

Process simulation_Base

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Célok

Szimuláció alapjai

Mikor/hol használunk szimulációt

Milyen modellek vannak

Modell felépítésének lépései

Egyszerű üzemi modell: GFR 106-112 j. kolonna

PFD (P&I)-ból szim modell

Mire jó a szimuláció ?

Miért, mikor?

Egyedi készülékek/egyszerűbb rendszerek

- Üzemi problémák megoldása
- Új javaslatok vizsgálata
- Mi lenne ha vizsgálatok
- Hogyan csináljuk, hogy
- Milyen hatása van ?
- Készülékek működésének vizsgálata

Bonyolultabb rendszerek....

Teljes üzemi modellek

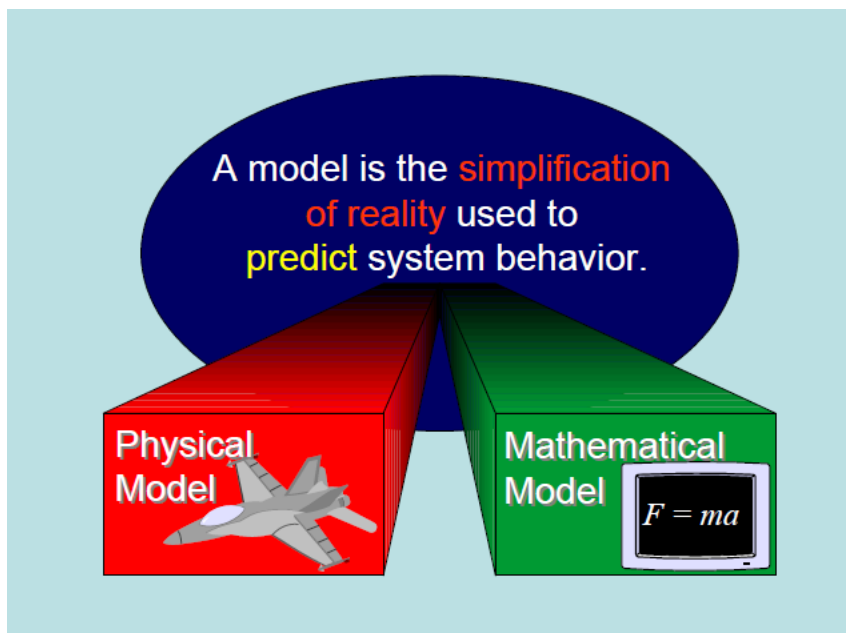
Hőintegráció

dinamikus modellek

OTS

Tervezési adatszolgáltatás (SCM)

Mi a szimuláció ?



Process simulation is a **model-based** representation of different type of processes.

Simulation programs perform **rigorous mass and energy balances** for wide range of chemical processes.

- Not necessarily a one-to-one correspondence between pieces of equipment in the plant and simulation model
- Always the task determine the depth of the model
- Always has to check the results are consistent and realistic
 - „Papír mindent elbír”

Szimuláció a Finomítóban

- Steady state szimuláció (állandósult állapot)
- Dinamikus szimuláció
- Hőcserélők/ hőátadás
- Hőintegráció
- Kemence
- Reaktor modellek
- Csővezetékek/Piping network
- Lefuvató rendszerek/Safety system

Szimuláció ?

Steady state szimuláció

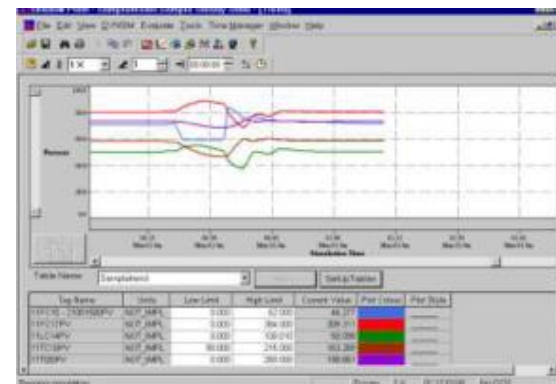
anyag és energia mérlegek
különböző esetek vizsgálata
szűk keresztmetszetek vizsgálata
nem mérhető paraméterek meghatározása

Dinamikus szimuláció

szabályozó rendszerek modellezése
paraméterek időbeli változásának vizsgálata

Időben állandó

Időben változó



Mit csinálunk?

Folyamat ábra/Process flowsheet
P&I /PID



Szimulációs folyamatábra/Simulation flowsheet

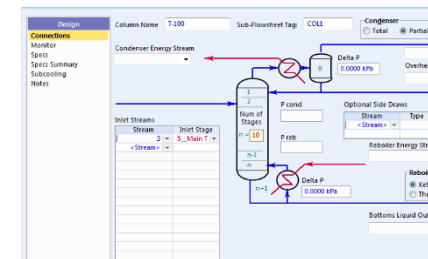
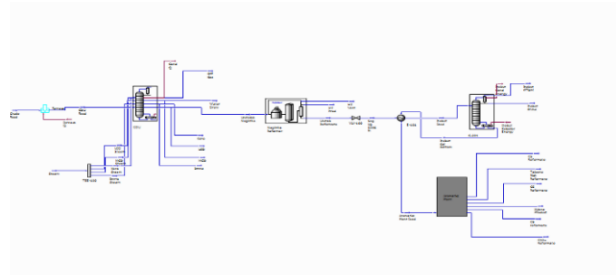
Equipments



Simulation unit

Mi kell hozzá?

- áram paraméterek
- Készülék paraméterek



Szimuláció lépései:



Gázfrakcionáló üzem

Üzem feladata:

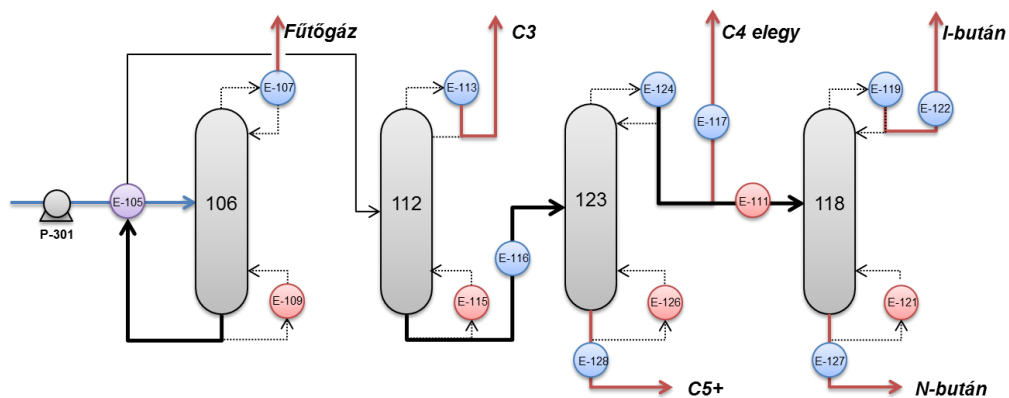
Az üzem a PB kénmentesítő termékét (az AV-1, AV-2, AV-3 üzemek valamint a HDS és BEK-2 üzemek kénmentesített PB-jét), a Reformáló-4 üzemi PB-t és stabilgázt, valamint (téli időszakban) a GOK-3 üzemből származó PB-t dolgozza fel, ill. frakcionálja.

A feldolgozás termékei:

- **Fűtőgáz:** a fűtőgáz gyűjtő és elosztó gerincvezetékbe adják ki.
- **Propán:** a propánt PB keveréshez használják, vagy PAM üzembe
- **Bután elegy:** a bután elegyet PB, illetve benzinkeveréshez használják. Lehetőség van a vegyipari benzinbe történő kitárolásra is.
- **Izobután:** az izobután a HF Alkilezőbe adható tovább vagy a bután elegyhez hasonlóan használható.
- **Normál-bután:** a normálbutánt az MSA üzembe adható ki vagy a bután elegyhez hasonlóan használható fel.
- **Pentán frakció (maradék):** a maradékot motorbenzinbe vagy vegyipari benzinbe keverik.

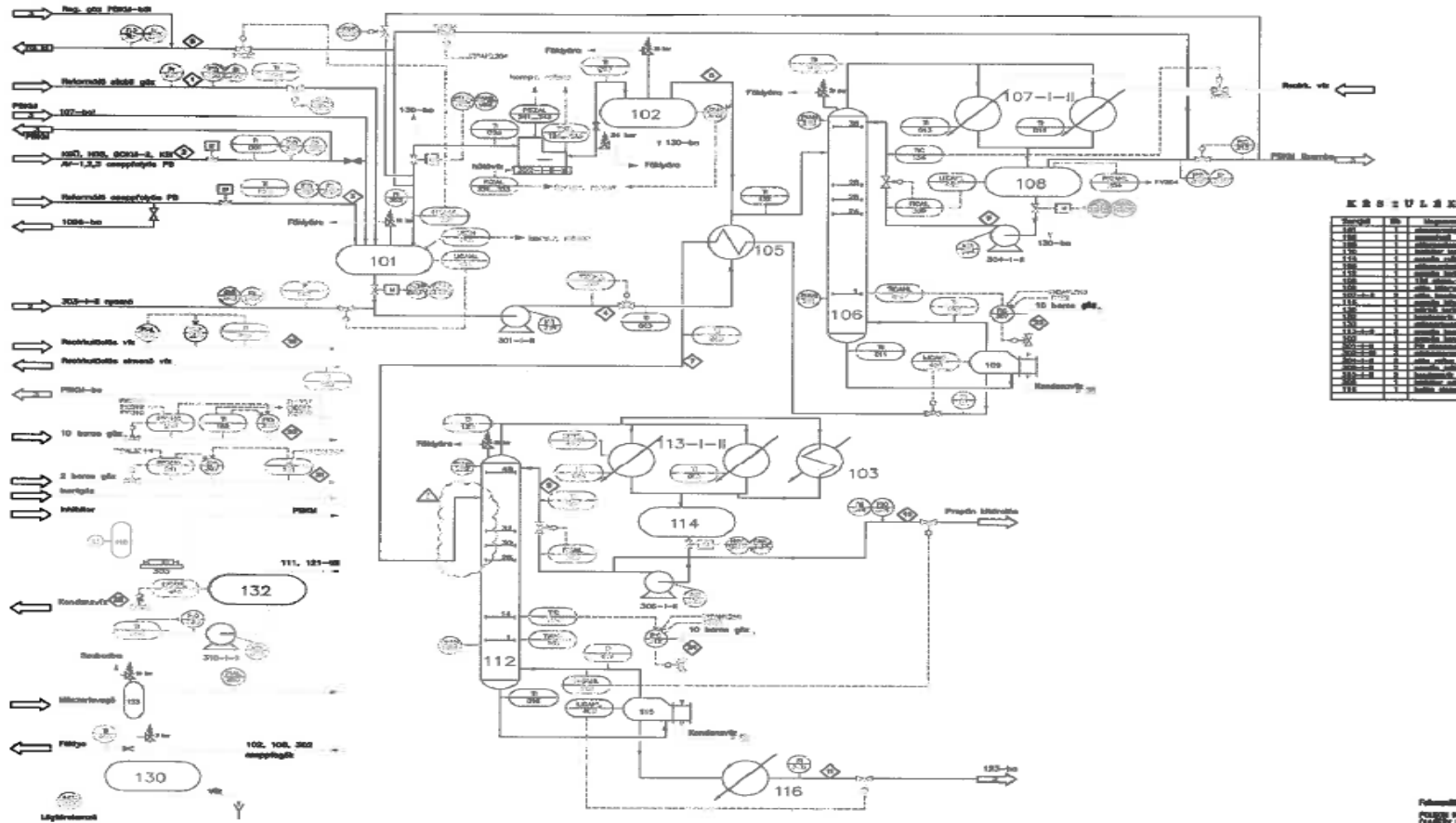
Feladat/gyakorlat

Feladat: GFR üzem első két kolonna modellezése



- PFD/P&I alapján rajzoljuk meg a sim, folyamatábrát, határozzuk meg mely készülékeket kell modellezni
- Indítsuk el a Petrosim-et
- Válasszuk ki az alkalmazott mértékegység rendszert (kg/h, C, barg)
- Válasszuk ki az alkalmazott termodinamikát
- Definiáljuk a komponenseket (következő slide, külön lap)

1. PFD –ből szimulációs folyamatábra



KÖSSZÖLÉS

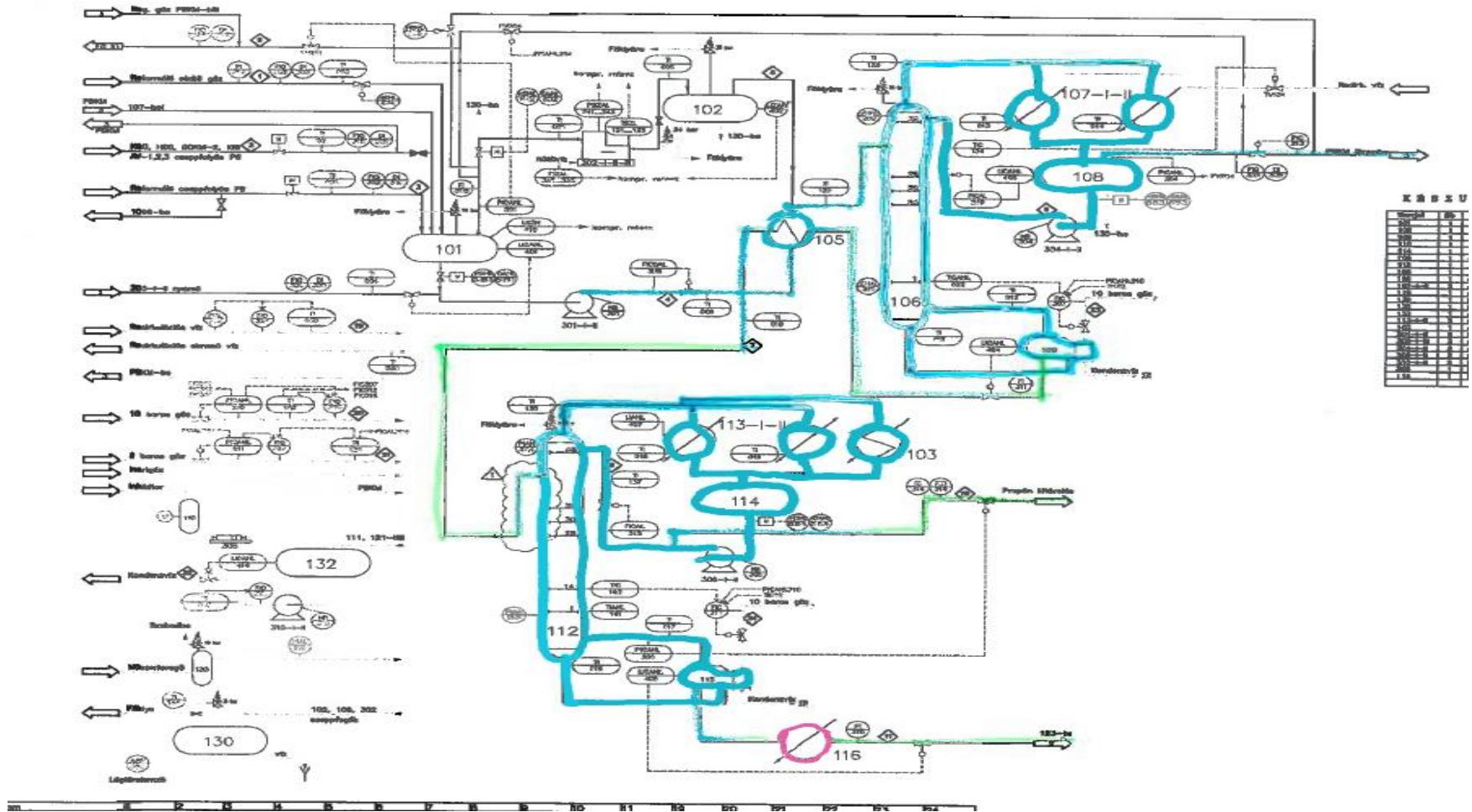
Szám	Név	Megjegyzés
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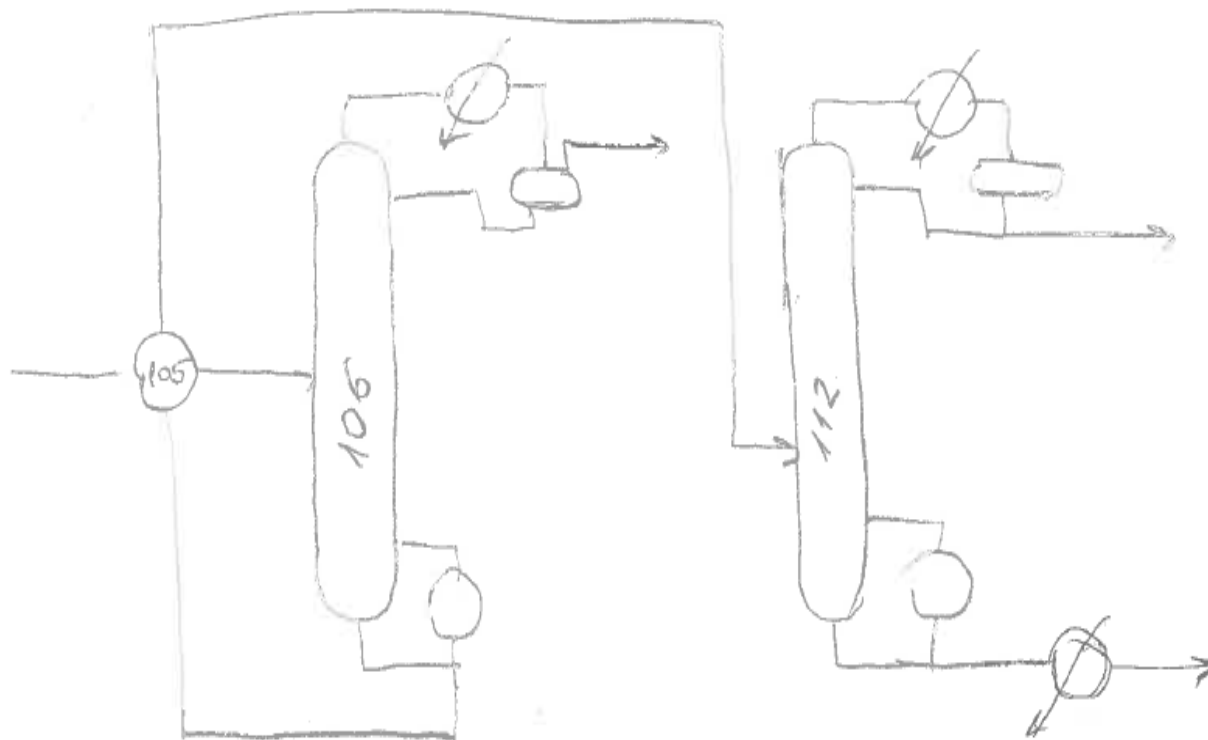
Technical drawing symbols and standards:

- ISO 704
- ISO 10668
- ISO 15926-2
- ISO 15926-3
- ISO 15926-4
- ISO 15926-5
- ISO 15926-6
- ISO 15926-7
- ISO 15926-8
- ISO 15926-9
- ISO 15926-10
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- ISO 15926-97
- ISO 15926-98
- ISO 15926-99
- ISO 15926-100

1. PFD –ből szimulációs folyamatábra



1. PFD –ből szimulációs folyamatábra



2. Mértékegységek



Több lehetőség:
default:

Unit Set	EuroSI	Field	RefineryField	RefineryMetric	SI
Temperature	C	F	F	C	K
Pressure	bar	psia	psig	bar_g	kPa
Flow	kgmole/h	lbmole/hr	MMSCFD	kNm3/h	kgmole/h
Mass Flow	kg/h	lb/hr	lb/hr	tonne/hr	kg/h
Liquid Volume Flow	m3/h	barrel/day	barrel/day	m3/h	m3/h
Energy	kcal/h	Btu/hr	MMBtu/hr	Gcal/hr	kJ/h
Molar Density	kgmole/m3	lbmole/ft3	lbmole/ft3	kgmole/m3	kgmole/m3
Heat Capacity	kJ/kgmole-C	Btu/lbmole-F	Btu/lbmole-F	kcal/kgmol-C	kJ/kgmole-C
Actual Liquid Flow	m3/s	USGPM	barrel/day	m3/s	m3/s
Length	m	ft	ft	m	m
Length Small	mm	in	in	mm	mm
Time	seconds	seconds	hours	hours	seconds

térfogat:

Std m3/h (15 C ,1 bar)

Actual: adott paraméterek (T,p) mellett (általában ezt mérik az üzemek)

Minden mértékegység módosítható, beállítható, egyéni rendszer elmenthető

3. Komponensek, áram összetételek



Komponens :

egyedi komponensek

jól definiált, többnyire ismert
szénhidrogén és egyéb egyedi
magas szénatomszámú komp (kevesebb)

pseudo(hypo) komponensek/petroleum/assay komponens

desztillációs görbe (több lehetőség)
sűrűség

Lehetséges problémák:

könnyű anyagáramok:

nehéz komponensek:

elemzési/mintavételi problémák

nem/nehezen beazonosítható komponensek,
nincs a rendszerben megfelelő komponens

Definiálható:

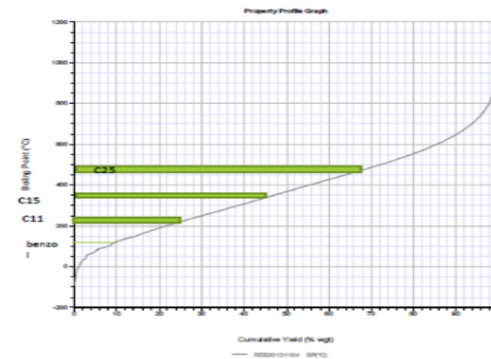
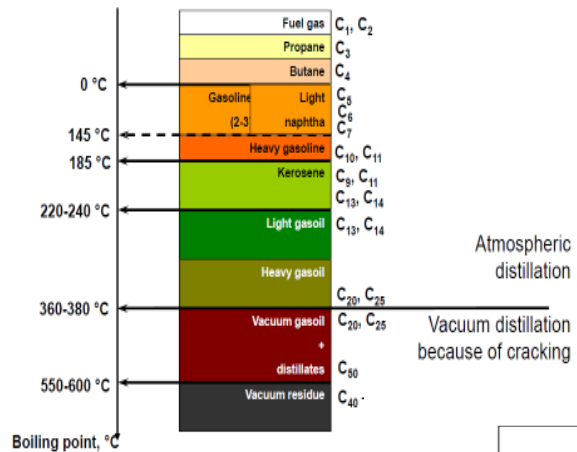
- név alapján
- képlet/összetétel alapján

3. Komponensek, áram összetételek

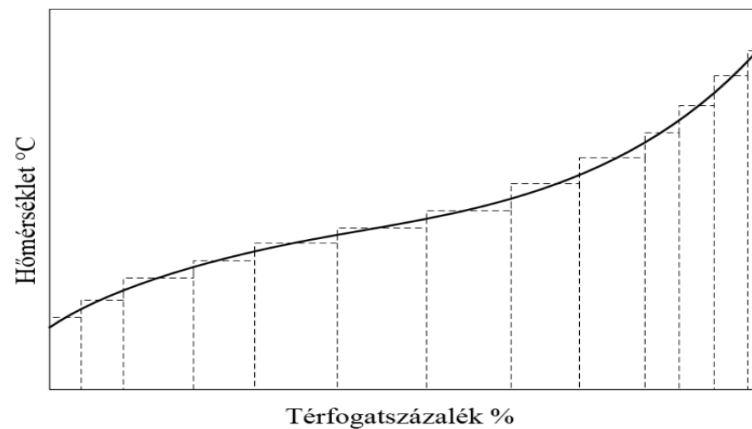
Hypo/pseudo/petroleum komponens

Komponensek generálása:

- sűrűség (sűrűség görbe)
- desztillációs görbe (ASTM D86,D1160,D2887..)
- könnyű komponensek (Lights end)
- viszkozitás(ok)



Pszedokomponensek



4. Termodinamika/fluidpackage



Paraméterek, komponensek alapján

Peng Robinson az alapértelmezett (HYSYS)

Type of stream	Recommended Method
Atmospheric towers	PR Options, GS, TST
Vacuum towers	PR Options, GS, TST, Braun K, Esso Tabular
High H2 System	PR, ZJ, GS, TST
Steam System	NBS Steam, ASME Steam, CS, GS
Compression	MBWR
Amine system	Amine Pkg, DBR Amine Package
Sour water	Sour PR, Sour SRK

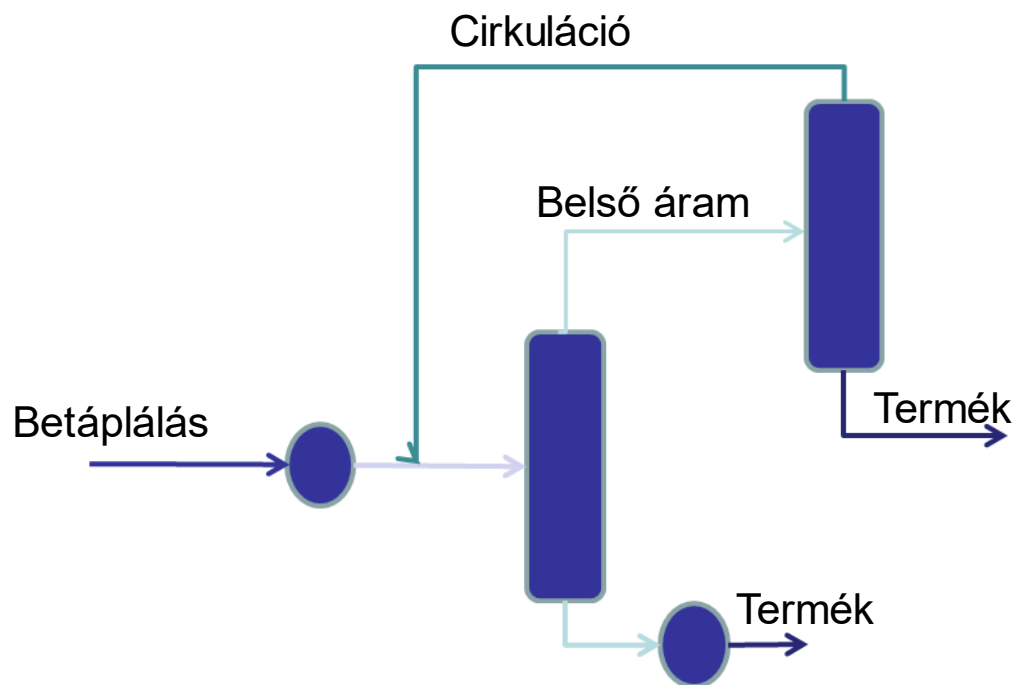
Komponens listához lehet/**kell** igazítani
egy modellen belül váltható
hőmérséklet és nyomástartomány is befolyásolja

5. Áramok



Áram típusok:

- Betáplálás
- Termék
- belső áram
- Cirkuláció
- reference áram



Referencia áram: más áramból vagy készülék belső pontja alapján definiált áram

5. Áramok



Áram tulajdonságok:

hőmérséklet
nyomás
mennyiség
összetétel



Betáplálás:

Termék/belső áram:
Cirkulációs áram

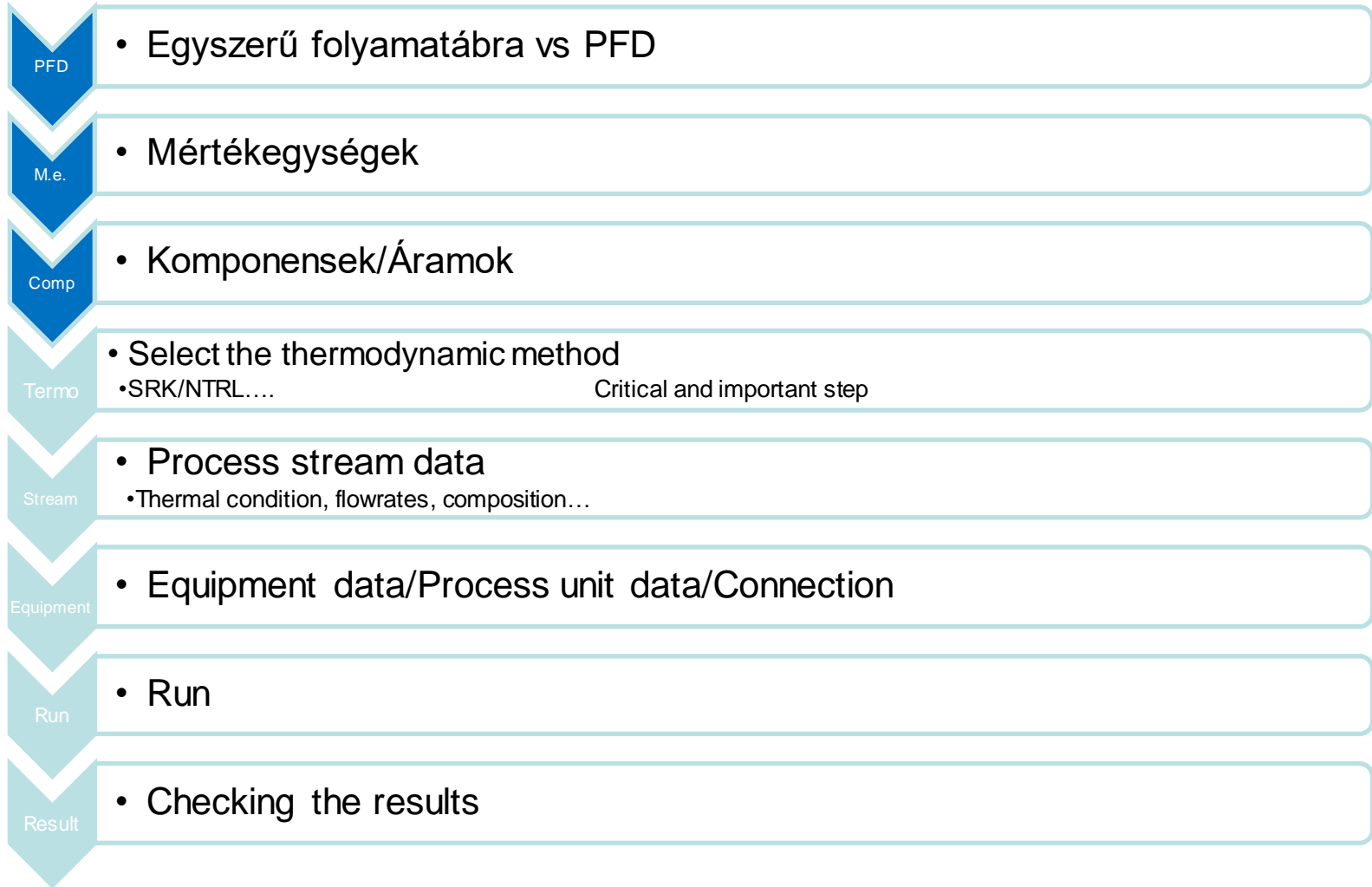
definiálni

számolt
indító érték

Számolt paraméterek

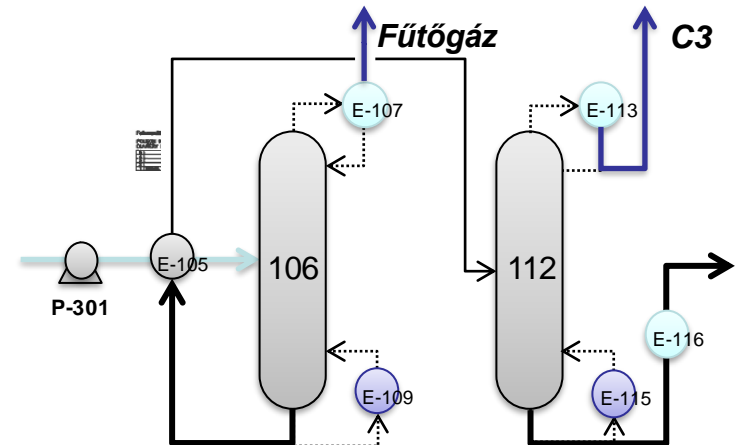
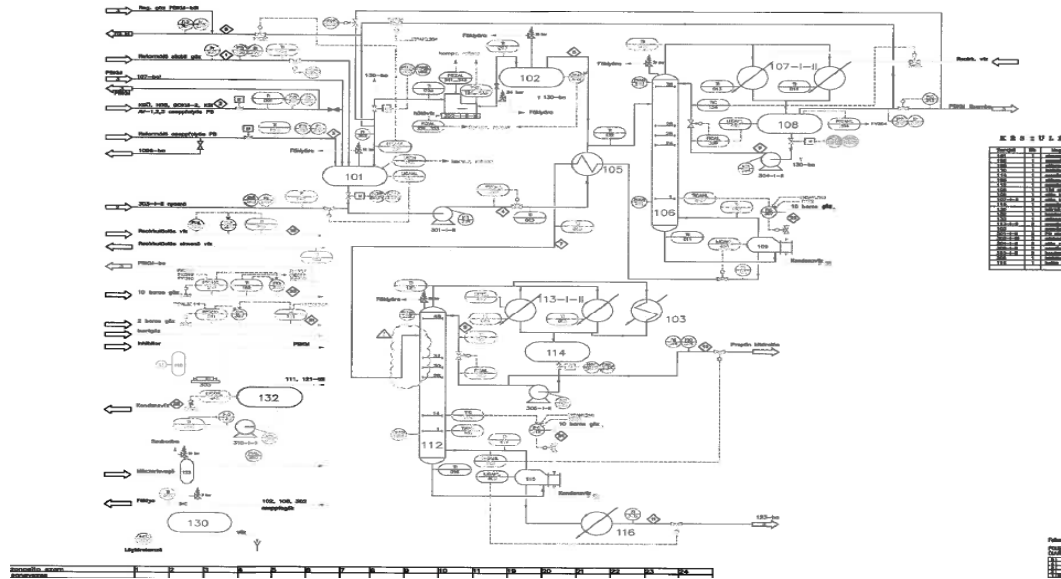
- fix tulajdonságok
 - MW,
 - Liq. Molar volume
 - Carbon Number
 - Chemical formula
 - Critical p, T
 - Critical volume
 - Flash point
 - Freezing point
 - GHT (gross heating value)
 - LHV (lower heating value)
 - Normal boiling point
 - Specific gravity
- hőmérséklet függő
 - Liquid density
 - Thermal conductivity
 - viscosity
 - Vapor pressure

Gyakorlat:



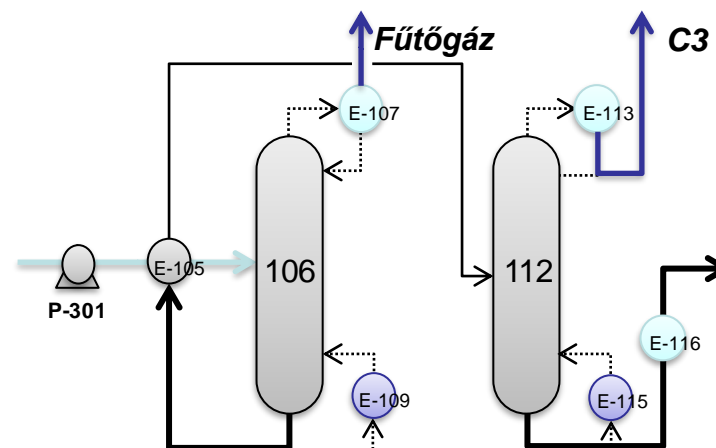


1. PFD – process flows simulation flowsheet



SIMULATION EXERCISE

	106_alapanyag	m/m%
HIDROGEN	0,089	
METAN	0,206	
ETAN	3,609	
ETILEN	0,003	
PROPAN	35,862	
PROPILEN	0,042	
I_BUTAN	20,950	
N_BUTAN	36,119	
I_BUTEN	0,100	
1_BUTEN	0,037	
CIS_2_BUTEN	0,020	
TR_2_BUTEN	0,038	
I_PENTAN	2,134	
N_PENTAN	0,473	
C6_ES_NEH_M	0,144	
SZENMONOXID	0,060	
NITROGEN	0,109	
H2S	0,003	

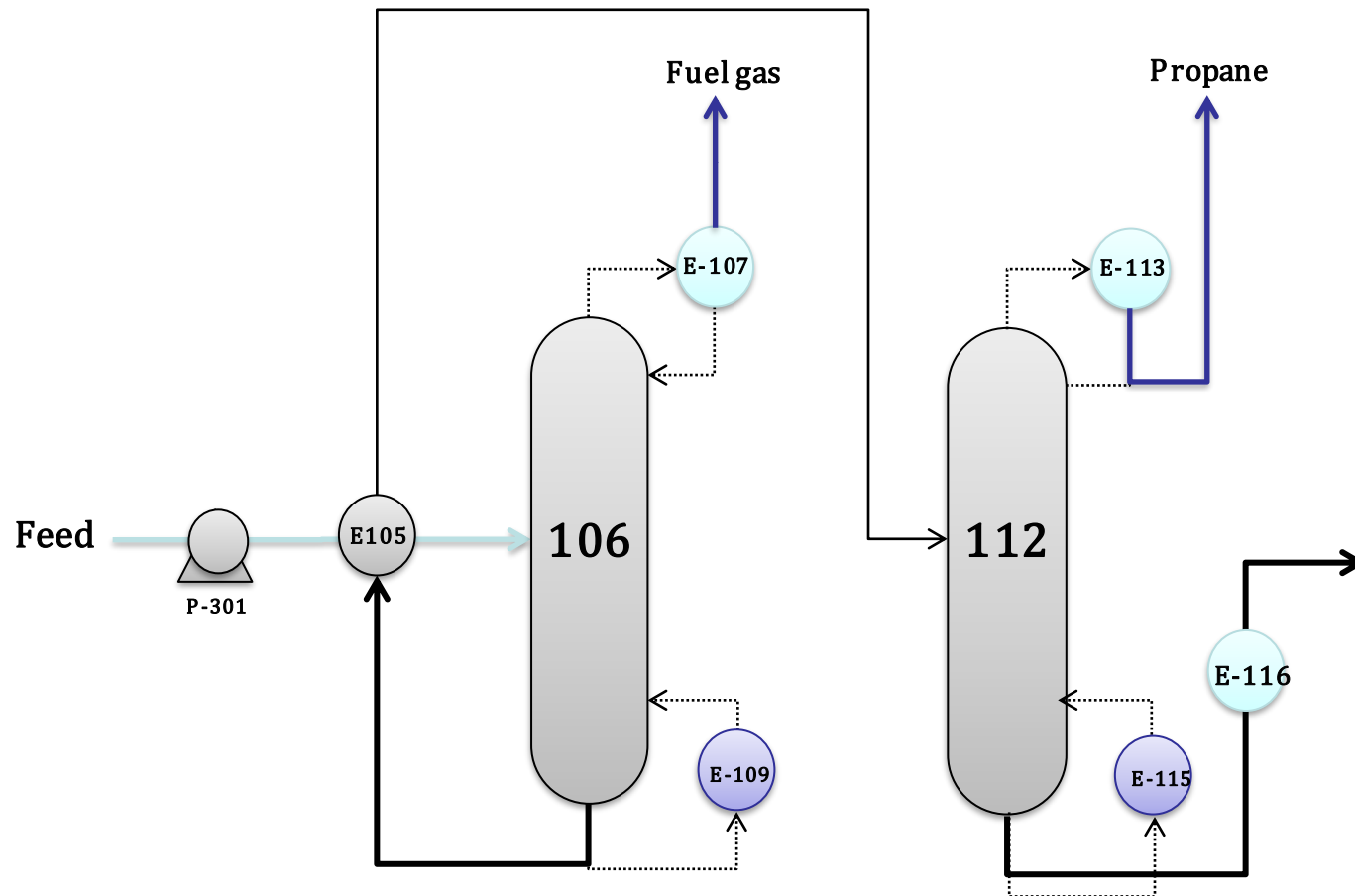


Betáplálás	kg/h	11701
	Cfok	15
	barg	28
Belépő nyomás	barg	32
Szivattyú hatások		0,7
106 belép hőmérséklet	Cfok	58

SIMULATION EXCERCISE

EXCERCISE

Modeling of deethenizer (Column 106) and depropanizer column (Column 112) of the Danube Refinery's Gas Fractionation Unit



GETTING START WITH ASPEN PLUS

- Open Aspen Plus V10
- Start:
 - **New simulation**
 - Aspen Plus template files (categorized by different applications)



Aspen Plus Templates

Category	Template	English Metric Met-C_bar_hr
Chemicals	Batch Polymers with English Units	
	Chemicals with English Units	
Gas Processing	Electrolytes with English Units	
Mining and Minerals	Polymers with English Units	
Refinery		
Specialty Chemicals and Pharmaceuticals		
User		

UNIT SETS



- Three default engineering unit sets:
 - SI
 - EuroSI (bar,kcal
 - Field(English)

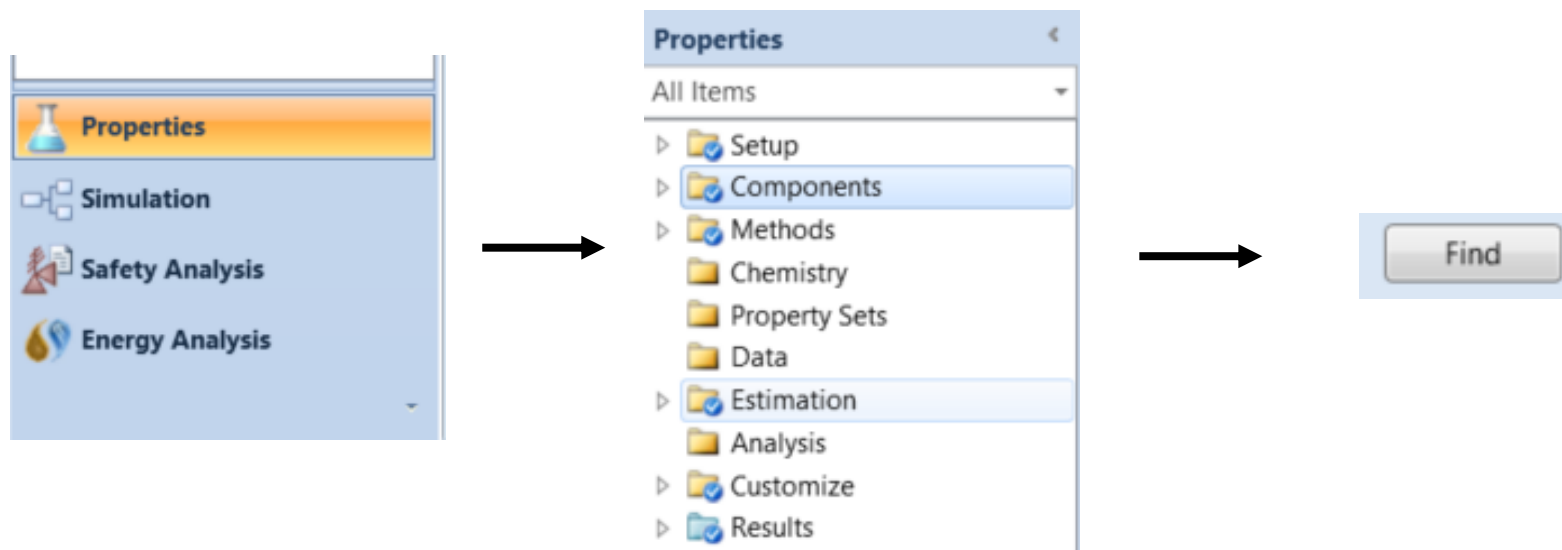
- Mostly used units:
 - mass: kg/h or t/h
 - temperature: C
 - pressure: barg
 - volume: m3/h

- Volume: Std m3/h (15 C ,1 bar) or actual m3/h (on actual T and p)

Component selection

Component selection:

- Properties → Components → Find



- **Pure component:**
 - Search by compound name/alternate name/formula
- **Assay/Blend definition:**
 - Generating pseudocomponents

Pure component selection

Search Criteria

Begins with

Name, Alias or CASRN: Contains

n-butane

Equals

Compound class:

All

Molecular weight:

From

To

Boiling point:

From

To

C

Find Now

New Search

Help

Compounds found matching the specified criteria

Compound name	Alias	Databank	Alternate name	MW	BP <C>	CAS number
BUTYRONITRILE	C4H7N	APV121.PU	N-BUTANENITI	69,10	117,6	109-74-0
DECAFLUOROBUT/	C4F10	APV121.PU	PERFLUORO-N	238,0	-1,299999	355-25-9
N-BUTANE	C4H10-1	APV121.PU	n-Butane	58,12	-0,5	106-97-8
N-BUTYL-MERCAP	C4H10S-D1	APV121.PU	n-Butanethiol	90,18	98,46	109-79-5
VALERYL-CHLORID	C5H9CLO	NISTV121.†	N-BUTANECAR	120,5	122,123	638-29-9

Pure component selection

Component list used in simulation

HIDROGEN
METAN
ETAN
ETILEN
PROPAN
PROPILEN
I_BUTAN
N_BUTAN
I_BUTEN
1_BUTEN
CIS_2_BUTEN
TR_2_BUTEN
I_PENTAN
N_PENTAN
N-HEXAN
SZENMONOXID
NITROGEN
H2S
VIZ



Component name	Alias
HYDROGEN	H2
METHANE	CH4
ETHANE	C2H6
ETHYLENE	C2H4
PROPANE	C3H8
PROPYLENE	C3H6-2
ISOBUTANE	C4H10-2
N-BUTANE	C4H10-1
ISOBUTYLENE	C4H8-5
1-BUTENE	C4H8-1
CIS-2-BUTENE	C4H8-2
TRANS-2-BUTENE	C4H8-3
2-METHYL-BUTANE	C5H12-2
N-PENTANE	C5H12-1
N-HEXANE	C6H14-1
CARBON-DIOXIDE	CO2
CARBON-MONOXIDE	CO
NITROGEN	N2
OXYGEN	O2
HYDROGEN-SULFIDE	H2S
WATER	H2O

THERMODYNAMIC METHODS

Fluid package/thermodynamic method

- to perform flash and physical property calculations

Method filter:
narrowing the methods
by grouping

Global | Flowsheet Sections | Referenced | Comments

Property methods & options

Method filter: COMMON

Base method: PENG-ROB

Henry components:

Petroleum calculation options

Free-water method: STEAM-TA

Water solubility: 3

Electrolyte calculation options

Chemistry ID:

Use true components

Method name: PENG-ROB [Methods Assistant...]

Modify

EOS: ESPRSTD

Data set: 1

Liquid gamma: 1

Data set: 1

Liquid molar enthalpy: HLMX106

Liquid molar volume: VLMX20

Heat of mixing

Poynting correction

Use liquid reference state enthalpy

Thermodynamic method
used in simulation
environment

THERMODYNAMIC METHODS

Select thermodynamic method according to process or component type

Specify component type:



Component system type	Thermodynamic methods
Chemical systems (low & high pressure)	Wong-Sandler, NRTL, Wilson, etc..
Hydrocarbon systems	Peng-Robinson, Chao-Seader, Grayson-Streed, etc..
Special (amine, sour water, electrolyte..)	Kent-Eisenberg, ELECNRTL, APISOUR, etc..
Refrigerants	REFRPOP

Specify process type:

Process type	Thermodynamic methods
Chemical	NRTL, Wilson, UNIQUAC
Refining	PR, Chao-Seader, Grayson-Streed, etc..
Gas processing	SRK, CPA, PR, etc..
Pharmaceuticals	RTL, UNIFAC, NRTL-SAC, COSMOSAC, etc..

SIMULATION ENVIRONMENT

The image shows a screenshot of a simulation software interface. The interface includes a menu bar at the top with options like File, Home, Economics, Batch, Dynamics, Plant Data, Equation Oriented, View, Customize, Resources, Modify, and Format. Below the menu bar is a toolbar with various icons for simulation control and analysis. The main workspace displays a simulation flowsheet with several units connected by streams. A left-hand pane lists simulation items, and a bottom pane shows a model palette with various unit icons. Callouts with blue boxes and arrows point to specific features: 'Run the simulation file' points to the 'Run' button in the toolbar; 'Simulation flowsheet' points to the main workspace area; 'List of simulation items' points to the left-hand pane; 'Checking simulation status' points to the 'Check Status' button at the bottom; and 'Selecting operation units' points to the 'Mixer' icon in the model palette.

Run the simulation file

Simulation flowsheet

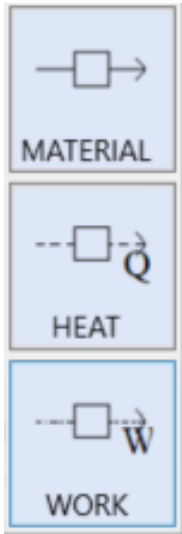
List of simulation items

Checking simulation status

Selecting operation units

DEFINING PROCESS STREAMS

Process streams



- **Material stream:**
 - Temperature, pressure/vapor fraction & composition
- **Heat stream**
 - Duty, start & end temperature
- **Work stream**
 - Power & speed

MATERIAL STREAM COMPOSITION AND CONDITIONS

Specifications

Flash Type: **Temperature** Pressure

State variables

Temperature: 15 C

Pressure: 28 barg

Vapor fraction: 0

Total flow basis: **Mass**

Total flow rate: 11701 kg/hr

Solvent:

Reference Temperature

Volume flow reference temperature: C

Component concentration reference temperature: C

Composition: **Mass-Frac**

Component	Value
HYDRO-01	0,089
METHA-01	0,206
ETHAN-01	3,609
ETHYL-01	0,003
PROPA-01	35,862
PROPY-01	0,042
ISOBU-01	20,95
N-BUT-01	36,119
ISOBU-02	0,1
1-BUT-01	0,037
CIS-2-01	0,02
TRANS-01	0,038
2-MET-01	2,134
N-PEN-01	0,473
N-HEX-01	0,144
CARBO-01	0
CARBO-02	0,06
NITRO-01	0,109
OXYGE-01	0
HYDRO-02	0,003
WATER	

Feed stream	Value	UoM
Mass flowrate	11701	kg/h
Temperature	15	°C
Pressure	28	barg

STREAM ANALYSIS

- Choosing mass density of mixture

Enter a search string Limit search to pure components properties
 Exclude Petroleum correlations

Select Property to include

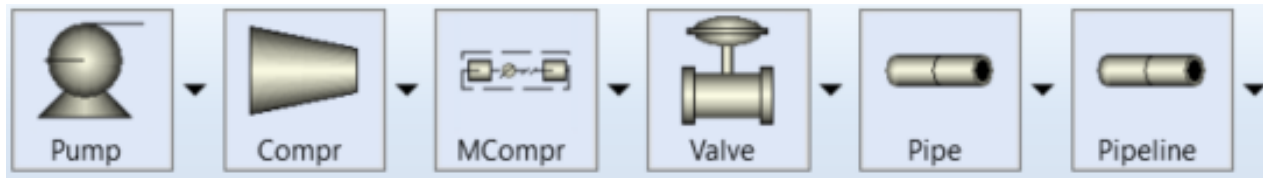
	Property name	Alias	
<input type="checkbox"/>	Mass density, pure component	MASSRHO	
<input checked="" type="checkbox"/>	Mass density, mixture	MASSRHOM	
<input type="checkbox"/>	Standard mass liquid density for a petrol	RHOSTD-R	
<input type="checkbox"/>	Standard mass density at 15C, reference	RHOST-15	
<input type="checkbox"/>	Standard mass density at 0C, reference 0	RHOST-0	
<input type="checkbox"/>	Mass standard liquid density	MRHOLSTD	

Property Set Contents

Property name	Alias		
Mass density, mixture	MASSRHOM		✗

PRESSURE CHANGER UNIT OPERATIONS

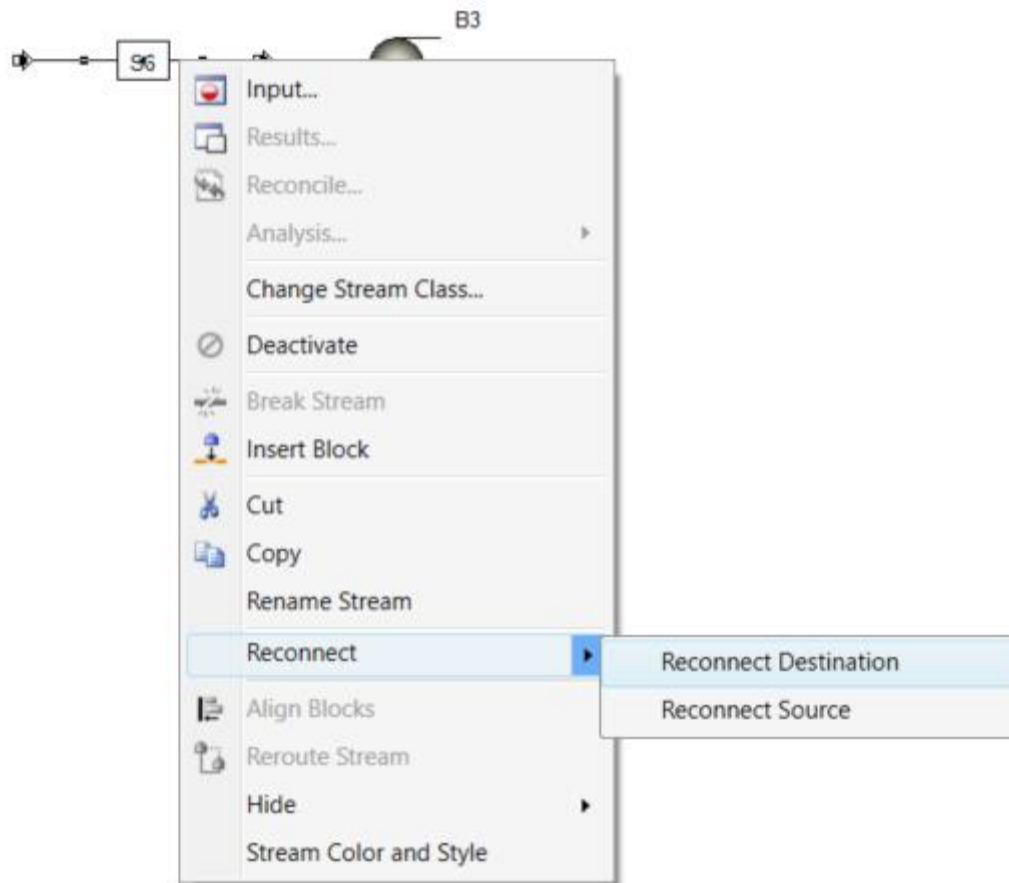
- Pressure changers:
 - Pump
 - Compressor
 - Multistage compressor
 - Valves
 - Pipe (single segment)
 - Pipeline (multiple segments)



PUMP

- **Stream connection to pump**

- Reconnect → Destination (for inlet streams) / source (for outlet streams)



PUMP

- Pump outlet specifications & efficiency

Model

Pump Turbine

Pump outlet specification

Discharge pressure barg

Pressure increase bar

Pressure ratio

Power required Watt

Use performance curve to determine discharge conditions

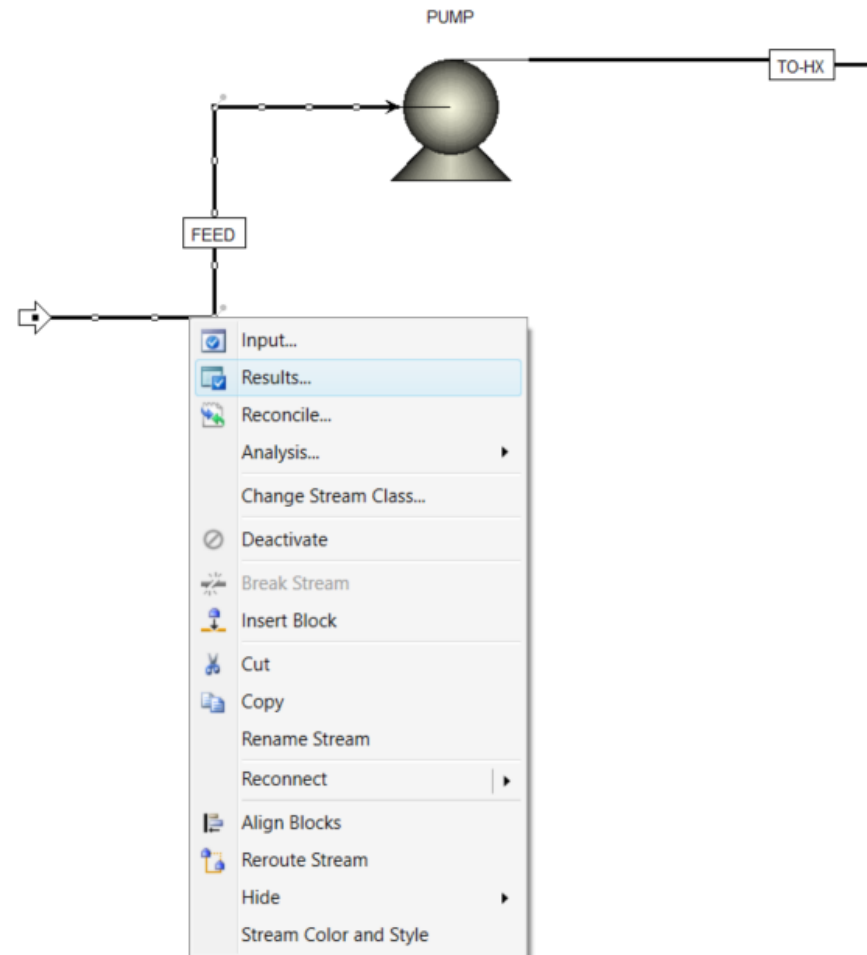
Efficiencies

Pump Driver

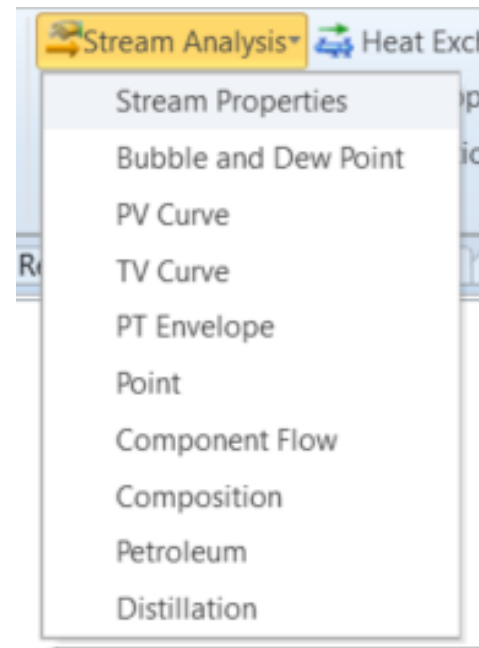
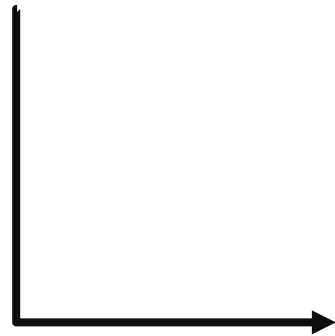
- Pump operation won't work if the inlet stream has vapor fraction

PUMP

- Run the simulation and check the calculated values



STREAM ANALYSIS



STREAM ANALYSIS

Stream chosen for analysis

Definition of dependent variables

Independent variable

The screenshot shows the 'Stream Property Analysis' software interface. At the top, there are tabs for 'Stream Property Analysis', 'Simulation Options', 'Diagnostics', 'Results', and 'Comments'. Below the tabs, the 'Reference stream' is set to 'FEED'. The 'Properties to Report' section contains a list of properties with navigation buttons (>, >>, <, <<, New) and up/down arrows. The 'Selected manipulated and parametric variables' section is expanded to show the 'Manipulated variable' settings: 'Temperature' is selected, with 'Equidistant' chosen as the method. The start point is 0 C, the end point is 100 C, and the number of intervals is 20. The 'Parametric Variable' section shows 'Pressure' selected with units 'barg', and a table for 'Enter Values' with a value of 0.

Stream Property Analysis | Simulation Options | Diagnostics | Results | Comments

Reference stream: FEED

Properties to Report

Selected manipulated and parametric variables

Manipulated variable: Temperature

Equidistant | Logarithmic | List of values

Start point: 0 C

End point: 100 C

Number of intervals: 20

Increment: 5 C

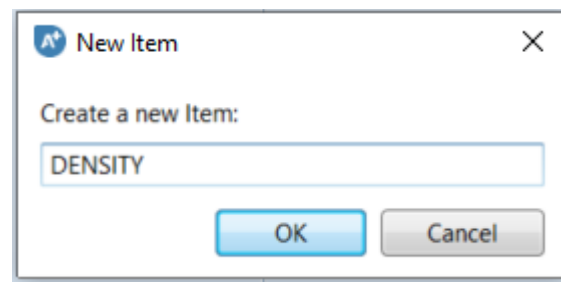
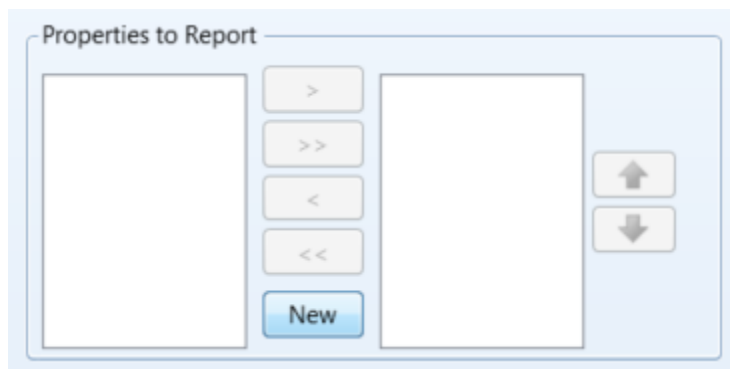
Parametric Variable: Pressure barg

Enter Values

>	
>	0
>	

STREAM ANALYSIS

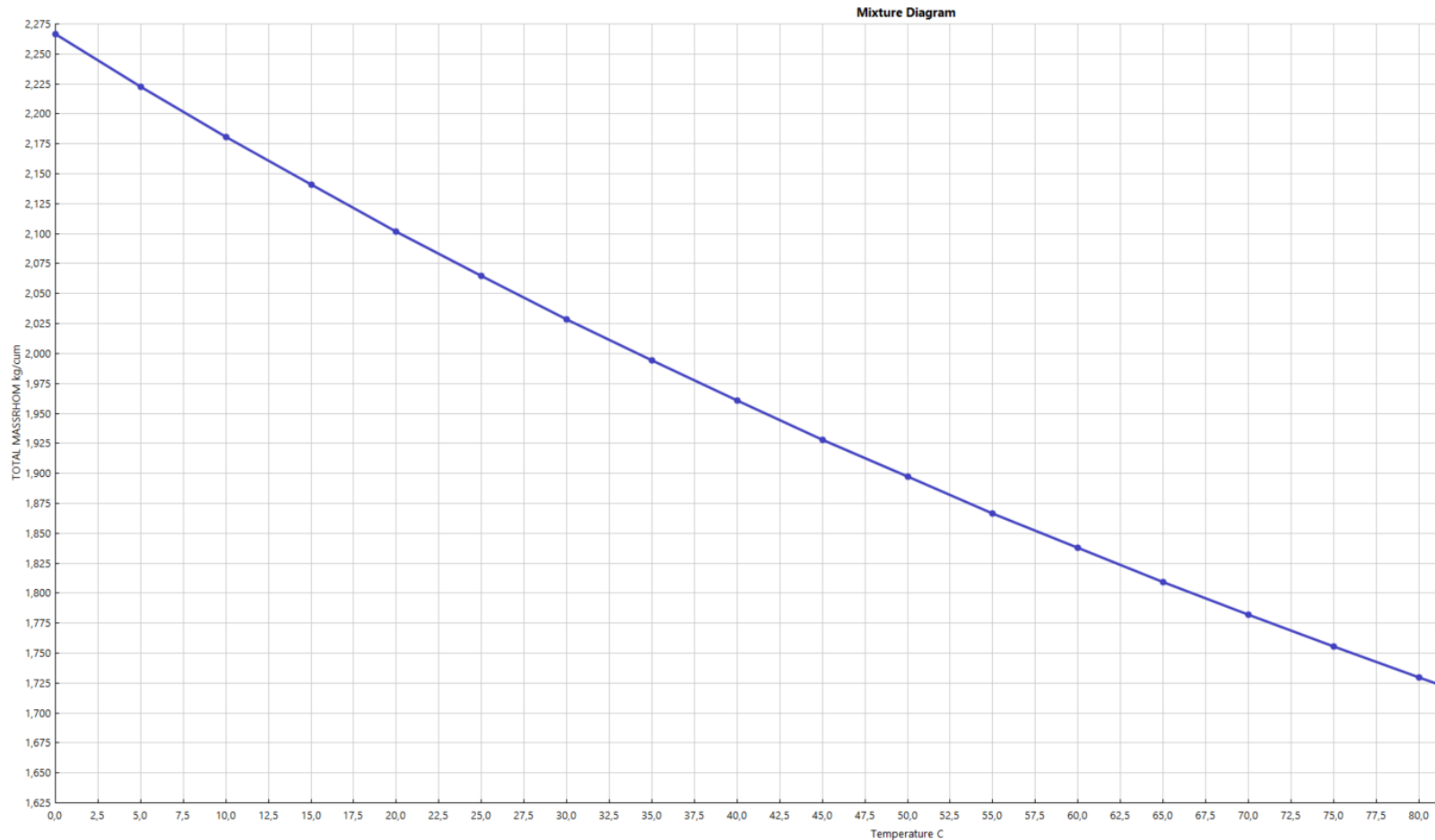
- Choosing properties to report



STREAM ANALYSIS

- After running analysis, results will be plotted

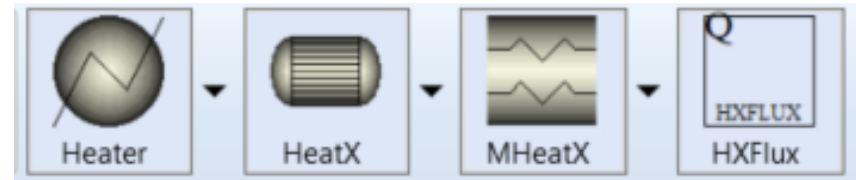
Run Analysis



HEAT EXCHANGERS

Exchanger models

- Simple heater/cooler
 - Simple heat transfer calculation for one stream
 - Pressure and outlet temperature, ΔT , degrees of superheating/subcooling or heat duty need to be specified
- Detailed heat exchanger (HeatX)
 - Heat transfer calculations between 2 material streams
 - Different types:
 - Shortcut (simple calculations)
 - Shell & Tube (detailed geometry)
 - Kettle reboiler
 - Thermosyphon
 - Air Cooled
 - Plate
 - Different calculation modes
 - Design
 - Rating
 - Simulation
 - Maximum fouling



HEAT EXCHANGERS

Simple heater specifications

Flash specifications

Flash Type **Temperature** ▾

Pressure ▾

Temperature **C** ▾

Temperature change C ▾

Degrees of superheating C ▾

Degrees of subcooling C ▾

Pressure **barg** ▾

Duty Watt ▾

Vapor fraction

Pressure drop correlation parameter

Always calculate pressure drop correlation parameter

Valid phases

Vapor-Liquid ▾

HEAT EXCHANGERS

Shell & tube heat exchanger sizing (EDR sizing console)

- Specifying detailed geometry

Calculation mode: **Rating / Checking** Recent Previous Setting Plan Tube Layout

Configuration

TEMA Type: **B -** **E -** **M -** BEM

Tube layout option: **New (optimum) layout**

Location of hot fluid: **Shell side**

Tube OD / Pitch: **in** **0,75** / **0,9375** 0,75 / 0,9375 /

Tube pattern: **30-Triangular** 30

Tubes are in baffle window: **Yes** Yes

Baffle type: **Single segmental** Single segmental

Baffle cut orientation: **Horizontal** H

Default exchanger material: **Carbon Steel** **1** Carbon Steel

Size

Specify some sizes for Design: **Set default** No

Shell ID / OD: **in** / 8,071 / 8,625 /

Tube length: **in** 165,3543

Baffle spacing center-center (Bc): **in** 3,5433

Number of baffles: 42

Number of tubes / Tube passes: / 40 / 2 /

Shells in series: 1

Shells in parallel: 1

Overall Results

Excess surface (%): 2

Dp-ratio Shellside / Tubeside: **0,6978** / **0,2932** /

Total cost (all shells): **Dollar(US)** 15189

Stream Temperatures vs Distance from End

Legend: **TS Bulk Temp. (F)** (Blue line), **SS Bulk Temp (F)** (Red line)

DISTILLATION COLUMNS

Different column types:

- DSTWU, Distl, SCFrac – shortcut columns with different calculation methods (Winn-Underwood-Gililand, Edmister...etc)
- **RadFrac** – rigorous 2 or 3 phase fractionation for single columns
- Extract – rigorous liquid-liquid extractor
- MultiFrac – rigorous fractionation for complex columns
- PetroFrac - rigorous fractionation for petroleum refining applications
- ConSep – feasibility and design calculations



RADFRAC COLUMN - CONFIGURATION

Distillation column 106 configuration

The screenshot displays the configuration interface for a distillation column. It is divided into several sections:

- Configuration tabs:** Configuration (selected), Streams, Pressure, Condenser, Reboiler, etc.
- Setup options:**
 - Calculation type: *Equilibrium*
 - Number of stages: **34** (with a 'Stage Wizard' button)
 - Condenser: **Partial-Vapor**
 - Reboiler: *Kettle*
 - Valid phases: *Vapor-Liquid*
 - Convergence: *Standard*
- Operating specifications:**
 - Distillate rate: **Mass**, **3868 kg/hr**
 - Reflux rate: **Stdvol**, **5 cum/hr**
 - Free water reflux ratio: (empty field)
 - Feed Basis: (button)
- Design and specify column internals:** (button)

Number of stages: column tray number + 2 (condenser & reboiler are defined as trays)

Condenser type (total, partial or none)

Operating specifications (distillate rate, reflux ratio, boilup, etc) – can be overwritten by design specifications

Specifying column internals (trays or packing type, tray spacing, column diameter, tray geometry details)

RADFRAC COLUMN - STREAMS

Defining column 106 streams (streams need to be put down to the flowsheet and connected to the column before defining)

Configuration Streams Pressure Condenser Reboiler 3-Phase Comments

Specifying feed stage number and feed convention

Feed streams

Name	Stage	Convention
TO-COL	14	Above-Stage

Product streams

Name	Stage	Phase	Basis	Flow	Units	Flow Ratio	Feed Specs
106VAP	1	Vapor	Mole		kmol/hr		Feed basis
106BTM	34	Liquid	Mole		kmol/hr		Feed basis

Pseudo streams

Name	Pseudo Stream Type	Stage	Internal Phase	Reboiler Phase	Reboiler Conditions	Pumparound ID	Pumparound Conditions	Flow	Units
106OH	Internal	2	Vapor		Outlet		Outlet		kmol/hr
106REB	Internal	33	Liquid		Outlet		Outlet		kmol/hr
106-REF	Internal	1	Liquid		Outlet		Outlet		kmol/hr
S1	Internal	5	Liquid		Outlet		Outlet		kmol/hr

Pseudo streams – exported internal streams (reflux, overhead vapors, pumparounds etc)

Specifying product stream stages and phases

► **MOL GROUP**

RADFRAC COLUMN - PRESSURE

Defining column 106 pressure

The screenshot shows the 'Pressure' configuration tab for a RADFRAC column. The 'View' is set to 'Top / Bottom'. The 'Top stage / Condenser pressure' is set to 22,37 barg. The 'Stage 2 pressure (optional)' is set to 22,47 barg. The 'Pressure drop for rest of column (optional)' is set to 0,52 bar.

Parameter	Value	Unit
Top stage / Condenser pressure	22,37	barg
Stage 2 pressure (optional)	22,47	barg
Pressure drop for rest of column (optional)	0,52	bar

- Top/bottom pressure & pressure drop
- Pressure profile
- Section pressure drop

RADFRAC COLUMN – CONDENSER

Specifying condenser parameters

Configuration Streams Pressure Condenser Reboiler 3-Phase Comments

Condenser specification

Temperature

Distillate vapor fraction

Mole 1

Subcooling specification

Subcooled temperature 33,7 C

Both reflux and liquid distillate are subcooled

Only reflux is subcooled

Utility specification

Utility

- In case of choosing Partial-Vapor condenser type in configuration tab, only subcooled temperature or degrees of subcooling can be specified
- In case on Partial-Vapor-Liquid condenser, temperature or vapor fraction need to be defined along with subcooling parameters

RADFRAC COLUMN – CONDENSER

Specifying reboiler parameters

Thermosiphon reboiler options

Specify reboiler flow rate

Specify reboiler outlet condition

Specify both flow and outlet condition

Reboiler Wizard

Flow rate

Mole kmol/hr

Outlet condition

Temperature C

Optional

Reboiler outlet pressure barg

Reboiler return feed convention Above-Stage

Utility

Reboiler configurations

Circulation without baffle

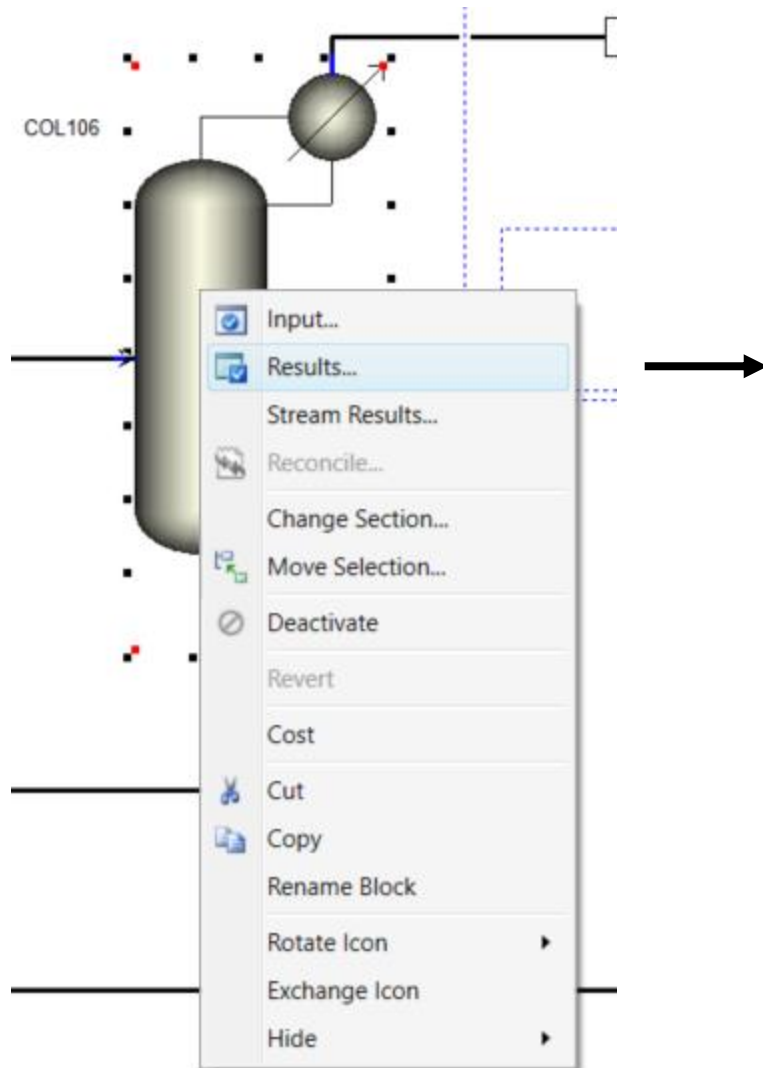
Circulation with baffle

Circulation with auxiliary baffle

- In case of choosing Kettle Reboiler, there's no parameter to be specified
- In case of thermosiphon reboiler, flowrate and/or outlet condition can be defined

RADFRAC COLUMN – RESULTS

After defining column specification simulation can run → results



Basis: Mass

Condenser / Top stage performance

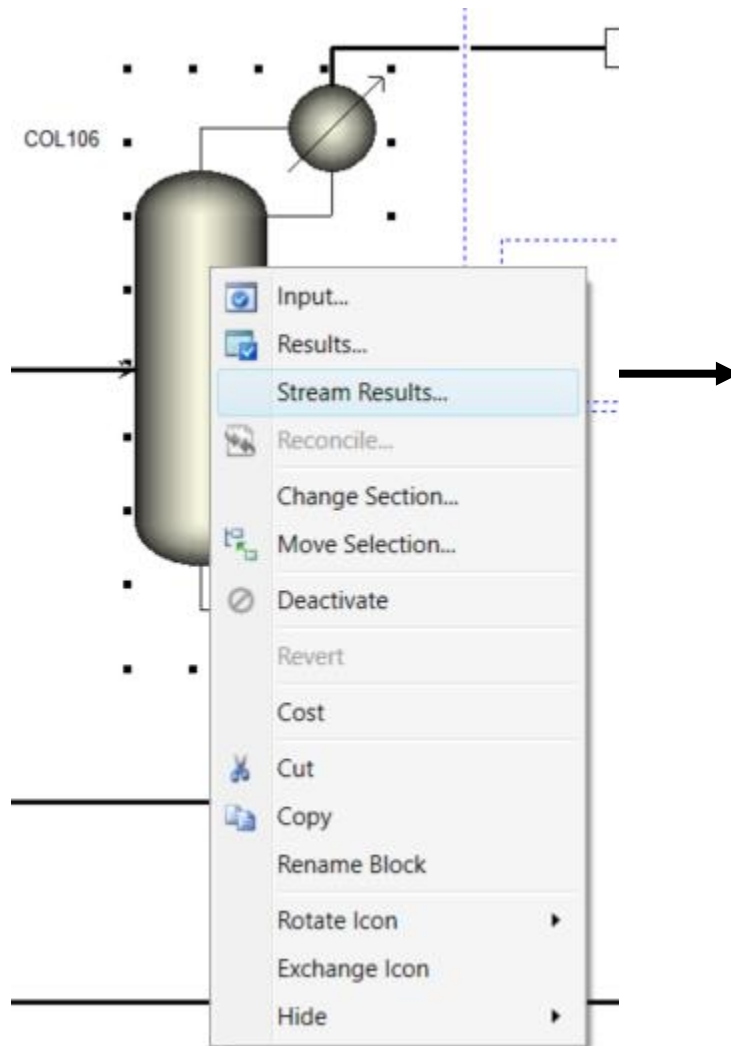
Name	Value	Units
Temperature	64,605	C
Subcooled temperature	33,7	C
Heat duty	-0,739834	GJ/hr
Subcooled duty	-0,241306	GJ/hr
Distillate rate	3868	kg/hr
Reflux rate	2591,25	kg/hr
Reflux ratio	0,66992	
Free water distillate rate		
Free water reflux ratio		
Distillate to feed ratio		

Reboiler / Bottom stage performance

Name	Value	Units
Temperature	103,823	C
Heat duty	3,31037	GJ/hr
Bottoms rate	7833	kg/hr
Boilup rate	14364	kg/hr
Boilup ratio	1,83378	
Bottoms to feed ratio		

RADFRAC COLUMN – STREAM RESULTS

Connected stream properties and compositions



	Units	TO-COL	106-REF
Description			
From		B5	COL106
To		COL106	
Stream Class		CONVEN	CONVEN
Maximum Relative Error			
Cost Flow	\$/sec		
- MIXED Substream			
Phase		Liquid Phase	Liquid Phase
Temperature	C	53,1641	33,7
Pressure	barg	35	22,37
Molar Vapor Fraction		0	0
Molar Liquid Fraction		1	1
Molar Solid Fraction		0	0
Mass Vapor Fraction		0	0
Mass Liquid Fraction		1	1
Mass Solid Fraction		0	0
Molar Enthalpy	J/kmol	-1,27326e+08	-1,2644e+08
Mass Enthalpy	J/kg	-2,57285e+06	-2,67562e+06
Molar Entropy	J/kmol-K	-359366	-353306
Mass Entropy	J/kg-K	-7261,63	-7476,35
Molar Density	kmol/cum	9,69643	10,5496
Mass Density	kg/cum	479,86	498,539
Enthalpy Flow	Watt	-8,36248e+06	-1,92589e+06
Average MW		49,4883	47,2564
+ Mole Flows	kmol/hr	236,44	54,8338
+ Mole Fractions			
+ Mass Flows	kg/hr	11701	2591,25
+ Mass Fractions			
Volume Flow	cum/hr	24,3842	5,19769

RADFRAC COLUMN – DESIGN SPECIFICATIONS

Distillation parameters (product qualities, component recoveries.etc) can be defined by design specifications (can be found on item list)

The image illustrates the process of defining design specifications in the software. On the left, a tree view shows the project structure under 'COL106', with 'Design Specifications' selected. A 'New' button is highlighted, leading to a configuration dialog box. The dialog box contains the following fields:

- Description:** C3 bottom recovery (User-defined)
- Design specification Type:** Mass recovery (Specification type)
- Specification Target:** 0,65 (Specified value)

RADFRAC COLUMN – DESIGN SPECIFICATIONS

Available components

- HYDRO-01
- METHA-01
- ETHAN-01
- ETHYL-01
- ISOBU-01
- N-BUT-01
- ISOBU-02
- 1-BUT-01
- CIS-2-01
- TRANS-01
- 2-MET-01
- N-PEN-01
- N-HEX-01
- CARBO-01
- CARBO-02
- NITRO-01
- OXYGE-01
- HYDRO-02
- WATER

Selected components

- PROPA-01
- PROPY-01

>
>>
<

Choosing components for specifications



Product streams

- 106VAP
- 106BTM

>
>>
<
<<

Choosing streams for specifications

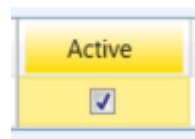
RADFRAC COLUMN – DESIGN SPECIFICATIONS

Vary – selecting adjusted variables in order to meet the specified target values

The screenshot shows a configuration window for a design specification. It includes the following fields and callouts:

- Description:** Vapor flowrate (Callout: User defined description)
- Adjusted variable Type:** Distillate rate (Callout: Adjusted variable type)
- Upper and lower bounds:**
 - Lower bound: 200 kg/hr
 - Upper bound: 5000 kg/hr (Callout: Bounds where the variable will be adjusted)
- Optional:** Maximum step size (empty field)

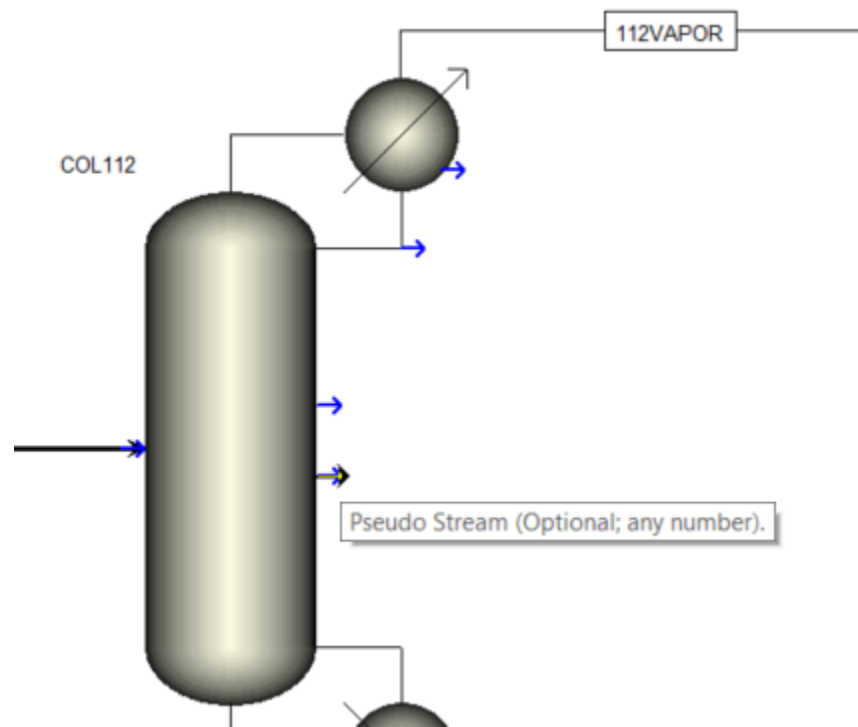
After definition, both design specification and vary have to be set active



RADFRAC COLUMN – PSEUDO STREAMS

Internal streams from column, which are not presented in mass balance but can be used for modeling exercises

Specification of pseudo streams: create a material stream in the simulation flowsheet by choosing the lower blue arrow on the column



RADFRAC COLUMN – PSEUDO STREAMS

Go to streams page inside the column block

Pseudo streams

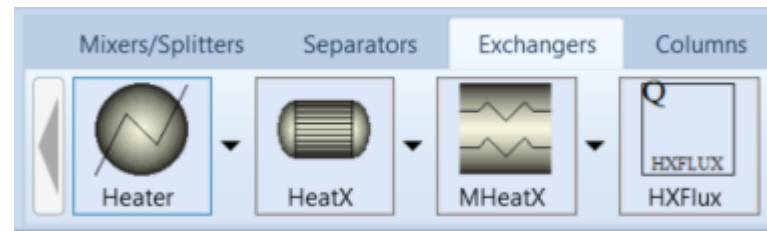
Name	Pseudo Stream Type	Stage	Internal Phase	Reboiler Phase	Reboiler Conditions	Pumparound ID	Pumparound Conditions	Flow	Units
S2	<i>Internal</i>	2	Vapor		Outlet		Outlet		<i>kmol/hr</i>

Liquid from Stage 2 (column's top stage) is specified, so after running simulation we have the column's overhead vapor as a pseudo stream

MODELING COLUMN'S OVERHEAD VAPOR SECTION

Buliding cooler heat exchanger and reflux drum in the column's overhead vapor section

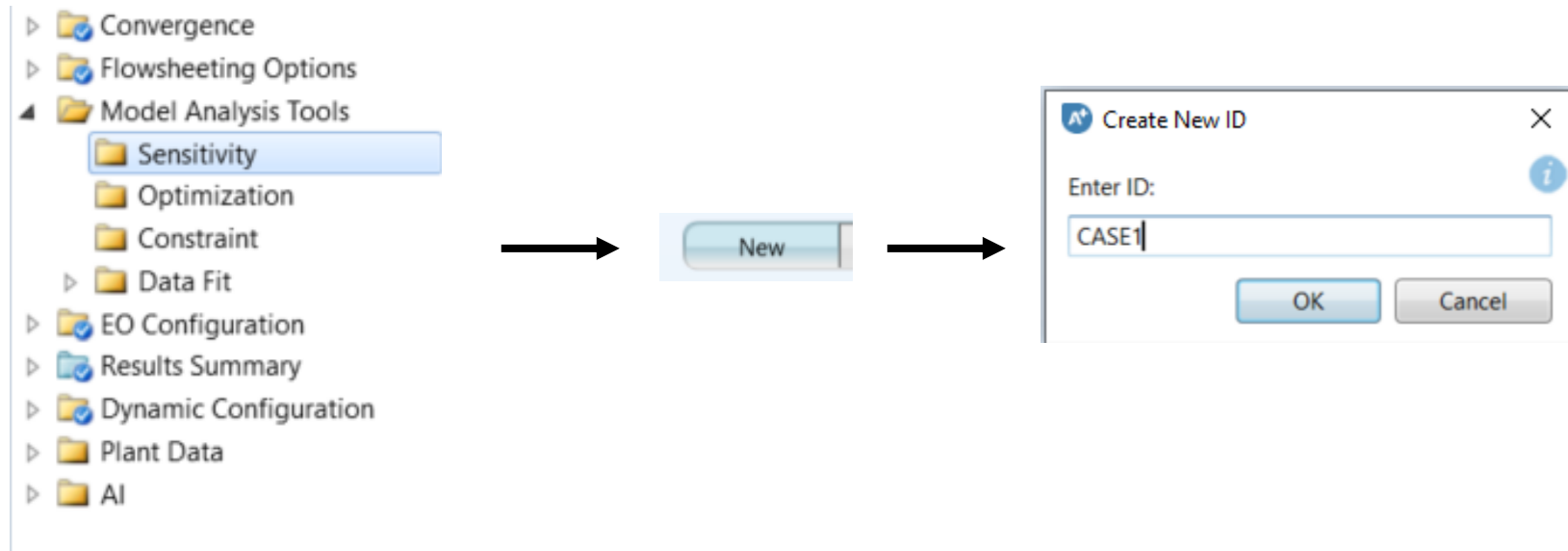
Creating simple heat exchanger for overhead cooling



CASE STUDY

Dependent variable analysis as a function of an independent variable

Case study creation:



CASE STUDY

Definition of independent (manipulated variable) – reflux rate of Column 106

The screenshot displays the Aspen Plus software interface for defining a manipulated variable. The 'Vary' tab is selected, and the 'Active' checkbox is checked. The 'Manipulated variables' section shows a table with one entry:

Variable	Active	Manipulated variable	Units
1	<input checked="" type="checkbox"/>	Block-Var Block=COL106 Variable=STDVOL-L1 Sent...	cum/hr

Below the table are buttons for 'New', 'Delete', 'Copy', 'Paste', and 'Send to Aspen Multi-Case'. The 'Edit selected variable' section is expanded, showing the following details:

Manipulated variable

- Variable: 1
- Type: Block-Var
- Block: COL106
- Variable: STDVOL-L1
- Sentence: COL-SPECS
- Units: cum/hr

Manipulated variable limits

- Equidistant (selected), Logarithmic, List of values
- Start point: 2 cum/hr
- End point: 30 cum/hr
- Number of points: 29
- Increment (selected): 1 cum/hr

Report labels are also visible at the bottom of the 'Edit selected variable' section.

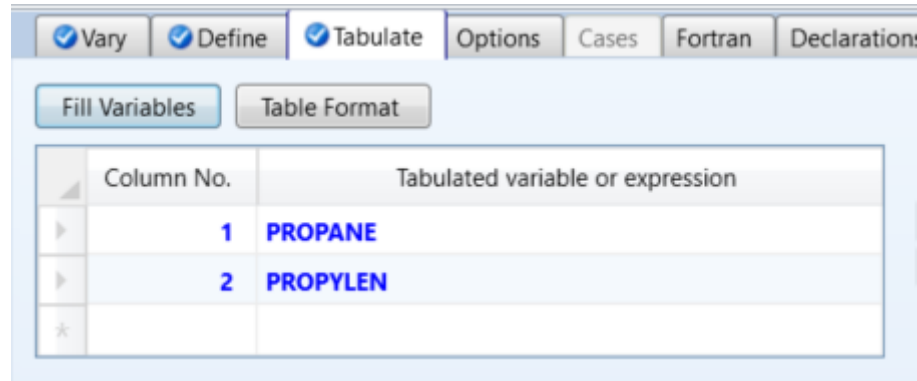
CASE STUDY

Definition of dependent variable– ethane mass fraction of Column 106 bottom

Software interface showing the definition of a dependent variable. The interface includes tabs for Vary, Define, Tabulate, Options, Cases, Fortran, Declarations, and Comments. The 'Define' tab is active, showing a list of sampled variables. The variable 'PROPANE' is defined as 'Mass-Frac Stream=106OH Substream=MIXED Component=PROPA-01'. Below the list are buttons for New, Delete, Copy, Paste, Move Up, Move Down, and View Variables. The 'Edit selected variable' section shows the variable 'PROPANE' selected, with a Reference section containing dropdowns for Type (Mass-Frac), Stream (106OH), Substream (MIXED), and Component (PROPA-01). A Category section has radio buttons for All, Blocks, Streams, Model Utility, Property Parameters, and Reactions, with Streams selected.

CASE STUDY

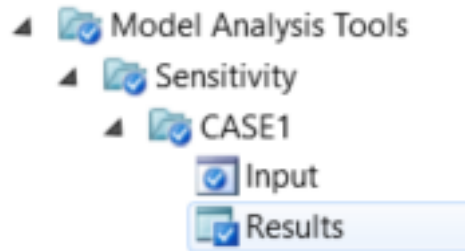
Tabulate – fill variables



Before running case study, make sure that RadFrac column's design specifications can be satisfied

CASE STUDY RESULTS

Checking case study results after running simulation



Row/Case	Status	Description	VARY 1 COL106 COL-SPEC STDVOL-L 1 CUM/HR	PROPANE
1	OK		2	0,530119
2	OK		3	0,56887
3	OK		4	0,617286
4	OK		5	0,673925
5	OK		6	0,734207
6	OK		7	0,788689
7	OK		8	0,822182
8	OK		9	0,836873
9	OK		10	0,844289
10	OK		11	0,848974
11	OK		12	0,852387
12	OK		13	0,855083
13	OK		14	0,857314
14	OK		15	0,859216
15	OK		16	0,860869
16	OK		17	0,862327
17	OK		18	0,863627
18	OK		19	0,864796

CASE STUDY RESULTS

Case study plots



CASE1 - Results Summary

