

Life Cycle Simulation using Bayesian Calculation

by Ferdinand Heru Utomo

Project Description

Initiatiate the Life Cycle simulation using the Bayesian Calculation

- Building Bayesian network model for a chemical process
- Modeling a database for the process
- Implement the simulation application
- Building a user interface for the application
- Add knowledge-rules for the decision advices

Area of Application

Hybrid Distillation and

Vapor Permeation Process

- Separation Process
- At a laboratory scale
- Pilot at Laboratory of Process Equipment, Delft University of Technology

Distillation Process





What is Life Cycle?



The Process Life Cycle



1. Process Design (using ASPEN)

- 2. Process Monitoring (using Honeywell, ERP, etc)
- 3. Costs, Maintenance and Effectiveness (using SAP)

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Modeling Uncertainty

- Fuzzy Logic
- Statistical Probabilities (Bayesian Technique)

Why not Fuzzy Logic?

- Misunderstood the term 'uncertain reasoning'
- No further facts examination
- Not wholy consistent

Bayesian Technique in contrast.....

- Represents Conditional independence information naturally
- Represents joint probability distribution
- Use a well-known statistical formula, based on the formula:

P(E|H) = P(H,E)/P(H)

The Bayes' Rule



$$P(E \mid H) = \frac{P(H \mid E).P(H)}{P(E)}$$

Finding the probability of the evidence based on the facts on the hypothesis when the conditional probabilities between the hypothesis en evidence is known.

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Simulation Application



Data Handling



Coversion Example

| 4 | | | | ~ | |
|------|--------------------|---------|---|----------|----------|
| 5 | Display | 17 | B1 (| 01 | E I |
| 6 | | PMIX | DIST1 | DIST1 | |
| 7 | Format: | MEM | 5.0° 0.000 000 000 000 000 000 000 000 00 | PRHEAT | MIX I |
| 8 | | VAPOR | LIQUID | VAPOR | LIQUID |
| 9 | Substream: MIXED | | | | |
| 10 | Mole Flow KMOL/HR | | | | |
| 11 | IPA | 0.000 | 0.000 | 31.641 | 30.829 |
| 12 | WATER | 0.000 | 174.498 | 25.888 | 174.700 |
| 13 | Mole Frac | | | | |
| 14 | IPA | 0.100 | 0.000 | 0.550 | 0.150 |
| 15 | WATER | 0.900 | 1.000 | 0.450 | 0.850 |
| 16 | Mass Flow KG/HR | | | | |
| 17 | IPA | 0.000 | 0.000 | 1901.479 | 1852.725 |
| 18 | WATER | 0.000 | 3143.634 | 466.377 | 3147.275 |
| 19 | Mass Frac | | | | |
| 20 | IPA | 0.270 | 0.000 | 0.803 | 0.371 |
| 21 | WATER | 0.730 | 1.000 | 0.197 | 0.629 |
| 22 | Total Flow KMOL/HR | 0.000 | 174.498 | 57.529 | 205,830 |
| 23 | Total Flow KG/HR | 0.000 | 3143.634 | 0.125 | 5000.000 |
| 24 | Total Flow CUM/HR | 0.000 | 3.567 | 612.571 | 6.163 |
| 25 | Temperature C | 116.058 | 100.000 | 111.059 | 111.521 |
| 26 | Pressure BAR | 0.150 | 3.000 | 0.970 | 3.000 |
| 27 | Vapor Frac | 1.000 | 0.000 | 1.000 | 0.000 |
| 28 | Liquid Frac | 0.000 | 1.000 | 0.000 | 1.000 |
| - 20 | loser- | 0.000 | 0.000 | 0.000 | 0.000 |

Column.Top_Temp=111

data from ASPEN

Simula Database

- Integration
- Standardization
- Uniformity
- Selected technique: Object-Oriented model

Database Model



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SmileX

- ActiveX component implementing Bayesian network
- Work with application GeNIe
- Basic Bayesian network operations

Enhanching SmileX(1)



- Restructuring the network into object classes
- Adding a conversion function

Enhanching SmileX(2)

Adding a conversion function



Applying The Bayesian Network Model

Design steps:

- Understanding the process principles
- Finding the variables
- Constructing the network
- Validate the model
- Fine tuning

Distillation Process

Reboiler:

- degrades \rightarrow bottom temperature lower
- lower temperature \rightarrow less vapor
- less vapor → lower vapor flowrate
 Condenser:
- degrades \rightarrow more vapor exiting the process
- more vapor \rightarrow less reflux
- less reflux \rightarrow less/more purity

Vapor Permeation

Membrane Unit:

- Low permeate pressure \rightarrow high quality
- Low distillate flowrate \rightarrow high quality

Bayesian Network Variables

Inputs:

- Bottom Temperature
- Bottom Water
 Concentration
- Distillate Flowrate
- Retentate Concentration
- Permeate Pressure

Outputs:

- Reboiler Degradation
- Condenser Degradation
- Membrane Degradation
- Performance

Bayesian Network Model for the Process



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Simulation User Interface (1)

Main window



Simulation User Interface (2)

Data tabs

| | Fields_1 | Fields_2 | Fields_3 | Fields_4 | Fields_5 | Fields |
|---|------------|-------------|----------|-------------|-----------|--------|
| | Steam Temp | Bottom Temp | Top Temp | Retent Temp | Top Press | Reter |
| 1 | 116.42 | 100.73 | 87.51 | 21.83 | 0.97 | -0.08 |
| 2 | 116.42 | 100.77 | 87.65 | 21.83 | 0.97 | -0.06 |
| 3 | 116.16 | 100.59 | 87.51 | 21.74 | 0.97 | -0.05 |
| 4 | 116.6 | 100.59 | 87.37 | 21.6 | 0.96 | -0.14 |
| 5 | 116.52 | 100.91 | 87.33 | 21.74 | 0.97 | -0.07 |
| 6 | 116.52 | 101.1 | 87.28 | 21.74 | 0.97 | -0.08 |
| 7 | 116.6 | 101.15 | 87.33 | 22.11 | 0.98 | -0.04 |

Simulation User Interface (3)

Analysis Results

| Failure | Failure | Failure | Temperature | Temperature | Temperature | FlowRate | FlowRate | FlowRate | Concentratio | C. | AVERAGES : |
|-----------|------------|---------------|-------------|-------------|-------------|----------|----------|----------|--------------|----|---|
| ОК | Fail | Contaminate | ок | VeryLow | Lower | OK | Low | High | Good | F. | Failure: 0K=46.63% |
| | | | 80.09322 | 80.09322 | 80.09322 | 5.582953 | 5.582953 | 5.582953 | | | Failure: Fail=17.03% Failure: Contaminated=36.34% |
| 0.18 | 0.37 | 0.45 | 0.28 | 0.38 | 0.34 | 0 | 1 | 0 | 0.53 | 0. | Temperature: UK=75.94% Temperature: VeryLow=12.7% |
| 0.18 | 0.37 | 0.45 | 0.28 | 0.38 | 0.34 | 0 | 1 | 0 | 0.53 | 0. | FlowRate: OK=0% |
| 0.18 | 0.37 | 0.45 | 0.28 | 0.38 | 0.34 | 0 | 1 | 0 | 0.53 | 0. | FlowHate: Low=100% FlowRate: High=0% |
| 0.18 | 0.37 | 0.45 | 0.28 | 0.38 | 0.34 | 0 | 1 | 0 | 0.53 | 0. | Concentration_Water: Good=83.63% Concentration_Water: Fair=3.67% |
| 0.18 | 0.37 | 0.45 | 0.28 | 0.38 | 0.34 | 0 | 1 | 0 | 0.53 | 0. | Concentration_Water: Poor=12.7% Membrane_Degradation: 0K=98% |
| 0.18 | 0.37 | 0.45 | 0.28 | 0.38 | 0.34 | 0 | 1 | 0 | 0.53 | 0. | Membrane_Degradation: Degradated=2% Condensor_Degradation: 0K=98.83% |
| 0.18 | 0.37 | 0.45 | 0.28 | 0.38 | 0.34 | 0 | 1 | 0 | 0.53 | 0. | Condensor_Degradation: Degradated=1.17% Permeate Pressure: 0K=99.73% |
| 0.18 | 0.37 | 0.45 | 0.28 | 0.38 | 0.34 | 0 | 1 | 0 | 0.53 | 0. | Permeate_Pressure: Higher=0.27% |
| 0.18 | 0.37 | 0.45 | 0.28 | 0.38 | 0.34 | 0 | 1 | 0 | 0.53 | 0. | ConcentrationIPA: Fair=1.01% ConcentrationIPA: Poor=1.03% |
| • | | | | | | | | | | • | Performance: Good=74.97% |
| Data Shee | t Aspen Sh | eet SAP Sheet | t Analysis | | | | | | | | |

Simulation User Interface (4)

Action window

| | There are a | There are a few pieces equipment that need maintenance job or replacement. | | | | | | | | |
|-----------|-------------|--|------------------|---------|--|--|--|--|--|--|
| Equipment | Degrad. (%) | Maintenance (\$) | Replacement (\$) | Action | | | | | | |
| HE01 | 82 | 120 | 750 | REPLACE | | | | | | |
| МЕМ | 2 | 500 | 1200 | ок | | | | | | |
| HE02 | 1 | 50 | 200 | ок | | | | | | |

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Simulation Testing

Assumptions:

- All in good condition
- Stable state
- Quality as reported
- No process control

Test Results



Reboiler Degrades?

- Againts the assumption
- Analysing the data file:
 - very large record file
 - may includes start-up and shut-down data



Conclusions

- It was possible to apply Bayesian techniques to the Life Cycle simulation
- The tested model lacks of accuracy because of limited measurement
- Although measurements are few, prelimenary result seems to be meaningfull

Further Research

- How to increase the accuracy for larger processes
- Supporting the Bayesian network with statistical correlation analysis (instead of expert review)
- Simulation based on online process data
- More compatible with commercial software pakages