



Optimal Design of Reliable Integrated Chemical Production Site

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In collaboration with The Dow Chemical Company



**Petrochemical JV
integrated** with refinery
complex ⁽¹⁾

60 production units ⁽²⁾

**28 commodities &
specialty chemicals** ⁽²⁾

**Will be one of the largest grassroots plastics and chemicals
production facilities in the world.** ⁽¹⁾

(1) http://news.dow.com/dow_news/corporate July 12, 2007

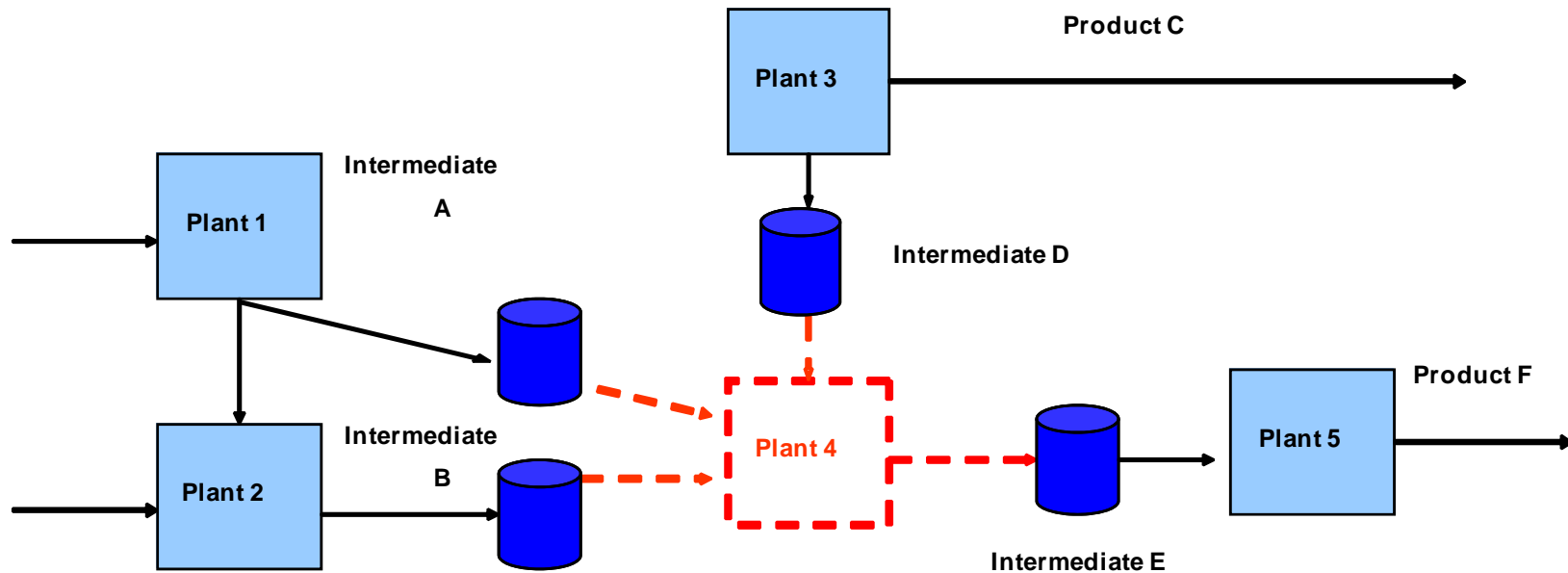
(2) <http://www.icis.com/Articles> February 2, 2010

Provide a **computational tool** that:

Optimizes the use of available capital for the design of an Integrated Site considering random equipment failures

With the objective of maximizing Service level **SL**

i.e., maximizing probability of meeting entire demand (while subject to discrete uncertainties).



Effects of intermediate storage:

Buffer of supply-demand mismatch

Material available if upstream plant fails

Upstream plant can keep running if downstream plant fails

Given

- The flowsheet of an integrated site
- A linear mass balance model
- Probability distributions of discrete uncertainties (plant failure modes).
- A cost function

Determine

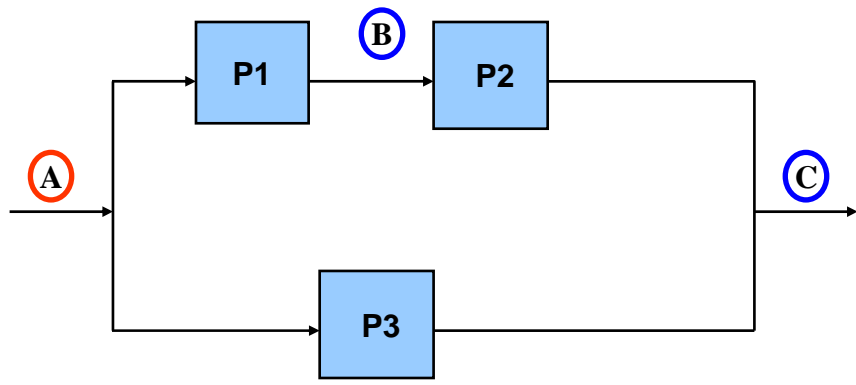
- Size of intermediate storage
- Average inventory (set point)
- Operation of intermediate storage during each failure mode scenario

Objective

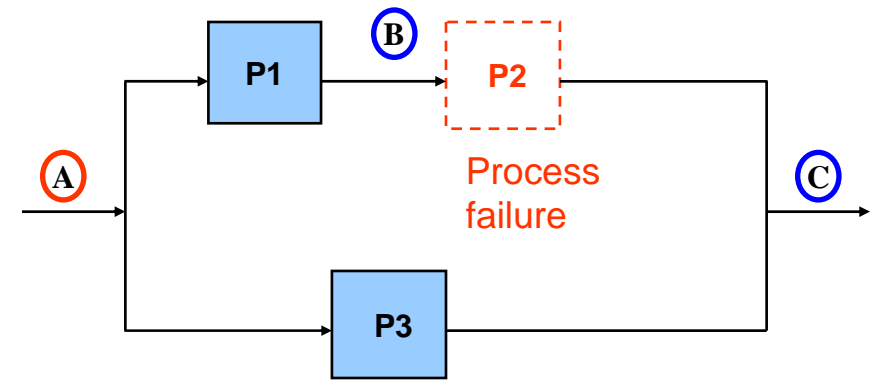
Maximize Service Level

Remark: This is a sub problem of the optimal design of reliable integrated chemical production sites

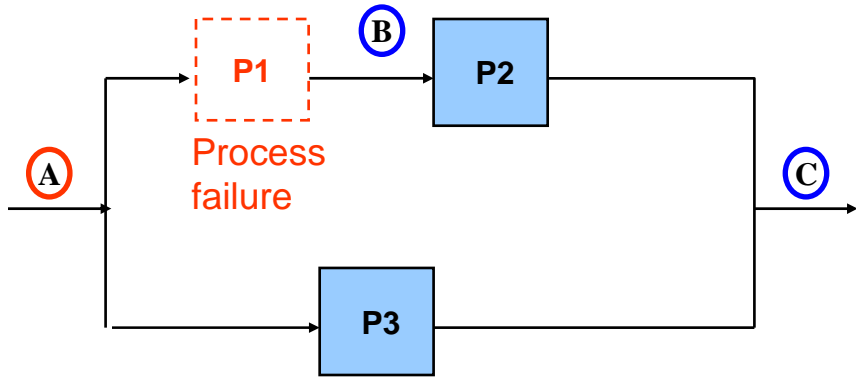
State 1



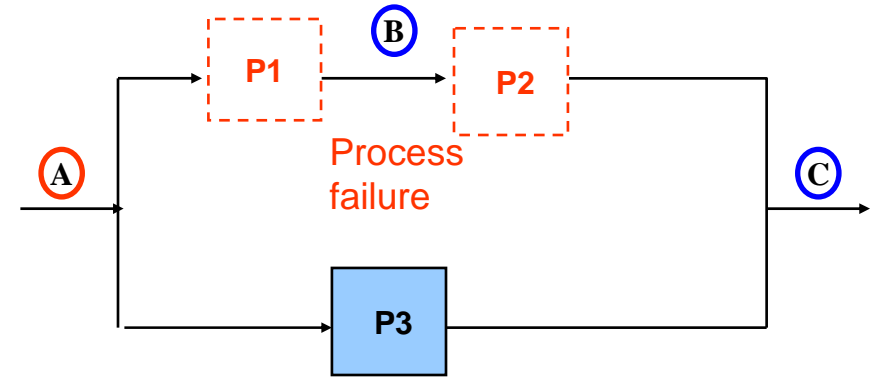
State 3



State 2



State 4

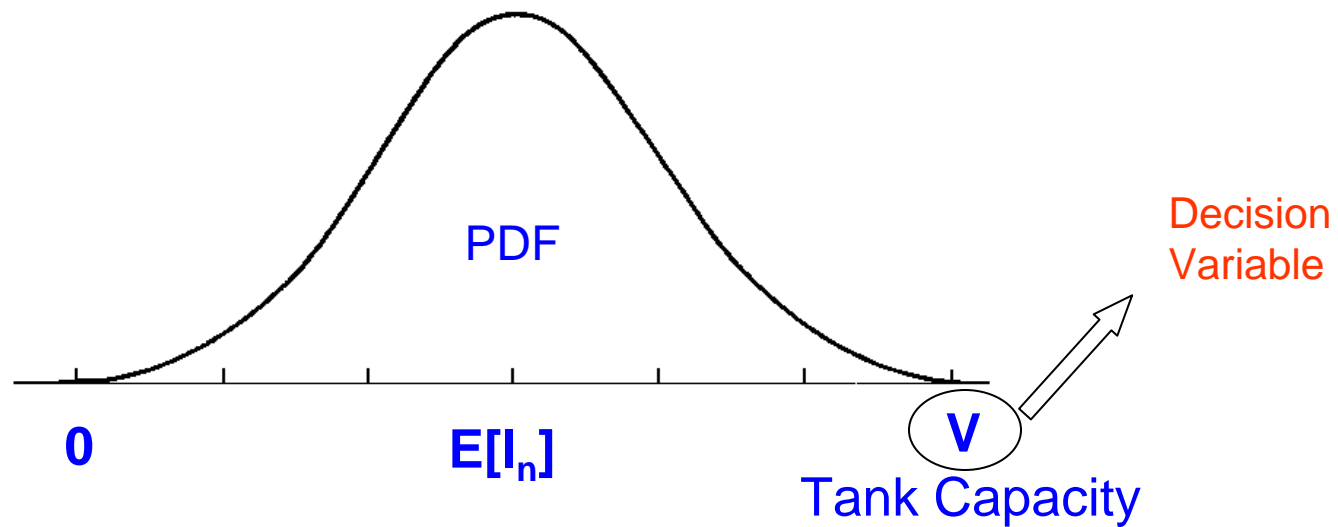
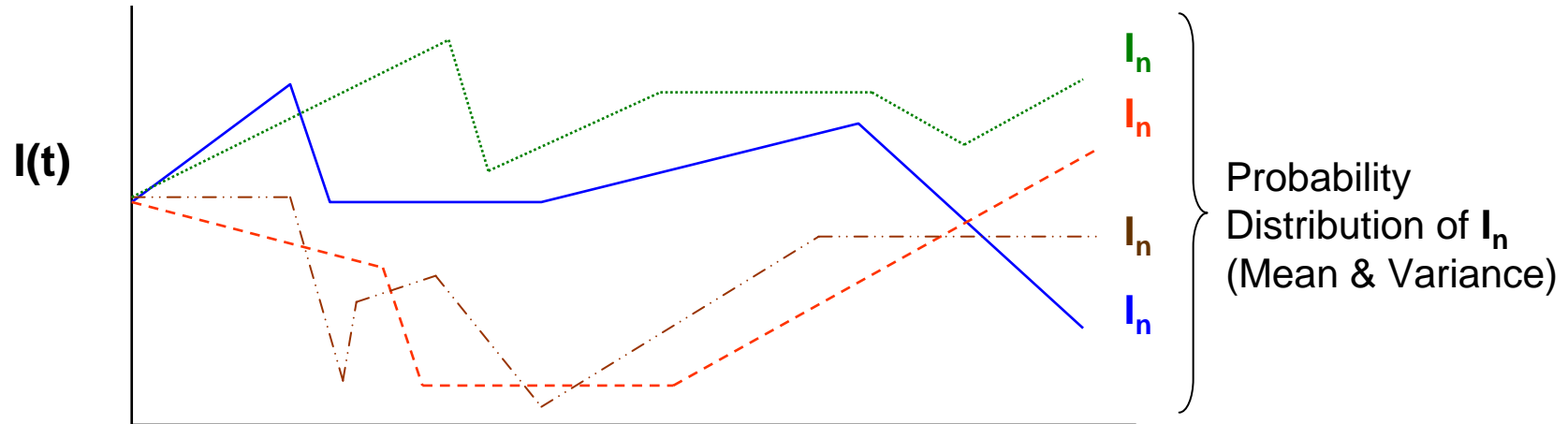


The system continuously transitions among states

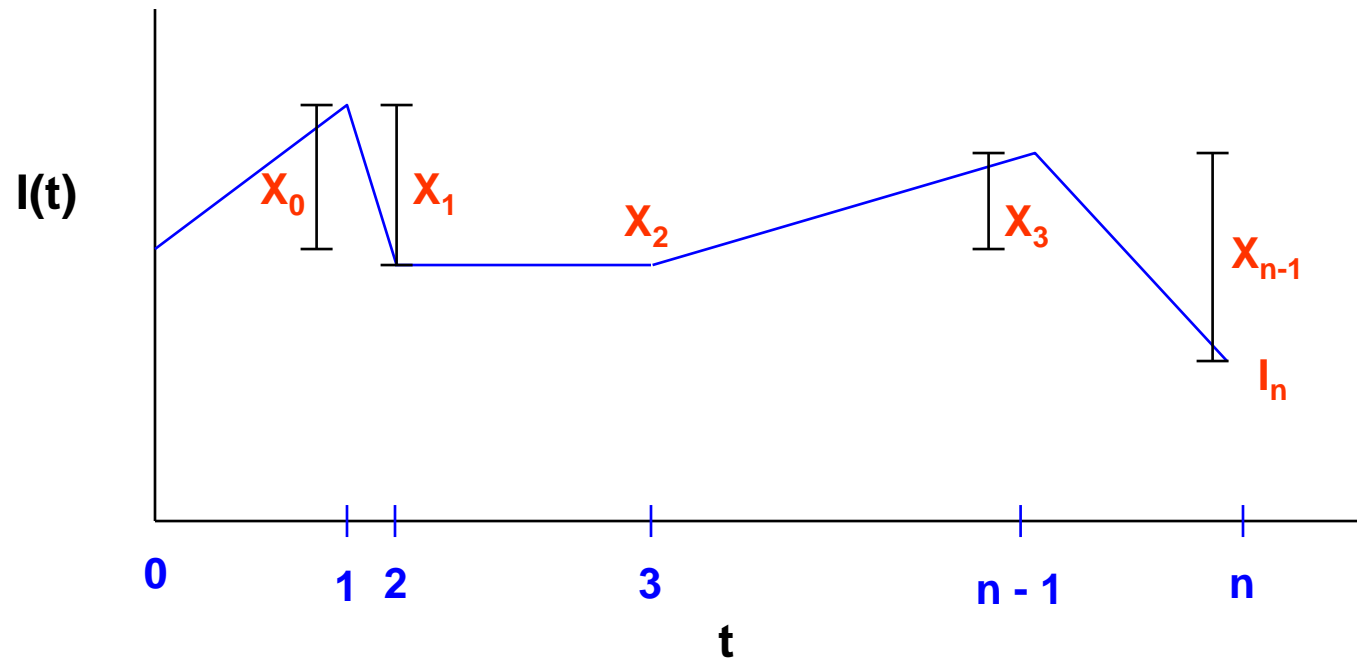
The following parameters are given for each state

- **$prob_s$ probability associated with each state**
How likely it is to find a combination of active and failed plants
- **fr_s frequency for visiting each state**
How often the system enters into a state (visits / unit time)
- **mrt_s mean residence time**
Average time spent in each state
- **vrt_s variance of residence time**
Dispersion for time spent in each state in different visits
- **tc_s cycle time**
Time interval between successive visits to a state

Each sequence of states results in a trajectory for inventory levels



Proposed approach: Describe inventory levels as a random variable



X_i := material consumed/replenished from epoch i to epoch $i+1$

X_i is a random variable

$$I_n = I_0 + \sum_{i=0}^{n-1} X_i$$

$$I_n = I_0 + \sum_{i=0}^{n-1} \delta_{s \text{ at } i} rt_{s \text{ at } i}$$

S set of discrete states

δ inventory rate

$$E[I_n] = I_0 + \sum_{i=0}^{n-1} \delta_{s \text{ at } i} E[rt_{s \text{ at } i}]$$

rt residence time

fr frequency for visiting each state

$$E[I_n] = I_0 + t \sum_{s \in S} \delta_s fr_s mrt_s$$

mrt mean residence time

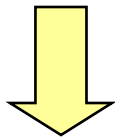
$$Var[I_n] = t \sum_{s \in S} \delta_s^2 fr_s vrt_s$$

vrt variance of residence time

fr, mrt, vrt are problem parameters

δ is a decision variable in the optimization formulation

$$E[I_n] = I_0 + t \sum_{s \in S} \delta_s fr_s mrt_s$$

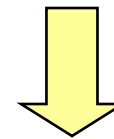


(A)
$$\sum_{s \in S} \delta_s fr_s mrt_s = 0$$

$$Var[I_n] = t \sum_{s \in S} \delta_s^2 fr_s vrt_s$$

$$\sqrt{Var[I_n]} \leq \sum_{s \in S} \delta_s \sqrt{vrt_s fr_s t}$$

Overestimation
of the variance

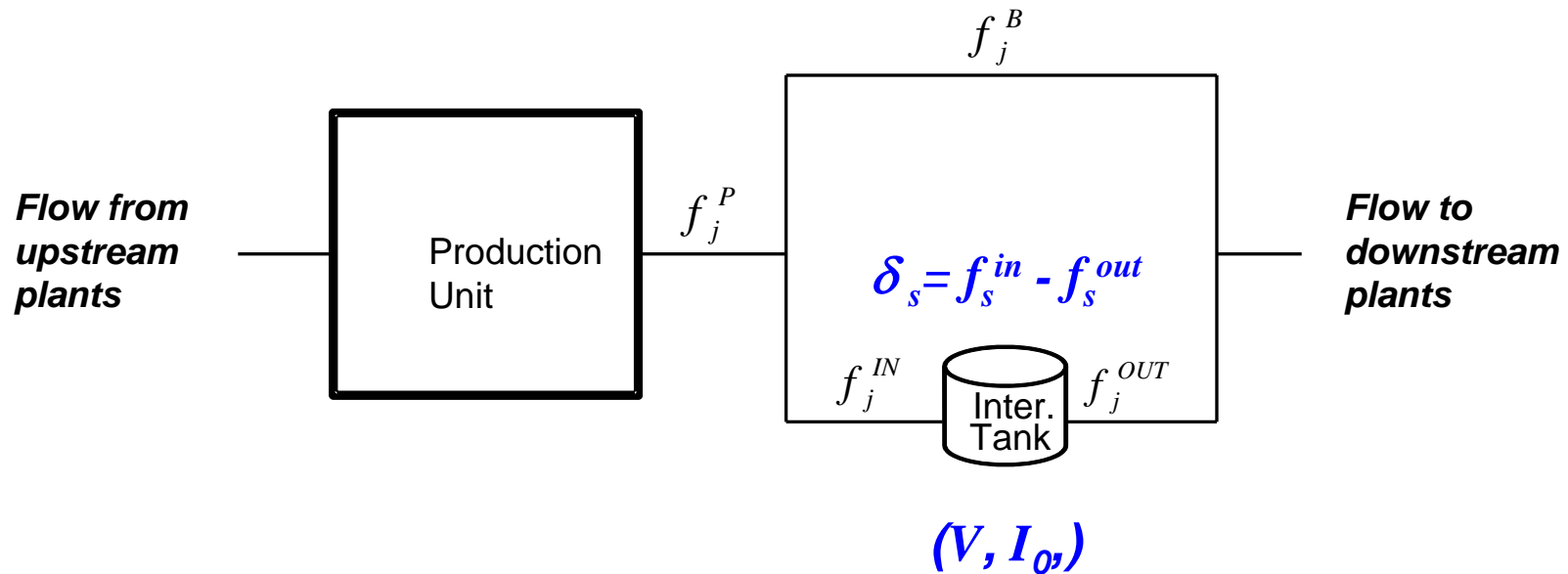


(B)
$$I_0 + \tau \sum_{s \in S} \delta_s \sqrt{vrt_s fr_s t} \leq V$$

$$I_0 - \tau \sum_{s \in S} \delta_s \sqrt{vrt_s fr_s t} \geq 0$$

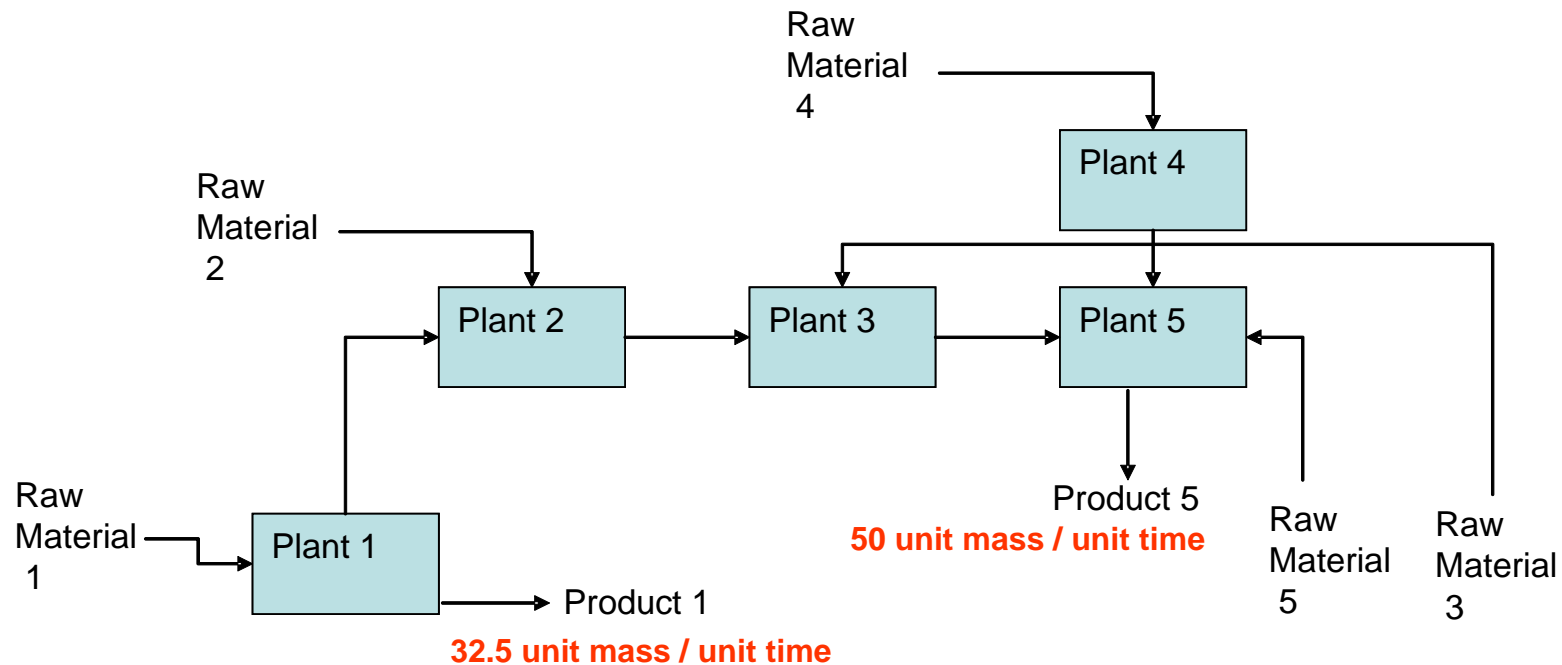
(A) and (B) are constraints in the optimization model

Each plant in the integrated is represented by a module



$$\begin{aligned} \max \quad & \text{Service Level}(V, I_0, \delta_s) \\ \text{s.t} \quad & \text{Capital Investment} \leq \varepsilon \\ & + \text{rest of model constraints} \end{aligned}$$

s/S: index/set of discrete states



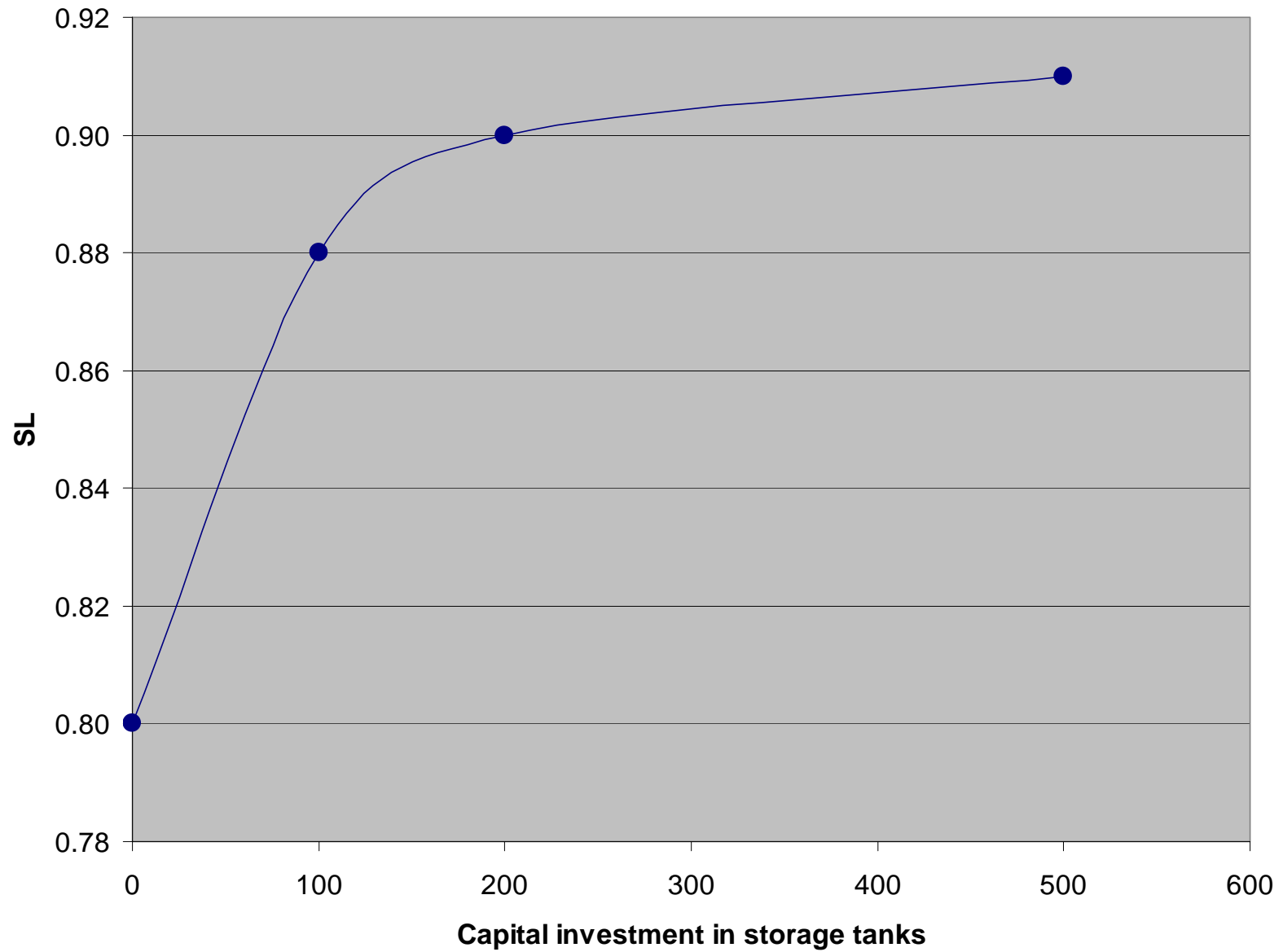
Multiple failure modes in each plant

Aprox. **160 discrete states** (combinations of failure modes)

5-plant example is a subset of 9-plant real industrial case study

Size of MILP: 0.5 M constraints; 0.2 M variables; 160 discrete variables

Example: Effect of intermediate storage



Example: Effect of intermediate storage

| Available Capital for storage tanks * | Tank 1 [mass units] | | Tank 2 [mass units] | |
|--|---------------------|---------------|---------------------|---------------|
| | Volume | Average Level | Volume | Average Level |
| 0 k | - | - | - | - |
| 100 k | - | - | 2465 | 1232 |
| 200 k | 4760 | 2380 | 7500 | 3750 |
| 500 k | 15000 | 7500 | 7500 | 3750 |

| Tank 3 [mass units] | | Tank 4 [mass units] | | Service Level |
|---------------------|---------------|---------------------|---------------|---------------|
| Volume | Average Level | Volume | Average Level | |
| - | - | - | - | 0.80 |
| 7500 | 3750 | - | - | 0.88 |
| 7500 | 3750 | 56 | 28 | 0.90 |
| 7500 | 3750 | 5000 | 316 | 0.91 |

Total CPU time : 240 s

* 1 unit of volume = 10 monetary units

- **The full problem of optimal design of integrated sites also includes process superstructure and variable production capacities.**

Paper submitted to Computers & ChemE

- **We are developing an algorithm for large-scale problems.**

Based on Benders Decomposition

10^6 total variables & constraints; 10^3 discrete variables

- **We have verified our results using state of the art discrete event simulation tools.**

ExtendSim from *Imagine That! Inc.*