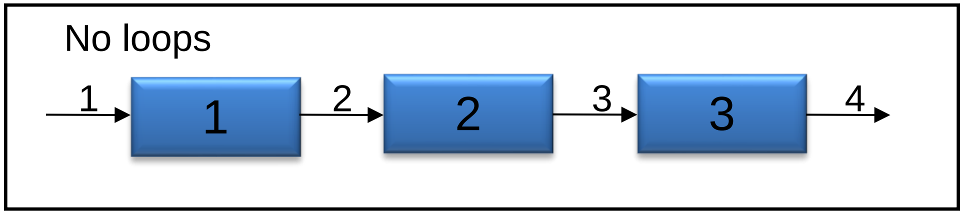
$$x_{k+1} = q \cdot x_k + (1-q)F(x_k)$$ $$q = \frac{s}{s-1}$$ $$s = \frac{F(x_k) - F(x_{k-1})}{x_k - x_{k-1}}$$

- Steffensen's method:

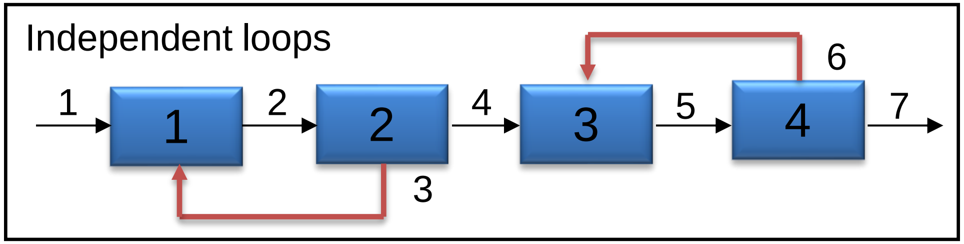
$$X_k = X_{k-3} - \frac{(X_{k-2} - X_{k-3})^2}{X_{k-2} - 2X_{k-2} + X_{k-3}}$$

Flowsheet simulation
Calculation sequence

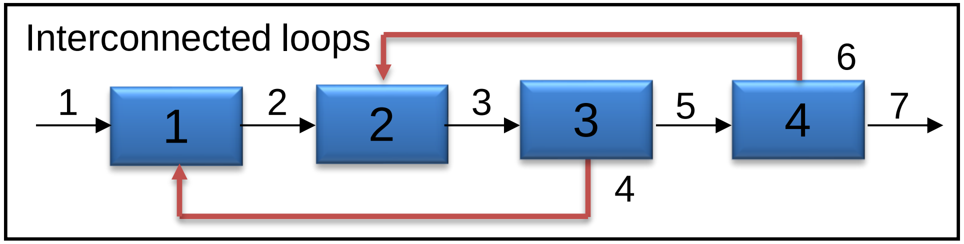
- Calculation sequence plays important role in the case of modular approach
- Recycle stream denotes process stream that returns material or enthalpy from downstream process unit back to upstream process unit
- Complex schemes, consisting of large number of recycle streams cannot be easily solved
- Units connected with recycle streams form loops
- Loops are solved iteratively via cutting of recycle streams
- Tearing - providing initial guess, such as total flow, PSD, composition, temperature, etc.
- A tear stream is not necessary recycle stream



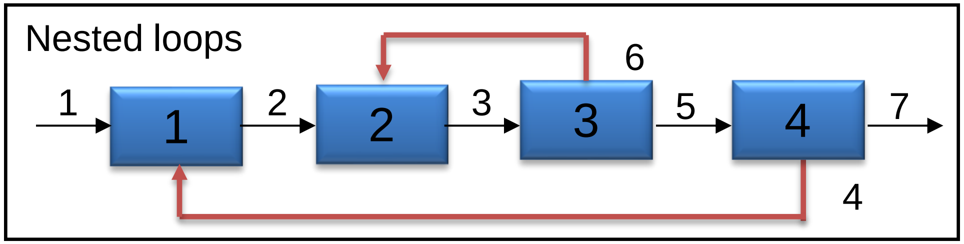
Flowsheet can be directly calculated without any iteration (no recycle streams)



Several recycle streams co-exist, however both loops can be solved separately

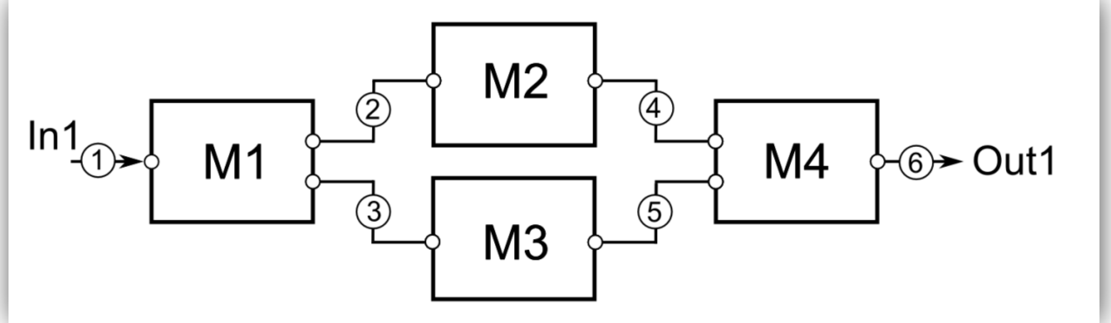


Several recycle streams co-exist, whole scheme should be solved iteratively



Recycle include another recycle stream

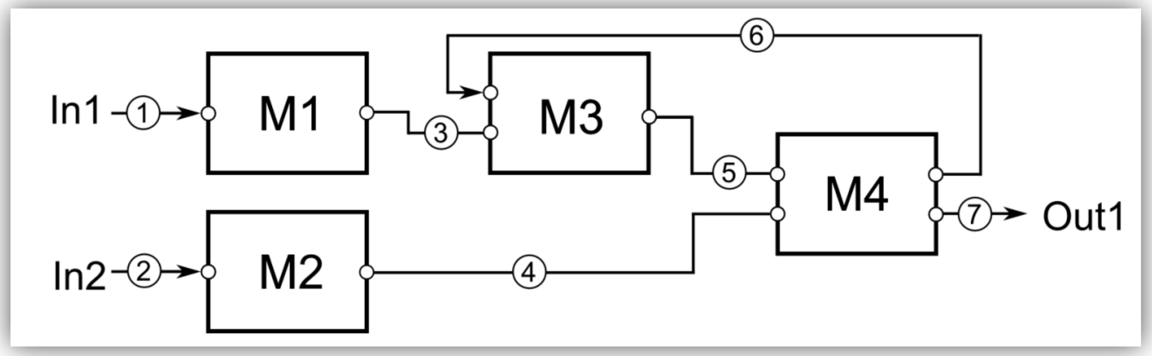
Example 1



Calculation sequence 1

Step 1	Step 2	Step 3	Step 4
M1	M2	M3	M4

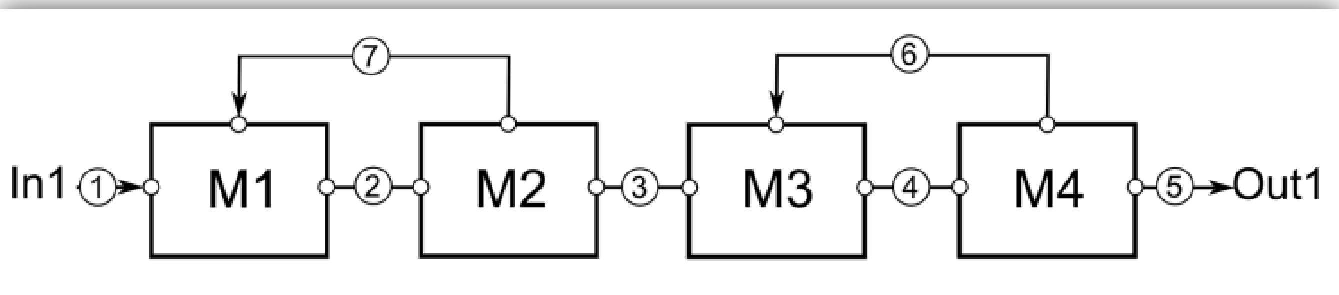
Example 2



Calculation sequence 2

Step 1	Step 2	**Step 3** *(iterative until convergence)*
M1	M2	M3; M4; *S6*

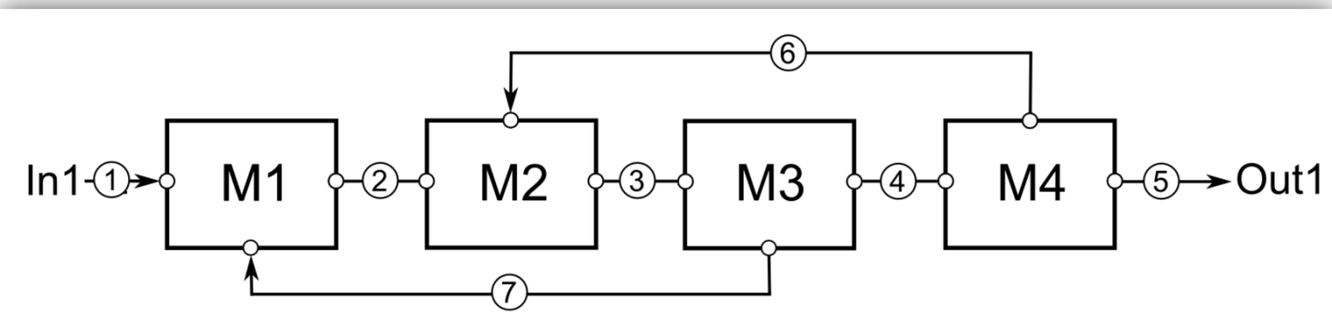
Example 3:



Calculation sequence 3

Step 1 *(iterative until convergence)*	**Step 2** *(iterative until convergence)*
M1; M2; *S7*	M3; M4; *S6*

Example 4:



Calculation sequence 4

Step 1 *(iterative until convergence)*
M1; M2; M3; M4; *S6; S7*

- Approximation of calculation sequence is performed in two steps:

1. Units which are related to one loop should be identified and combined in separate blocks

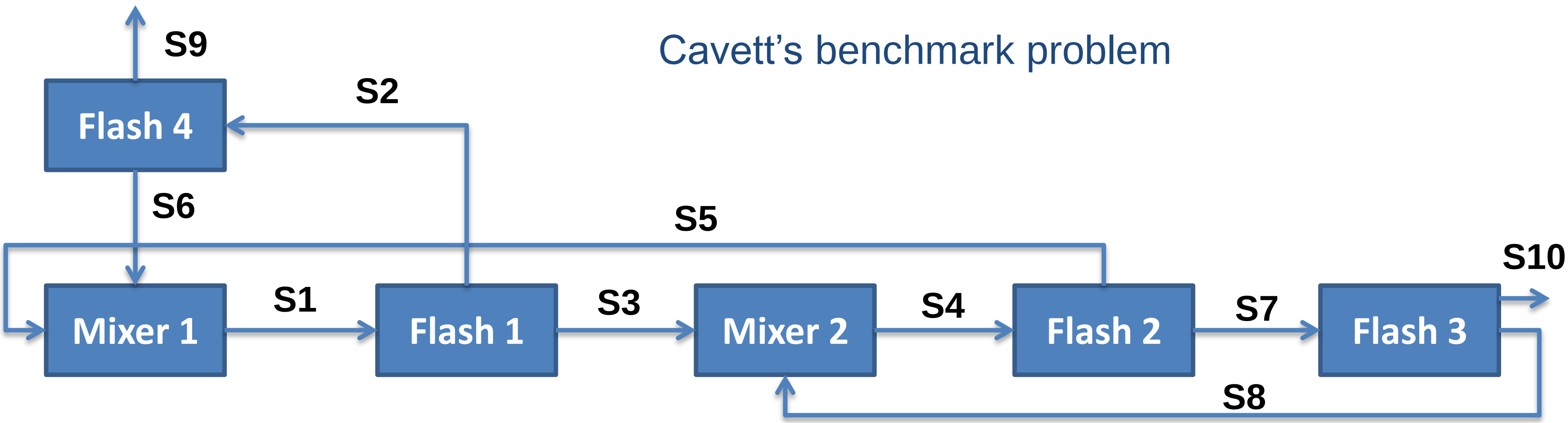
    - Existing algorithms
        - Sargent und Westerberg algorithm
        - Loopfinder algorithm according to Forder und Hutchinson
        - …

2. Specification of tear streams on optimal position

    - Criteria for selection of tear streams
        - Minimal number of tear streams
        - Availability of initial data for first iteration
    - Existing algorithms
        - Barkley und Motard algorithm
        - ItFinder-algorithm according to Forder und Hutchinson
    - …

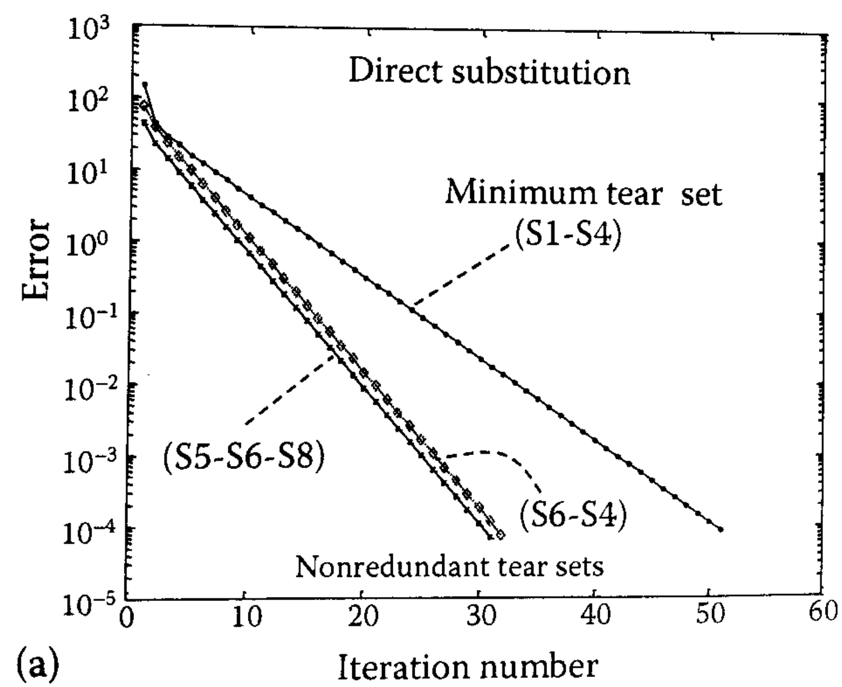
Tarjan's algorithm for partitioning

- Main idea of algorithm – path tracing and identifying information paths
- The stack of visited nodes is built
- Each cycle appears as a group of nodes



Cavett's benchmark problem

- Three different sets of tear streams are possible:
  - S1-S4
  - S5-S6-S8
  - S6-S4



R.H. Cavett (1963). Application of numerical methods to the convergence of simulated processes involving recycle loops.