Module A Conceptual design

Thursday: The process of designing
Friday: Process synthesis

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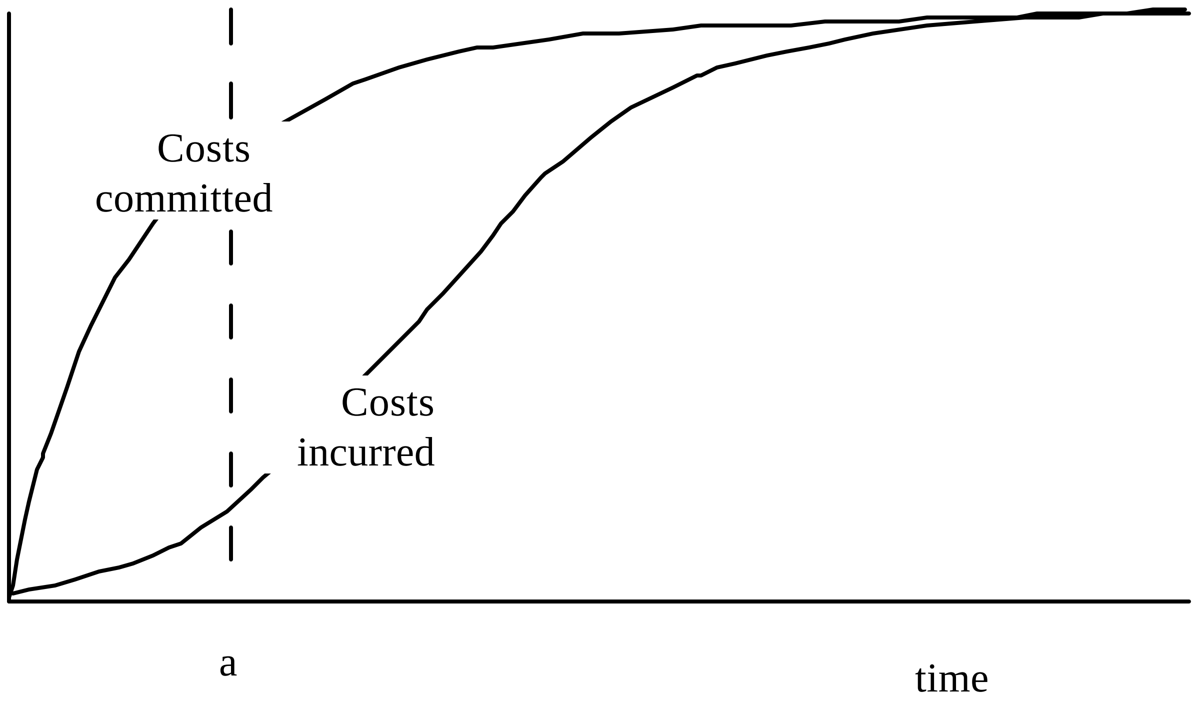
Outline

The design process

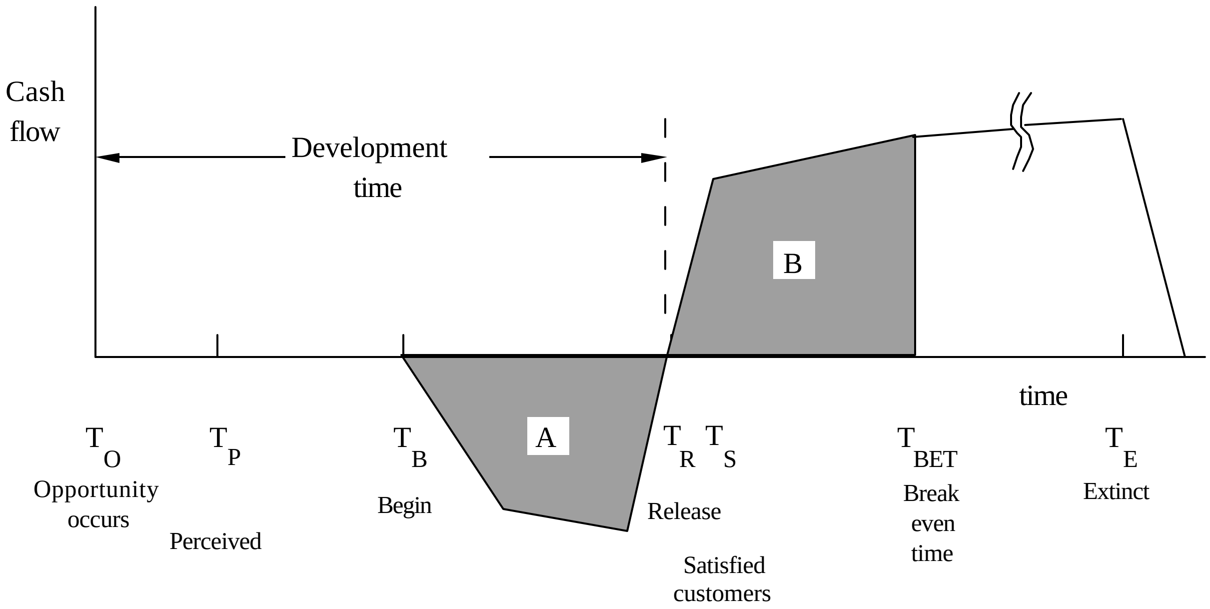
- Our experiences
  - + Design problem formulation
  - + Designing of products
- Tools to support designing
- Designing the design process

Why is design so important?

Design costs are small relative to impact



Typical cash flow for a project



Impact of delays and cost overruns on profits

In 1991, M. Patterson, then Director of Corporate Engineering at HP computed sensitivity of profits in two projects to three factors related to the development time:

- running late
- creating a design with higher production costs
- spending more funds on design and development

Higher production costs and being late -- especially for the first project -- were the big losers.

Table 1: Change in profits

	First shipment 6 months late	Production costs 9% higher	Development cost 50% higher
5 yr project	-33%	-22%	-3.5%
10 yr project	-7%	-45%	-1.8%

Project(1) assumptions

- units sold increases 20% per year
- price per unit declines 12% per year

Project (2) assumptions

- steady price per unit
- 7% annual market growth

Design is ubiquitous

We design

- engineering systems
- reports -- when we organize them
- short courses
- weekly menus
- experiments
- shelving for our basement workshop
- our kitchens

Some typical maxims

- Know the customer
- Know the competition
- Design quality into products and process
- Use rating systems - even simple ones -- to assess manufacturability, simplicity, etc
- Use rating systems for the process too (e.g., continually update the estimate for life cycle)
- Continually study and improve design process
- Deliver on time
- Use modern statistical experimental designing

A look at designing

There are many variations in the nature of the artifact and the process by which it will be designed. Thus designing is a widely varying process. For example --

Ethylene to ethanol chemical process

Design process: Fairly routine; highly modular - often in terms of well understood unit operations; significant regulation involved -- but design is not all in response to regulation; activity is significantly computerized; of the order of 5000 engineer hours from concept through to PIDs; mostly ChEs, some MEs, EEs in early stages

Artifact: large but not huge, geometry plays a minor role, only one to be built, will not be very novel, 5 decade lifetime

New laser tape measure

Design Process: innovative; highly modular - use of existing chips, separate interface, etc; some but not much regulation; highly computerized activity; 2000 engineering hours; involves circuit designers, product designers

Artifact: very small; little to modest amount of geometry involved in the designing; tens of thousands to be manufactured; would be quite novel; maximum lifetime of five years

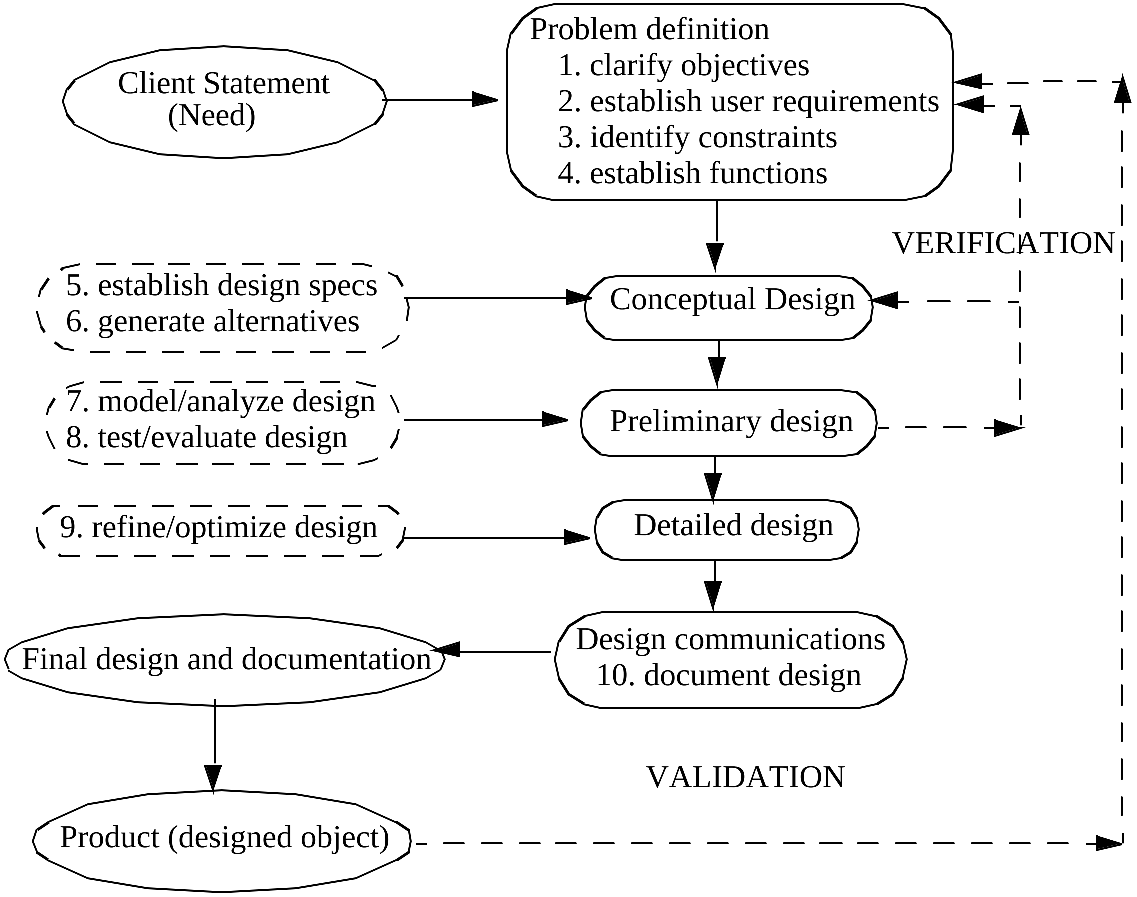
We can characterize designing along many axes

Design process - 6 axes

1. Activity type (routine, innovative or creative)
2. Degree of modularity (decomposes nicely or not)
3. Degree of regulatory constraints (regulations drive all decisions or only play a minor role)
4. Type of information flow (computer, pencil & paper, ...)
5. Magnitude of design activity (one up to millions of engineering hours)
6. Diversity of domains involved

Artifact - another 5 axes

7. Magnitude (very small to immense in size)
8. Role geometry plays in designing
9. Quantity (1 or a million)
10. Novelty
11. Longevity (days to decades)Steps in designing - formal description



Client Statement
(Need)

Problem definition
1. clarify objectives
2. establish user requirements
3. identify constraints
4. establish functions

VERIFICATION

5. establish design specs
6. generate alternatives

Conceptual Design

7. model/analyze design
8. test/evaluate design

Preliminary design

9. refine/optimize design

Detailed design

Design communications
10. document design

Final design and documentation

VALIDATION

Product (designed object)

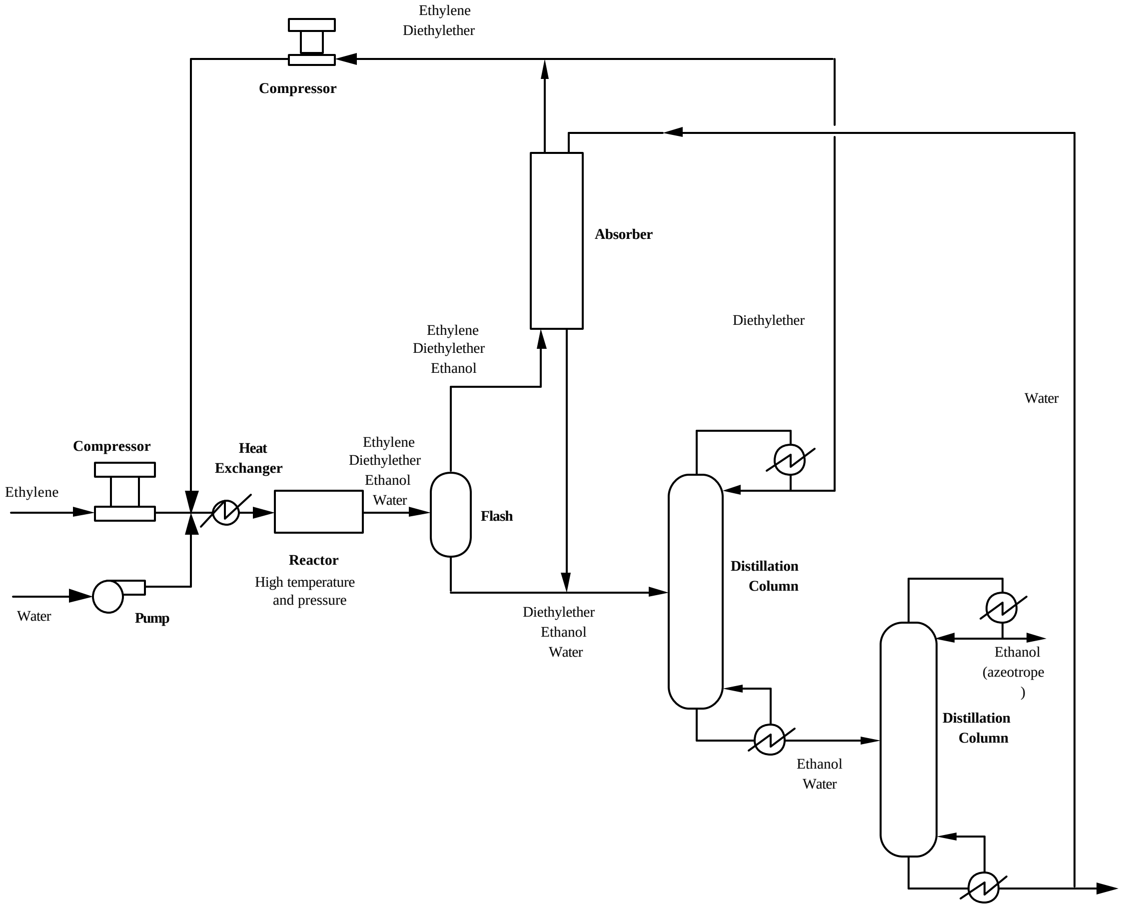
A model of the design process
(alla Dym and Little)

Slight variation on the labeling

- **Formulation**
  - \+ Goals
  - \+ Tests
  - \+ Design space
  - \+ Starting points
- **Design specifications**
  - \+ Functional specifications
  - \+ Performance specifications
- **Synthesis**
  - \+ Generate
  - \+ Analyze
  - \+ Evaluate
  - \+ Refine
- **Report**

Stages in design a chemical process

- preliminary design
- basic process design
- final process design
- equipment and detailed project design
- startup and plant operation



Steps in designing - informal

No design process ever follows a formal description of it -- except for truly routine (cookbook) designs.

Bucciarelli (Louis L. Bucciarelli, Designing Engineers, MIT Press, 1996) describes design as a social process. There are two aspects to its being social

1. the beliefs/values of the participants significantly affect the design outcome and
2. the interactions among the participants will affect the designing activities -- negatively and positively.

Designing can fail because of these interactions, even when the expertise is present to do it right.

Two views of design (Bucciarelli)

Savant: Scientific principles establish the form of a design. Given the principles, the design follows. One can take a final product, dissect it and ascertain the design decisions that led to its creation.

Utilitarian: The consumer demands a product, which will then be designed. Every society gets the technology it deserves. Smarter consumers will lead to better products.

Is either right? Let's discuss.

He observed and reported on three design projects:

- Designing a photovoltaic array for supplying a highway lighting system in Saudi Arabia
- Resolving a quality problem called “dropout” in a printed image that arose during their new product called Atlas
- Designing a new cargo inspection system capable of handling a whole truck

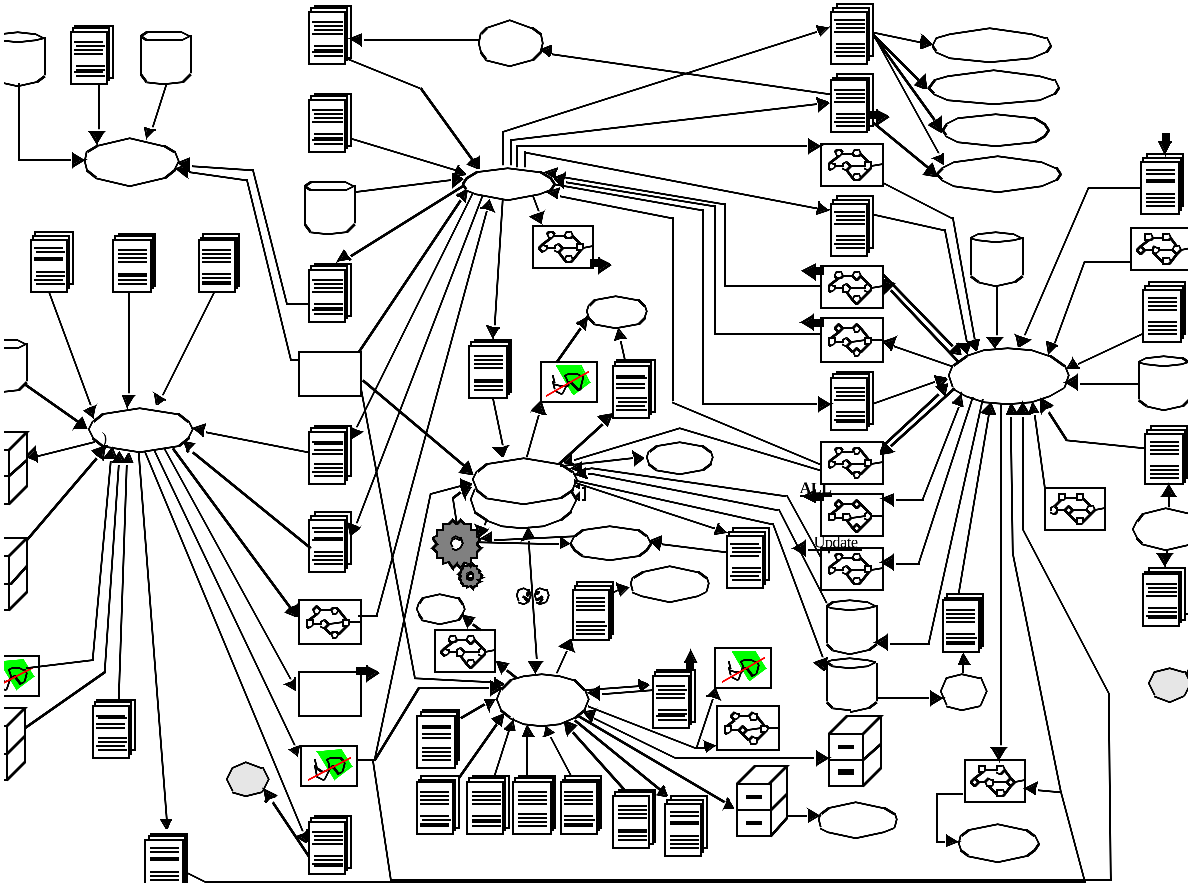
The reporting includes the times spent in the hallways, in meetings, on the phone etc., with many participants being very frustrated and feeling they were wasting time -- but he argues they were not.

He states that designing is the bringing together and rationalizing the differert “object worlds” of the participants. In other words, the participants have to develop a new special purpose language in which to converse (let’s call it a “pidgin” or a “creole” language). A major part of their activities is involved in developing that language.

He also points out that design occurs in a context and is significantly impacted by that context.

His final paragraph is: “The realization that design is a social process, that alternative designs are possible, and that a design’s quality is as much a question of culture and context as it is of a thing in itself or of the dictates of science or market forces -- all this is a prerequisite to moving beyond simplistic images and myths about technology and doing better as designers, as corporate strategists, as government regulators, as consumers, and as citizens.”

A modern design organization is complex

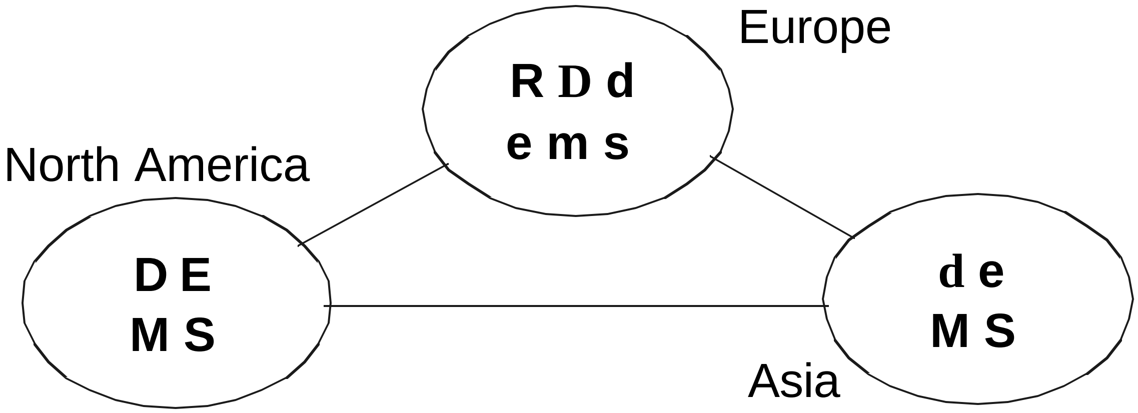


People and the information they share when designing a relatively routine product in a major European company. Ovals are people; other icons different types of information. Developed using questionnaires and personal interviewing.

International teaming for designing -- today’s experience for many

- Research: R, r
- Development: **D**, **d**
- Design: D, d
- Engineering: E, e
- Manufacturing: M, m
- Sales: S, s

These are often distributed internationally



Europe

R D d
e m s

North America

D E
M S

Asia

d e
M S

Differences caused by distribution of activities

- Over long links
  - + Language (e.g., English/German)
  - + Time zone differences (a major problem)
  - + Domain vocabulary (e.g., sales/research)
  - + Regional knowledge (e.g., there’s mildew in Florida)
  - + Expensive face to face meetings
- Over short links
  - + Domain vocabulary

Putting a structure on problem formulation

- State the goals
- For each goal, propose a test
- Determine the design space
- State the starting points

Problem: Find the “best” route for us to drive from here to the airport.

Convert this into a math programming problem

Goals

A first question that should occur to you is - what do we mean by “best?”

- Minimum time
- Most comfortable
- Most reliable
- Most scenic
- Shortest distance
- Uses only main roads
- Normally takes less than 35 minutes

All design problems have multiple competing goals (including the design of chemical processes)

Tests

Which test would you use for the fastest route?

- Drive them all and time each, selecting fastest
- Use a good map and estimate times. Select fastest

The second option one can do quickly (with a program) and while in one’s office

How would you propose to test a proposed design for a chemical process for its safety? for its economic return? for its reliability?

What is the design space?

- Your ideas?

My proposal

A design is a proposed route to the airport as an unambiguous naming of all of the roads segments along which one will travel

Starting points

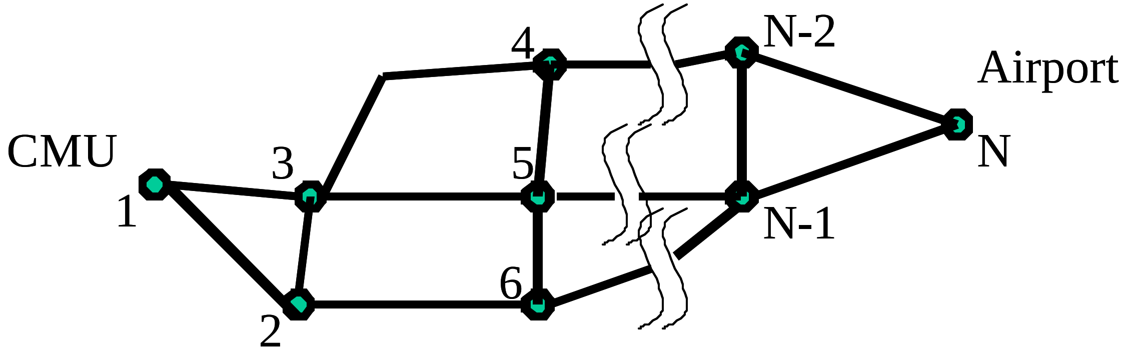
- Use existing maps
- Devise your own maps
- Use the solution method that yellow cab uses for this problem
- Use the solution methods for another city
- Use the methods Delorme uses for their USA maps

Formulating as a math model

Use a graph model

Graphs have nodes (intersections)

Edges (road segments)



Intersections

Define a set of intersections

$$I = \{1, 2, 3, \ldots\ldots.N\}$$

where 1 = CMU and N = Airport

Connection matrix

Define connection matrix C with elements c[i,j] where

- c[i,j] = 1 if there is a simple road segment from intersection i to intersection j
- c[i,j] =0 otherwise – e.g., c[3,4]=1, c[1,4]=0

Binary variables y[i,j]

- Let y[i,j] = 1 if the road segment from intersection i to j is part of the current proposed route
- Else y[i,j] = 0

Question: what are the design variables for this problem?

There are NxN variables y[i,j] and each can take on one of two values: 0 or 1

- Size of the design space is 2^{NxN}
- If N = 10 intersection, we can generate $2^{100} > 10^{31}$ alternatives (there are about 10^{21} grains of sand in the world)

Constraints

Not all designs as we just defined them are feasible. What constraints can we write to assure

- each design alternative is a simple path from CMU to the airport?
- Can’t use nonexistent roads

  y[i,j] $\leq$ c[i,j] for all i, j in I
- Route starts at CMU

  sum(y[1,j], j in I) = 1

  sum(y[i,1], i in I) = 0
- Route ends at airport

  You figure these out

- Must be a connected path
  + At most one road segment into any intersection k

    sum(y[i,k] for i in I) < 1
  + At most one road segment out of any intersection

    sum(y[k,j] for j in I) < 1
  + We must select a road segment out of each intersection k if and only if we select one in, except for intersections 1 and N

    sum(y[i,k], i in I-{1,N}) = sum(y[k,j], j in I-{1,N})

Are we done?

You think about it – try out some small examples

Tests

How can we evaluate the metrics that measure the worth of our goals -- e.g., distance, time, reliability, …. of the route?

- Length of the route

Let d[i,j] be the known length of the road segment from intersection i to intersection j

Then the length of the selected route is

sum(d[i,j]*y[i,j], all i and j in I)

- Reliability

Let’s brainstorm this one

Some other example design problems - think about the goals, tests, design space, starting points

- Write a paper for presentation at a conference
- Construct new shelving for your basement

Goals for the design of chemical processes

Economics is NOT the only goal for process design. It is not difficult to generate many other goals which are competing with each other.

For her PhD, Paulien Herder (Process Design in a Changing Environment: Identification of Quality Demands Governing the Design Process, PhD Thesis, Delft University Press, Delft, Netherlands (1999)) used two industrial panels to identify important “quality” factors for process design. The first panel comprised industrial professionals from operating companies, engineering contractors and academic institutions, all involved in the design and constructing of processes. Members for the second were from the metallurgical and pharmaceutical industries, government agencies and public interest groups.

The panels developed the following two “top ten” lists:

1. Safety during operation
2. Operability of the plant
3. Acceptability for environment
4. Safe startup and shutdown
5. Fit for purpose
6. Efficient use of raw materials
7. Design should meet location specific demands
8. Control of product quality and quantity
9. Maintenance
10. Total life span aspects

and environment requirements

3. Reliability
4. Sustainability
5. Operability
6. High feedstock efficiency
7. Clear project and communication structure
8. Environmental constraints
9. Safety for employees and environment
10. Adequate use of knowledge and experience of designers, operators and maintenance services

Homework: Select one of these goals and propose a test for it. Remember, you must apply the test to select the better solutions while searching among design alternatives -- of which there could be millions.

An aside: solving multiobjective problems

How does one solve a problem with competing goals. The following are steps one could take.

- Create the list of goals
- Tentatively categorize into two classes
  - + Objectives to be maximized or minimized
  - + Inequality or equality constraints to be satisfied

Ex 1: Find process having maximum present worth that can manufacture at least 1000 kg/day of product.

Ex 2: Maximize the production capacity of a plant that will have a present worth of at least $10 million.

Ex 3: Maximize the production capacity and present worth of the plant.

Ex 4: Find a design that can manufacture 1000 kg/day of product and that has a present worth of at least $10 million.

Note: Each of these is a very different problem. It is a lot of work to maximize or minimize compared to satisfying a constraint. One typically converts goals to constraints to reduce the search effort BUT one takes a chance of missing a great nearby solution when doing so.

- Choose perhaps two or three of the most important goals to consider at first, leaving the remaining ones to be examined later.
- For the objectives, find the Pareto set of solutions. A solution is in the Pareto set if no other solution is better in one objective and at least as good in all others.

Example

Find the Pareto set among the following investment opportunities for a married couple.

Max F1:Rate of return

Min F2: % of time all money is totally lost

leads to following proposed solution points

F1, %	F2, %
10	7
5	6
10	4
9	2
6	4
3	0

- Have whoever makes the final decisions select the solution. The exact choice is a value judgement where here one is trading rate of return for risk. Older people near to retirement would abhor risk while 20 year olds might willingly take a chance.

Uses for a proper formulation

- It gives a formalized description of what you think the problem is about, a description you can use to negotiate among the stakeholders. When you state a test for the investment cost of a process will be to simulate using AspenPlus, then to size using a prescribed set of guidelines, and then use Guthrie cost models, your client may or may not like this approach.
- It makes you be much more precise in your thinking so you can better plan what tools you may need, etc., to carry out the design process.

The design of products

Examples of products

- Portable enriched oxygen device
- Tape that peels off without taking off the paint
- Drug to combat Parkinson’s disease
- Nonfat replacement for cooking oil
- Fuel for race cars
- Disposable diaper
- Hand warmer

Examples of processes

- Deliver 1000 tonnes/day of ammonia
- Manufacture 30% of current demand for vitamin C
- Produce the racing fuel mentioned above

References

MechE Product Design

- Dym and Little, 2000
- Ulrich and Eppinger, 2nd Ed, 2000

Chemical Product Design

- Cussler and Moggridge, 2001

Why chemical product design?

- ~50% BS ChEs entering product related industry
- Many companies now aiming at high value added chemicals -- e.g., specialties and products
- Commodity manufacture can often be bought and put anywhere - easy to lose edge
- It has always been with us -- 3M, Kodak, ...

- Basis for most startup companies

A prototypical process design course

- Create plant to make 1000 tonnes/day of ammonia
- Find a good low cost solution
- Rate safety, environmental impact
- Possibly develop preliminary control structure

Problem characteristics

- Generally large-scale manufacture, continuous plants
- Lifetime often measured in decades

Approach

- Create base case (from literature)
- Invent process alternatives for separation
- Carry out heat and material balance (by hand or simulate or both)
- Heat integrate (using pinch technology)
- Perform simple economic analysis

Outcomes desired

Have our students

- put their “chemical engineering” all together
- learn to function in teams (3 to 5 ChEs each)
- learn to make technical presentations

Our product design course

Given a one line idea -- and little else

- a tape that peels off without taking off the paint
- a teaching module for air separation
- a product to teach young asthma patients how to control their affliction
- a laser-based replacement for a tape measure

Problem characteristics

- First to market is the big winner
- Lifetime measured in months
- Manufacturing can often be contracted to others
- Design of interfaces plays key role

Approach -- and here it is really different

- Must find out what the stakeholders want - customers, manufacturers, designers, investors, ...
- Must set design goals - economics may not be prime
- Must establish how to rate proposed designs -- what will one do for testing?
- Must establish the design space of allowable alternatives

Students learn

- to work on multidisciplinary teams
- the best technology improperly packaged is valueless
- to present both orally and in writing
- what it could take to make it in a start-up

The many talents needed for product design

Business

- Which decision is worth more: Optimize a refinery OR buy the right tanker of crude oil?
- Understanding supply/value chains
- How does one establish the price - head off competitors, make a quick killing, or what?
- What is a business plan?

Industrial design

- Products have to appeal - color and shape have major impact on customer appeal
- Non-intuitive interfaces to computer aids are a disaster
- What buttons are needed on a laser tape measure, where should they be placed, what should they do?

Social sciences

Sociology, anthropology, psychology, linguistics, history of technology provide methods to

- enhance understanding and execution of product design
- identify customer needs
- make qualitative evaluation assessments
- understand consequences of decisions on people

And, of course, excellent science and engineering

=> A product design team should be a well thought out mix of persons from many backgrounds

Characteristics of chemical products

At least three classes of products

- Products that are chemicals - pharmaceuticals, proteins, insecticides, cleaning fluids, lubricants
- Products that require chemistry in their manufacture - computer chips, layer manufactured products
- Products whose functioning involves chemistry - portable oxygen generator, lens that change color

General characteristics

- High value added
- Lifetime measured in months
- Often small volume
- Manufactured in existing multipurpose plants
- Often produced as solids
- Often electromechanical too

Manufacturing facility design

- Retrofit of existing plant
- Design of new multipurpose plant - with unknown future products (equip a kitchen)

Aids for the product design process

- Establishing multiple goals (brainstorming, interviewing)
- Organizing goals (goal, subgoal hierarchies, objectives, constraints)
- Managing the design process (work breakdown structures, Microsoft Project tools, etc)
- Establishing the design function (“verb object” pairs -- e.g., deliver physical strength)
- Estimating levels required for performance ($1 savings is useless, $5 is fantastic)
- Develop tests (simulations, prototypes)
- And so forth

Ties to current process design technology

Examples

- Find chemicals having desired functionality
- Use group contribution methods backwards
- Rapid “Edisonian experimentation” using combinatorial chemistry
- Extending simulators to handle product
- Manufacturing in existing facilities related to scheduling and planning
- Retrofit design

Educating chemical engineers in the future

We should think seriously about redirecting effort toward product design

Possible recommendations

- Continue current process design class - perhaps as a more conventional course
- Add a product design course as the capstone that uses all of a student’s educational experience
- Have students learn to function on multidisiplinary teams

Discipline specific recommendations

- Teach more on solids handling
- Add more material on batch processes in unit operations course
- And for fun in thermo, occasionally ask students to do the inverse problem - e.g., find chemicals with desired properties

Support tools for designing

- Team building
- Collaboration
- Project management
- Information management
- Problem formulation

Tools for team building

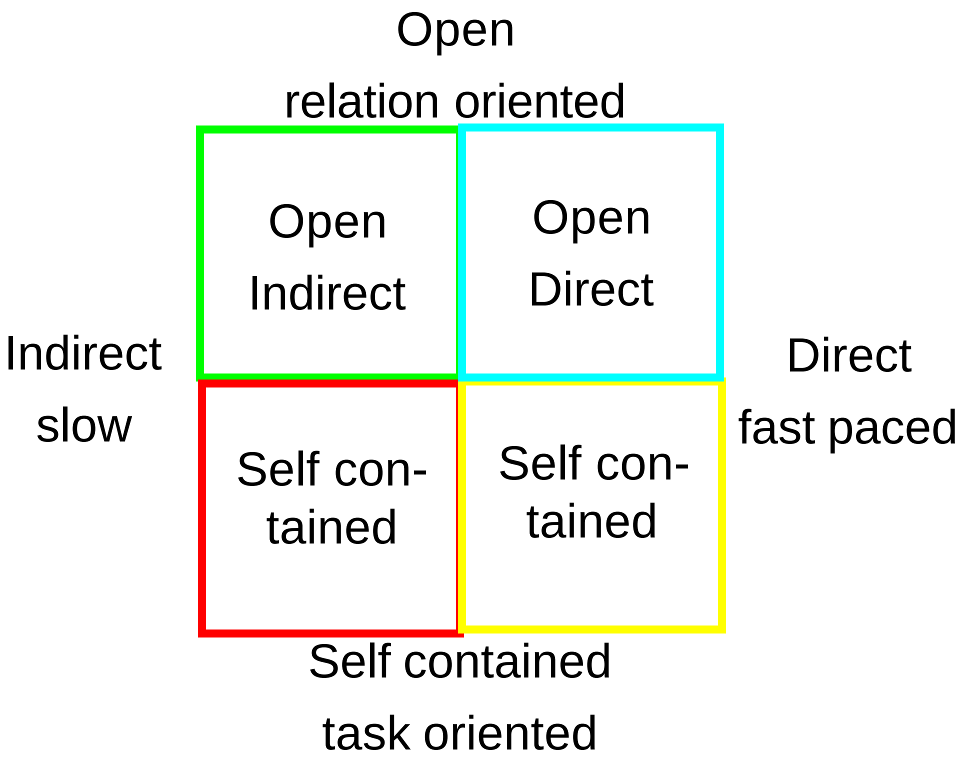
- How groups operate
- Personality types
- Forming groups

How groups operate

Four stages of group behavior

- Honeymoon - wow, this is great! Let’s get going.
- Anger - hey, why is she so bossy? Often the final stage for a group.
- Tolerance - things get done but can be unpleasant
- Harmony - the group starts to hum. People allowed to do things they like and are good at doing.

Personality types (a first, simple classification system



Open

relation oriented

Open

Indirect

Open

Direct

Indirect

slow

Direct

fast paced

Self con-
tained

Self con-
tained

Self contained

task oriented

Open/Indirect

- Amiable
- Steadiness, cooperating with others
- Slow and easy
- Values relationships
- Dislikes pushy behaviorOpen/Direct
- Expressive
- Influences others, forms alliances
- Fast paced
- Values relationships
- Dislikes boring tasks
- Good at socializing
- “Let me tell you what happened …”

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Self-contained/Indirect

- Analytical
- Compliance – existing conditions
- Slow, steady, methodical
- The task in important
- Does detail well
- Dislikes surprises
- Good at the process, systems
- “Can you document your claims”

Self-contained/Direct

- Driver
- Likes to dominate
- Fast pace
- The task is very important
- Focuses on the results
- Hates to waste time
- Good at being in control
- “I want it done right and done right now”

The Myers-Briggs test

Useful link for reading material:

http://www.teamtechnology.co.uk

Douglass Wilde’s ME210 test

http://me210.stanford.edu/98-99/index.html

=> Most important: Tells you how you prefer to operate, NOT how you operate.

The four dimensions

- Extrovert vs. Introvert
- Sensing vs. iNtuitive
- Thinking vs. Feeling
- Judgement vs. Perception

=> 16 different classifications, e.g., ESTJ, ENFJ, ISFP

My scores: 0, 40, 10, 0 (-NF-)

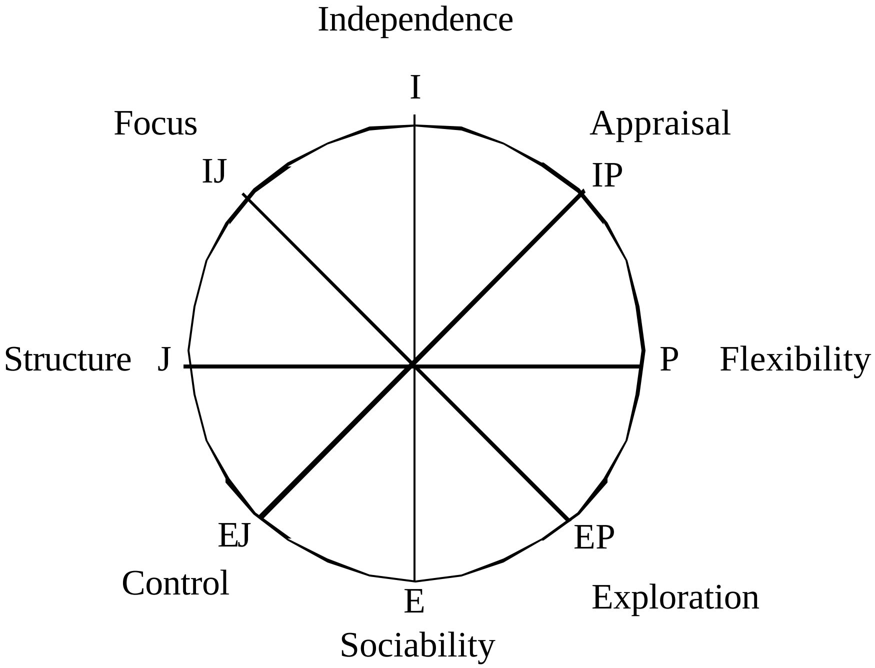
For example: INFP

Full of enthusiasms and loyalties, but seldom talk of these until they know you well. Care about learning, ideas, language, and independent projects of their own. Tend to undertake too much, then somehow get it done. Friendly, but often too absorbed in what they are doing to be sociable. Little concerned with possessions or physical surroundings.

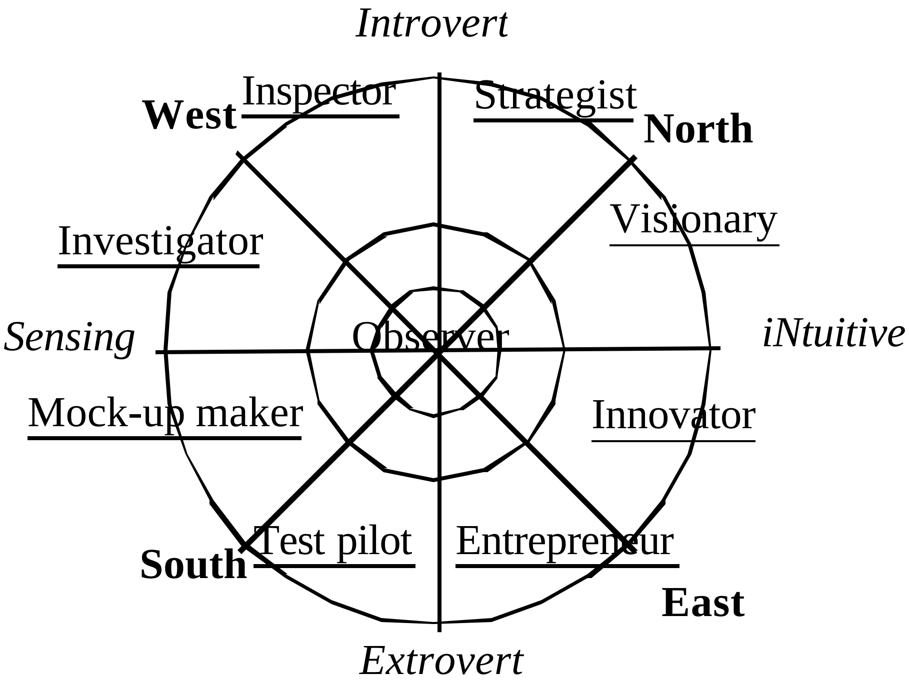
Or ENFJ

Responsive and responsible. Generally feel real concern for what others think or want, and try to handle things with due regard for the other person's feelings. Can present a proposal or lead a group discussion with ease and tact. Sociable, popular, sympathetic. Responsive to praise and criticism.

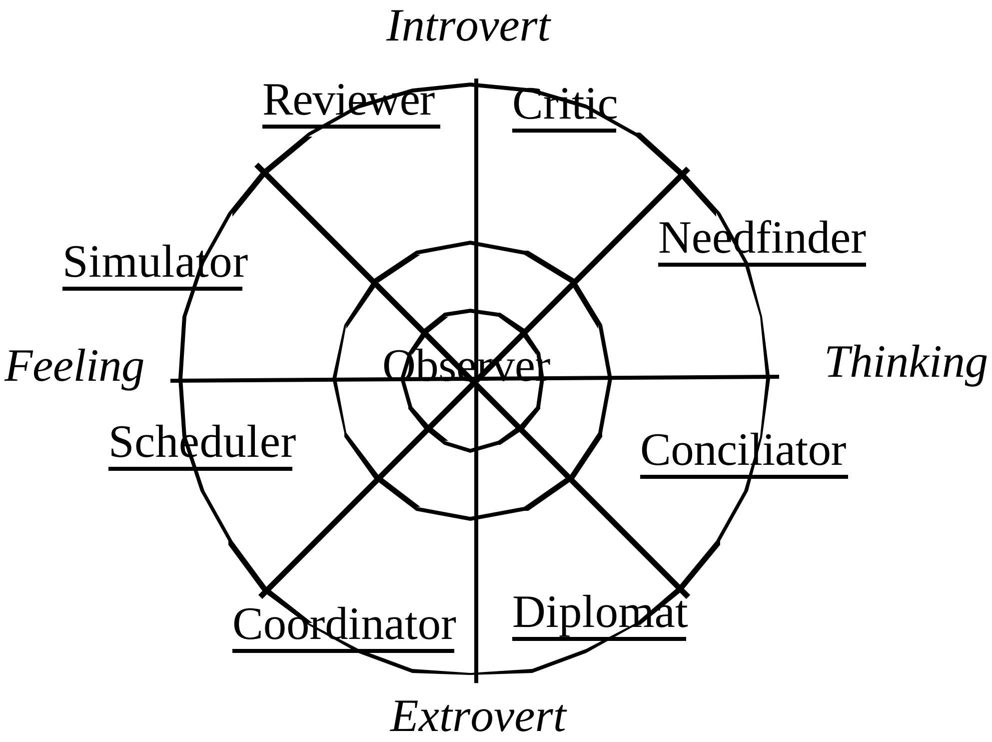
Transforming the axes - Wilde's attitude map



Perception domain roles



Judgment domain roles



Forming groups: Use the compass points...

- Really should have
  - + EN = East: Innovation (often not enough of these among engineers)
    - => pulls ideas together, the starter
  - + IS = West: Knowledge (often a lot of these among engineers)
    - => gets things right, the closer
- Great to have
  - + IN = North: Imagination
    - => dreams things up, offers a different perspective
  - + ES = South: Experimenter
    - => tries things out, hands on

A group formation process

Find someone not known

Take 5 minutes. In pairs, exchange following info:

- Names
- Occupations
- One thing each dislikes and one thing each likes
- Places in which each has lived
- How well each likes to use the computer
- Is other person a north, east, west or south

Each introduces his/her new friend

Tools for collaboration

Three questions we will ask throughout

- What should we do?
- What can we do
- How should we do what we should do?

NOTE: there are things we should do and can, should do and cannot, and can do and should not.

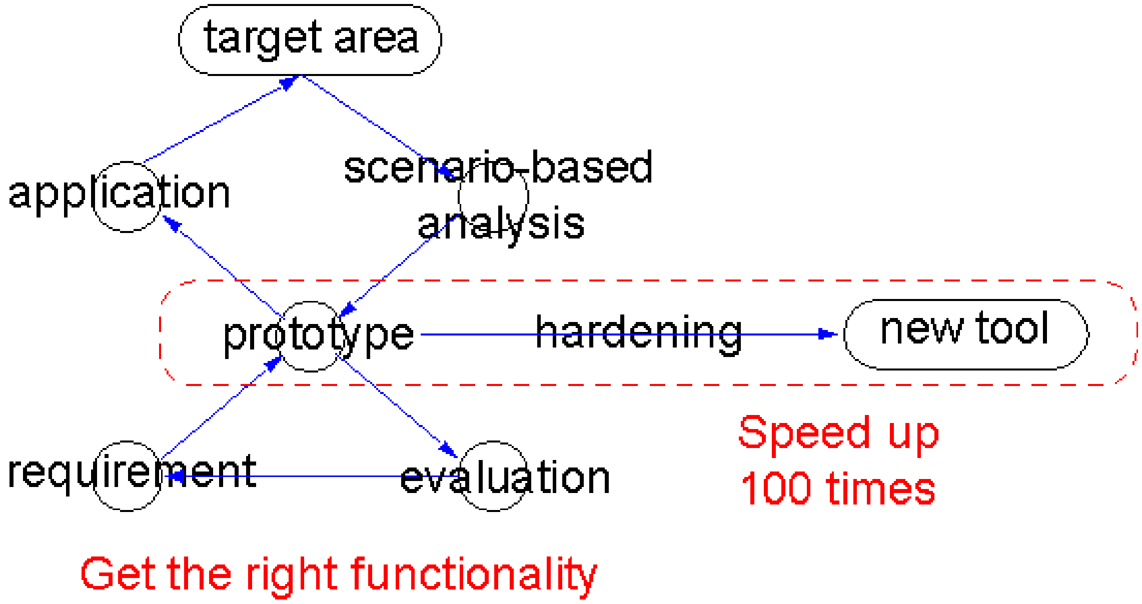
Goals

- To understand how to support worldwide, continually changing and rapidly formed virtual teams
- To support the three types of activities (the three O's)
  - \+ Ordinary
  - \+ Onerous
  - \+ Original

The "SEEM" hypotheses

- S:Design is a Social process
- E:Design is a continual Evolution
- E:Let the End user do the evolving
- M:Designers are continually constructing Models

An approach


target area
application
scenario-based analysis
prototype
hardening
new tool
requirement
evaluation
Speed up
100 times
Get the right functionality

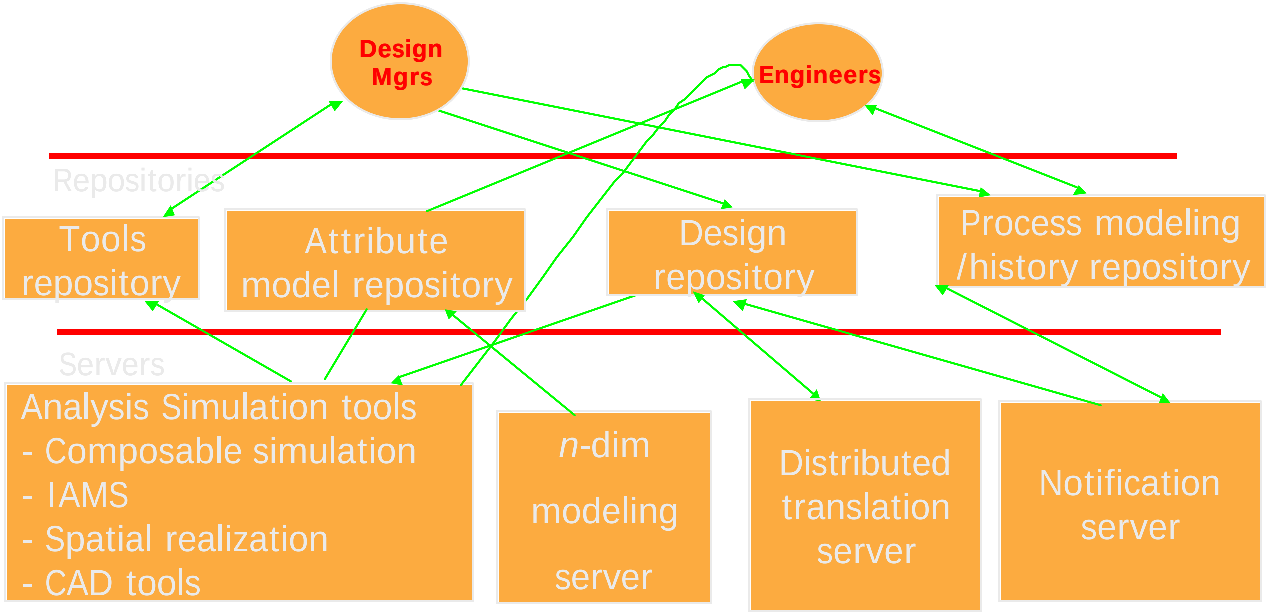
Software servers we have developed

- ***n*-dim** – general information modeling system ? rapid software prototyping system
- **LIRE’**– document repository / document converter for viewing and search
- **Babel** – document repository / document converter for viewing and search
- **AWARE** – general notification server

Current activities - combining these servers into larger tools

An example of putting all together in a system

A tool repository for mechanical design



Design Mgrs

Engineers

Repositories

Tools repository

Attribute model repository

Design repository

Process modeling /history repository

Servers

Analysis Simulation tools
- Composable simulation
- IAMS
- Spatial realization
- CAD tools

n-dim modeling server

Distributed translation server

Notification server

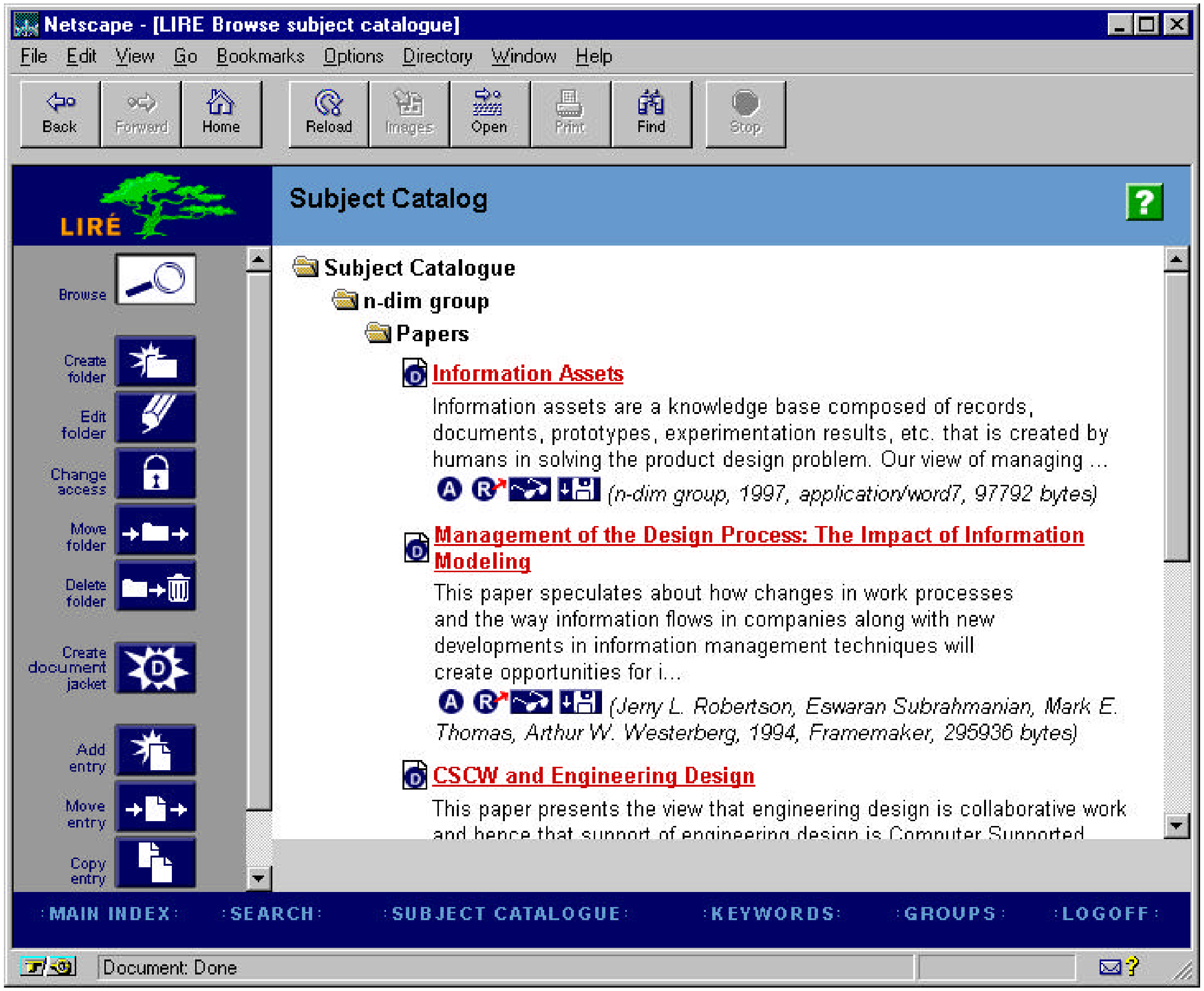
LIRE’ – LIving REpository

Features

- Accessible through Web
- Documents in flat file
- Folders and subfolders
- Access management
- Notification
- Annotations
- Keyword network
- Arbitrary relationships between docs
- Search over document contents and attributes
- NO LIBRARIAN (major hypothesis)

Some screen dumps

One organizes files in directories much like a PC



Subject Catalogue

n-dim group

Papers

Information Assets

Information assets are a knowledge base composed of records, documents, prototypes, experimentation results, etc. that is created by humans in solving the product design problem. Our view of managing ...

(n-dim group, 1997, application/word7, 97792 bytes)

Management of the Design Process: The Impact of Information Modeling

This paper speculates about how changes in work processes and the way information flows in companies along with new developments in information management techniques will create opportunities for i...

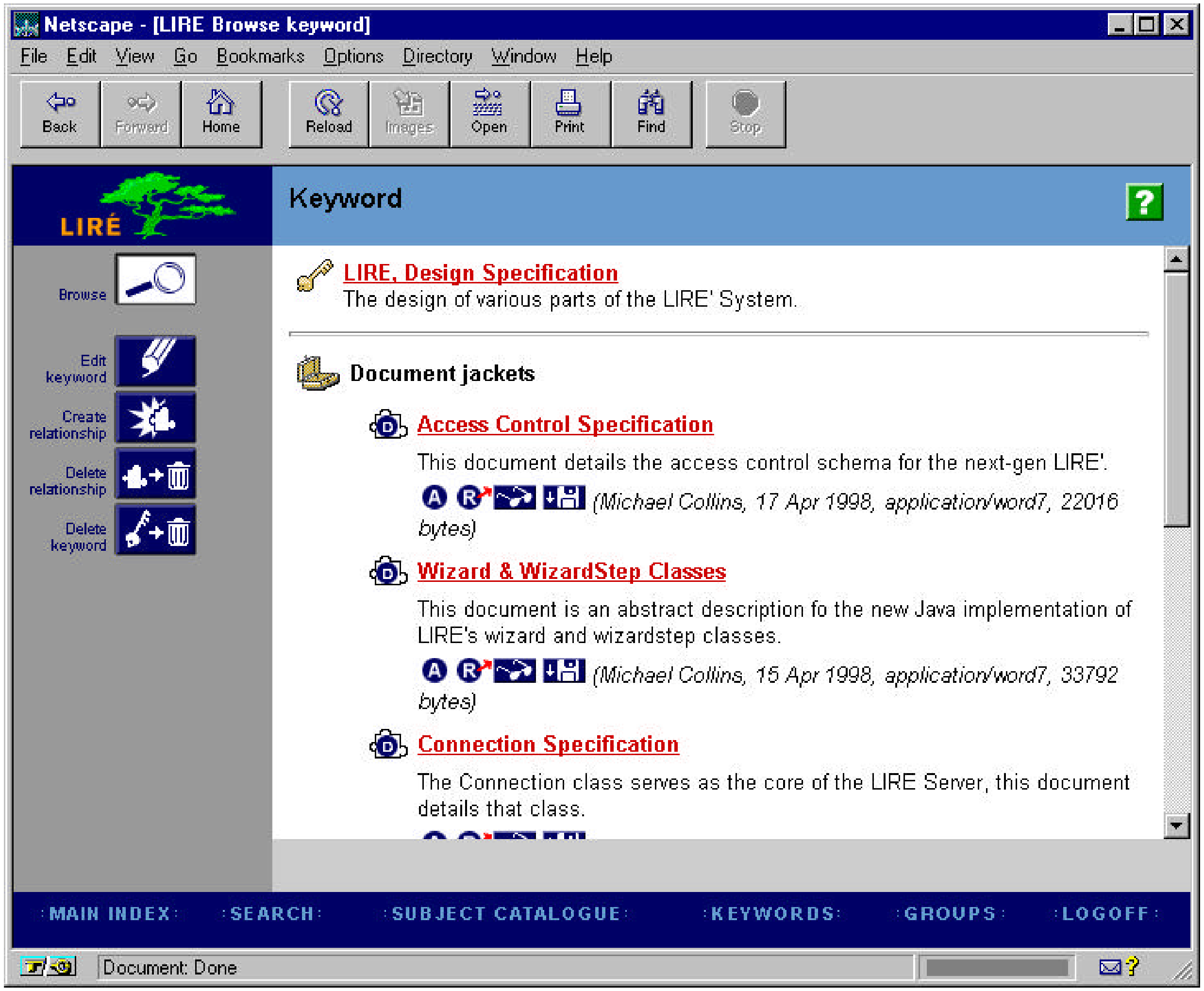
(Jerry L. Robertson, Eswaran Subrahmanian, Mark E. Thomas, Arthur W. Westerberg, 1994, Framemaker, 295936 bytes)

CSCW and Engineering Design

This paper presents the view that engineering design is collaborative work and hence that support of engineering design is Computer Supported

Document: Done

One can relate files through use of keywords (work/definition pairs organized in terminology hierarchy)



Keyword

LIRE, Design Specification
The design of various parts of the LIRE' System.

Document jackets

Access Control Specification

This document details the access control schema for the next-gen LIRE'.

(Michael Collins, 17 Apr 1998, application/word7, 22016 bytes)

Wizard & WizardStep Classes

This document is an abstract description fo the new Java implementation of LIRE's wizard and wizardstep classes.

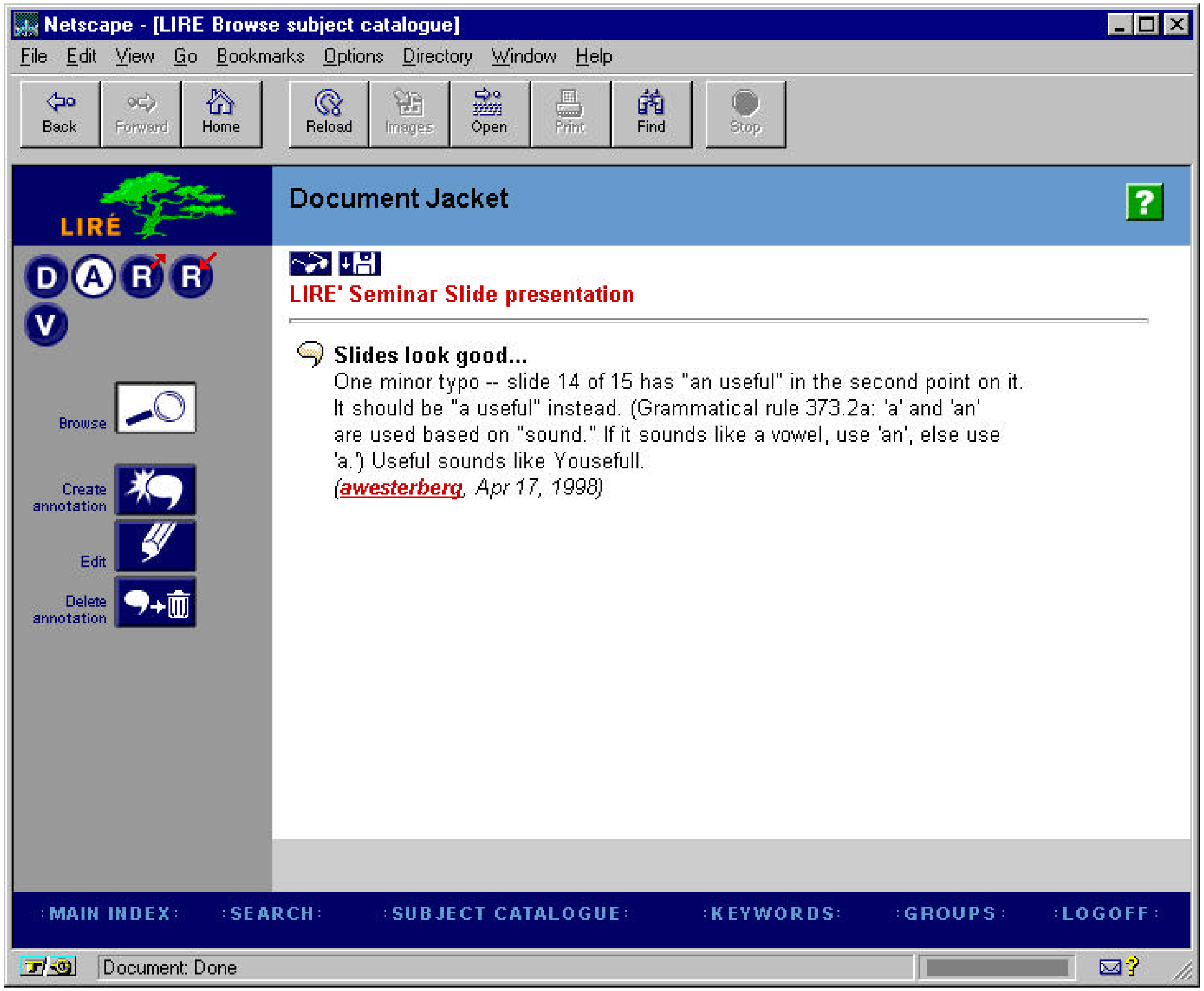
(Michael Collins, 15 Apr 1998, application/word7, 33792 bytes)

Connection Specification

The Connection class serves as the core of the LIRE Server, this document details that class.

Document: Done

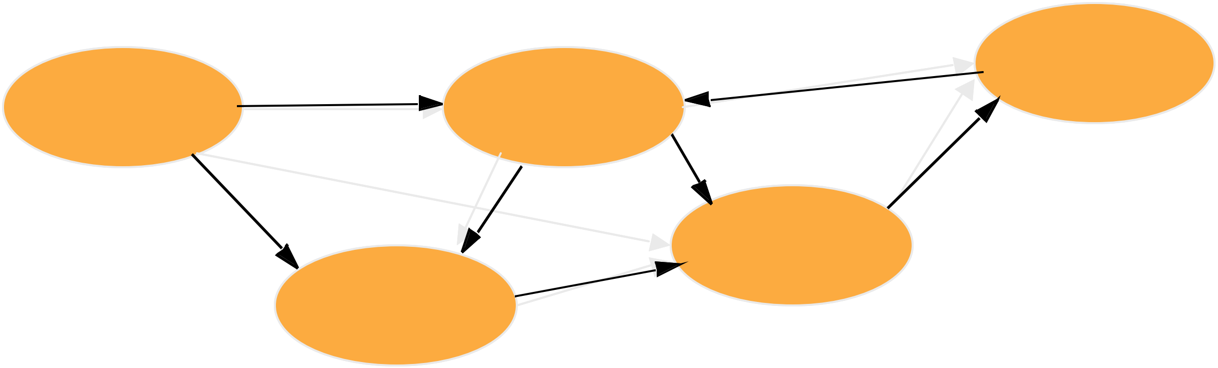
One can annote documents



LIRE' Seminar Slide presentation

Slides look good...
One minor typo -- slide 14 of 15 has "an useful" in the second point on it. It should be "a useful" instead. (Grammatical rule 373.2a: 'a' and 'an' are used based on "sound." If it sounds like a vowel, use 'an', else use 'a.') Useful sounds like Yousefull.
(awesterberg, Apr 17, 1998)

Babel – document translation server

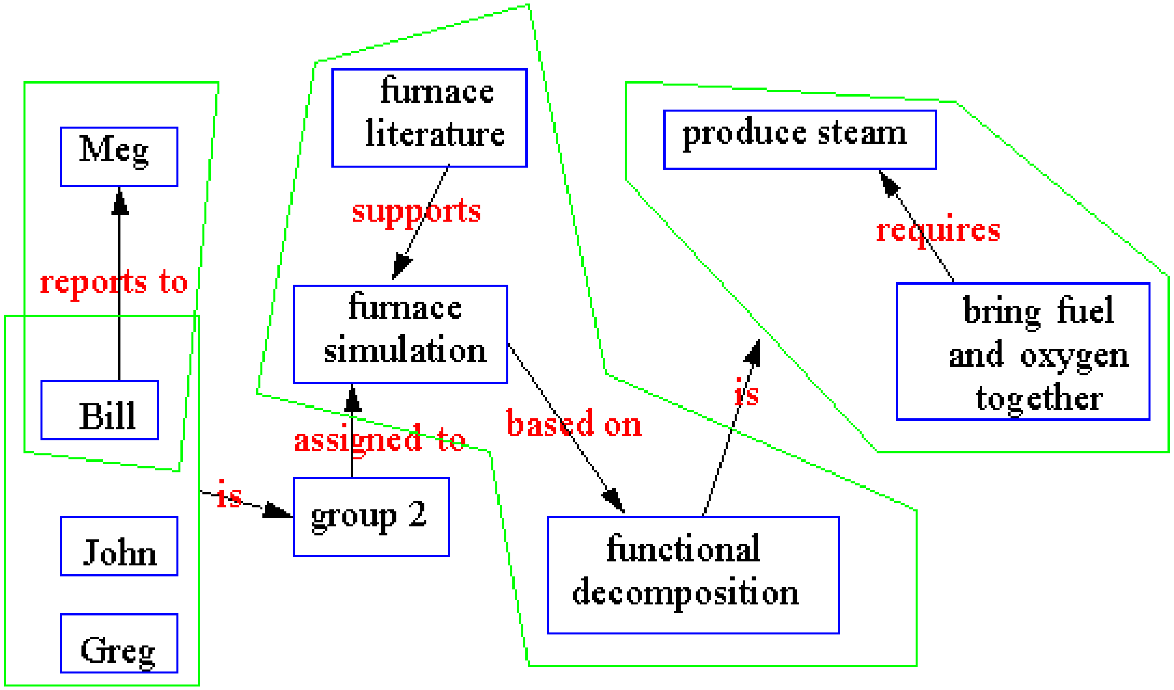


- Translates virtually any source into PDF and text files
- Can be separate multiple servers for reliability and speed

n-dim – n-dimensional information modeling

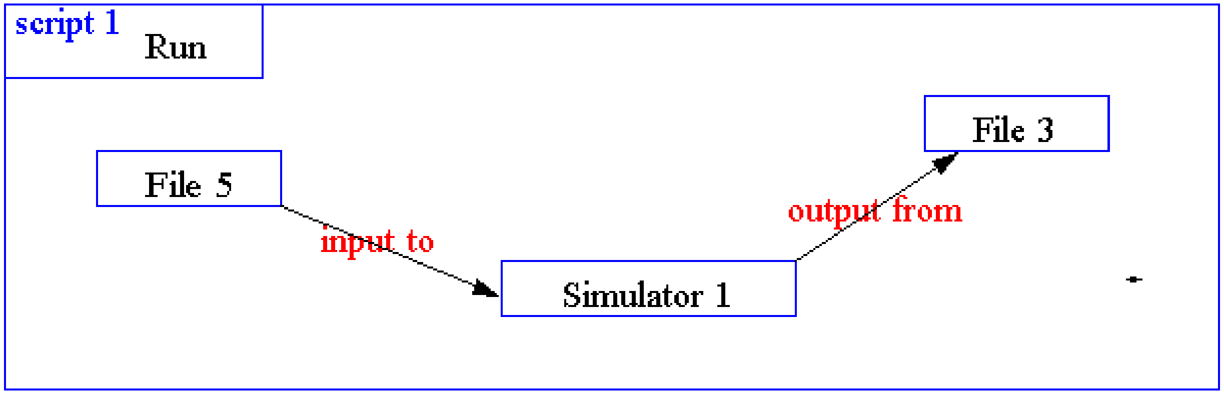
Arbitrary organization of information

In *n*-dim, one can organize any type of electronic information in an arbitrary fashion by grouping and relating with labeled links

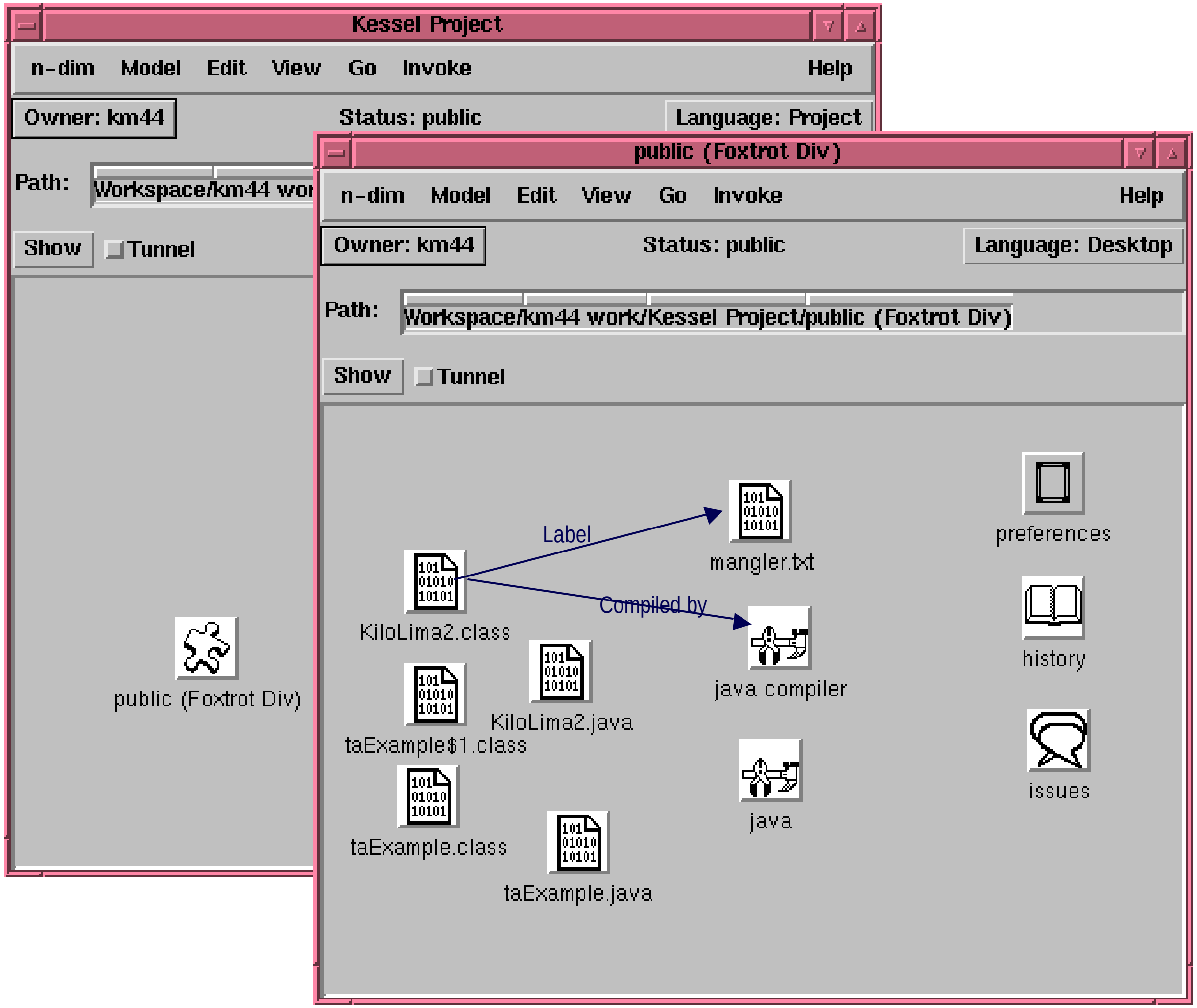


Operations in *n*-dim

One can run a script of instructions over any *n*-dim models



Screen dump of *n*-dim

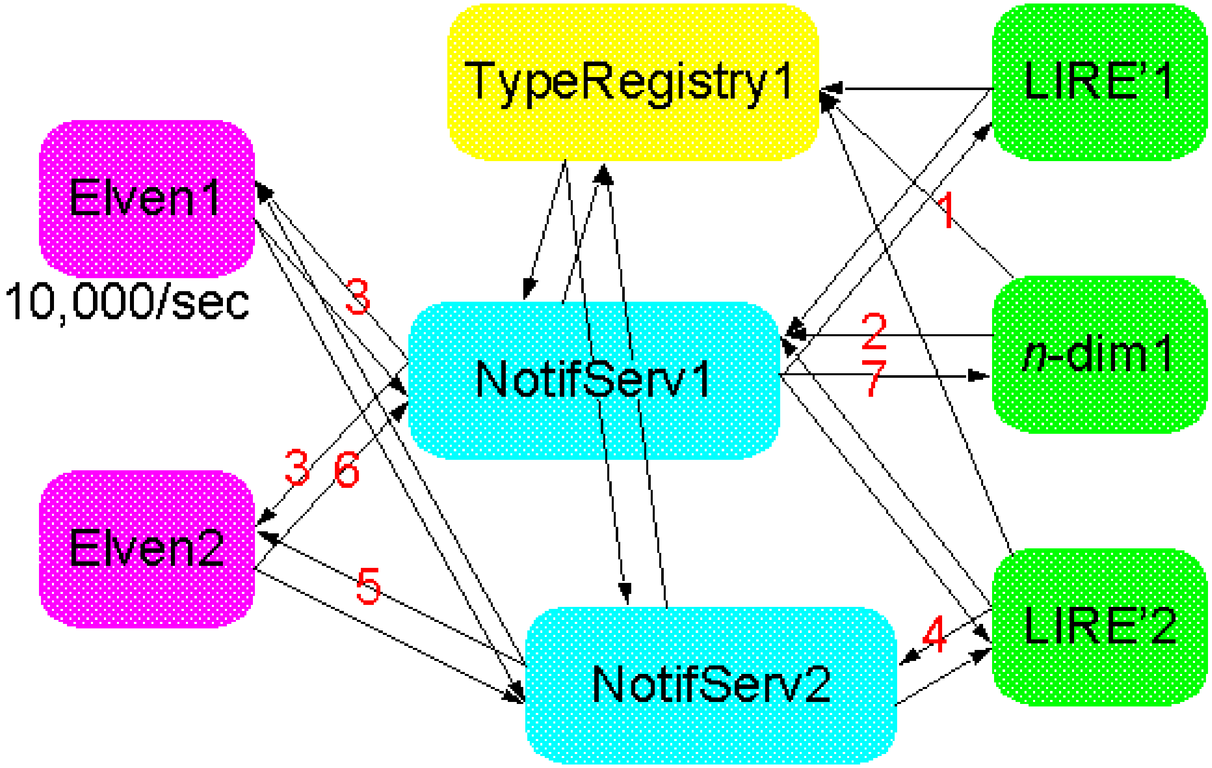


Owner: km44
Status: public
Language: Project
Path: Workspace/km44 wor

Owner: km44
Status: public
Language: Desktop
Path: Workspace/km44 work/Kessel Project/public (Foxtrot Div)

Notification Server (AWARE)

AWARE provides an event detection service. It can handle complex events distributed over the net (e.g., if someone changes a document in LIRE’ in Japan and then someone else from Europe annotates it, tell me)/



1. LIRE’1 registers LIRE’ with system, passing along a list of all events any LIRE’ server will report
2. *n*-dim1 posts request to be notified of future LIRE’ event
3. NotifServ1 posts event with all Elvens in system
4. LIRE’2 has event (e.g., someone changes a documents and then annotates it) which it passes to NotifServ2.
5. NovifServ2 passes event to Elven2.
6. Elven2 tells NotifServ1 one of its events has occurred.
7. NotifServ1 tells *n*-dim1 its event has occurred.

Features

- All NotifServ's can be duplicated to increase system capacity.
- Elven's can process 10,000 simple events/second.
- Elven software available over net from Australia.

Integrations we have completed among servers

Current

- LIRE' uses Babel for translations
- LIRE' uses NotiS for notifications

Almost completed

- *n*-dim model as stored object in LIRE'
- LIRE' objects as objects in *n*-dim

Tools for preliminary design

- Coming up with new ideas, setting some goals
  - + Quality Functional Deployment (QFD)
  - + Pugh’s method
- Emphasizing quality
  - + Taguchi’s method
- Setting goals -- what stakeholders want
- Managing time (as in Microsoft Project)

Quality function deployment

Ex: Create a new candy for children

Goals

- Maximize appeal to children
- Maximize appeal to the parents who buy the candy
- Be nutritionally acceptable

Creating a first House of Quality matrix

In the QFD method, one creates any number of HoQ matrices to rate how well competitors meets goals, to rate how well certain ways to implement product meets goals, etc. One should construct such a matrix to rate anything against anything else related to the design.

Example 1: HoQ for competitive products

- One column for each existing competitive product
- One row for each of the above goals
- In each cell for the above, rate how well each product meets each goal using scores from -5 (antithesis of goal), 0 (neutral in meeting goal) to +5 (meets goal in outstanding fashion)

- Highlight best in row in red
- Add in a column of row averages and a row of column averages
- Finally add in a column giving target for our new candy

=> Purpose of HoQ matrix: make you think about every cell in matrix.t

Example 1: Competitors vs. goals

	Pqws Chocolate Drops	Mnys Bars	Xyz Fruit Drops	Row average	Our Company Target
Appeal to Children	-2	3	0	0.33	3
Appeal to Parents	3	-1	4	2	5
Nutritional acceptable	-1	-1	-2	-1	0
Column average	0	0.33	0.67	0.4	2.67

The final column makes us think about what will be better about our product that would make it sell.

Example 2: Features vs. goals

We may wish to list possible features that could affect goals to aid us to select which features we wish to use.t

Example 2: Features vs. goals

	Sugar content	**Shape**	**Size**	**Color**	**Row average**
Appeal to Children	3	5	2	4	3.5
Appeal to Parents	-3	3	4	2	1.5
Nutritional acceptable	-4	0	-2	0	-1.5
Column average	-1.3	2.7	1.3	2	

General HoQ matrices

One can develop a very general form for an HoQ matrix, which becomes a matrix of matrices. A prototypical form is as follows. The added rows in this matrix give matrices of things we can rate vs. possible technical specifications, for example. Often one gets caught up in the “rules” of construction. Instead, simply think of using matrices like this to list things against things and rate them in some useful fashion. It is the thoroughness of thought that matters, which comes from filling in each rating for each option.

Supermatrix for HoQ analysis to set design specifications

	List of technical specifications	Column for each competitor (as with candy example) 1 2 3 ....n	Our product targets (alla Pugh)
List of functional requirements	Sensitivities indicating how the technical specs affect the functional requirements	Competitor scores - how well each meets functional requirements	Values we are targeting

Supermatrix for HoQ analysis to set design specifications

	List of technical specifications	Column for each competitor (as with candy example) 1 2 3 ....n	Our product targets (alla Pugh)
Rows for: * Column Weights * Competitor 1 * Competitor 2 . * Competitor n	Specifications used by all our competitors		
Rows for: Technical difficulty. Cost. Target cost.	Product goals for technical specs we should use		

Pugh’s method for concept generation

Pugh proposes one set up a House of Quality matrix with the intent to expose where one needs to develop new technology or technologies if one wishes to have a really good new product.

- rows: goals for product
- columns: known technologies for creating products that meet these goals
- matrix elements rate how well each technology meets said goal
- final column is a set of target element values for the new product. One or more of those elements will be “out of range” for any of the known technologies. It is here that one needs new technologies.

Example - homework

Set up such a matrix for designing a new device to remove corks from wine bottles. Discover where some new technological breakthrough would make a real improvement in such a product. Brainstorm on how you might create this technological breakthrough.

Taguchi's method

=> Proposition: Quality equates to product consistency

Classic example

- Start to tile your kitchen counter area
- Purchase added tiles to finish job

The irritation starts if tile sizes and colors do not match exactly

=> Proposal: modify manufacturing methods to reduce product feature variation while manufacturing -- i.e., can one reduce variations by how one manufactures the tiles?

Answer: If one increases the clay content of the tile, the tiles are much more uniform in size and just as nice in appearance, in spite of uncontrolled variations that occur in ambient temperature, humidity and in clay and sand compositions.

The Taguchi procedure to find this answer

Conjecture why tile size varies?

- Uncontrolled and unmeasurable variations in
  - materials used (variability in raw materials supply)
- Uncontrolled but measurable variations in
  - ambient humidity while glazing
  - ambient temperature while glazing
- Controlled and measurable variations in
  - oven temperature
  - glazing time
  - relative amounts of clay, sand, ...

One is creating a so-called “fish” diagram here in which one conjectures an effect and then diagrams all possible causes for that effect. Here one is conjecturing what causes product variability while manufacturing.

Determine sensitivies quantitatively

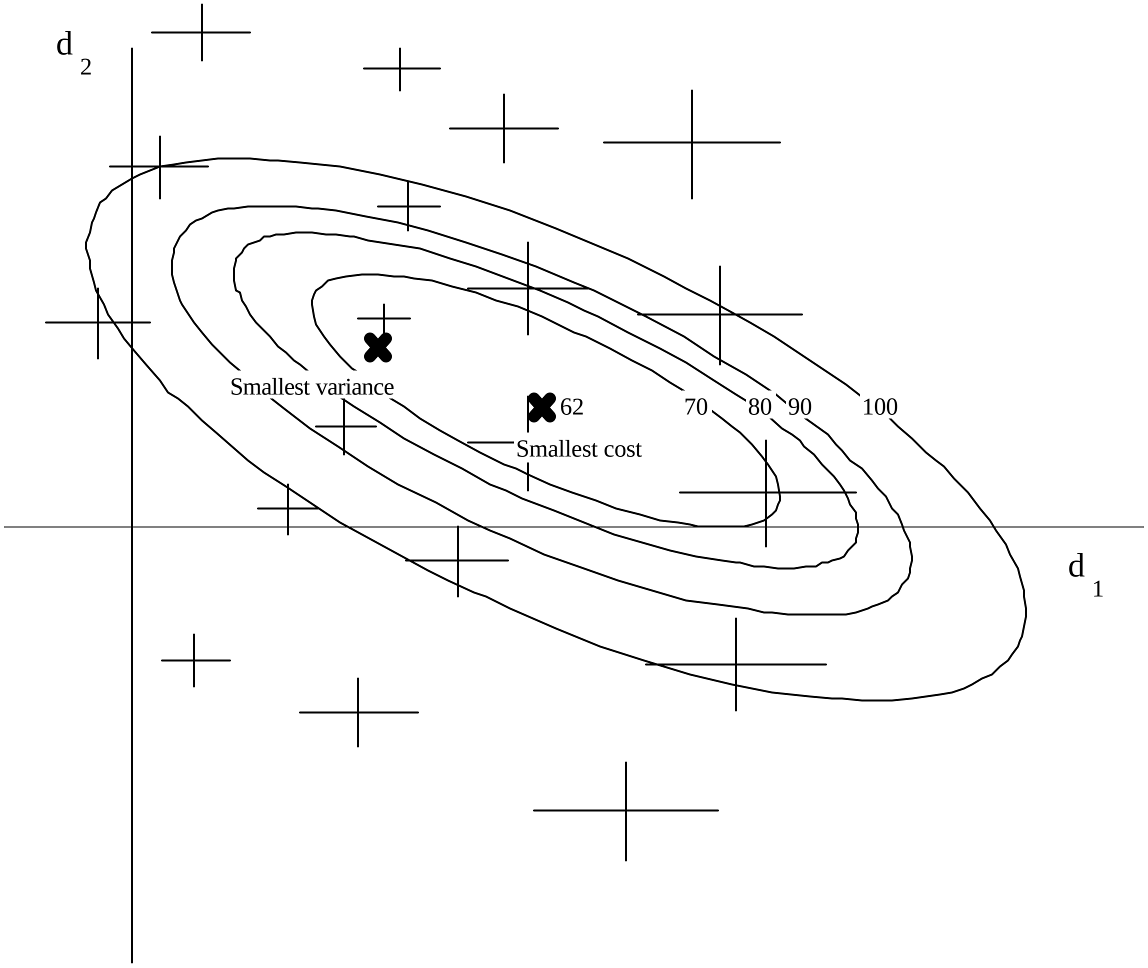
- Through well designed experiments, determine impact on uncontrolled variances of tile size to each of the measurable variations. Using repeated experiments estimates variances due to all variables one cannot measure. *(Use good experimental design techniques -- e.g., factorial designs -- here. Find a company expert to help on this. Experiments are generally very time consuming and expensive. Good design minimizes the number of experiments needed to get the quantitative estimates one seeks.)* Discover sensitivities by varying controllable variables and by measuring uncontrollable but measureable variables.

Set minimizing product variability as one of the design goals

- Use as one of the goals for the design to minimize variance in product size by choice of controlled variable values.

Example of results

The following diagram has two goals simultaneously included. The contours indicate costs to manufacture while the crosses indicate product variability. Clearly one has to trade off cost and variability.



Final comment

Taguchi pointed out that one can set up very crude measures for variability and still get much reduced manufacturing variances. So do not get sidetracked here by trying to be too precise.

Simple support tools to aid in meeting customer needs

Ref: Dym and Little, Preliminary Product Design (2001).

- Discovering and organizing what stakeholders want
  - Objective trees
- Organizing effort
  - Work breakdown schedules (WBS)
  - Linear responsibility charts (LRC)

Objectives trees -- for creating and organizing objectives

Example

Design of a Device for Teaching Asthma Management and Control

Client’s Statement

It is desired to develop a teaching mannequin, and/or torso and head, with the following characteristics:

- show simplified respiratory system (section)
- upon application of a trigger (cigarette) airways contract, produce mucus, wheezing, retraction
- upon application of rescue inhaler, airways open up, mucous stops, no wheezing, no retraction
- include breathing sounds (wheezing)
- include skin retraction
- size of a 5 year-old’s torso (big enough to clearly show the effects of asthma)

The production specifications for the device are:

- durable (can withstand moving and rough handling)
- keep production cost at or around $500

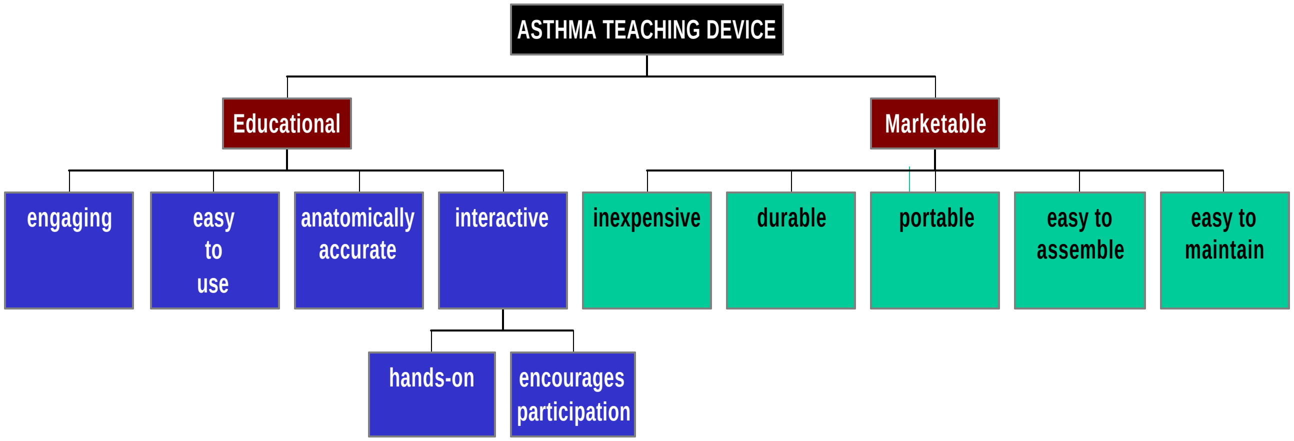
Clarification of the Need Statement

“Design a device for teaching asthmatic and non-asthmatic children how to manage and control asthma.”

Attributes List

- Interactive
- Educational
- Engaging
- Easy to use
- Easy to assemble
- Easy to maintain
- Safe/non-toxic
- Anatomically accurate
- Aesthetically pleasing
- Durable
- Inexpensive
- Portable

Preliminary Objectives Tree

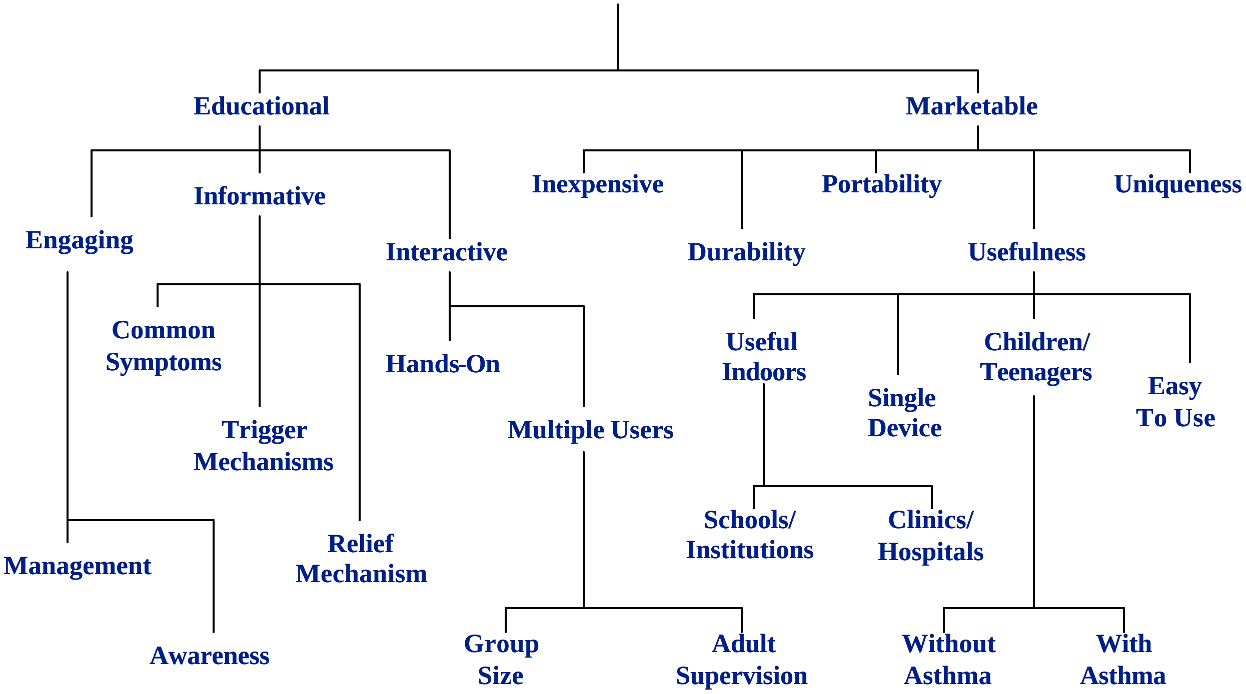


- ASTHMA TEACHING DEVICE
  - Educational
    - engaging
    - easy to use
    - anatomically accurate
    - interactive
      - hands-on
      - encourages participation
  - Marketable
    - inexpensive
    - durable
    - portable
    - easy to assemble
    - easy to maintain

Constraints

- Used for children ages 6 to 18 years old
- Sales price <$500
- Prototype price <$1000
- Must be portable
- Entire device should be lighter than 25 lbs
- Removable parts must be lighter than 3 lbs

Objectives Tree



Why Create an Objectives Tree?

- To clarify and organize goals for the project
- To keep the design team focused
- To have a written record of agreed-upon goals
- It can be modified as the project progresses

Guidelines

- Do not limit your preliminary attributes list
- Include everything you can think of
- Then separate the list into:
  - + Attributes
  - + Functions and implementations
  - + Constraints
- Include goals for the object being designed, not for the design process itself
- In the objectives tree, list only attributes
- When you start listing functions, you’ve gone too far!

What needs to be done and who will do it?

Advice -- spend no more than 10% of your time organizing your time

Work Breakdown Schedules (WBS)

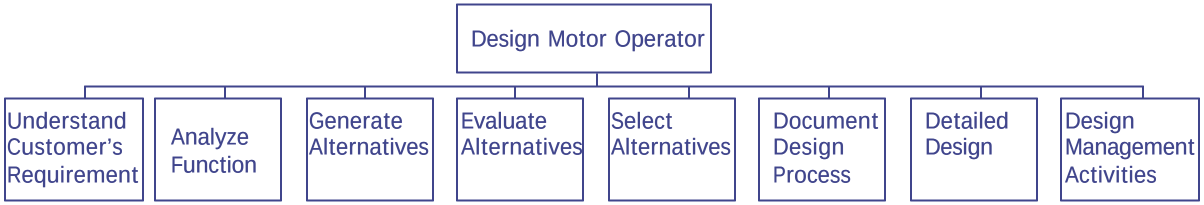
Best guess as to the breakdown of everything that has to be done for the project into discrete, measurable tasks

Linear Responsibility Chart (LRC)

Assignment of responsibilities for each item in WBS

Examples

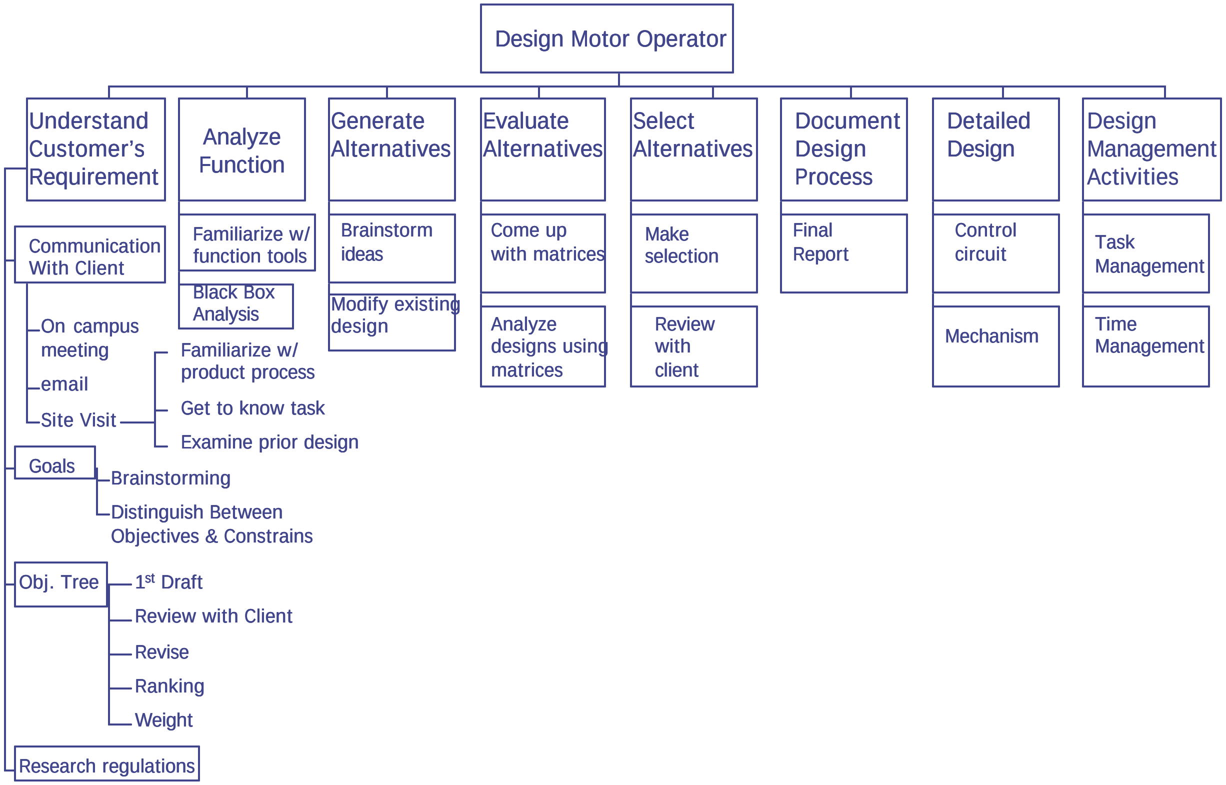
High level tasks conjectured early in design process for a circuit breaker design project



Design Motor Operator

- Understand Customer's Requirement
- Analyze Function
- Generate Alternatives
- Evaluate Alternatives
- Select Alternatives
- Document Design Process
- Detailed Design
- Design Management Activities

Fleshing out the tasks - a more complete WBS



- Design Motor Operator
  - Understand Customer's Requirement
    - Communication With Client
      - On campus meeting
      - email
      - Site Visit
        - Familiarize w/ product process
        - Get to know task
        - Examine prior design
    - Goals
      - Brainstorming
      - Distinguish Between Objectives & Constrains
    - Obj. Tree
      - 1st Draft
      - Review with Client
      - Revise
      - Ranking
      - Weight
    - Research regulations
  - Analyze Function
    - Familiarize w/ function tools
    - Black Box Analysis
  - Generate Alternatives
    - Brainstorm ideas
    - Modify existing design
  - Evaluate Alternatives
    - Come up with matrices
    - Analyze designs using matrices
  - Select Alternatives
    - Make selection
    - Review with client
  - Document Design Process
    - Final Report
  - Detailed Design
    - Control circuit
    - Mechanism
  - Design Management Activities
    - Task Management
    - Time Management

Linear responsibility chart

	Chris	Li	Mike	Anne	Daniel	Sittan	Lutz
Understanding Customer Requirements							
Goals	1		1				
Brainstorming		2		3	3	3	3
Distinguish Obj.& Constr.		2		3	3		
Objectives Tree	1		1				
1st Draft	2	2	2			3	3
Review with client		2	1		3		
Revise	1			3	3	3	
Ranking		2	1			3	
Weight	1	2	1	3			3
Research Regulations					3		3

1: Approval, 2: Consult, 3:Work

Some time management tools (e.g., using Microsoft Project)

Questions to be addresses

- What do we have to do when?
- When are things due?
- Where are we in this process?
- What do we do next?
- Who will do what?
- Is there time to relax?

Tools one can use

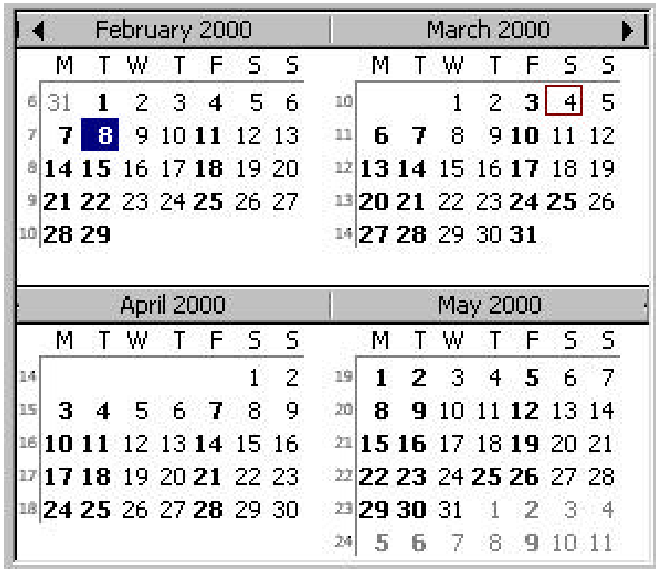
- Calendar
- Activities Network
- Gantt Chart
- Percent-Complete Matrix
- Budgets

Calendar

Place on calendar the following items --

- Due Dates
- External & Internal Deadlines
- Meeting Dates
- Vacations / Illness

Hard to see order of tasks



February 2000

	M	T	W	T	F	S	S
6	31	1	2	3	4	5	6
7	7	8	9	10	11	12	13
8	14	15	16	17	18	19	20
9	21	22	23	24	25	26	27
10	28	29					

March 2000

	M	T	W	T	F	S	S
10			1	2	3	4	5
11	6	7	8	9	10	11	12
12	13	14	15	16	17	18	19
13	20	21	22	23	24	25	26
14	27	28	29	30	31		

April 2000

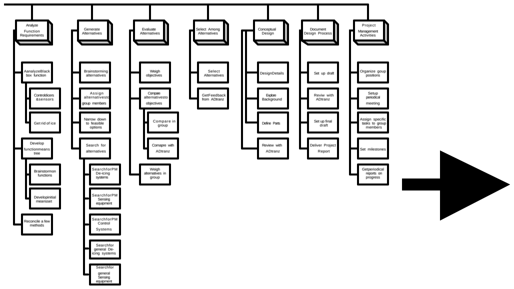
	M	T	W	T	F	S	S
14						1	2
15	3	4	5	6	7	8	9
16	10	11	12	13	14	15	16
17	17	18	19	20	21	22	23
18	24	25	26	27	28	29	30

May 2000

	M	T	W	T	F	S	S
19	1	2	3	4	5	6	7
20	8	9	10	11	12	13	14
21	15	16	17	18	19	20	21
22	22	23	24	25	26	27	28
23	29	30	31	1	2	3	4
24	5	6	7	8	9	10	11

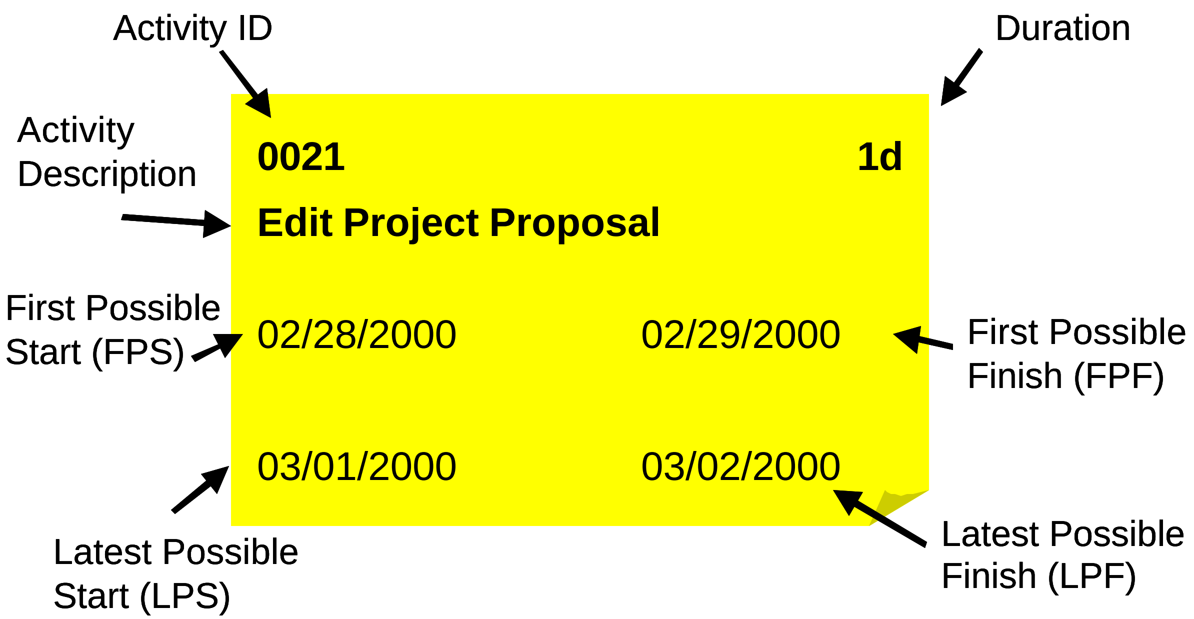
Activity networks, Gantt charts, and the like

- Using WBS, estimate time duration for tasks



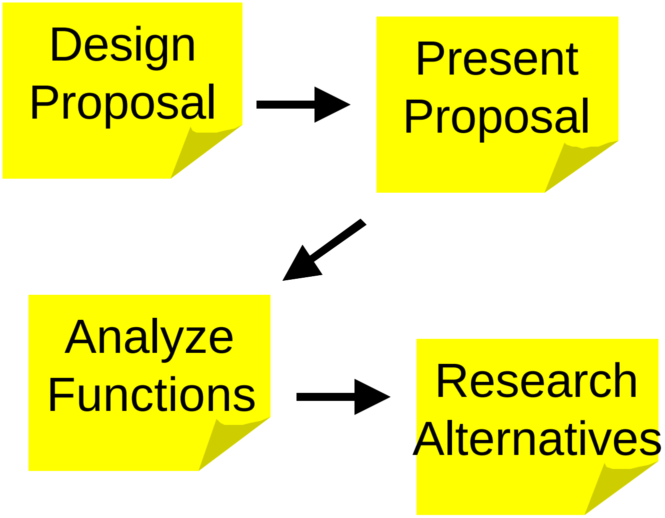
Design Proposal Paper	9d
Presentation of Proposal	8h
Analyzing the deicing functions	3d
Analyzing Communications Functions	3d
Brainstorming for Necessary Function	1d
Choosing deicing & communication methods	1d
Brainstorm for alternatives	1d
Research alternatives	6d
Evaluate alternatives against objectives	1d

- Create Post-Its for each task



“Latest” - “First” = “Slack”

- Place an partial ordering over the tasks



- Enter into Microsoft Project or equivalent software and create
  - Activity network (above partial ordering)
  - a Gantt chart which indicates graphically among the projects

Description

Duration

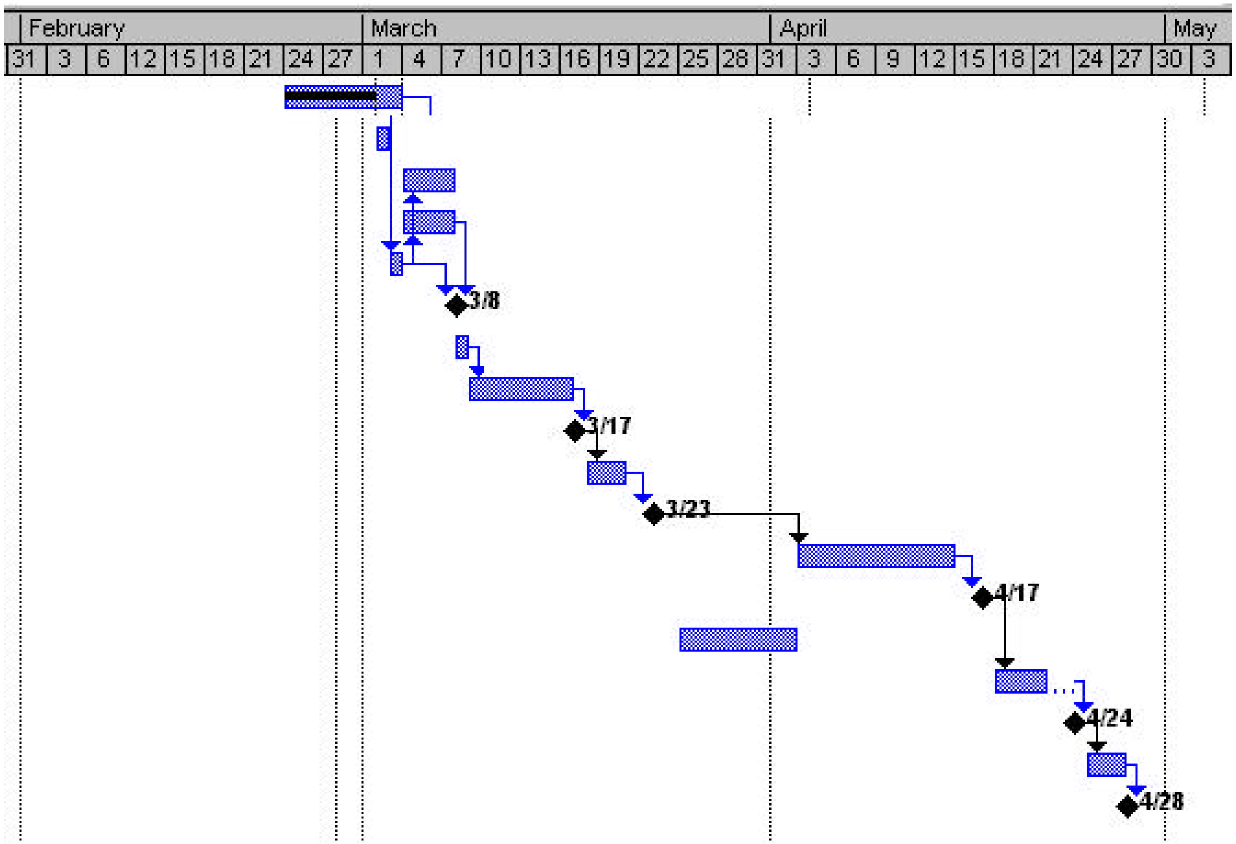
Start/Finish Date

Duration Bar

Critical Point

Milestone

Logical relationships



- a textual output showing start and finish time

Task Name	Start	Finish
Design Proposal Paper	2/21/2000 8:00	2/29/2000 17:00
Presentation of Proposal	3/2/2000 8:00	3/2/2000 17:00
Analyzing the deicing functions	3/4/2000 8:00	3/7/2000 17:00
Analyzing Communications Functions	3/4/2000 8:00	3/7/2000 17:00
Brainstorming for Necessary Function	3/3/2000 8:00	3/3/2000 17:00
Chosing a few methods for deicing and communications	3/8/2000 8:00	3/8/2000 17:00
Brainstorm for alternatives	3/8/2000 8:00	3/8/2000 17:00
Reseach alternatives	3/9/2000 8:00	3/16/2000 17:00
Evaluate Alternatives against weighed objectives	3/17/2000 8:00	3/17/2000 17:00
Weighing alternatives	3/18/2000 8:00	3/20/2000 17:00
Selecting Alternatives with Adtranz	3/23/2000 8:00	3/23/2000 17:00
Creating a conceptual design	4/3/2000 8:00	4/14/2000 17:00
Review conceptual design with Adtranz	4/17/2000 8:00	4/17/2000 17:00
Spring Break	3/25/2000 8:00	4/2/2000 17:00
1st Draft of Conceptual Design	4/18/2000 8:00	4/23/2000 17:00
Review with Draft with Adtranz	4/24/2000 8:00	4/24/2000 17:00
Finalize Document	4/25/2000 8:00	4/27/2000 17:00
Final Meeting with Adtranz	4/28/2000 8:00	4/28/2000 17:00

Percent-complete matrix (PCM)

What is it?

- Tracks how team performs according to plan
- Uses information from WBS
- Relates extent of work done to status of entire project
  - + Money
  - + Physical measures
  - + Time

How to construct it

- Use estimated time duration of activities to track progress
  - + Time estimates must be accurate
- Simple rules for implementation
  - + 33% complete when activity started
  - + At completion, remaining 67% awarded
  - + No more than 100% credit awarded

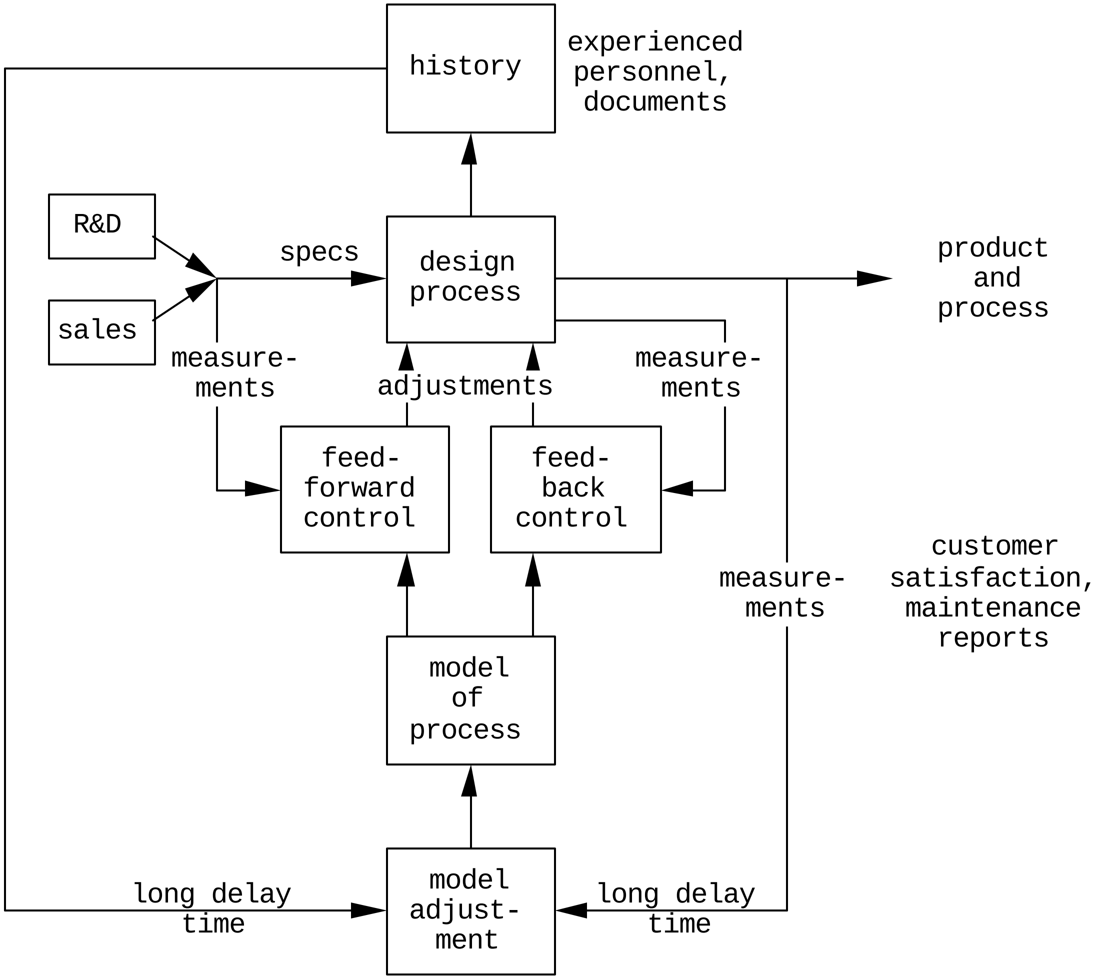
The completion percentages show up on an updated Gantt chart

Budget

Using above information, one should estimate expenditure of resources to date and cost of resources to complete if one wishes to track this information. When budget estimates change signficantly, one has an indicator that a project is likely in trouble.

Designing the design process

What is the design process -- a “control loop” view



Design of a chemical process vs design of a design process

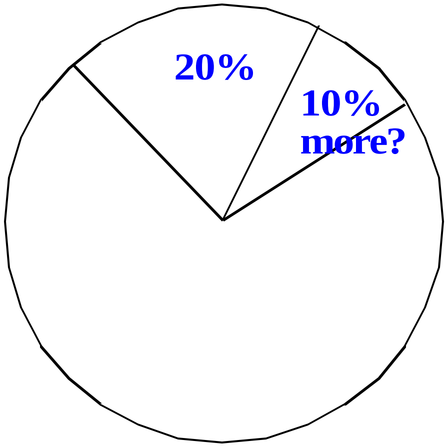
Design of a chemical process

- Goals
  - + Profitable
  - + Safe
  - + Flexible
  - + Operable
- Tests
  - + Simulations
  - + Committee reviews
  - + Hazops
- Design space
  - + From existing unit operations
- Starting points
  - + Previous design
  - + Entirely new design

Design of a design process

- Goals
  - + Effectiveness
  - + Do not destroy morale
- Tests
  - + Predict performance
  - + Committee reviews
- Design space
  - + Hierarchical teams
  - + Asynchronous teams
- Starting points
  - + Existing policies and procedures
  - + Entirely new approach

Potential for improvement



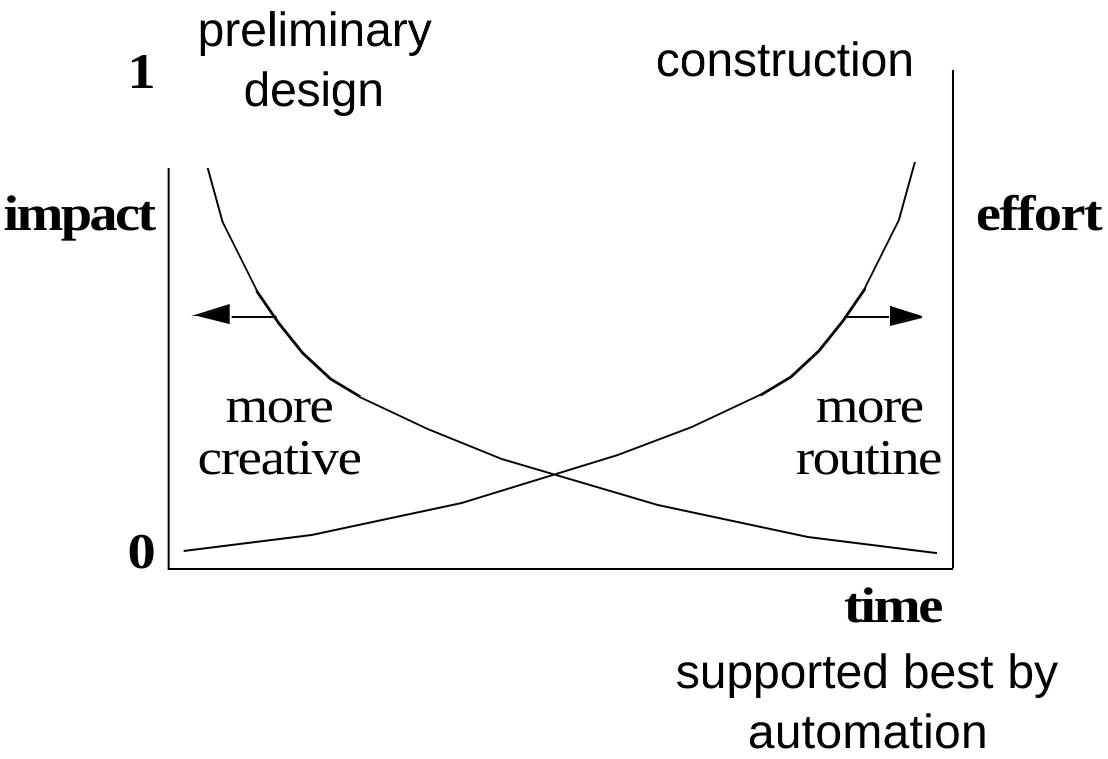
Companies capture only about 20% of their intellectual capital created when designing

Who designs design processes?

- Re-engineering “experts”
- Preparers of policy/procedure manuals
- Technical support environment creators
- Developers of “Colab”
- Design framework/planner creators
- CSCW efforts
- Empirical studies
- INPRO group at Trondheim

- Actually -- maybe we all do

Impact vs. effort

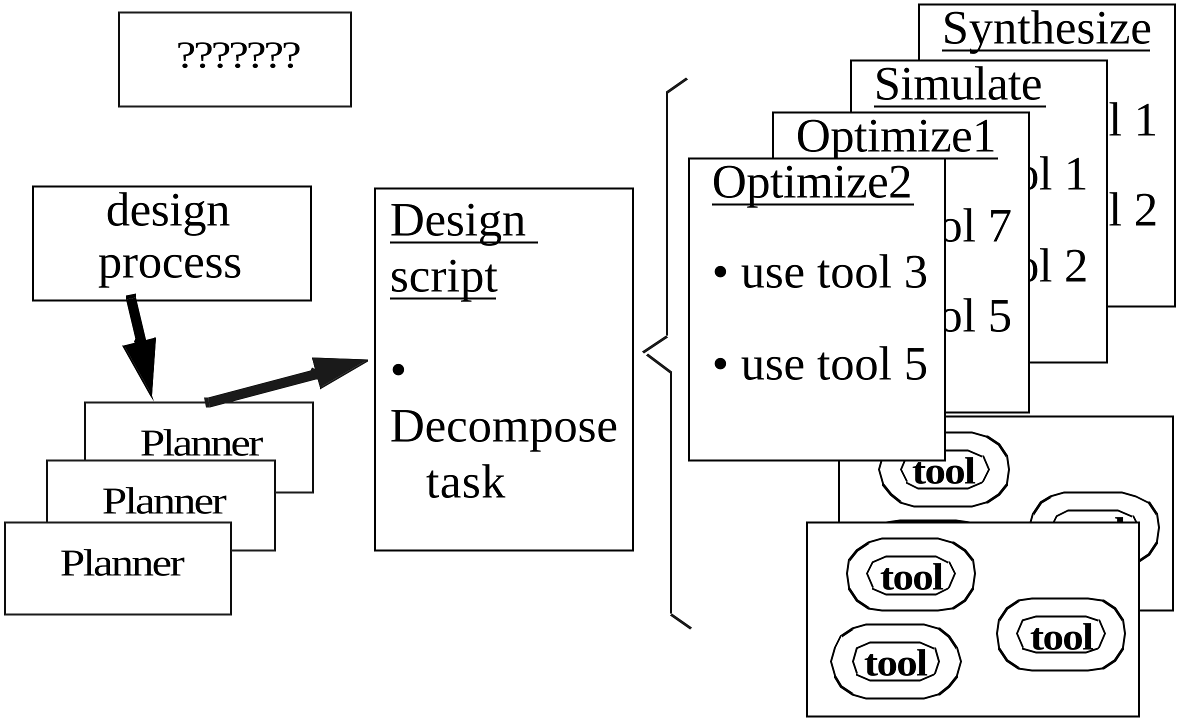


preliminary
design

construction

supported best by
automation

Advanced design frameworks -- for routine design



???????

design process

Planner

Planner

Planner

Design script

• Decompose task

Synthesize

Simulate

Optimize1

Optimize2

• use tool 3

• use tool 5

But will this framework support non-routine design? (No.)

Need for anarchy and standardization


anarchy - personal views

standardized structuring of information

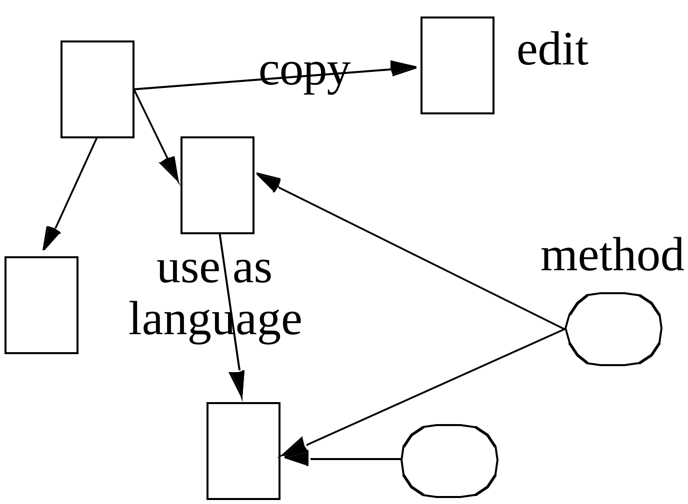
learning

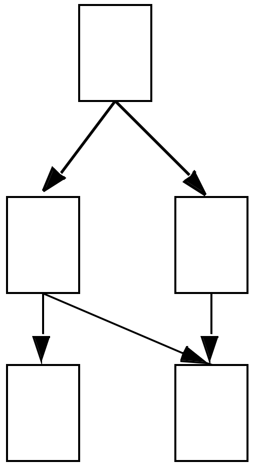
automation

=> anarchy allows end users to participate in creating and modifying standards, policies, procedures, etc.

Prototype-based vs class-based inheritance for design

Design is prototype-based -- class-based suggests routine and well understood behavior





- Methods attached (and removed) from instances (very powerful programming paradigm)

And some technical issues we must resolve

- Approach to organize information
- Providing standardization
- Managing data storage and retrieval
- Providing private and public access mechanisms
- Providing history maintenance
- Managing revisions
- Handling events
- Supporting end user addition of “operations”

The Creation of ASCEND, a Modeling System for Hard Science and Engineering Problems

by

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USA

*** Demo first ***

ASCEND

- Why we developed ASCEND
- Features of the ASCEND system
  - + language
  - + solvers
  - + interactive user interface
  - + debugging aids

Modeling - general discussion

- Modeling is a product design problem
  - Modeling is more than
  - writing down some equations
  - coding
  - solving
- Modeling is hard
  - Writing a correct model
  - Writing a maintainable model: the issues of elegance and reuse
  - Correctly handling degrees of freedom
  - Dealing with different ways models fail to converge
  - Thou shalt not divide

Acknowledgements

Pre ASCEND III

Dean Benjamin
Larry Gaydos

ASCEND III

Peter Piela
Tom Epperly
Karl Westerberg
Roy McKelvey
Joseph Zaher
Oliver Smith
Neil Carlberg

ASCEND IV

Kirk Abbott
Ben Allan
Tom Epperly
Robert Huss
Vicente Rico Ramirez
Mark Thomas
Boyd Safrit
Kenneth Tyner

Why did we develop ASCEND?

Because modeling is extremely hard.

- Graduate students can take several months to over a year to develop what look like simple models

We want this process to take one tenth this time.

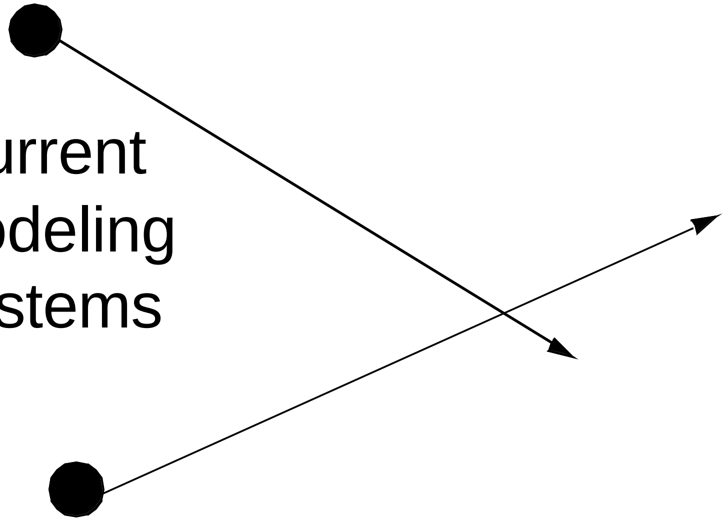
ASCEND related Ph.D. projects (date started)

Approach: ask hard questions about modeling

- **1984**: (Piela) Reduce modeling effort by order of magnitude
- **1988**: (Zaher) Formulate and solve regional models
- **1991/2**: (Abbott and Allan) Increase size of model we can solve by order of magnitude (on same workstation)
- **1992**: (Allan) Give typical end user the possibility to reuse complex models developed by others
- **1993**: (Rico-Ramirez) Continue work on regional models
- **1993**: (Tyner) Significantly improve solver reliability

Goals for ASCEND

- To provide scientists and engineers with a modeling system for very hard science and engineering problems
- To be a modeling environment that pushes the limits of what is possible

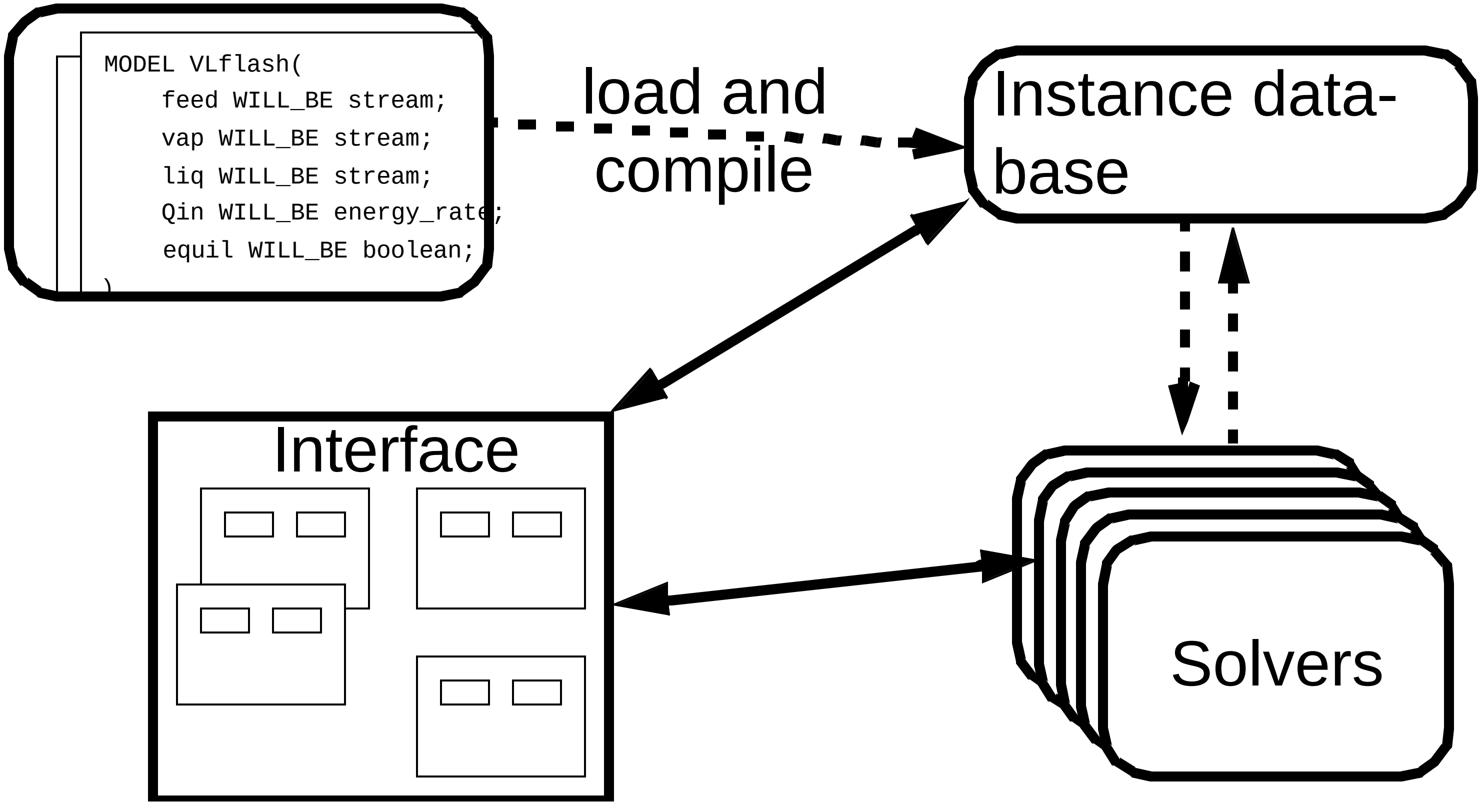


current modeling systems

ASCEND: push on the edges to find out what is possible

What is the ASCEND system?

- A modeling language
- An interactive interface
- A suite of solvers



```
MODEL VLflash(
    feed WILL_BE stream;
    vap WILL_BE stream;
    liq WILL_BE stream;
    Qin WILL_BE energy_rate;
    equil WILL_BE boolean;
)
```

load and compile

Instance database

Interface

Solvers

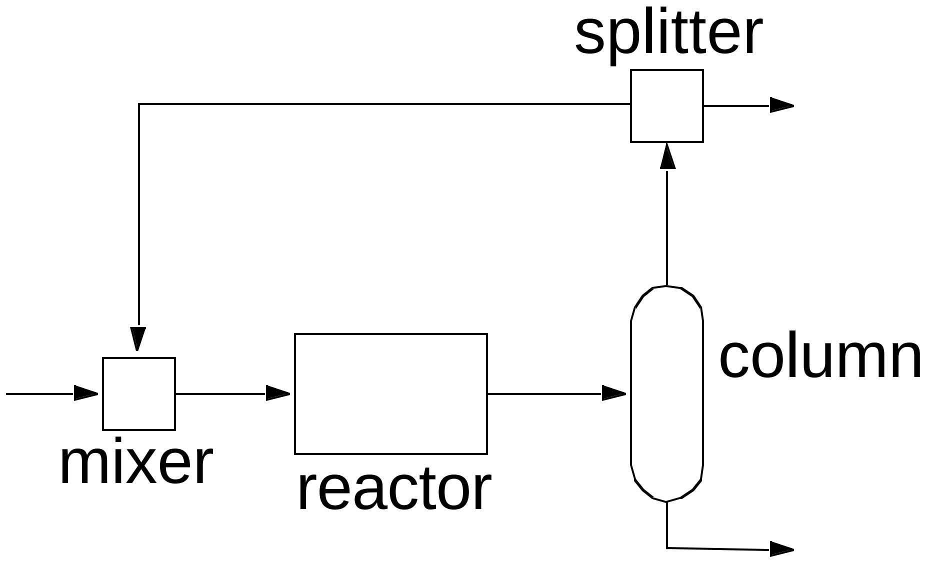
Typical execution of an ASCEND model

(Debugging aids at every step)

- Using editor, create text file containing model
- Load text file
- Compile instance of one of the types in the text file
- Browse instance to examine it for correctness
- Run methods belonging to model that prepare it for solving (make it well-posed, establish initial values, establish scaling)
- Pass any part of model to solver
- Solve
- Browse instance to see results

Capabilities of ASCEND

Example



Language (based on object-oriented principles)

Elementary types

Reals
Booleans
Integers
Symbol

Sets

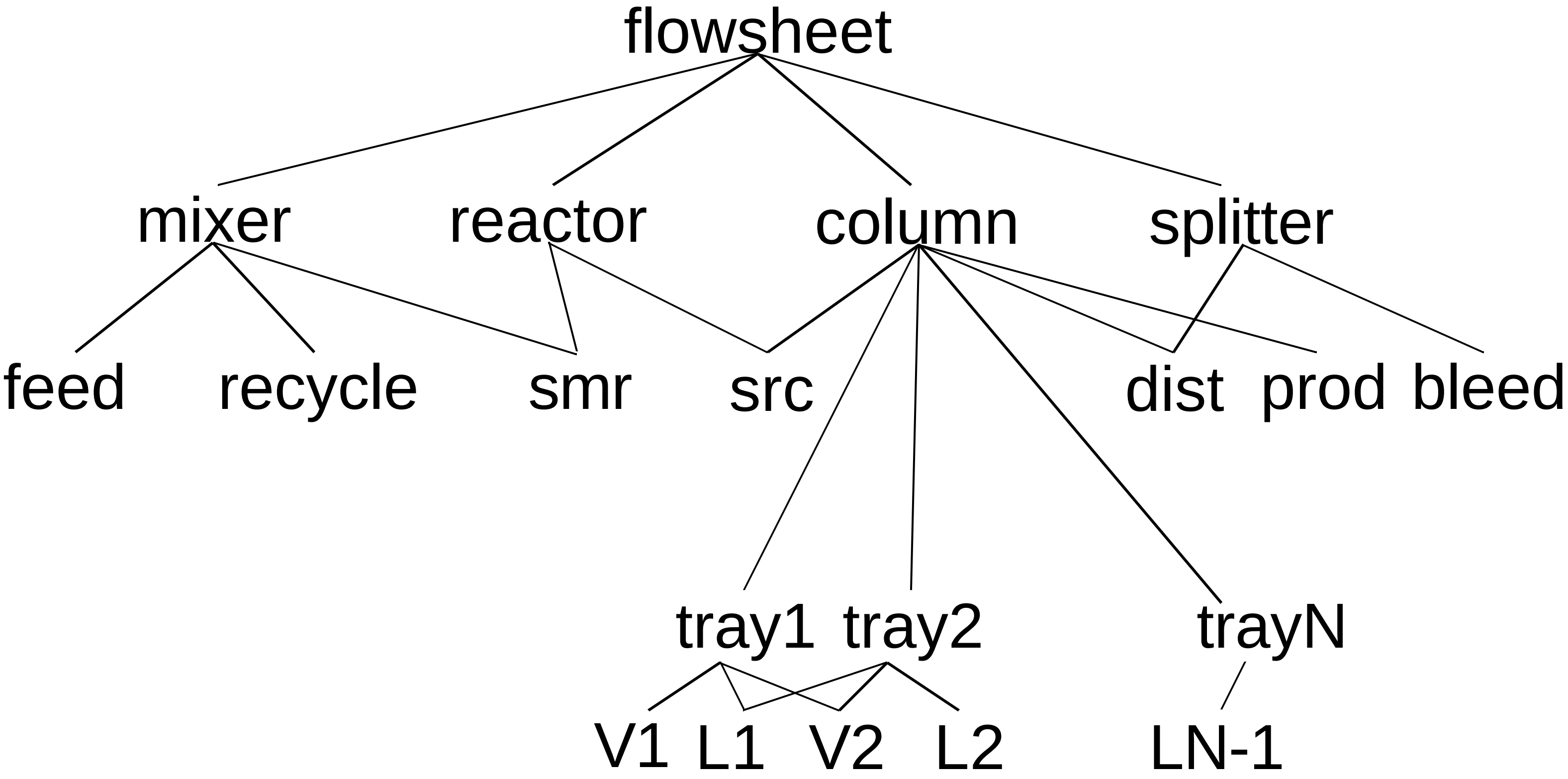
Equations
Sparse associative arrays (of anything)

When
Select
Loops
Models/atoms
Methods

Language concepts

Part/whole modeling to

- control complexity



flowsheet

mixer reactor column splitter

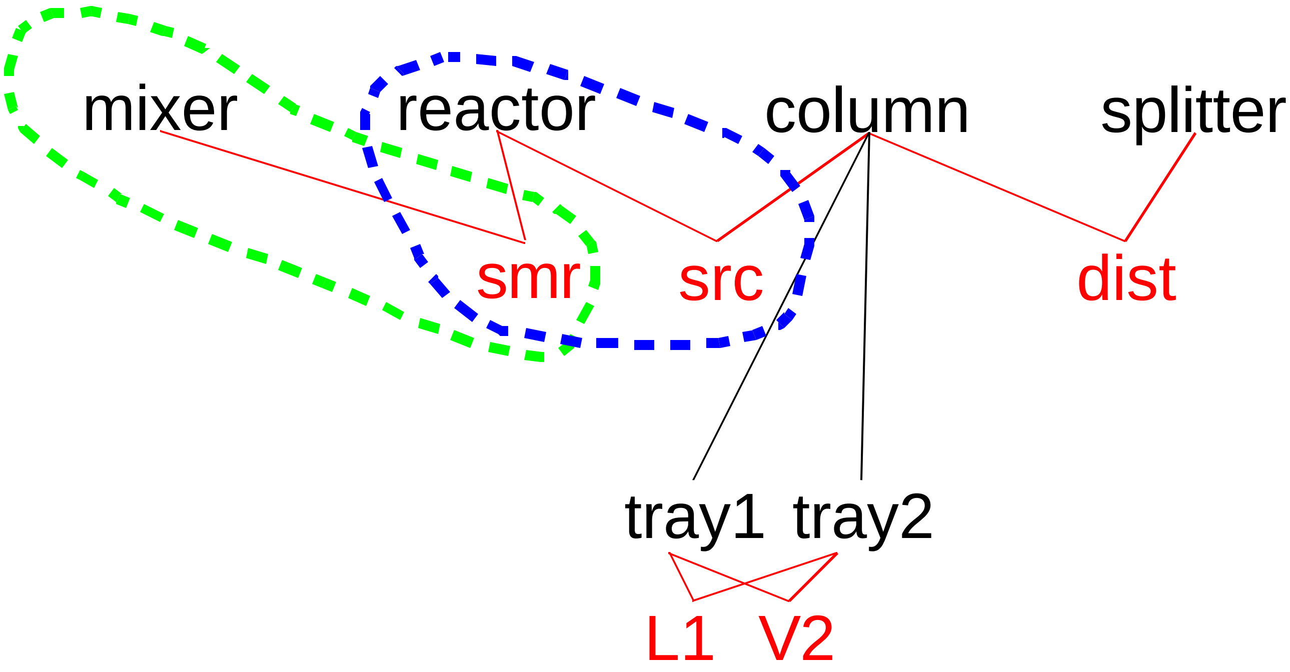
feed recycle smr src dist prod bleed

tray1 tray2 trayN

V1 L1 V2 L2 LN-1

Sharing of parts to

- configure complex models in a natural way
- permit solving of isolated parts



Parameterized types to

- allow sharing of parts
- aid user to see exactly what must be defined to use this model

```
MODEL VLflash(
  feed WILL_BE stream;
  vap WILL_BE stream;
  liq WILL_BE stream;
  Qin WILL_BE energy_rate;
  equil WILL_BE boolean;
)
```

- allow modeler to supply constraints to the compiler to reduce misuse

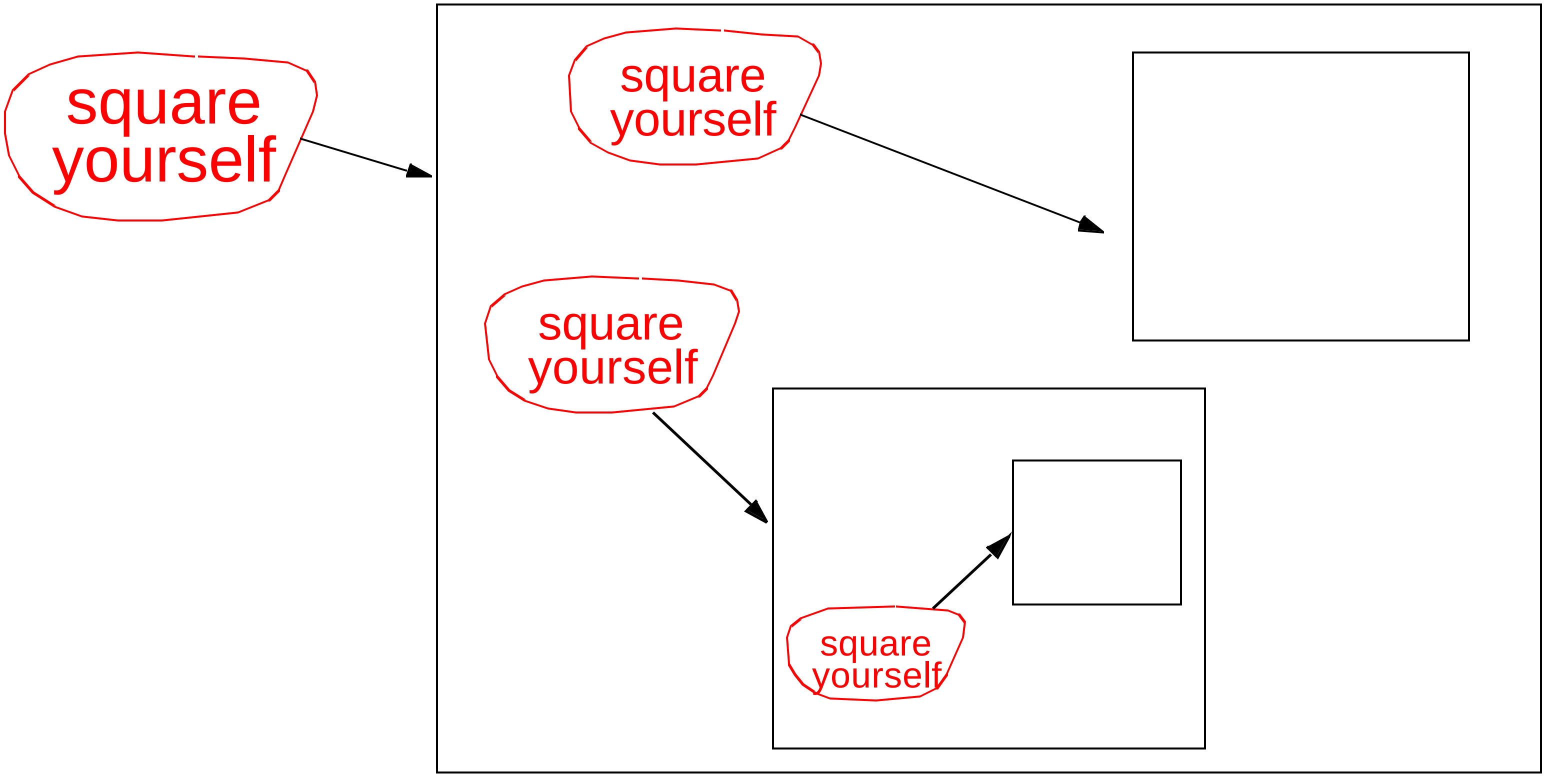
```
WHERE(
  feed, vap, liq WILL_NOT_BE_THE_SAME;
  (feed.pd.phase_indicator IN
        ['V','L','VL','VLL']) == TRUE;
  (vap.pd.phase_indicator IN ['V']) == TRUE;
  (liq.pd.phase_indicator IN ['L']) == TRUE;
);
```

Methods to

- carry out pre- and post-processing of variable values
- prepare model for solving (done recursively through all the model parts): clear, specify (square yourself), values, scale

```
METHOD specify;
        RUN feed.specify;
        RUN vap.specify;
        RUN liq.specify;
        Qin.fixed := TRUE;
        RUN st.specify;
END specify;
```

or in pictures to illustrate recursive nature --



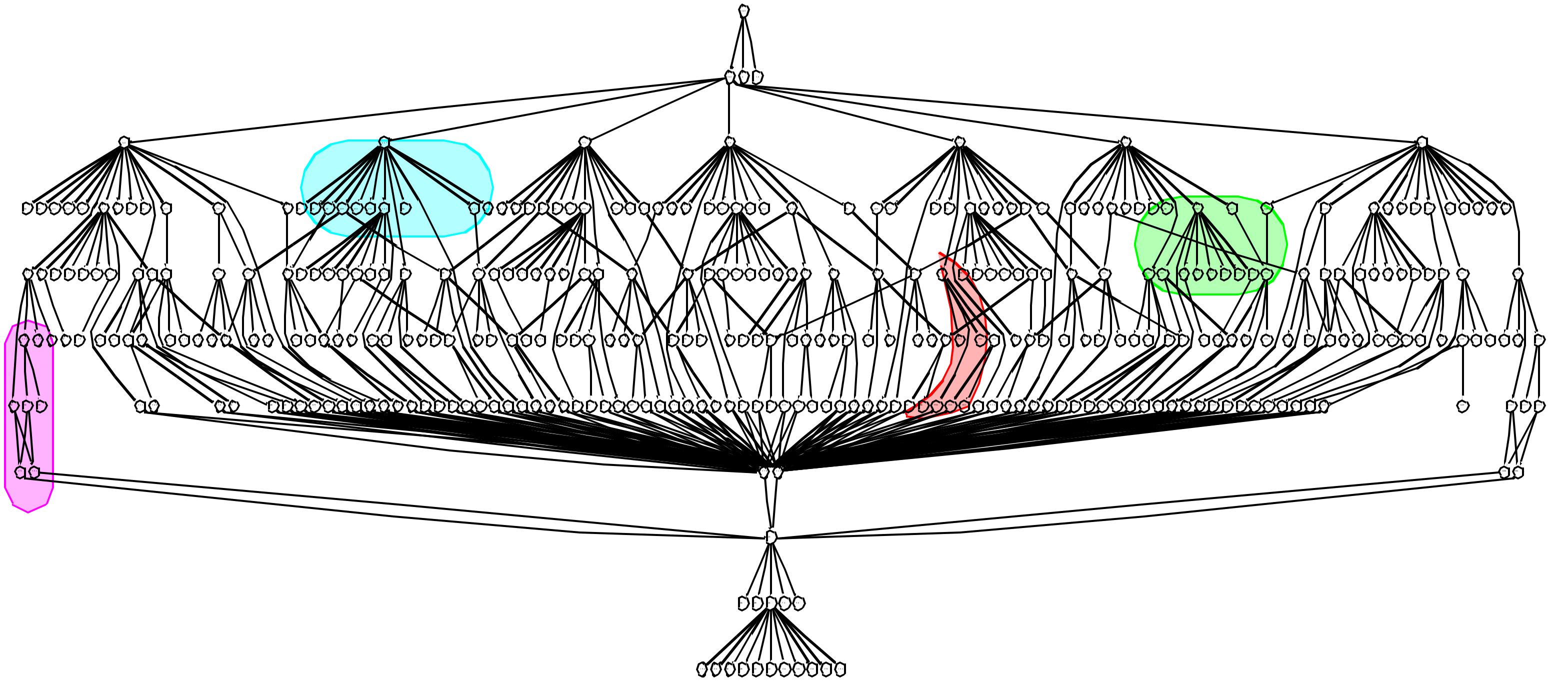
Very fast compile times

We now compile at the rate of 120,000 equations/minute on 200 megahertz pentium PC

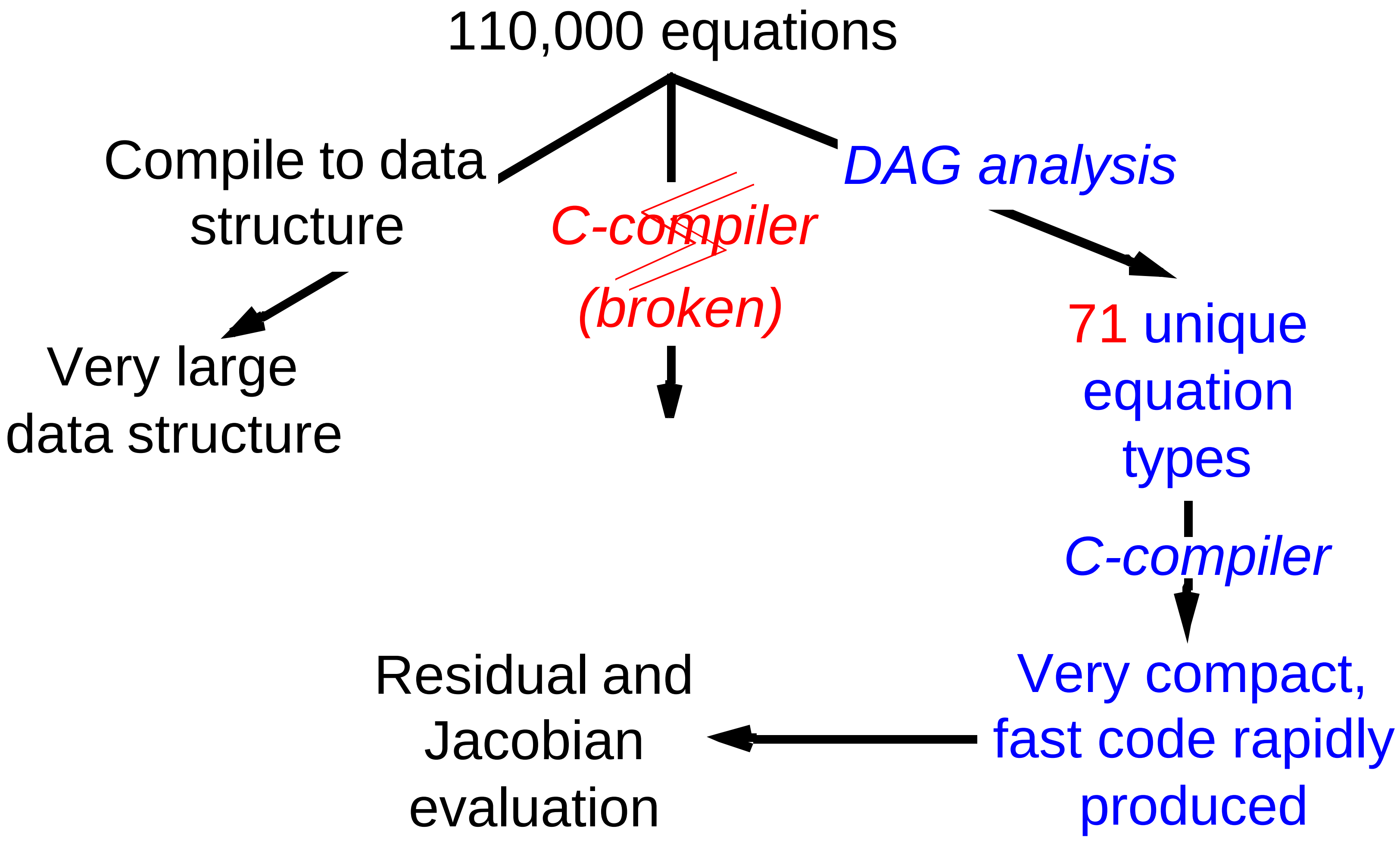
Approach

- Analyze part/whole structure (a Directed Acyclic Graph (DAG)) to discover unique equation types in model
- Compile only each unique equation type
- Equation instances become pointers to variables and type

The DAG for a seven tray column



Why so fast?



110,000 equations

Compile to data structure

Very large data structure

~~C-compiler~~ (broken)

DAG analysis

71 unique equation types

C-compiler

Very compact, fast code rapidly produced

Residual and Jacobian evaluation

Faster solve times

Requires

- very fast residual and Jacobian evaluation

Residual evaluation is at
230,000 equations/second on
200 megahertz pentium PC

AND

- faster factorization times for solving Newton equations
  - + Very simple and fast global preordering algorithm - also based on analyzing DAG
    - => Four columns with recycle: 83,000 equations (53,000 equation partition)

      Preorder time - 15.5 sec

      L/U factor time - 4 sec

Related to tearing in sequential modular

Kinds of solvers

- Normal simulation (solve *n* equations in *n* unknowns) but with bounds on variables (for example, to prevent mole fractions from being negative) - our solvers
- Optimization (using CONOPT, working on OPT)
- Dynamic simulation (using LSODE)
- Conditional models (*Vicente Rico-Ramirez*) -- is it a sub-cooled liquid, two phase, three phase or a superheated vapor stream? - our solvers

Generation of output files for other solvers

- Output for a GAMS model

Had following at one time and need to reimplement

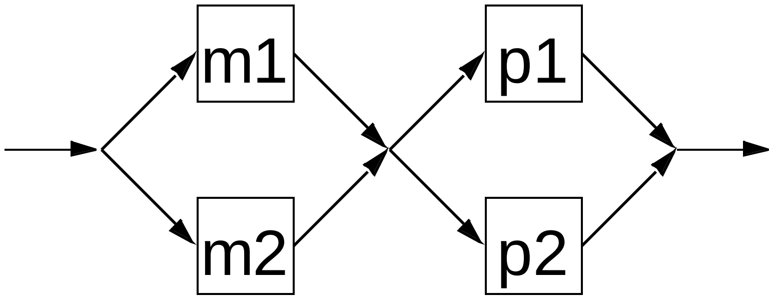
- Automatic generation of linearized *mixed integer linear program* - as extended MPS input file

More on conditional models

Equations defining model depend on where solutions occurs

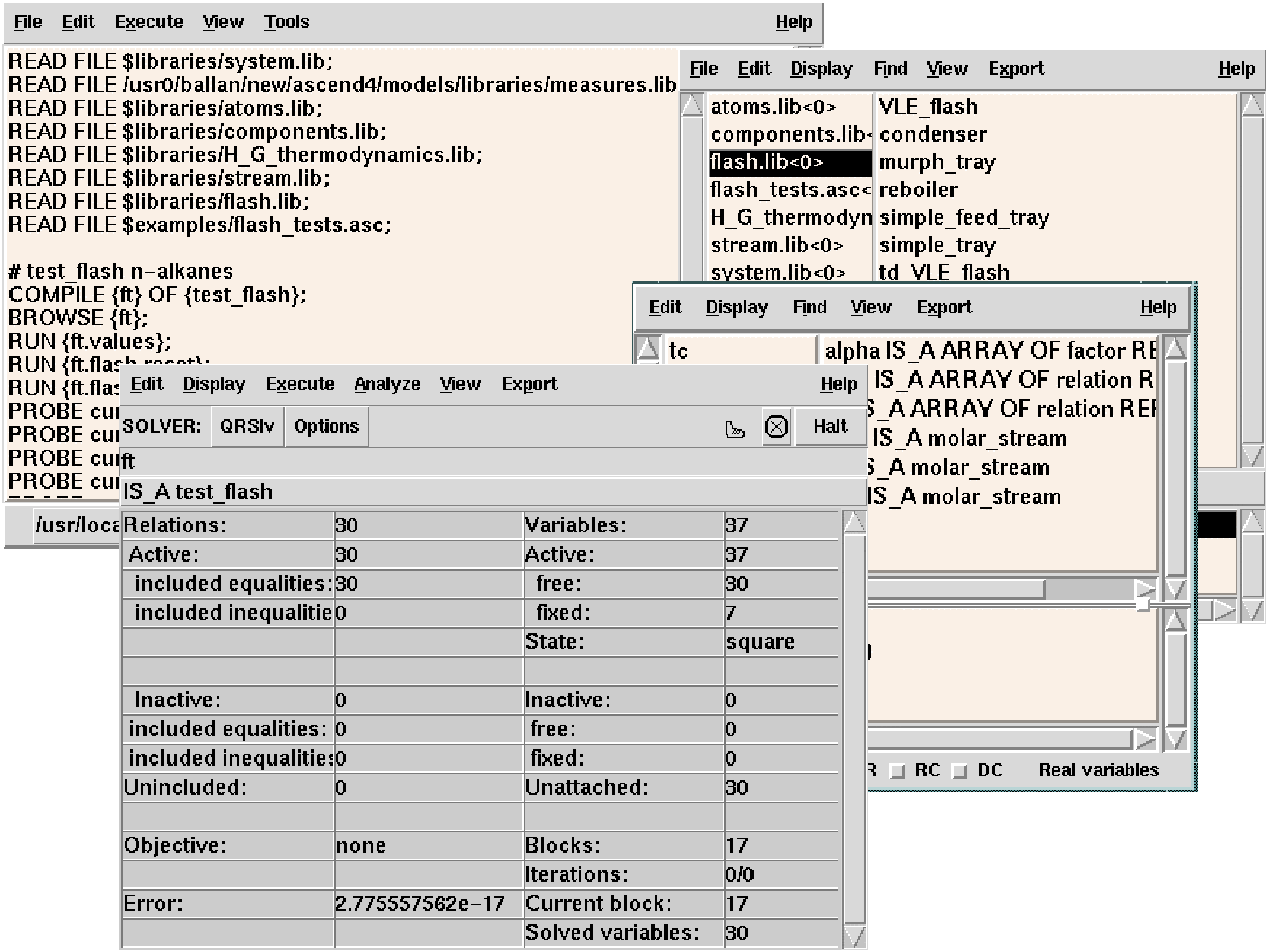
Ex. "laminar vs. turbulent flow"

- Language constructs (**WHEN** and **SELECT**)
  - + Replace/drop model parts (e.g., in superstructure optimization) based on value of discrete variable



- New regional model solvers (including optimization)
  - \+ Based on complementarity formulations
    - => formulations by others are incomplete and allow spurious solutions
  - \+ Based on boundary crossing
    - => Newton/gradient based method to cross boundaries mid-iteration -- steps over boundaries without region convergence

Interactive user interface for ASCEND



```
READ FILE $libraries/system.lib;
READ FILE /usr0/ballan/new/ascend4/models/libraries/measures.lib
READ FILE $libraries/atoms.lib;
READ FILE $libraries/components.lib;
READ FILE $libraries/H_G_thermodynamics.lib;
READ FILE $libraries/stream.lib;
READ FILE $libraries/flash.lib;
READ FILE $examples/flash_tests.asc;

# test_flash n-alkanes
COMPILE {ft} OF {test_flash};
BROWSE {ft};
RUN {ft.values};
RUN {ft.flash.reset};
RUN {ft.flas
PROBE cur
PROBE cur
PROBE cur
PROBE cur
/usr/loca
```

atoms.lib<0>
components.lib<
flash.lib<0>
flash_tests.asc<
H_G_thermodyn
stream.lib<0>
system.lib<0>

VLE_flash
condenser
murph_tray
reboiler
simple_feed_tray
simple_tray
td_VLE_flash

tc

alpha IS_A ARRAY OF factor RE
IS_A ARRAY OF relation R
S_A ARRAY OF relation REI
IS_A molar_stream
S_A molar_stream
IS_A molar_stream

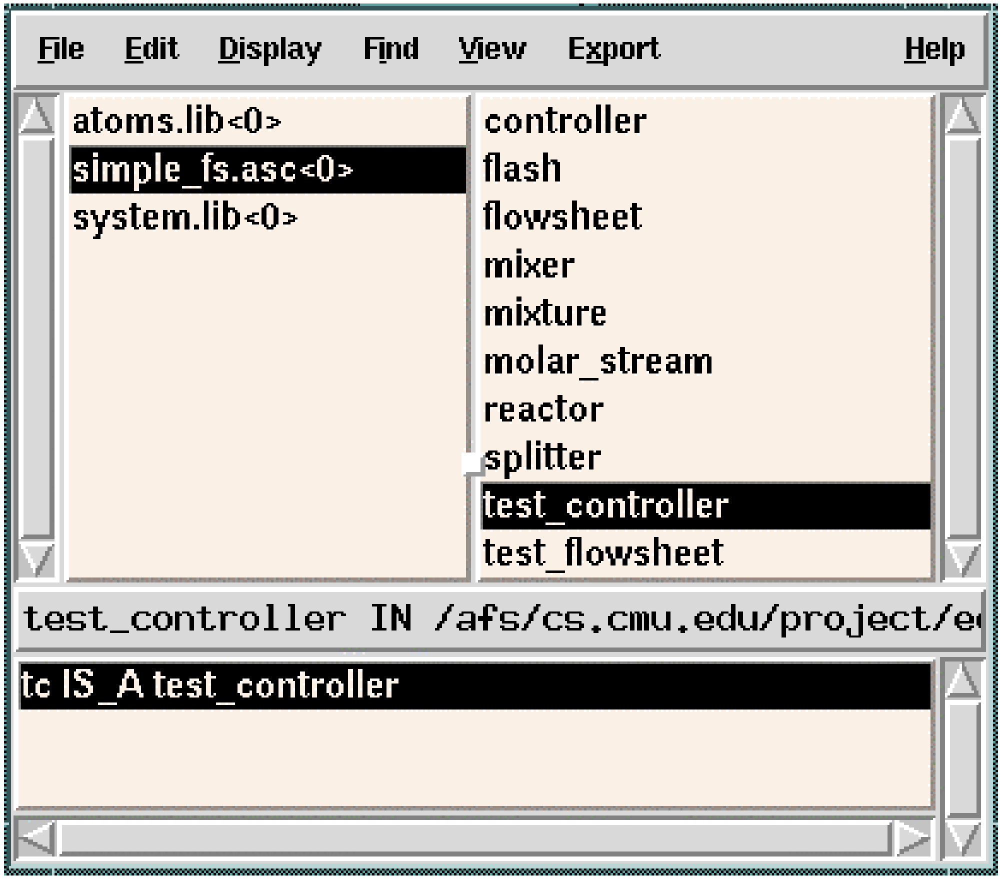
ft

IS_A test_flash

Relations:	30	Variables:	37
Active:	30	Active:	37
included equalities:	30	free:	30
included inequalitie	0	fixed:	7
		State:	square
Inactive:	0	Inactive:	0
included equalities:	0	free:	0
included inequalitie:	0	fixed:	0
Unincluded:	0	Unattached:	30
Objective:	none	Blocks:	17
		Iterations:	0/0
Error:	2.775557562e-17	Current block:	17
		Solved variables:	30

Some of the steps in modeling

Load and compile a text file containing model



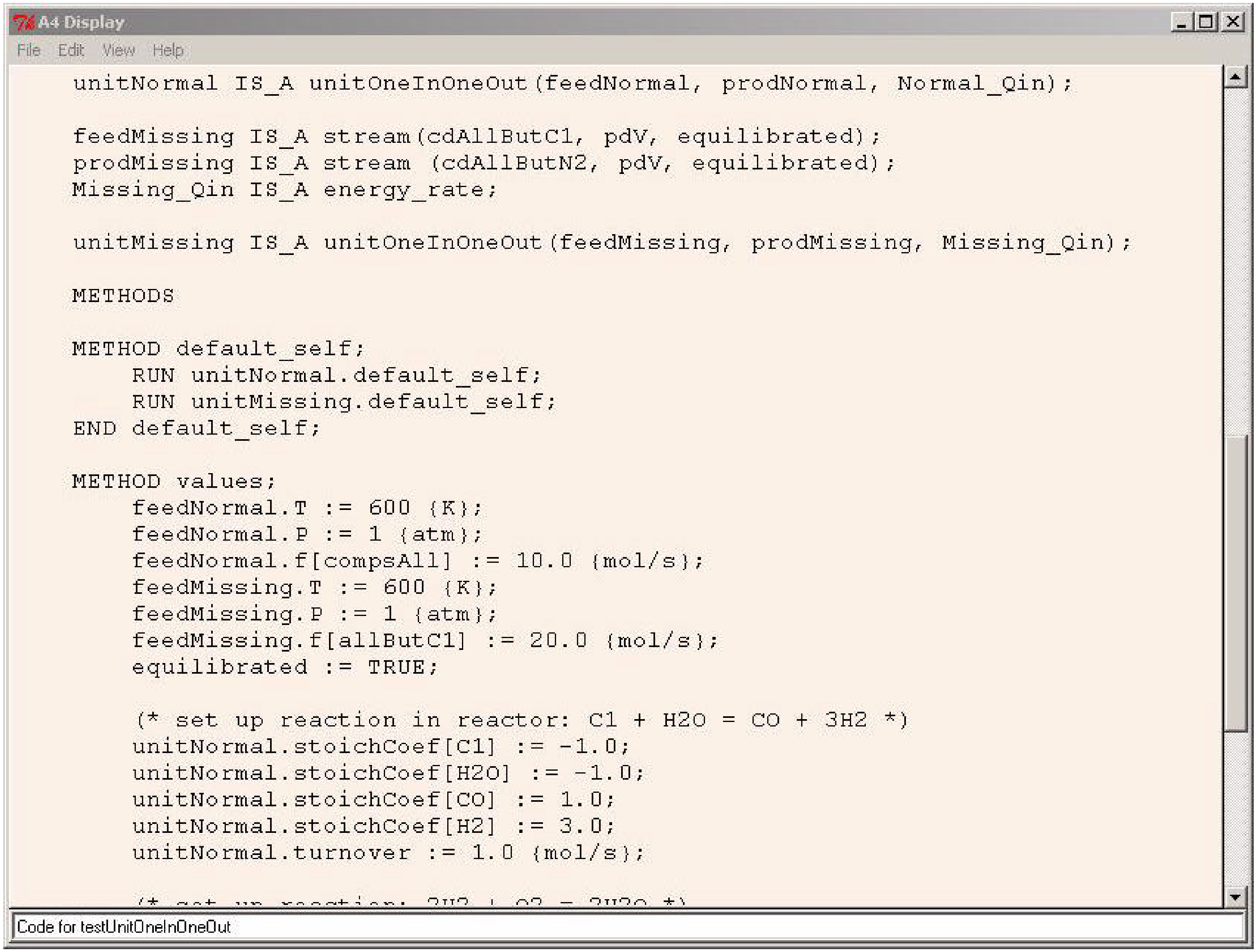
```
atoms.lib<0>
simple_fs.asc<0>
system.lib<0>
```

```
controller
flash
flowsheet
mixer
mixture
molar_stream
reactor
splitter
test_controller
test_flowsheet
```

```
test_controller IN /afs/cs.cmu.edu/project/e
```

```
tc IS_A test_controller
```

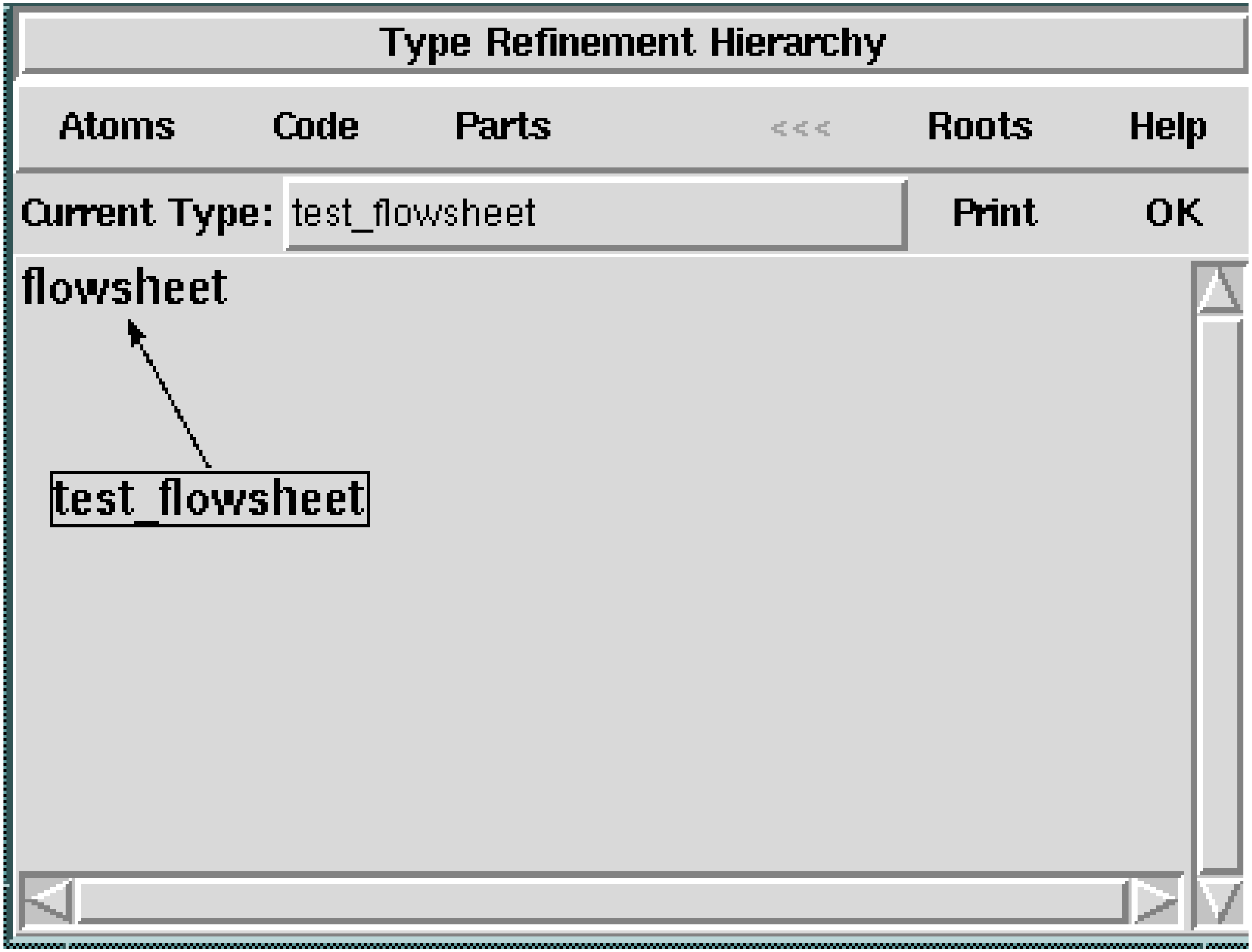
View the code for a loaded type



```
unitNormal IS_A unitOneInOneOut(feedNormal, prodNormal, Normal_Qin);

feedMissing IS_A stream(cdAllButC1, pdV, equilibrated);
prodMissing IS_A stream (cdAllButN2, pdV, equilibrated);
Missing_Qin IS_A energy_rate;

unitMissing IS_A unitOneInOneOut(feedMissing, prodMissing, Missing_Qin);

METHODS

METHOD default_self;
    RUN unitNormal.default_self;
    RUN unitMissing.default_self;
END default_self;

METHOD values;
    feedNormal.T := 600 {K};
    feedNormal.P := 1 {atm};
    feedNormal.f[compsAll] := 10.0 {mol/s};
    feedMissing.T := 600 {K};
    feedMissing.P := 1 {atm};
    feedMissing.f[allButC1] := 20.0 {mol/s};
    equilibrated := TRUE;

    (* set up reaction in reactor: C1 + H2O = CO + 3H2 *)
    unitNormal.stoichCoef[C1] := -1.0;
    unitNormal.stoichCoef[H2O] := -1.0;
    unitNormal.stoichCoef[CO] := 1.0;
    unitNormal.stoichCoef[H2] := 3.0;
    unitNormal.turnover := 1.0 {mol/s};
```

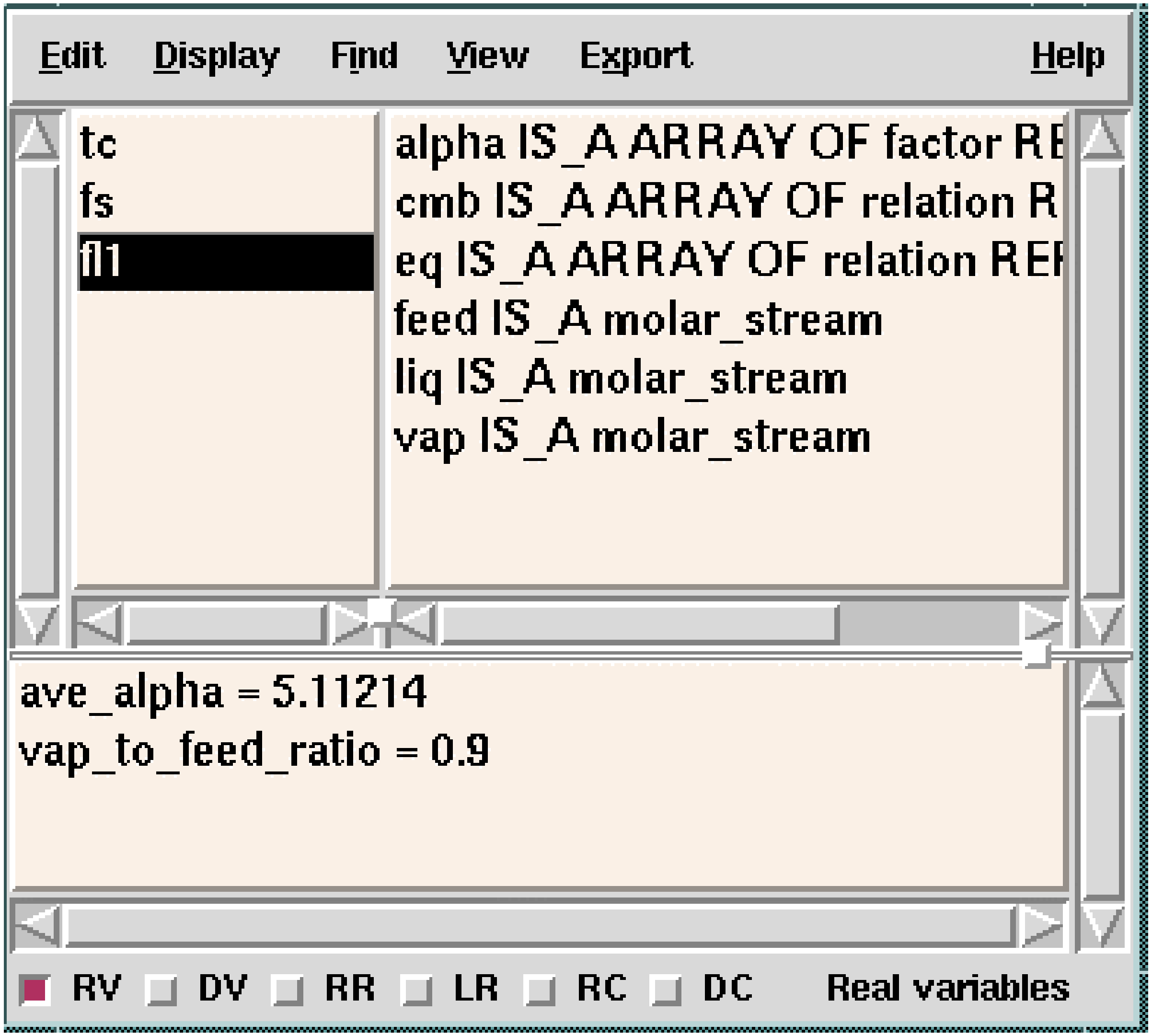
Code for testUnitOneInOneOut

Look at the type hierarchy of loaded models



Current Type: test_flowsheet

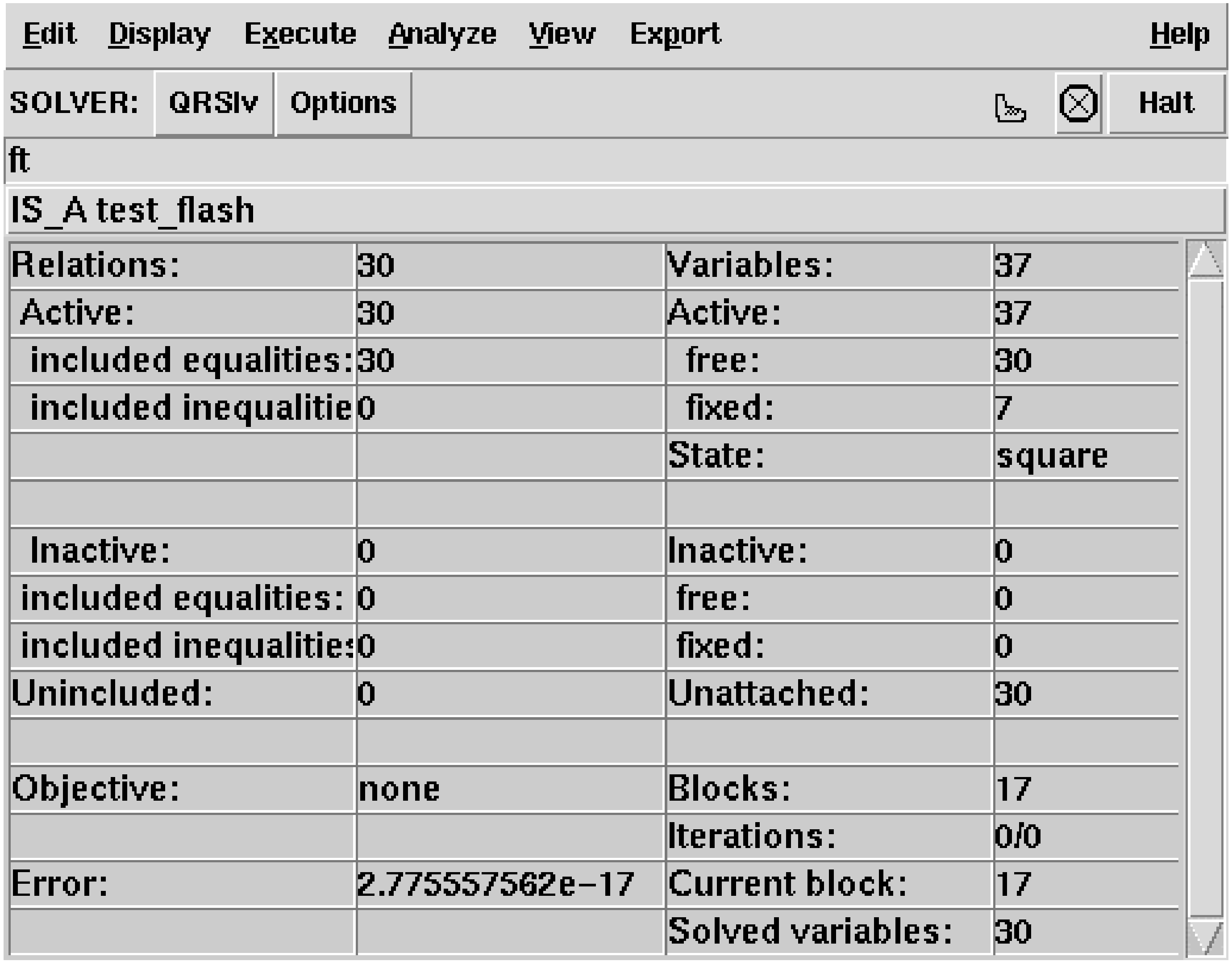
Browse the current compiled instance



alpha IS_A ARRAY OF factor RE
cmb IS_A ARRAY OF relation R
eq IS_A ARRAY OF relation REI
feed IS_A molar_stream
liq IS_A molar_stream
vap IS_A molar_stream

ave_alpha = 5.11214
vap_to_feed_ratio = 0.9

Solve

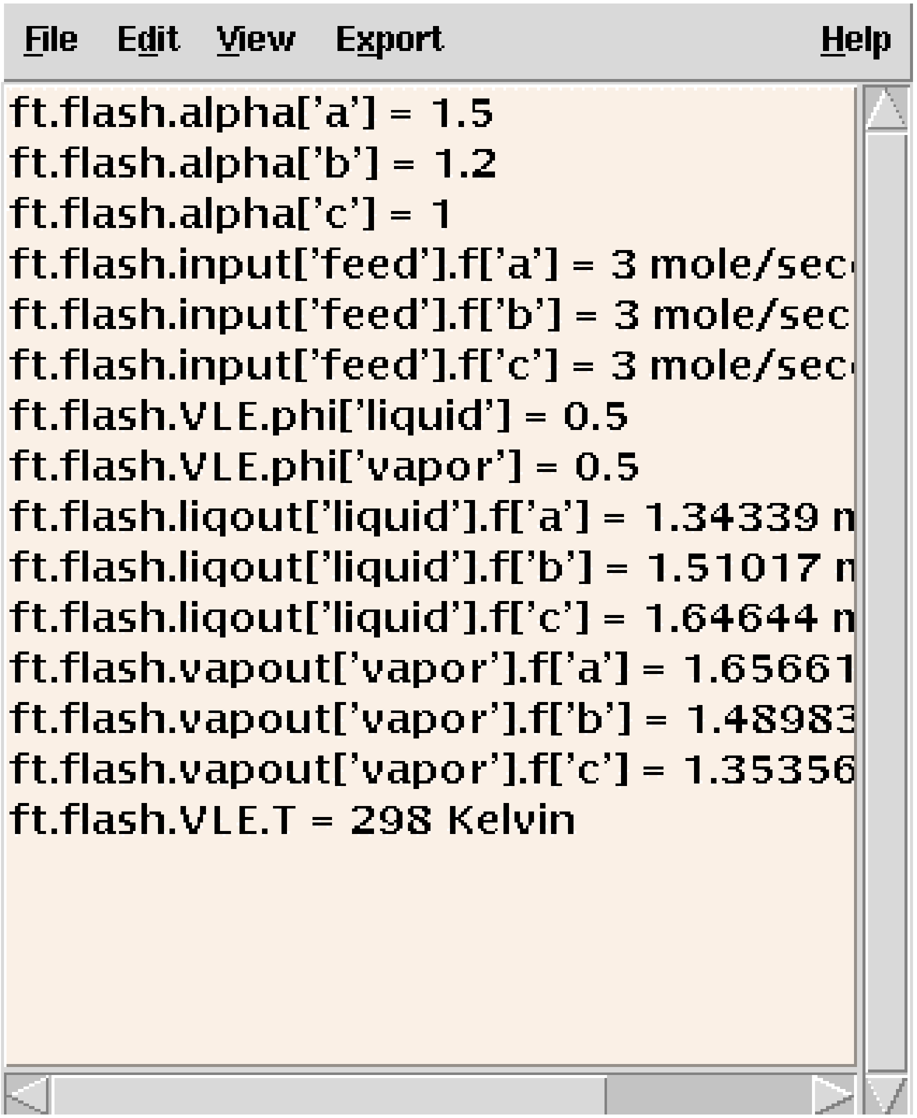


ft

IS_A test_flash

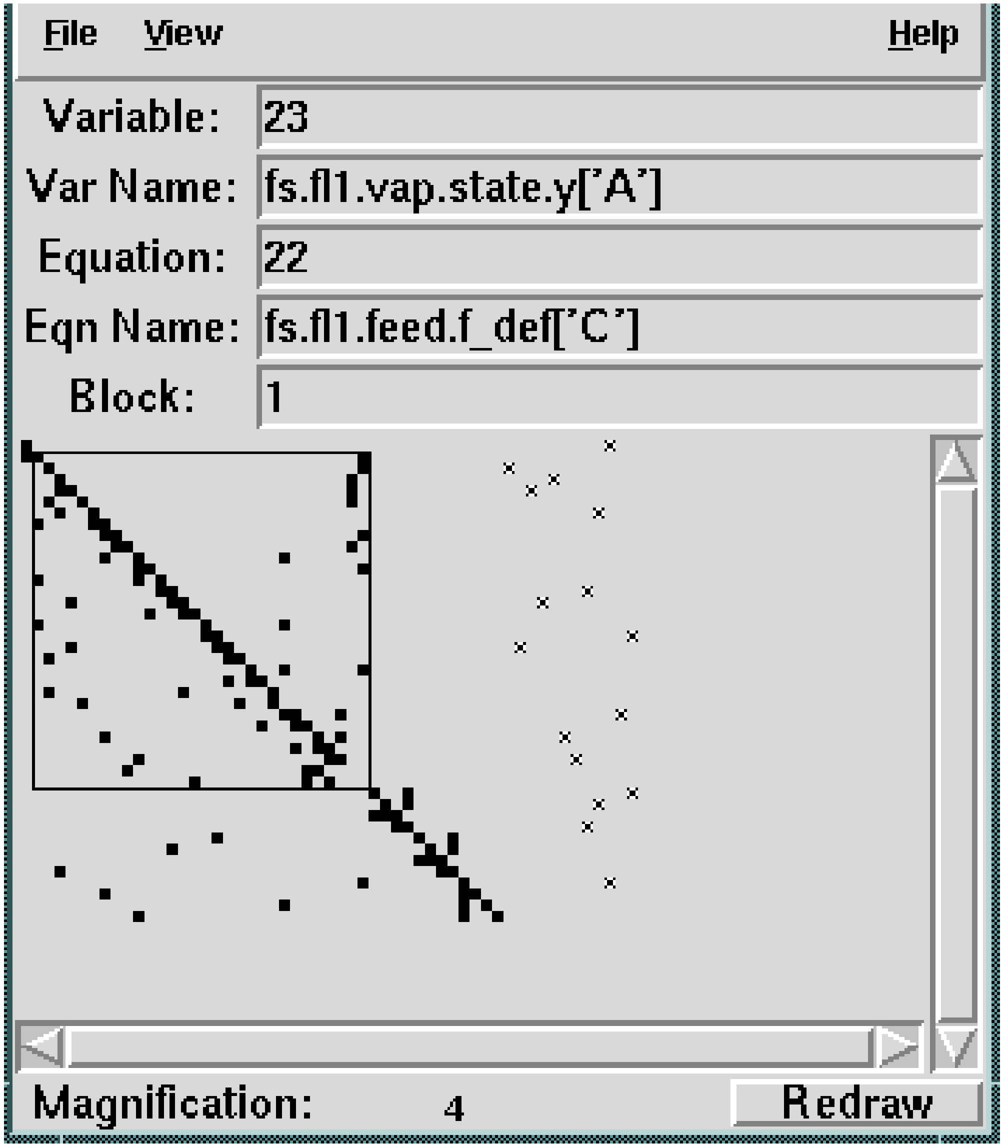
Relations:	30	Variables:	37
Active:	30	Active:	37
included equalities:	30	free:	30
included inequalitie	0	fixed:	7
		State:	square
Inactive:	0	Inactive:	0
included equalities:	0	free:	0
included inequalitie:	0	fixed:	0
Unincluded:	0	Unattached:	30
Objective:	none	Blocks:	17
		Iterations:	0/0
Error:	2.775557562e-17	Current block:	17
		Solved variables:	30

View results in Probe



```
ft.flash.alpha['a'] = 1.5
ft.flash.alpha['b'] = 1.2
ft.flash.alpha['c'] = 1
ft.flash.input['feed'].f['a'] = 3 mole/sec
ft.flash.input['feed'].f['b'] = 3 mole/sec
ft.flash.input['feed'].f['c'] = 3 mole/sec
ft.flash.VLE.phi['liquid'] = 0.5
ft.flash.VLE.phi['vapor'] = 0.5
ft.flash.liqout['liquid'].f['a'] = 1.34339
ft.flash.liqout['liquid'].f['b'] = 1.51017
ft.flash.liqout['liquid'].f['c'] = 1.64644
ft.flash.vapout['vapor'].f['a'] = 1.65661
ft.flash.vapout['vapor'].f['b'] = 1.48983
ft.flash.vapout['vapor'].f['c'] = 1.35356
ft.flash.VLE.T = 298 Kelvin
```

Debugging tools - view incidence matrix



Variable: 23

Var Name: fs.fl1.vap.state.y['A']

Equation: 22

Eqn Name: fs.fl1.feed.f_def['C']

Block: 1

Magnification: 4

And many other such tools

- Browse to see if configured correctly
- Find within any part variables eligible to be fixed
- Send any part to solver to be solved
- Ask if any part is numerically singular -- answer indicates which (if any) equations are locally dependent in their linearized form
- Find all variables which are close to their bounds
- List all variables which are currently fixed within any part
- List the equations for any part
- List the variables for any part

And tools to aid in solving numerically hard problems

- Send any sequence of parts to solver to be solved one at a time
- Recompute model scaling (send "rescale yourself" message to instance)
- Change value for variable that picks which form of model is active
- Change type of a part to be more refined -- causes compiler to restart and incrementally compile in the refinements

In conclusion

- Demo of ASCEND
  - creating a simple flowsheet
- Why we developed ASCEND
- Features of the ASCEND system
  - language
  - solvers
  - interactive user interface
  - debugging aids

Graphical Methods for Reactive Distillation

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Coworkers

- Jae Woo Lee, my Ph.D. student (finished April, 2000)
- Kristian Lien, Trondheim
- Steinar Hauan (completed Ph.D. with Kristian, joined our faculty in 1999)
- Amy Ciric, University of Cincinnati

History of reactive distillation

- A few early papers
- Industry often uses batch reactive distillation (pot with refluxed trays above it and possibly below it)
- Eastman’s methyl acetate process (1985) spurs real interest
- Simulation companies added reaction to trays
- Doherty and students discover very clever variable transformation - and start to discuss reactive azeotropes
- Attempts to aid finding if reaction can be feasible -- with ∞ trays, ∞ reflux, rxn equilibrium, 3 components
- Approach has been “simulate/optimize and see”
- Hauan and Lien identify vector additive nature of reaction, mixing, distillation

Outline

- Why reactive distillation
- Reaction, separation and mixing vectors, design in transport space
- Difference points
- McCabe-Thiele diagram
- Non-intuitive behavior
- Ponchon-Savarit diagram
- Examples
  + diluted ternary: MTBE
  + quaternary (using projection): methyl acetate

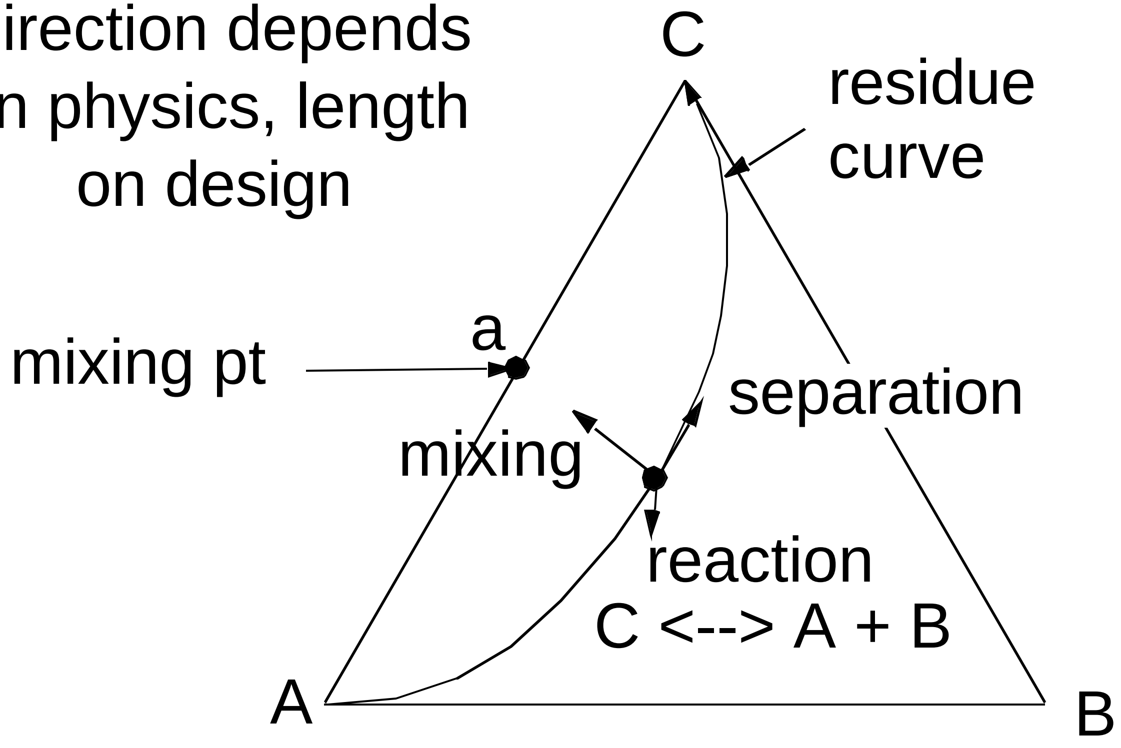
Why reactive distillation

Methyl acetate process (Eastman Chemicals, ~1985)

- 1 reactor and 6 separation devices ==> 1 reactive extractive distillation column
- Costs drop to 16% of previous process (not to 95%)

Reaction, separation and mixing vectors

Examining processes in “composition” space



Direction depends
on physics, length
on design

Example

Separation

$$\frac{\mathrm{d}}{\mathrm{d}t}\underline{x} = \frac{V}{M}\cdot(\underline{x}-\underline{y})$$

- $\frac{V}{M}$ set by design and operation
- If $(\underline{x}-\underline{y}) = \underline{x}-K\underline{x}$, then direction set by vapor-liquid equilibrium

Mixing

- Mixing is along the line joining the two mix points
- Length depends on quantities selected to be mixed.

Useful geometry in "transport space"

Straight lines

Given a set of balances of the form

$$a\underline{u} \; = \; b\underline{v} + c\underline{w}$$

If

$$\sum_i u_i \; = \; \sum_i v_i \; = \; \sum_i w_i$$

Then we see

$$a \; = \; b + c$$

And

$$\underline{u} = \frac{b}{b+c} \cdot \underline{v} + \frac{c}{b+c} \cdot \underline{w} = \alpha \cdot \underline{v} + (1-\alpha) \cdot \underline{w}$$

i.e., points satisfying these balances are on a straight line in this vector space

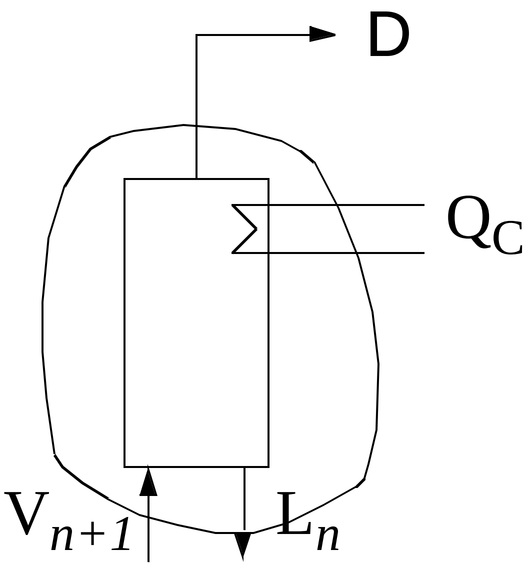
Augmenting this space

Adding another dimension that satisfies

$$au_{new} = bv_{new} + cw_{new}$$

leads to straight lines in this augmented space

Consider the top of a column



Composition space

$$V_{n+1} \cdot \underline{y}_{n+1} = L_n \cdot \underline{x}_n + D \cdot \underline{x}_D$$

Augmented with molar enthalpy

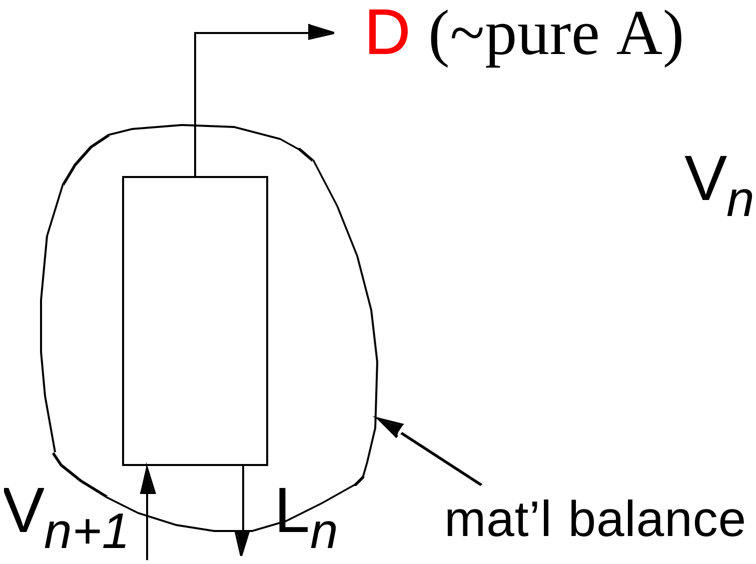
$$V_{n+1} \cdot H_{n+1} = L_n \cdot h_n + D \cdot \left(h_D + \frac{Q_C}{D} \right)$$

Thus balances in a composition space and in an augmented molar enthalpy + composition space both give rise to points on straight lines. (Is there a way to include momentum?)

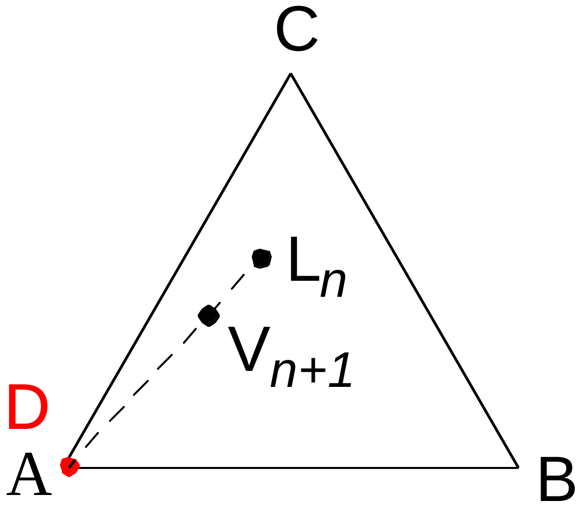
Difference points

Sum of flows

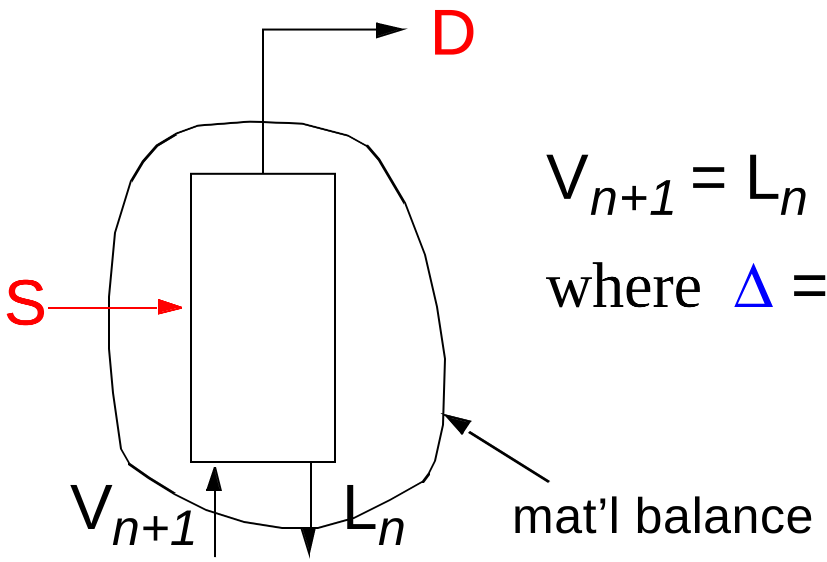
- V_{n+1} is the mixing of two positive flows, L_n and D
- The lever rule indicates relative amounts



$$V_{n+1} = L_n + D$$

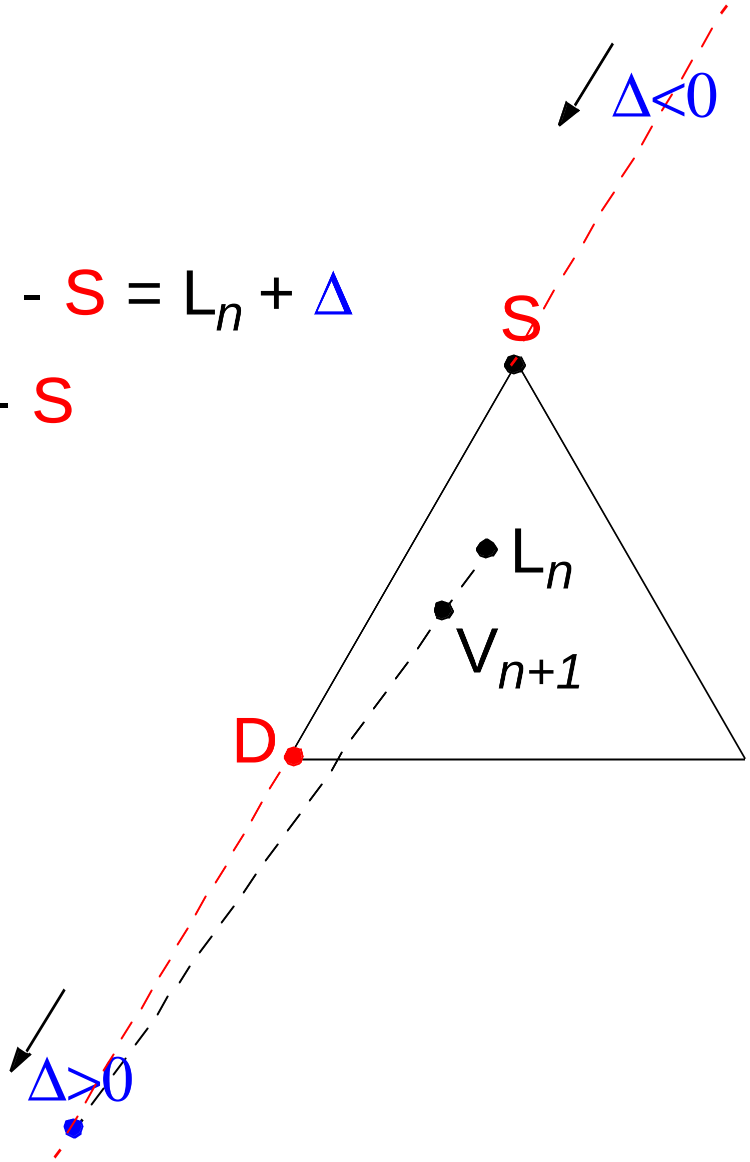


Difference of flows, extractive distillation



$$V_{n+1} = L_n + D - S = L_n + \Delta$$

where $\Delta = D - S$



Reaction "flow" and "composition"

A + B <--> C <==> -1 A -1 B + 1 C = 0; ν^T =[-1, -1, 1]

- Flow: Everytime reaction "turns over" (ξ mol/s), we lose one mol/s of material

flow = (-1 + (-1) + 1) $\xi = -1\ \xi$ (mol/s) = $\nu_T\ \xi$

- Composition: We lose one mol/s of A, one mole of B and gain one mole of C

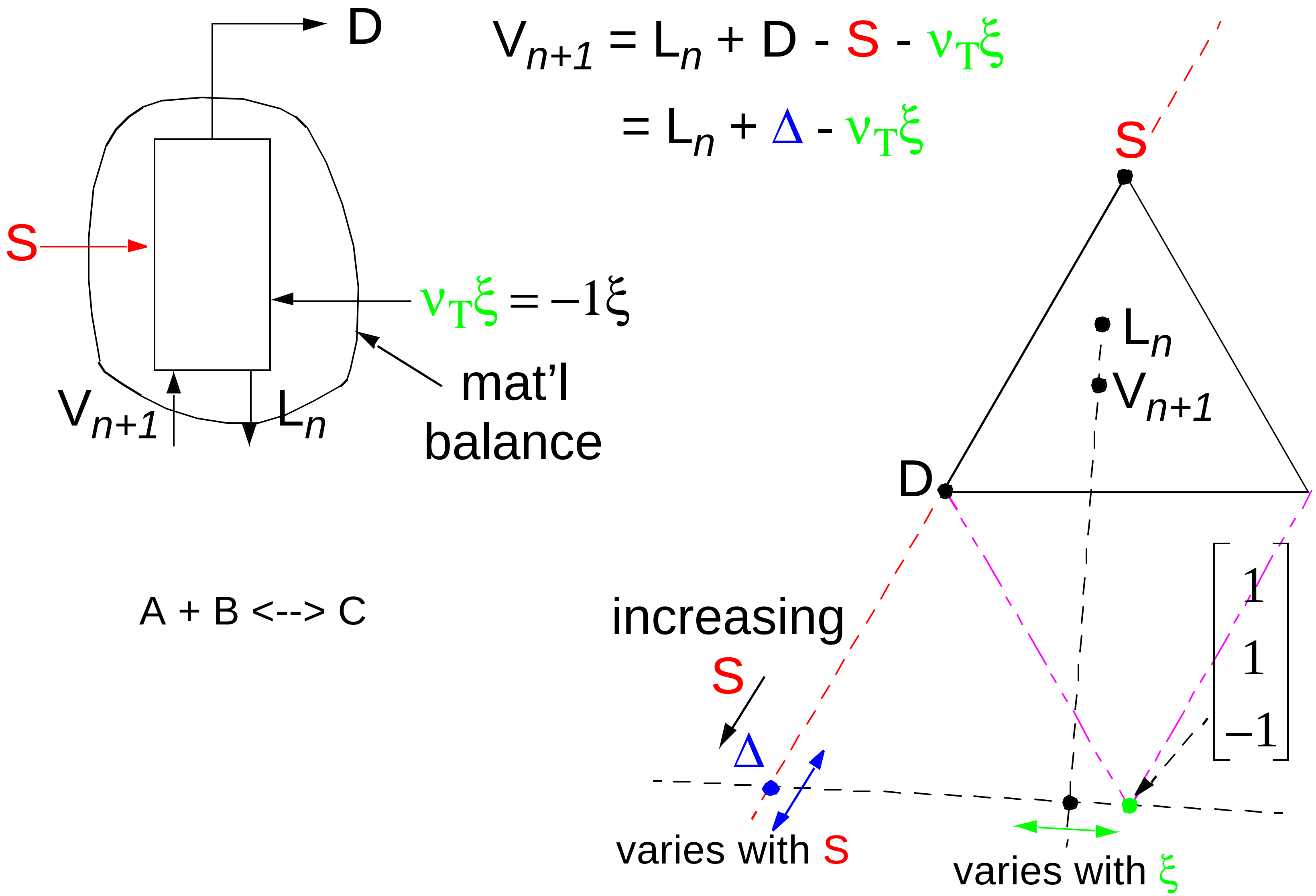
$$\text{composition} = \left(\begin{bmatrix} -1 \\ -1 \\ 1 \end{bmatrix} / (\nu_T) \right) = \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix}$$

Note: composition sums to one but lies outside composition triangle

The reaction difference point

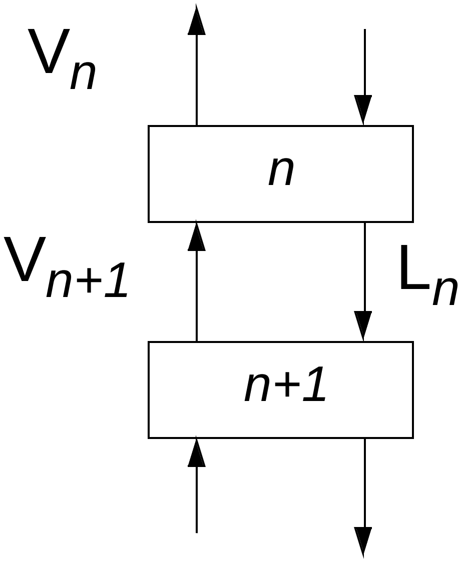
$$V_{n+1} = L_n + D - S - \nu_T \xi$$

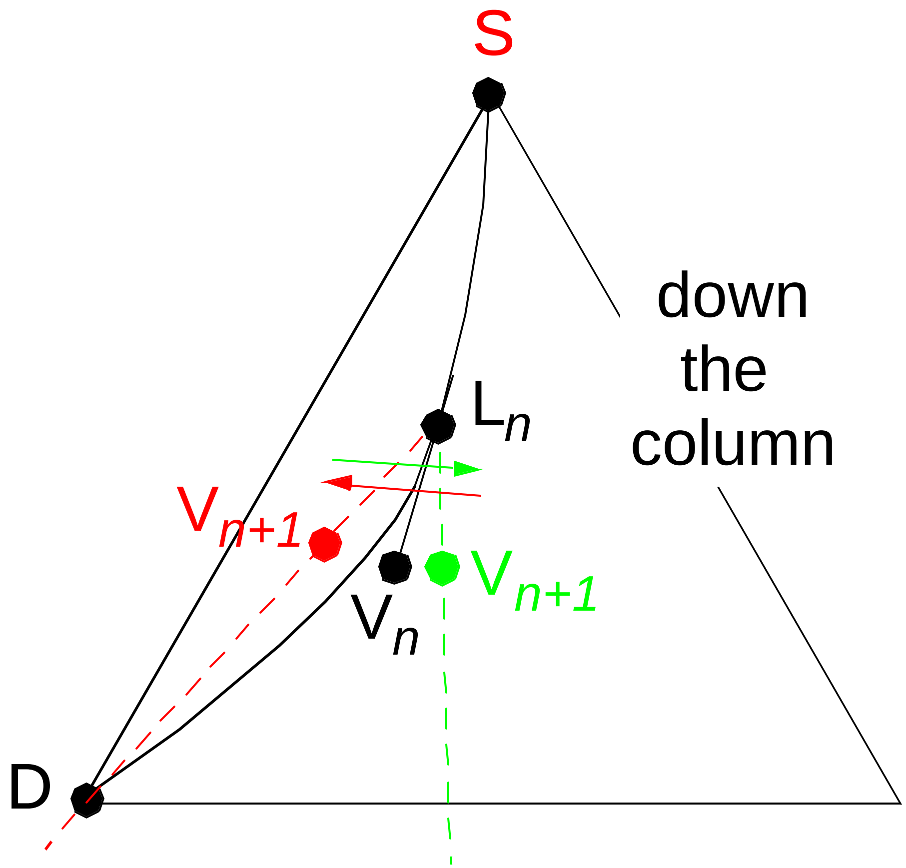
$$= L_n + \Delta - \nu_T \xi$$



A + B <--> C

Steering tray compositions in column





Note: altered material balance can make temperature changes reverse in column

Binary diagrams

- Reactions possible
  - + Isomerization

    B --> A (A is more volatile)
  - + Decomposition

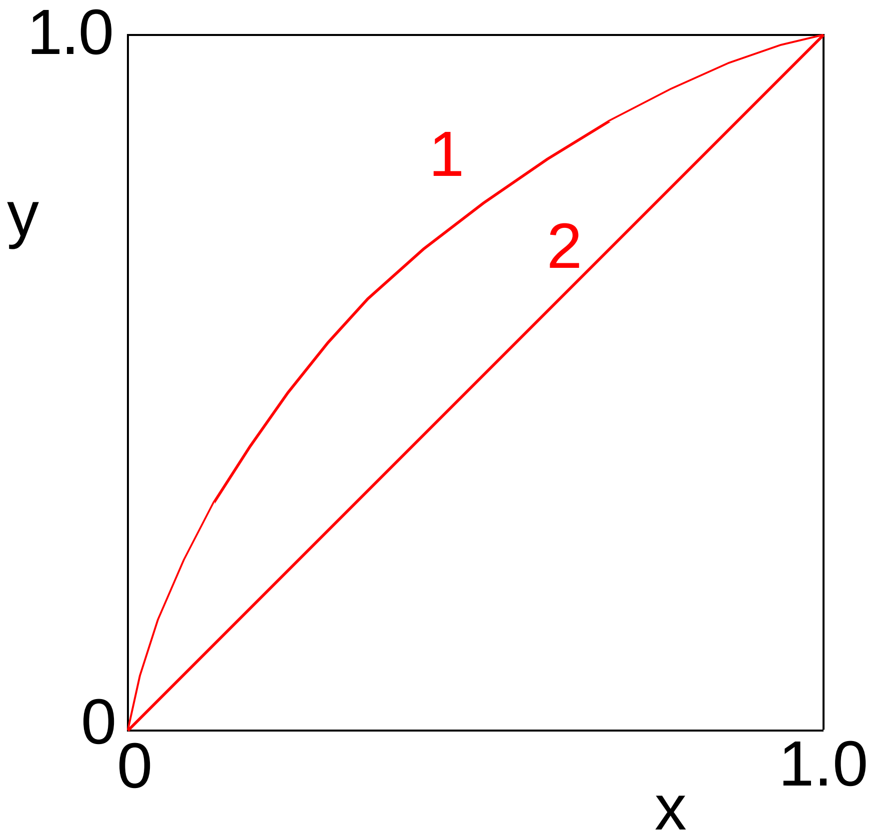
    B --> 2A

Review of McCabe-Thiele Diagram

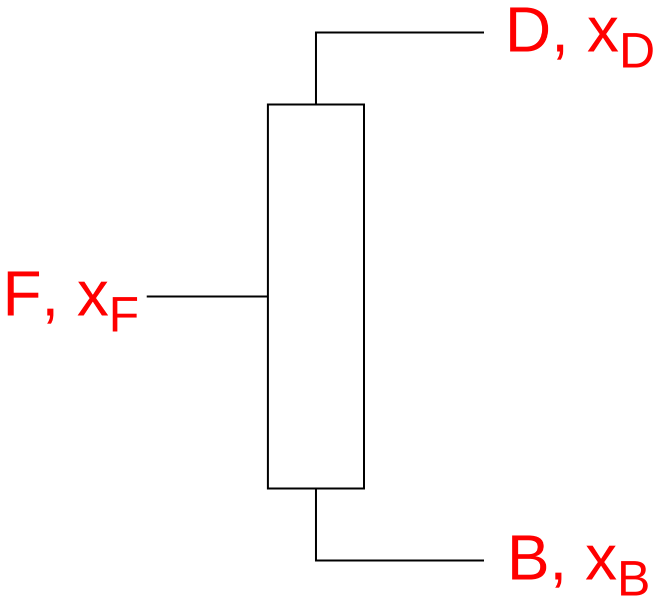
- y vs. x plot for binary column
- Can be used to design number of stages required in column
- Major use - for practiced engineers, to develop insights into column behavior

Quick review

1. Plot equilibrium curve
2. Add 45 degree line (y=x line)



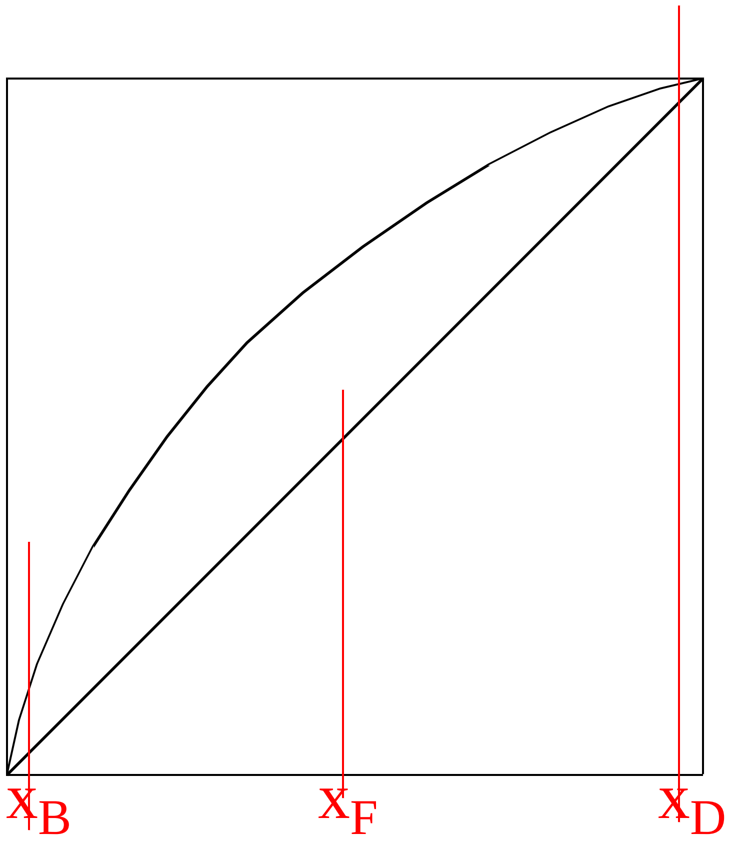
3. Indicate feed, bottoms, and distillate compositions



D, x_D

F, x_F

B, x_B

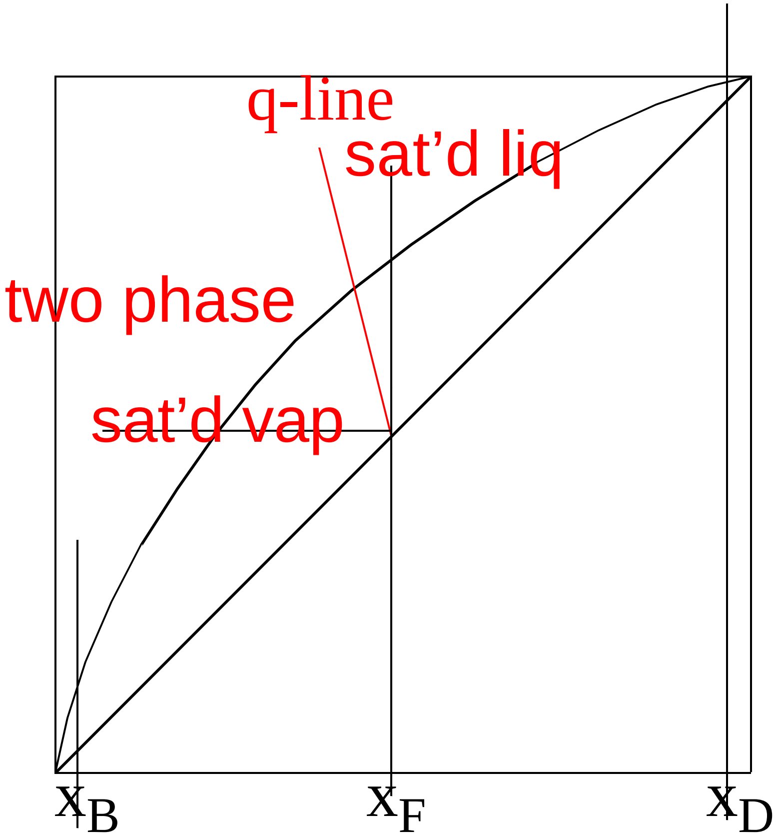


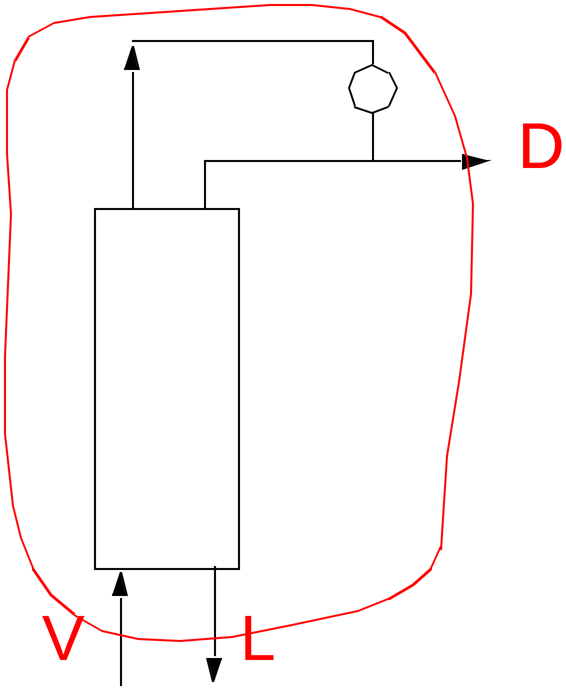
x_B x_F x_D

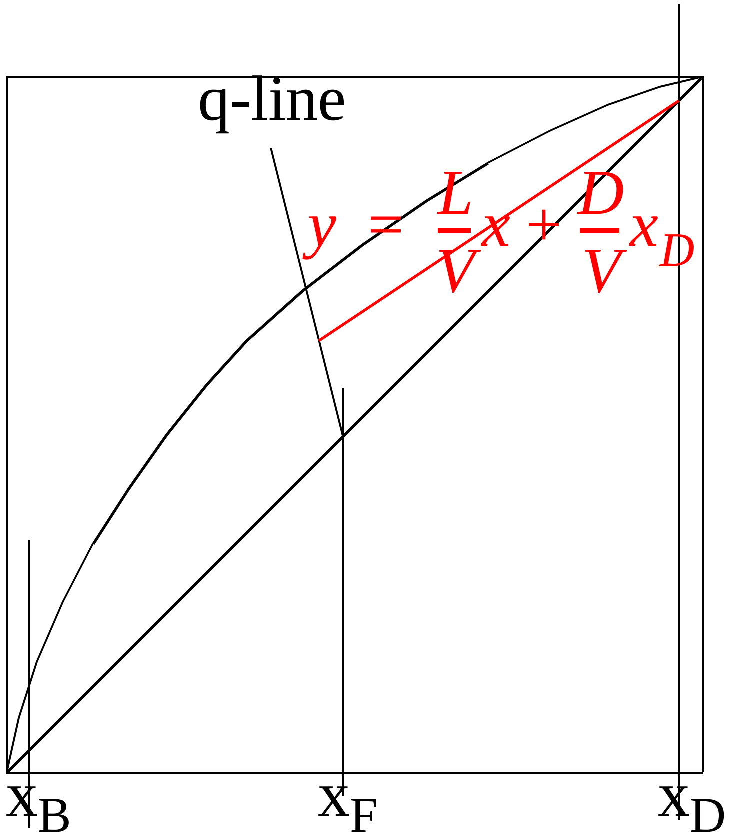
3. Plot q-line

   + intersection of operating lines

   + function of thermal condition of feed

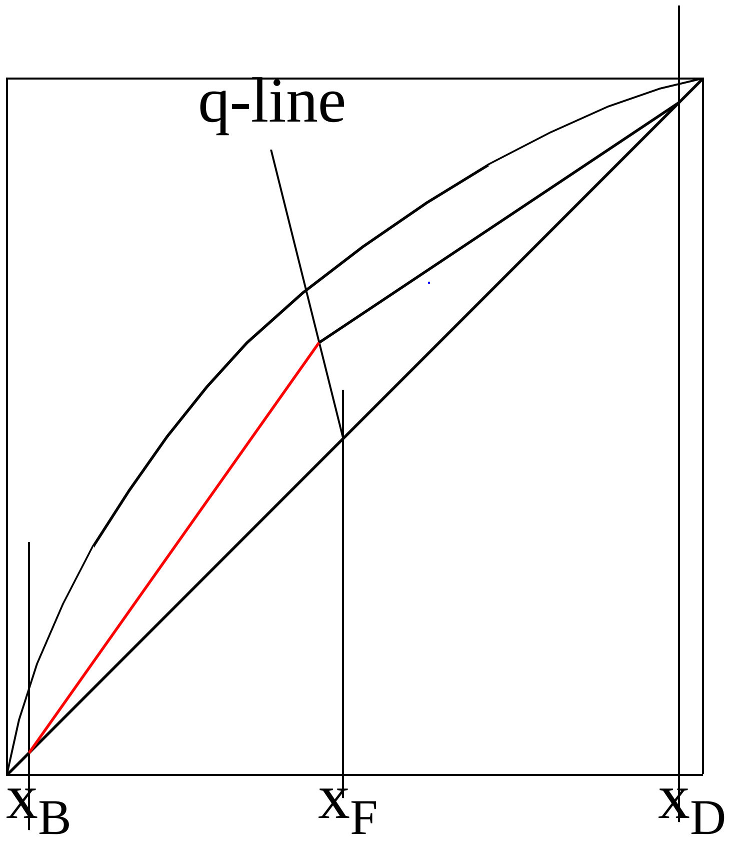


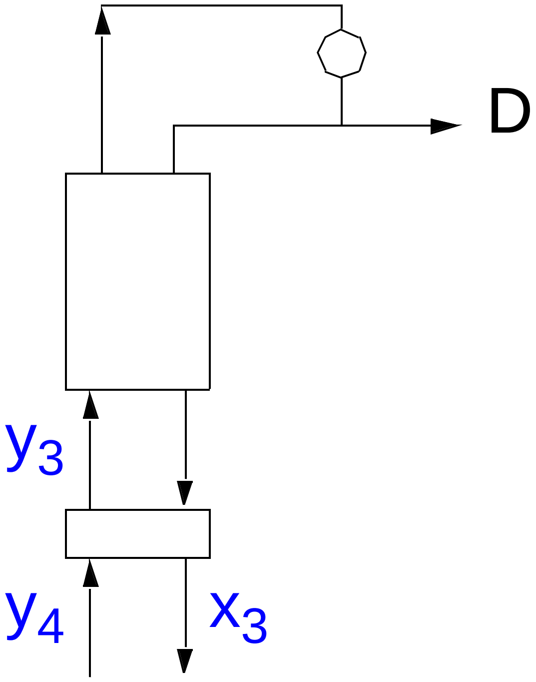


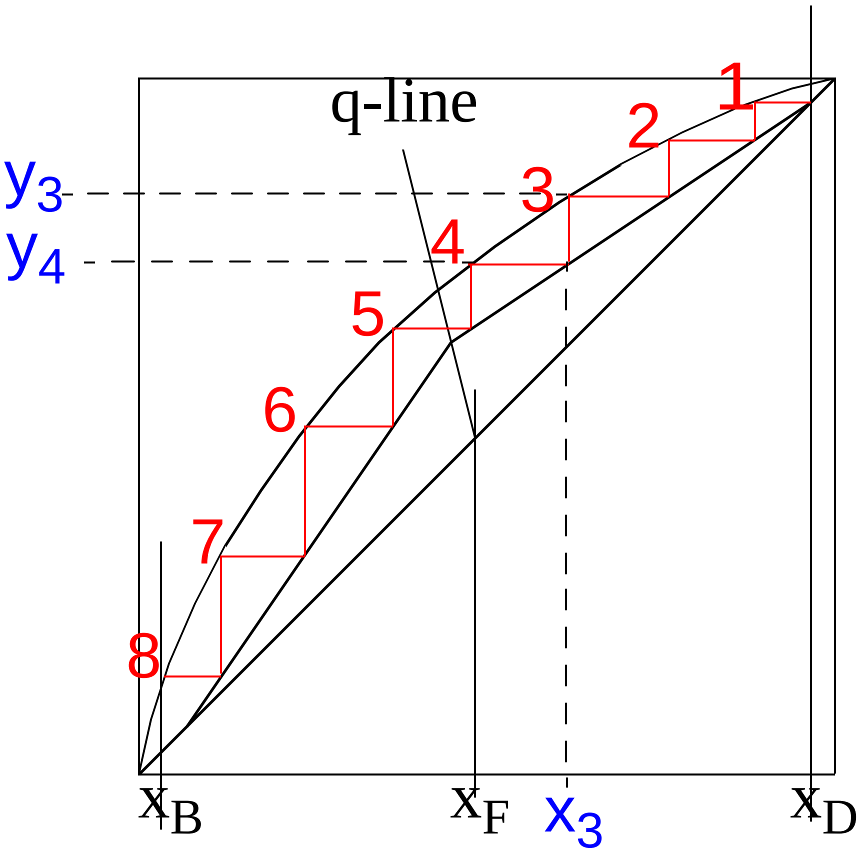


4. Plot top operating line
(based on mat’l balance)

5. Plot bottom operating line (connects x_B on 45 degree line to point where top line intersects q-line -- also based on material balance)





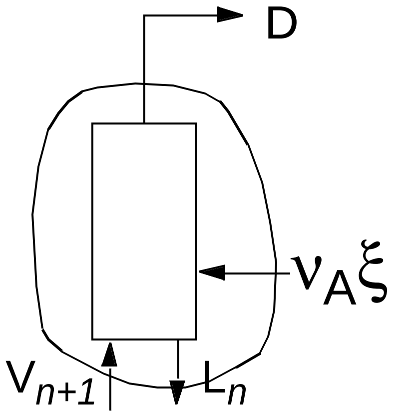


6. Step off stages

Effect of reaction in top of column

Material balance with reaction (-B + A = 0) for species A only

$$Vy = Lx + Dx_D - \xi\, \nu_A, \text{ where } \upsilon_A = 1$$



Let y = x and solve

$$(V-L)x = (D-\nu_T\xi)x = Dx$$

$$= D(x_D - \frac{x}{D})$$

or on 45 degree line where y=x, we have

$$x = x_D - \frac{x}{D}$$

Thus intersection shifts down by $\frac{x}{D}$

Typical values (flows in mol/time)

	B (Reactant)	A (Product)	
ν	-1	1	
x_D		0.99	
Feed	50	50	
ξ	Bott	Dist	diff pt
5	45	55	0.899
25	25	75	0.657
45	5	95	0.516
50	0	100	0.490

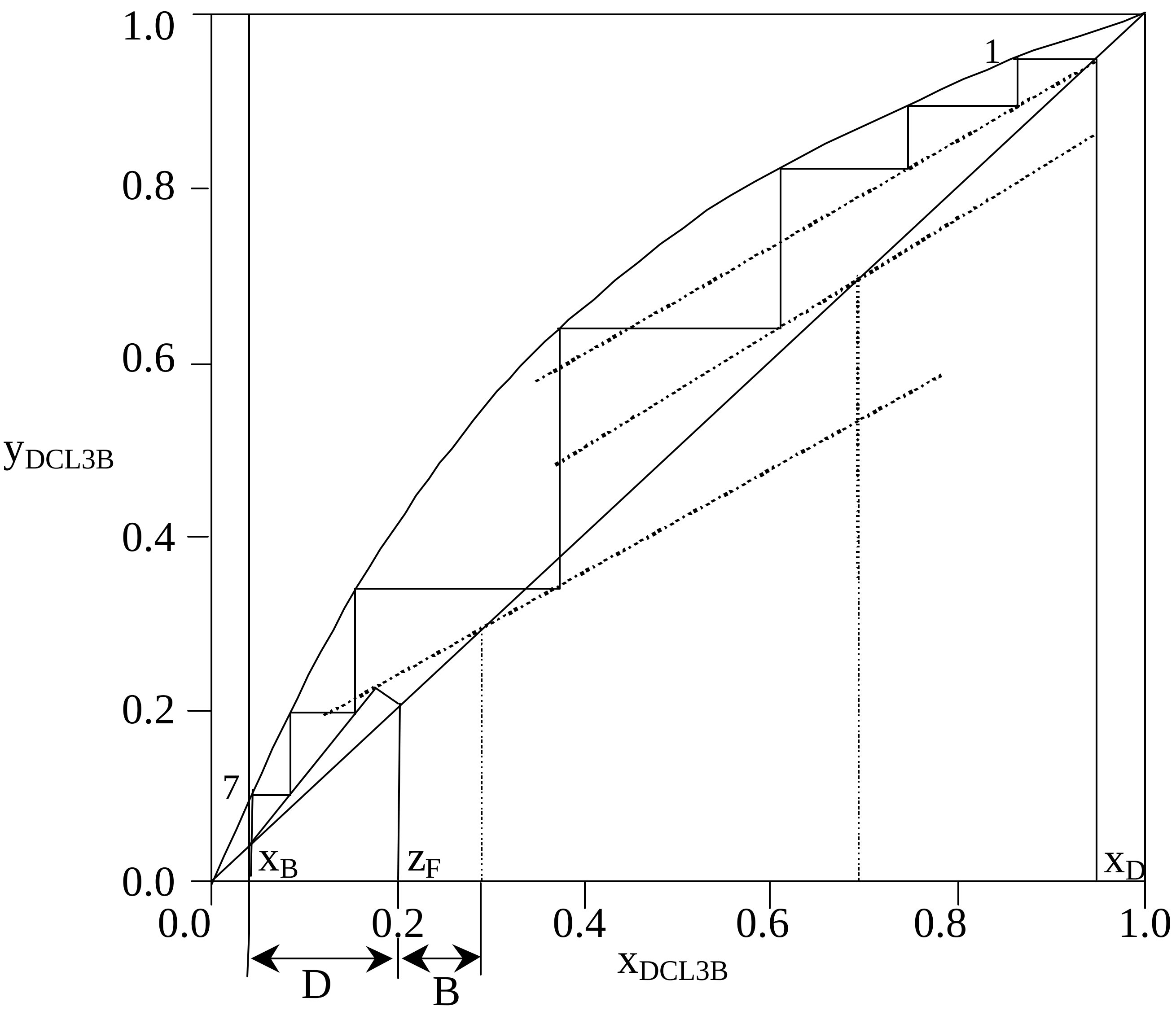
	B (Reactant)	A (Product)	
ν	-1	1	
x_D		0.99	
Feed	90	10	
ξ	Bott	Dist	diff pt
9	81	19	0.516
45	45	55	0.172
81	9	91	0.100
90	0	100	0.090

Typical values (cont'd)

	B (Reactant)	A (Product)	
ν	-1	1	
x_D		0.99	
Feed	100	0	
ξ	Bott	Dist	diff pt
10	90	10	-0.010
50	50	50	-0.010
90	10	90	-0.010
100	0	100	-0.010

Note, we get negative values here

MT plot: 1,4 dicloro-2 butene--> 1,2 dicloro-3 butene



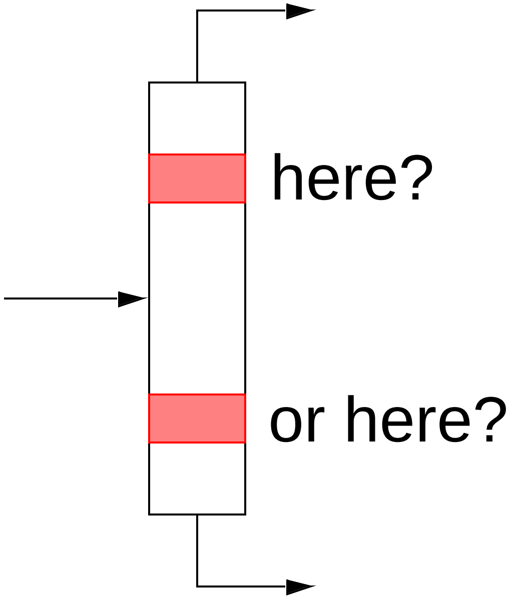
Short quiz

Given

B --> A

A is the light component

Should you put reaction in top or bottom section of the column?

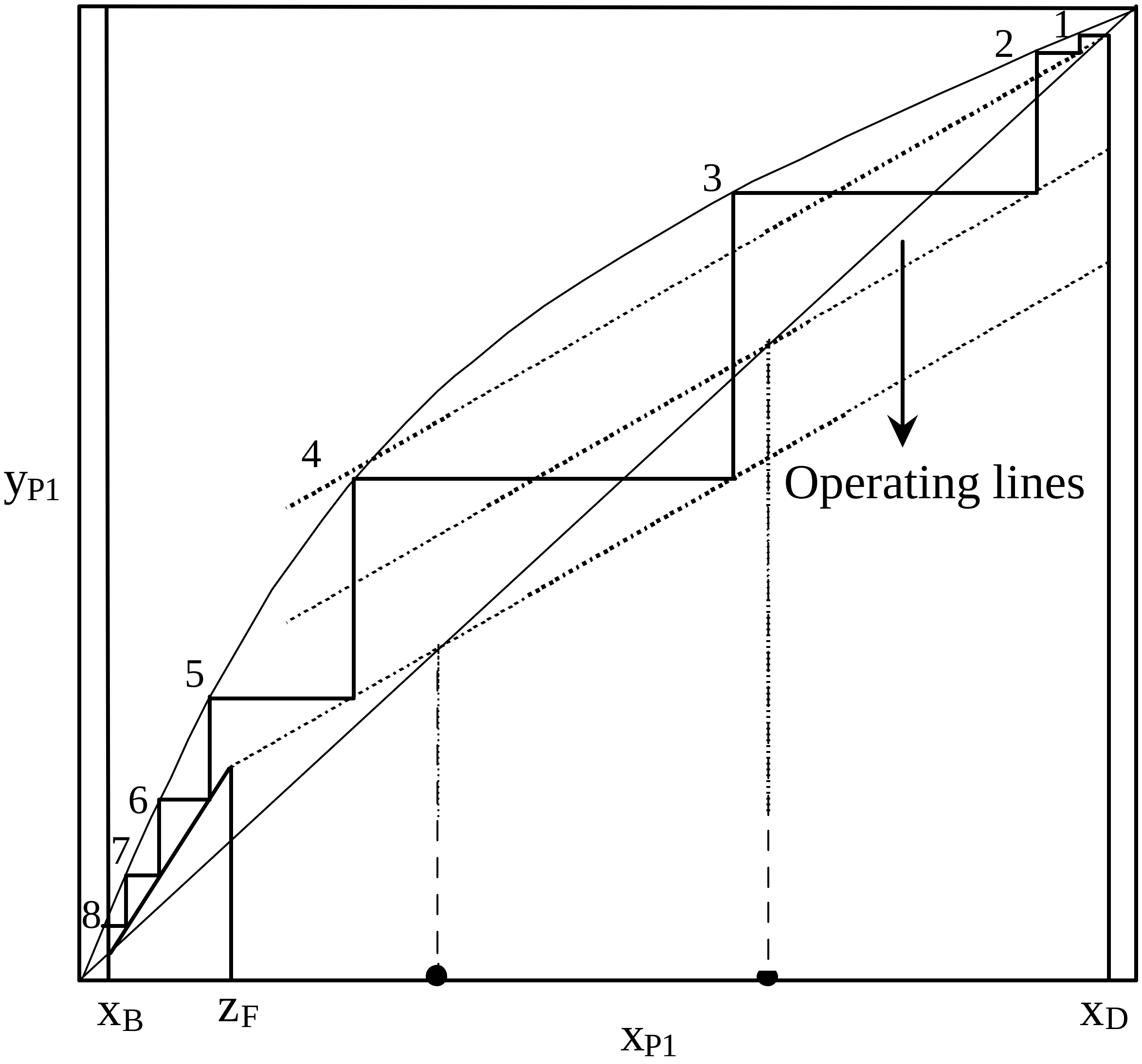


Arguments for bottom

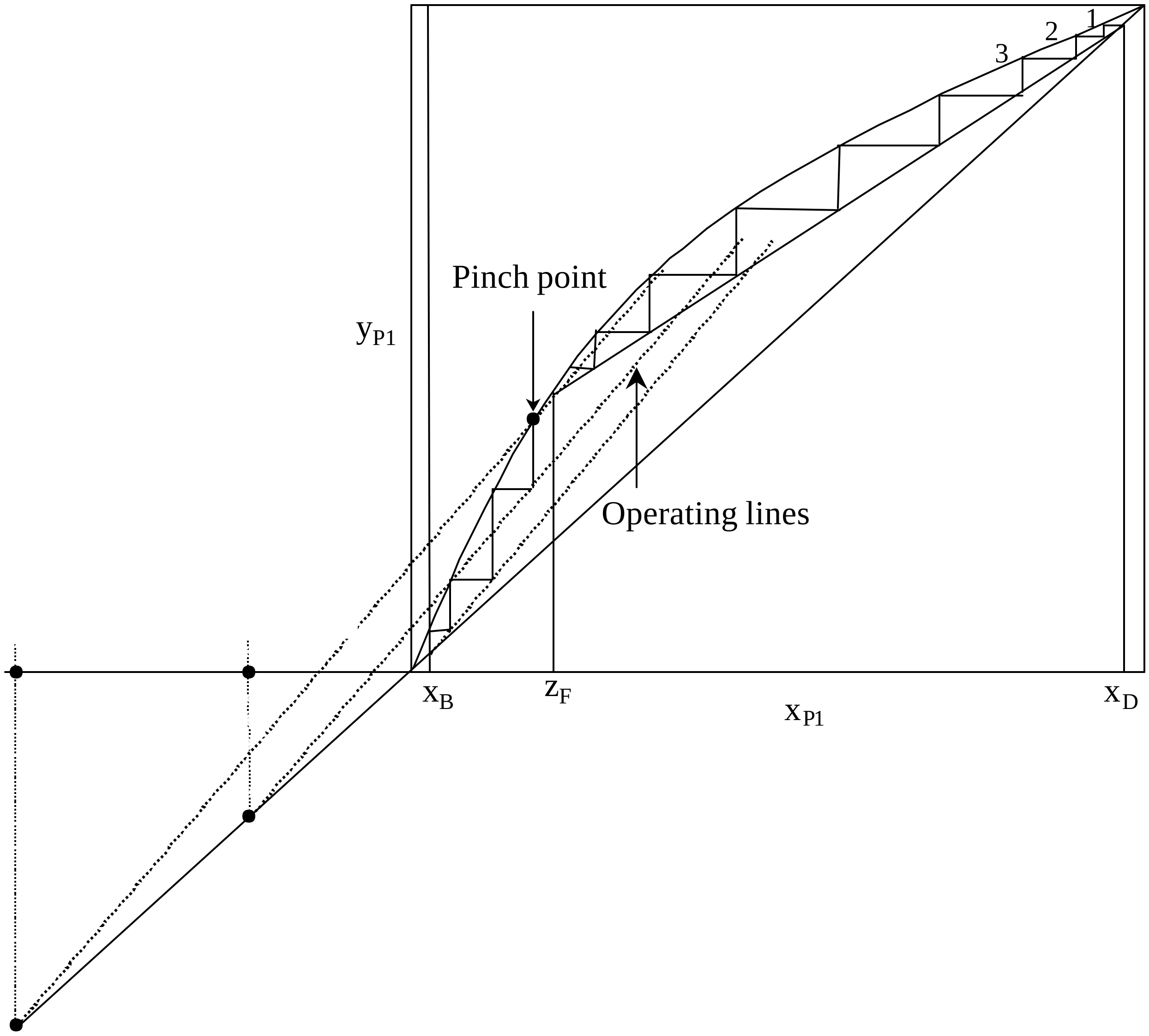
- Heavy reactant will go down, react in lower section, and form light product which is driven up the column
- Kinetics may be enhanced by hotter temperatures in the bottom
- Reaction equilibrium may be shifted -- higher temperatures are better for endothermic (bottom) and worse for extho-thermic (top)

The first observation above suggests how separation will be affected

Reaction in top section makes separation easier



Reaction in bottom section makes separation harder

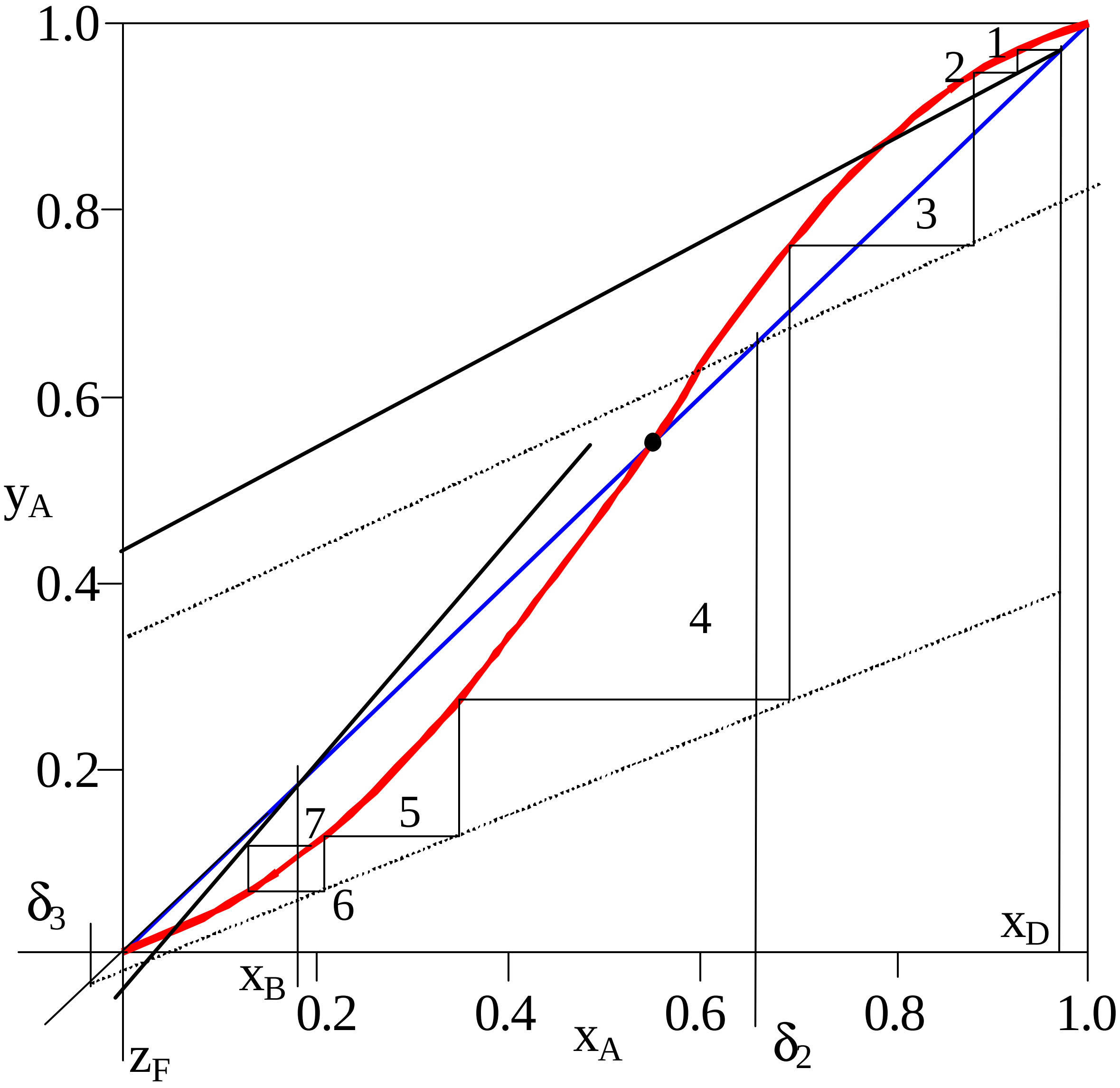


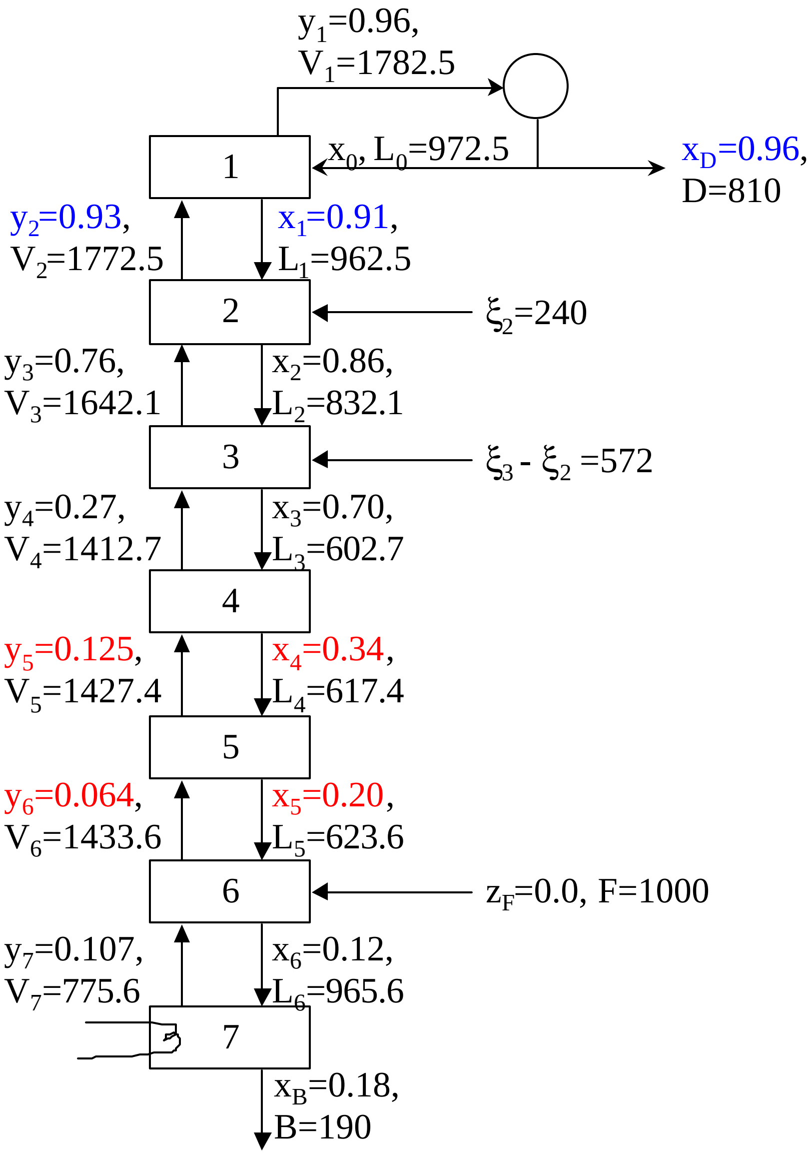
Arguments for bottom

- Heavy reactant will go down, react in lower section, and form light product which is driven up the column
- Kinetics may be enhanced by hotter temperatures in the bottom
- Reaction equilibrium may be shifted -- higher temperatures are better for endothermic (bottom) and worse for extho-thermic (top)

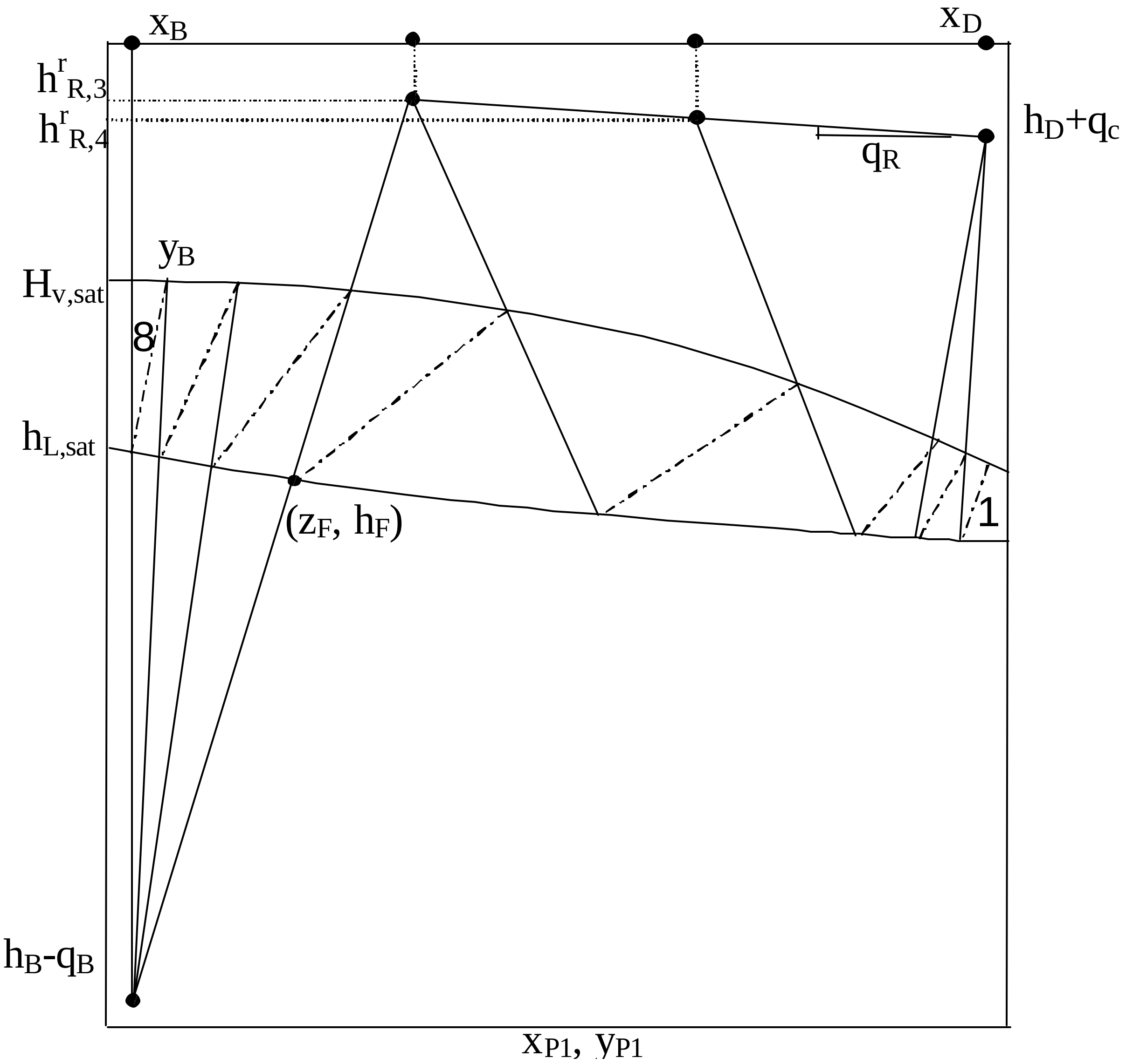
The first insight *appears to be an invalid insight*

Breaking an azeotrope



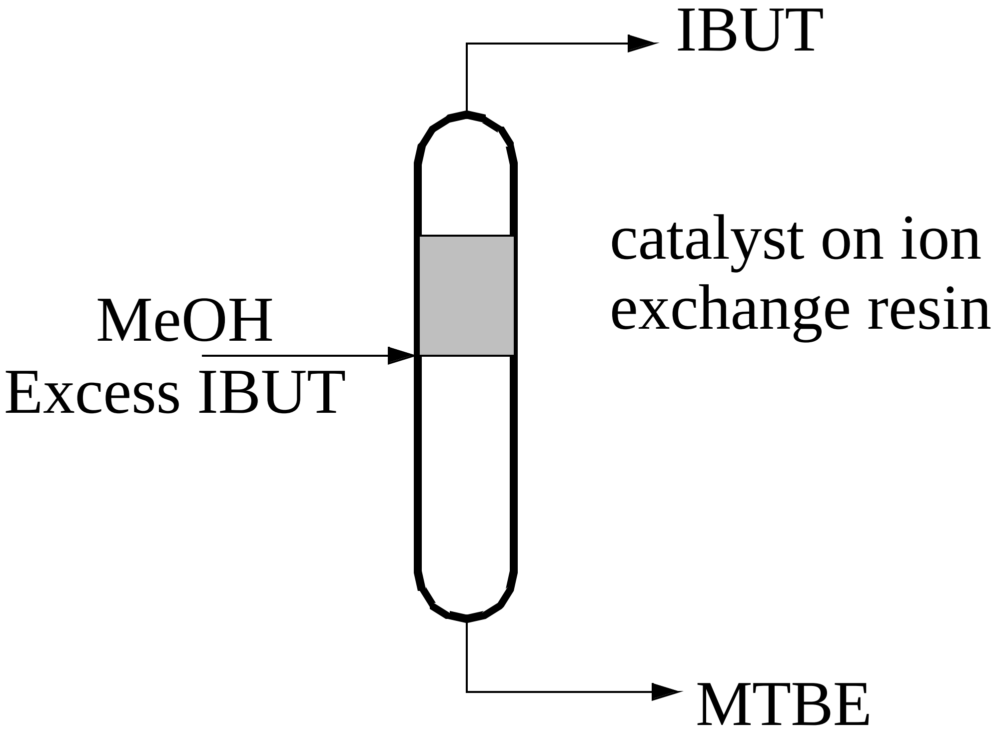

y_1=0.96,
V_1=1782.5
1
x_0, L_0=972.5
x_D=0.96,
D=810
y_2=0.93,
V_2=1772.5
x_1=0.91,
L_1=962.5
2
ξ_2=240
y_3=0.76,
V_3=1642.1
x_2=0.86,
L_2=832.1
3
ξ_3 - ξ_2 =572
y_4=0.27,
V_4=1412.7
x_3=0.70,
L_3=602.7
4
y_5=0.125,
V_5=1427.4
x_4=0.34,
L_4=617.4
5
y_6=0.064,
V_6=1433.6
x_5=0.20,
L_5=623.6
6
z_F=0.0, F=1000
y_7=0.107,
V_7=775.6
x_6=0.12,
L_6=965.6
7
x_B=0.18,
B=190

Ponchon-Savarit Diagram



Ex: MeOH + IBUT <==> MTBE

Why did industry settle
on this design?



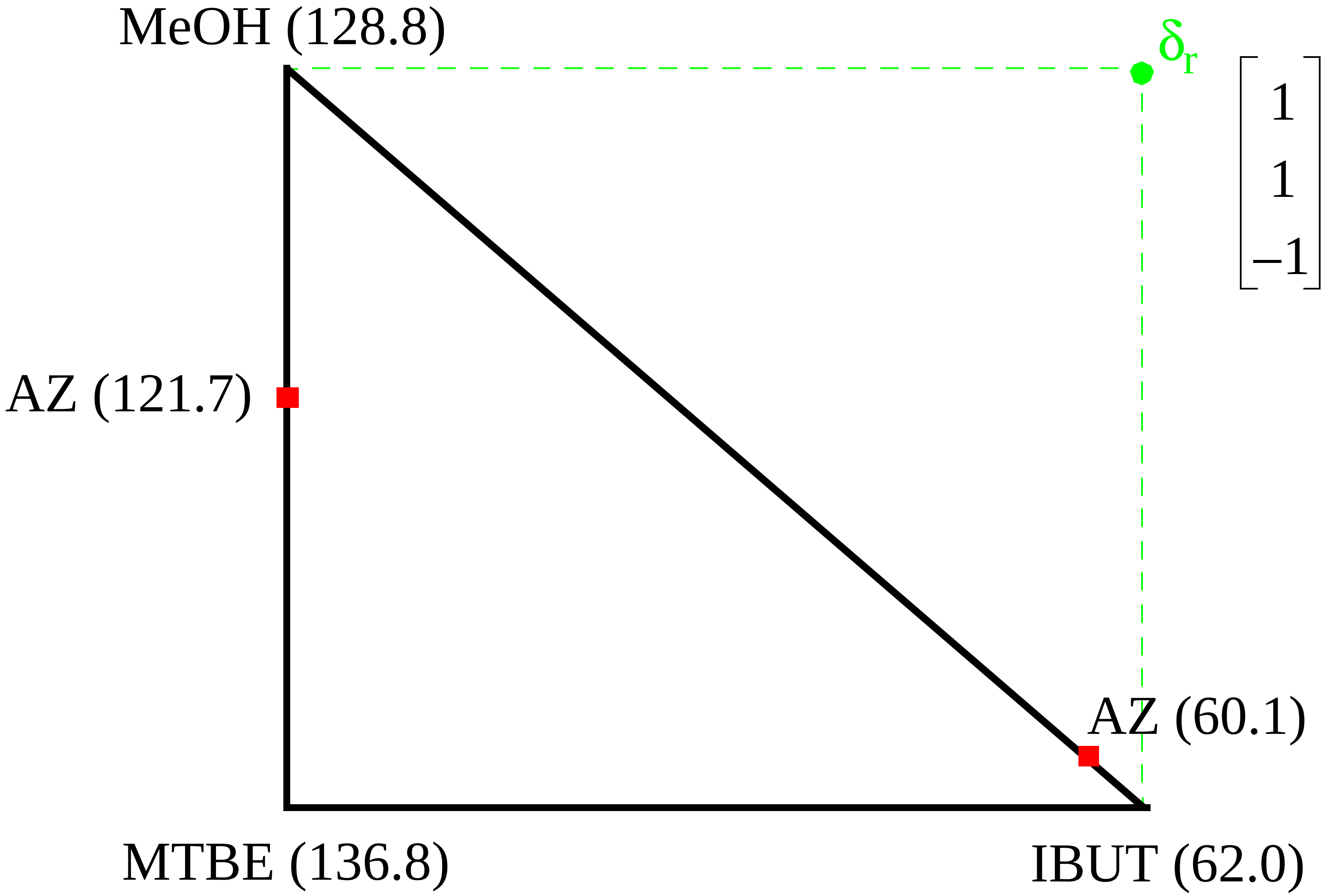
IBUT

catalyst on ion
exchange resin

MeOH
Excess IBUT

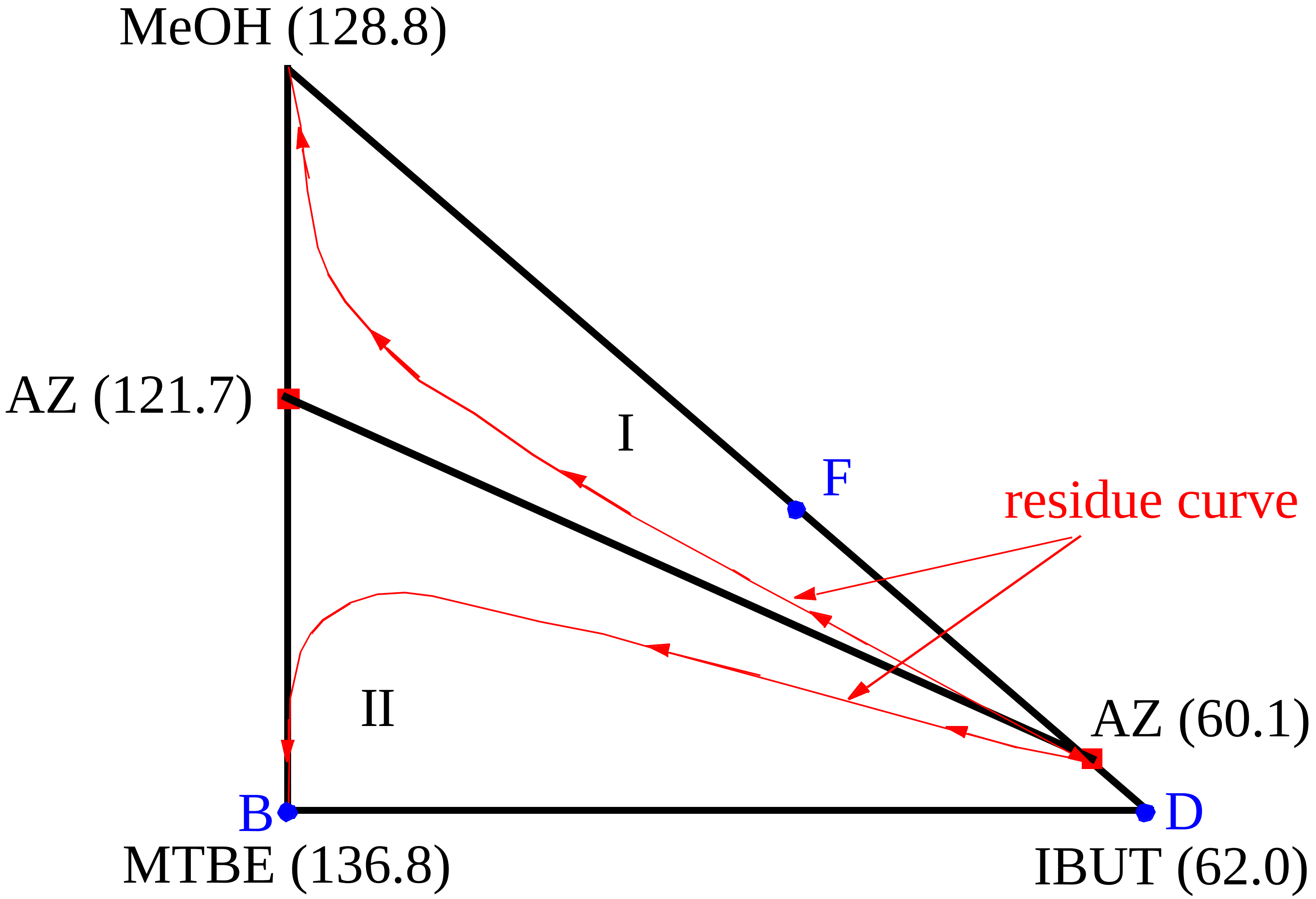
MTBE

Reaction difference point (MeOH + IBUT <==> MTBE)

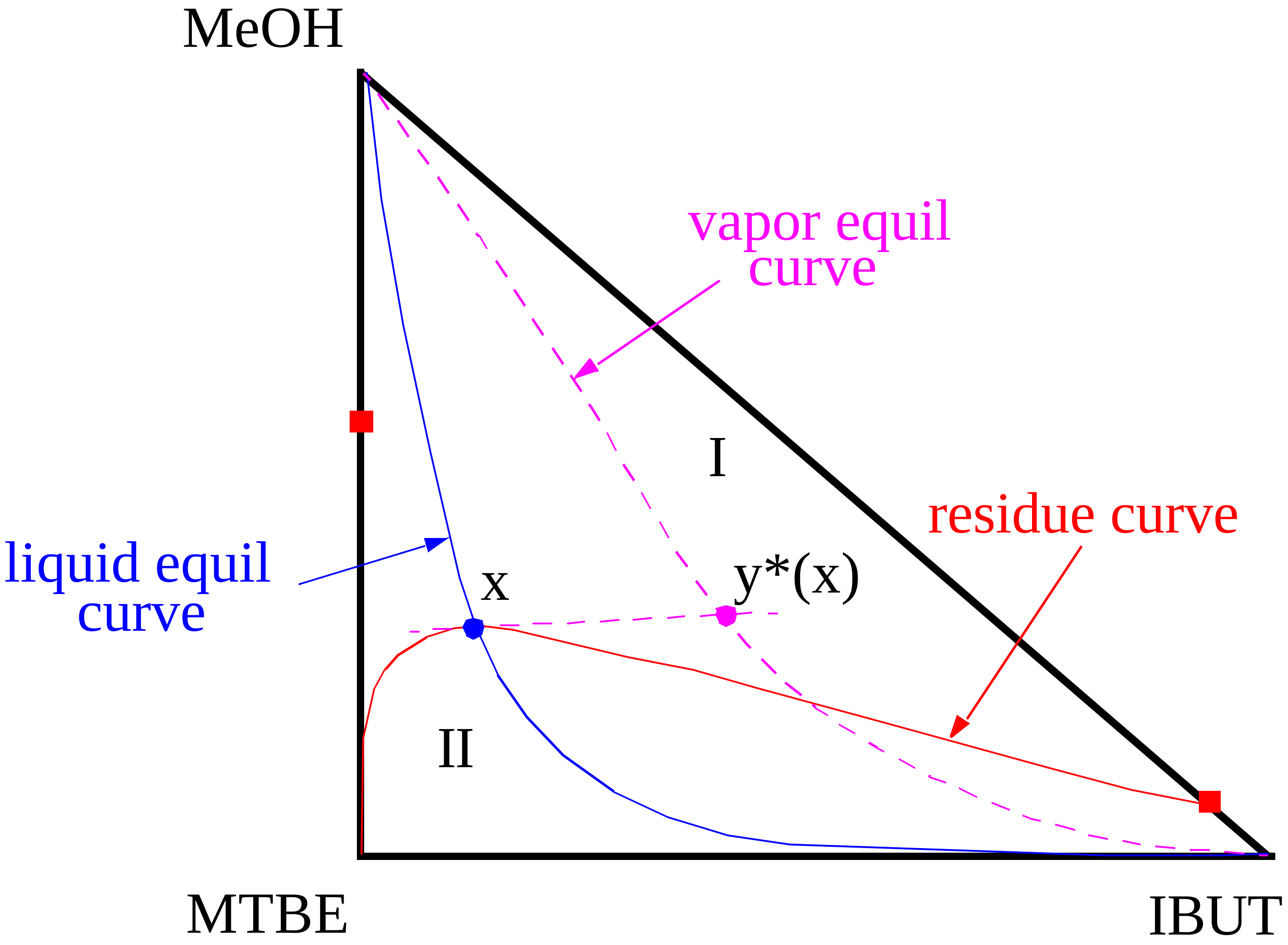


$$\begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix}$$

Two distillation regions



Liquid and vapor (rxn) equilibrium curves



Reactive diff pt and lever rule ==> little reaction in bottom

In bottom

$L_n = V_{n+1} + \Delta$

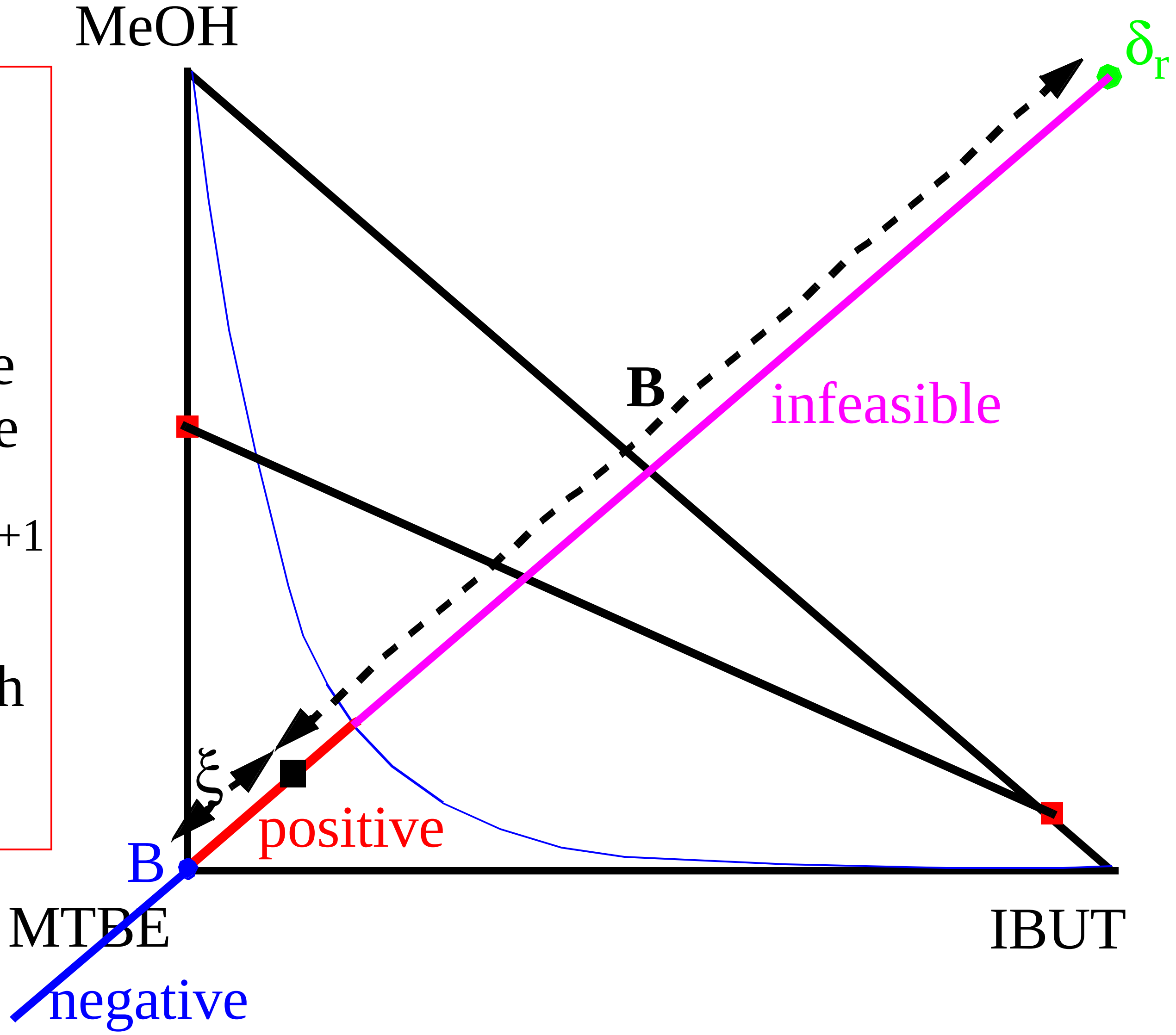
$\Delta = B + \xi$

Want ξ positive

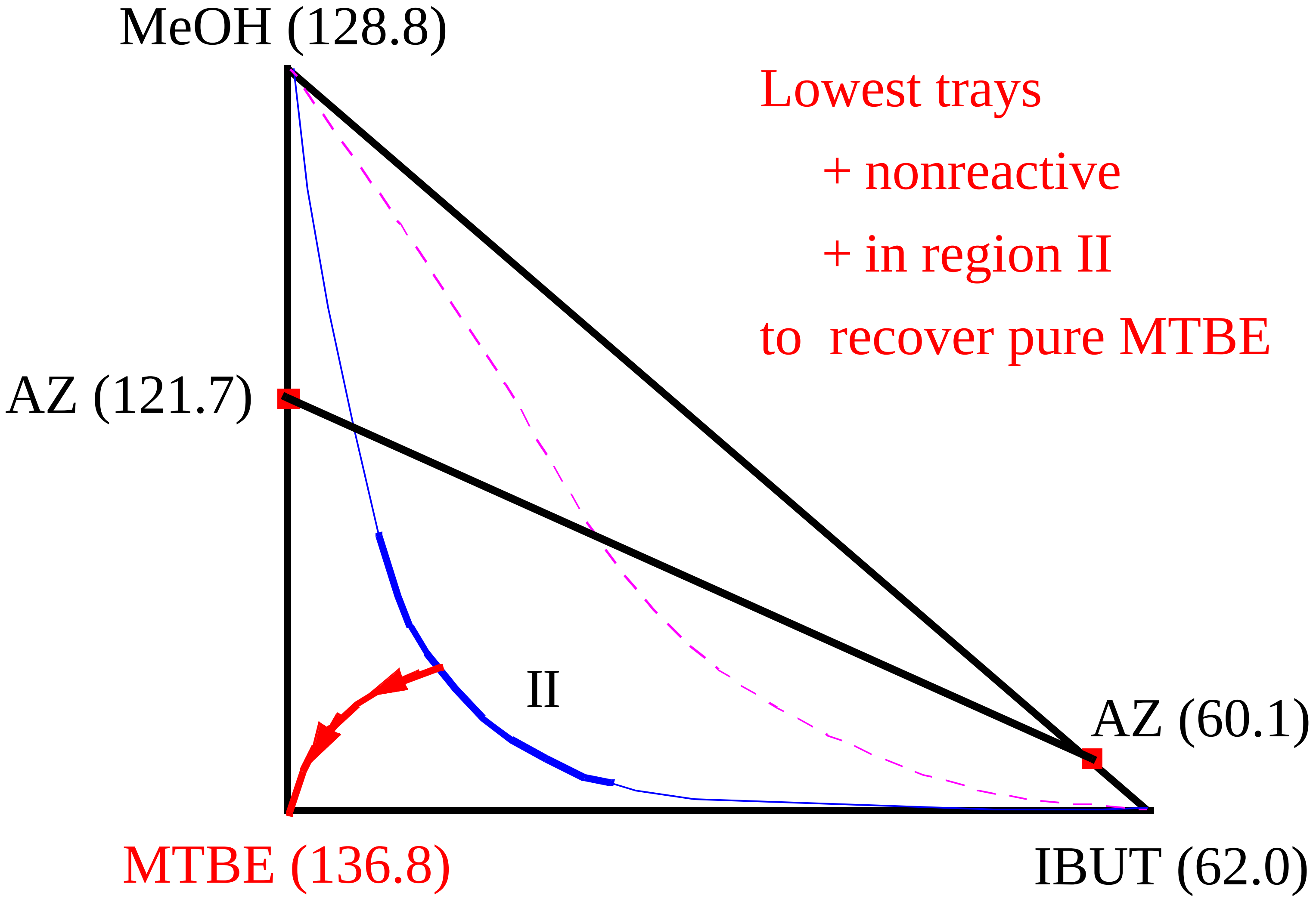
==> Δ positive

L_n between V_{n+1} and Δ

Cannot be much reaction in bottom



Nonreactive bottom section required



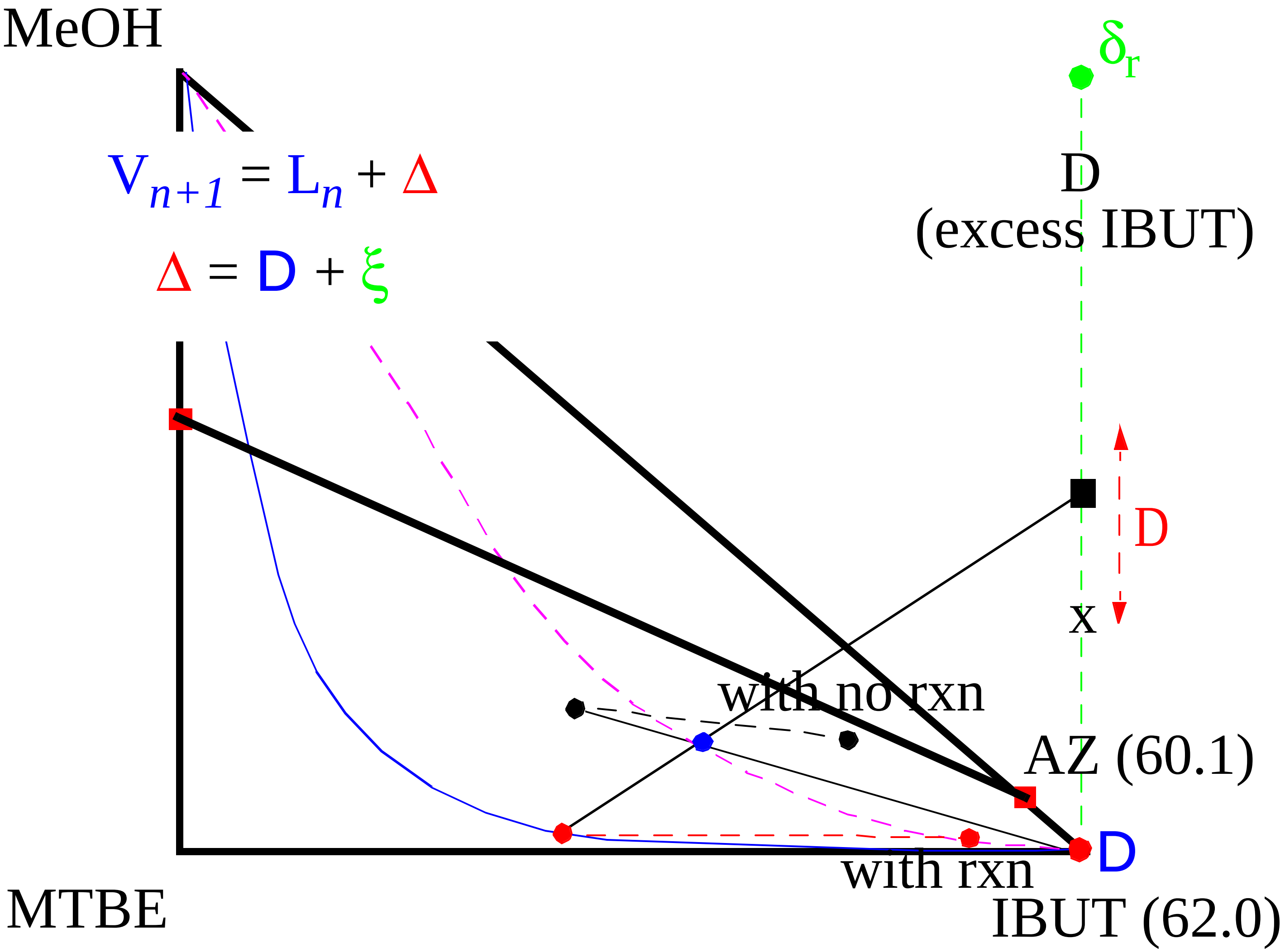
Lowest trays

+ nonreactive

+ in region II

to recover pure MTBE

Major reaction possible and needed in top section



$$V_{n+1} = L_n + \Delta$$

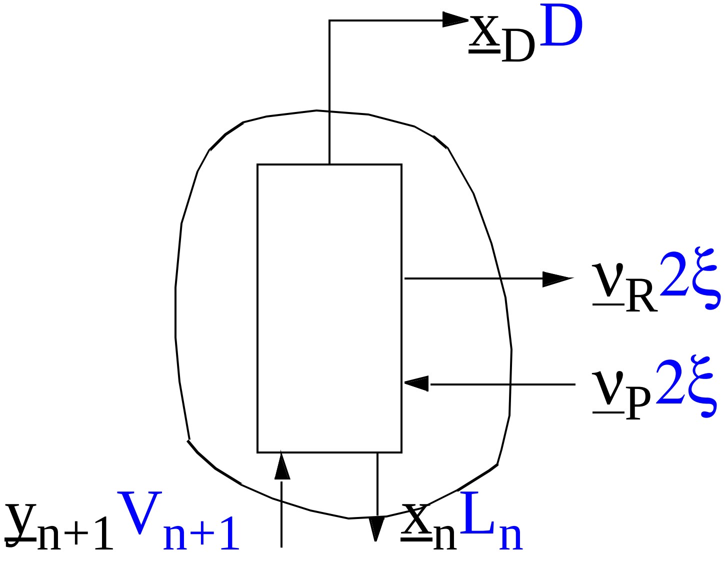
$$\Delta = D + \xi$$

A “split” lever rule

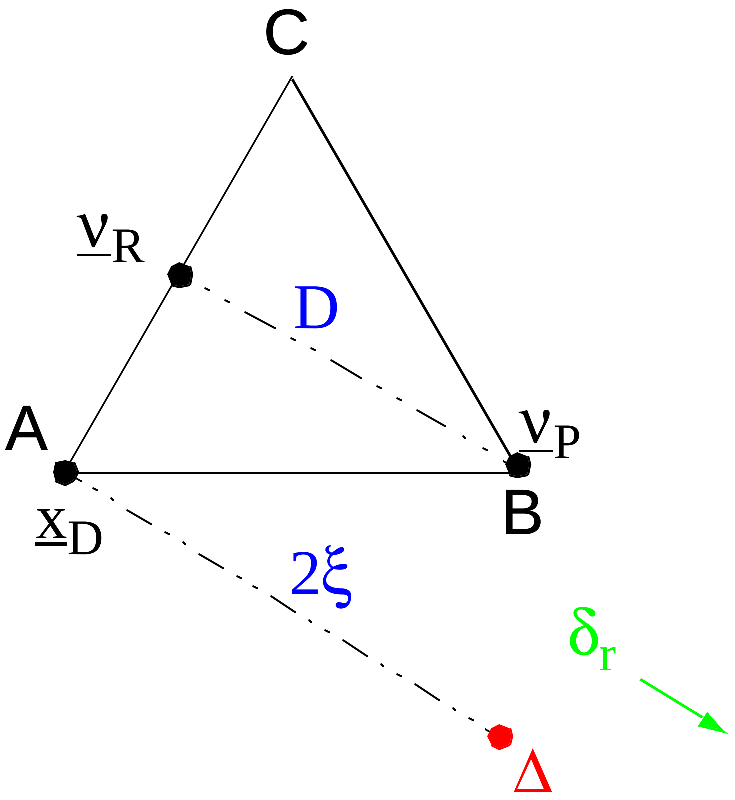
$\nu_T = -1-1+2 = 0$

$$\underline{y}_{n+1} V_{n+1} = \underline{x}_n L_n + \underline{x}_D D + (\underline{\nu}_R - \underline{\nu}_P) 2\xi$$

$$==> \underline{x}_\Delta \Delta = \underline{x}_D D + (\underline{\nu}_R - \underline{\nu}_P) 2\xi$$

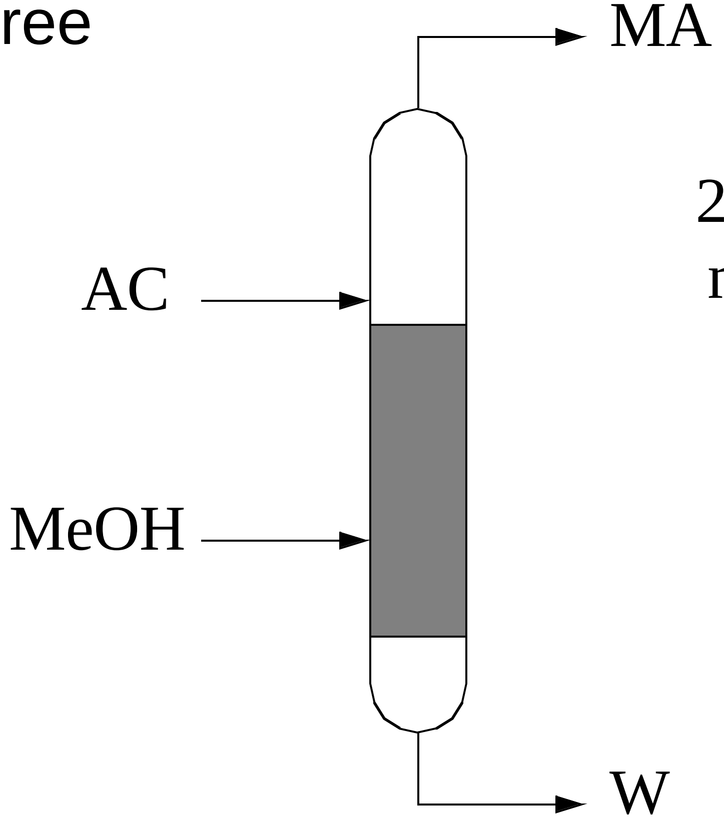


A+C <==> 2B



Ex: Methyl acetate, MeOH + AC = MA + W

A way to handle more than three components



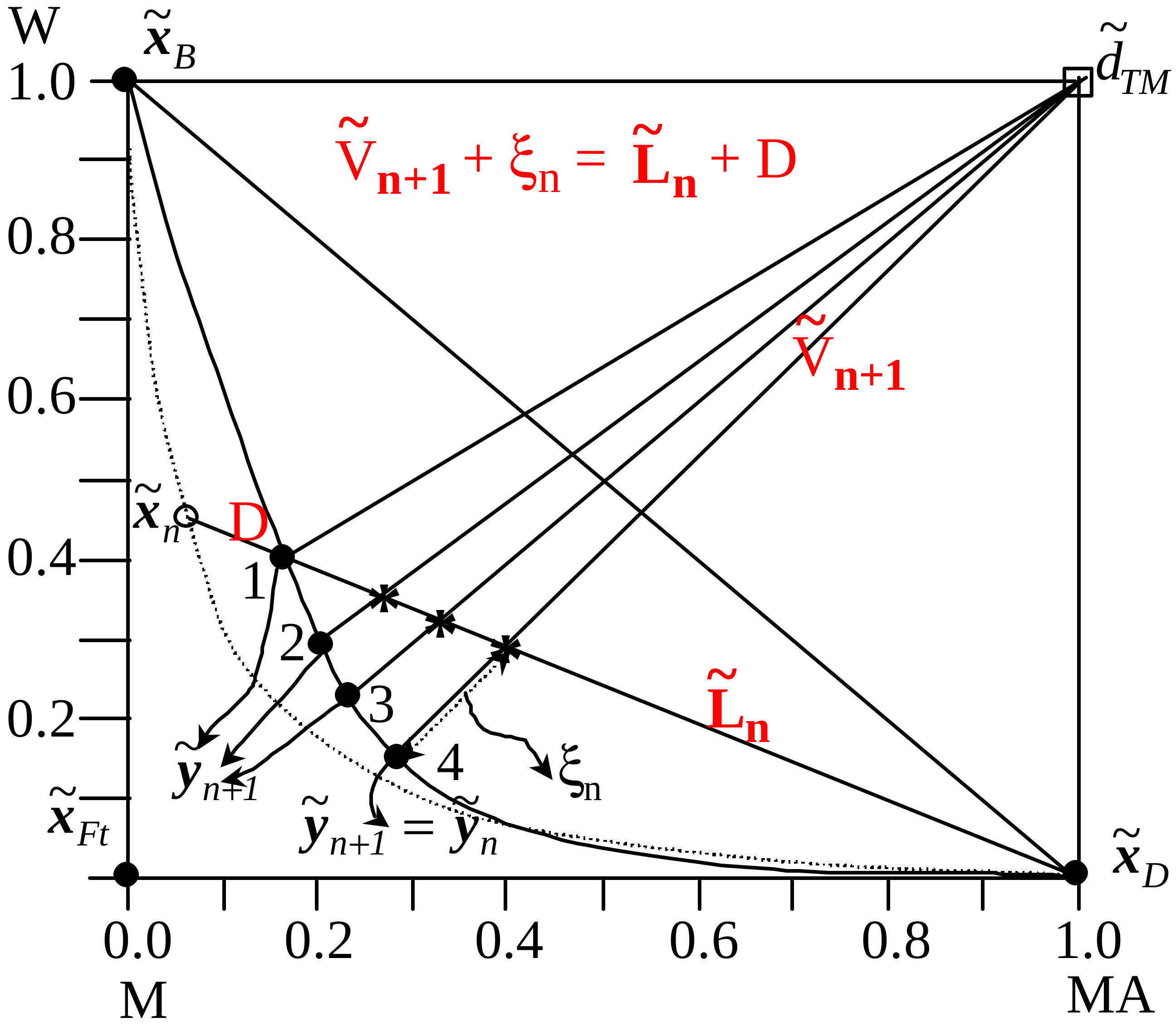
2 moles produce 2 moles so reaction point at infinity

Four components - use following projection

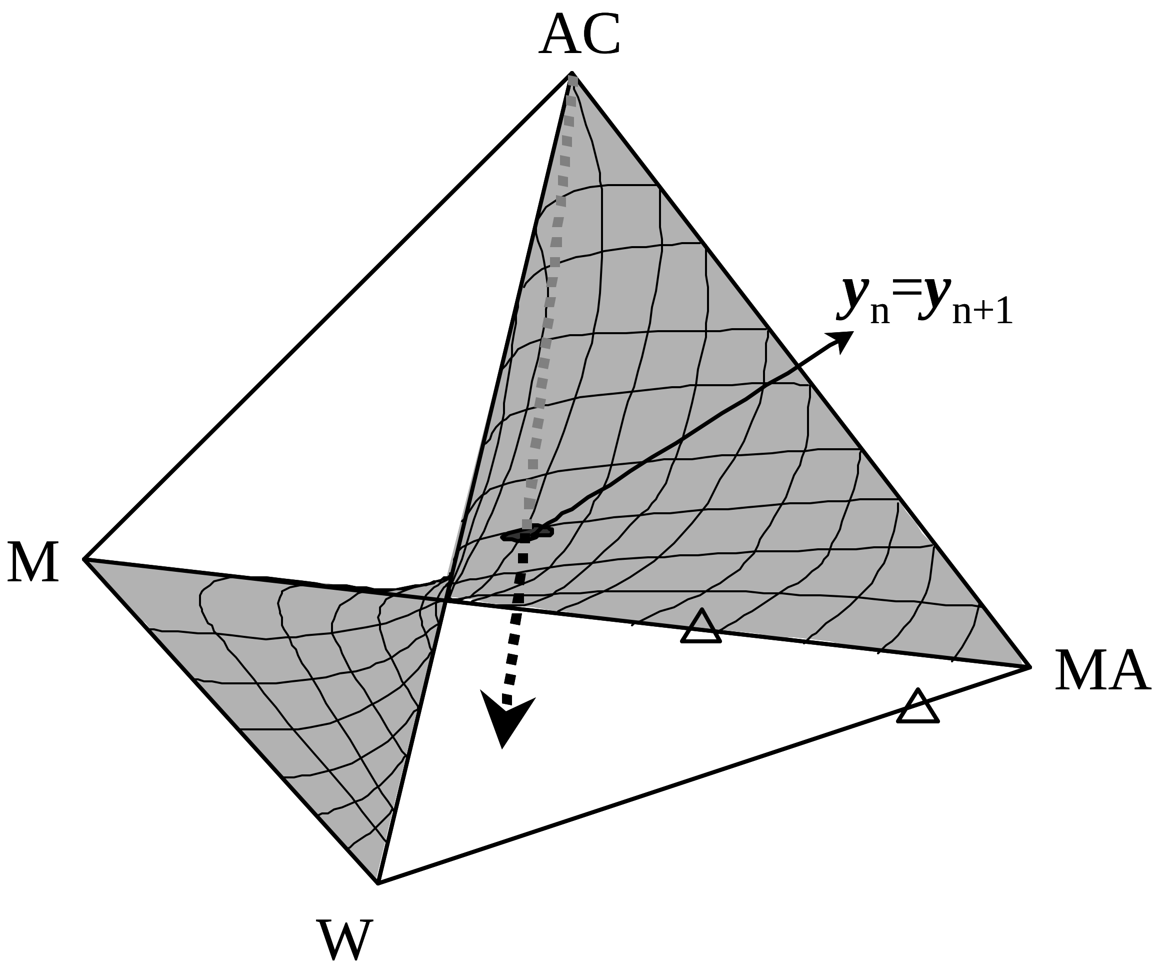
- Set acetic acid concentration to a low value (say 5%) and fix it
- Map to acetic acid free basis
- All equations transform nicely
- On acetic acid free basis
  - MeOH = MA + W
  - reaction difference point moves to finite location

Question: Why does the amount of reaction that can occur in the column *decrease* with large reflux ratios? This is counterintuitive.

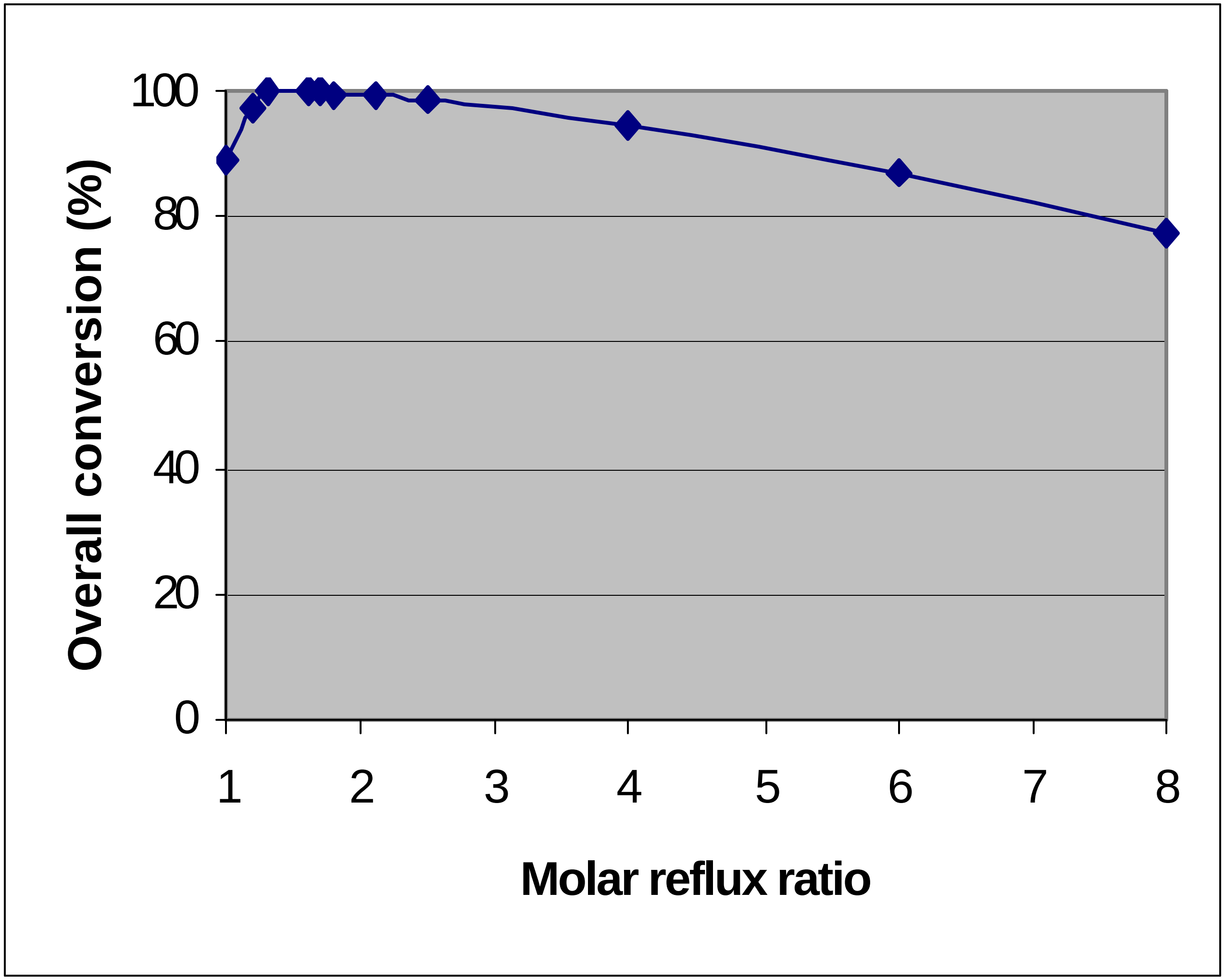
Geometry


W
$\tilde{x}_B$
$\tilde{d}_{TM}$
1.0
0.8
0.6
0.4
0.2
$\tilde{V}_{n+1} + \xi_n = \tilde{L}_n + D$
$\tilde{V}_{n+1}$
$\tilde{x}_n$
D
1
2
3
4
$\tilde{L}_n$
ξ_n
$\tilde{y}_{n+1}$
$\tilde{x}_{Ft}$
$\tilde{y}_{n+1} = \tilde{y}_n$
$\tilde{x}_D$
0.0
0.2
0.4
0.6
0.8
1.0
M
MA

Projection of equilibrium vapor composition



Maximum in conversion vs. reflux ratio



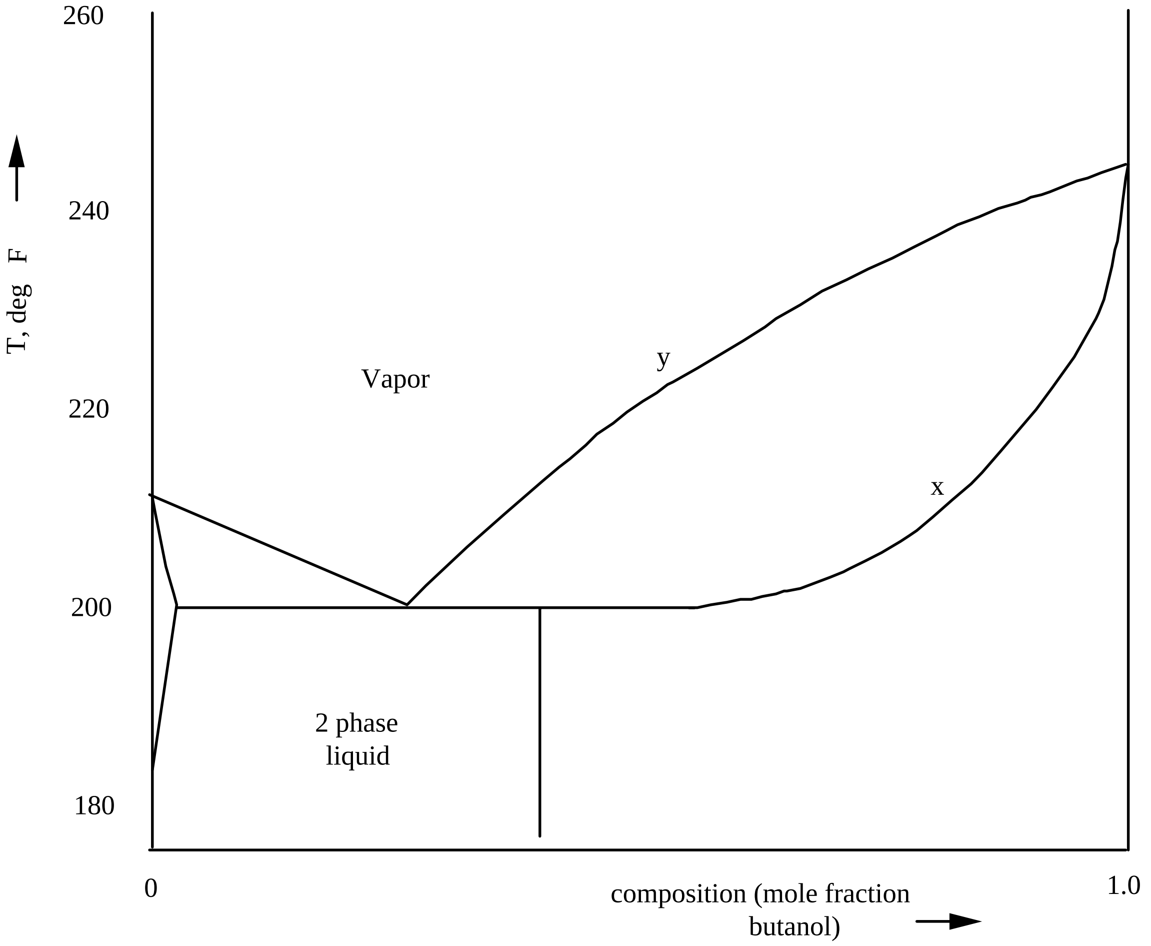
Conclusions

- Why reactive distillation
- Reaction, separation and mixing vectors, design in transport space
- Difference points
- McCabe-Thiele diagram
- Non-intuitive behavior
- Ponchon-Savarit diagram
- Examples
  - + diluted ternary: MTBE
  - + quaternary (using projection): methyl acetate

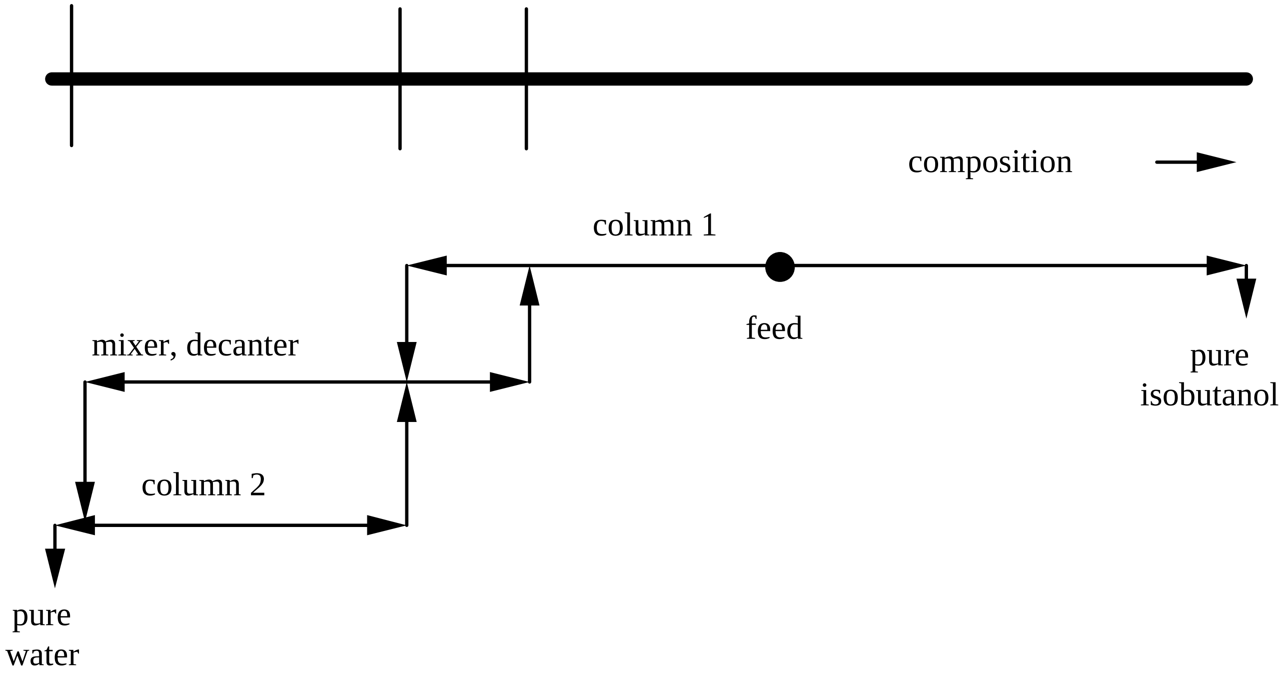
Azeotropic distillation

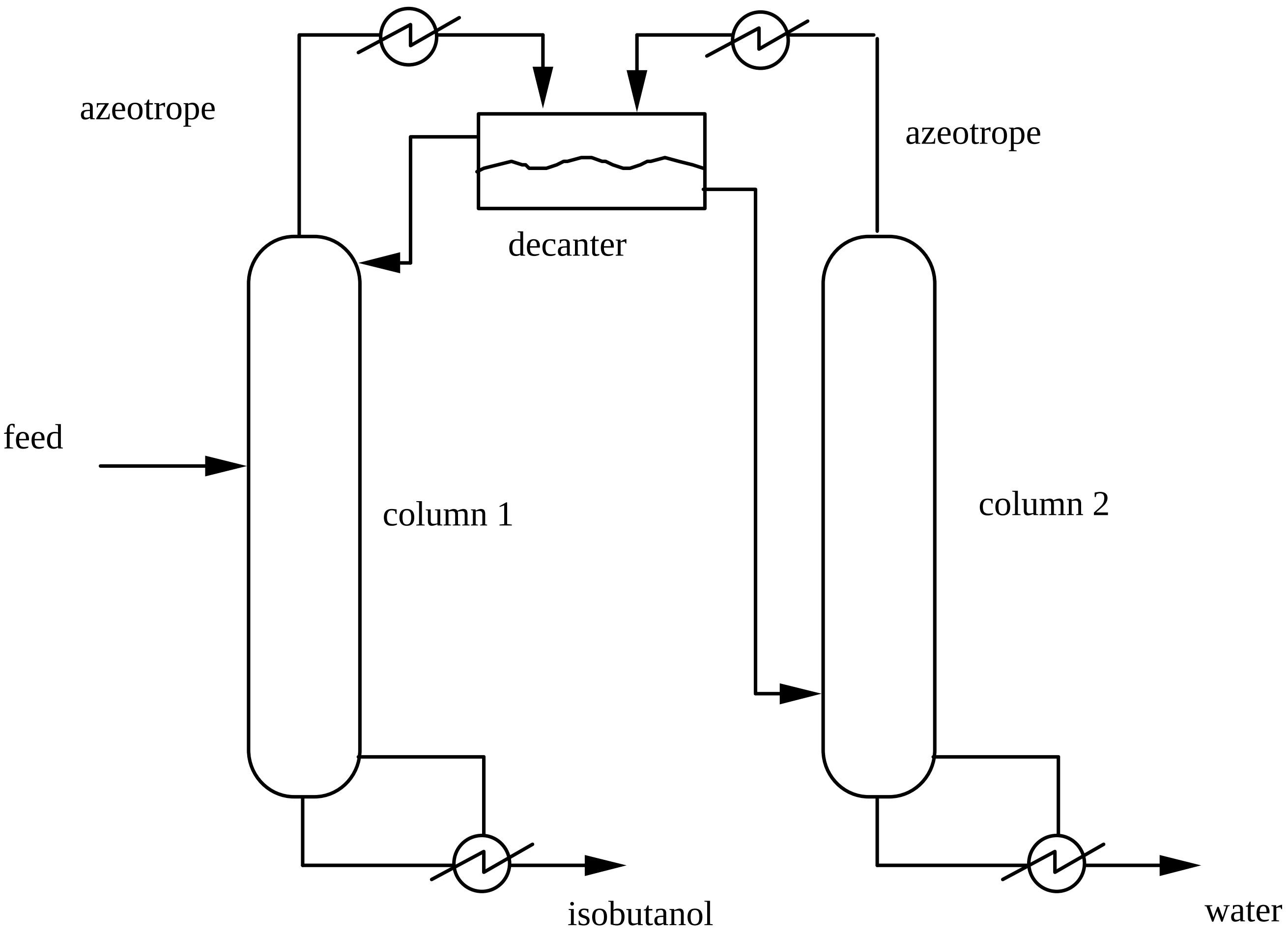
Example 1

Separate water from iso-butanol. The phase behavior for this mixture is interesting. There is a minimum boiling azeotrope formed as well as a liquid-liquid phase separation when the liquid is cooled enough.

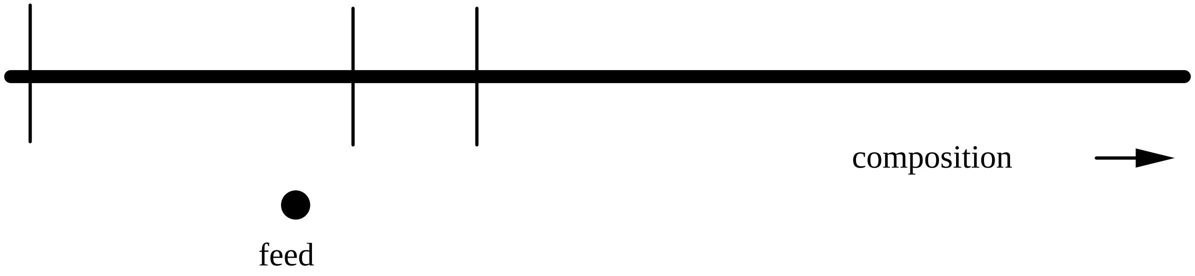


A convenient representation to look at this problem is the following which shows the key points along the composition axis




azeotrope
azeotrope
decanter
feed
column 1
column 2
isobutanol
water

Question: how would you design the system for the following feed?



Residue curves and distillation boundaries

Doherty and coworkers and Stichlmair and Fair described residue curves, and as we shall see shortly, distillation boundaries for azeotropic mixtures. They describe them almost exclusively for three component mixtures. The two approaches are similar but not exactly the same.

Doherty et al

Integrate the trajectory in composition space described by the equations

$$\frac{dx_1}{dt} = x_1 - y_1 = x_1 - K_1 x_1$$

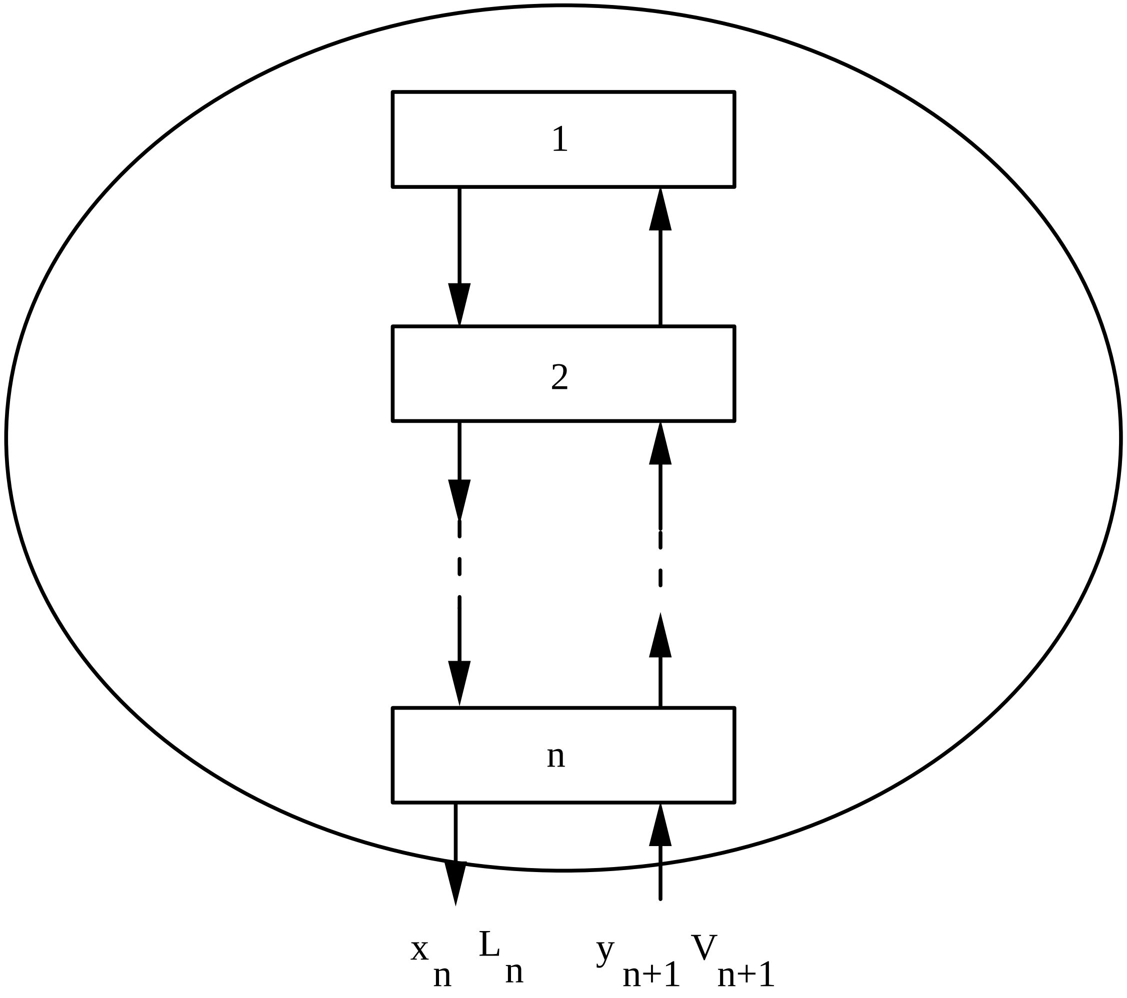
$$\frac{dx_2}{dt} = x_2 - K_2 x_2$$

$$\frac{dx_3}{dt} = x_3 - K_3 x_3$$

and plot on a triangular diagram. Note, the x_i's sum to unity so one of these equations is not independent.

Stichlmair and Fair

Step from any point to another by assuming one is operating a total reflux column.



Total reflux column (no feed or product)

Material balance equations

$V_{n+1} = L_n$ $\qquad$ $y_{n+1,i} V_{n+1} = x_{n,i} L_n$

therefore

$$y_{n+1,i} = x_{n,i} \qquad (1)$$

Equilibrium gives

$$y_{n+1,i} = K_{n+1,i} x_{n+1,i} \qquad (2)$$

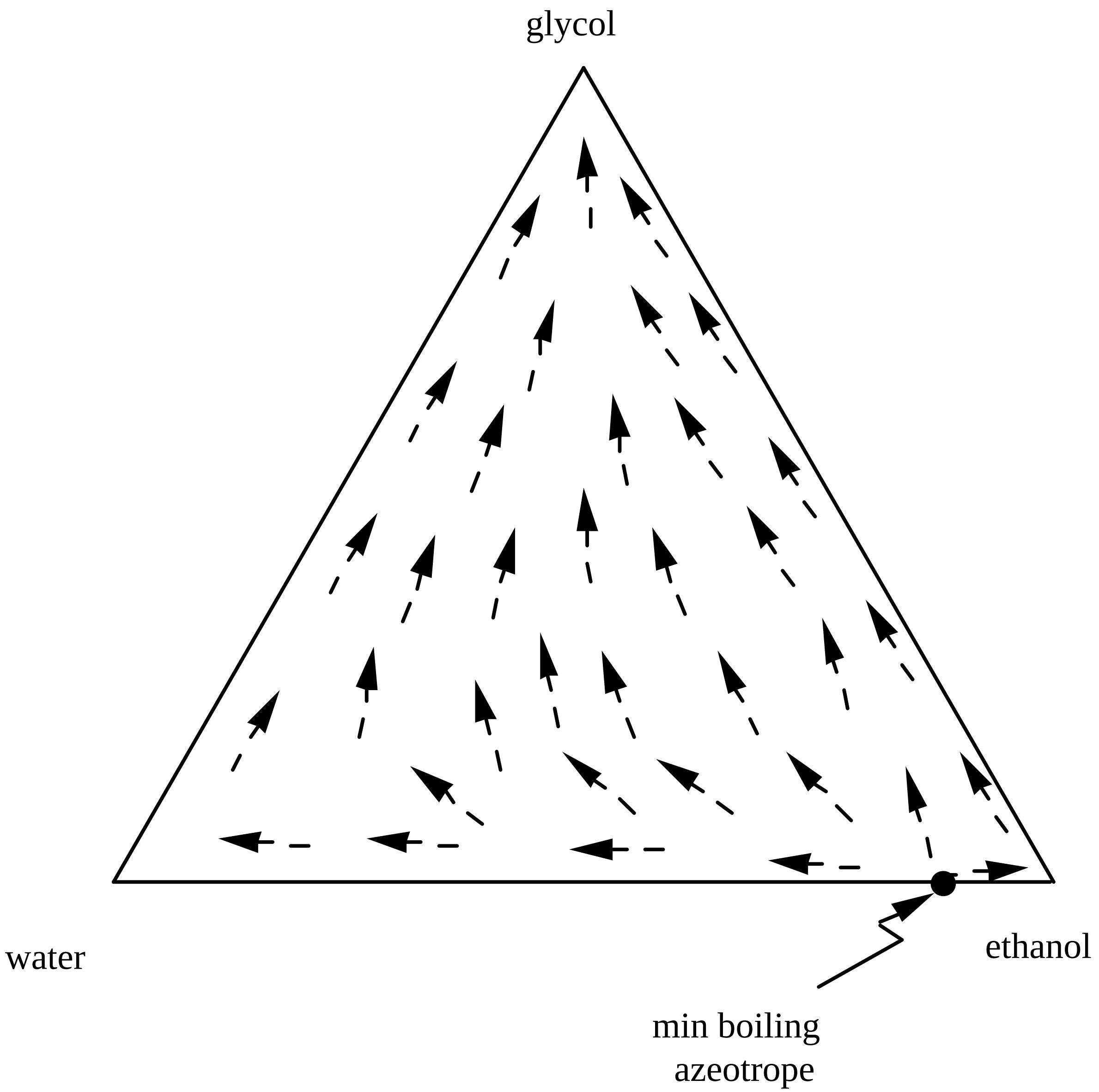
Propagation from one point to the next therefore combines (1) and (2)

$$x_{n,i} = K_{n+1,i} x_{n+1,i}$$

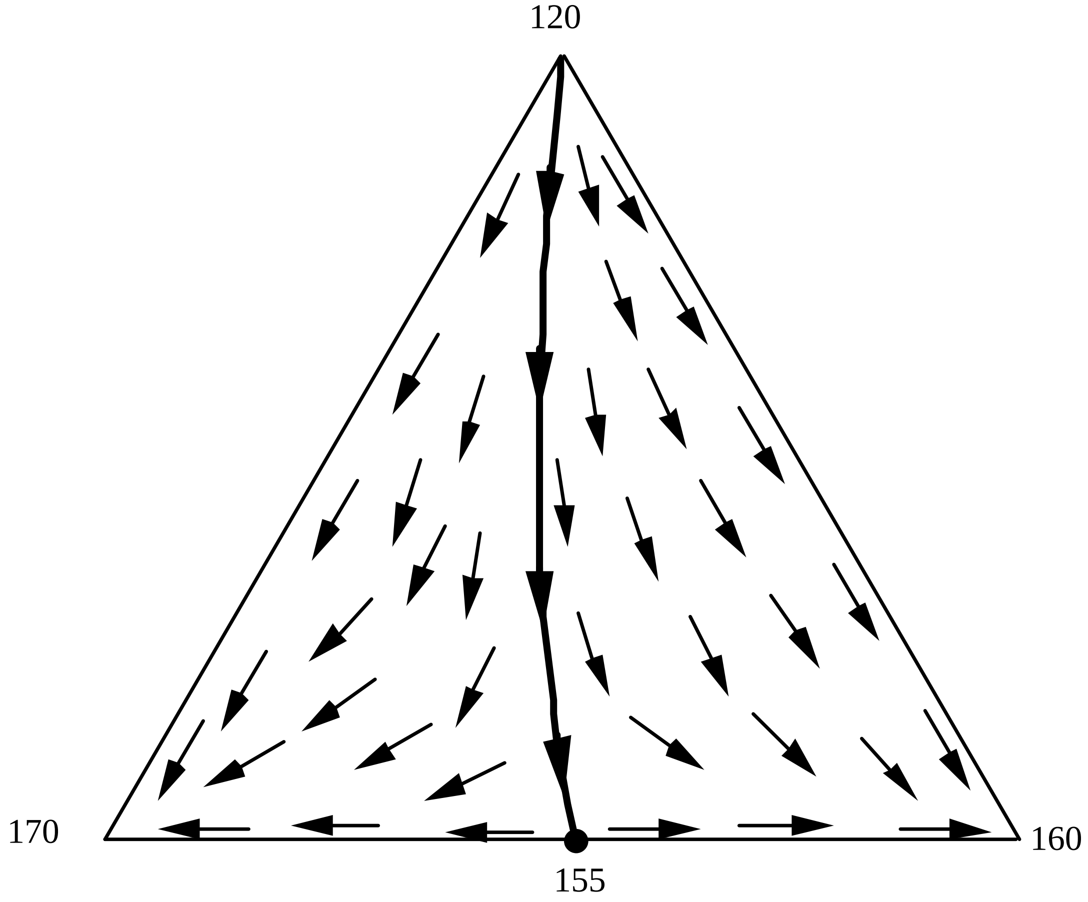
to propagate up the column.

Plotting the results from developing these solutions creates trajectories on a triangular composition diagram.

- These trajectories always move from low boiling mixtures to higher boiling ones.


glycol
water
ethanol
min boiling
azeotrope

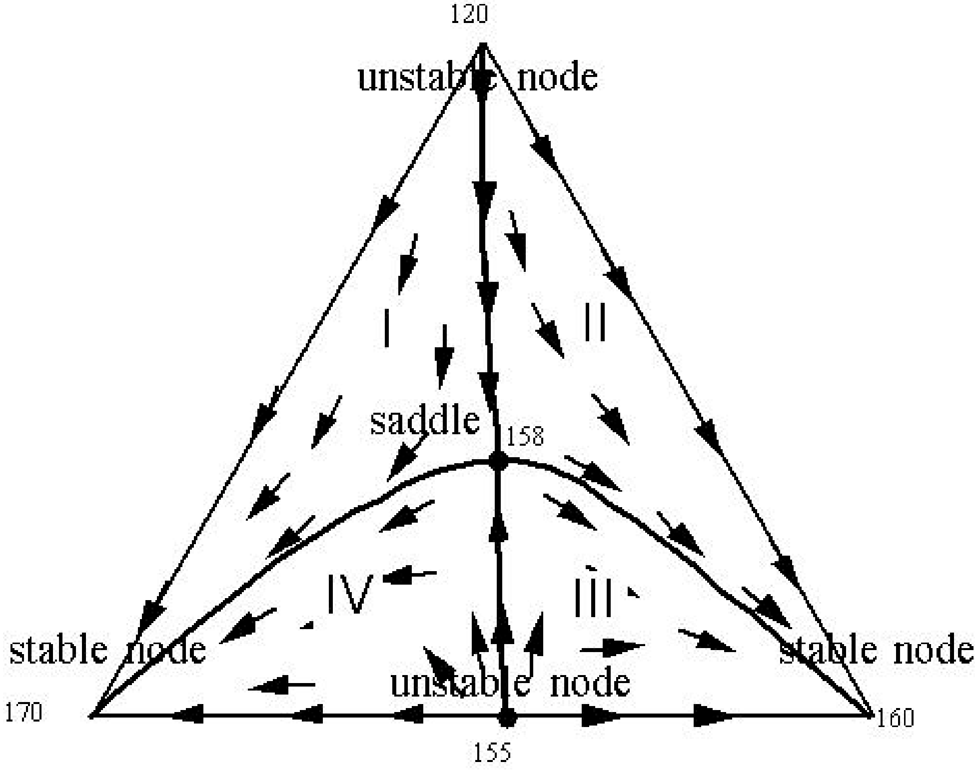
There are examples where these trajectories break the triangle into regions.



The claim is that one cannot cross these boundaries using distillation columns, at least not by enough to make it useful. It would be impossible therefore to break the minimum boiling azeotrope (155 deg point) with the low boiling component (120 deg component) indicated using ordinary distillation columns.

Nodes and saddles

In a residue map, the pure component and azeotrope points are of three types: stable nodes, unstable nodes and saddle. All trajectories enter a stable node (it is a local high temperature point), all trajectories leave an unstable node (it is a local low temperature point), and some trajectories enter while others leave a saddle.



In this case there are four distillation regions. Note the nodes and saddles. Why is the ternary azeotrope a saddle?

One can check if a ternary diagram is topologically legal by using the following formula (Doherty and Perkins, 1975):

$$4*(N3-S3)+2*(N2-S2)+(N1-S1) = 1$$

where

N3 is the number of ternary azeotropes that are nodes
S3 the number that are saddles
N2 the number of binary azeotropes that are nodes
S2 that are saddles
N1 the number of pure component nodes
S1 the number of pure component saddles

If you create a sketch that violates this equation, the diagram is not legal.

For the above examples

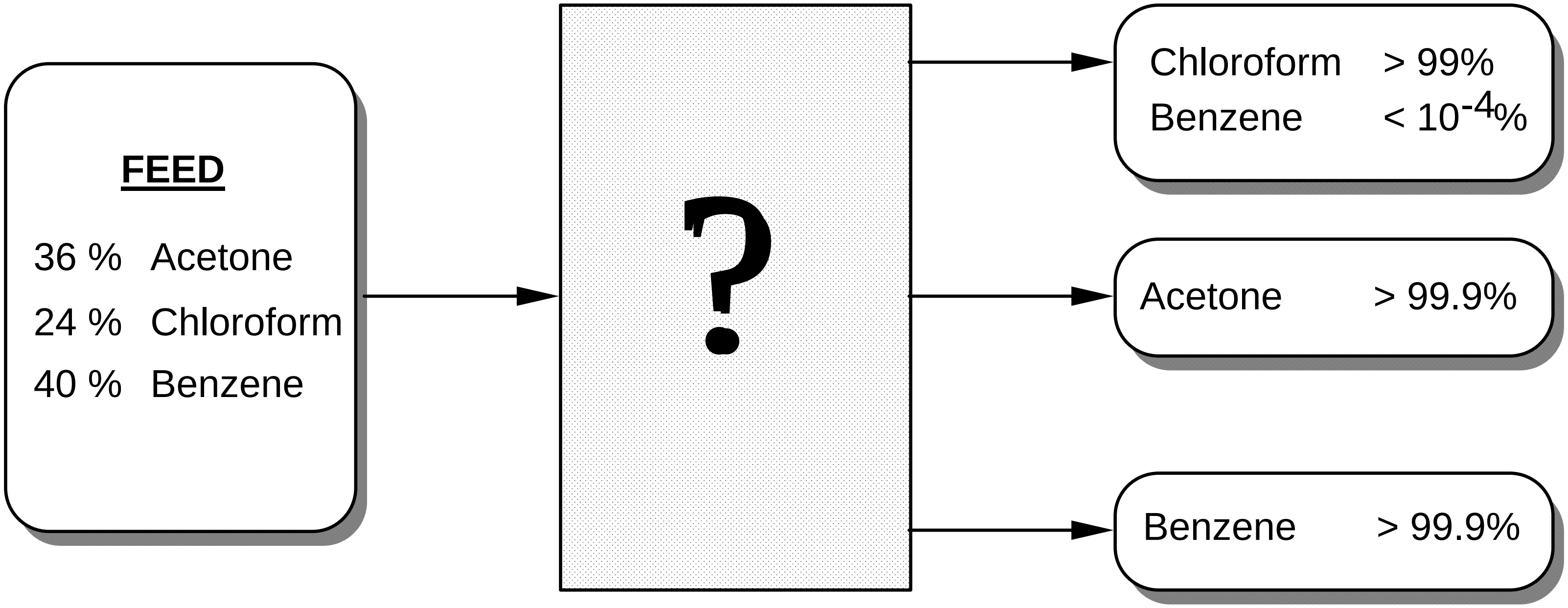
Ethanol, water, glycol: $(4(0-0) + 2*(1-0) + (1-2) = 2-1=1$
Next figure: $4(0-0) + 2(0-1) + (3-0) = -2+3 = 1$
Last figure: $4(0-1) + 2(1-0) + (3-0) = -4+2+3=1$

and all three are topologically legal.

Homework: Suppose you have the following data for the pure components and all the binary azeotropes that exist (but none for ternary azeotropes) – pure component BP: A:190, B:200, C:220; binary azeotropes AB:185, BC:195. Assume at most one ternary azeotrope can exist. How many different ways can you sketch a residue curve that would be topologically legal for these temperatures? Prove a ternary azeotrope is not possible?

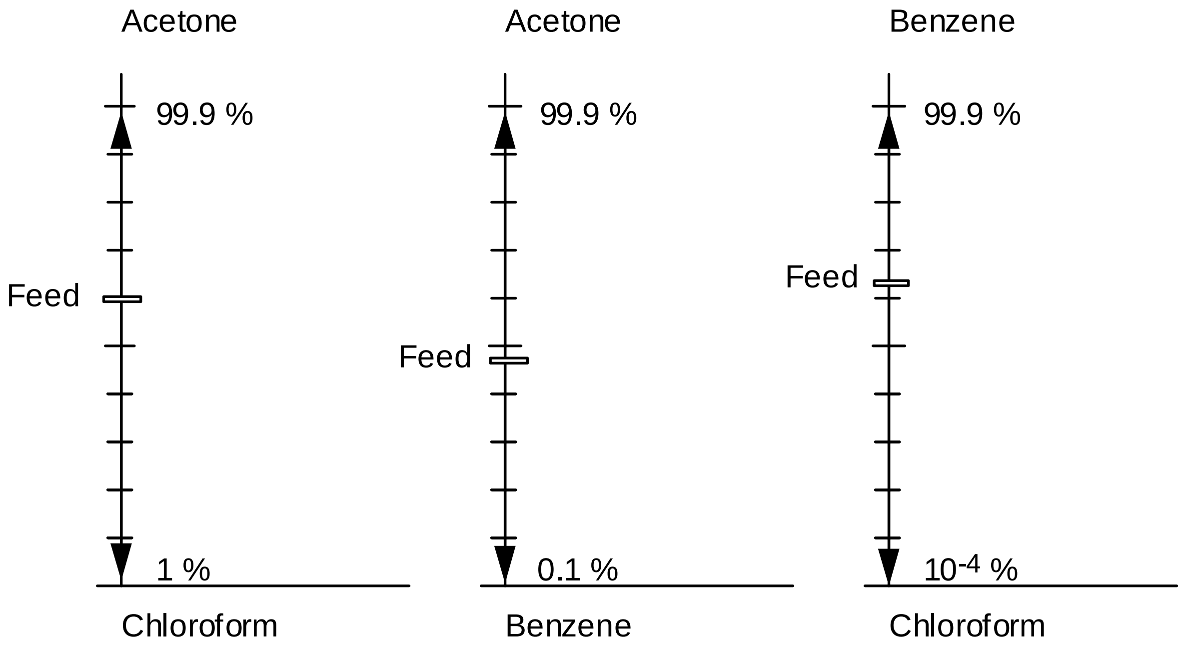
Example 2

Separate a mixture of acetone, chloroform and benzene. We shall show how to generate alternative structures systematically for solving this problem.



Note we will allow the chloroform to have up to about 1% acetone in it. We will use this higher level of contamination later to our advantage.

We can show the "binary separation tasks" for this problem as follows. As we suggest separations, we can keep track of which portions of these tasks they accomplish.



First we need to estimate the ideal/nonideal behavior of these species. We can use infinite dilution K-values as follows. (One could also develop T vs x,y plots using a flowsheeting system for each binary pair.)

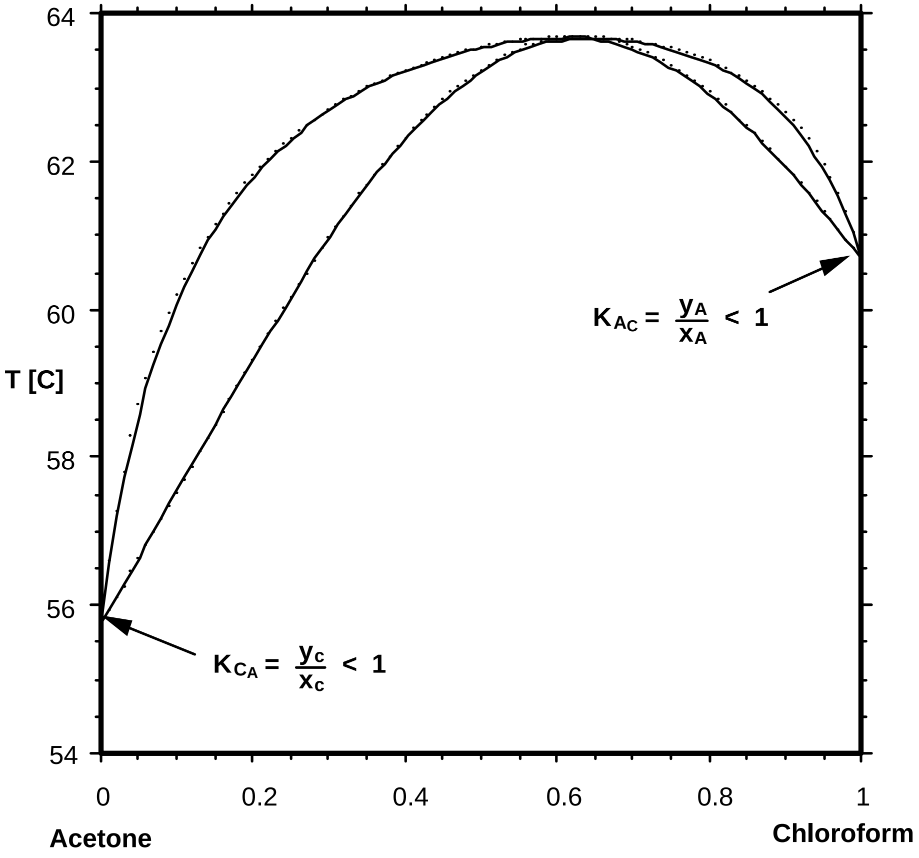


Fig. Liquid and vapor mole fractions vs T at equilibrium for Acetone and Chloroform

We can predict azeotropic behavior as follows from infinite dilution K-values. These in turn are readily available by performing a small set of flash calculations using any flowsheeting system.

$$K_{12} = \frac{y_1}{x_1} = \frac{\gamma_1 \bullet p_1^o}{p} ; \quad K_{21} = \frac{y_2}{x_2} = \frac{\gamma_2 \bullet p_2^o}{p}$$

Max. boiling azeotrope: $K_{12} < 1 \wedge K_{21} < 1$

Min. boiling azeotrope: $K_{12} > 1 \wedge K_{21} > 1$

Heteroazeotrope: $K_{12} > 10 \wedge K_{21} > 10$

Applying these ideas to our problem

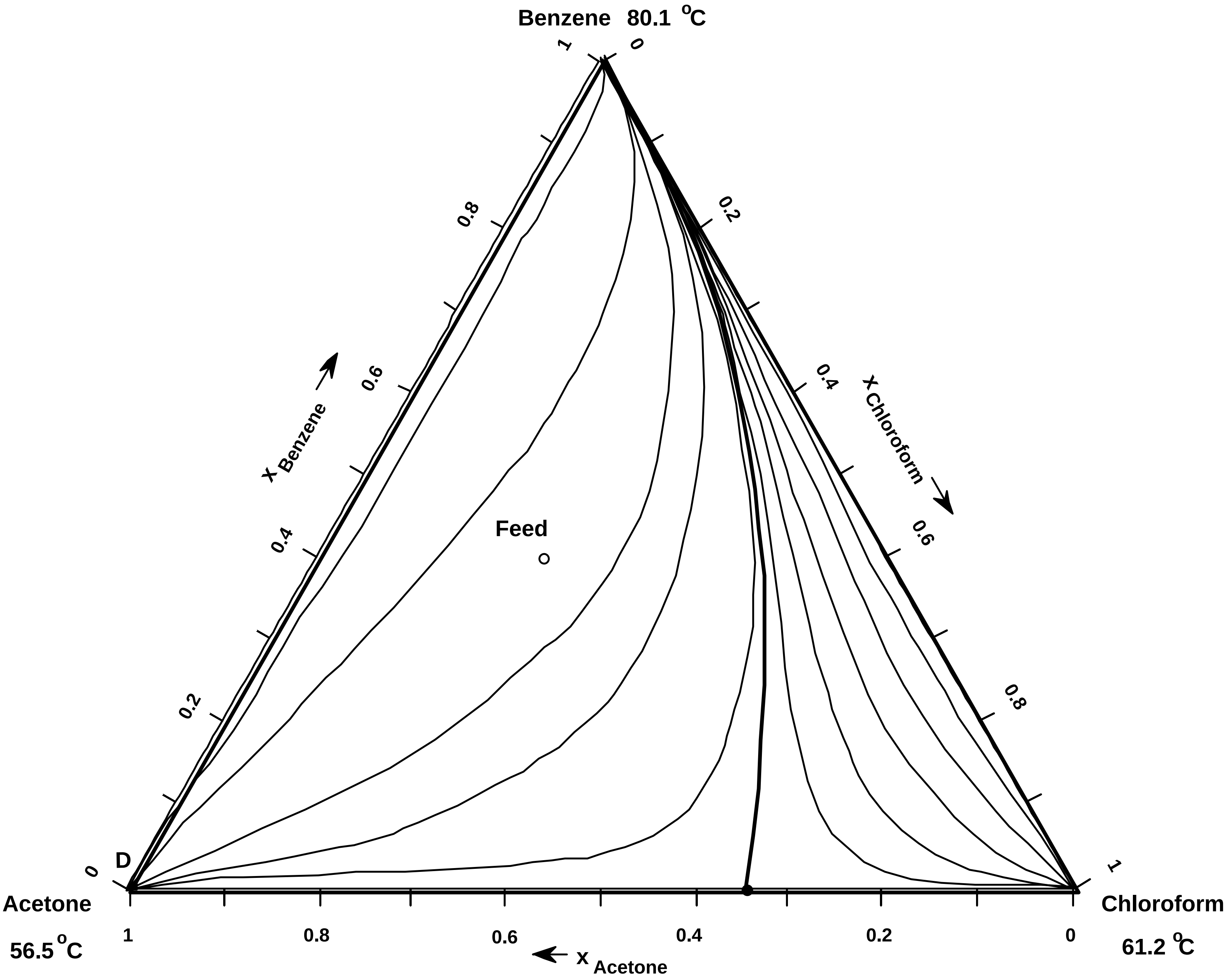
K^{ω} of ----- in	Acetone	Chloroform	Benzene
Acetone	1.0	0.4 **(max)**	0.7 **(normal)**
Chloroform	0.6	1.0	0.4 **(normal)**
Benzene	3.0	1.5	1.0

With this information and that for pure component boiling points at the pressure of interest, we can sketch the ternary diagram for this mixture. We can also use a computer code to generate it, which was done for the following figure. We see that there is one maximum boiling azeotrope between Acetone and Chloroform.

Two things we can put on this diagram when sketching

1) a distillation boundary exits, which we deduce when attempting to explain the azeotropic behavior determined using infinite dilution K-values.

2) the boundary is curved. This, too, can be predicted by noting that the infinite dilution K-values for Acetone and Chloroform in lots of Benzene indicate that Acetone is more volatile. Therefore, Chloroform acts like an intermediate component in the benzene rich end of the diagram. The residue curves start out aiming at Chloroform from Benzene.


Benzene 80.1 °C
1
0
0.8
0.6
0.4
0.2
0
x Benzene
0.2
0.4
0.6
0.8
1
x Chloroform
Feed
D
Acetone
56.5 °C
Chloroform
61.2 °C
1
0.8
0.6
0.4
0.2
0
x Acetone

If we distill the feed, **what products might we expect to be able to produce** in the column?

We can carry out the following experiment.

- Run a column with the given feed.
- Use lots of trays top and bottom
- Use a large reflux rate
- Draw off one drop of top (distillate) product, with the rest drawn off as a bottoms product.

The top product will be the extreme we can get from distillation – the composition corresponding to the lowest temperature in this distillation region. That is, it will be pure acetone. The bottoms will be the entire feed.

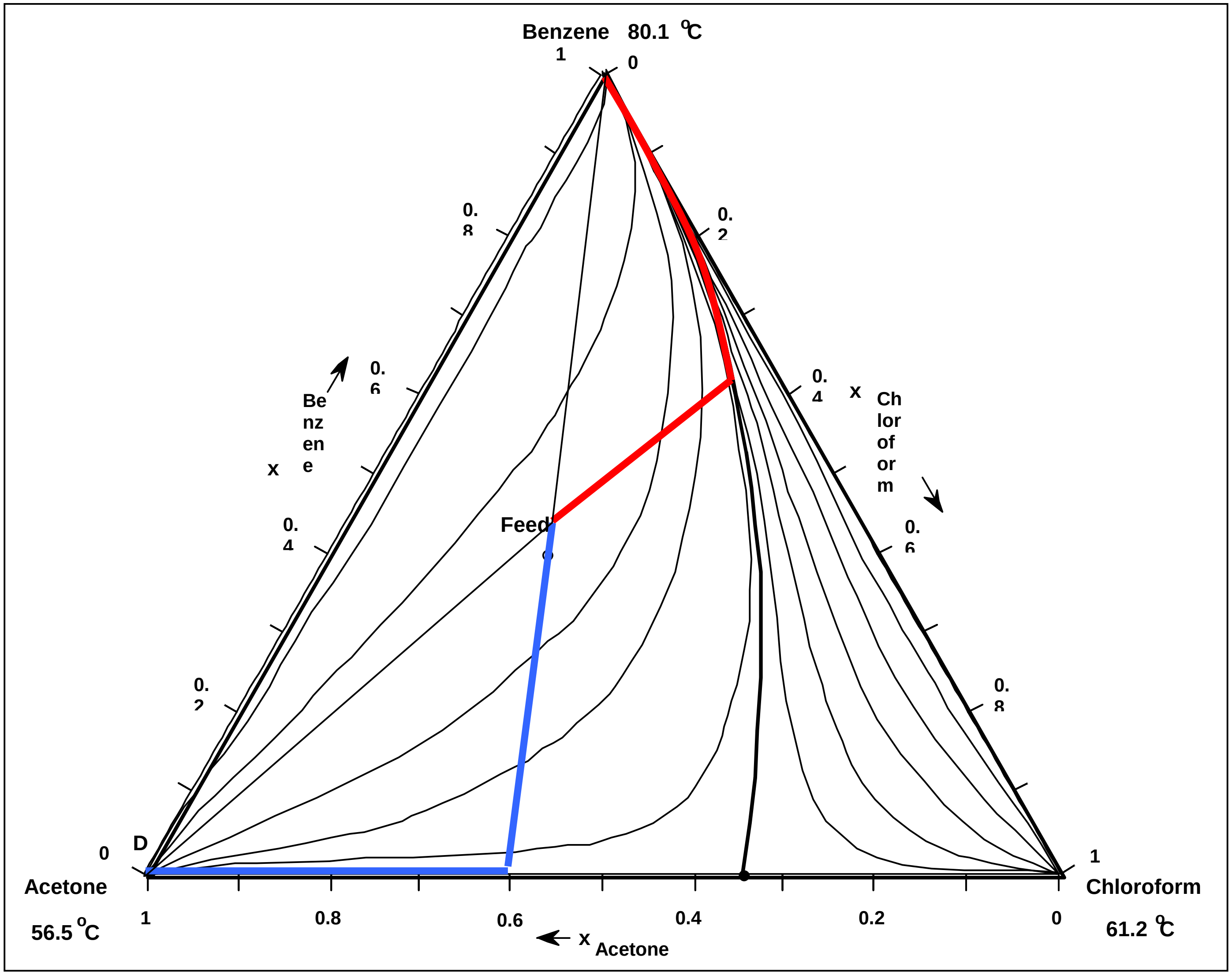
Next draw off 1% of the feed as a top product. It too will be pure acetone, but the bottom product will be the feed less this acetone. Its composition is on a straight line from the acetone through the feed and slightly to the other side.

Draw off 2%, 3% etc. Continue until the top product is no longer pure acetone. This will happen when one draws off 31% of the feed as top product. At this point the bottoms product will hit the distillation boundary for the region.

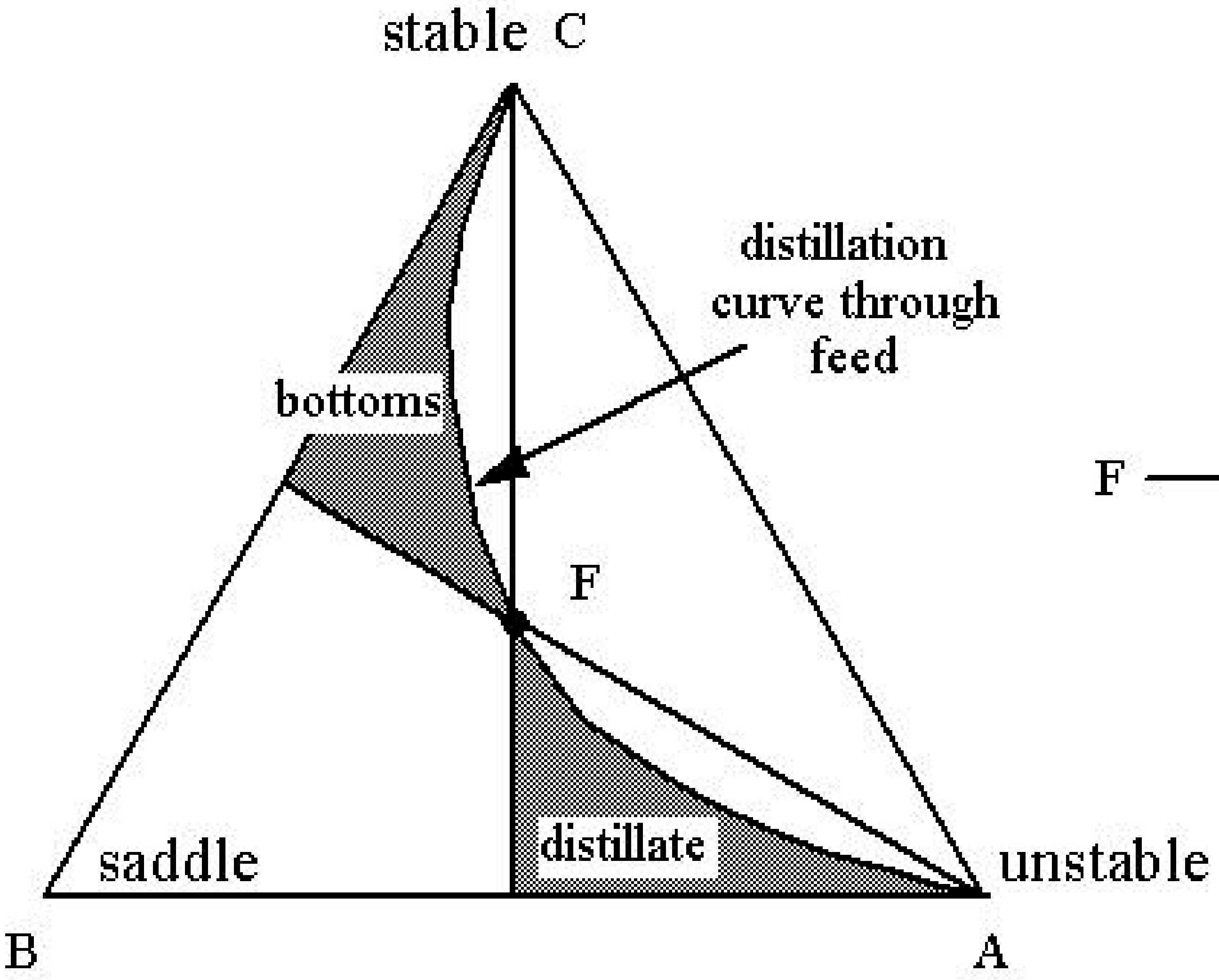
Draw off 32% and one will take chloroform with the acetone. As one increases from here one draws off more and more chloroform, and the top product composition moves along the lower edge while the bottoms moves along the distillation boundary.

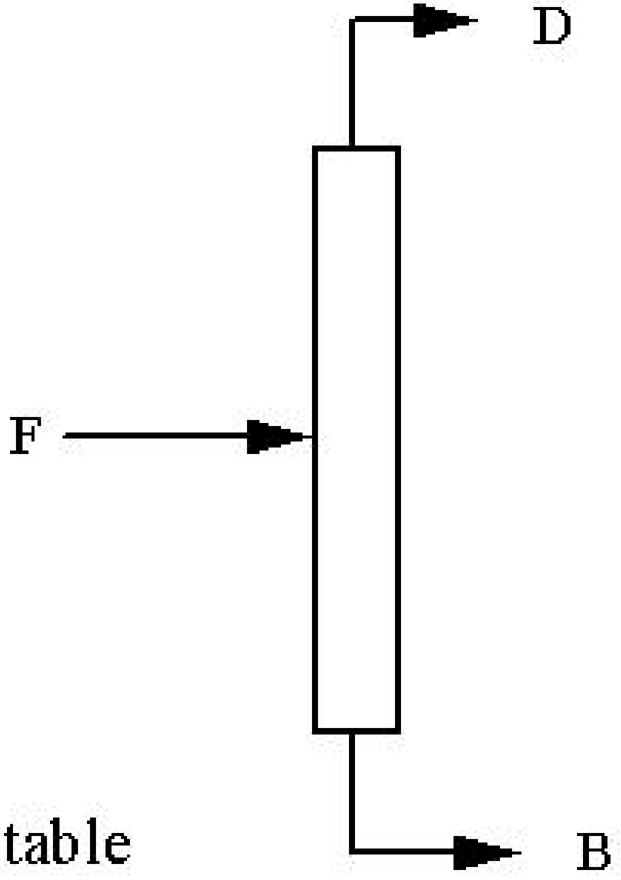
At 60%, the top will be all the acetone and all the chloroform and the bottoms will be all the benzene. If one draws off 61%, one must take some benzene overhead. The bottoms will remain pure benzene, but it will not be all of it.

The following figure illustrates.

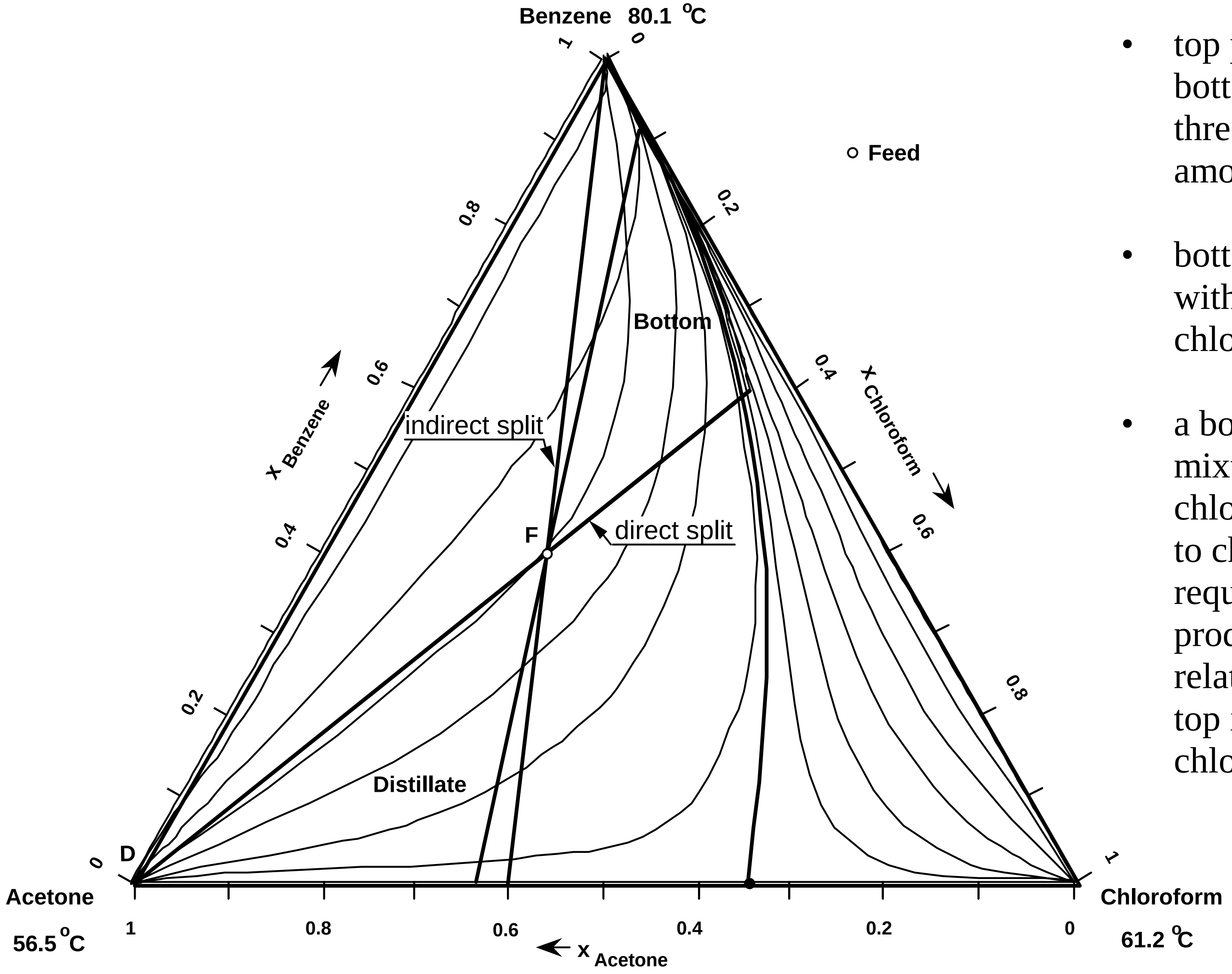


Note the “bow tie” shape to this region. A good first approximation to what can be reached is to draw a line from the lowest boiling point through the feed until hitting a distillation region boundary or the edge of the composition triangle. Also draw a line from the highest boiling point through the feed as far as possible while staying within the same distillation region. The “bow tie” region represents a good approximation of what one can reach for products in a column. For nearly ideal components, the picture is as follows:


stable C
distillation
curve through
feed
bottoms
F
saddle
distillate
unstable
B
A


D
F
B

To see some of the possibilities for benzene, acetone and chloroform, look for interesting products we can reach. They include:

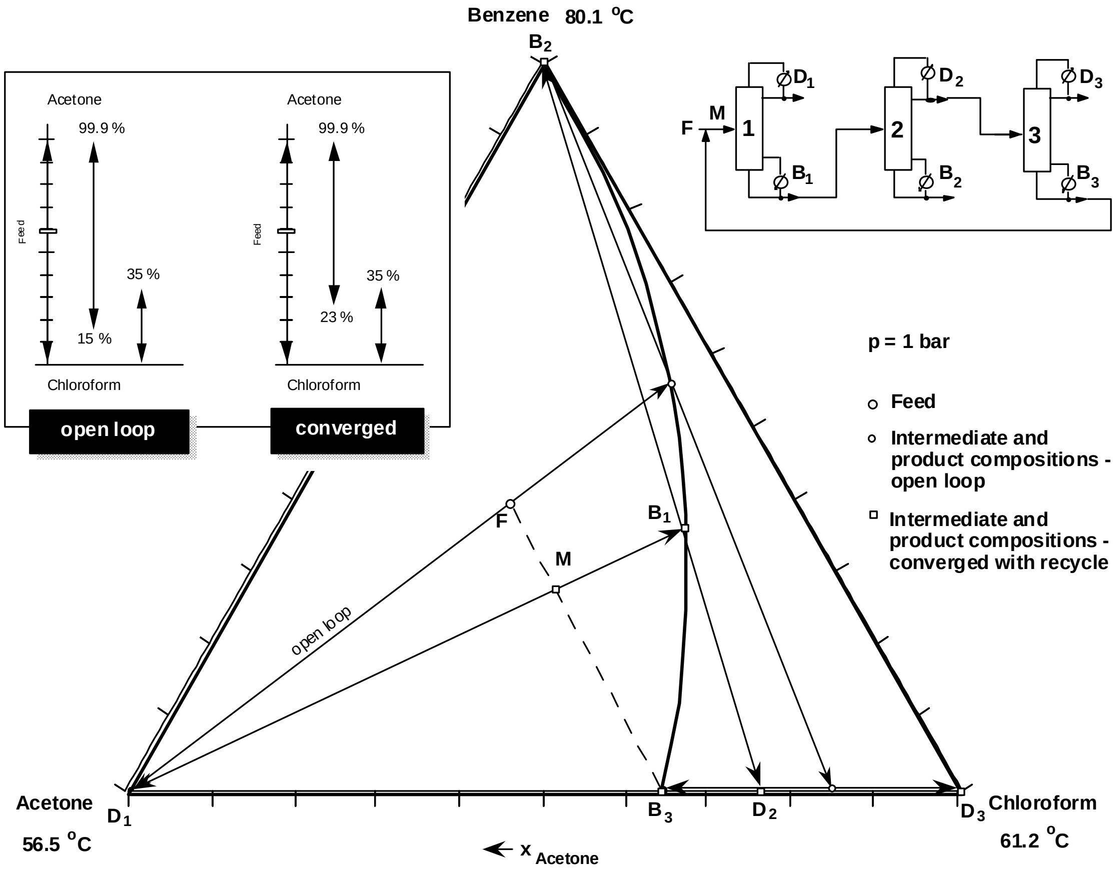


- top product of pure acetone with a bottoms being a mixture of all three species in significant amounts - the direct split

- bottom product of pure benzene with a top that is only acetone and chloroform - the indirect split

- a bottom product, which is a mixture of benzene and chloroform. The ratio of acetone to chloroform is lower than required for the chloroform product - less that 1% acetone relative to the chloroform. The top is a mixture a acetone and chloroform - an intermediate split

We can start with the direct split, which produces nearly pure acetone from the top of the first column. A second column separates benzene (bottoms) from a mixture of acetone and chloroform. The mixture of acetone and chloroform is separated into pure chloroform (top) and the maximum boiling azeotrope (bottoms) between acetone and chloroform. The azeotrope can be mixed with the original feed to complete the flowsheet.

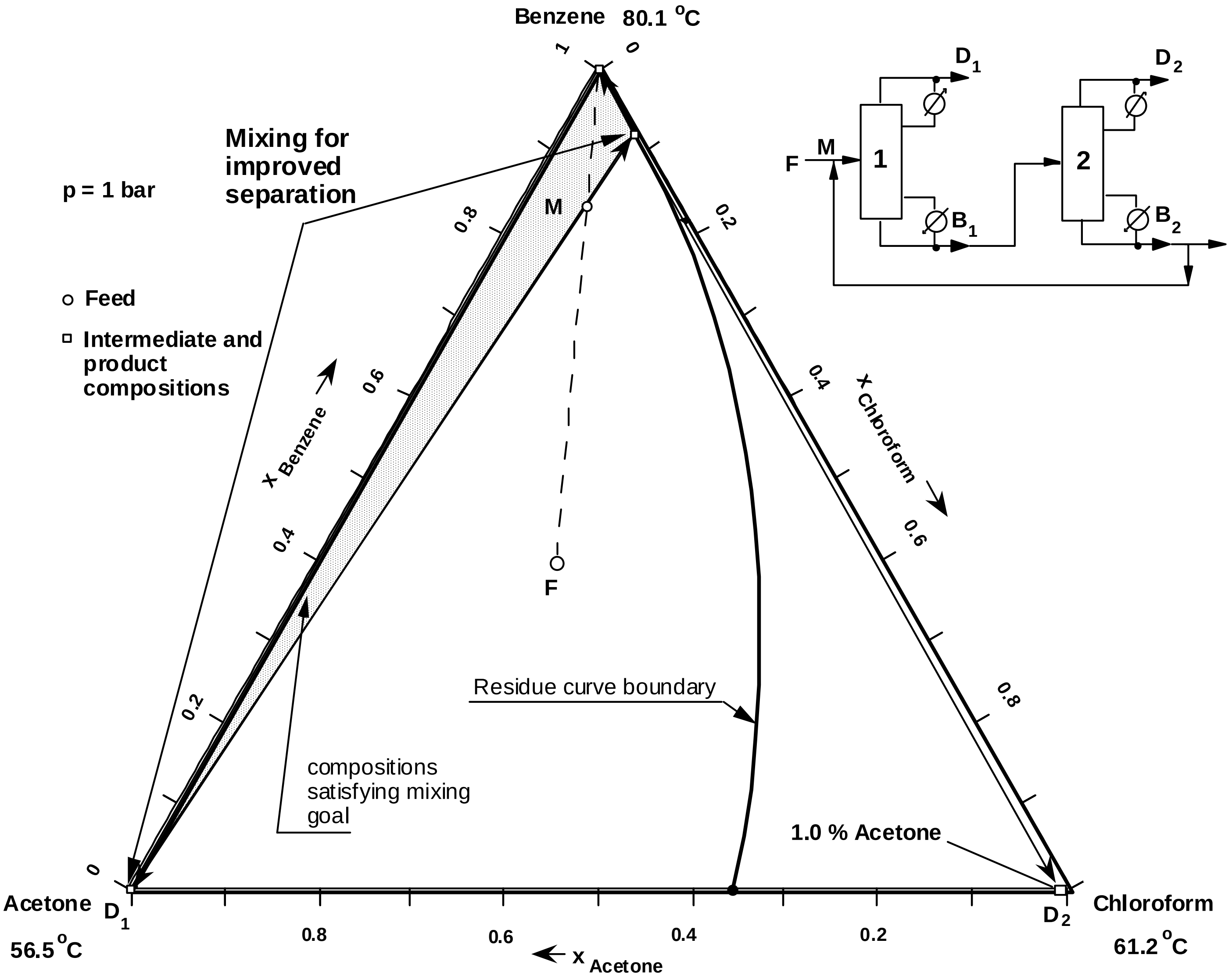


Benzene 80.1 °C
B2
Acetone
99.9 %
Feed
35 %
15 %
Chloroform
open loop
Acetone
99.9 %
Feed
35 %
23 %
Chloroform
converged
D1
D2
D3
F
M
1
2
3
B1
B2
B3
p = 1 bar
○ Feed
○ Intermediate and product compositions - open loop
□ Intermediate and product compositions - converged with recycle
F
M
B1
open loop
Acetone
D1
56.5 °C
B3
D2
D3
Chloroform
61.2 °C
← x Acetone

The indirect split is not a useful starting point as benzene is needed to separate acetone from chloroform and removing it first is counterproductive.

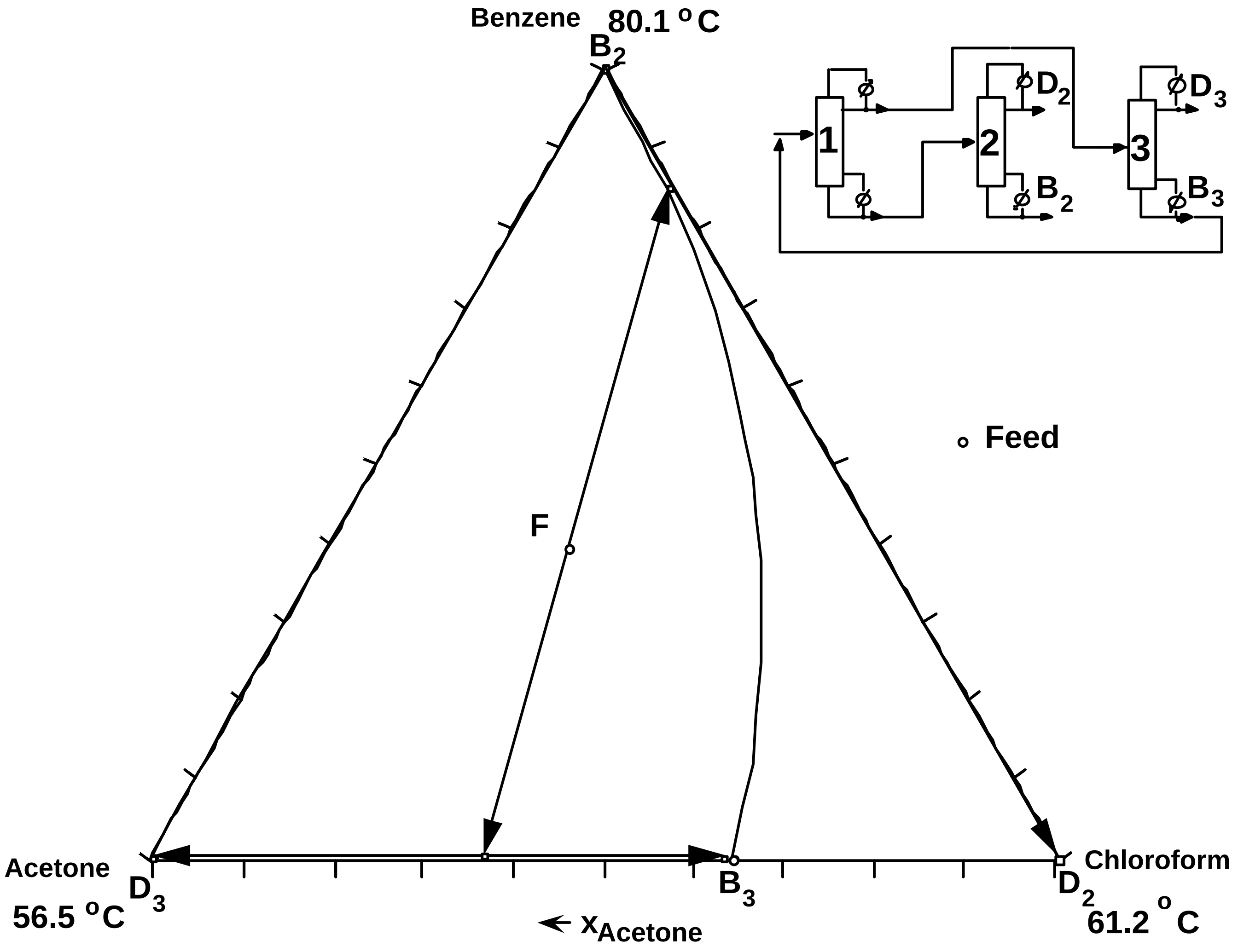
Mixing to improve separation: We can propose using mixing to get two interesting products from a single separation - a contradiction. However, it can be done. Propose mixing benzene with the original feed to move the material balance line so it permits acetone as a top product and the benzene/chloroform mixture that has very little acetone as the bottoms.

Doing so means we can get a solution to our problem that involves only two columns, as follows.

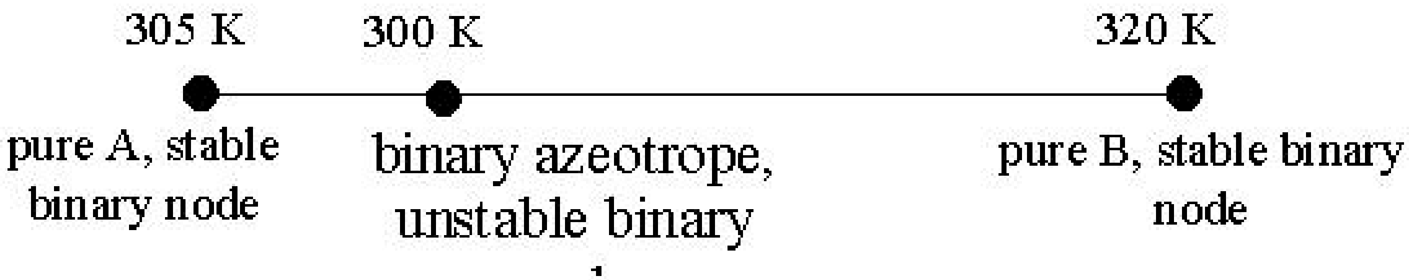


The first column produces pure acetone at the top and an nearly acetone free bottoms. The second column separates benzene (bottom) from chloroform. Part of the benzene recycles to shift the feed to the first column.

Finally, we can start with the intermediate split. In this solution, we separate the feed into a bottom product that has little acetone in it. The bottom is separated into benzene and chloroform. The top is a mixture of acetone and chloroform that we separate in a third column into acetone and the azeotrope between the acetone and chloroform. The azeotrope can again be mixed with the feed.



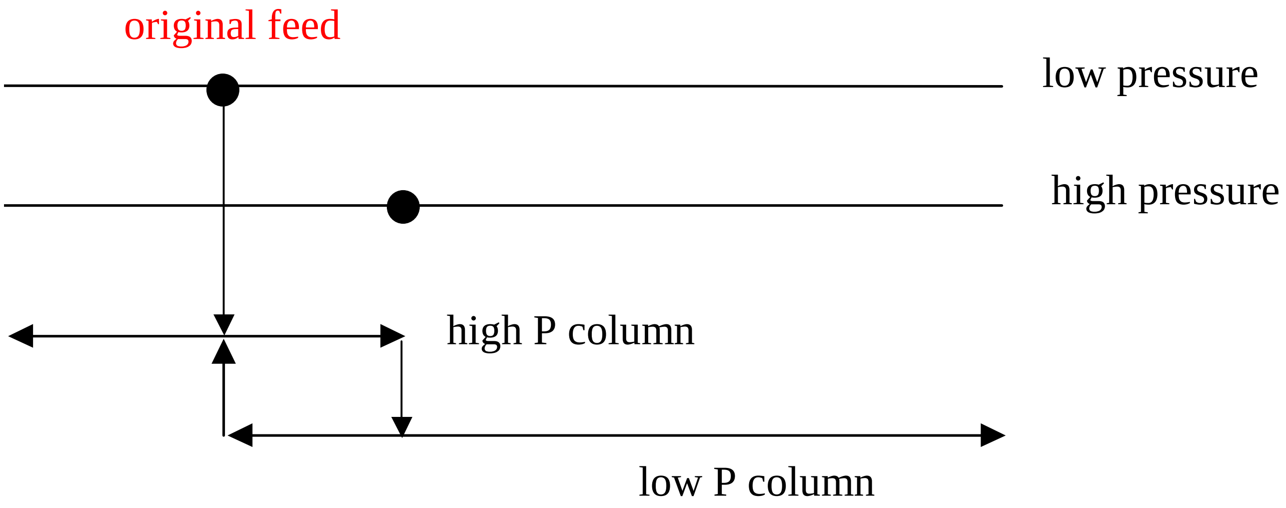
Example 3. Breaking a binary azeotrope: You have been given the following binary azeotrope. How would you synthesize a process to break it into pure A and pure B products? You are allowed to use a third species to help.



We cannot break it as it is using binary distillation because we cannot get past the azeotrope. The best top product from a column will be arbitrarily close to the binary azeotrope. The best bottom products will be arbitrarily close to either of the stable nodes – pure A if the column is to the left of the binary azeotrope or pure B otherwise.

What could be your thought processes to accomplish a separation here?

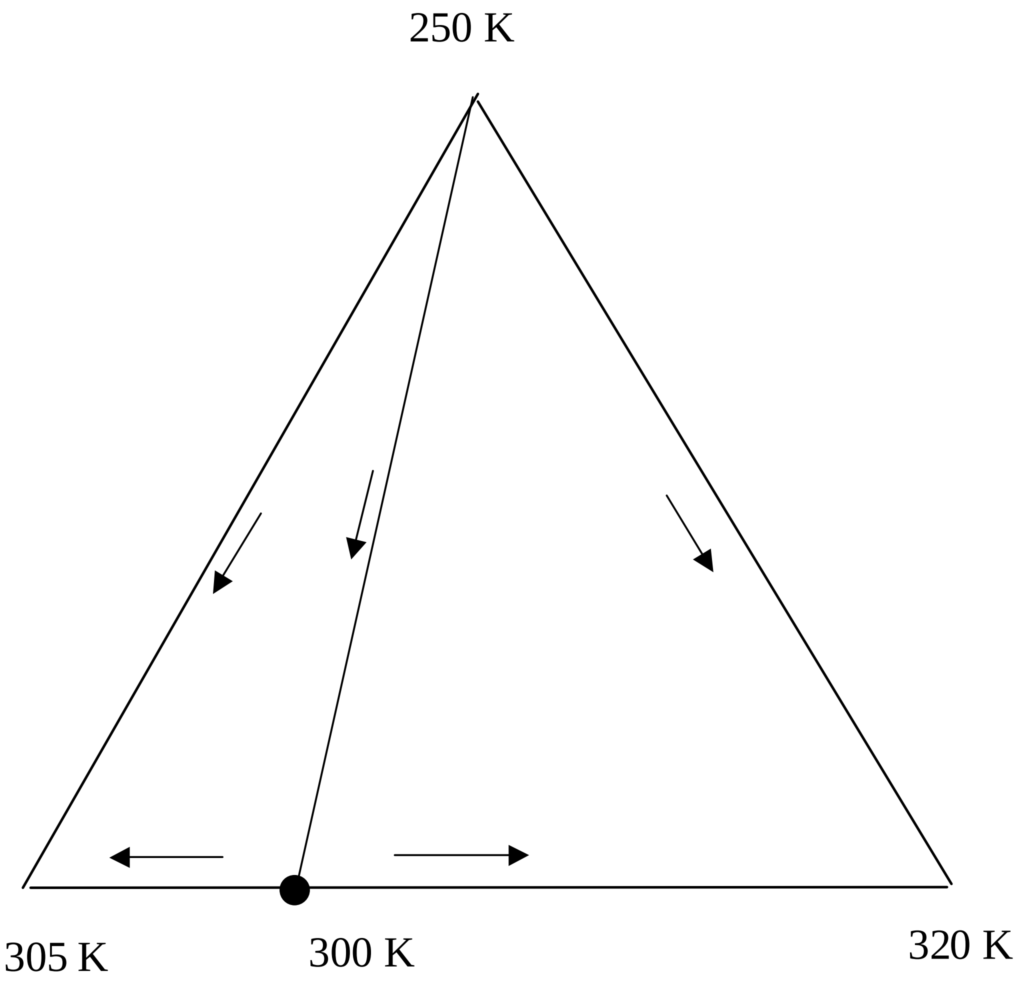
How about checking if the pressure has an effect on the composition at which the azeotrope boils? This would be the easiest way to break it. For example, suppose at high pressure the azeotropic composition shifts as shown here. We can quickly sketch a process using this representation.



First feed the azeotrope to the high pressure column, getting the separation shown here. The two products will be pure left most product and high pressure azeotrope. Feed the high pressure azeotrope to a low pressure column and in that column product pure right most product and low pressure azeotrope. Recycle this low pressure azeotrope back to feed the high pressure column.

Let’s think of adding a third component. What properties must it have? **Any thoughts?**

How about mixing with a third component and using distillation? Suppose we do and choose one that boils below the other two.

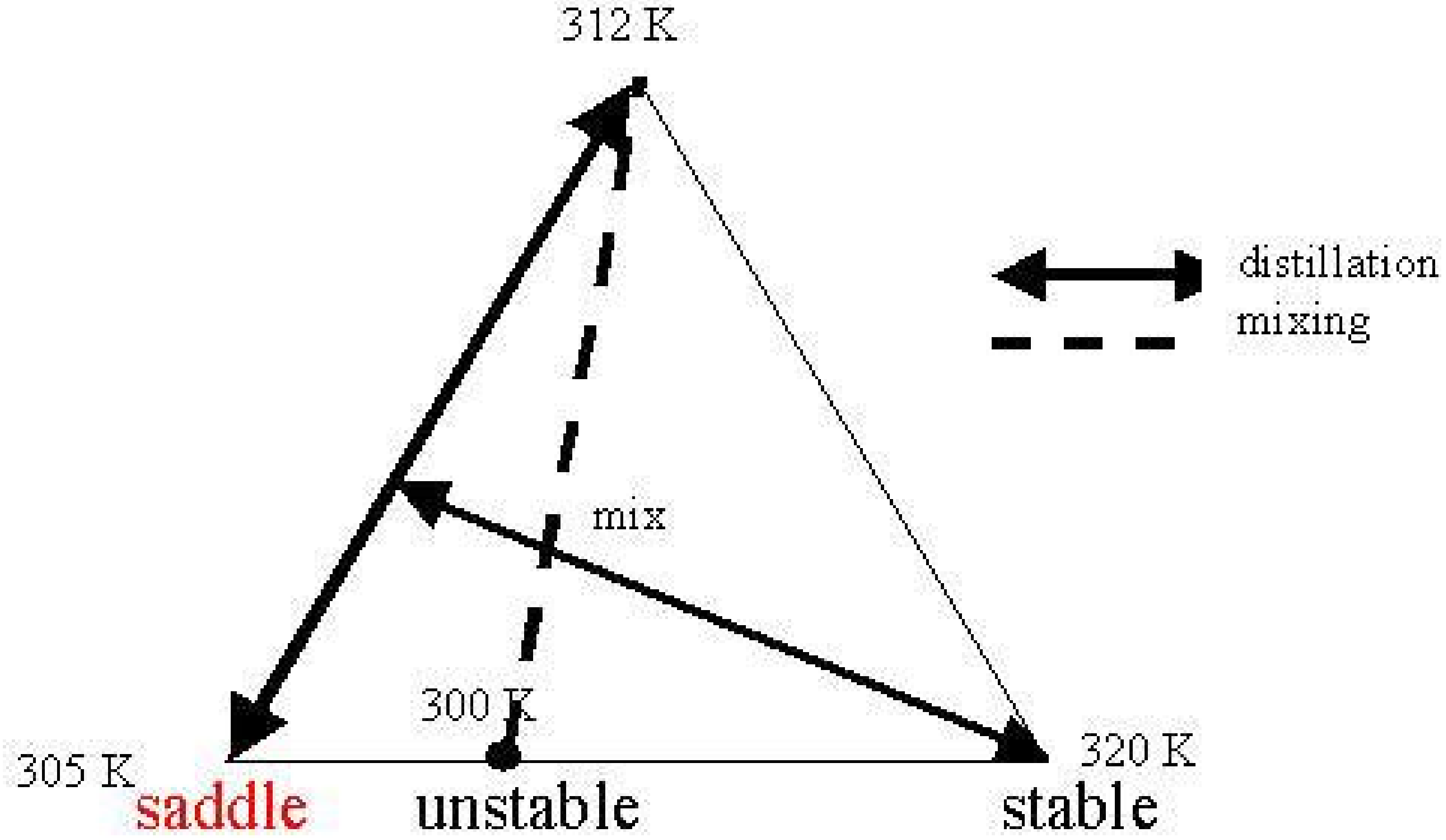


Then there will be a distillation boundary created with the 305 and 320 points being stable nodes – i.e., the best bottom product in any separation we might propose. The best top product is again the azeotrope, the lowest temperature point in our diagram.

How about if the top temperature is 350 K? Then it becomes the stable node and converts the previous two to saddles. They can never be products in any column.

Okay, what might you try next?

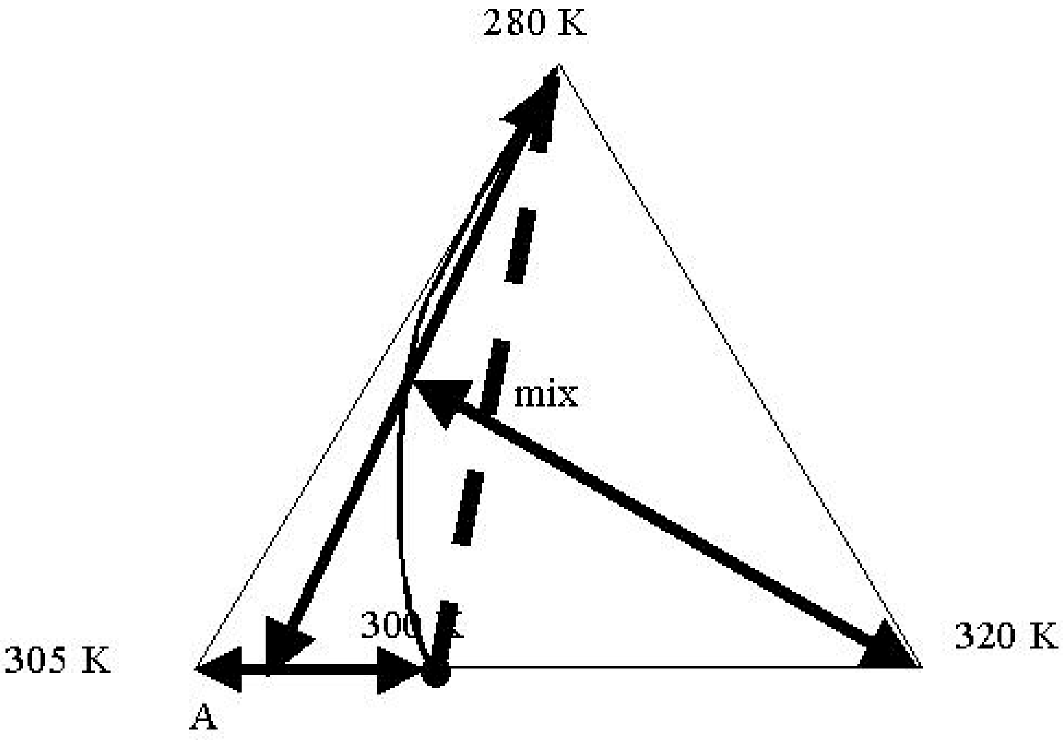
What if you convert one of the stable nodes to an intermediate one? We can do this by choosing the third component to be one that boils between the other two. No distillation boundary results. Do you agree?



Now we can mix the azeotrope we are trying to break so we can feed a column that can have the stable node as the bottom product and the left edge as the top product. A second column will recover the third component and the component that boils at 305 K in as pure a form as desired. This is a general way to think about breaking a binary azeotrope.

Are there any other “general” approaches to break a binary azeotrope?

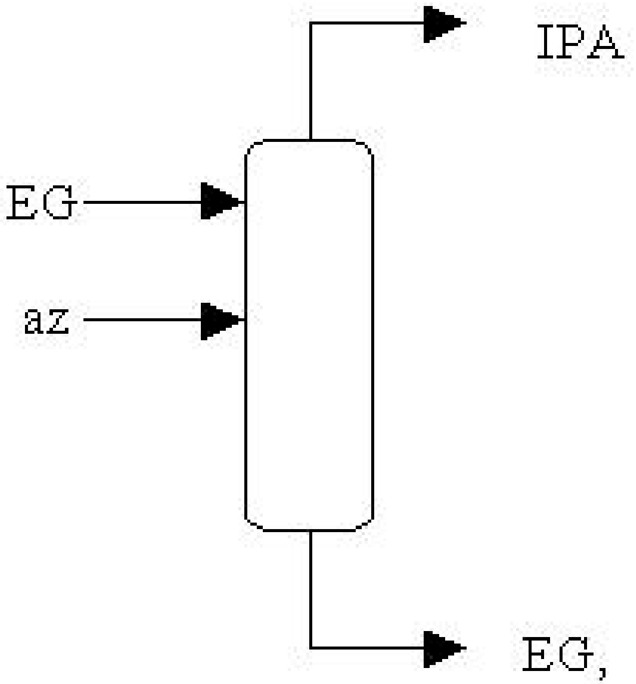
How about adding a low boiling third component that gives us a very curved boundary?

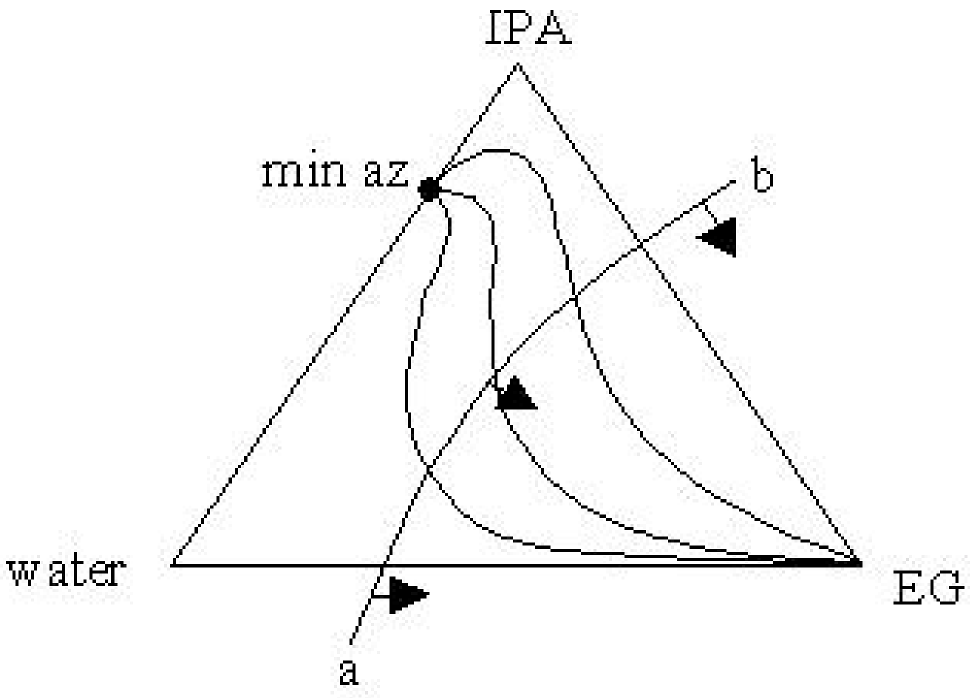


This is suggested by the acetone, chloroform, benzene example. As here we have a min boiling azeotrope, the other species must boil at a lower temperature. It will create a distillation boundary – something we just suggested we wanted to avoid. But do we really need to?

How do we assure ourselves of a curved boundary? We need a third component that has very different infinite dilution K-values with the two original species. Thus in lots of the third component, the 320 K component should be a lot less volatile (have a low K value) relative to the 305 K component – or vice versa.

And yet another way to think about this problem – **use extractive distillation**. In this case we feed the column with a second feed, generally with a heavy component above the azeotrope feed. An example is to separate water (W) from isopropylalcohol (IPA) using ethylene glycol (EG). In lots of ethylene glycol, water is an intermediate component and IPA a light. We operate to have lots EG in most of the column by feeding it near the top of the column. It is heavy and will be on all trays below its feed, leaving at the bottom. The residue curves for these three species for a ternary diagram are as shown to the right here.

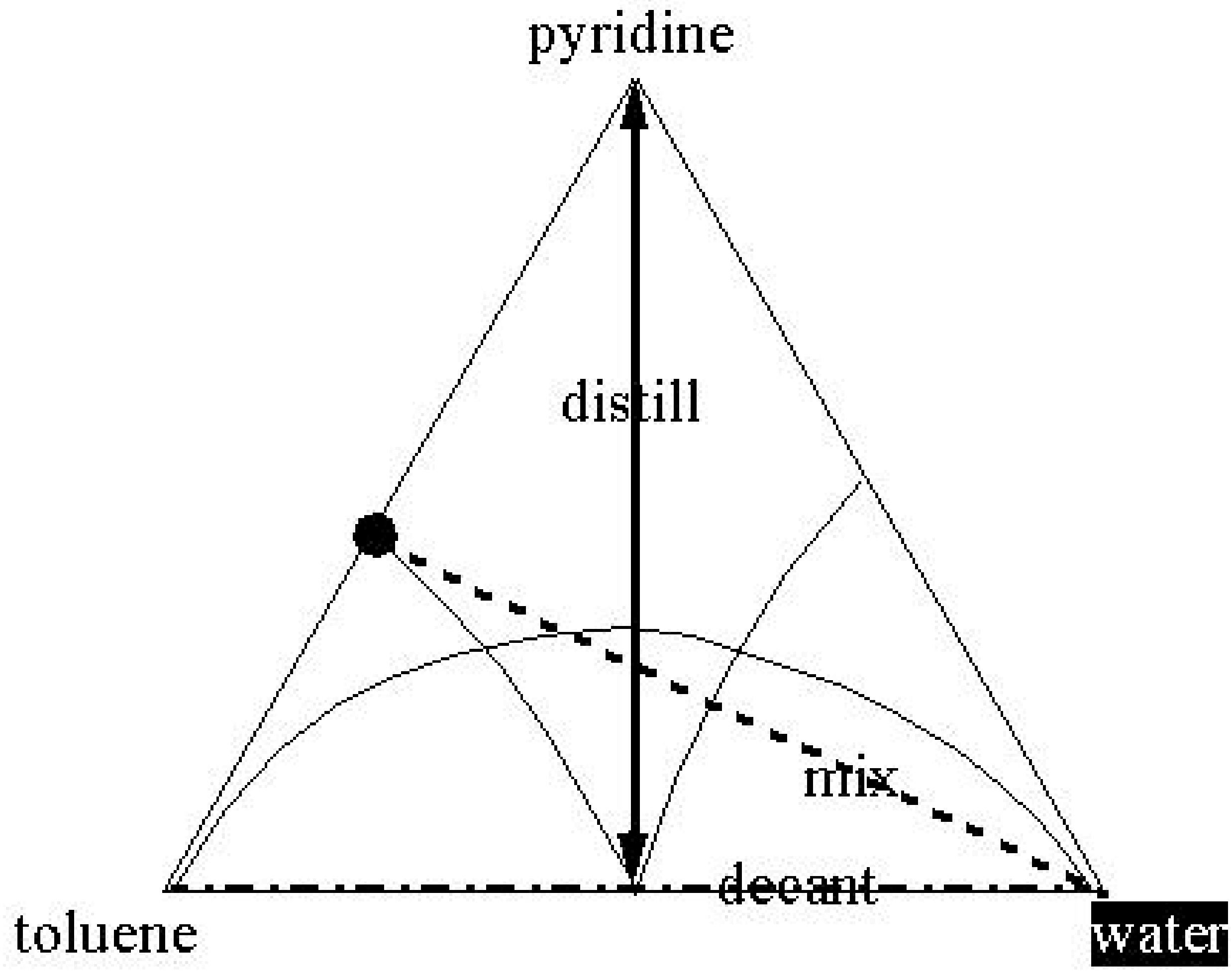




Note, to the right of the a-b line, where lots of EG is present, the residue curves give one the impression that EG is the heavy component, water the intermediate and IPA the light.

In the bottom of this column, below the feed, one is separating the IPA from the water. The water makes it to the bottom product but not the IPA. Above the azeotrope feed, one is separating the water from the IPA, with the IPA making it to the EG feed but not the water. Above the EG feed, we simply separate the very heavy EG from IPA in one or two trays, as all the water is gone by this point.

And yet another thought on this. How about using **liquid-liquid behavior** if it is available?



Suppose we have the pyridine, toluene azeotrope to break. We can do it using water. Add water until the mixture allows a column to separate pyridine from the azeotrope between toluene and water on the lower edge. Then decant the toluene from the water.

So then, what should you look for in a solvent to break a minimum boiling azeotrope?

- If the solvent is lighter than the other two, look for a very curved distillation boundary – you will get a boundary.

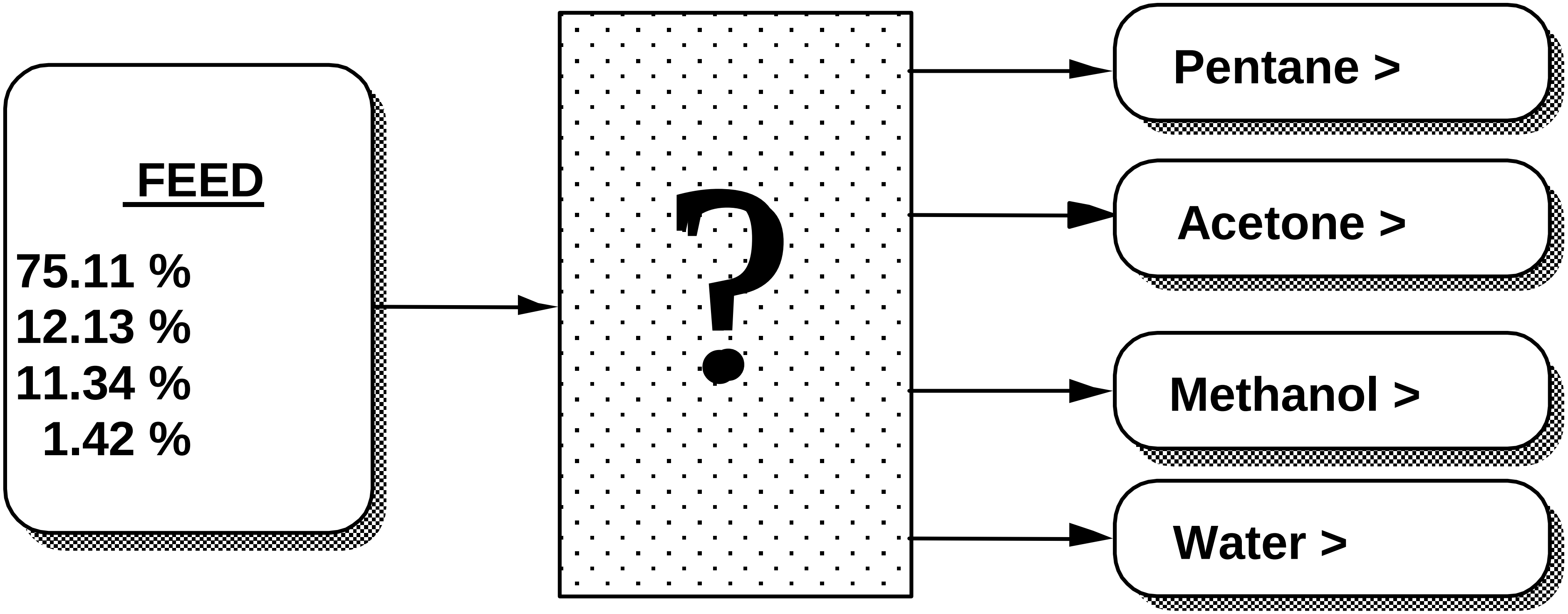
- If the two original species boil at quite different temperatures, look for a solvent that boils between.

- If you can find a suitable heavy solvent, think to use extractive distillation.

- If a solvent yields favorable liquid/liquid behavior, consider using it as illustrated for breaking the toluene/pyridine azeotrope.

By analogy, you should be able to invent the rules to break a maximum boiling azeotrope. Total symmetry is not possible, however, as a three component liquid/liquid region that starts at a binary edge always has a binary minimum boiling azeotrope in it.

Example 3: A tough four component separations problem



This one is tough because it was deliberately constructed to have species that “hate” each other. They form all sorts of azeotropes. Also we see water and pentane, which almost certainly will form two liquid phases.

Finally, the feed is the hydrocarbon rich phase of doing a decantation of an equal molar mixture of the four species. So decanting it to get started has already been done.

Alternative separation options

Let’s examine K-values and activity coefficients at infinite dilution

a drop of in lots of	pentane	acetone	methanol	water
pentane	K = 1	3 (min)	5.9 (min)	71.4 (het)
	$\gamma = 1$	6.6	23.1	1537
acetone	7.9	1	1.3	1.05 (min)
	4.7	1	2	7.4
methanol	29.6	2.4	1	0.4 (ok)
	14.4	2.0	1	1.6
water	8106	38.5	7.8	1
	3213	11.5	2.2	1

First, why not distillation? There are a lot of azeotropes.

Then how about extractive distillation using water? Acetone and methanol have very different K-values (38.5 and 7.8) in water and would seem to be separable? Also both are much lighter (K-values much larger than unity) than water. But water will break into a separate liquid phase if added.

So then, how about liquid-liquid extraction?

Equilibrium for liquid-liquid extraction. Equate fugacities of a component i in two liquid phases I and II

$$x^{I}[i]\gamma^{I}[i]f^{Io}[i]= x^{II}[i]\gamma^{II}[i]f^{IIo}[i] \Rightarrow x^{I}[i]\gamma^{I}[i] = x^{II}[i]\gamma^{II}[i] \rightarrow x^{I}[i]/x^{II}[i] = \gamma^{II}[i]/\gamma^{I}[i]$$

as the pure component i fugacity at T and P, $f^{Io}[i] = f^{IIo}[i]$.

We define a separation factor between two species i and j as their mole fraction ratios in the two phases.

$$S^{I/II}[i,j] = (x^{I}[i]/x^{II}[i])/ (x^{I}[j]/x^{II}[j]) = (\gamma^{II}[i]/\gamma^{I}[i])/(\gamma^{II}[j]/\gamma^{I}[j]),$$

which we can evaluate at infinite dilution in the phases I and II. We assume I = n-pentane and II = water are the major components in the two phases and estimate the following limiting separation factor for how methanol and pentane will split between these two phases:

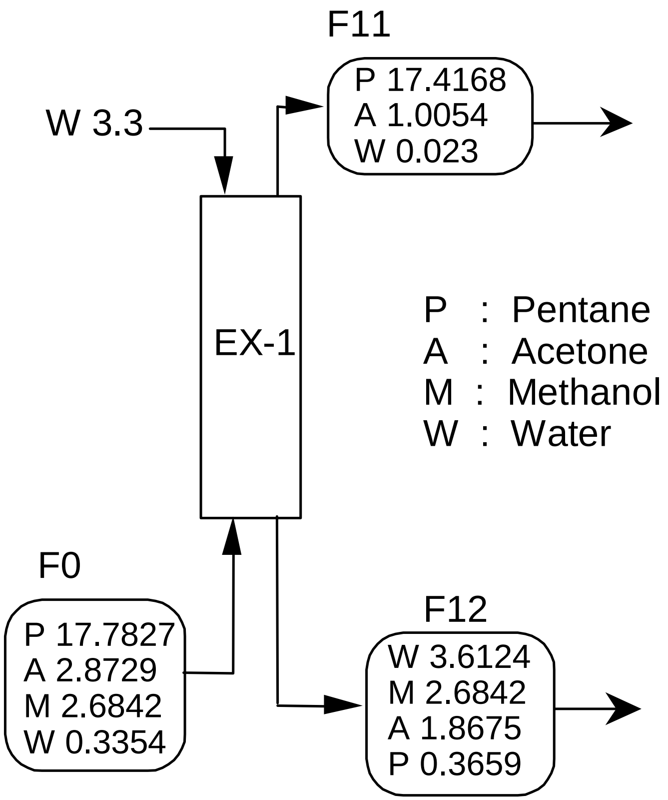
$$S^{water/pentane}[methanol, pentane] = (23.1/2.2)/(1.0/3213) = 33{,}740,$$

which is a large separation factor. In other words methanol likes water a lot more than it likes pentane and will go largely into the water phase.

$$S^{water/pentane}[acetone, pentane] = (6.6/11.5)/(1.0/3213) = 1850,$$

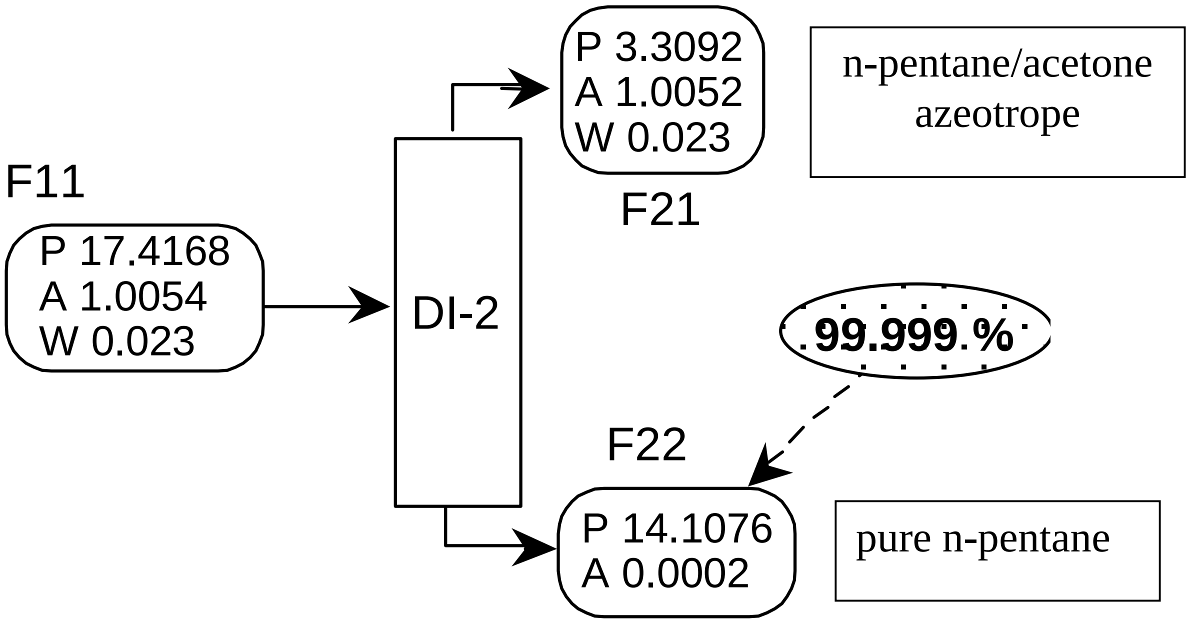
which says acetone also much prefers water but not as much as methanol prefers water to pentane.

We propose as a first separation device, liquid-liquid extraction. Analyzing using Aspen gives:



The n-pentane rich product F11 has essentially no methanol and very little water.

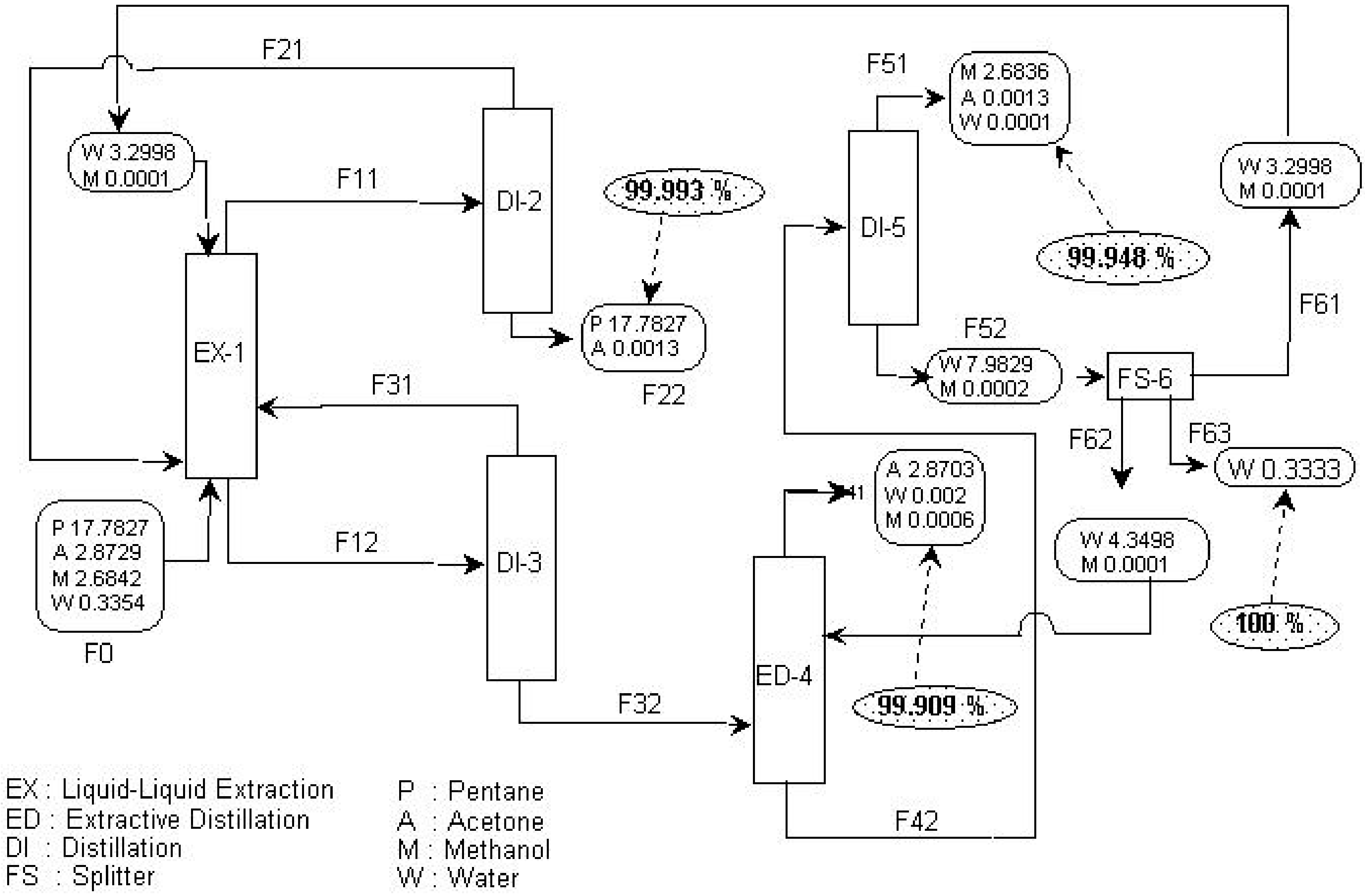
This unit also took a large part of the acetone out with the water, leaving a pentane rich phase with little of acetone and a water rich one with a mot of it. Distilling the pentane-rich phase lets us obtain a bottom product which is essentially pure n-pentane and a top which is the pentane/acetone azeotrope.



Distilling the bottom product gives us again the azeotrope as the top product but this time we get all the water out the bottom. It has both acetone and methanol in it.

We recycle the azeotropes back to the liquid/liquid extraction unit.

We now have a mixture of methanol, acetone and water to separate, and methanol and acetone form a min boiling azeotrope. Water and methanol on the other hand do not. In lots of water, methanol is the intermediate (K-value of 7.8) and acetone the light (K value of 38.5). We can easily use extractive distillation with water to separate acetone from methanol, getting acetone out the top of the column and methanol with the water out the bottom. The last step is to distill to separate the methanol and water. The final flowsheet is as follows.


F21
W 3.2998
M 0.0001
F11
DI-2
99.993 %
P 17.7827
A 0.0013
F22
EX-1
F31
P 17.7827
A 2.8729
M 2.6842
W 0.3354
F0
F12
DI-3
F32
ED-4
A 2.8703
W 0.002
M 0.0006
99.909 %
F42
F51
M 2.6836
A 0.0013
W 0.0001
DI-5
99.948 %
F52
W 7.9829
M 0.0002
FS-6
F61
W 3.2998
M 0.0001
F62
W 4.3498
M 0.0001
F63
W 0.3333
100 %
EX : Liquid-Liquid Extraction
ED : Extractive Distillation
DI : Distillation
FS : Splitter
P : Pentane
A : Acetone
M : Methanol
W : Water