Optimal Design of Reliable Integrated Chemical Production Site

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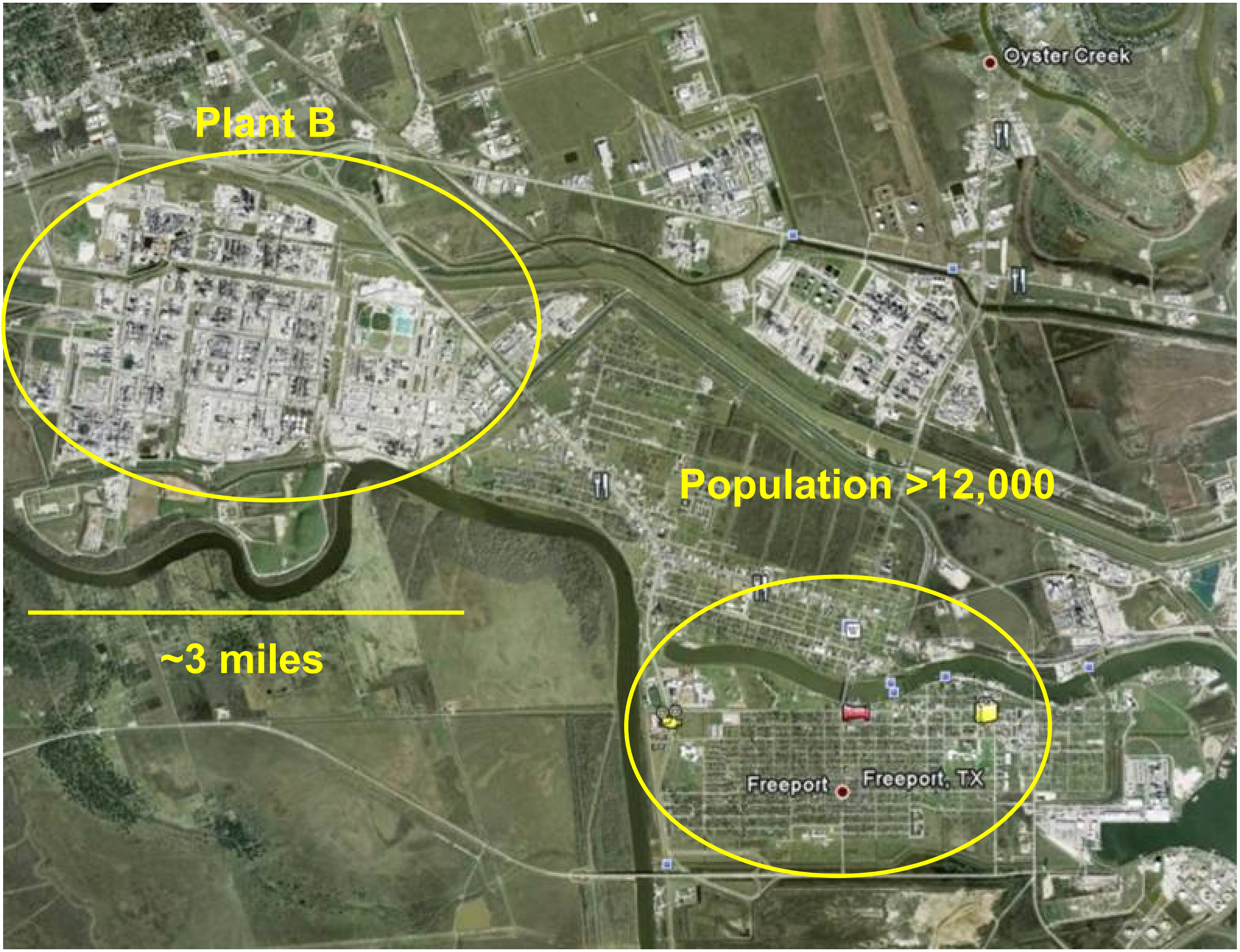
Motivation

Large scale chemical companies operate integrated chemical complexes for the manufacture of many products

Dow's Texas Operations (huge chemical complex) manufactures 21% of Dow products sold globally

Contents of this slide based on: Wassick , J. M. *Computers & Chemical Engineering* , 2009

Motivation


Oyster Creek
Plant B
Population >12,000
~3 miles
Freeport
Freeport, TX

Motivation

These type of sites should deliver their target production capacity in spite of uncertain events (plant outages)

There is a need to develop systematic design methods to optimize the reliability and flexibility of integrated sites

Contents of this slide based on: Wassick , J. M. *Computers & Chemical Engineering* , 2009

Goal

Provide a computational tool that:

Optimizes the use of available capital for the design of an Integrated Site

With the objective of:

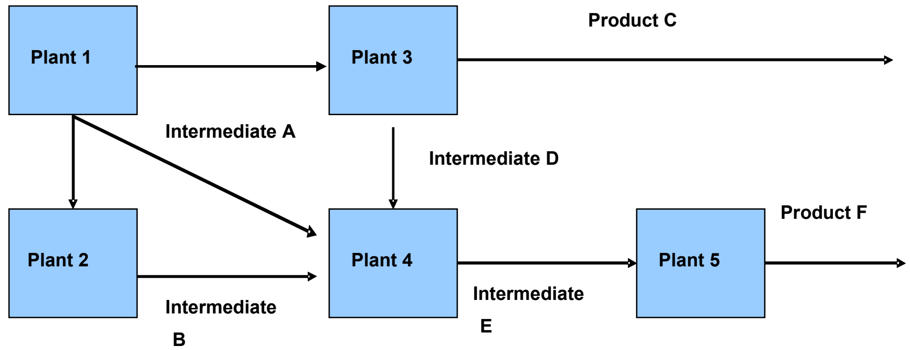
Maximizing the probability of meeting operational targets consistently

An integrated site (IS) is a large network of processes

Design challenge: Different uncertainties affect an IS

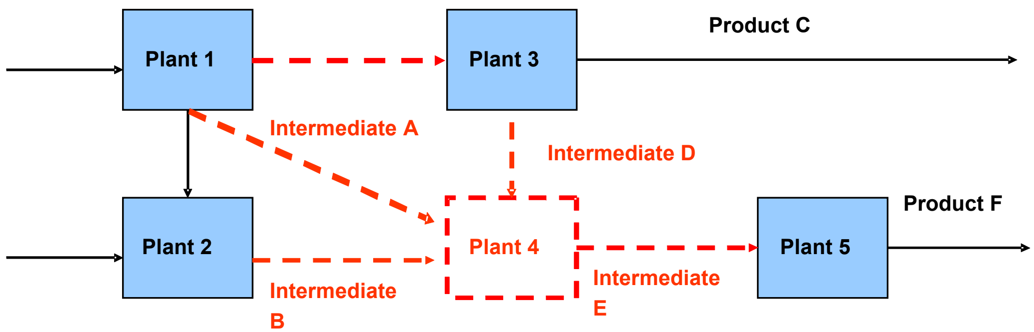
Continuous uncertainties

Uncertain Supply



Uncertain demand

Discrete uncertain events



Plant failure

E(SF) useful metric. Interpret as Service Level

Expected stochastic flexibility E(SF)[1]

Probabilistic measure of a system's ability to tolerate discrete and continuous uncertainties

Service level SL[2]

Probability of meeting entire demand
(while subject to discrete and continuous uncertainties).

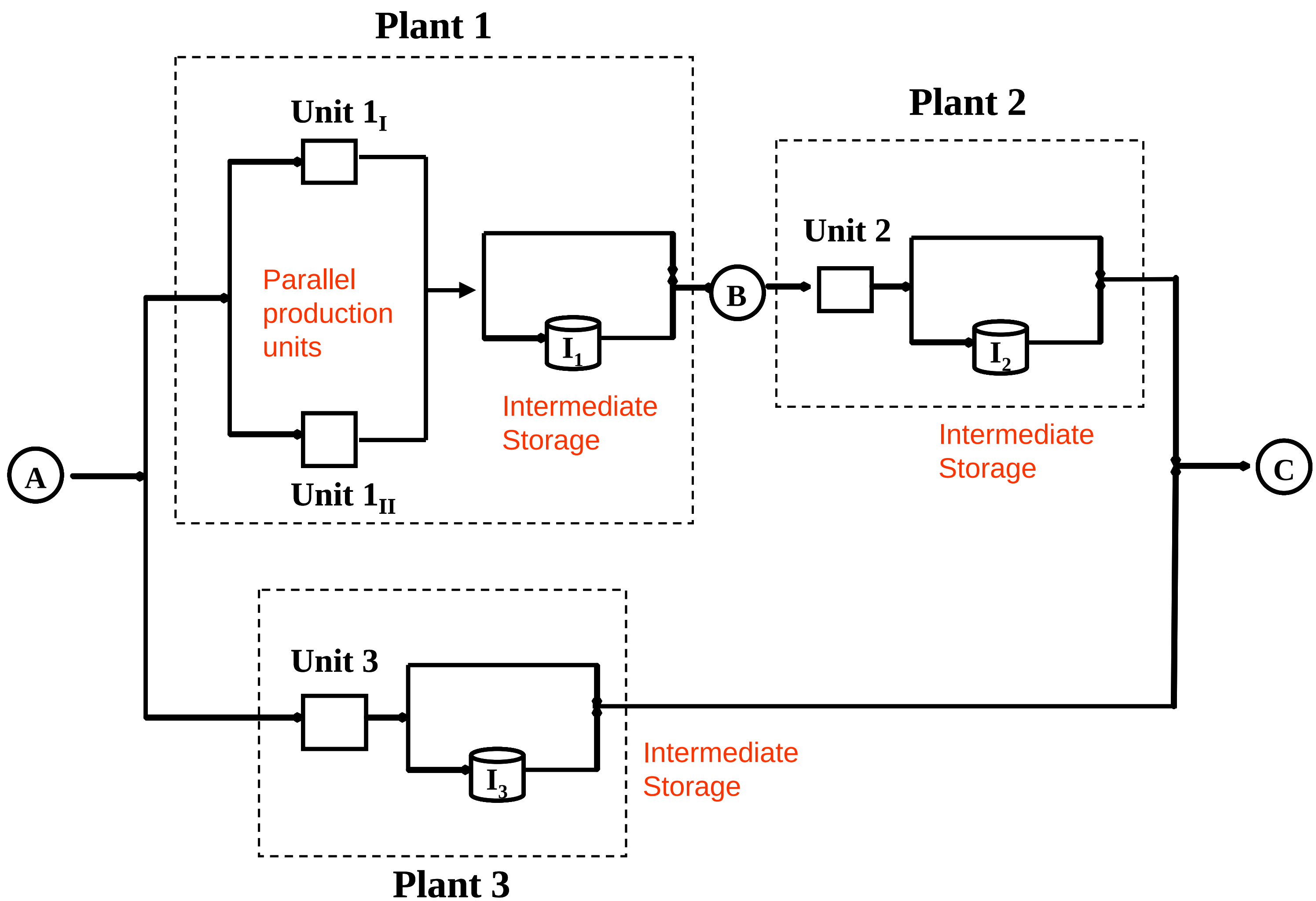
<u>In this problem</u>

E(SF) ≈ Service Level (SL)

(1) Straub D. A., I. E. Grossmann. *Computers & Chemical Engineering* , 1990

(2) Gupta A., C. D. Maranas. *Computers & Chemical Engineering* , 2003

Parallel production units, intermediate storage and spare production capacity increase service levels



But require extra capital investment

Problem statement

Given	Determine
•The superstructure of an integrated site	• The selection of production units
•Materials consumed and produced.	• Total production capacity of each unit
•Unit ratios (yield coefficients)	
•Supply and demand probability distributions	• Size of intermediate storage
•Reliability data	• Average inventory (set point)
•A cost function	

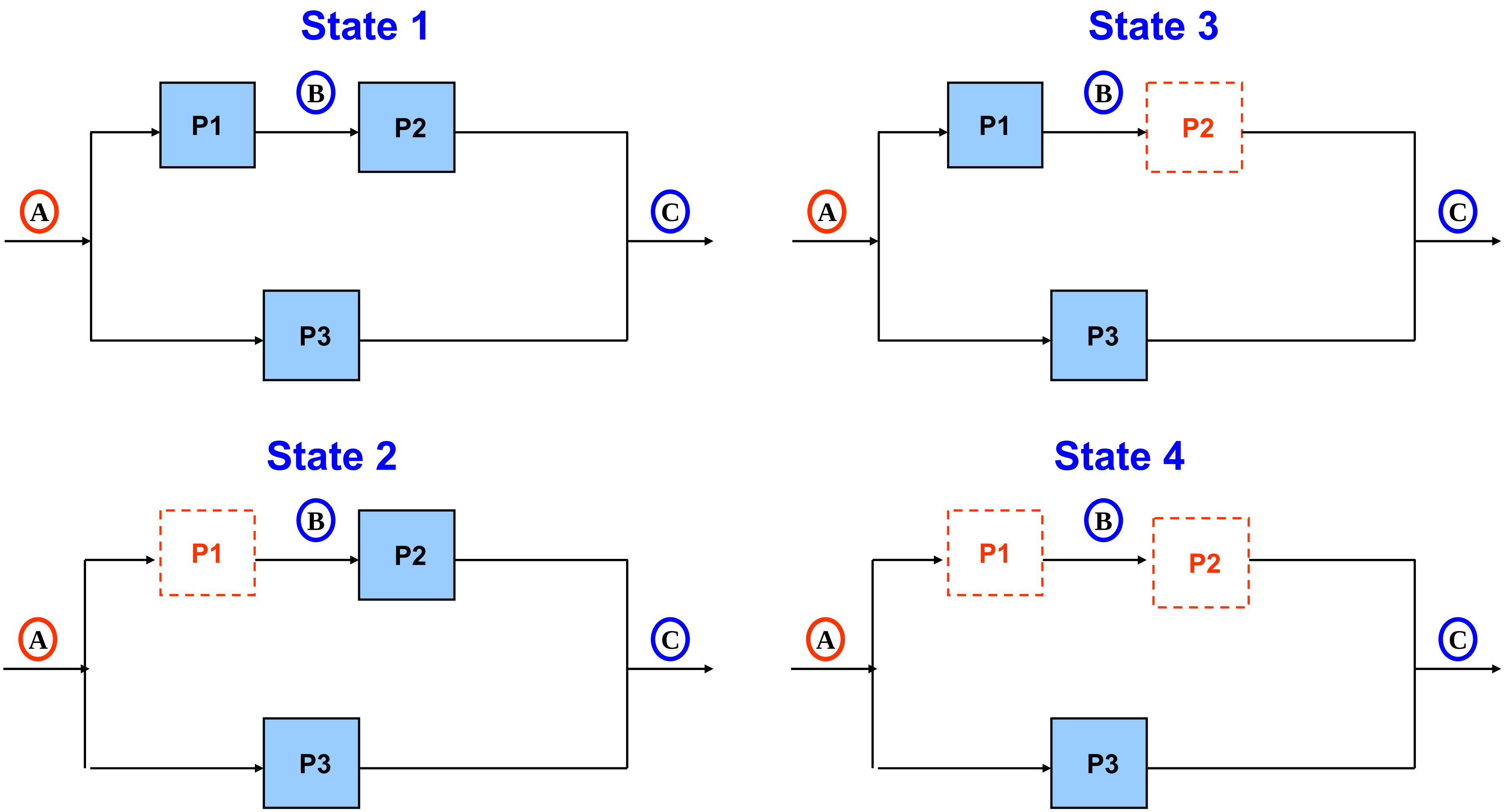
Objectives

Maximize Service Level

Minimize capital investment

Bi-criterion optimization model

Our modeling approach uses a state space representation



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

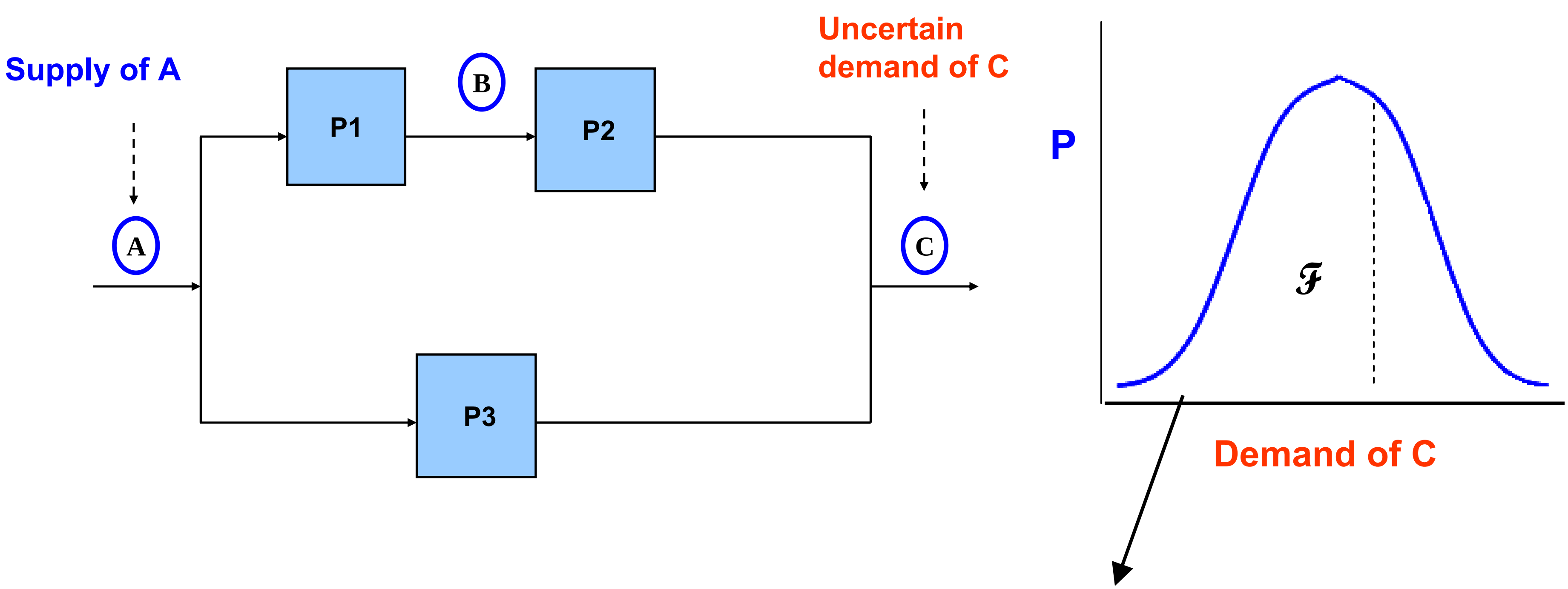
- ***fr_s*** **frequency for visiting each state**
  How often the system enters into a state (visits / unit time)

- ***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

Stochastic flexibility: Ability to operate under cont. uncertainties

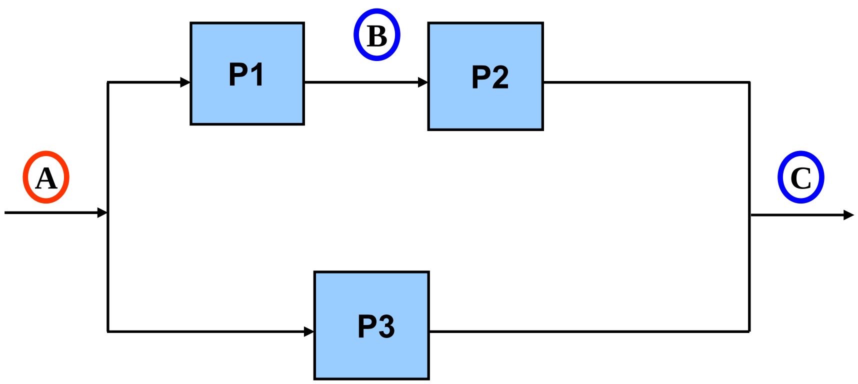


Stochastic Flexibility (SF) represents area of feasible operation under probability distribution

e.g. SF = 0.67

Expected Stochastic Flexibility E(SF) ≈ Service Level

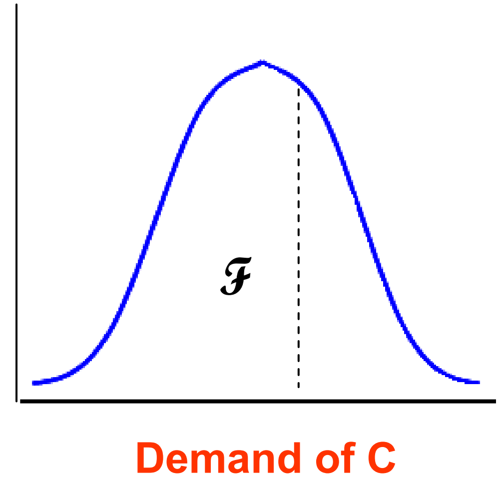
State 1



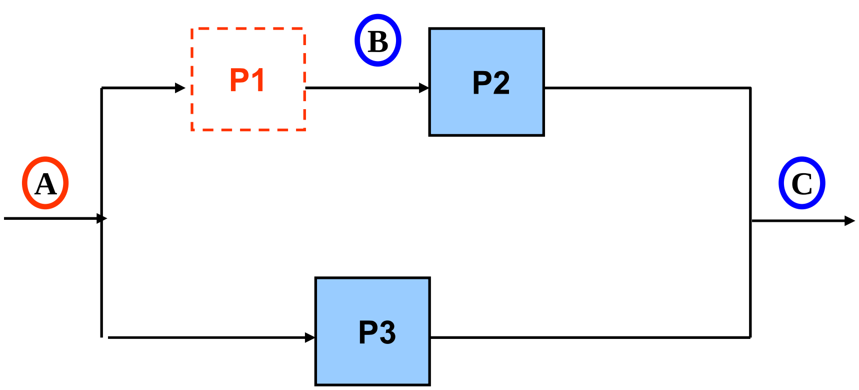
Define:

prob$_1$: probability of finding system in State 1

SF$_1$: Stochastic Flexibility in State 1

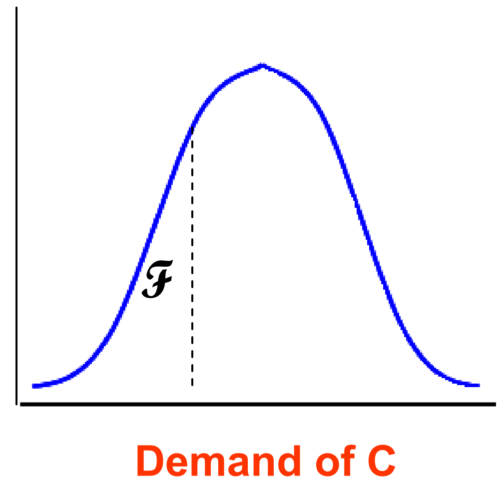


State 2



prob$_2$: probability of finding system in State 2

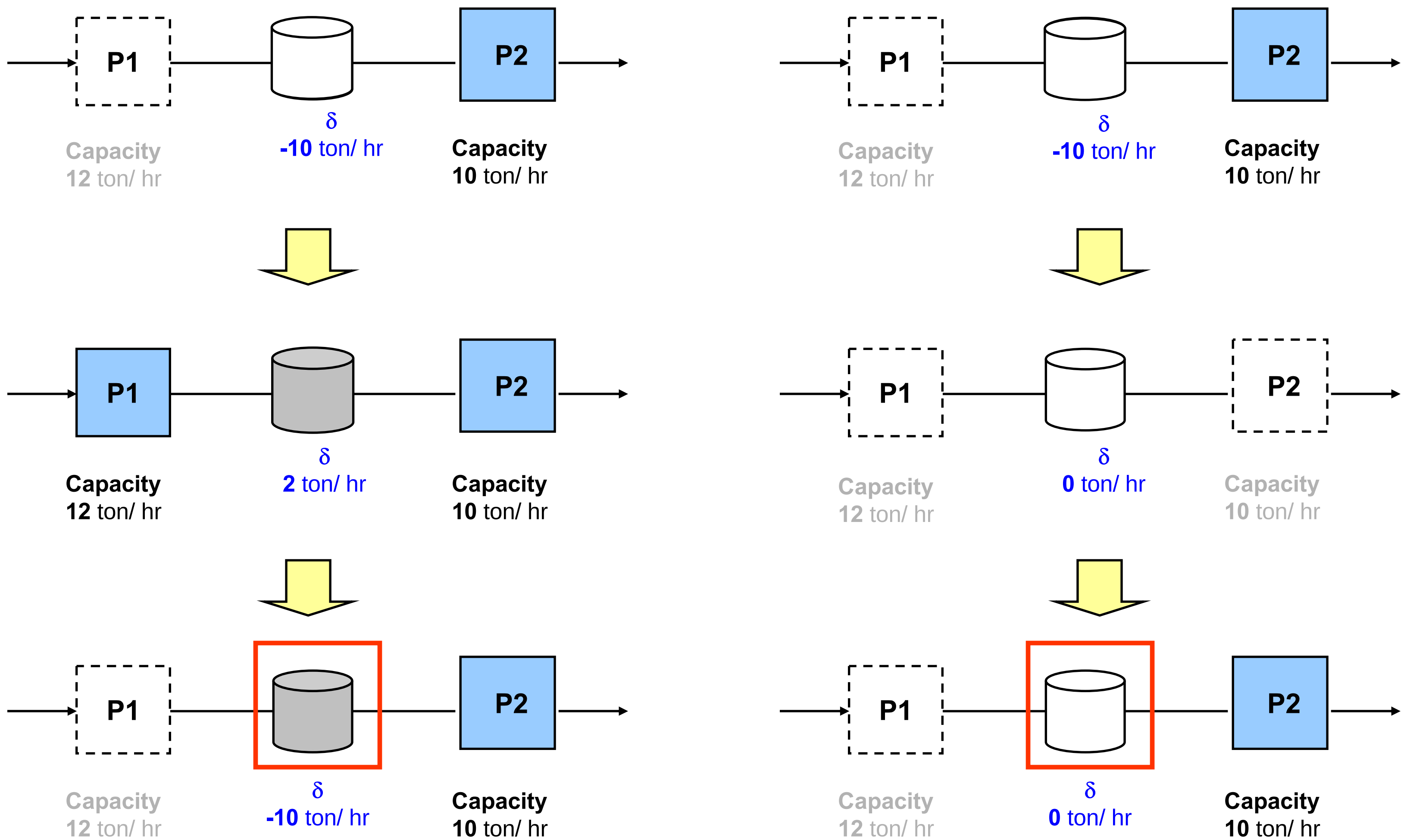
SF$_2$: Stochastic Flexibility in State 2



Service Level ≈ E(SF)

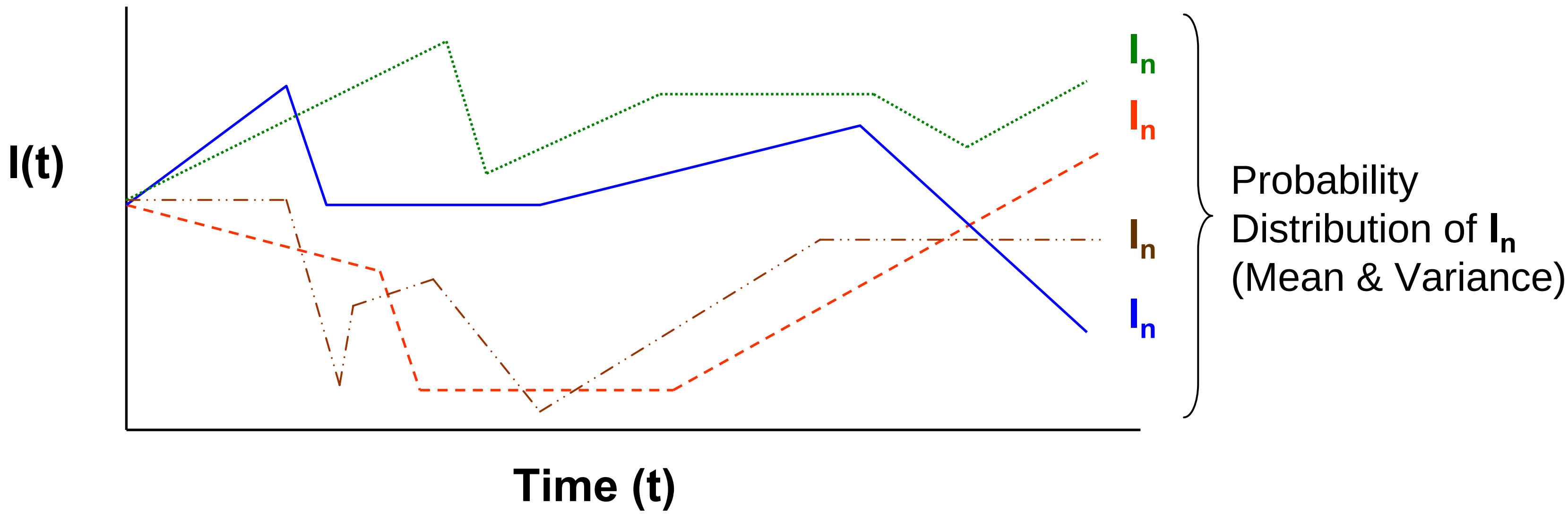
$$= prob_1 SF_1 + prob_2 SF_2$$

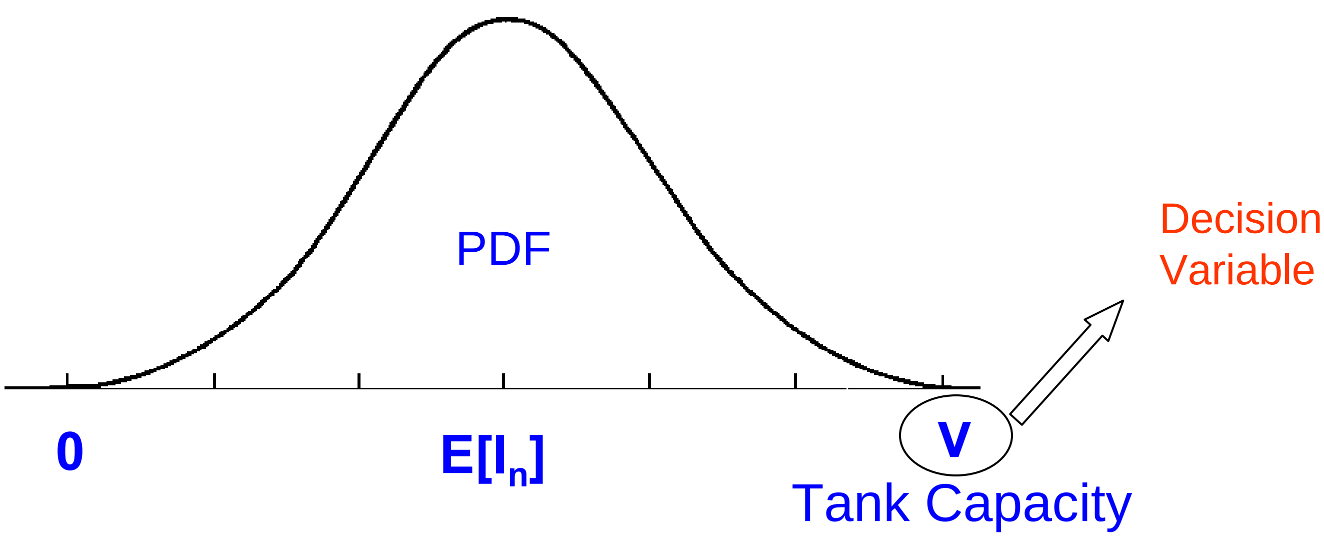
Intermediate storage is affected by the sequence and duration of discrete states



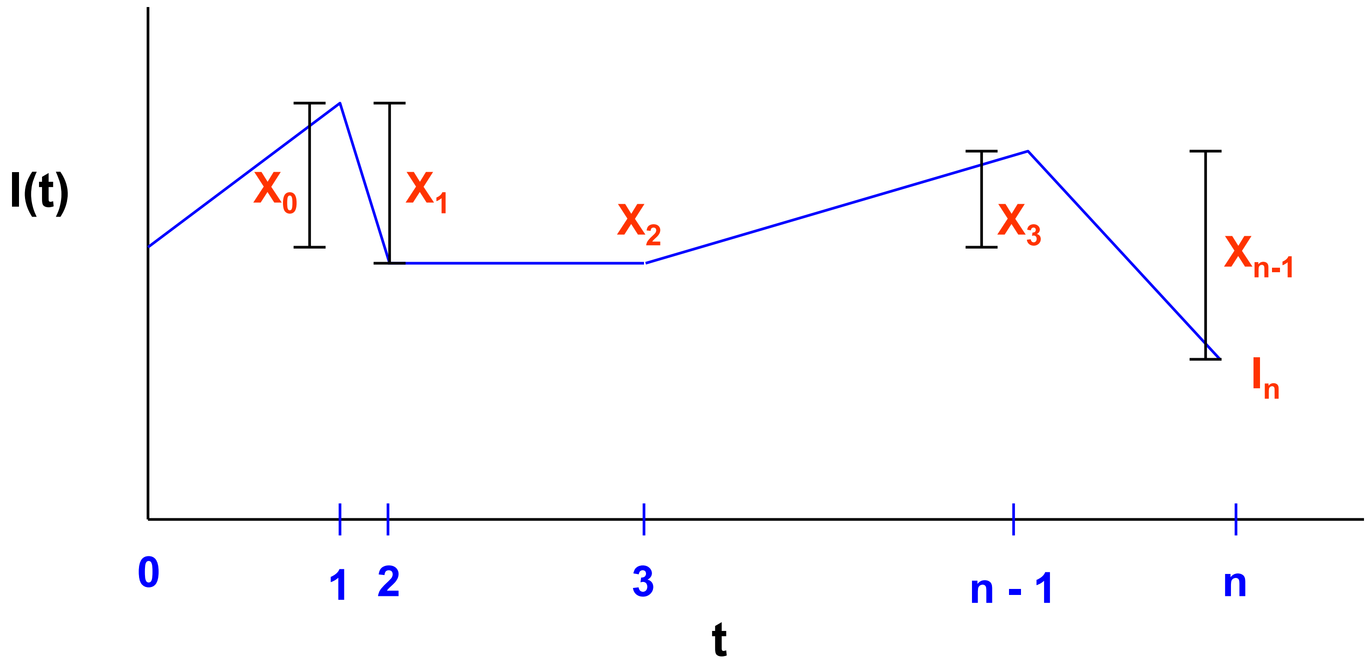
The exact inventory levels depend on the sequence of system states

Each sequence of events results in a trajectory for inventory levels





Proposed approach: Describe inventory levels as a random variable



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

Calculations of inventory set point and required tank size

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

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

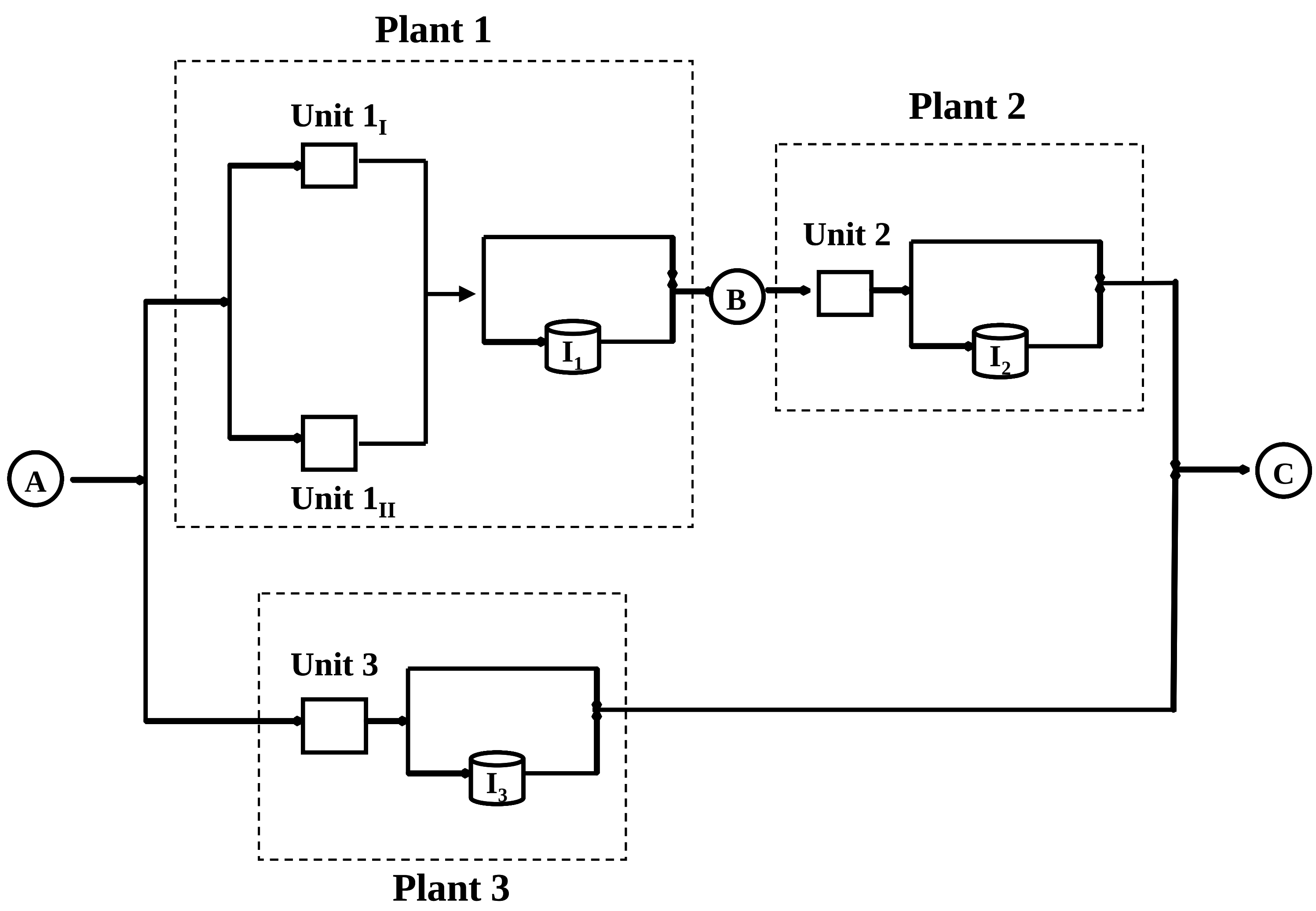
⇓

$$E[I_n] + \tau \sum_{s \in S} \delta_s \sqrt{vrt_s \, fr_s t} \leq V$$

$$E[I_n] - \tau \sum_{s \in S} \delta_s \sqrt{vrt_s \, fr_s t} \geq 0$$

S	**set of discrete states**
δ	**inventory rate**
rt	**residence time**
fr	**frequency for visiting each state**
mrt	**mean residence time**
vrt	**variance of residence time**

A case study adapted from Straub & Grossmann (1990)



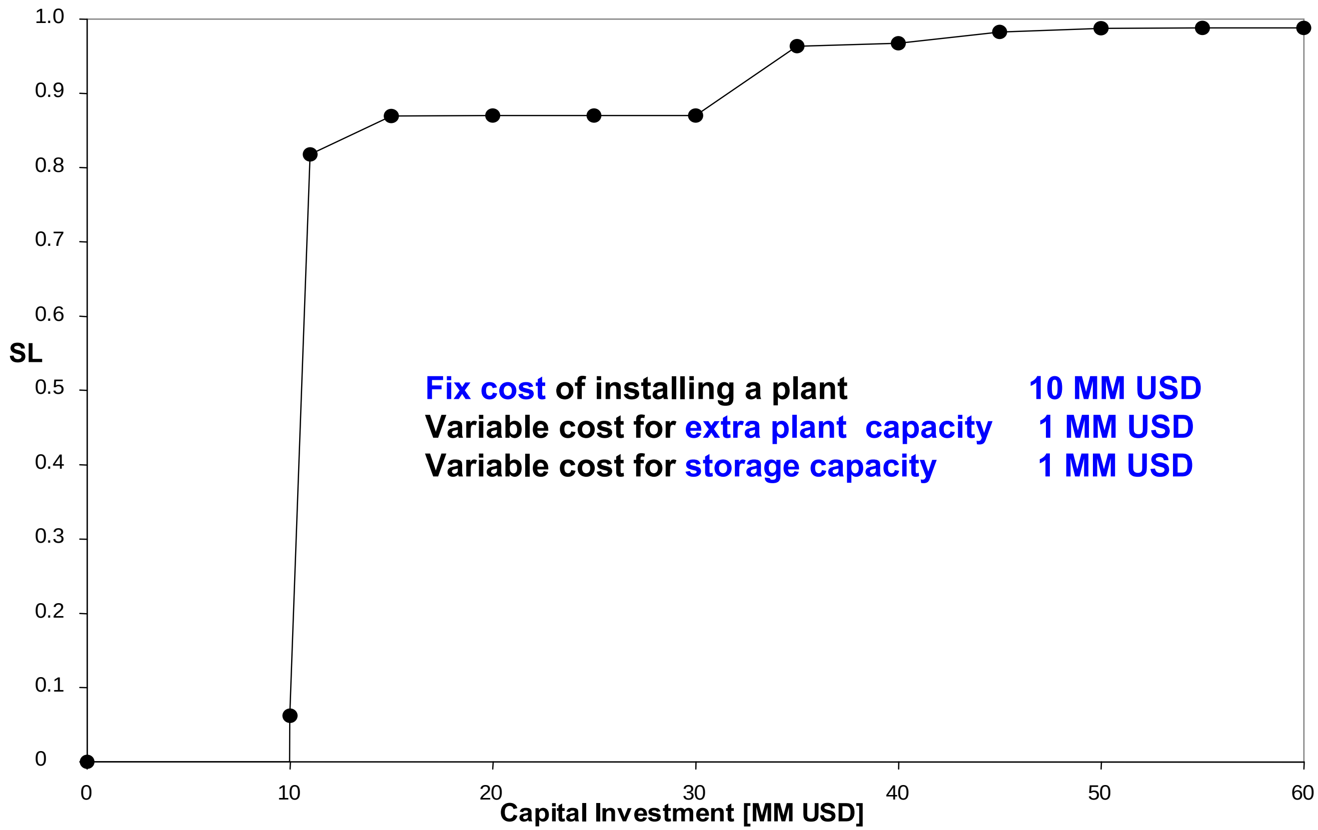
Problem parameters

Input (given) data

Supply of A [10^3 *ton / day*]	Mean = 12	Stand. Dev = 1		
Demand of C [10^3 *ton / day*]	Mean = 7	Stand. Dev = 1		
Probability of operation	*Unit* 1_I 0.95	*Unit* 1_{II} 0.95	*Unit 2* 0.92	*Unit 3* 0.87
Mass balance coefficient	α_{1I}=0.92	α_{1II}=0.92	α_2=0.85	α_3=0.75
Base capacity [10^3 *ton / day*]	5	5	7	9
Mean time to repair [*day*]	0.25	0.25	0.25	0.25
Mean time to failure [*day*]	4.75	4.75	2.88	1.67

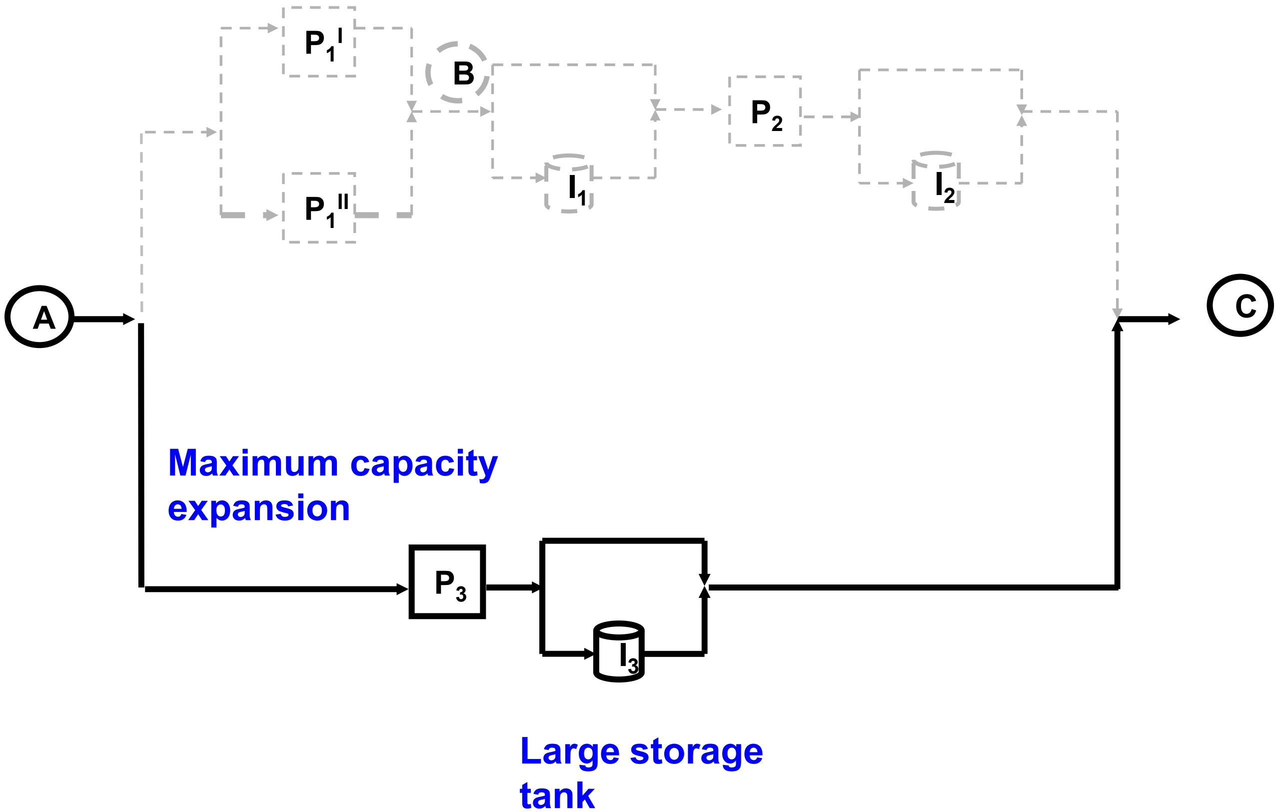
Results: set of Pareto-optimal solutions

$$\max \quad \textit{Service Level}$$
$$s.t \quad \textit{Capital Investment} \leq \varepsilon$$
$$+ \textit{rest of model constraints}$$



Results: Details of some of the designs in the Pareto-optimal set

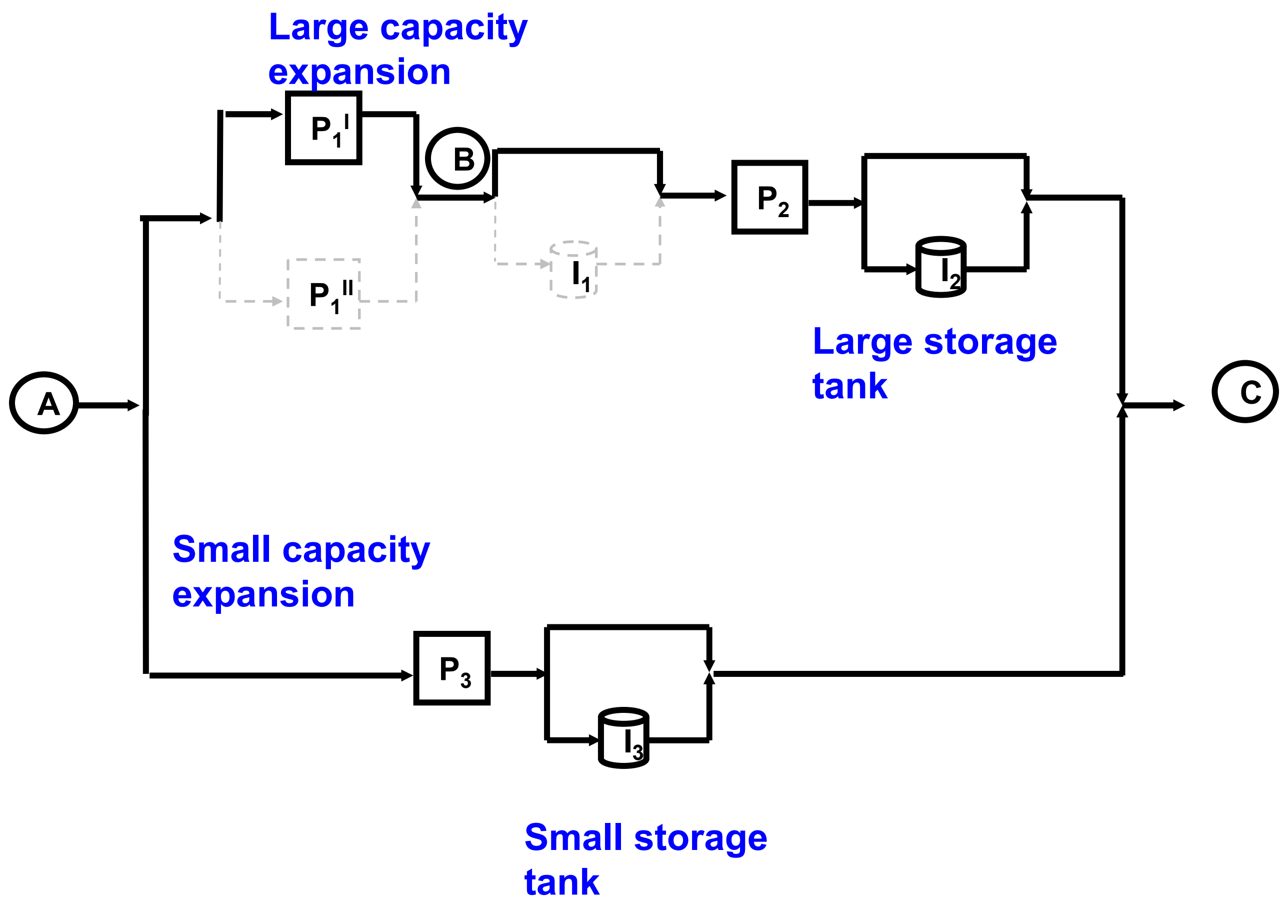
Capital Investment =25 MM USD
SL = 0.87



Results: Details of some of the designs in the Pareto-optimal set

Capital Investment =35 MM USD

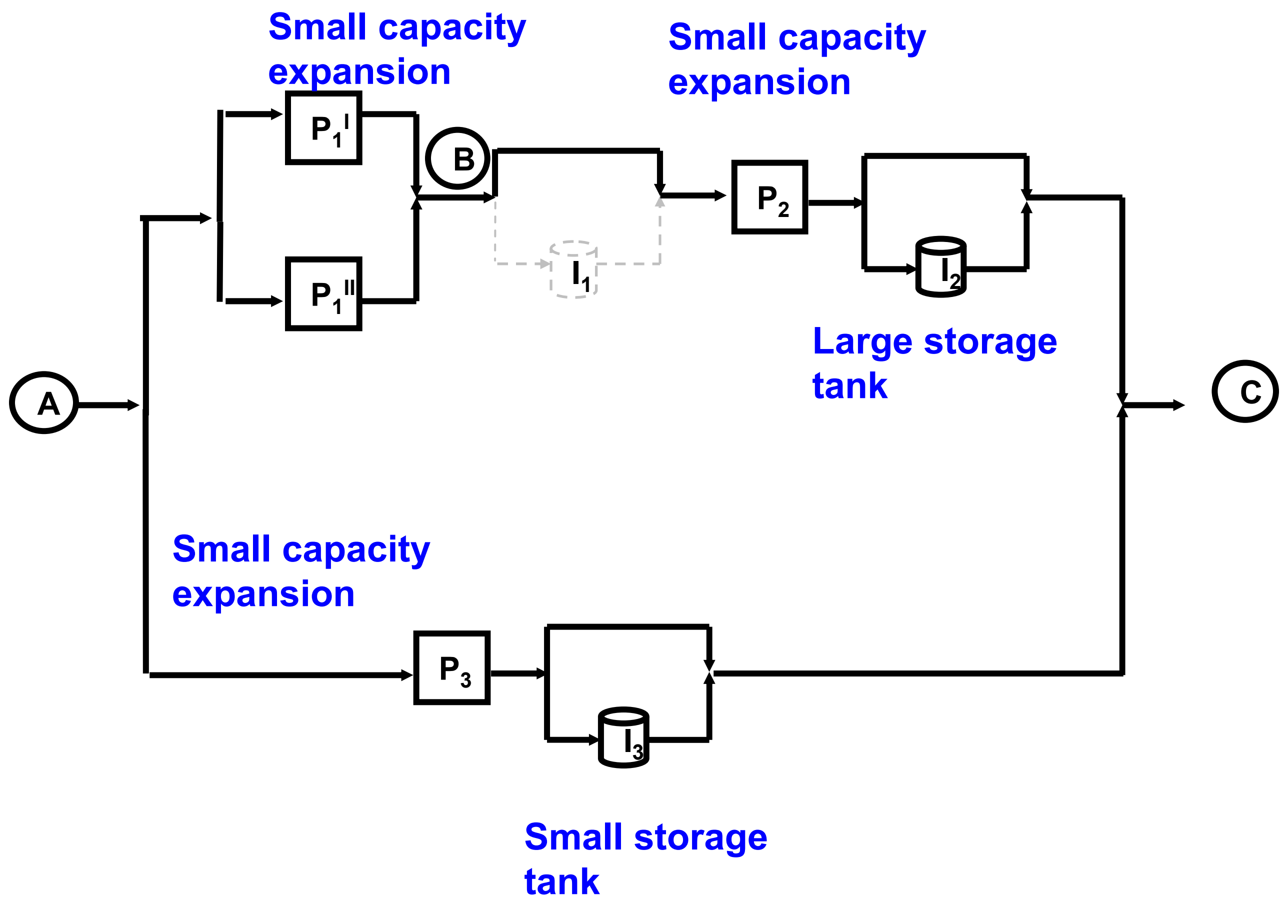
SL = 0.96



Results: Details of some of the designs in the Pareto-optimal set

Capital Investment =45 MM USD

SL = 0.98



Summarizing: current capabilities and limitation of the proposed approach

- Mathematical formulation captures the main trade-off between performance (service level) and capital investment.
- The effect of intermediate storage on service level is included.
- A superstructure approach is used for integrated site design
- Algorithmic techniques are required to solve large-scale problems
- Extend model to include schedule maintenance

Acknowledgements

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