MultiBatch DS: Professional MultiBatch Distillation Systems for multiple column configurations, multiple operating modes, multiple fractions, and multiple products -- with multiple levels of models

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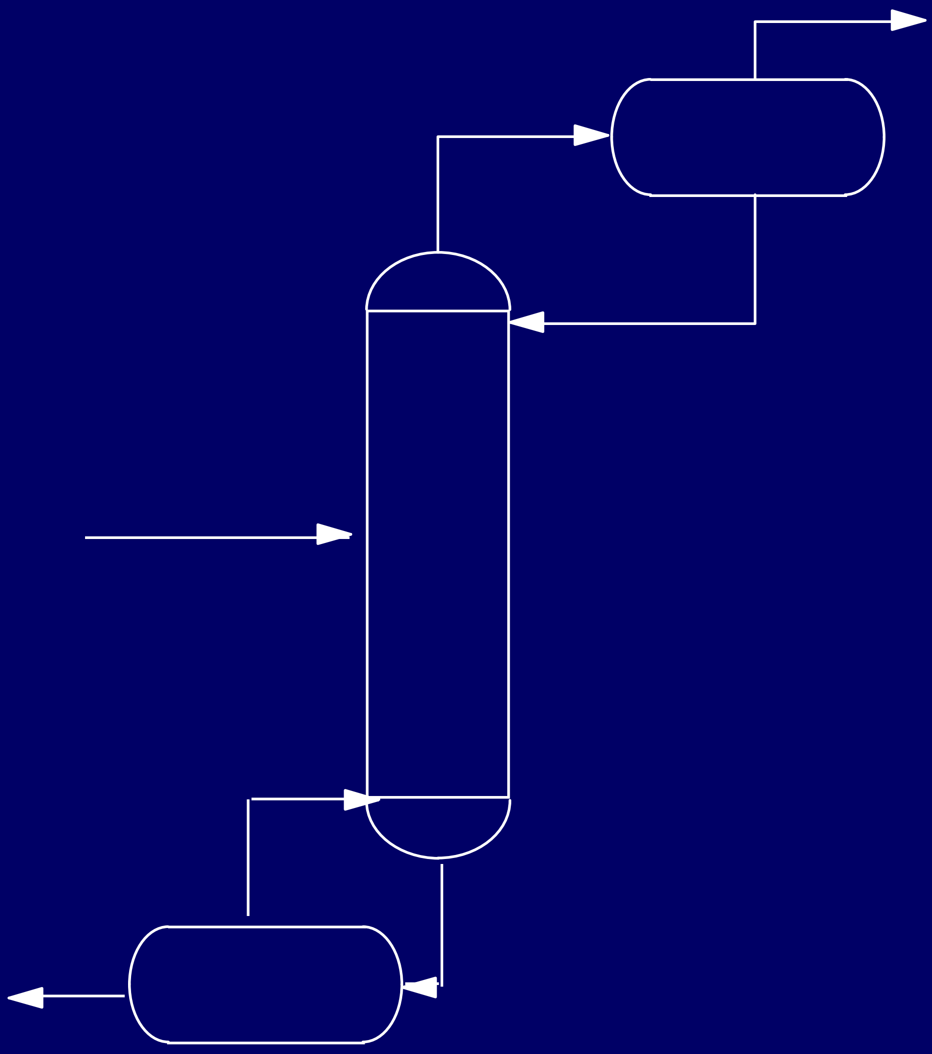
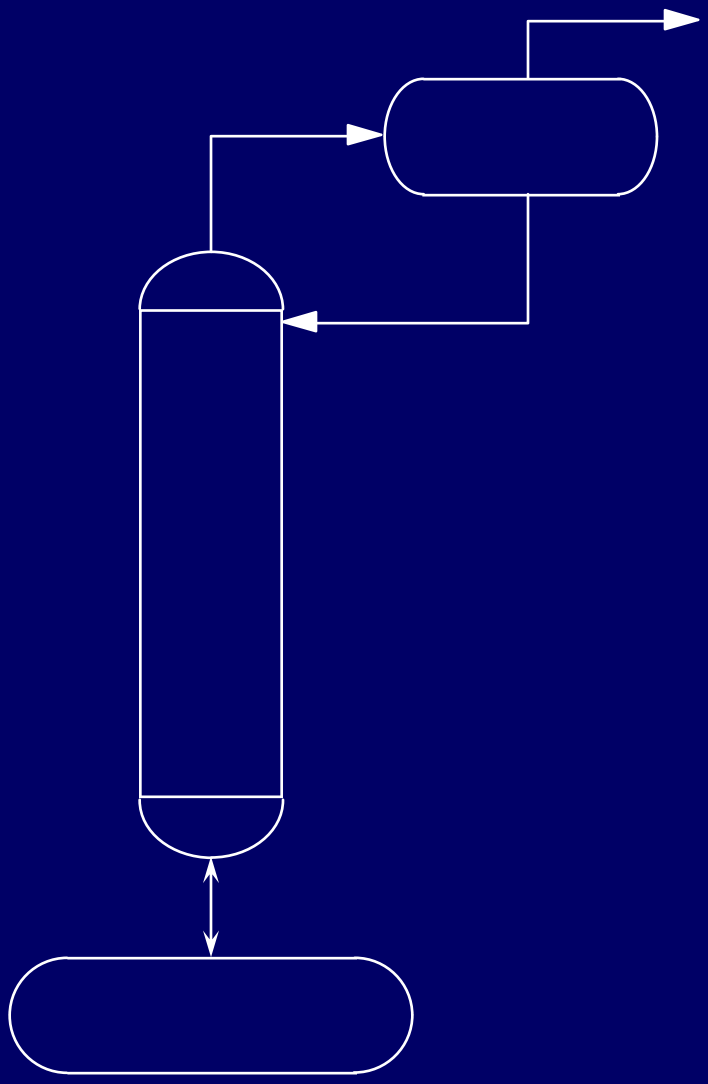
Why Batch Distillation?

Unsteady State Nature of Batch Distillation

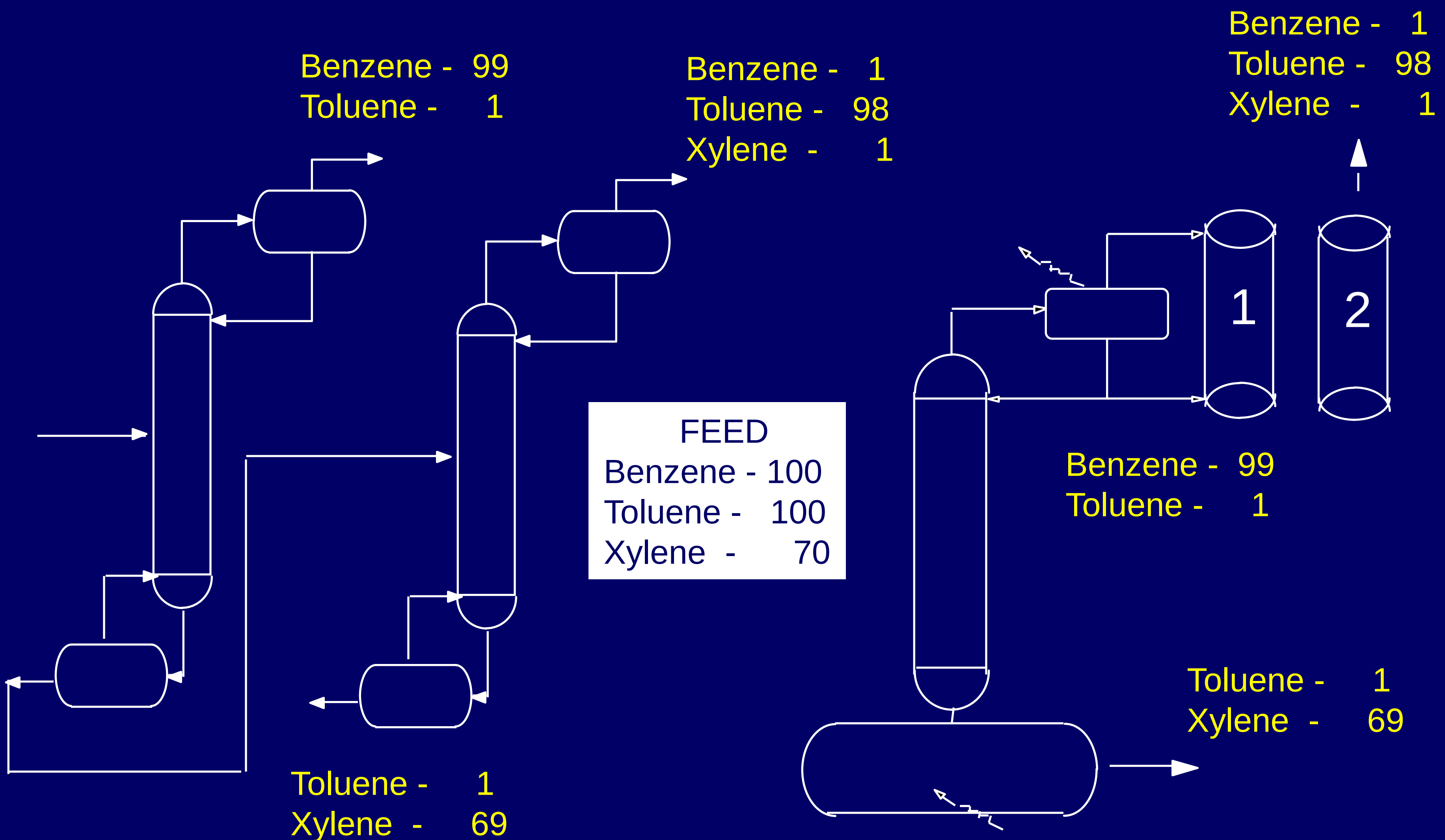


Continuous Distillation

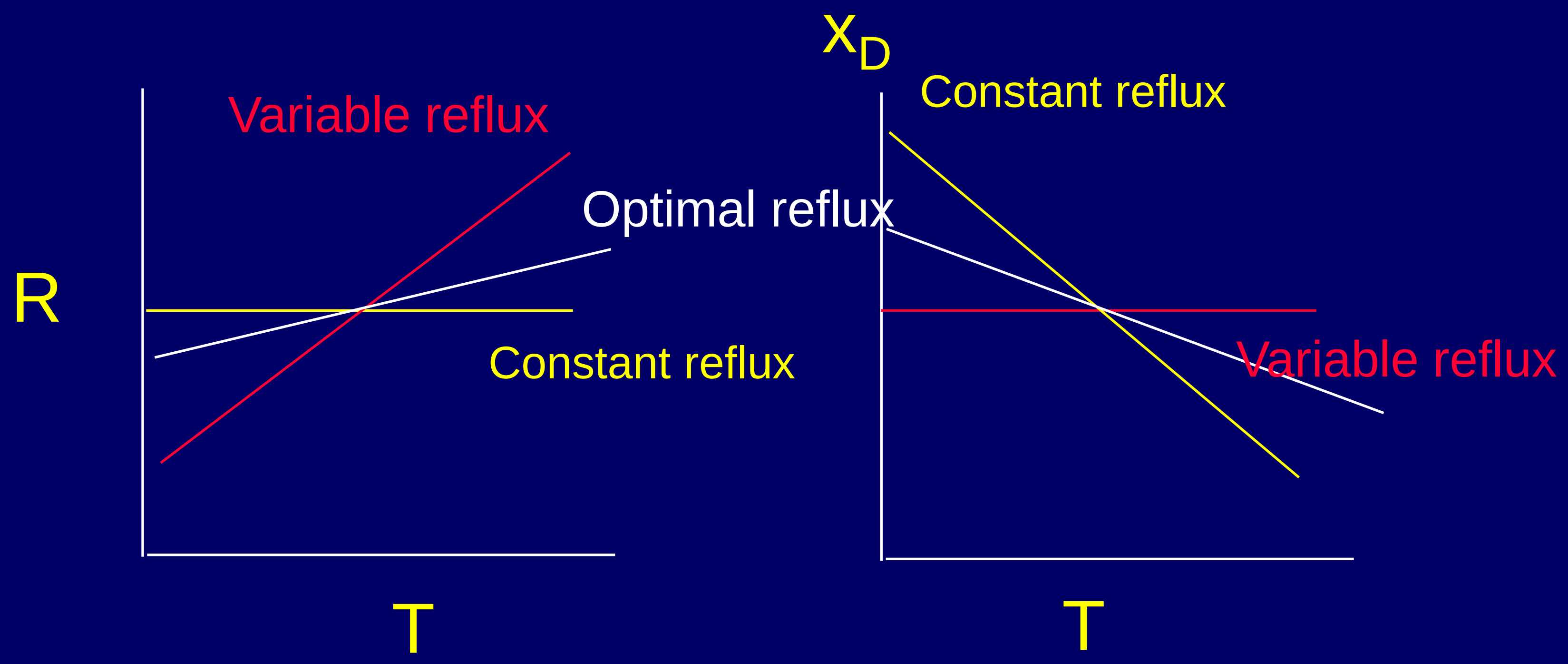


Batch Distillation

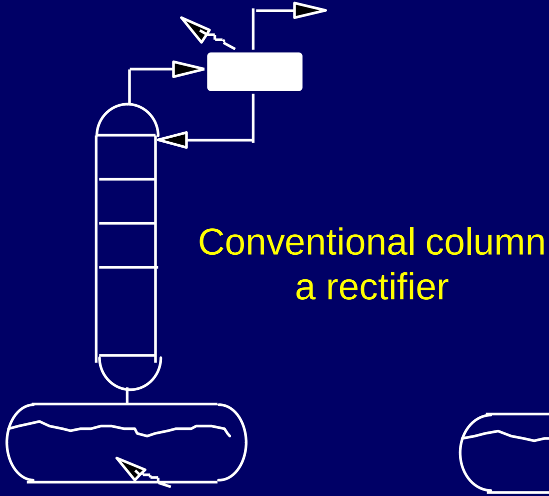
Flexibility



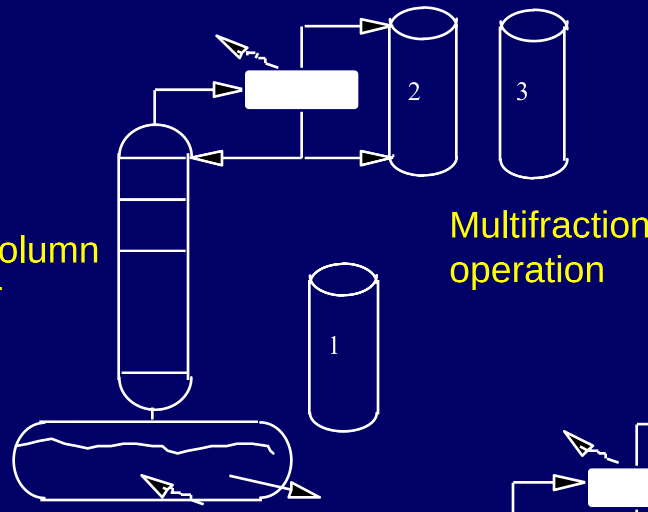
Operating Modes
(linear representation)



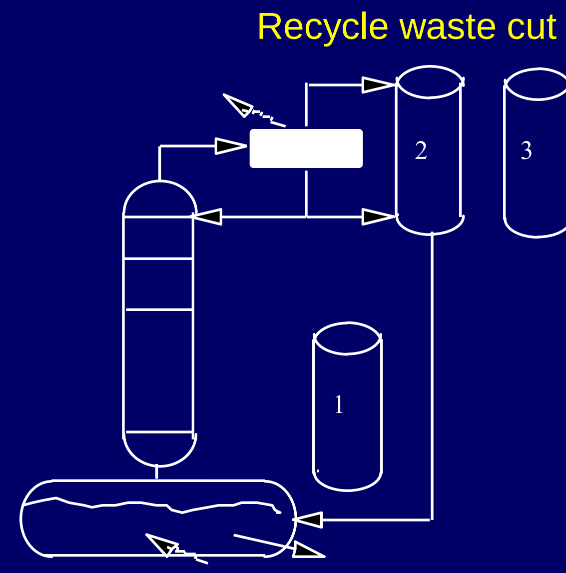
Different column configurations including emerging designs



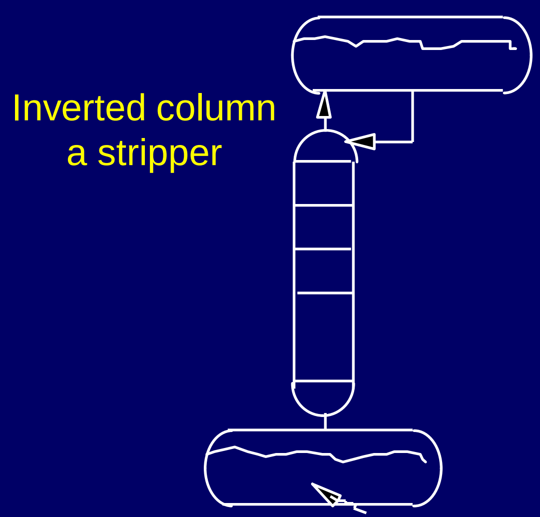
(a)



(b)



(c)



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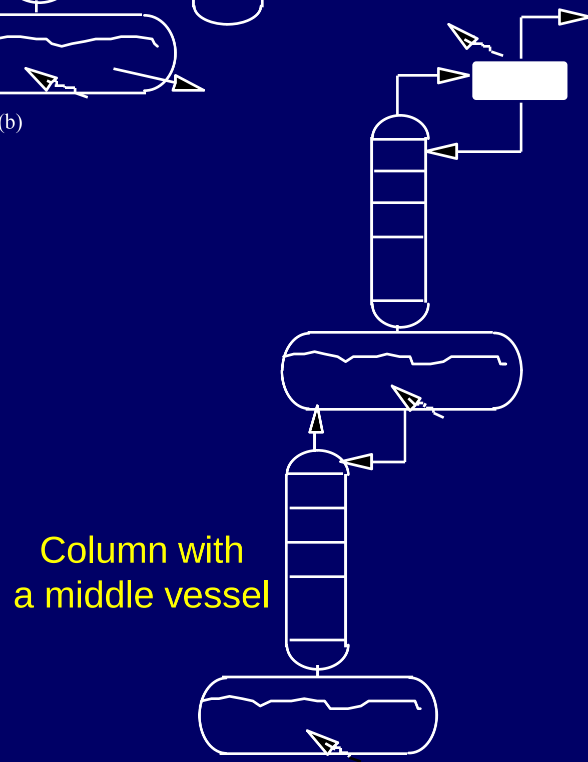
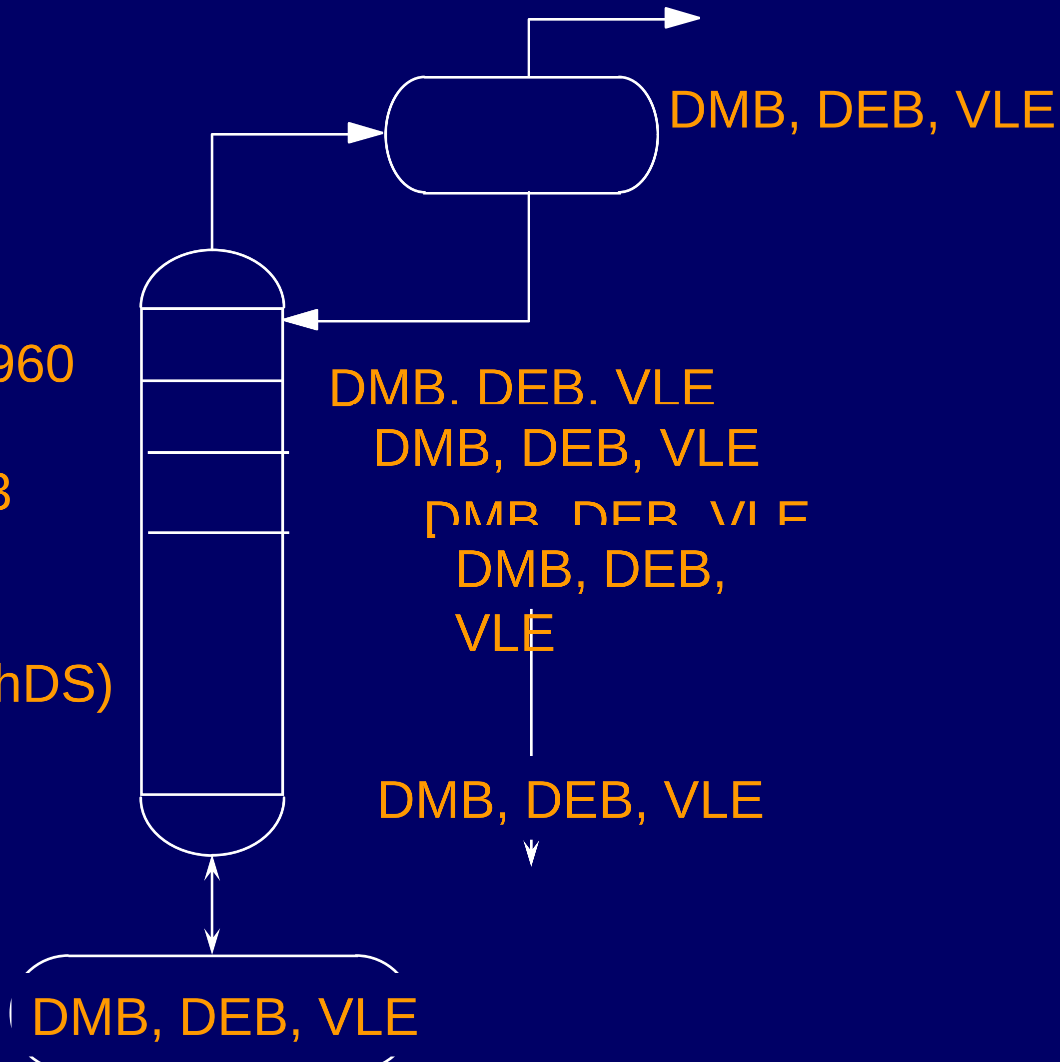


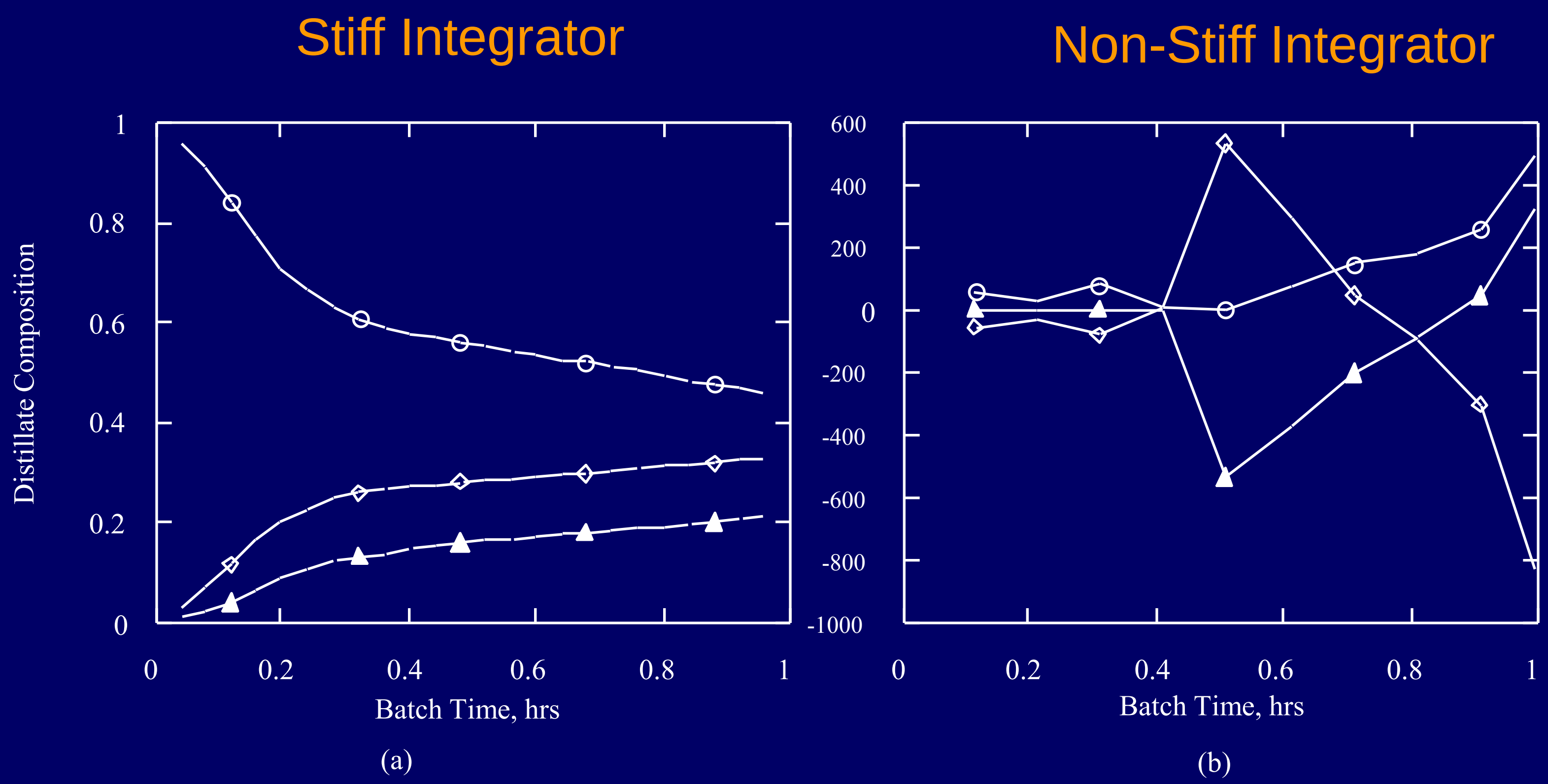
(e)

Rigorous Models



Huckaba & Danly, 1960
Distefano,1969
Boston et al., 1983
(BATCHFRAC)
Diwekar, 1988
(Batch-Dist, MultiBatchDS)

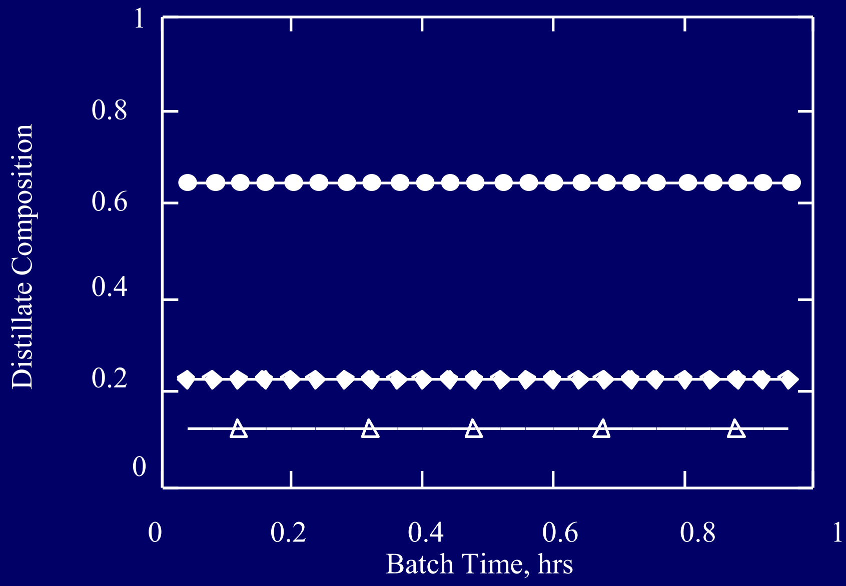
Numerical Integration (contd.)



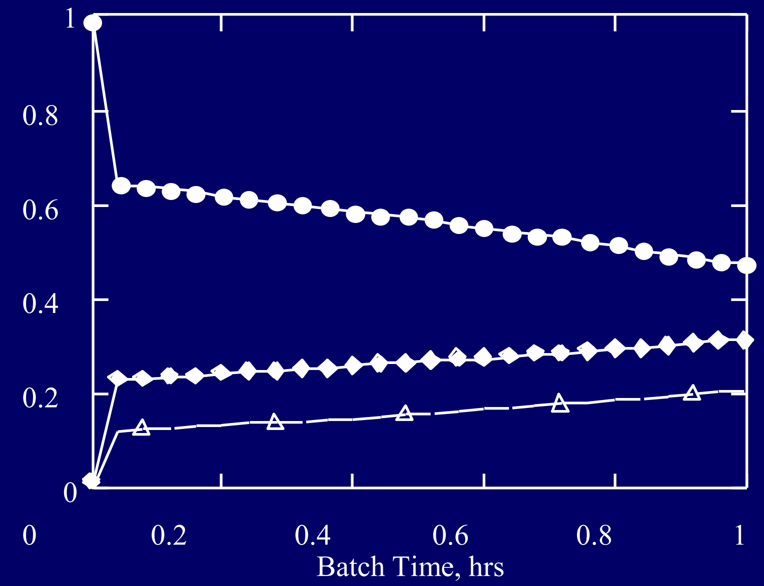
10 % Holdup on plates

Numerical Integration (contd.)

Stiff Integrator



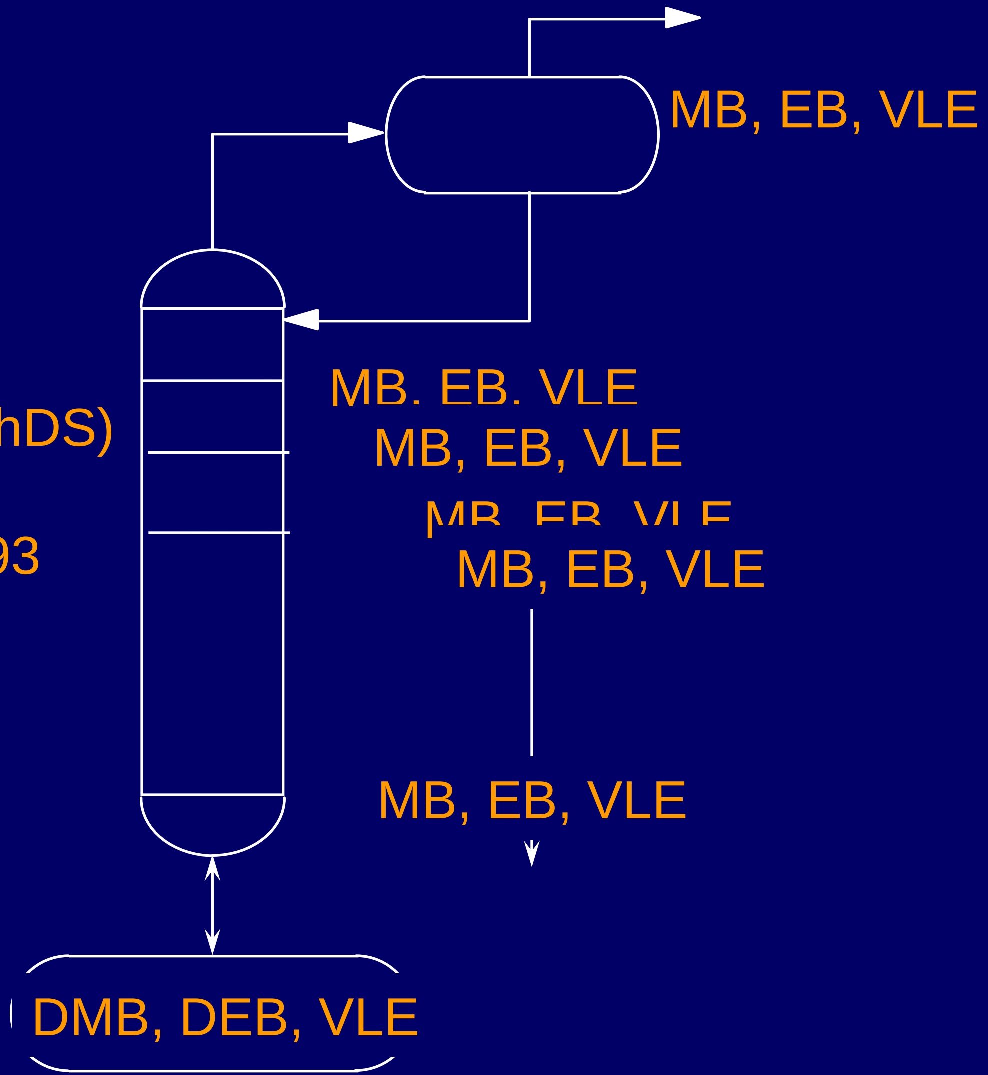
Model Change



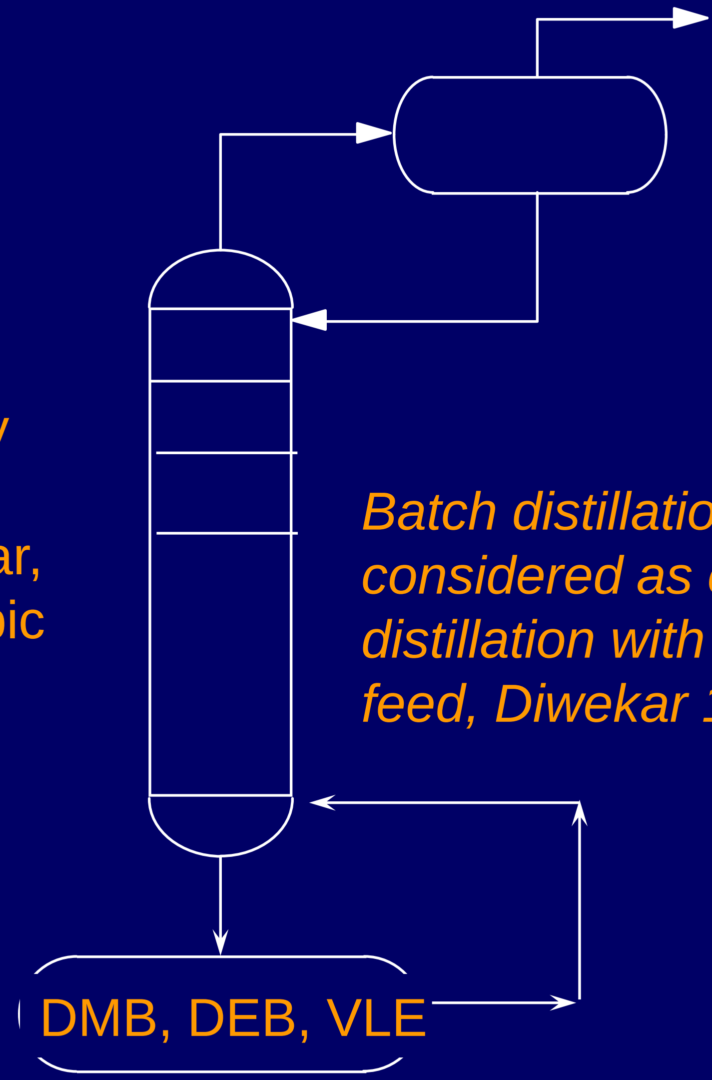
1 % Holdup on plates

Semi-rigorous Models

Diwekar, 1988
(Batch-Dist, MultiBatchDS)
Doherty &
co-workers, 1990-93



Shortcut Model



Diwekar, 1988
Diwekar, 1991 Binary Azeotropic Systems
Kalagnanam & Diwekar, 1993,Ternary Azeotropic Systems

Batch distillation can be considered as continuous distillation with changing feed, Diwekar 1988

Batch Distillation Column Software Requirements

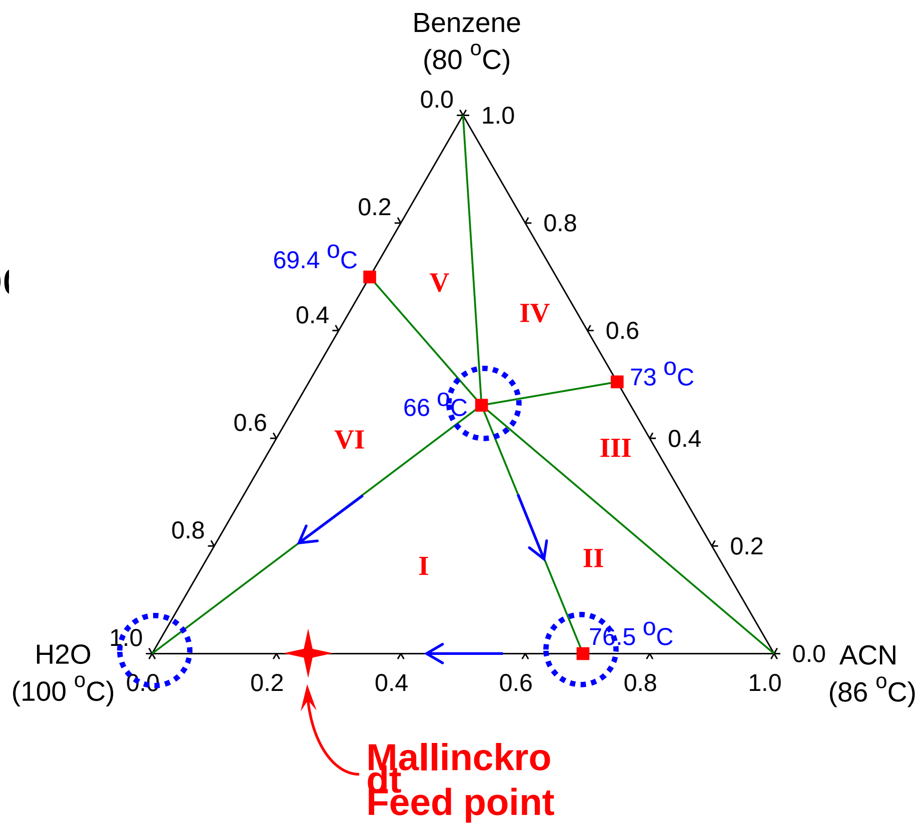
Features	Why
Windows	User friendly state of the art input/output interface
Databank	Ability to generate data from structural information
Operations Constant Reflux Variable Reflux Fixed Eqn. Optimal Optimal Reflux	Yield improvement due to operational flexibility and systematic optimization/optimal control methods
Models Shortcut Semirigorous Reduced Order Rigorous	Hierarchy of models for numerical stability, design feasibility, and advanced system designs.
Options Design Feasibility Optimization Reactive Distillation 3 phase Distillation Uncertainty Analysis	Advanced features
Configurations Semi-batch Recycle waste cut Rectifier Stripper Middle Vessel	Emerging designs provide promising directions for cost effective designs to obtain purer products

TABLE 10.1
Comparison of Software Packages

Features	CHEMCAD BATCH	BATCHSEP	MultiBatch*DS*
Databank	CHEMCAD	ASPEN PLUS	CRANIUM
Operations			
Constant Reflux	Yes	Yes	Yes
Variable Reflux	No	Yes	Yes
Optimal Reflux	No	No	Yes
Optimal Reflux Fixed Equation	No	Yes	Yes
Models			
Shortcut	No	No	Yes
Low Holdup Rigorous/Semirigorous	Yes	No	Yes
Reduced Order	No	No	Yes
Rigorous	Yes	Yes	Yes
Configurations			
Rectifier	Yes	Yes	Yes
Semi-batch	No	Yes	Yes
Recycle waste cut	No	Yes	Yes
Stripper	No	No	Yes
Middle Vessel Column	No	No	Yes
Options			
Design Feasibility	No	No	Yes
Optimization	No	Yes	Yes
Reactive Distillation	No	Yes	Yes
3 phase Distillation	Yes	Yes	Yes
Uncertainty Analysis	No	No	Yes

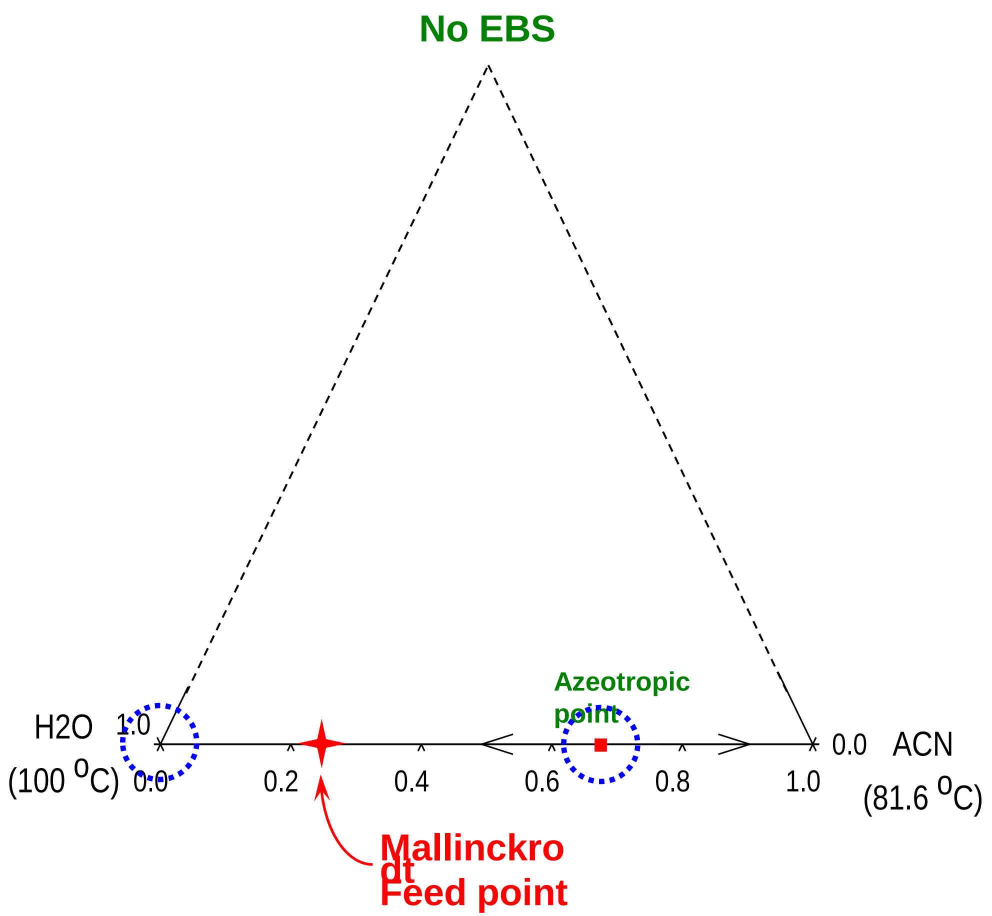
Industrial Case Study 2 (MALLINCKRODT)
Green Solvent Selection & Solvent Recycling

- Acetonitrile(ACN)/Water mixture from peptide drug processes
- Complex thermodynamic system
- Azeotropic agents (Smallwood 1993)
  - Benzene
  - Trichloroethylene
  - Diisopropyl ether
- ***Integrated approach***
  - Batch column configuration
  - using MultiBatchDS
  - EBS selection - Discrete optimization



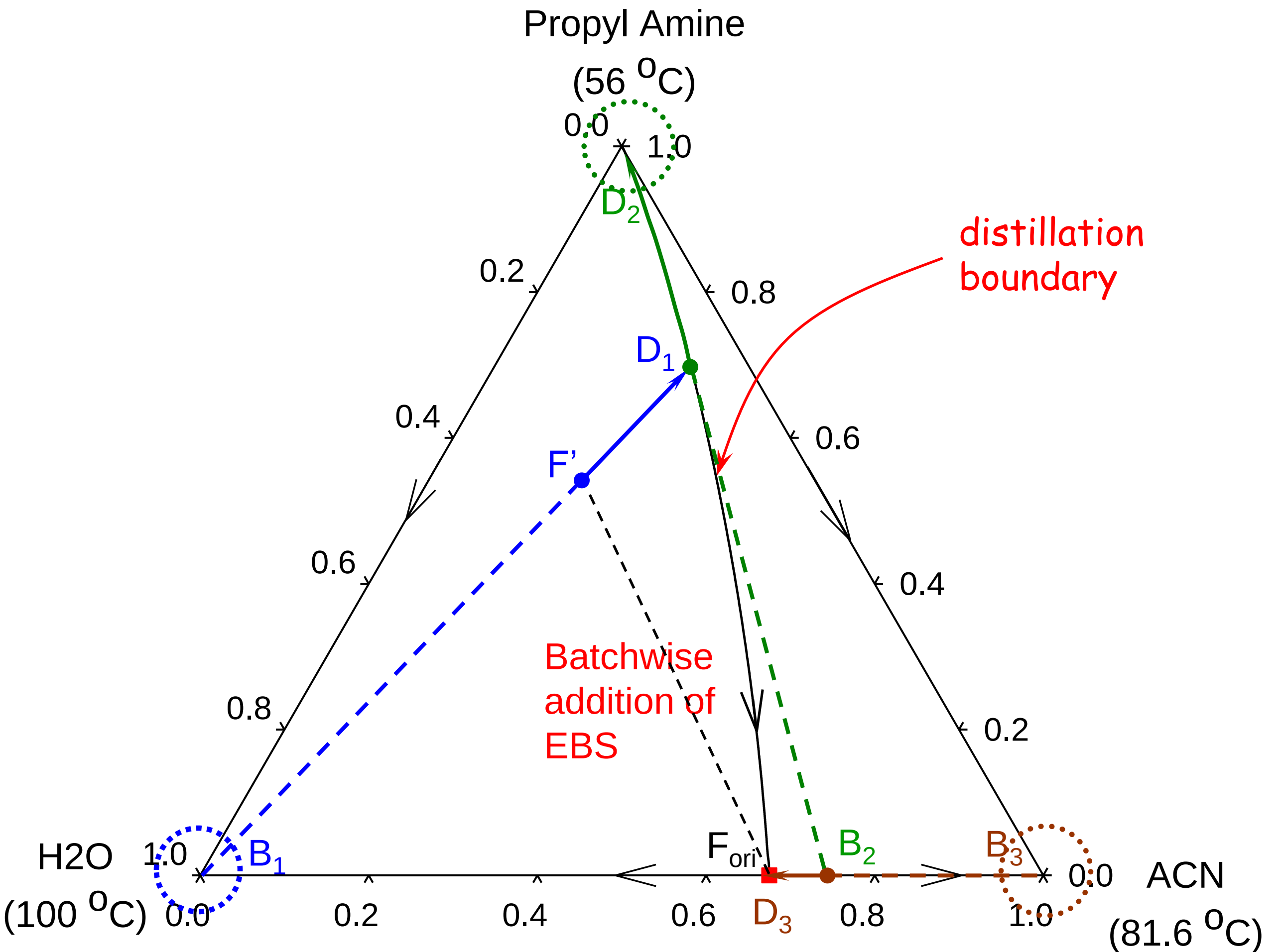
Two Campaigns

- Campaign I
  - Pure water removal
  - Optimal configuration⇨ middle vessel column
  - H_2O recovery = 86% (Waste reduced)
  - *H_2O recovery in a rectifier at Mallinckrodt experiments = 61%*



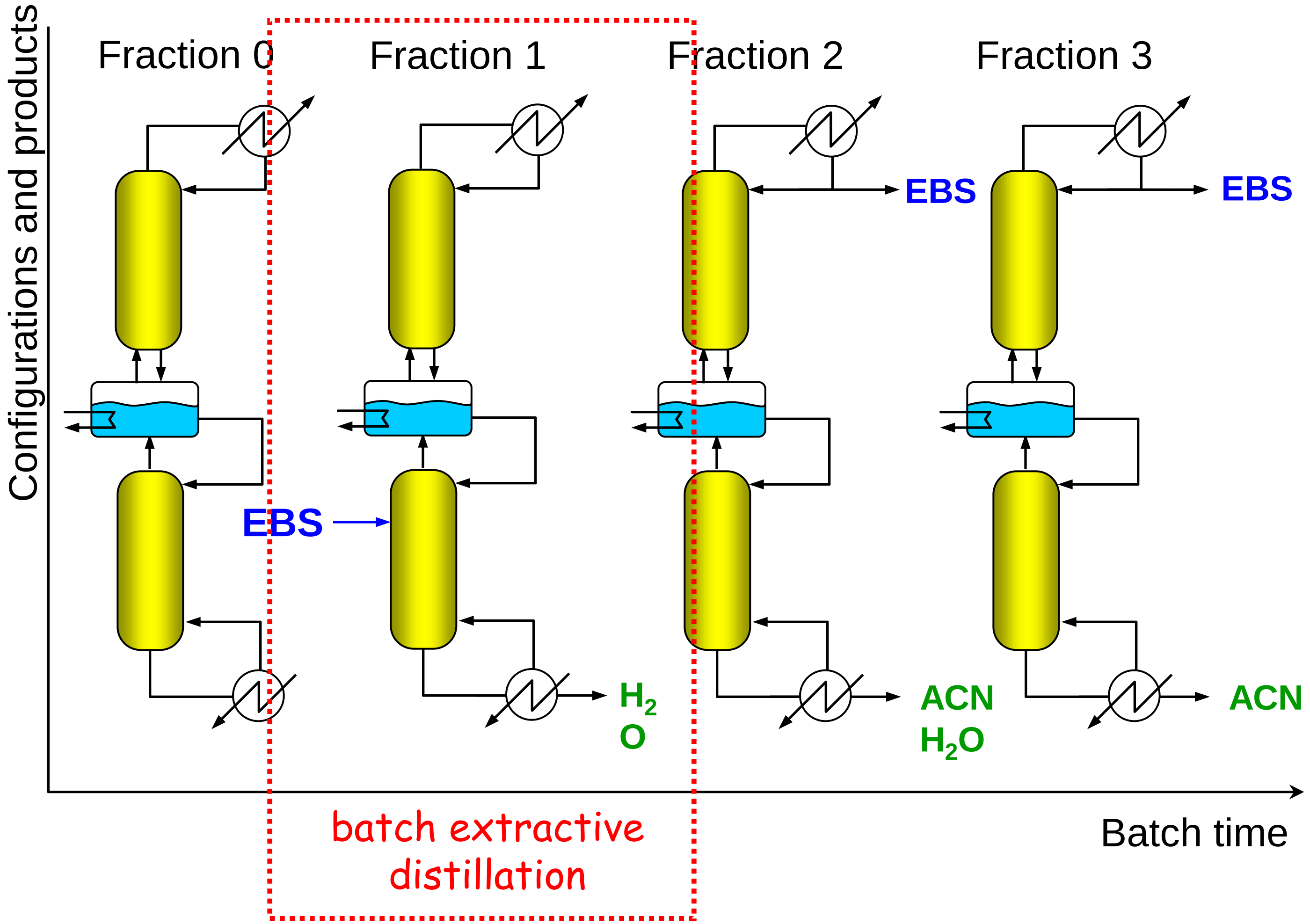
Two Campaigns… cont'd

- Campaign II
  - ACN recovery
  - EBS selection
    - **Propyl amine**
    - **Acetone**
  - Product sequences ⇨ middle vessel column



CAMD

Operations for Campaign II



Comp I
Comp II

Results and Conclusions of Case Study

- The ***first*** analysis for the integration of EBS selection and IPS recycling in batch processes
- Optimal configuration: Middle vessel column
- EBS selection for batch extractive distillation ⇨ Pareto solution
  - Propyl amine (Recovery: H_2O=98% and ACN=49%)
  - Acetone (Recovery: ACN=68% and H_2O=43%)

Summary

- Batch Distillation Column Design
  - Unsteady state nature
    - Number of models
  - Flexibility
    - Different modes of operation
    - Different column configurations
- *MultiBatch*DS offers **multiple column configurations, multiple operating modes, multiple fractions, and multiple products -- with multiple levels of models**