

# An efficient algorithm for designing reliable large-scale process networks

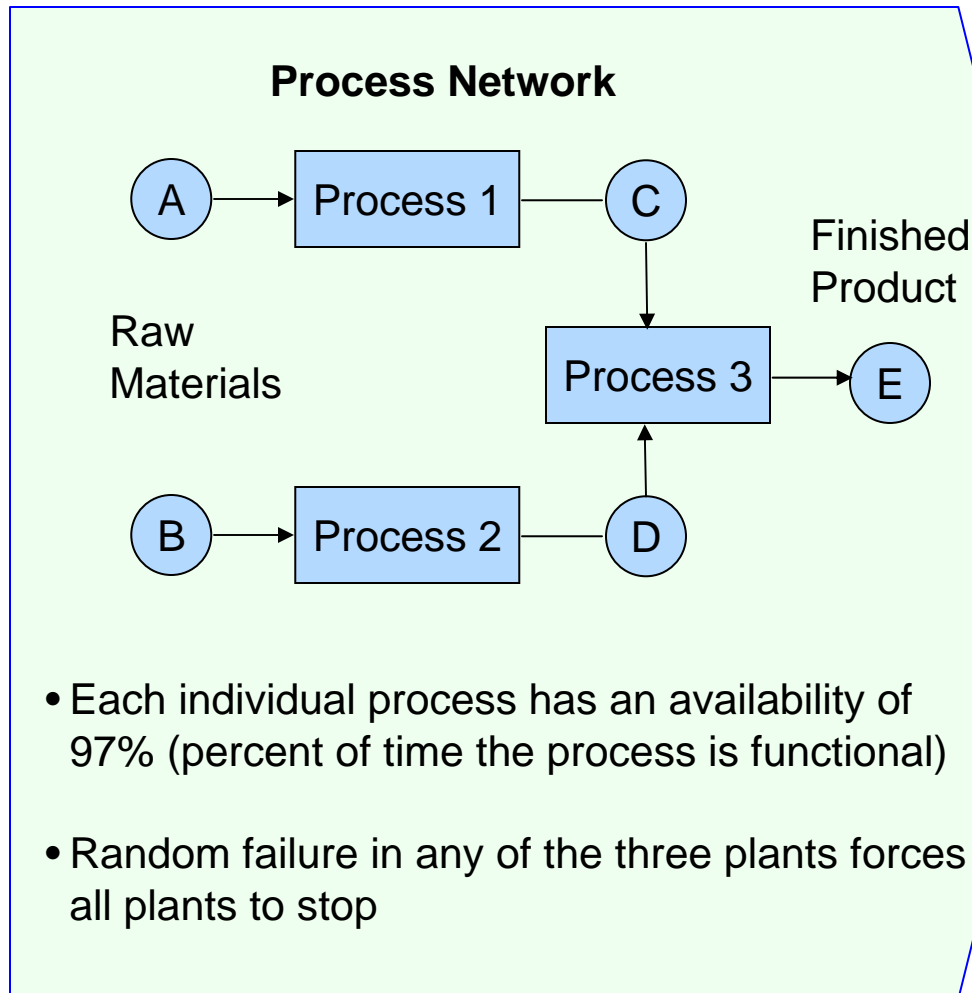
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**EWO Meeting**  
**Carnegie Mellon University**  
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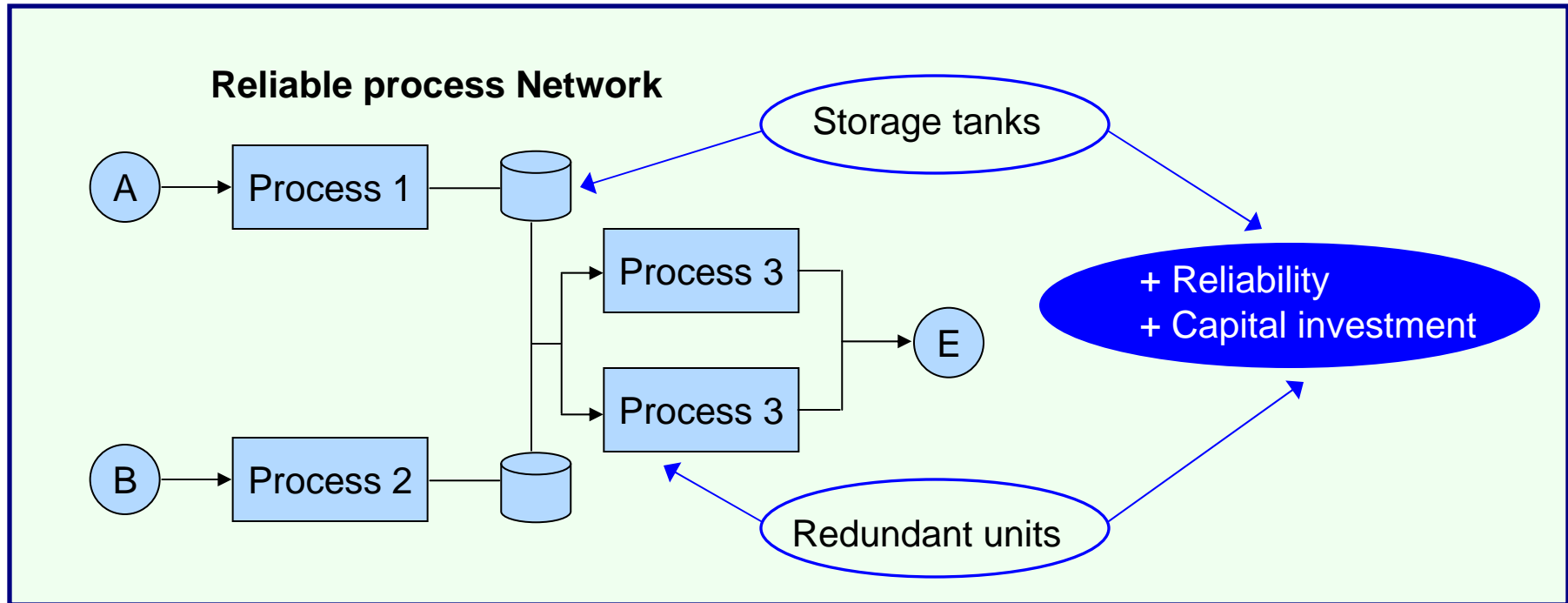
In collaboration with The Dow Chemical Company



- Chemical plants are networks of processes
- All processes in real plants are subject to stochastic (random) failures
- The network has to be designed so that failures do not propagate (think about bullwhip effect in a supply chain).



Without **intermediate storage** or **redundant parallel** units the network is NOT functional ~ 10% of the time



**Challenges** involved in designing reliable process networks:

- How much investment is required to ensure certain reliability ?
- How to invest a given amount of capital in the best possible way ?
  - Redundancies vs. storage tanks
  - There are 27 combinations of redundancies and storage tank configurations in the simple network above



## Mathematical optimization provides a systematic method for achieving the objective of reliable design



### Given:

- The superstructure of an integrated site
- Process specifications (maximum allowable capacities, supply of raw material, etc.)
- Number of failure modes and their corresponding probability

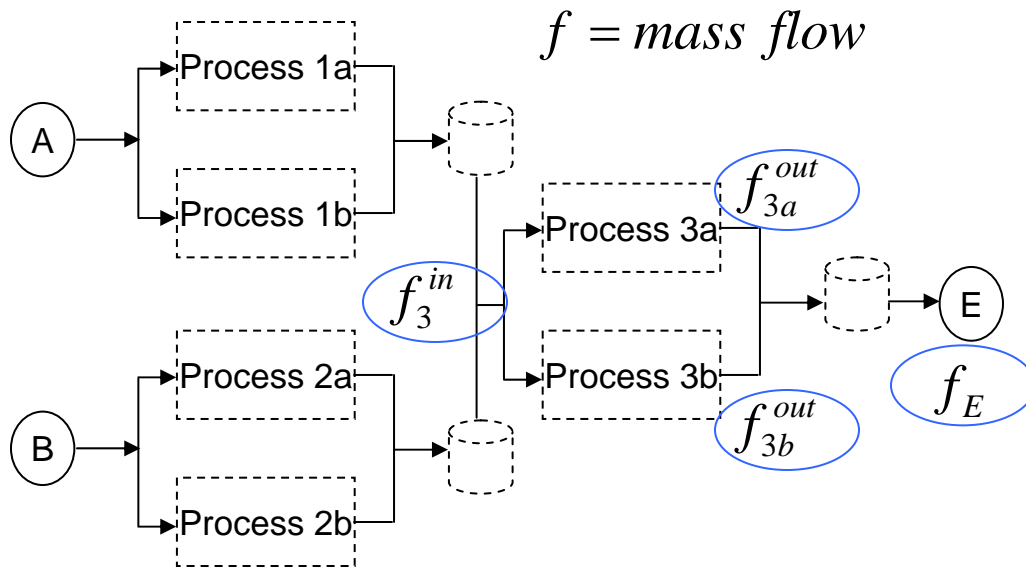
### Determine:

- The number of parallel production units for each process.
- Sizes of intermediate storage between processes.

### With the objective of:

- Maximizing the average production rate (function of reliability)
- Minimizing the capital investment.

## Postulate a *superstructure*



## Superstructure constraints

$$f_{3a}^{out} \leq y_{3a} \text{Capacity}_{3a}$$

$$f_{3b}^{out} \leq y_{3b} \text{Capacity}_{3b}$$

$$(f_{3a}^{out} + f_{3b}^{out}) - f_E \leq \frac{v_3}{\text{repair time}}$$

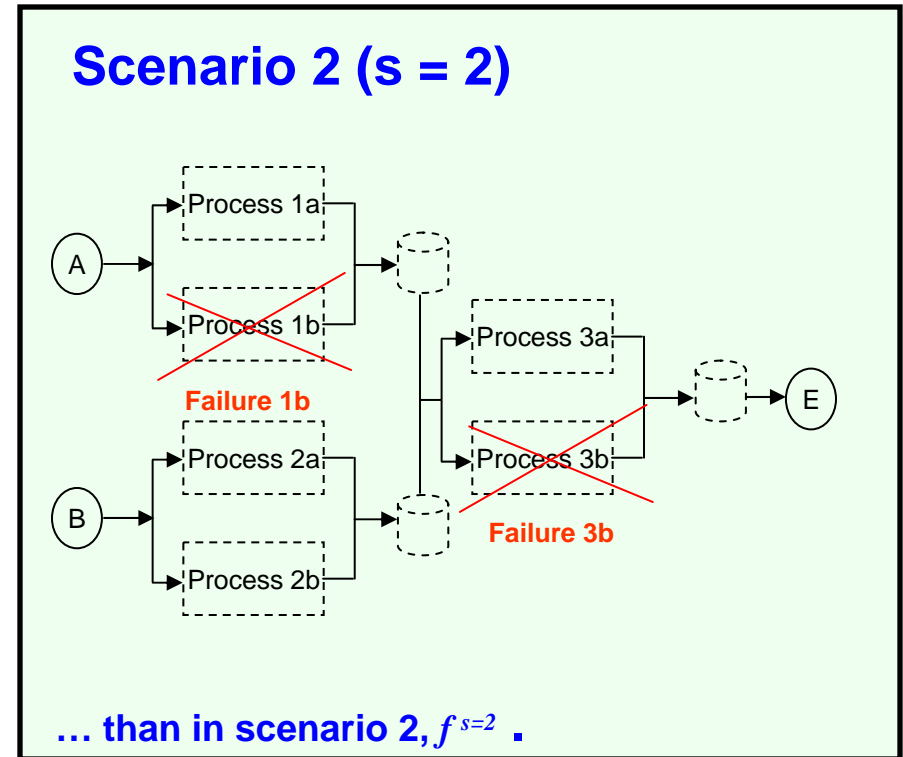
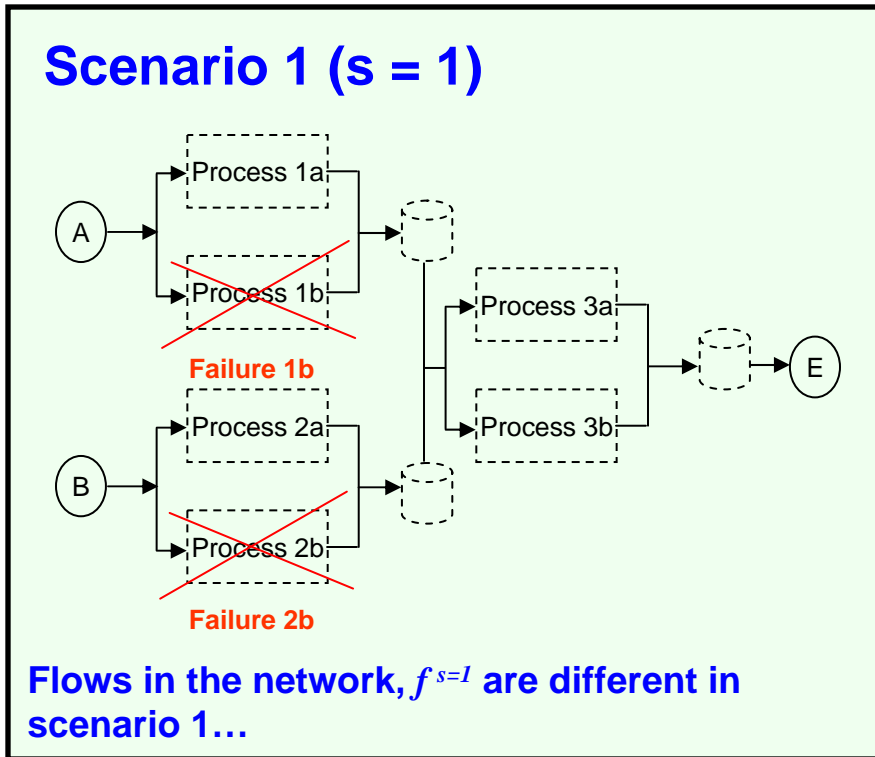
Assign **decision variables** to redundancies and tanks

$y_{3a}$  1 if process 3a is installed; 0 otherwise

$y_{3b}$  1 if process 3b is installed; 0 otherwise

$v_3$  Size of storage tank (0 if tank is not included)

The network is subject to failures; in each failure scenario the model of the network (mass balance, superstructure constraints, etc.) has a different solution, i.e.:



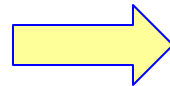
The mass balance equations in the model are repeated for each scenario:

$$m^s(f^s, y, v, \theta^s) \leq 0 \quad \Rightarrow$$

*Compact representation of the equations in the model for each scenario*

## Two-stage stochastic programming formulation

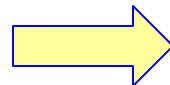
$$\max \sum_s p_s f_E^s$$



- $p_s$ : probability of each scenario
- $f_E^s$ : flow of finished product

*s.t.*

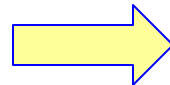
$$m^s(f^s, y, v, \theta^s) \leq 0$$



- Flow variables  $f^s$  are assigned to each scenario
- Design variables  $y, v$ , are not a function of the scenario

$$investment(y, v) \leq \varepsilon$$

$$s = 1, 2, \dots, S$$



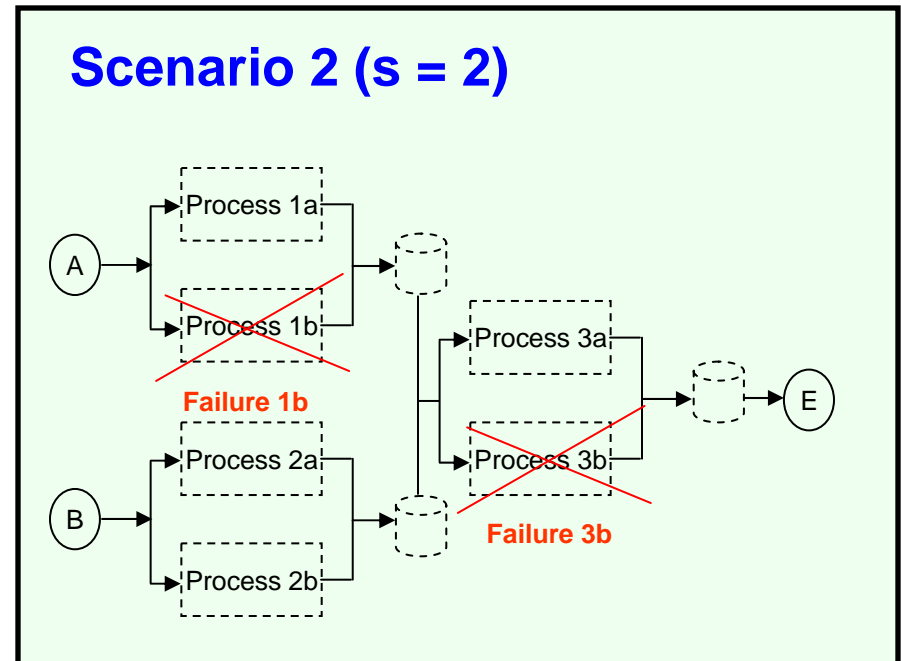
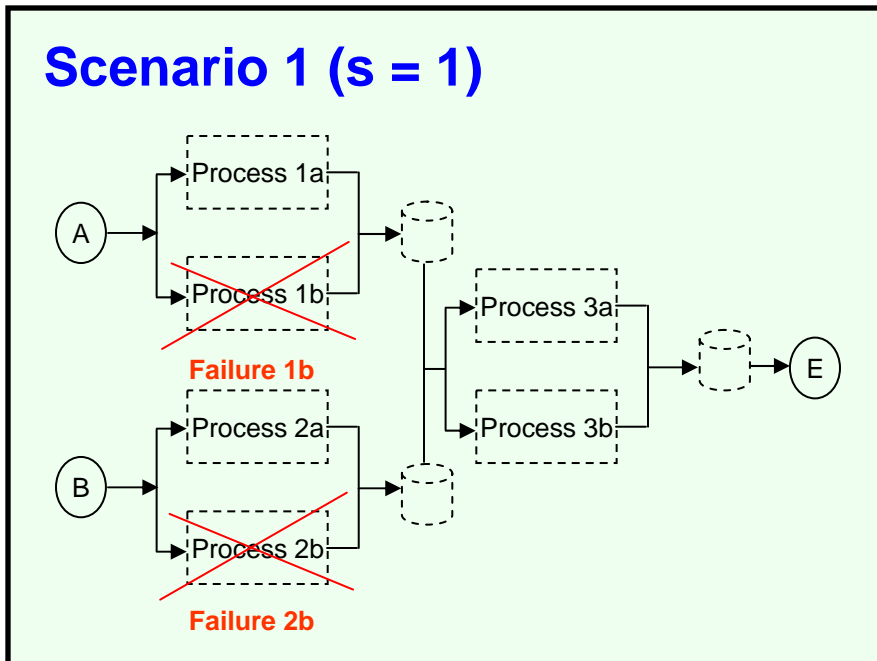
- One scenario for each combination of failure modes ***in the superstructure***

- Objective function represents the **average productivity**
- We want to **determine the design that maximizes** the average productivity



We still need more constraints...

Scenarios 1 and 2 are indistinguishable **IF** Process 1b, 2b, and 3b are not chosen from the superstructure



$$\left. \begin{aligned} \text{IF } y_{1b}, y_{2b}, y_{3b} &= 0 \\ f^{s=1} &= f^{s=2} \end{aligned} \right\}$$

- Equation for each possible pair of scenario
- Equation is activated or deactivated as a function  $y$
- These are Non-anticipativity constraints

$$\max \sum_s p_s f_E^s$$

*s.t.*

$$m^s(f^s, y, v, \theta^s) \leq 0$$

$$\text{investment}(y, v) \leq \varepsilon$$

$$f^s \leq f^{s'} + \alpha(y)$$

$$f^s \geq f^{s'} - \alpha(y)$$

$$s = 1, 2, \dots, S$$

$$s' = 1, 2, \dots, S$$

## Remarks about formulation

- **Optimizes the average performance** of network
- The probability of each scenario is affected by the design decisions: **endogenous uncertainty**.
- To model endogenous uncertainty we need **non-anticipativity (NA) constraints**
- Solve for different values of  $\varepsilon$  to obtain **Pareto-optimal solutions**

# The number of NA constraints turns most industrial applications into large-scale optimization problems

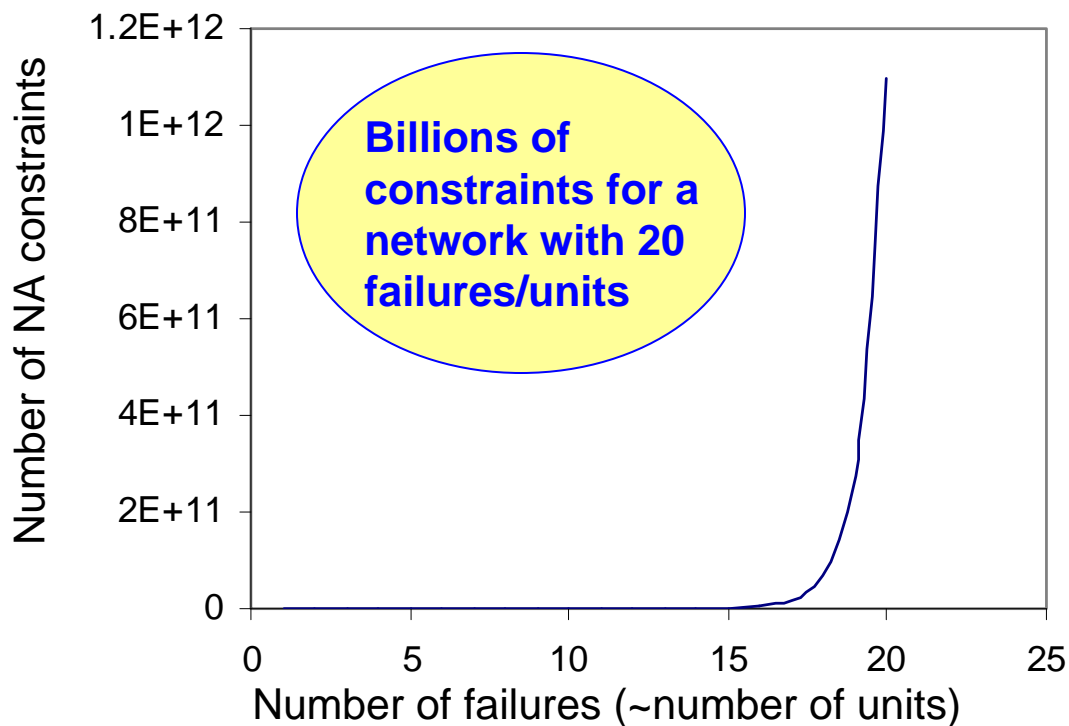
- Number of scenarios as a function of possible failures in the network:

$$scenarios = 2^n$$

$n$  = Number of possible failures

- Number of non-anticipativity constraints required

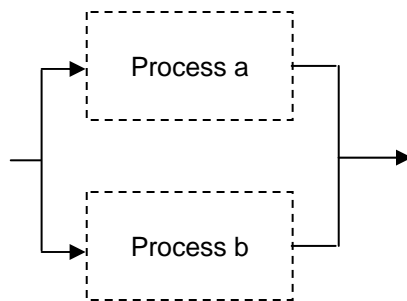
$$\# NA = s^2 = 2^{2n}$$



**Largest Mixed-integer**  
(continuous and discrete variables) problems can involve a **few million constraints**

**Basic idea: If design variables are fixed there is NO need for NA constraints**

For a *superstructure* with two parallel redundant units we have 4 scenarios:



Scenario	Process A	Process B
1	Functional	Functional
2	Failure	Functional
3	Functional	Failure
4	Failure	Failure

and two NA constraints\*

$$f^{s=1} \leq f^{s=2} + \alpha(y_1, y_2)$$

$$f^{s=1} \geq f^{s=2} - \alpha(y_1, y_2)$$

**Basic idea: If design variables are fixed there is NO need for NA constraints**

But if the designed is fixed we need only construct the scenarios relevant for the process installed



and we don't need NA constraints

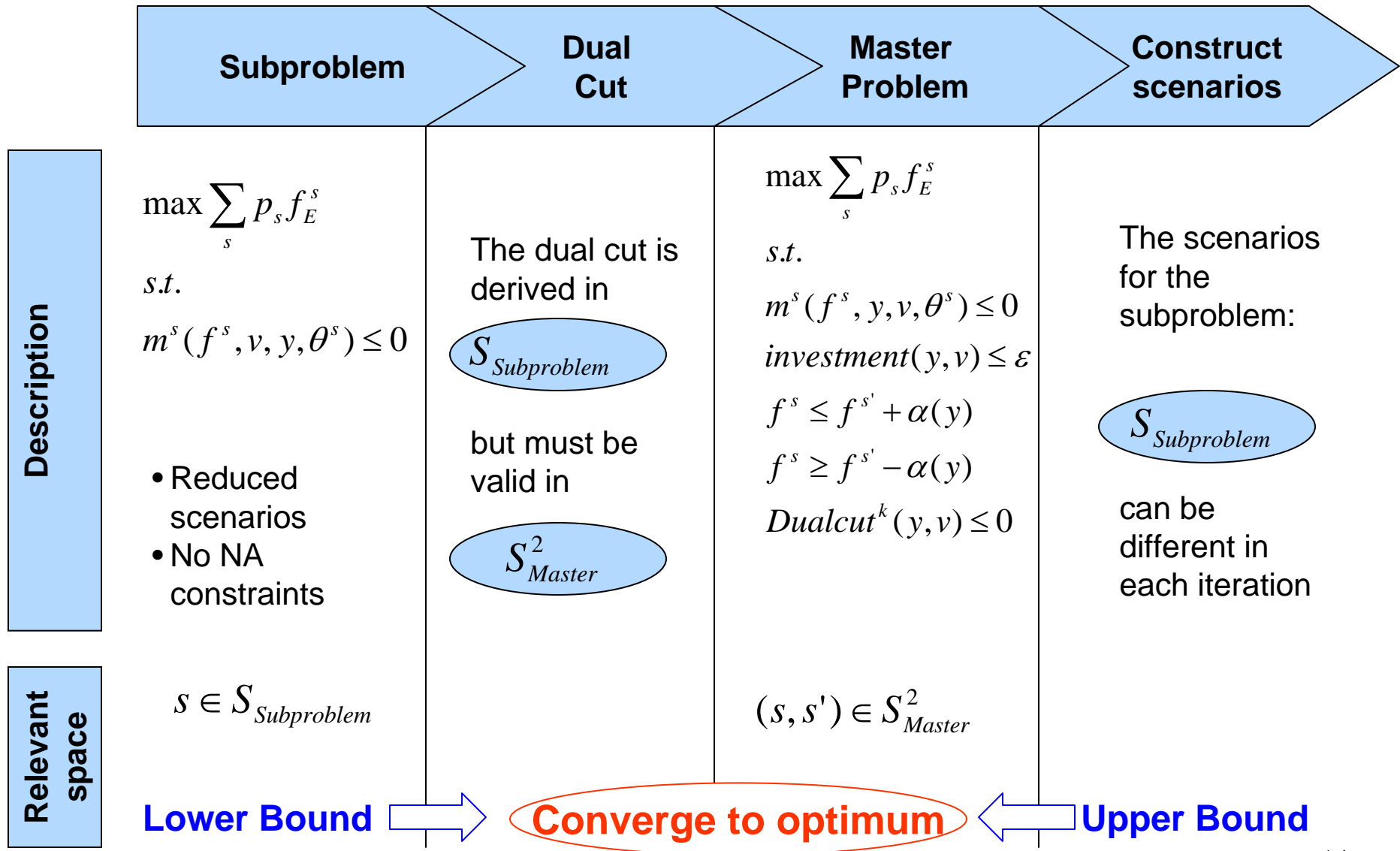
**Fewer scenarios, no NA constraints:  
Problem smaller by orders of magnitude**

## Proposed algorithm:

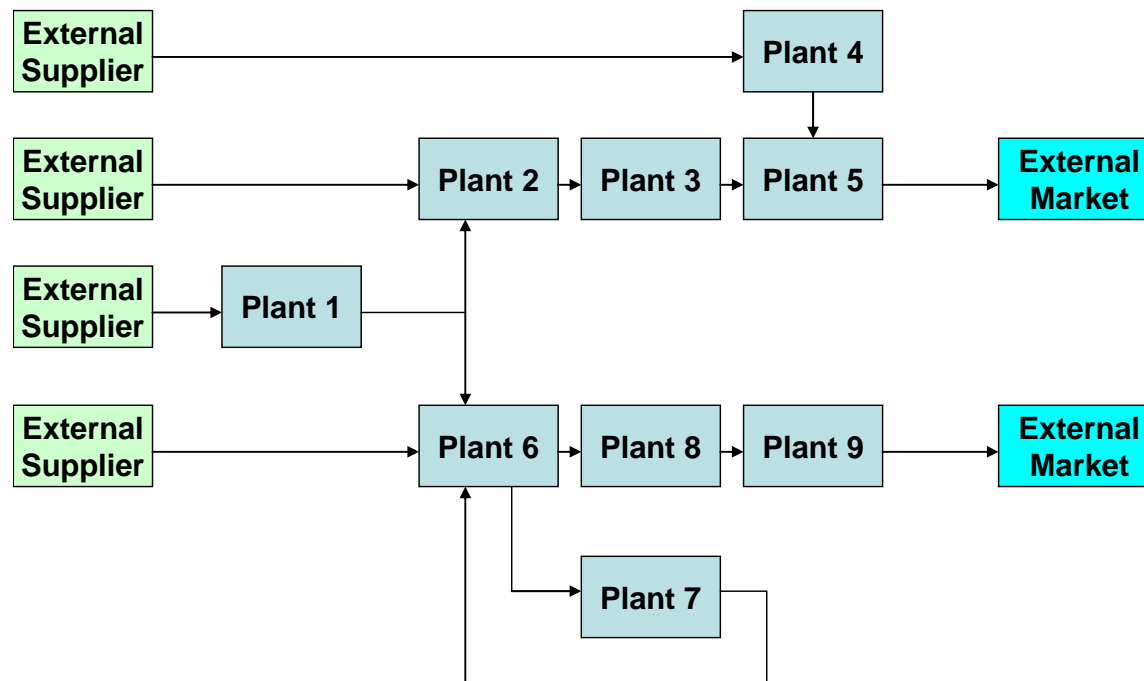
1. Fix design variables  $y, v$
2. Construct only the scenarios relevant for the processes included in the design
3. Optimize the network for the given design
4. Use a different trial value for  $y$  and  $v$

Add dual cut between steps 3.  
and 4.

The resulting algorithm is equivalent to  
**Benders Decomposition**



## Case study provided by Dow

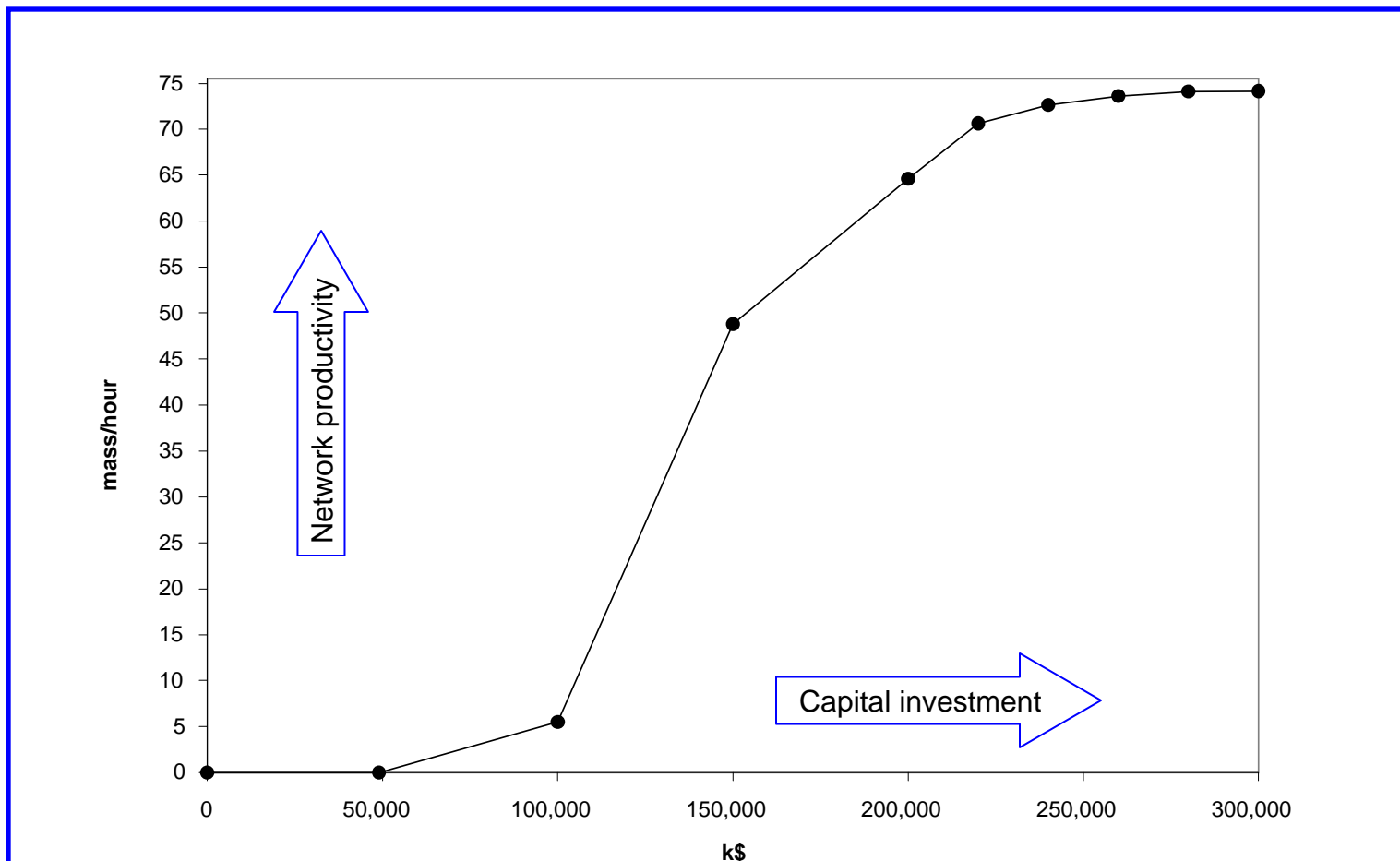


- Real integrated process called a product “envelope”
- 1000 failure scenarios were included in the problem formulation
- Work station (2G RAM) is not able to generate the model in GAMS



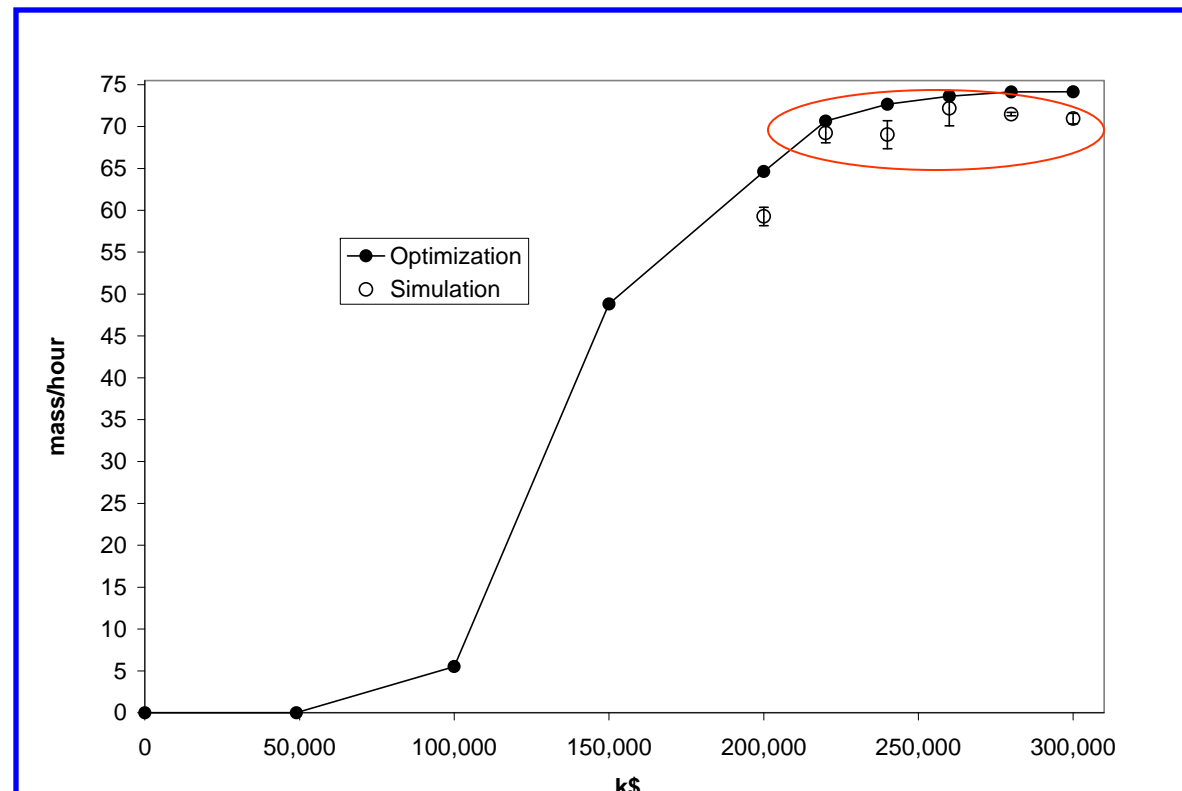
## An industrial case study illustrates the impact of using the proposed algorithm (2/2)

- Problem cannot be solved in workstation (2G RAM) due to insufficient memory
- A complete Pareto front for 10 values of available capital for investing (problem solved 10 times) can be generated in less than 6 hrs



## We validated the design obtained using the proposed decomposition technique

- Dow provided us with a simulation model that has been validated internally as an adequate representation of the real system
- We use this simulation to test the optimal designs found by the two-stage stochastic simulation



- Results of simulation validate the accuracy of the optimization model

- We formulated the design of reliable process networks under uncertainty as a two-stage stochastic program with endogenous uncertainties
- This a powerful representation that can be used to model a variety of problems that arise in industrial practice
- We proposed an algorithm to partly overcome the computational burden associated with this type of formulation
- We successfully applied this algorithm to the bi-criterion optimization of an industrial case study
- Next steps involve extending the modeling framework and solution methodology to batch and discrete manufacturing processes in multiproduct process networks