

# UniSim Design



- steady state modelling -

BME Kémiai és Környezeti Folyamatmérnöki Tanszék  
Dr. Mizsey Péter, Dr. Benkő Tamás, Dr. Mészéna Zsolt

# Áttekintés

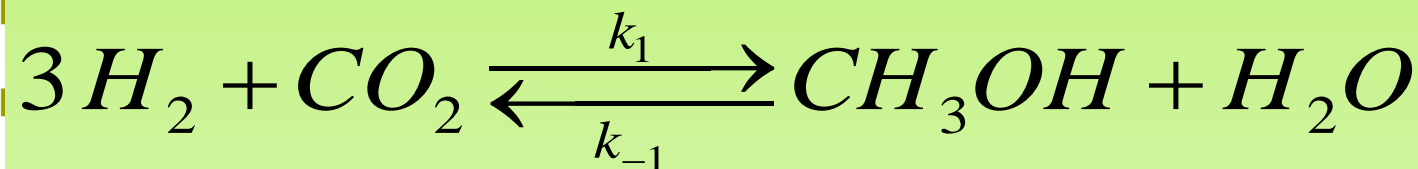
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- A metanol gyártó folyamat bemutatása.
- A folyamat modellezése – instruktorkor segítségével.

# Metanol gyártás

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- Egyszerűsített folyamat



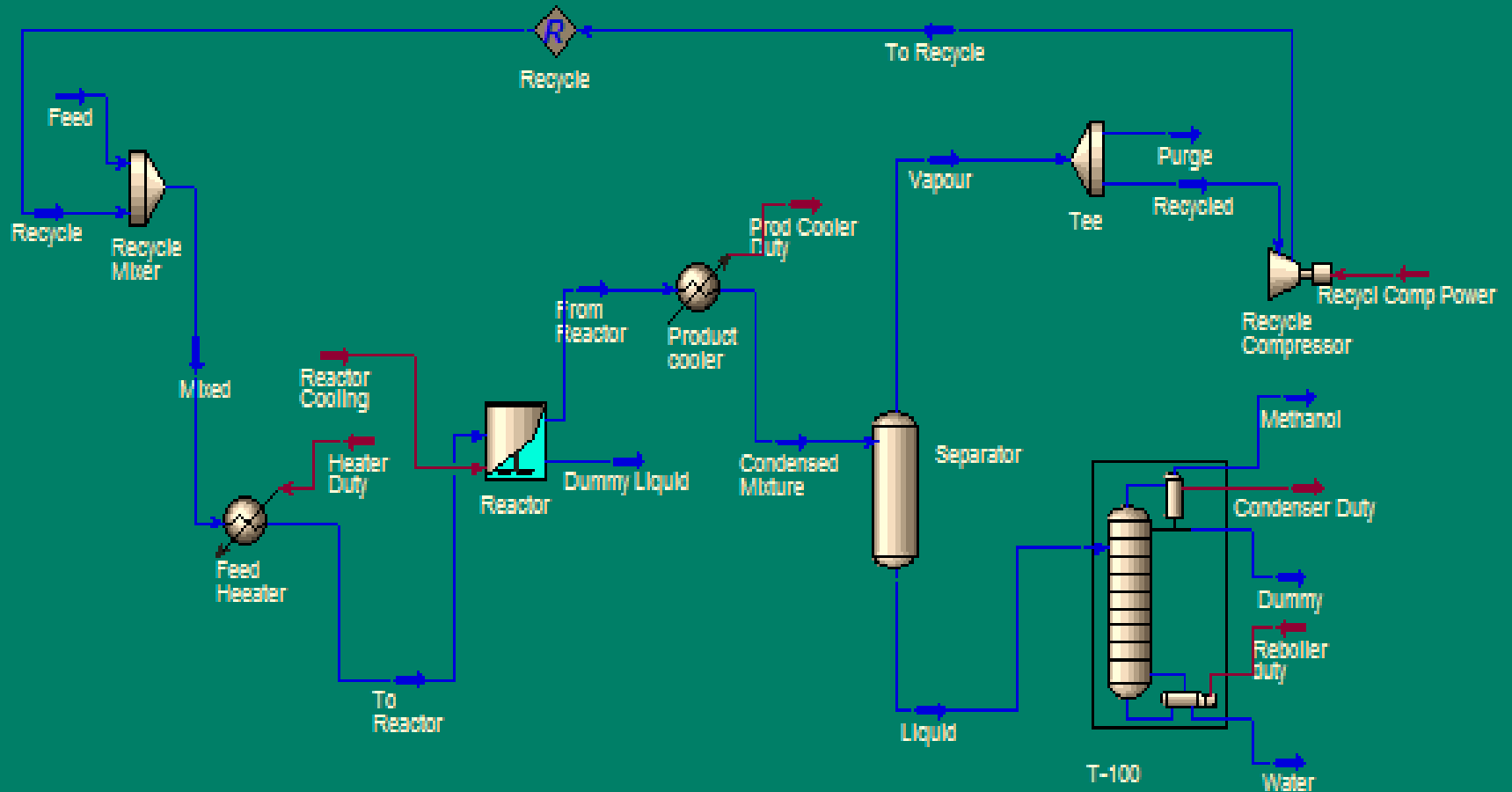
$$r_i = k_i \cdot c_1^a \cdot c_2^b$$

$$k_i = A \cdot \exp\left(-\frac{E}{RT}\right)$$

$$A = 1.04 \cdot 10^{22} \quad E = 1.7 \cdot 10^5 \text{ kJ / kmol}$$

$$A' = 2.6 \cdot 10^{28} \quad E' = 2.2 \cdot 10^5 \text{ kJ / kmol}$$

# Folyamatábra

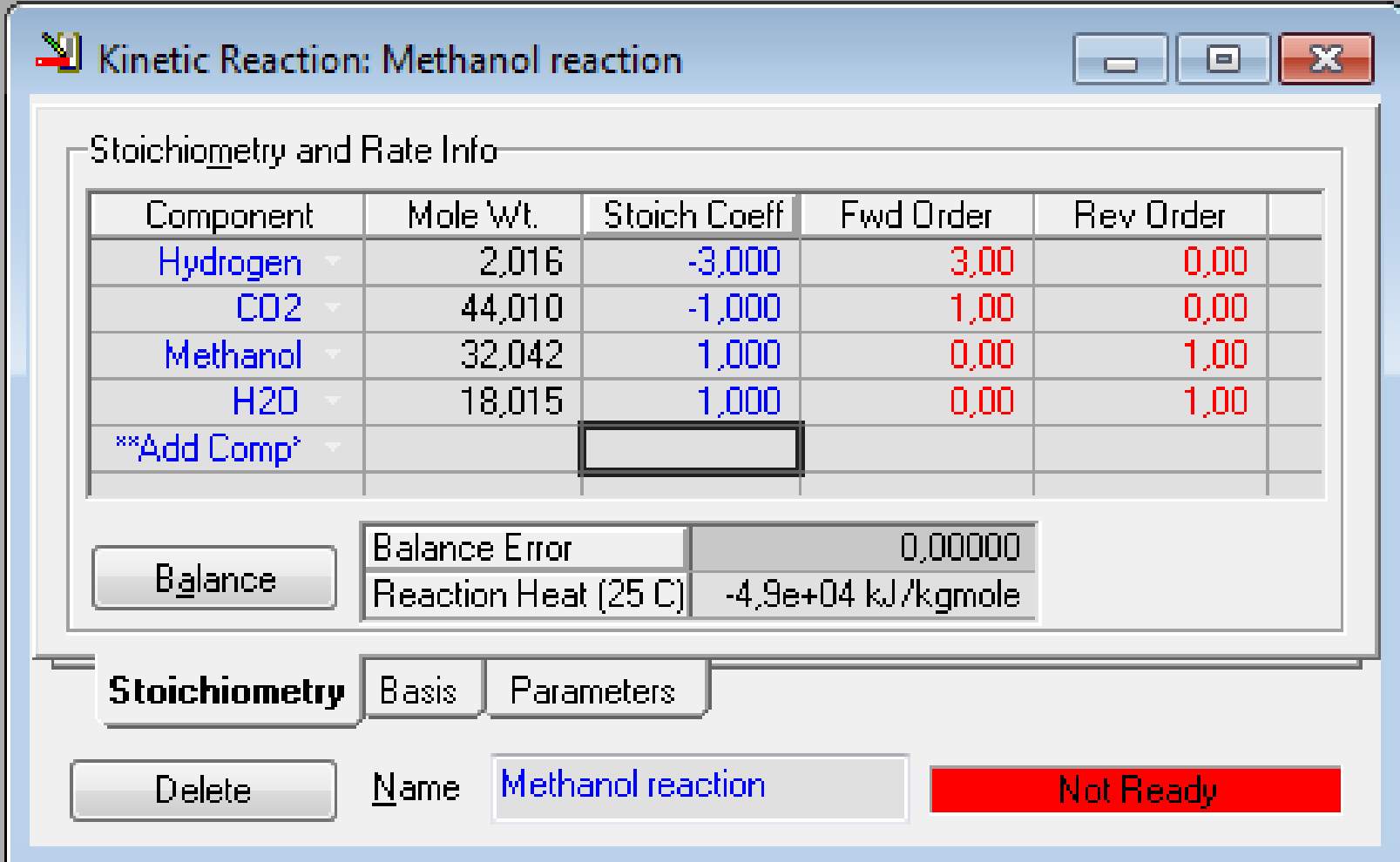


# Units, Thermodynamics

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- SI mértékegységrendszer
- Komponensek: MeOH, víz, CO<sub>2</sub>, H<sub>2</sub>
- Modell: UNIQUAC
- Reakció-kinetikai adatok bevitele
  - Simul. Basis manager: Reactions tab
  - Új reakció: Add Rxn (Kinetic)

# Reaction kinetics

A software window titled "Kinetic Reaction: Methanol reaction" with standard window controls (minimize, maximize, close). The window contains a table for "Stoichiometry and Rate Info" with columns for Component, Mole Wt., Stoich Coeff, Fwd Order, and Rev Order. Below the table are fields for Balance Error (0,00000) and Reaction Heat (25 C) (-4,9e+04 kJ/kgmole). At the bottom, there are tabs for "Stoichiometry", "Basis", and "Parameters", a "Delete" button, a "Name" field containing "Methanol reaction", and a red "Not Ready" status indicator.

**Kinetic Reaction: Methanol reaction**

Stoichiometry and Rate Info

Component	Mole Wt.	Stoich Coeff	Fwd Order	Rev Order
Hydrogen	2,016	-3,000	3,00	0,00
CO2	44,010	-1,000	1,00	0,00
Methanol	32,042	1,000	0,00	1,00
H2O	18,015	1,000	0,00	1,00
**Add Comp*				

Balance Error: 0,00000  
Reaction Heat (25 C): -4,9e+04 kJ/kgmole

**Stoichiometry** | Basis | Parameters

Delete | Name: Methanol reaction | **Not Ready**

# Reaction kinetics

Kinetic Reaction: Methanol reaction

Basis	
Basis	Molar Concn
Base Component	CO2
Rxn Phase	VapourPhase
Min. Temperature	-273,1 C
Max Temperature	3000 C

Basis Units: kgmole/m3

Rate Units: kgmole/m3-h

Stoichiometry **Basis** Parameters

Delete Name: Methanol reaction

Not Ready

Three green arrows point to the 'Base Component', 'Rxn Phase', and 'Rate Units' fields.

# Reaction kinetics

**Kinetic Reaction: Methanol reaction**

**Forward Reaction**

A	1,0400e+022
E	1,7000e+005
$\beta$	<empty>

**Reverse Reaction**

A'	2,6000e+028
E'	2,2e5
$\beta'$	<empty>

kJ/kqmole

**Equation Help**

$$r = k \cdot f(\text{Basis}) - k' \cdot f'(\text{Basis})$$
$$k = A \cdot \exp \{ -E / RT \} \cdot T^{\beta}$$
$$k' = A' \cdot \exp \{ -E' / RT \} \cdot T^{\beta'}$$

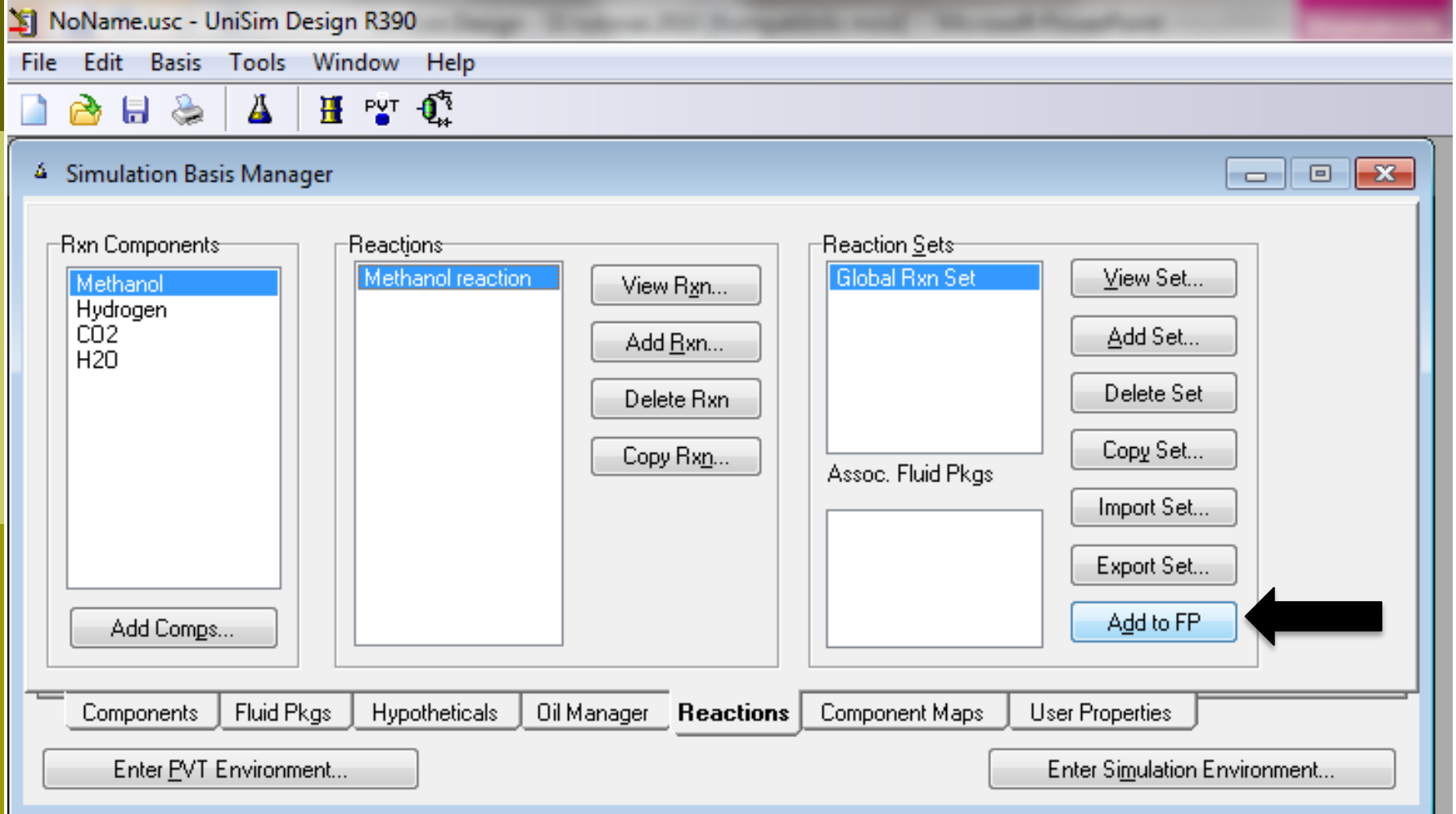
T in Kelvin

Stoichiometry   Basis   **Parameters**

Delete   Name   Methanol reaction   **Not Ready**



# Reaction kinetics



# Feed

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## □ Conditionss

- Stream name: Feed
- Temperature: 40°C
- Pressure: 4000 kPa
- Mass flow: 1000 kg/h

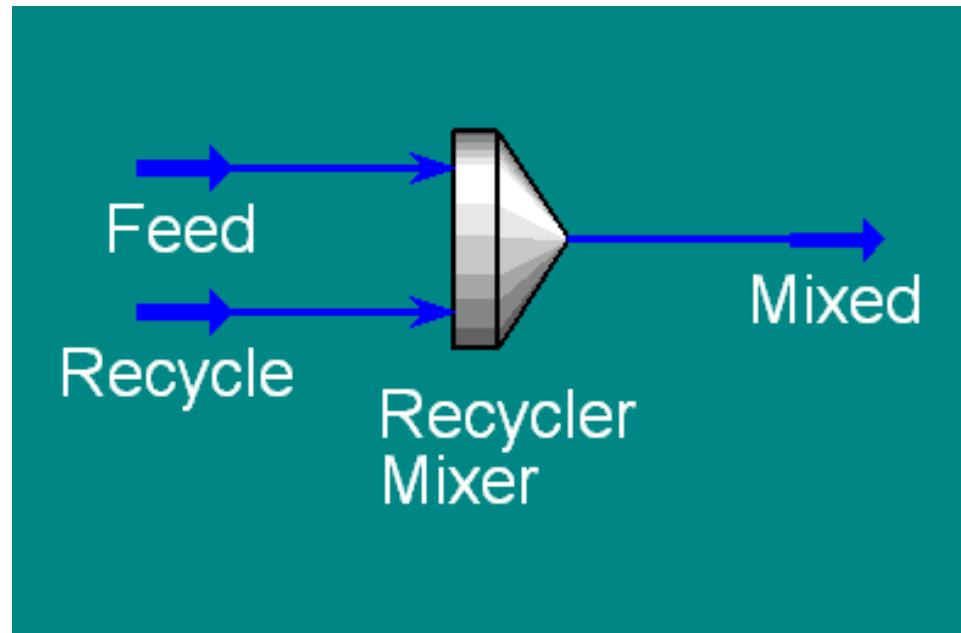
## □ Composition

- CO<sub>2</sub> = 0.25 n/n
- H<sub>2</sub> = 0.75

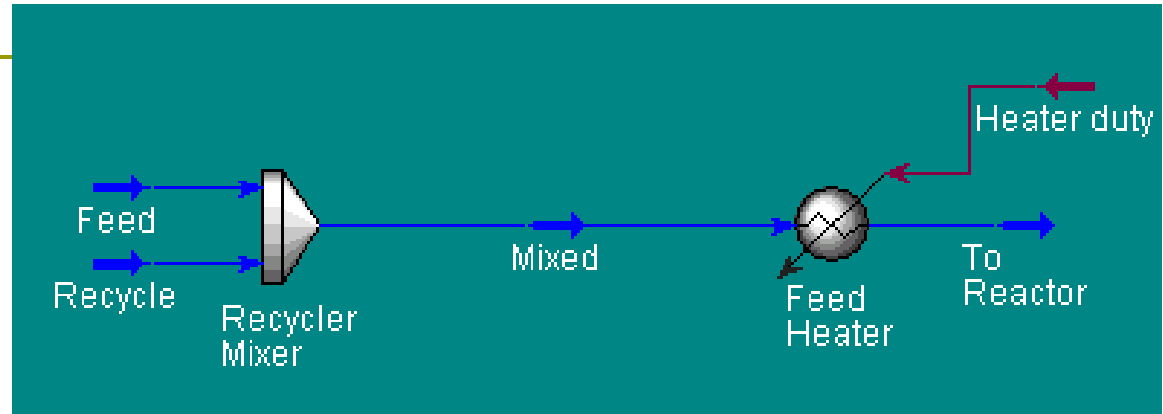
# Recycle Mixer

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- In: „Feed“, „Recycle“
- Out: „Mixed“
  - „Recycle“: T&p mint Feed, Molar flow: 200 kmol/h
  - CO<sub>2</sub>:0.1 n/n, H<sub>2</sub>:0.9 n/n



# Feed Heater



- Name: „Feed Heater“
- Inlet: „Mixed“
- Energy: „Heater duty“
- Outlet: „To Reactor“
  - Parameters - Pressure drop: 50 kPa
  - Worksheet - Output temp.: 200 °C

# Reactor

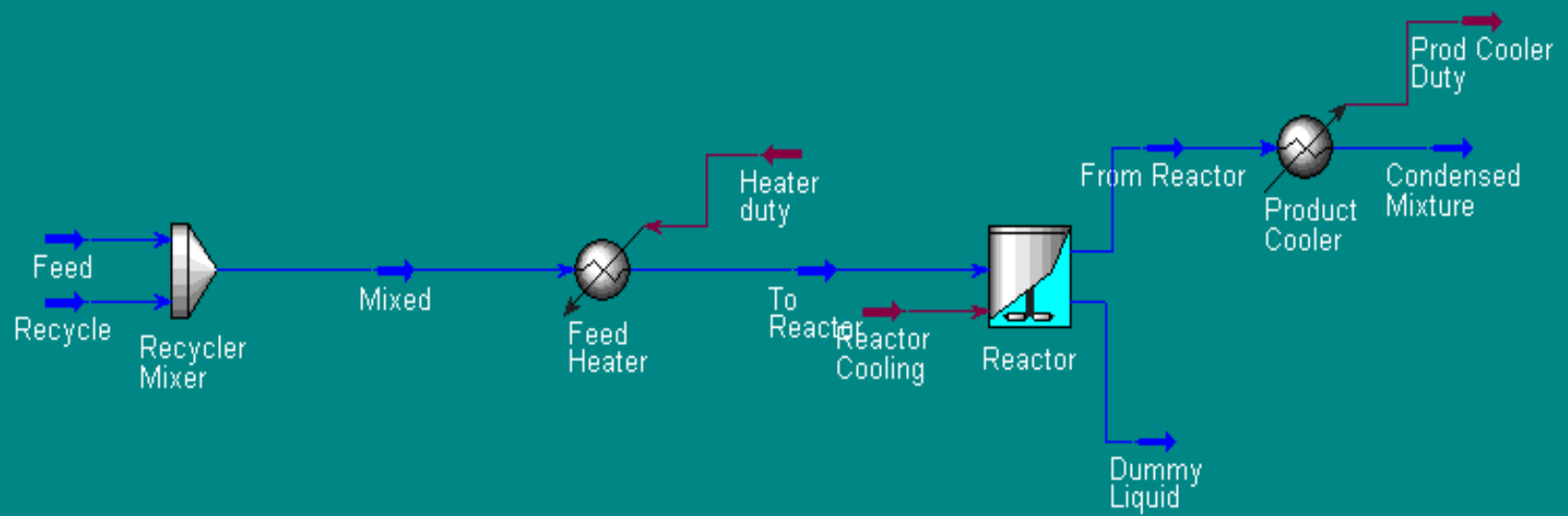
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- CSTR modell
- Inlets: To Reactor
- Vapour Outlet: From Reactor
  - $T = 200^{\circ}\text{C}$
- Liquid outlets: Dummy Liquid
- Energy: Reactor Cooling
  
- Nyomáskeresés: 100 kPa
- Geom. adatok:
  - átmérő: 10 m
  - magasság: 10 m
- Reakció kiválasztása

# Product cooler

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- Termékáram H<sub>2</sub> és CO<sub>2</sub> tartalmának recirkulációja = metanol leválasztása a gőzfázisból ← hűtés 40°C-ra
- In: From Reactor
- Out: Condensed Mixture
- Energy: Prod Cooler Duty
- Nyomásesés: 50 kPa



# Reaktorméretezés

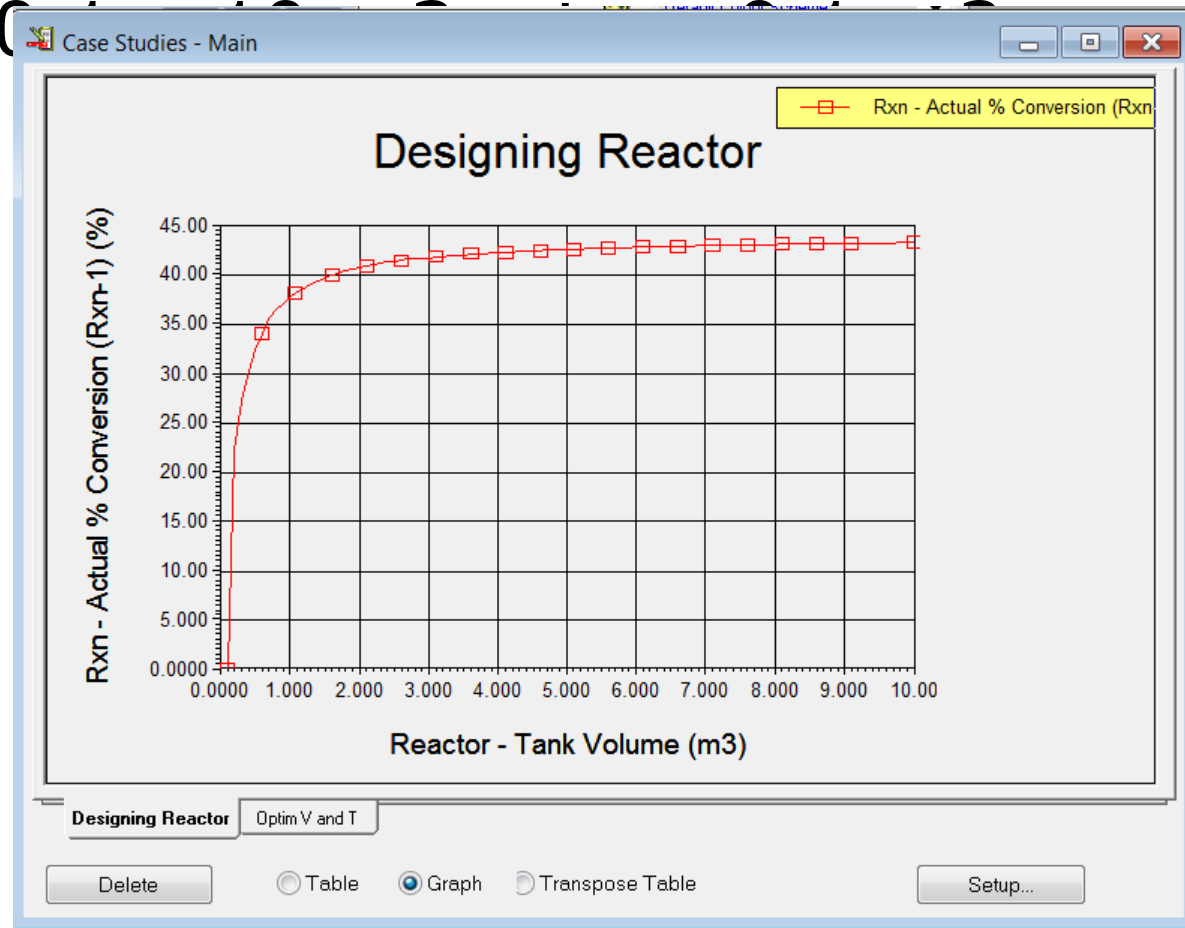
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- Korábban indokolatlanul nagy reaktort terveztünk. ( $V = 10 \text{ m}^3$ )
- Tool/Databook
- Insert variables:
  - Reactor/Tank Volume
  - Reactor/Rxn-Actual % conversion
- Case Studies – Add : „Designing reactor”
  - Ind: Tank Volume
  - Dep: Conversion



# Reaktorméretezés

- View..
- Tank volume (C)
- Start.
- Results..
  - $V \approx 3 \text{ m}^3$



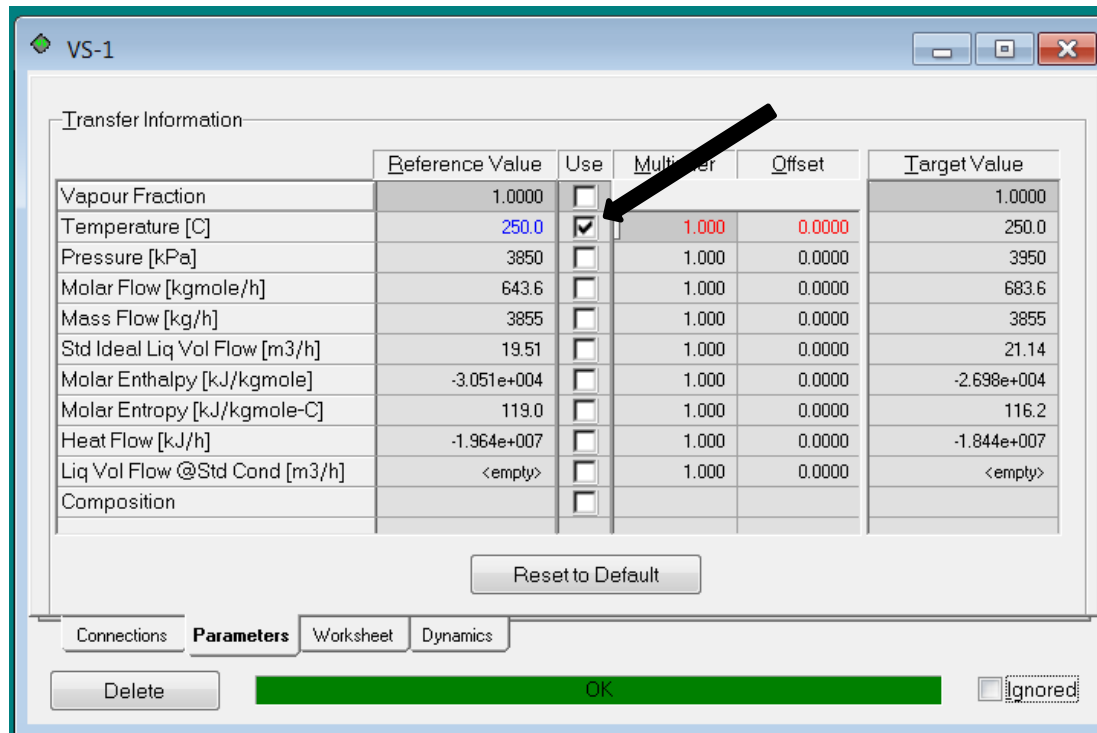
# Optimális hőmérséklet + térfogat

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- A kétváltozós optimum keresés problémás feladat
  - A lépések sorrendje nem mindegy (solver leállítása is szükséges)
- Első lépés: mentés! 😊
- A reaktor belépő és kilépő áramának összekapcsolása: *Virtual stream*

# Virtual stream

## □ Először: Parameters tab!



VS-1

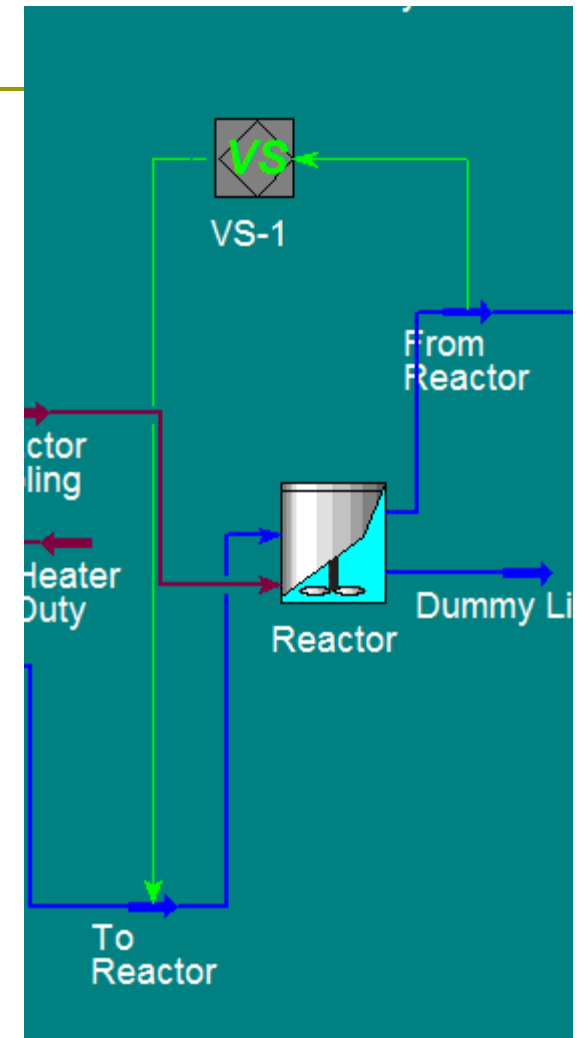
Transfer Information

	Reference Value	Use	Multiplier	Offset	Target Value
Vapour Fraction	1.0000	<input type="checkbox"/>			1.0000
Temperature [C]	250.0	<input checked="" type="checkbox"/>	1.000	0.0000	250.0
Pressure [kPa]	3850	<input type="checkbox"/>	1.000	0.0000	3950
Molar Flow [kgmole/h]	643.6	<input type="checkbox"/>	1.000	0.0000	683.6
Mass Flow [kg/h]	3855	<input type="checkbox"/>	1.000	0.0000	3855
Std Ideal Liq Vol Flow [m3/h]	19.51	<input type="checkbox"/>	1.000	0.0000	21.14
Molar Enthalpy [kJ/kgmole]	-3.051e+004	<input type="checkbox"/>	1.000	0.0000	-2.698e+004
Molar Entropy [kJ/kgmole-C]	119.0	<input type="checkbox"/>	1.000	0.0000	116.2
Heat Flow [kJ/h]	-1.964e+007	<input type="checkbox"/>	1.000	0.0000	-1.844e+007
Liq Vol Flow @Std Cond [m3/h]	<empty>	<input type="checkbox"/>	1.000	0.0000	<empty>
Composition		<input type="checkbox"/>			

Reset to Default

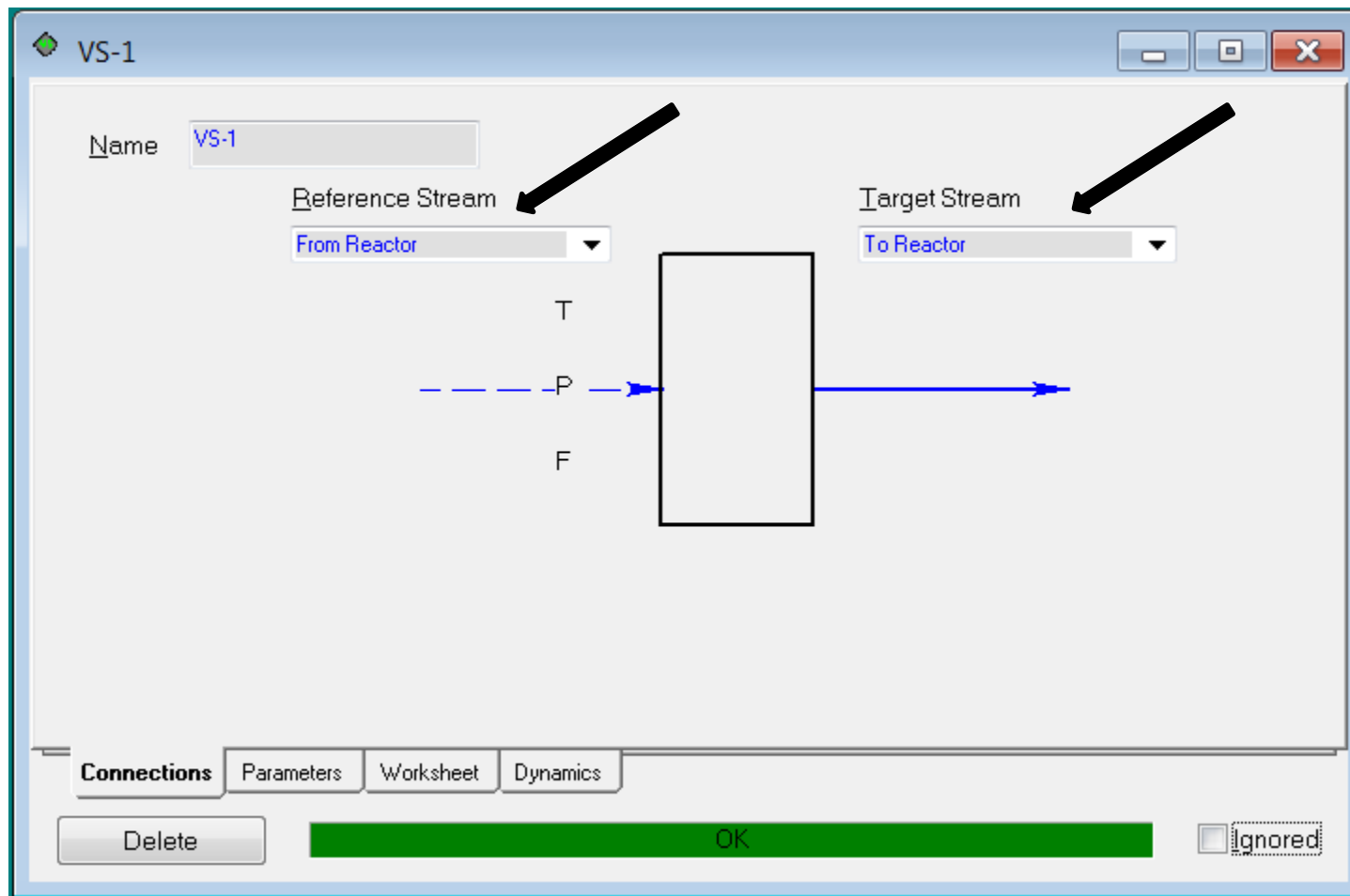
Connections Parameters Worksheet Dynamics

Delete OK Ignored



# Virtual stream

- Második lépésben: áramok megjelölése



# Case study 2

The screenshot shows the DataBook software interface. The window title is "DataBook". It is divided into several sections:

- Available Case Studies:** A list box contains "Designing Reactor" and "Reactor Temp+Vol" (which is selected). To the right are buttons for "Add", "Delete", and "View...".
- Available Displays:** Three radio buttons are present: "Table", "Transpose Table", and "Graph" (which is selected). A "Results..." button is located to the right.
- Case Studies Data Selection:** A text box labeled "Current Case Study" contains "Reactor Temp+Vol". Below it is a table with columns "Object", "Variable", "Ind", and "Dep".

Object	Variable	Ind	Dep
From Reactor	Temperature	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Reactor	Tank Volume	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Reactor	Rxn - Actual % Conversion (Rxn-1)	<input type="checkbox"/>	<input checked="" type="checkbox"/>

At the bottom of the window, there is a tabbed interface with the following tabs: "Variables", "Process Data Tables", "Strip Charts", "Data Recorder", "Case Studies" (which is the active tab), and "Spec Scenarios".

# Case study 2

- Hőmérséklet: 150 – 250°C, lépésköz: 10°C
- Térfogat: 5 – 50 m<sup>3</sup>, lépésköz 5 m<sup>3</sup>

Case Studies Setup - Main

Case Studies

- Designing Reactor
- Optim V and T

Optim V and T

Number of States: 110

State Input Type: Nested

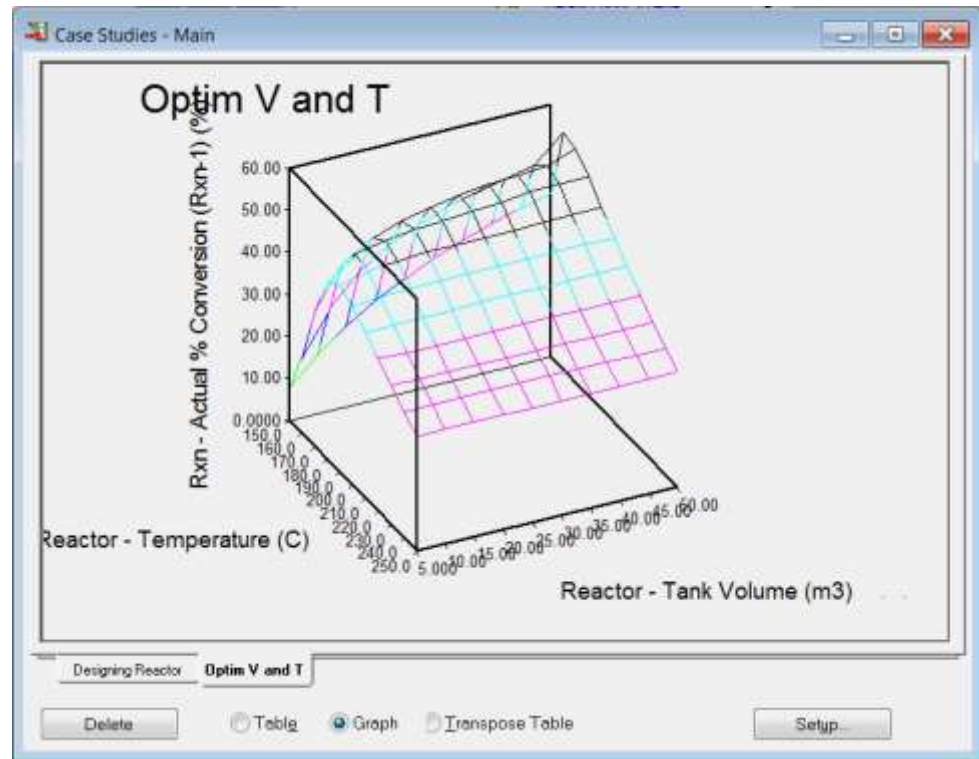
Step Downward

Variable	Low Bound	High Bound	Step Size	Use Log Step	No. of Points
Reactor - Tank Volume	5.000 m3	50.00 m3	5.000 m3	<input type="checkbox"/>	10
From Reactor - Temperature	150.0 C	250.0 C	10.00 C	<input type="checkbox"/>	11

Independent Variables Setup | Display Properties | Failed States

Add | Delete | Results... | Start

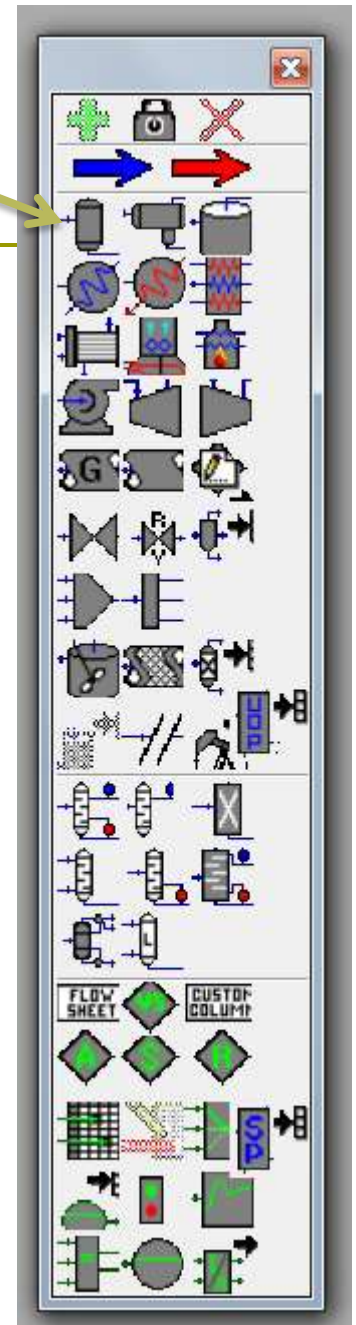
# Case study 2 - eredmények



- Optimális hőmérséklet:  $\sim 190^{\circ}\text{C}$
- Optimális térfogat:  $\sim 5 \text{ m}^3$

# Separator

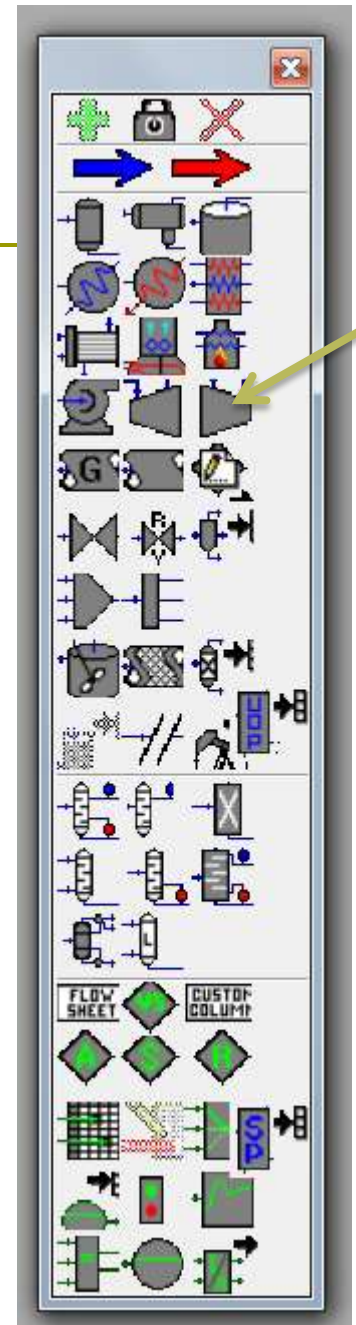
- A „condensed mixture” áram kétfázisú, a két fázist el kell választani: szeparátor
- In: Condensed Mixture
- Out: Vapour, Liquid





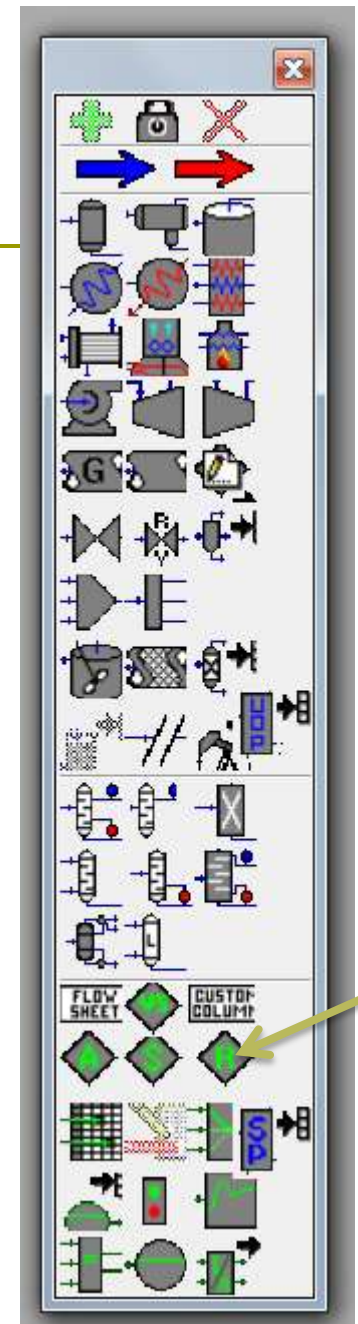
# Recycle Compressor

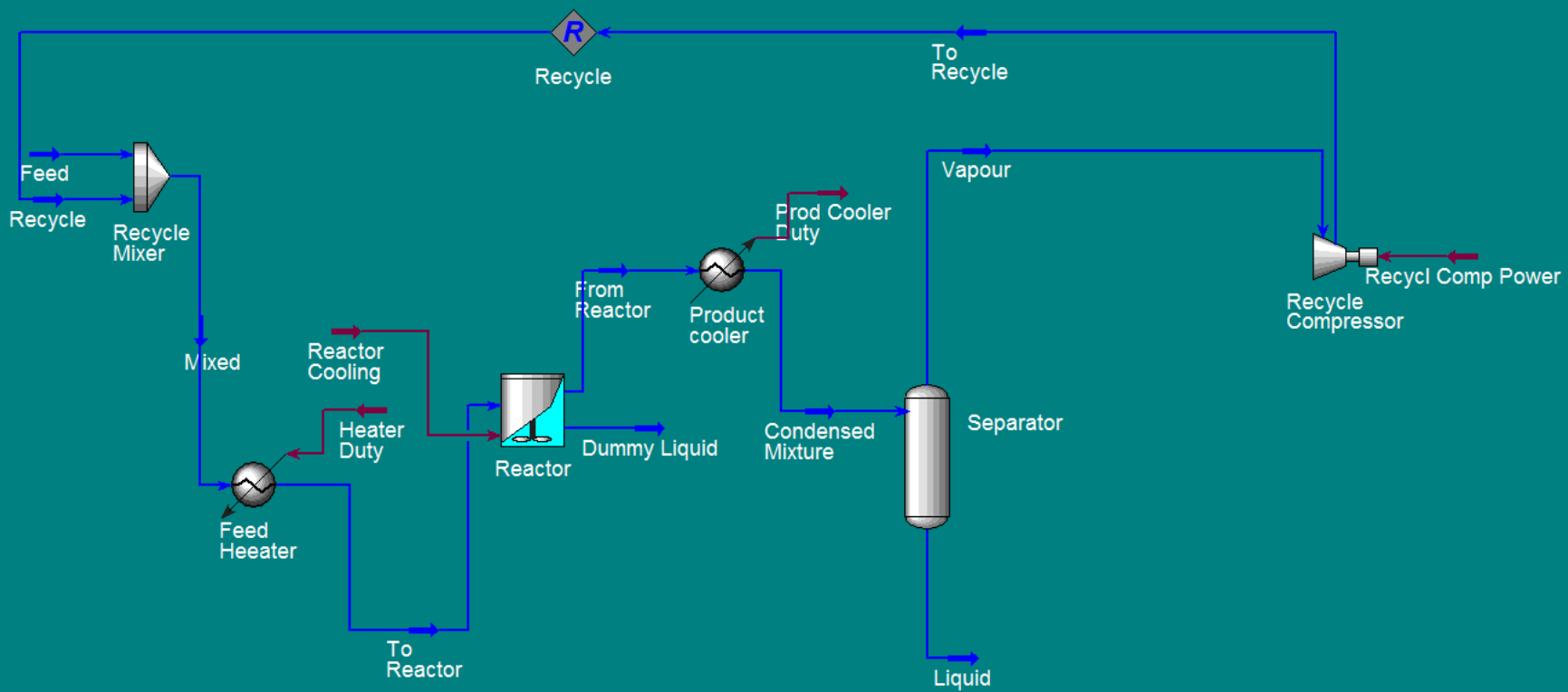
- A visszavezetendő áram nyomása alacsonyabb, mint a „Feed” áramé: komprimálás szükséges
- In: Vapour
- Out: To Recycle ( $p=4000$  kPa)
- Energy: Recycl Comp Power
- Adiabatic Efficiency: 75%



# Recycle

- A recirkuláció bekötése – modellezés közben- gyakran okoz instabilitást: mentés.
- In: To Recycle
- Out: Recycle





# Főtermék tisztítása: desztilláció

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- „Liquid” áram metanol mellet vizet is tartalmaz
- Tisztasági követelmények:
  - a kolonnába lépő MeOH 97% kerüljön a végtermékbe
  - a végtermék víztartalma max. 1 m/m%.

# Főtermék tisztítása: desztilláció (2)

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- In: Liquid
- N: 10
- Betáp. helye: 5
- Kond. típusa: parciális
- Kond. Hőáram: Condenser duty
- Out: Methanol, Dummy
- Visszaforraló: Reboiler duty
- Out: Water

# Distillation – pressure profile

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- Kondenzátor: 1000 kPa
- Visszaforraló: 1015 kPa

# Distillation – specifications

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- Vapour rate: 20 kmol/hr
- Liquid rate: 0 kmol/hr
- Reflux ratio: 3

# Distillation – specifications

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- Állítsuk be a terméktisztasági követelményeket:
  - **Column Component Recovery**,  
Methanol@COL1,  
Spec value 0.97, Methanol
  - **Column Component Fraction**,  
Methanol@COL1,  
Mass fraction, Spec value: 1e-2, H2O
  - Inaktiváljuk a következő specifikációkat:
    - Ovhd Vap Rate
    - Reflux Ratio
  - Run.



# Distillation

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- Tekintsük át az eredményeket.
  - Milyen töménységű a metanol áram?
  - Mi a halmazállapota?
  - Mennyi metanol megy el a fenékben?
    - kg/h-ban
    - a belépő metanolhoz képest (D/F arány)
- Hogyan lehetne töményebb metanolt kinyerni ebből az oszlopból?

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□ Köszönöm a figyelmet