



UNIVERSIDADE FEDERAL DO RIO DE JANEIRO  
ESCOLA DE QUÍMICA



## EQE776 Modelagem e Simulação de Processos

### Aula 07. Modelo customizado de separador por membrana em Aspen Plus

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# Recapitulando

- Craqueamento a vapor do etano em DWSIM

# Temas da aula

- Modelo customizado de separador por membrana em Aspen Plus

# Apresentação do problema

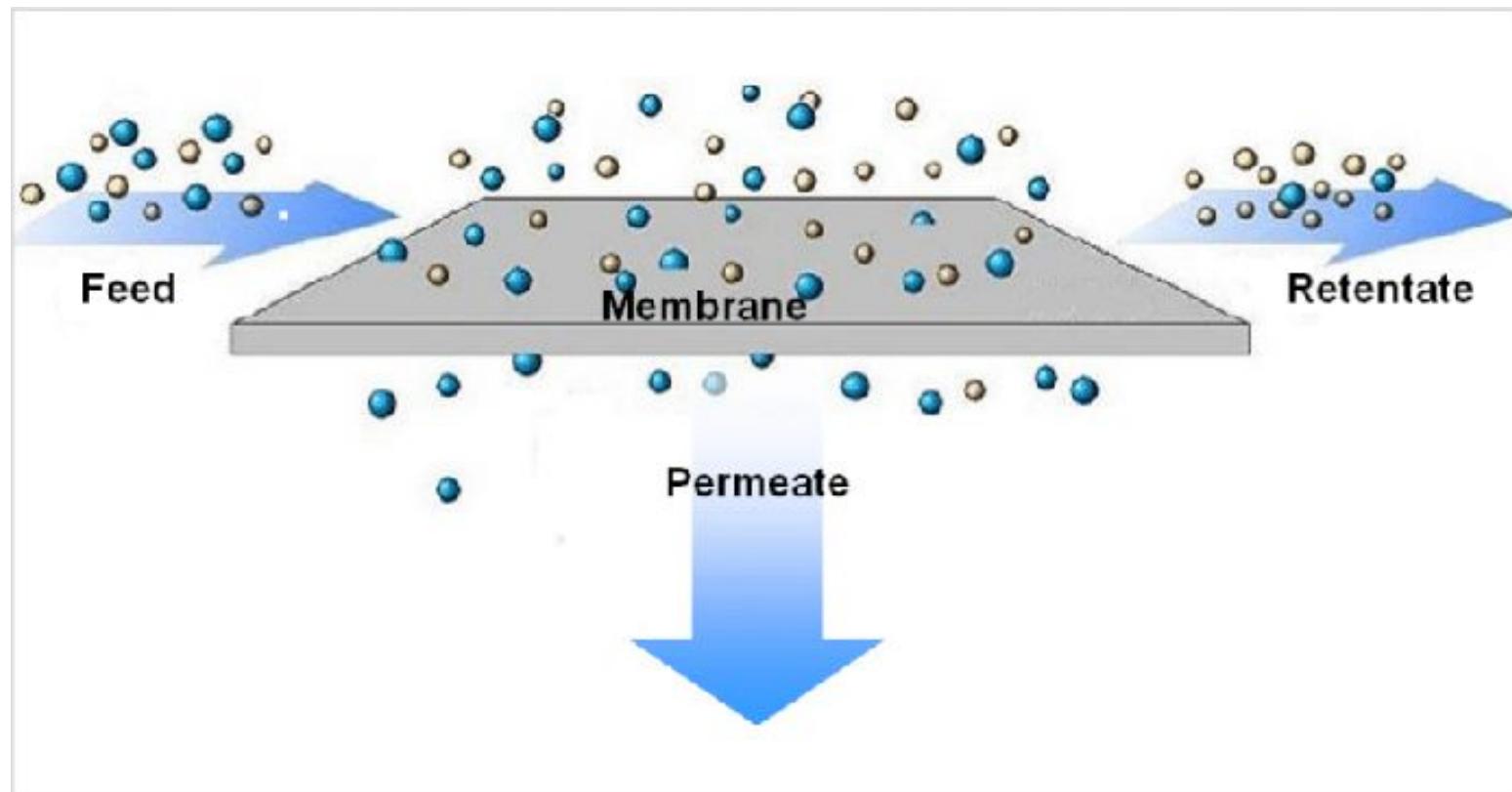
Sistemas de separação por membranas são amplamente utilizados para a remoção de  $\text{CO}_2$  e  $\text{H}_2\text{S}$  do gás natural.

Simuladores mais comuns não apresentam módulo de separador por membranas.

Neste exemplo será criado um modelo simplificado de separador por membrana utilizando o “Aspen Custom Modeler”, de forma tal que possa ser integrado em simulações de Aspen Plus.

# Apresentação do problema

Esquema simplificado do separador por membrana



# Apresentação do problema

## Condições da corrente de alimentação:

- Temperatura: 323 K
- Pressão:  $5 \times 10^5$  Pa
- Vazão: 100 kmol/s
- Fração molar  $\text{CO}_2$ : 0,20
- Fração molar de  $\text{CH}_4$ : 0,60
- Fração molar de  $\text{C}_2\text{H}_6$ : 0,15
- Fração molar de  $\text{C}_3\text{H}_8$ : 0,05

# Apresentação do problema

## Modelo simplificado:

### Parâmetros:

$L = 3 \times 10^{-3}$  m; espessura da membrana

$A = 10$  m<sup>2</sup>; área útil da membrana

$P_{ratio} = 0,8$ ; razão de pressão (P de Permeado / P de alimentação)

$K_{CO_2} = 4,6 \times 10^{-8}$  kmol.s<sup>-1</sup>.m<sup>-1</sup>.Pa<sup>-1</sup> ; permeabilidade de CO<sub>2</sub>

$K_{CH_4} = 1,8 \times 10^{-8}$  kmol.s<sup>-1</sup>.m<sup>-1</sup>.Pa<sup>-1</sup> ; permeabilidade de CH<sub>4</sub>

$K_{C_2H_6} = 6,1 \times 10^{-9}$  kmol.s<sup>-1</sup>.m<sup>-1</sup>.Pa<sup>-1</sup> ; permeabilidade de C<sub>2</sub>H<sub>6</sub>

$K_{C_3H_8} = 8,2 \times 10^{-10}$  kmol.s<sup>-1</sup>.m<sup>-1</sup>.Pa<sup>-1</sup> ; permeabilidade de C<sub>3</sub>H<sub>8</sub>

# Apresentação do problema

## Modelo simplificado:

### Variáveis:

$J_{CO_2}$ ; kmol.s<sup>-1</sup>.m<sup>-2</sup>; fluxo molar de CO<sub>2</sub> através da membrana

$J_{CH_4}$ ; kmol.s<sup>-1</sup>.m<sup>-2</sup>; fluxo molar de CH<sub>4</sub> através da membrana

$J_{C_2H_6}$ ; kmol.s<sup>-1</sup>.m<sup>-2</sup>; fluxo molar de C<sub>2</sub>H<sub>6</sub> através da membrana

$J_{C_3H_8}$ ; kmol.s<sup>-1</sup>.m<sup>-2</sup>; fluxo molar de C<sub>3</sub>H<sub>8</sub> através da membrana

# Apresentação do problema

## Modelo simplificado:

### Equações:

Permeate.T = Inlet.T;

Retentate.T = Inlet.T;

Permeate.P = P\_ratio\*Inlet.P;

Retentate.P = Inlet.P;

$J_i = K_i * (Inlet.P - Permeate.P) / L;$

$Permeate.F * Permeate.z_i = J_i * A;$

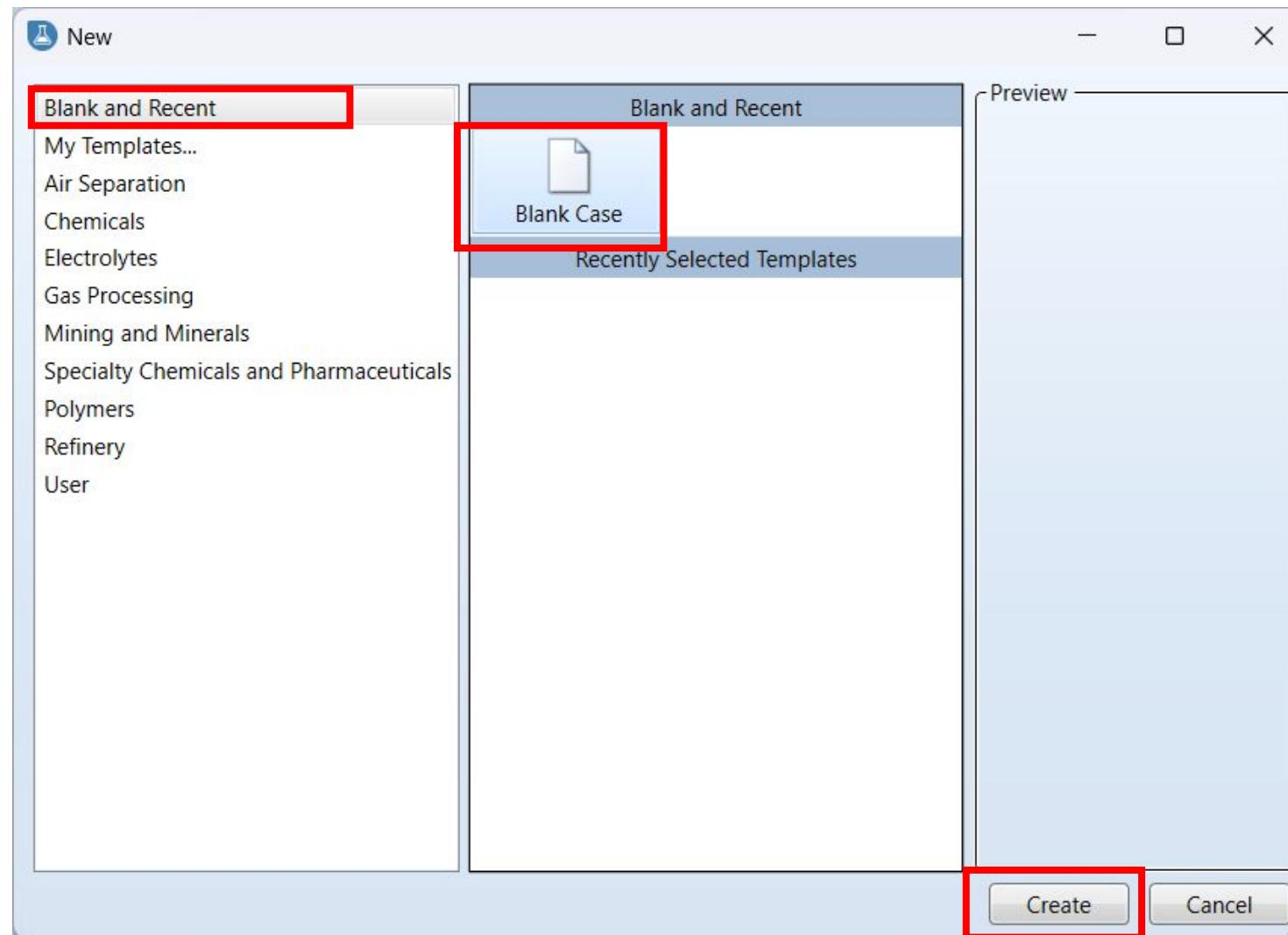
$Inlet.F * Inlet.z_i = Retentate.F * Retentate.z_i + Permeate.F * Permeate.z_i;$

$\text{sum}(Retentate.z_i) = 1;$

$\text{sum}(Permeate.z_i) = 1;$

# Criação do arquivo de propriedades

Criar um novo arquivo de “Aspen Properties”



# Criação do arquivo de propriedades

## Escolher os componentes

The screenshot shows the Aspen Properties V14 software interface with the title bar "Case 1 - Aspen Properties V14 - aspenONE". The menu bar includes File, Home, View, Customize, and Get Started. The toolbar contains various icons for setup, chemistry, methods, analysis, and input. The left sidebar shows a tree view of properties like Components, Methods, and Results. The main window displays the "Components - Specifications" dialog box, which lists four components: CARBO-01 (CO<sub>2</sub>, CAS 124-38-9), METHA-01 (CH<sub>4</sub>, CAS 74-82-8), ETHAN-01 (C<sub>2</sub>H<sub>6</sub>, CAS 74-84-0), and PROPA-01 (C<sub>3</sub>H<sub>8</sub>, CAS 74-98-6). A red box highlights the component list table.

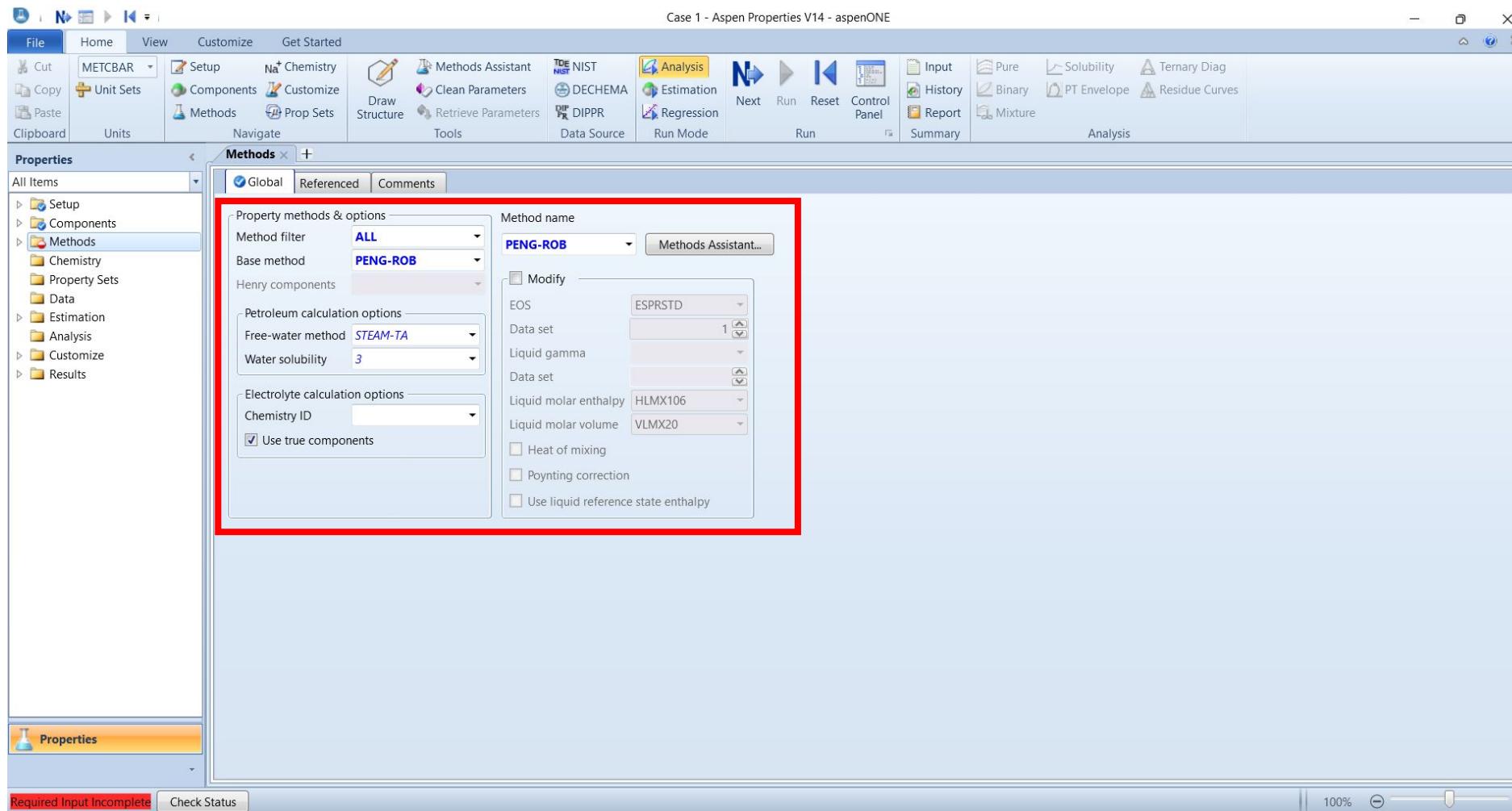
Component ID	Type	Component name	Alias	CAS number
CARBO-01	Conventional	CARBON-DIOXIDE	CO2	124-38-9
METHA-01	Conventional	METHANE	CH4	74-82-8
ETHAN-01	Conventional	ETHANE	C2H6	74-84-0
PROPA-01	Conventional	PROPANE	C3H8	74-98-6

Required Input Incomplete Check Status

11

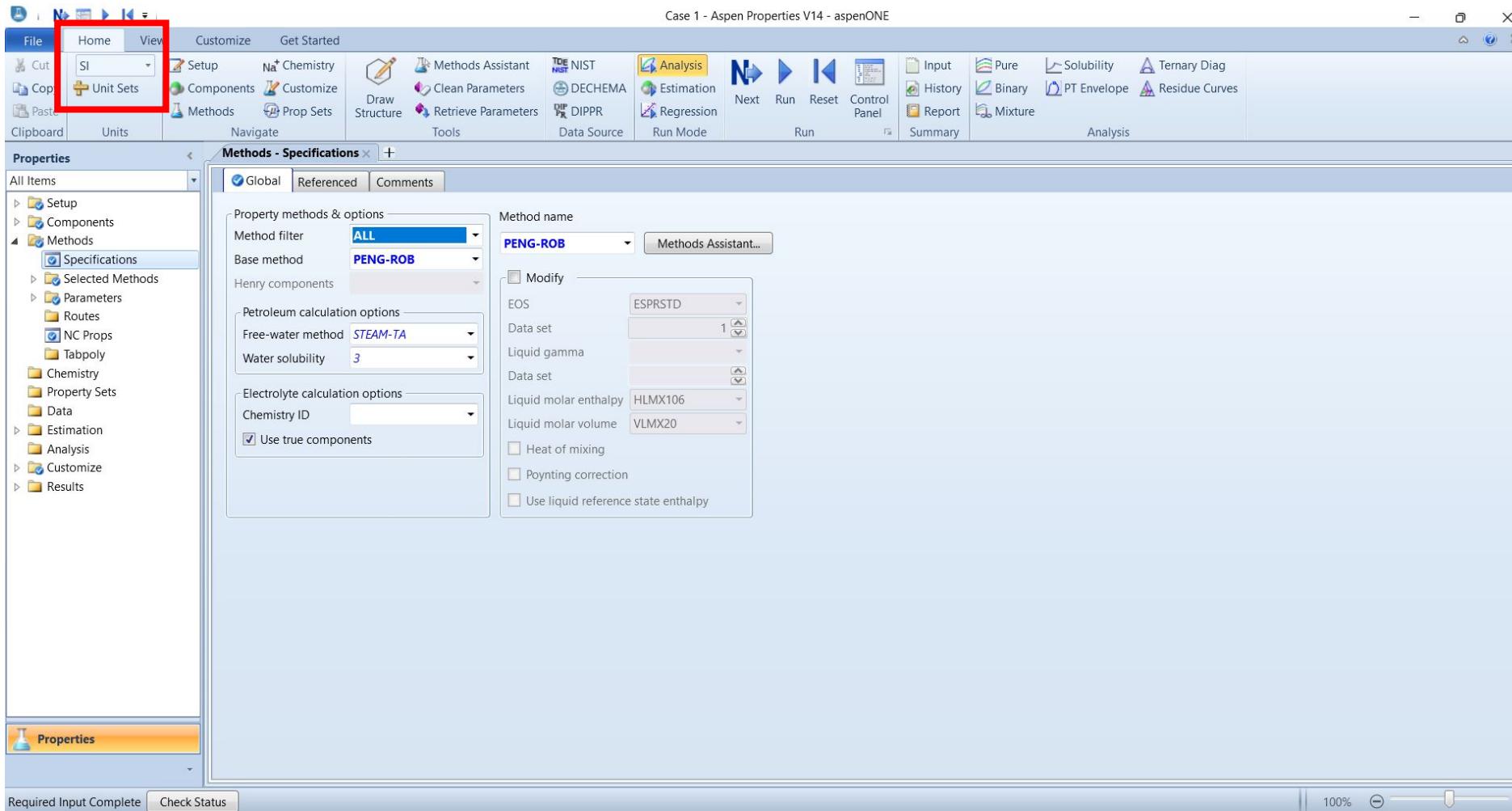
# Criação do arquivo de propriedades

## Escolher o modelo termodinâmico



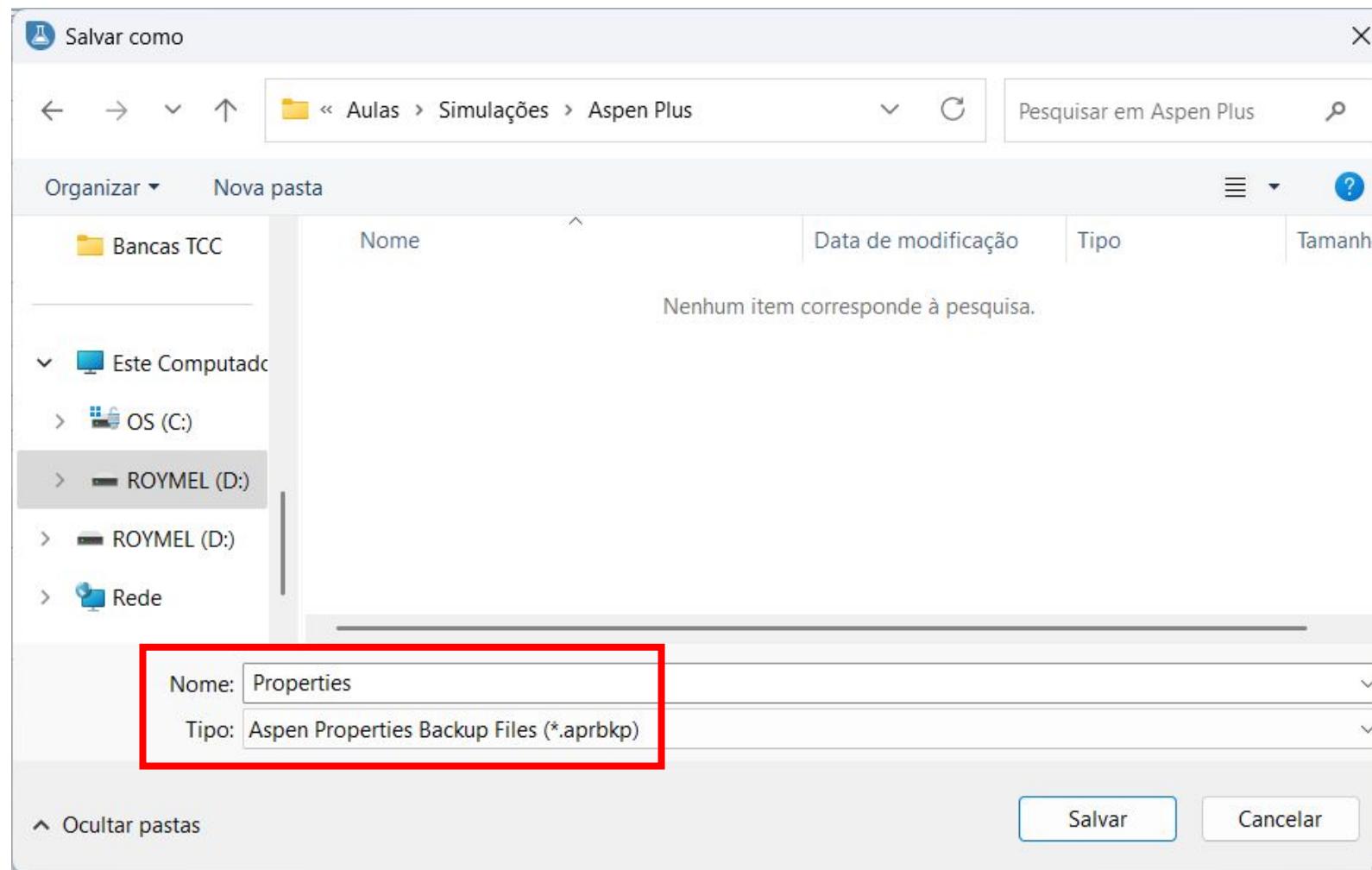
# Criação do arquivo de propriedades

Escolher sistema internacional de unidades



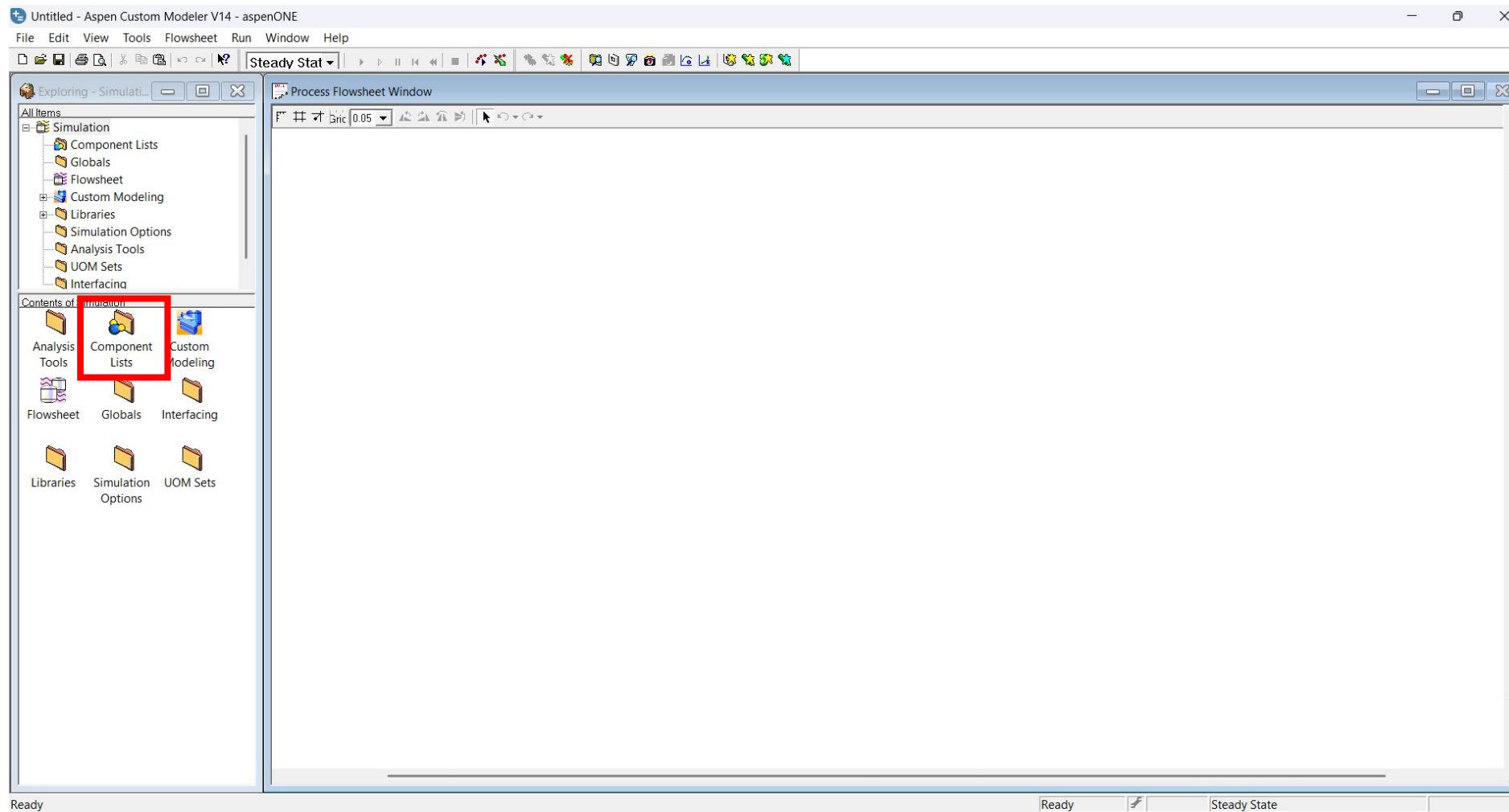
# Criação do arquivo de propriedades

Salvar o arquivo com o formato “\*.aprbkp”



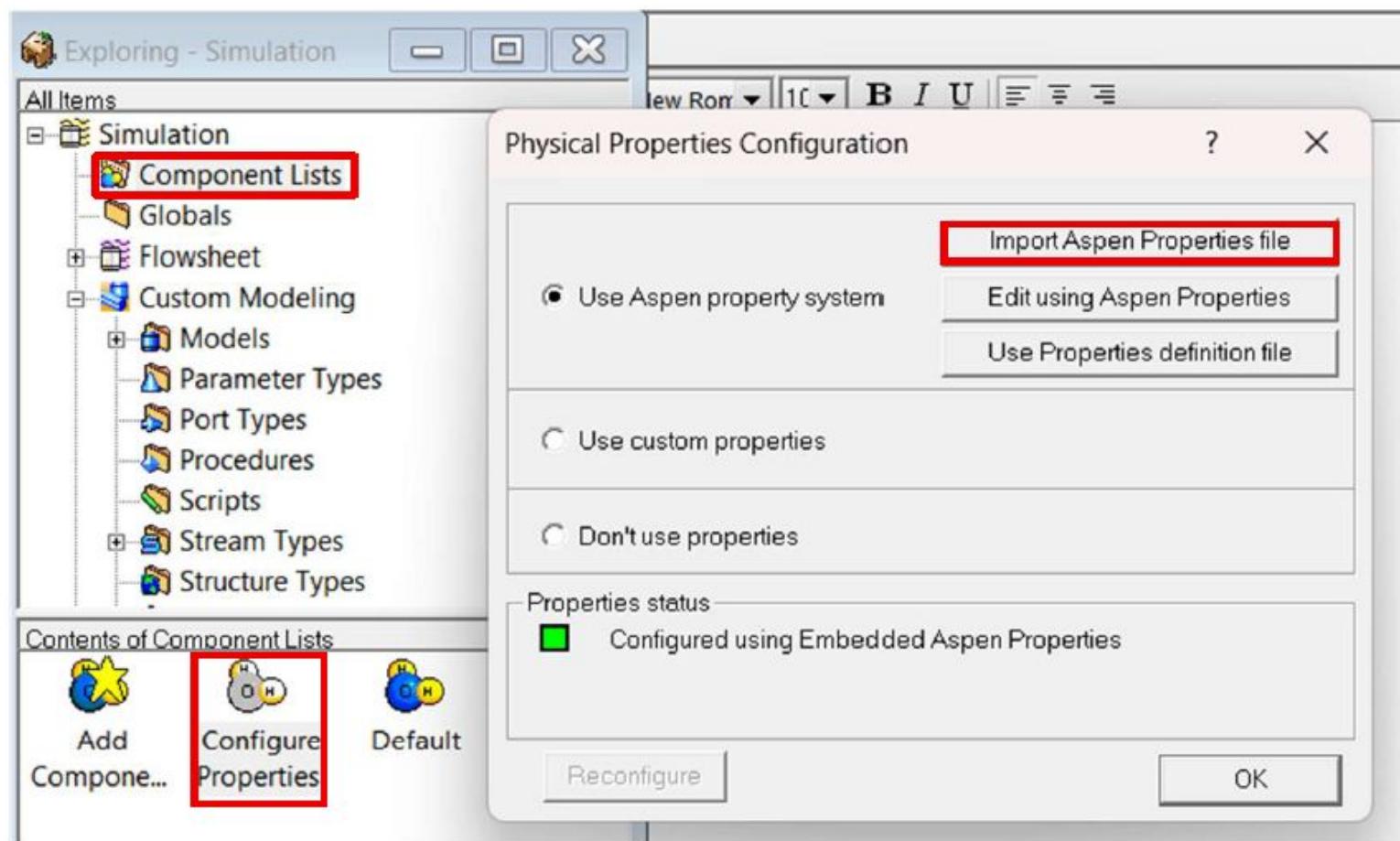
# Trabalhando com Aspen Custom Modeler

Abrir o “Aspen Custom Modeler”



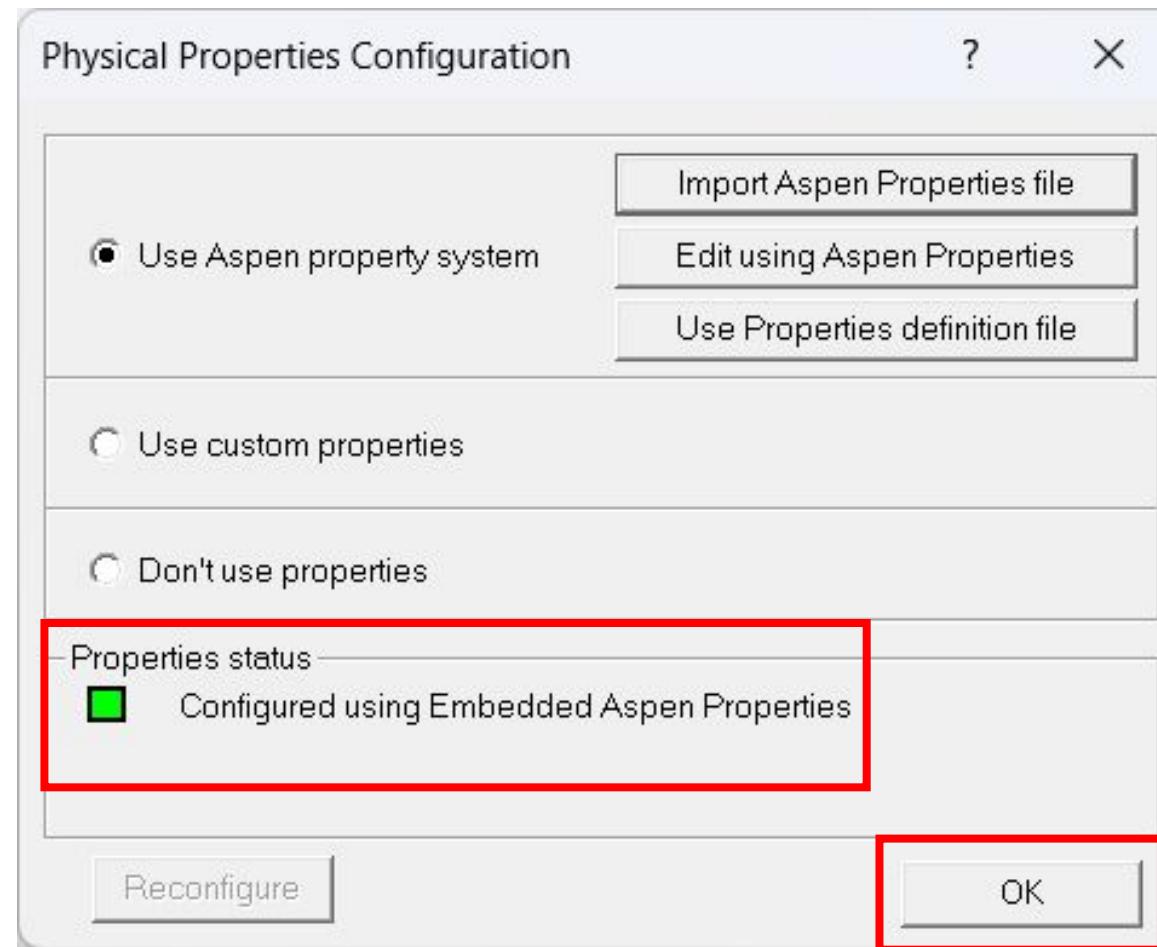
# Trabalhando com Aspen Custom Modeler

Importar o arquivo de propriedades criado anteriormente



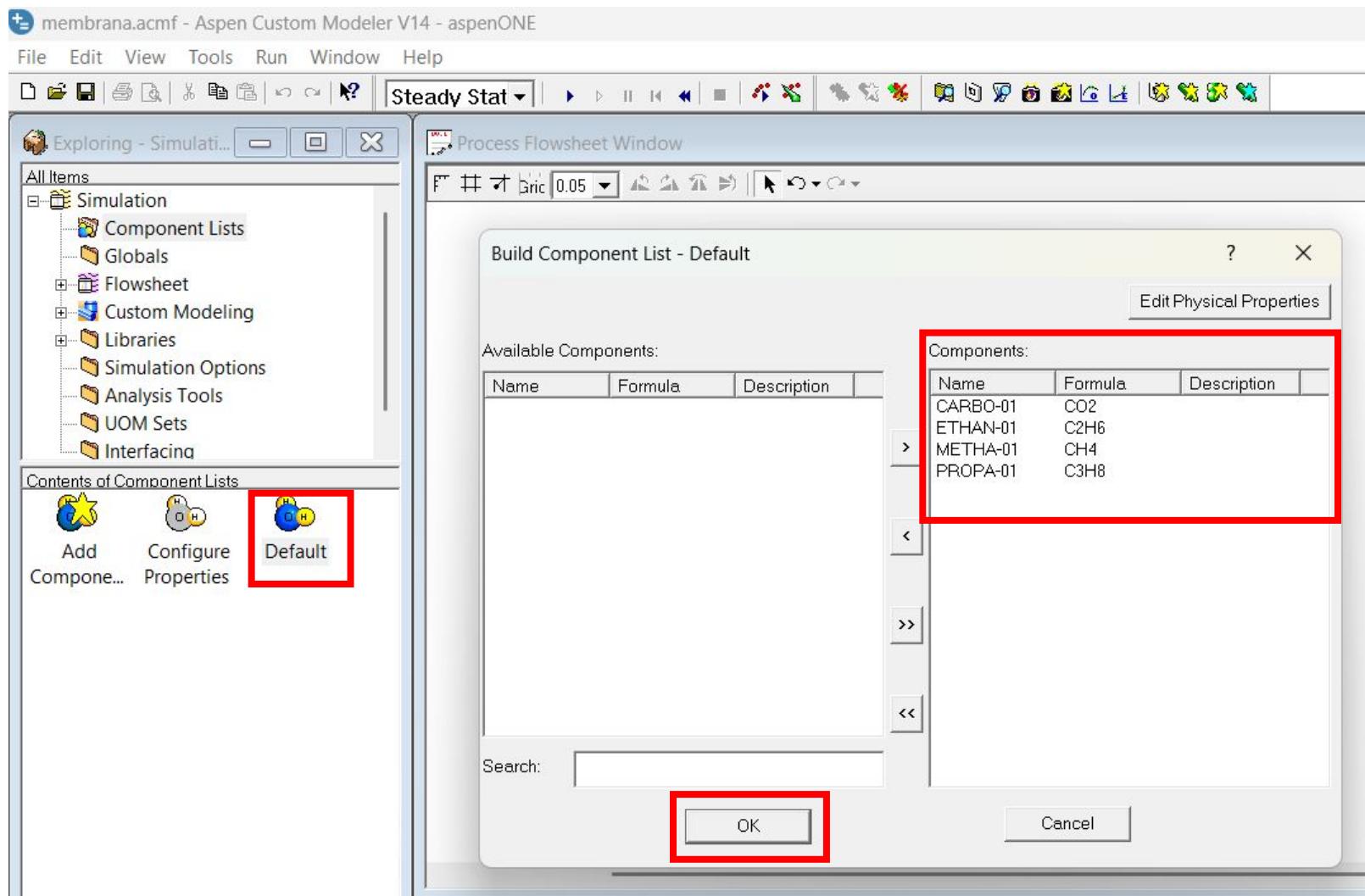
# Trabalhando com Aspen Custom Modeler

Propriedades configuradas satisfatoriamente



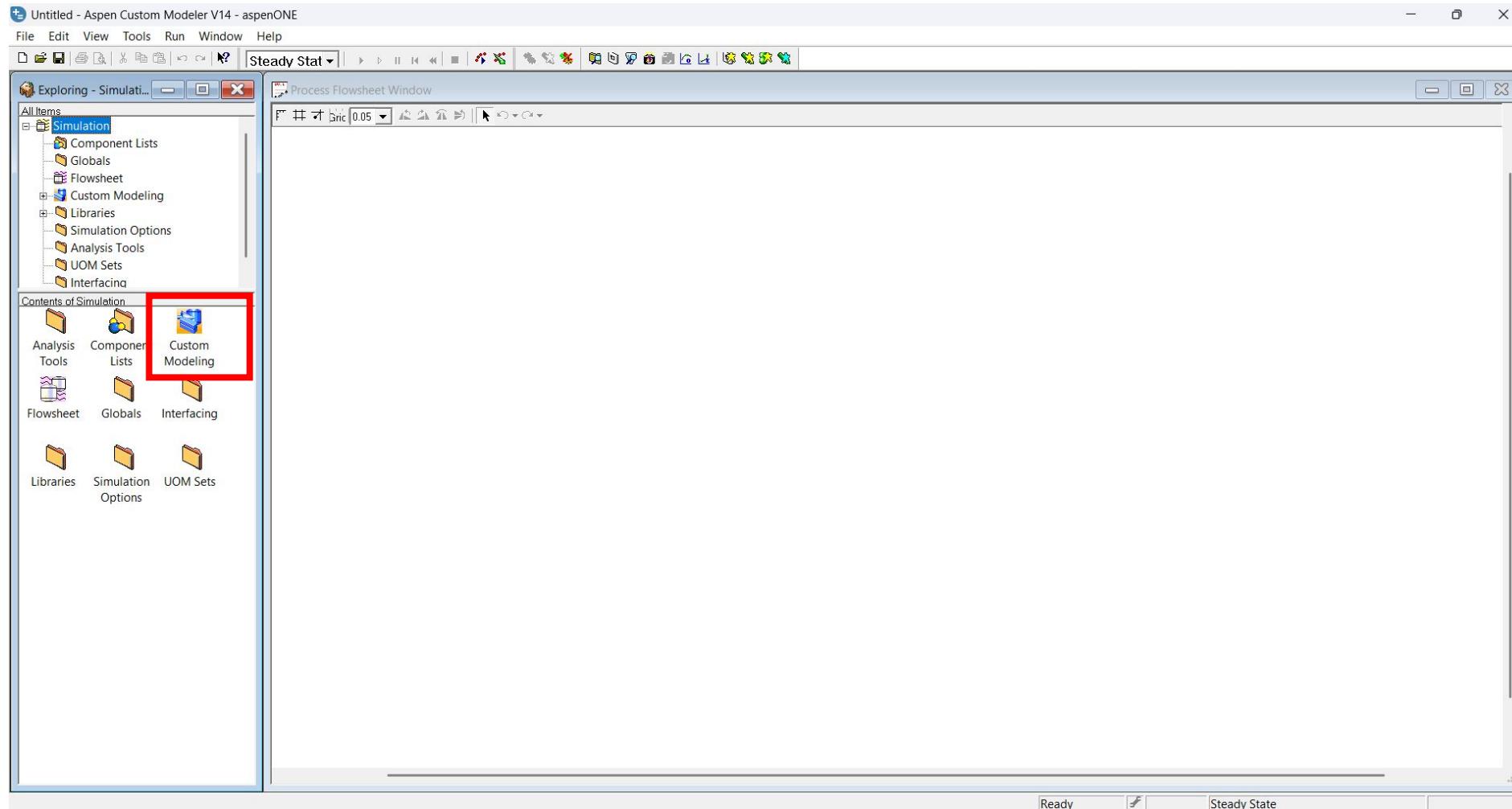
# Trabalhando com Aspen Custom Modeler

Adicionar os componentes à lista padrão de componentes



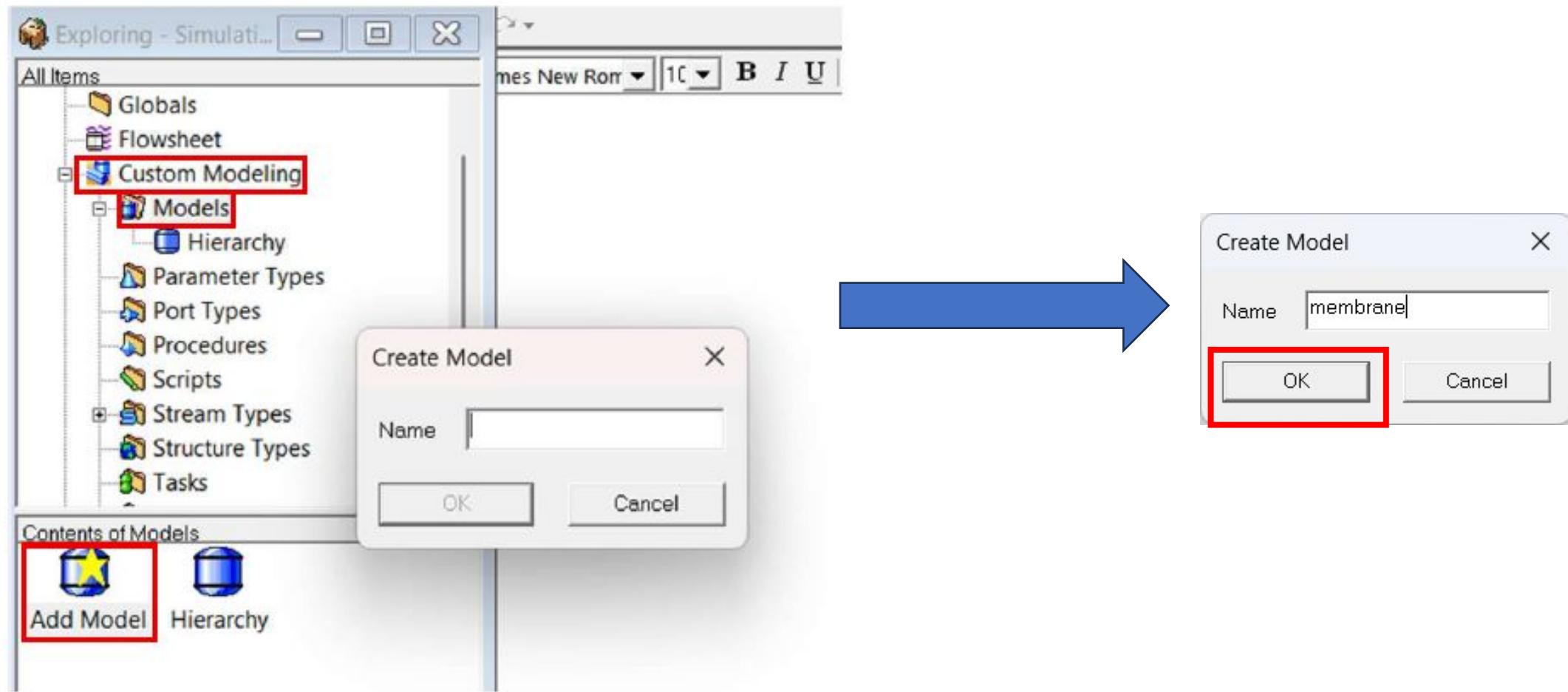
# Trabalhando com Aspen Custom Modeler

## Modelo customizado



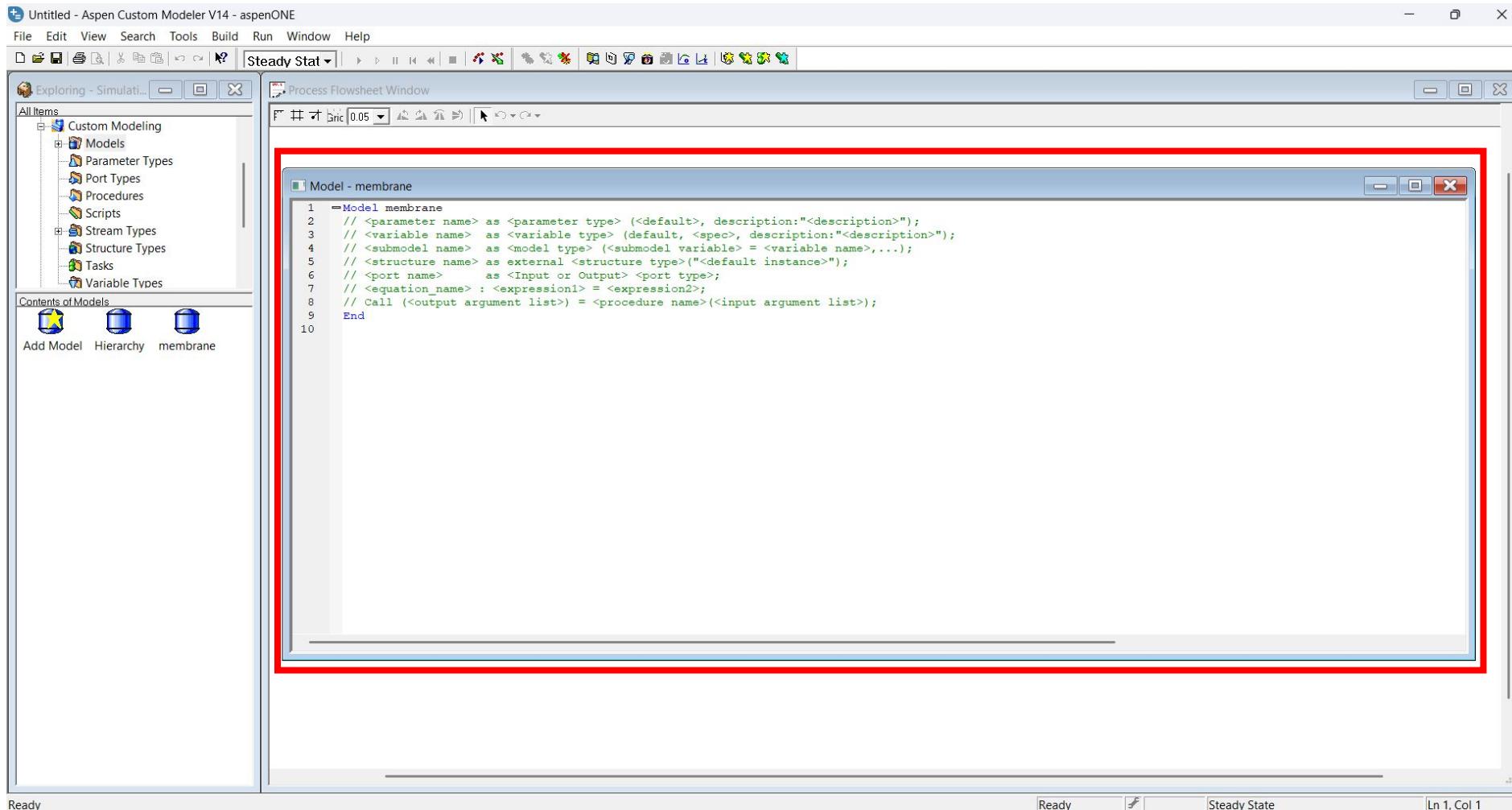
# Trabalhando com Aspen Custom Modeler

## Adicionar modelo



# Trabalhando com Aspen Custom Modeler

Área para escrever o modelo



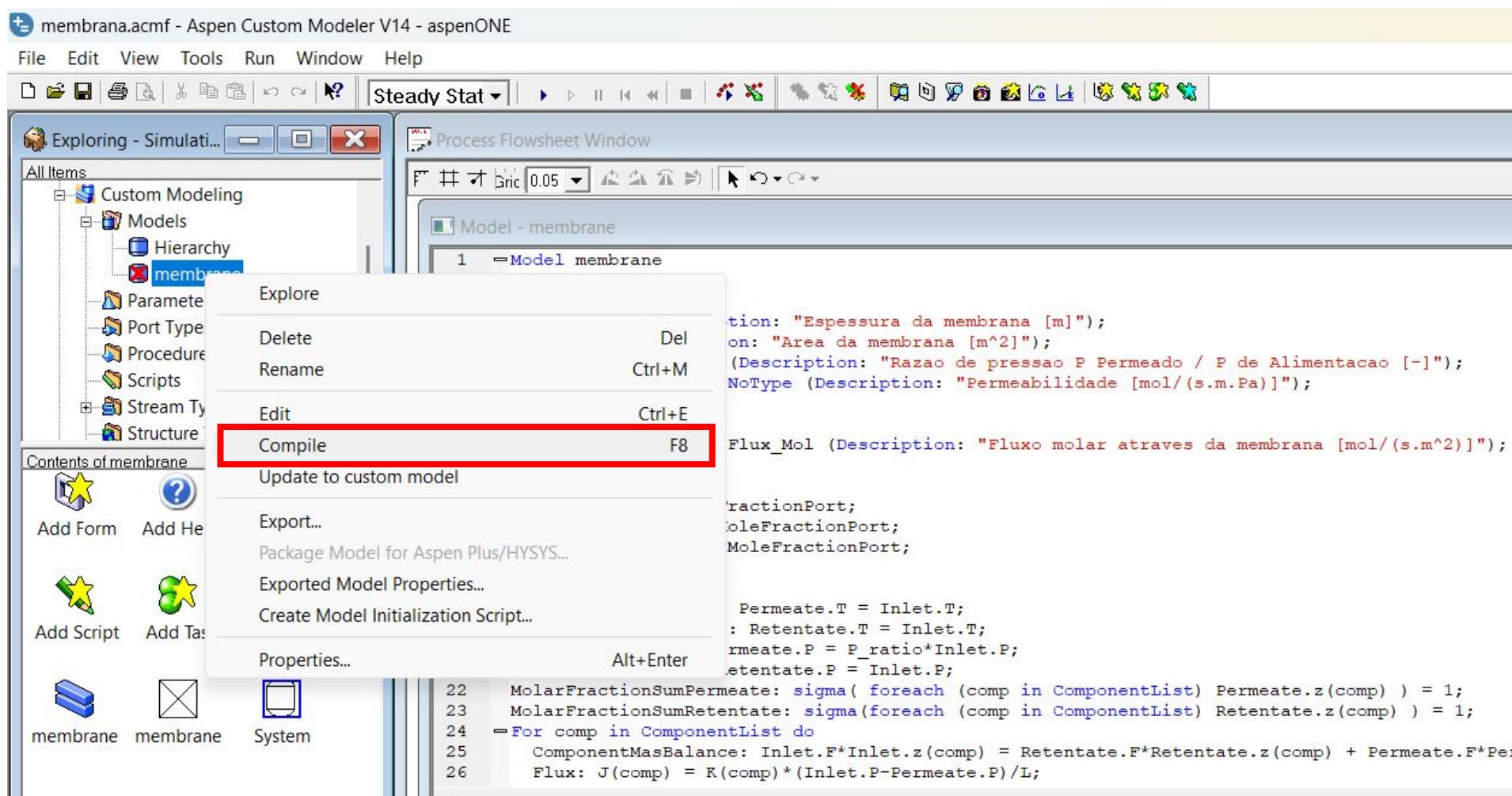
# Trabalhando com Aspen Custom Modeler

## Modelo implementado

```
1  =Model membrane
2
3  // Parameters
4  L as Length (Description: "Espessura da membrana [m]");
5  A as Area (Description: "Area da membrana [m^2]");
6  P_ratio as Fraction (Description: "Razao de pressao P Permeado / P de Alimentacao [-]");
7  K(ComponentList) as NoType (Description: "Permeabilidade [kmol/(s.m.Pa)]");
8
9  // Variaveis
10 J(ComponentList) as Flux_Mol (Description: "Fluxo molar atraves da membrana [kmol/(s.m^2)]");
11
12 // Conexoes
13 Inlet as Input MoleFractionPort;
14 Permeate as Output MoleFractionPort;
15 Retentate as Output MoleFractionPort;
16
17 // Equacoes
18 PermeateTemperature: Permeate.T = Inlet.T;
19 RetentateTemperature: Retentate.T = Inlet.T;
20 PermeatePressure: Permeate.P = P_ratio*Inlet.P;
21 RetentatePressure: Retentate.P = Inlet.P;
22 MolarFractionSumPermeate: sigma( foreach (comp in ComponentList) Permeate.z(comp) ) = 1;
23 MolarFractionSumRetentate: sigma(foreach (comp in ComponentList) Retentate.z(comp) ) = 1;
24 =For comp in ComponentList do
25   ComponentMasBalance: Inlet.F*Inlet.z(comp) = Retentate.F*Retentate.z(comp) + Permeate.F*Permeate.z(comp);
26   Flux: J(comp) = K(comp)*(Inlet.P-Permeate.P)/L;
27   PermeateMolarFlow: Permeate.F*Permeate.z(comp)= J(comp)*A;
28 EndFor
29
30 End
```

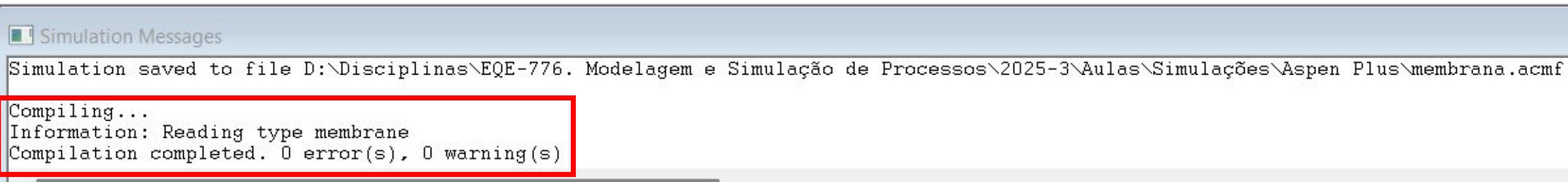
# Trabalhando com Aspen Custom Modeler

## Salvar e compilar



# Trabalhando com Aspen Custom Modeler

Conferir que não há erros de compilação



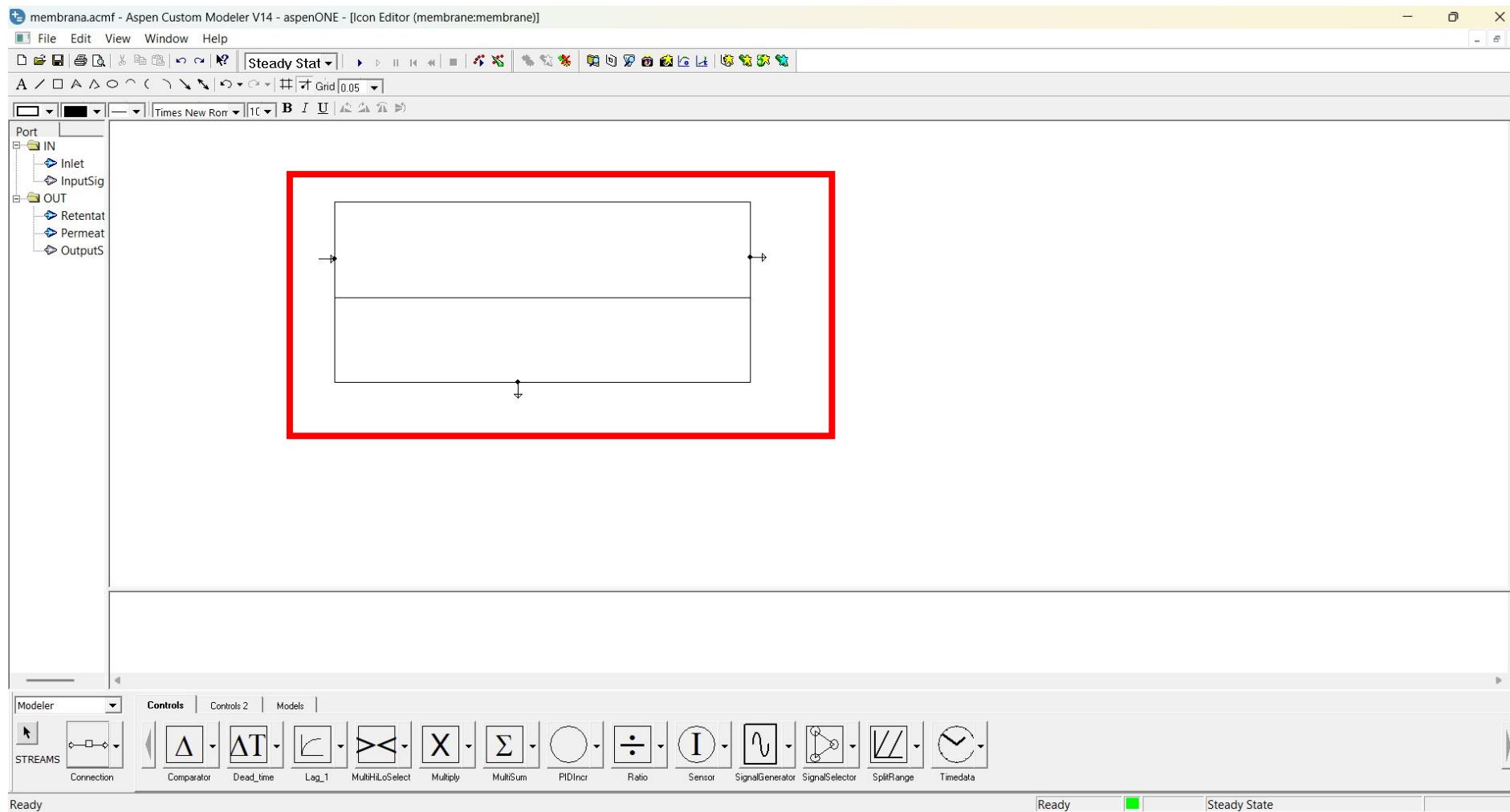
The screenshot shows a software window titled "Simulation Messages". The message log displays the following text:

```
Simulation saved to file D:\Disciplinas\EQE-776. Modelagem e Simulação de Processos\2025-3\Aulas\Simulações\Aspen Plus\membrana.acmf
Compiling...
Information: Reading type membrane
Compilation completed. 0 error(s), 0 warning(s)
```

The text from "Compiling..." to "Compilation completed." is highlighted with a red rectangular box.

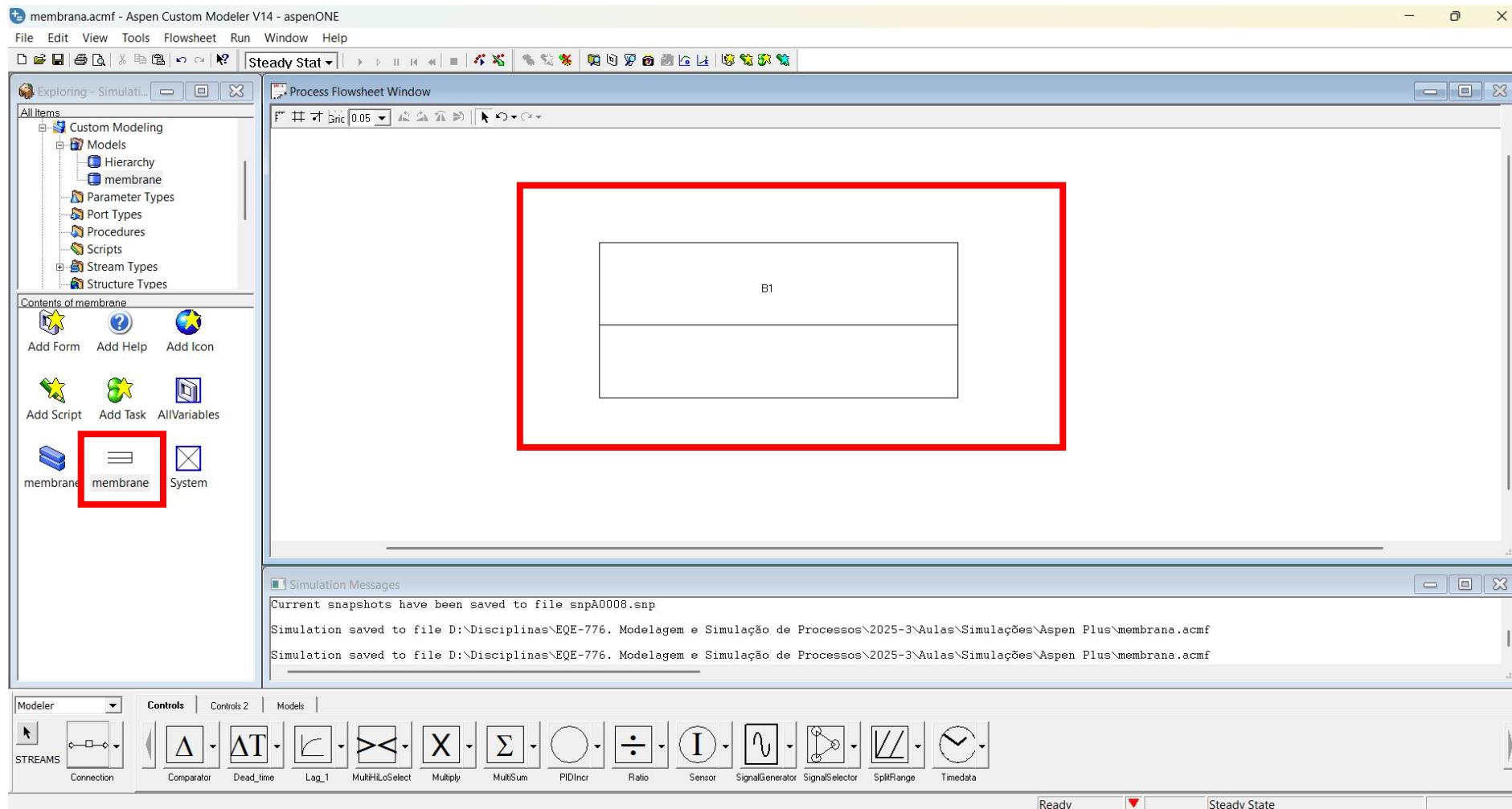
# Trabalhando com Aspen Custom Modeler

## Criando um ícone



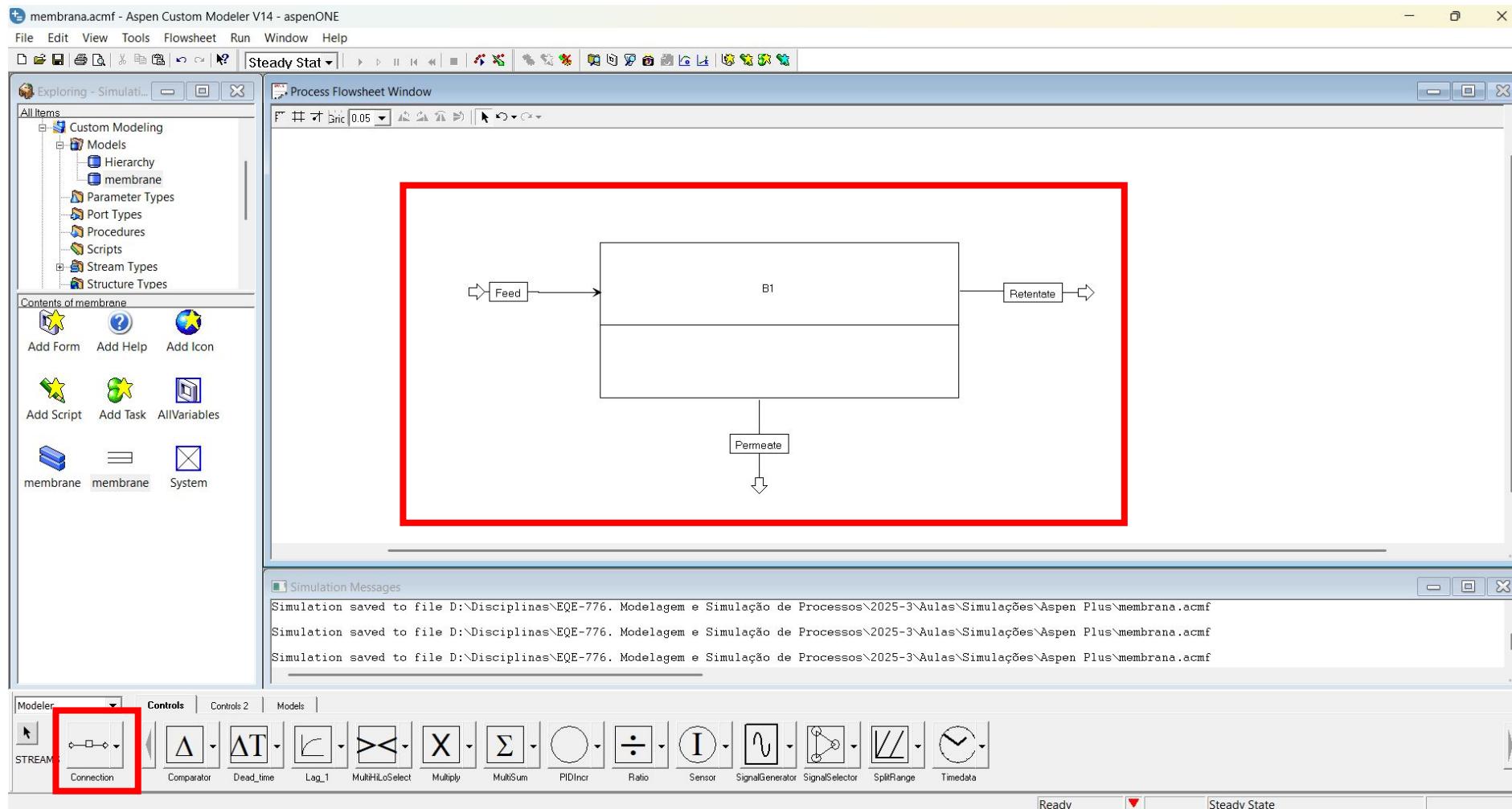
# Trabalhando com Aspen Custom Modeler

Arrastrando ícone para a janela de Flowsheet



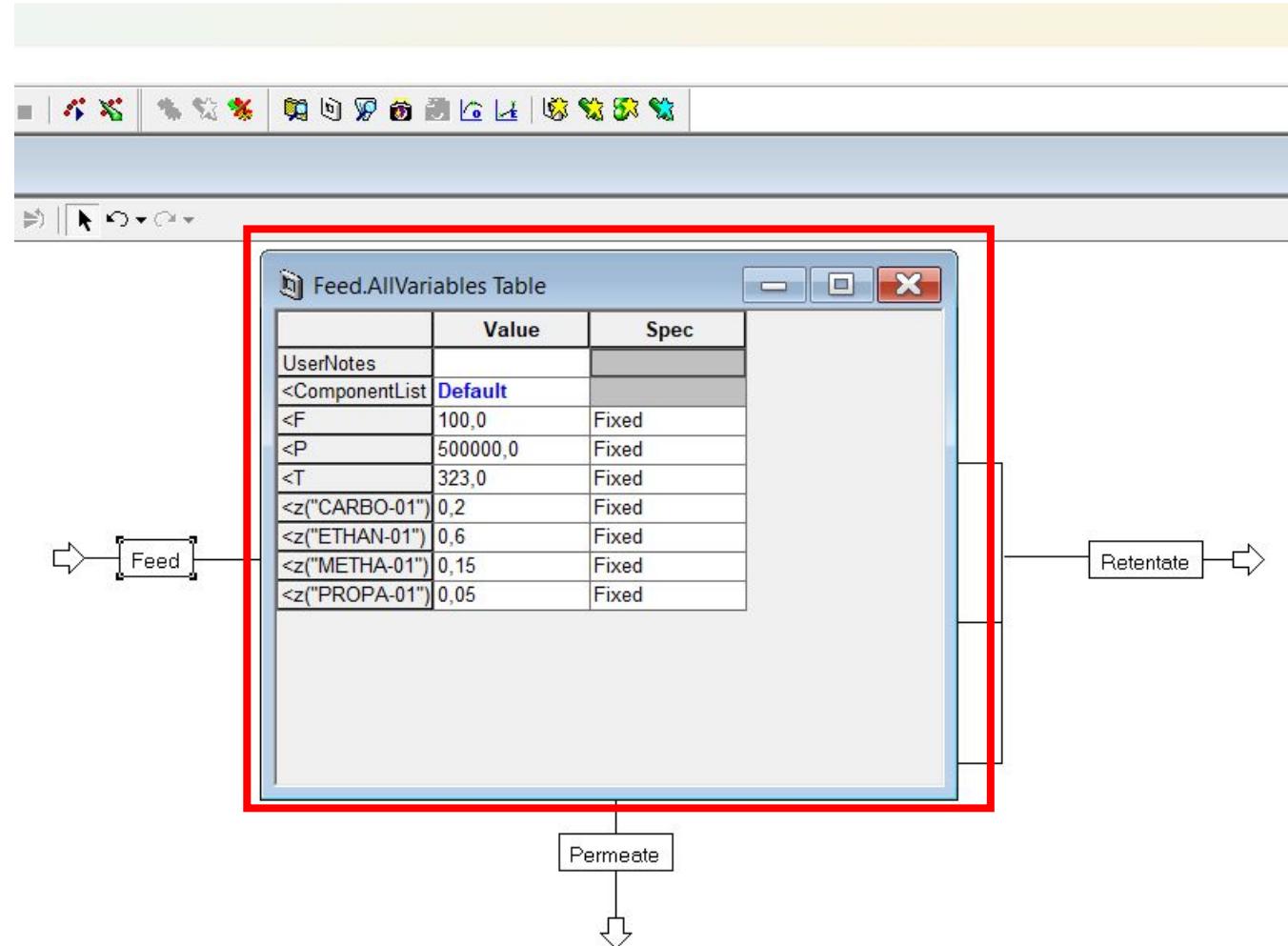
# Trabalhando com Aspen Custom Modeler

Conectando as correntes de entrada e saída



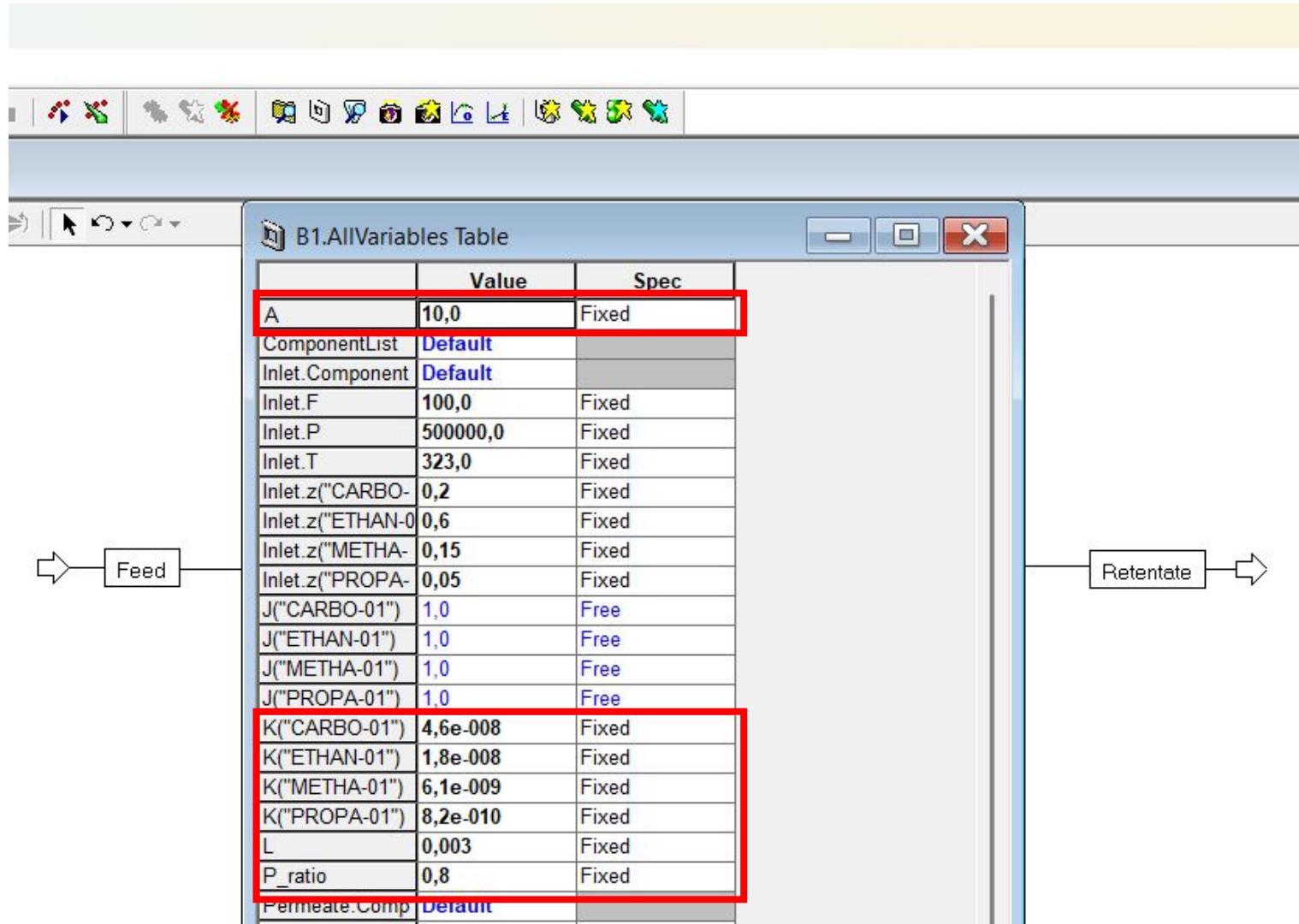
# Trabalhando com Aspen Custom Modeler

Especificando os valores da corrente de entrada



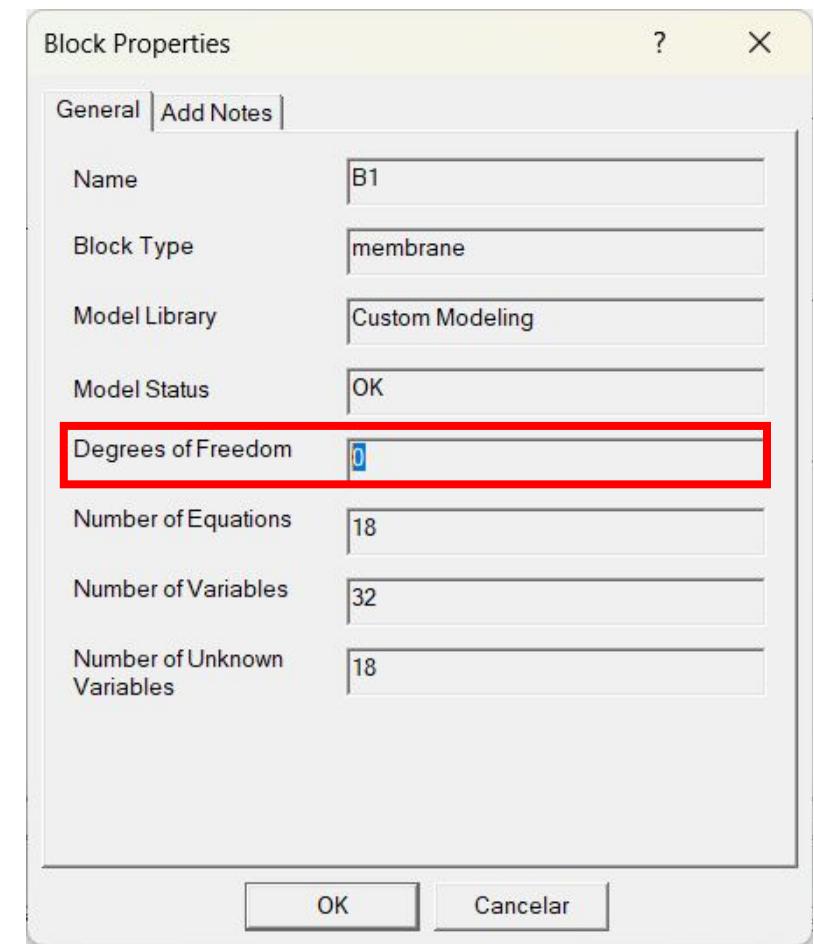
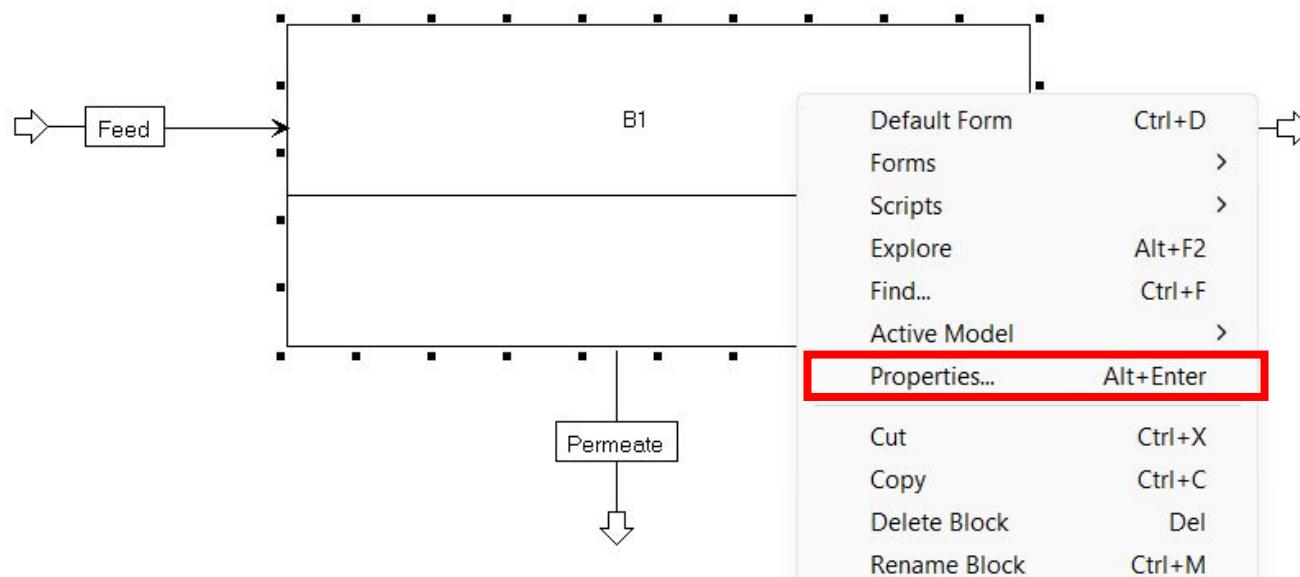
# Trabalhando com Aspen Custom Modeler

Especificando os parâmetros do modelo de separador por membrana



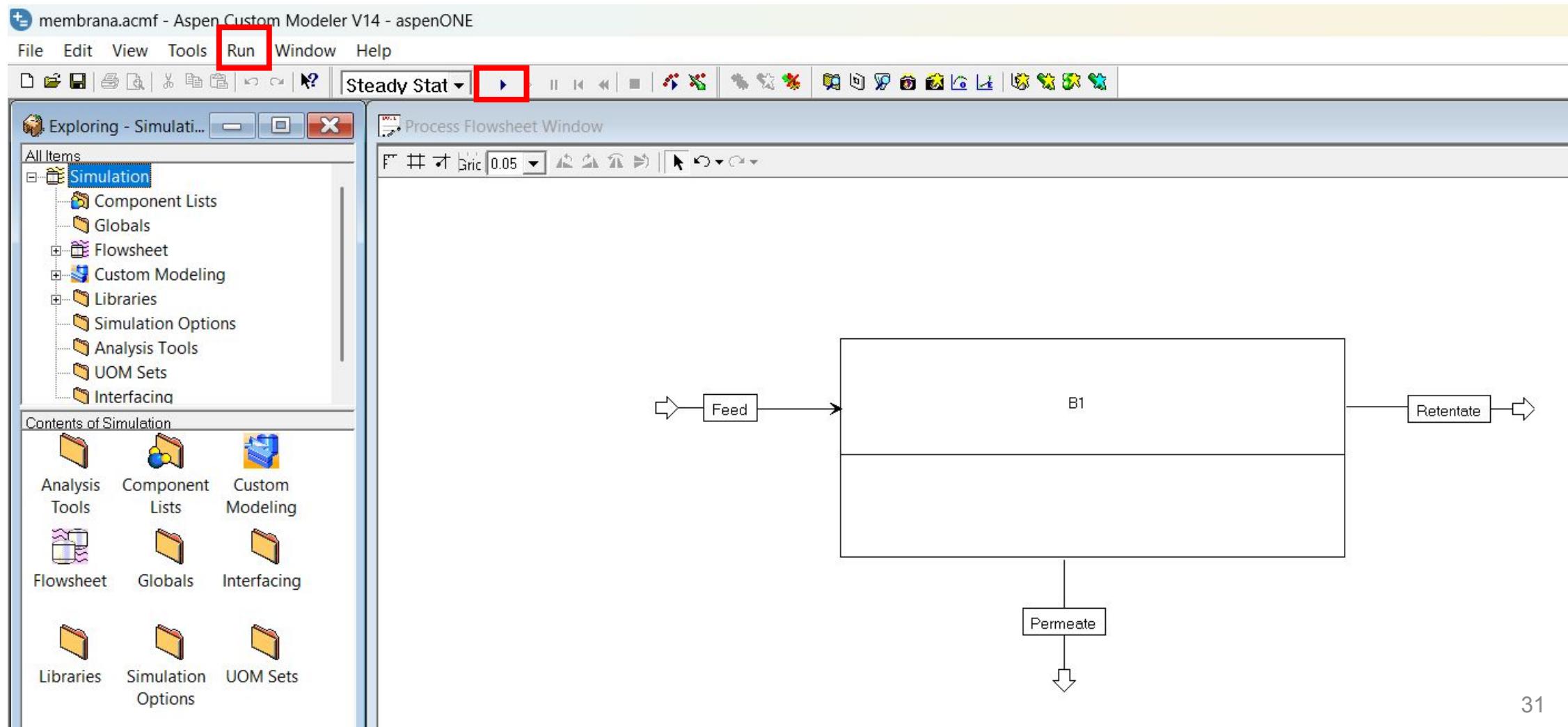
# Trabalhando com Aspen Custom Modeler

Conferindo se os graus de liberdade estão zerados



# Trabalhando com Aspen Custom Modeler

## Executando a simulação



# Trabalhando com Aspen Custom Modeler

## Conferir mensagem da simulação

```
Starting run at 13:42:28
Solving steady state ...
Decomposition:
    Total number of equations      = 18
    Total number of groups        = 10
    Number of explicit groups     = 8
    Number of nonlinear groups   = 2
    Largest group size           = 5
Solving group 6, size 5, type Nonlinear
SPARSE: Iteration 0, Var. Norm= 0.000e+00, Eqn. Norm= 1.283e+01 (best 1.283e+01)
Check bounds: Step cut by 4.43525e-01 due to B1.Permeate.z("PROPA-01")
          below lower bound 0.00000e+00
SPARSE: Iteration 1, Var. Norm= 1.240e+00, Eqn. Norm= 4.613e+00 (best 4.613e+00)
SPARSE: Iteration 2, Var. Norm= 4.452e-01, Eqn. Norm= 2.161e-01 (best 2.161e-01)
SPARSE: Iteration 3, Var. Norm= 5.576e-03, Eqn. Norm= 8.882e-16 (best 8.882e-16)
SPARSE: Residual convergence after 3 iterations
Solving group 8, size 5, type Nonlinear
SPARSE: Iteration 0, Var. Norm= 0.000e+00, Eqn. Norm= 5.150e+01 (best 5.150e+01)
Check bounds: Step cut by 1.73330e-01 due to B1.Retentate.z("CARBO-01")
          below lower bound 0.00000e+00
SPARSE: Iteration 1, Var. Norm= 6.033e+00, Eqn. Norm= 3.561e+01 (best 3.561e+01)
SPARSE: Iteration 2, Var. Norm= 2.438e+00, Eqn. Norm= 2.871e+01 (best 2.871e+01)
SPARSE: Iteration 3, Var. Norm= 1.167e+00, Eqn. Norm= 1.974e+00 (best 1.974e+00)
SPARSE: Iteration 4, Var. Norm= 1.538e-02, Eqn. Norm= 8.882e-16 (best 8.882e-16)
SPARSE: Residual convergence after 4 iterations
Steady state solution complete
Run complete at 13:42:28
```

# Trabalhando com Aspen Custom Modeler

## Resultados

Corrente “Permeate”

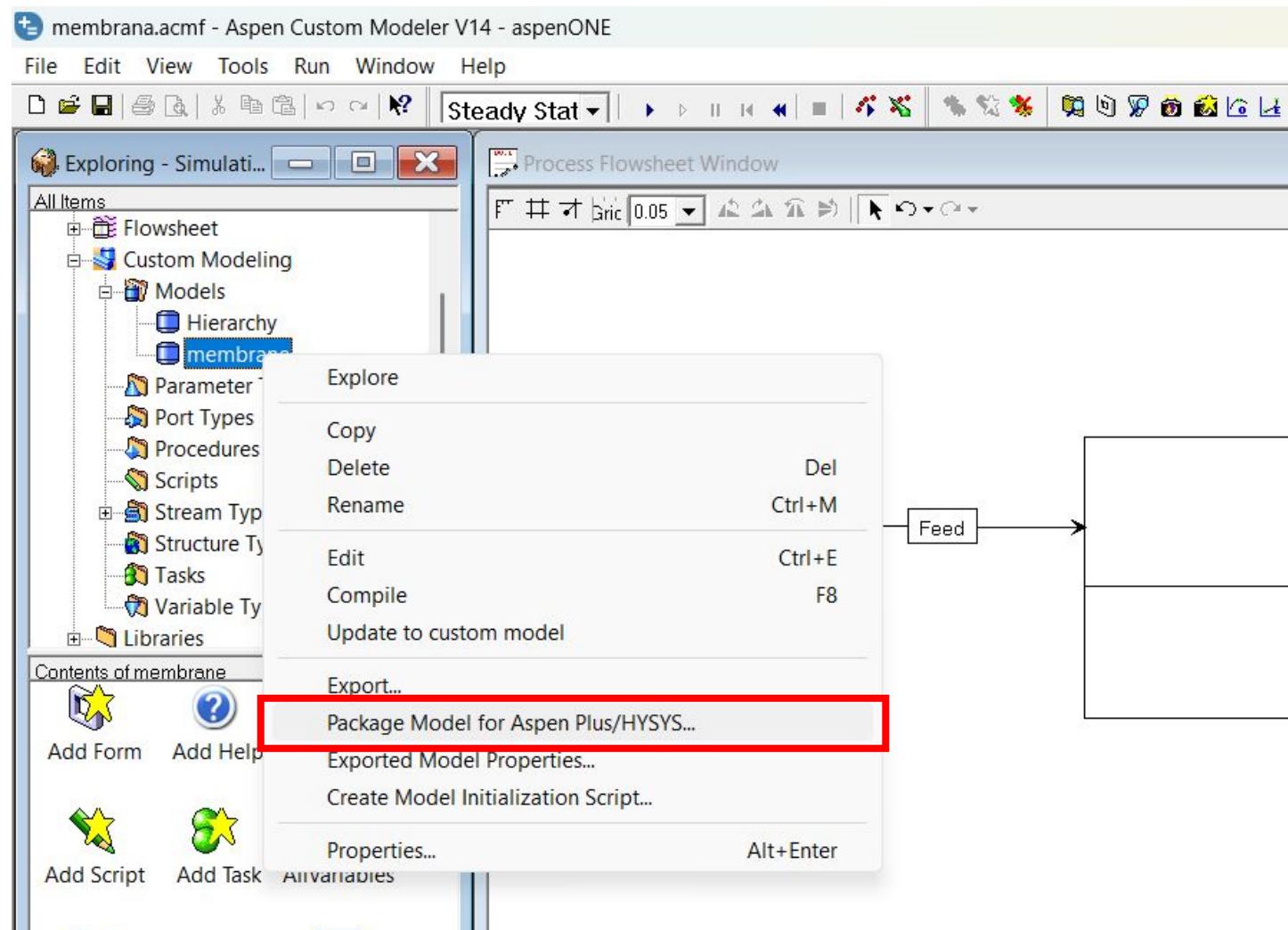
	Value	Spec
UserNotes		
>ComponentList	Default	
>F	23,64	Free
>P	400000,0	Free
>T	323,0	Free
>z("CARBO-01")	0,648618	Free
>z("ETHAN-01")	0,253807	Free
>z("METHA-01")	0,0860124	Free
>z("PROPA-01")	0,0115623	Free

Corrente “Retentate”

	Value	Spec
UserNotes		
>ComponentList	Default	
>F	76,36	Free
>P	500000,0	Free
>T	323,0	Free
>z("CARBO-01")	0,061114	Free
>z("ETHAN-01")	0,707177	Free
>z("METHA-01")	0,16981	Free
>z("PROPA-01")	0,0618998	Free

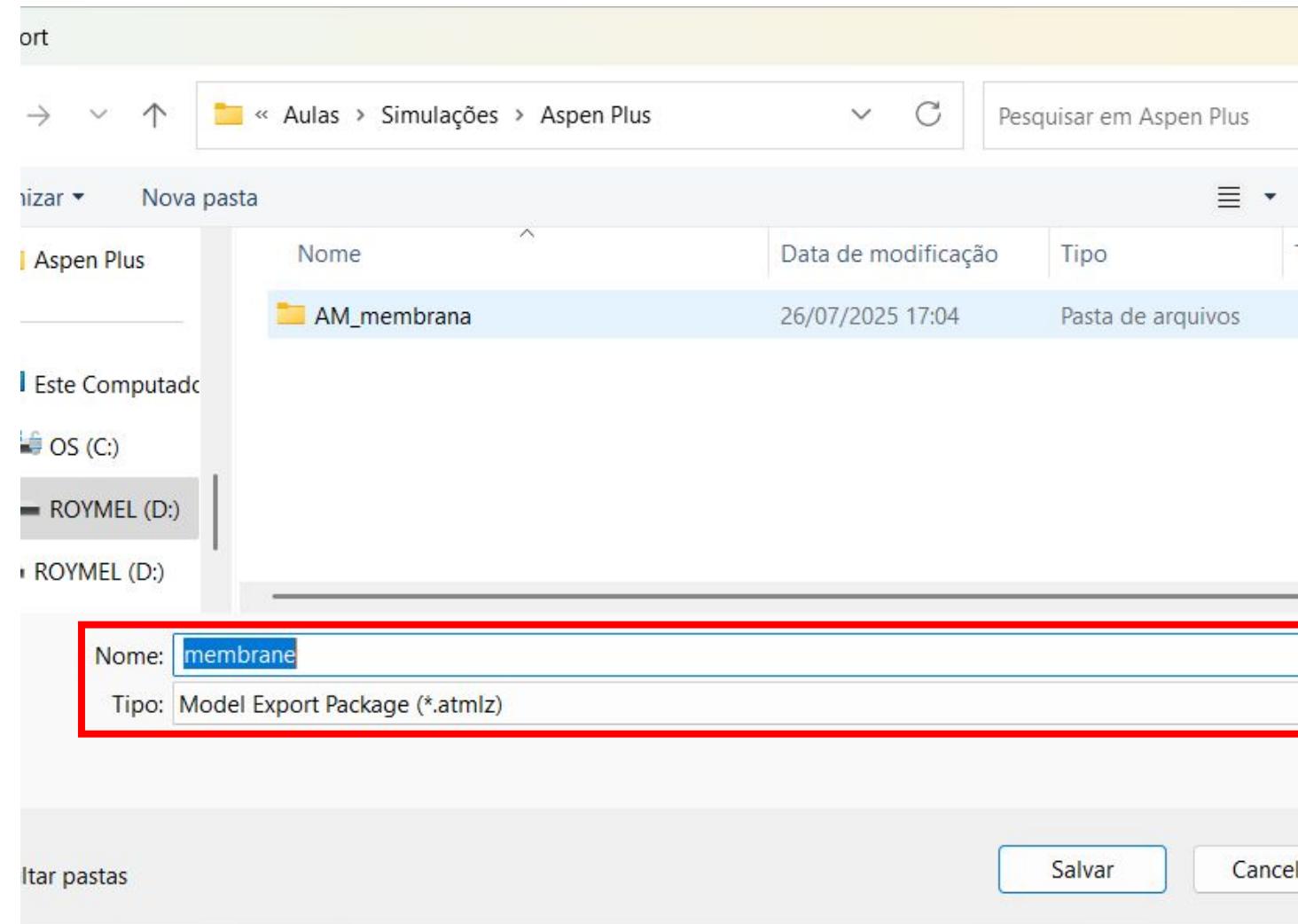
# Trabalhando com Aspen Custom Modeler

## Exportando o modelo para ser usado no Aspen Plus



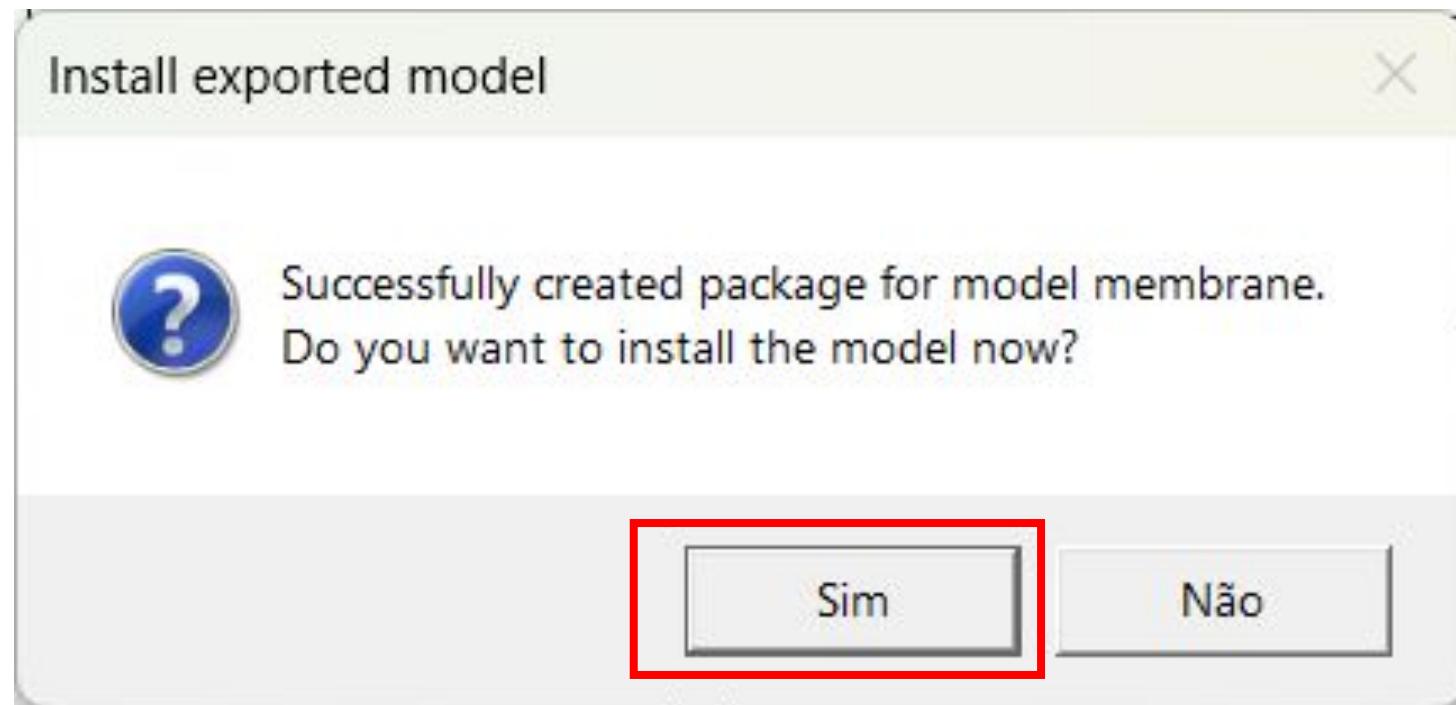
# Trabalhando com Aspen Custom Modeler

Salvar modelo no formato “\*.atmlz”



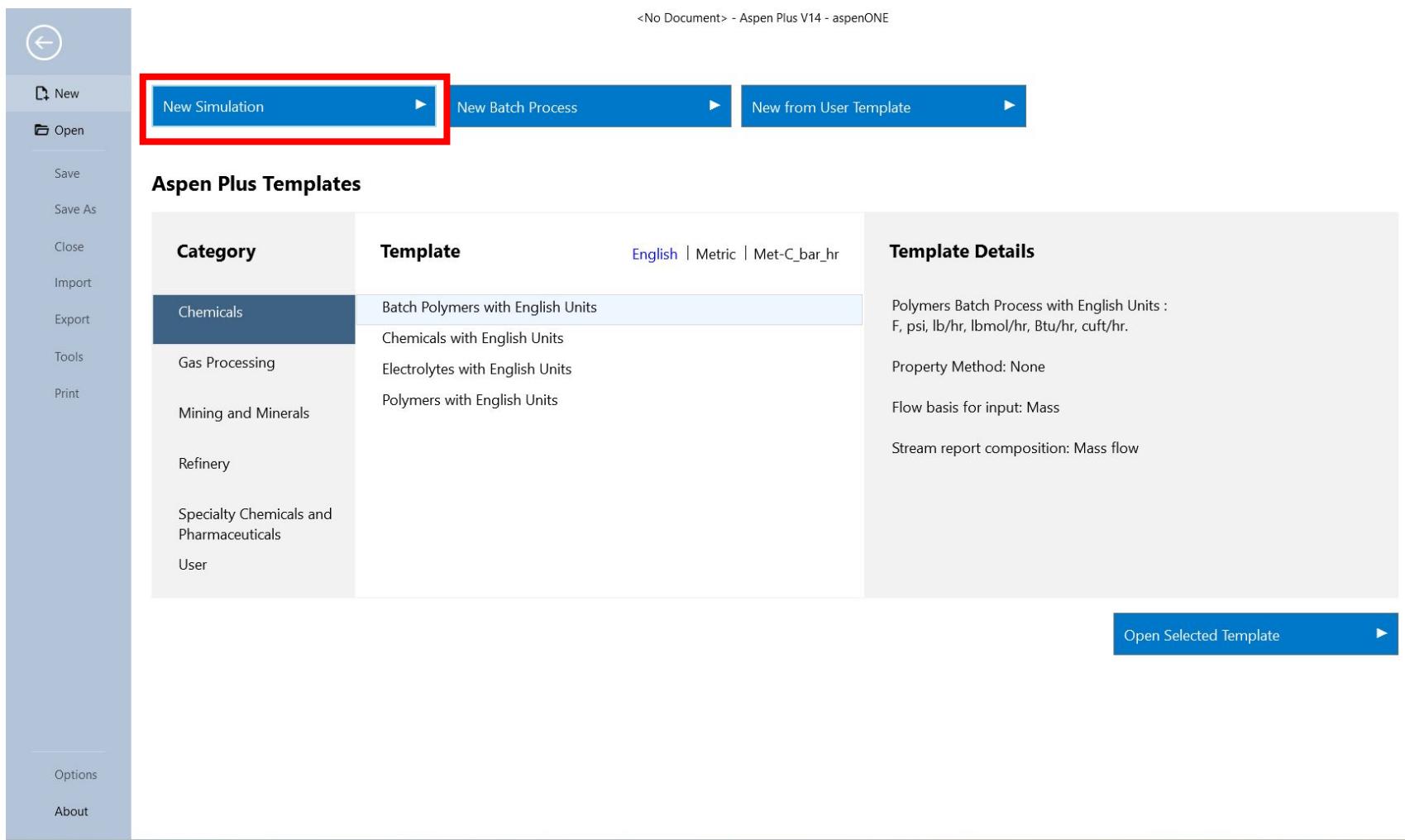
# Trabalhando com Aspen Custom Modeler

Instalar o modelo exportado



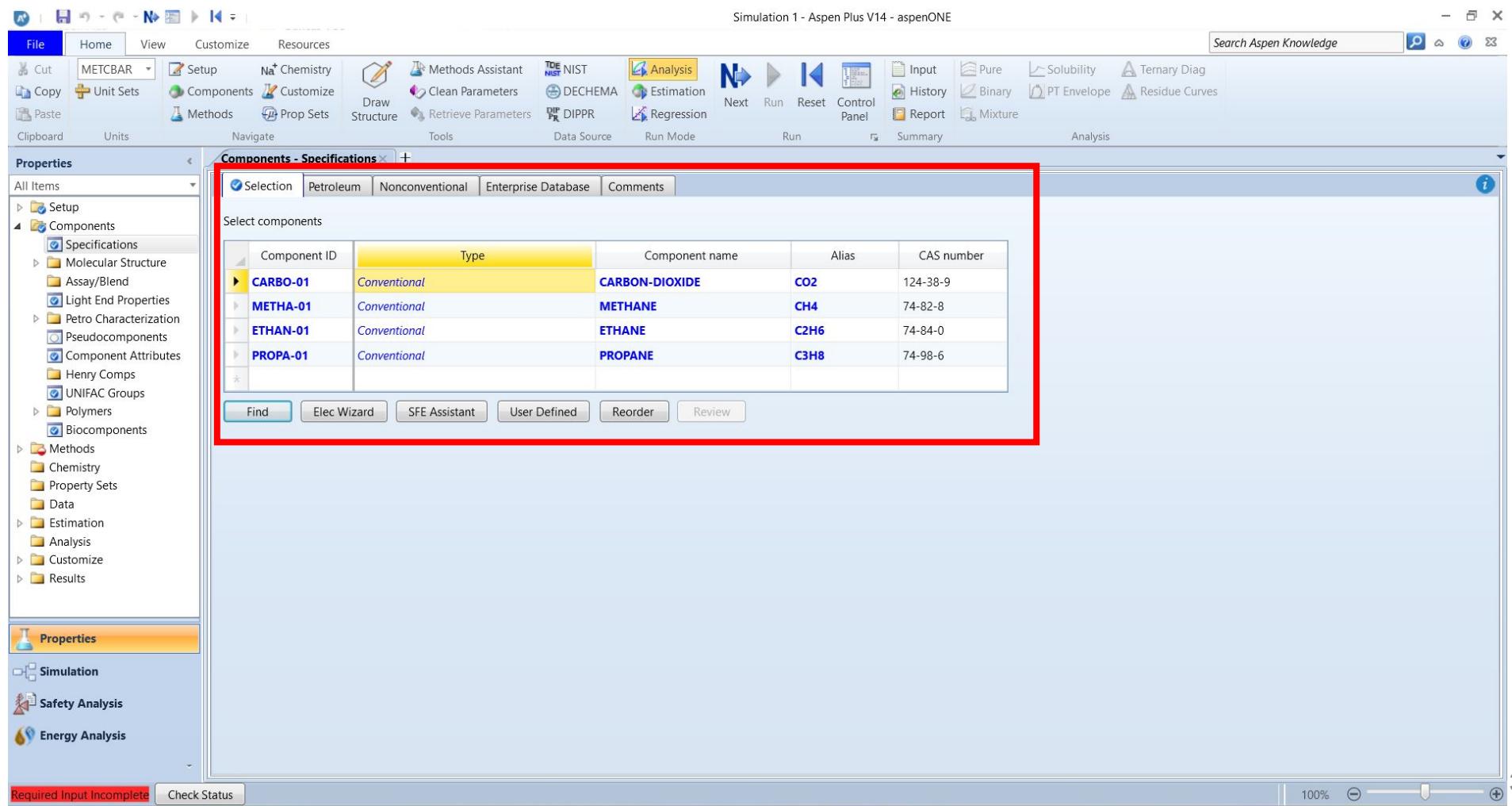
# Utilizando em Aspen Plus o modelo criado

## Criar uma nova simulação de Aspen Plus



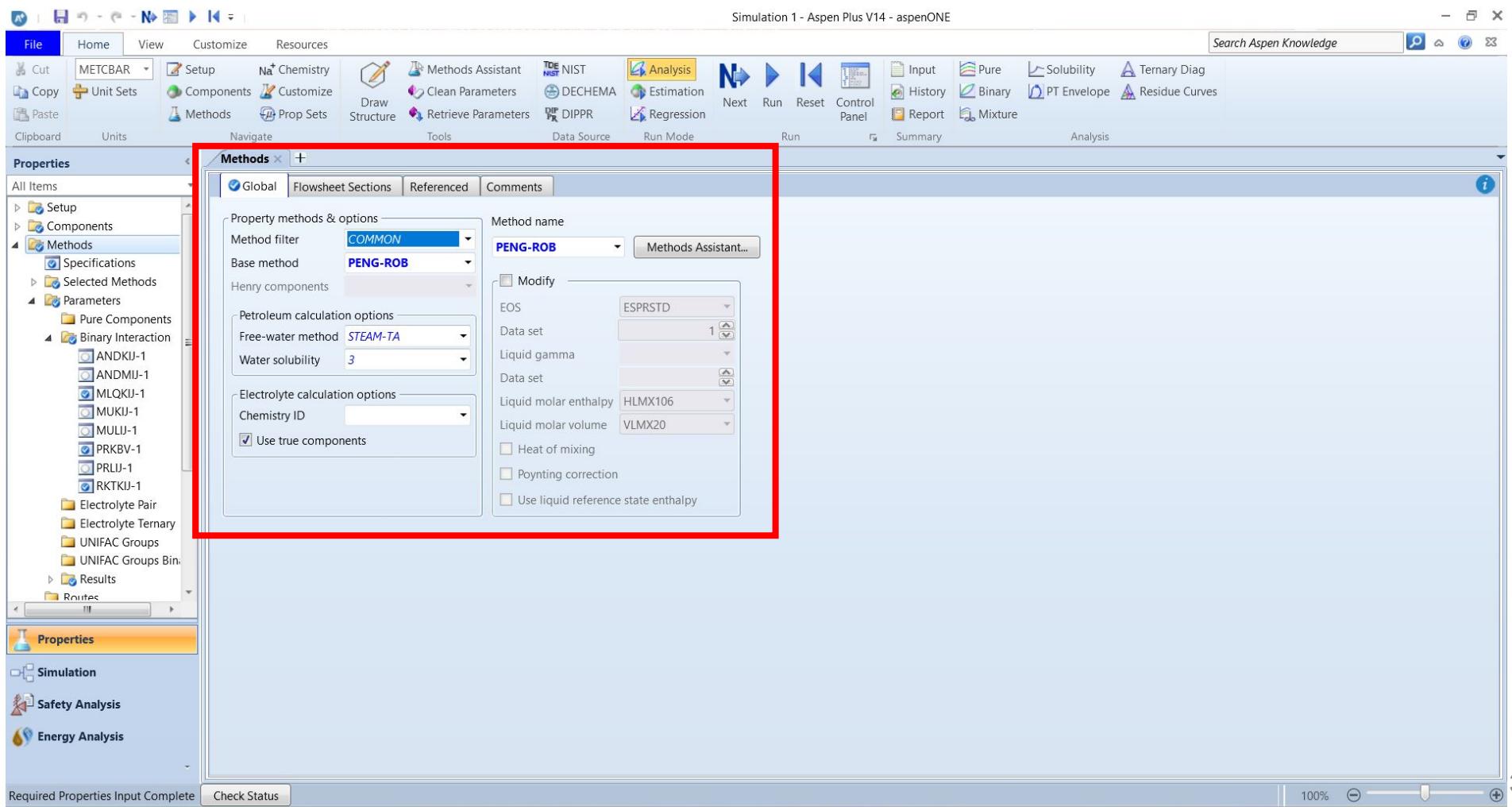
# Utilizando em Aspen Plus o modelo criado

## Escolher os componentes



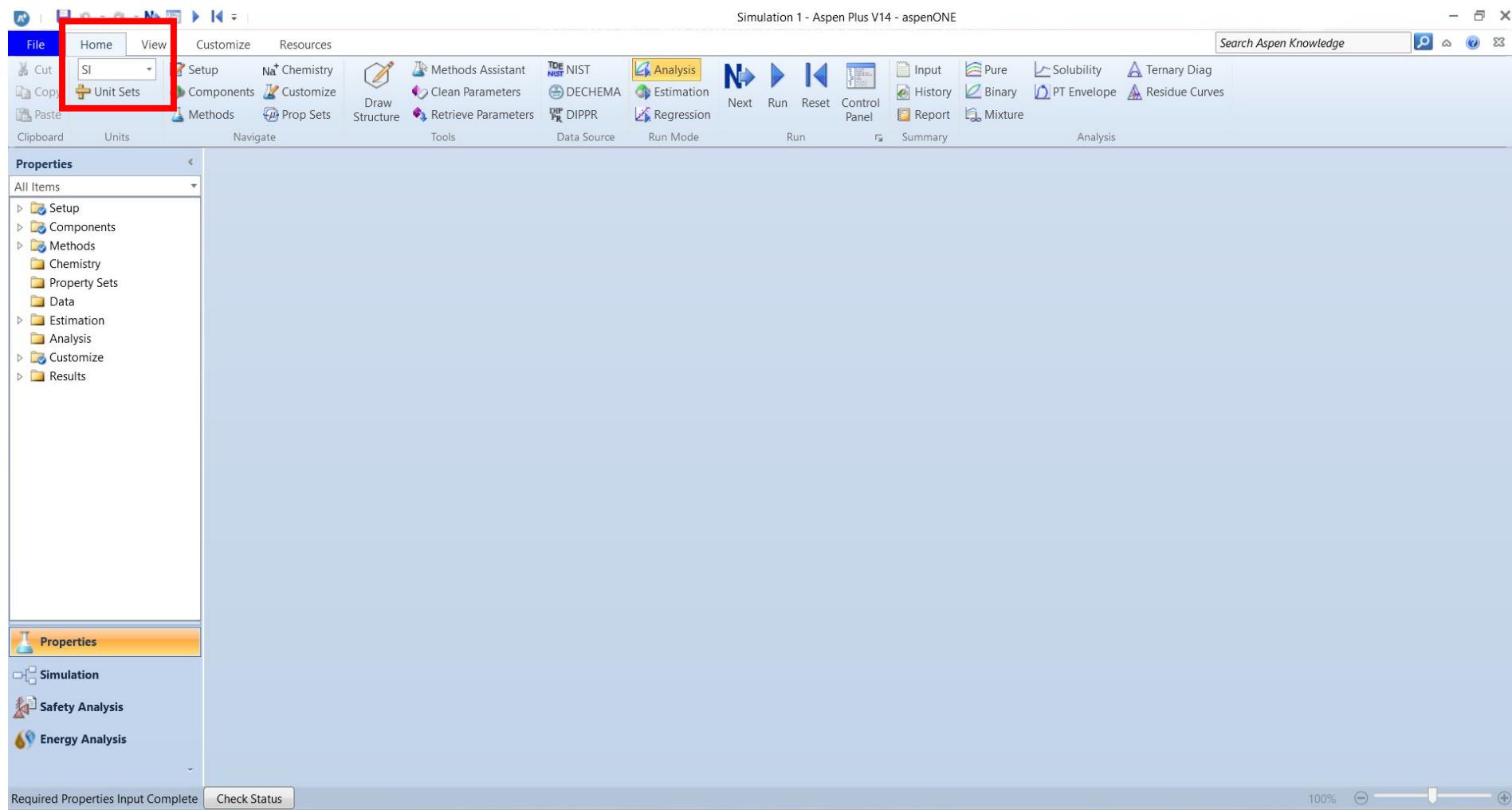
# Utilizando em Aspen Plus o modelo criado

## Escolher o modelo termodinâmico



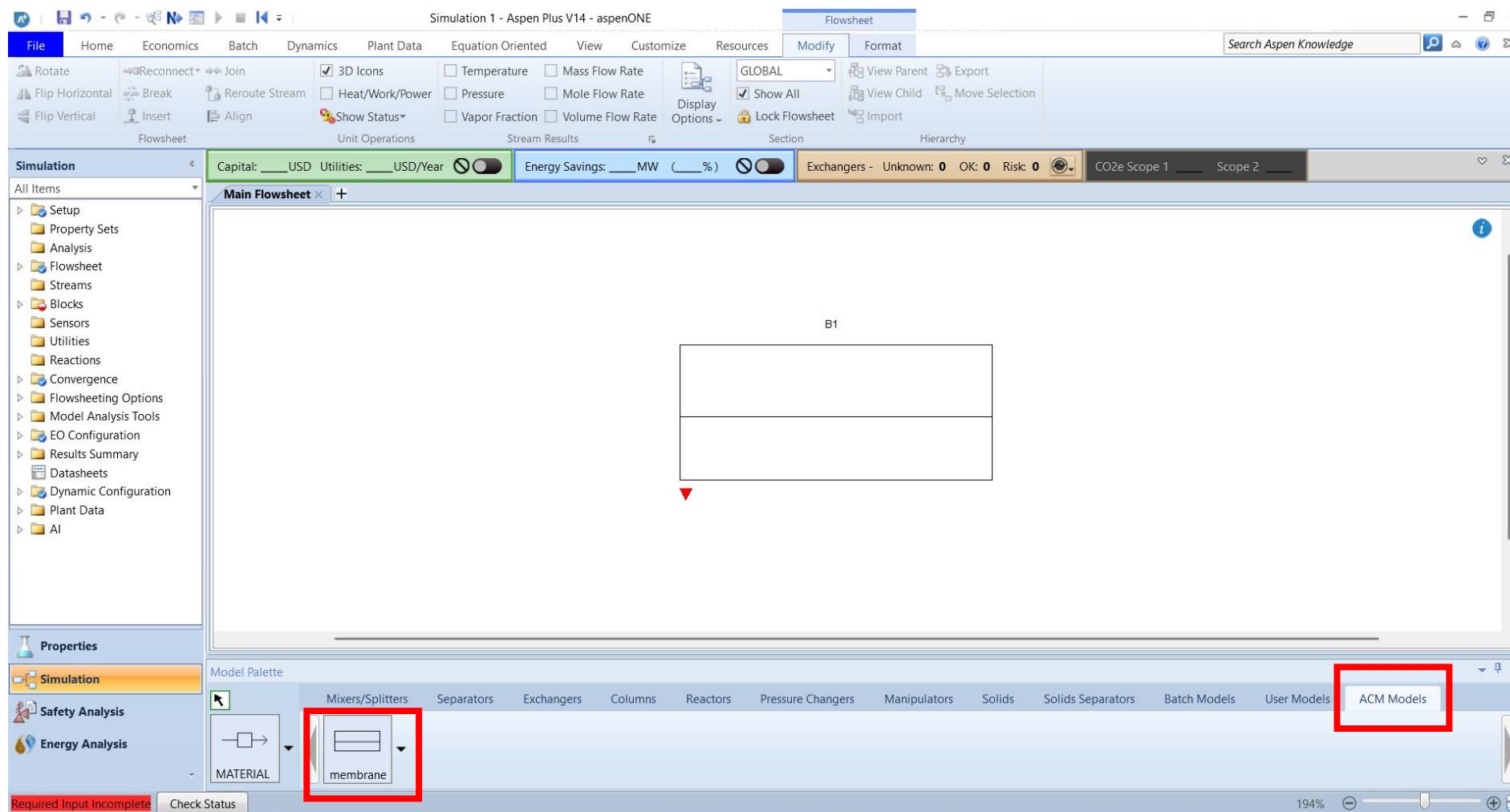
# Utilizando em Aspen Plus o modelo criado

Escolher o sistema de unidades



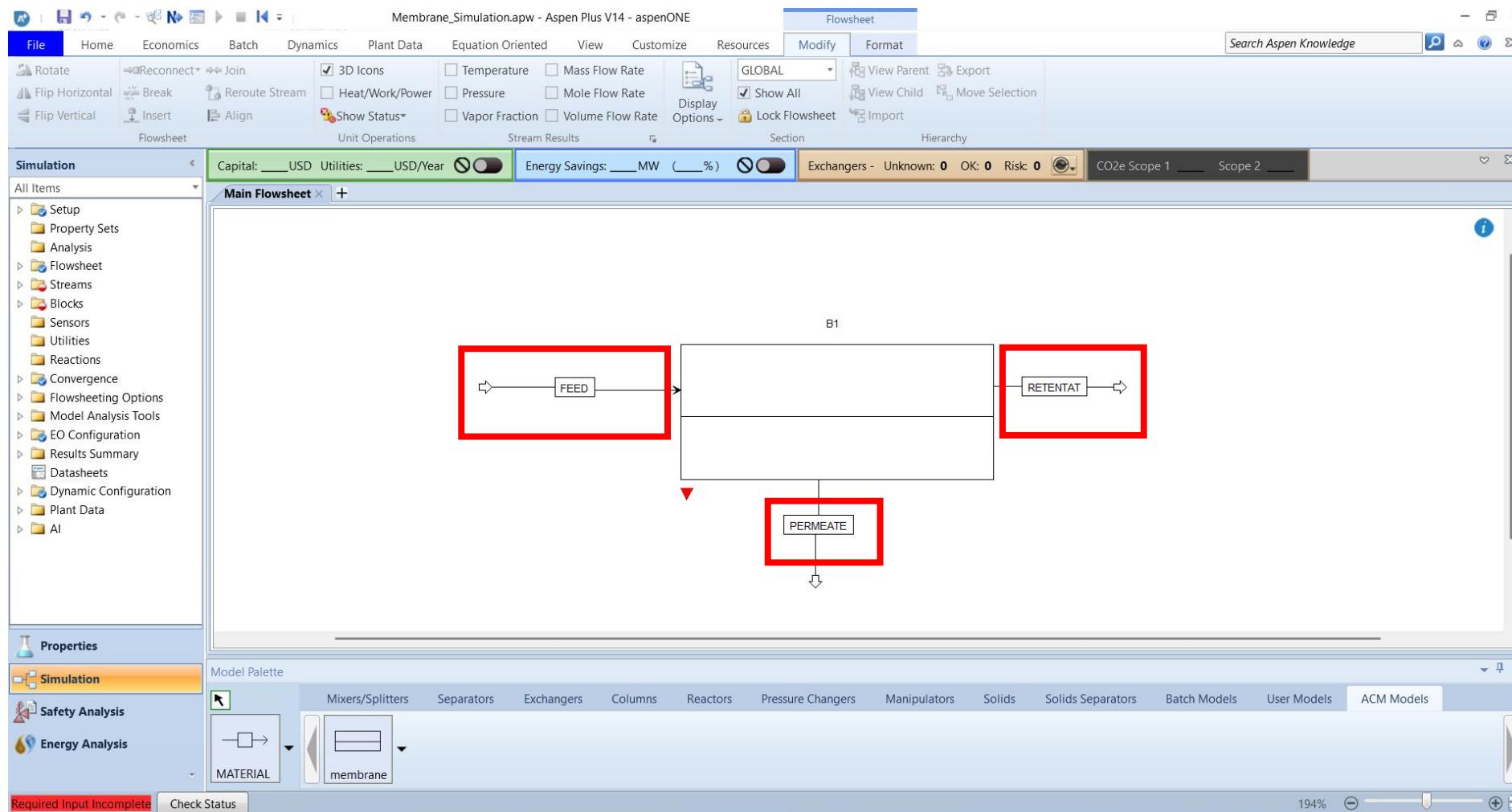
# Utilizando em Aspen Plus o modelo criado

## Inserir o modelo criado



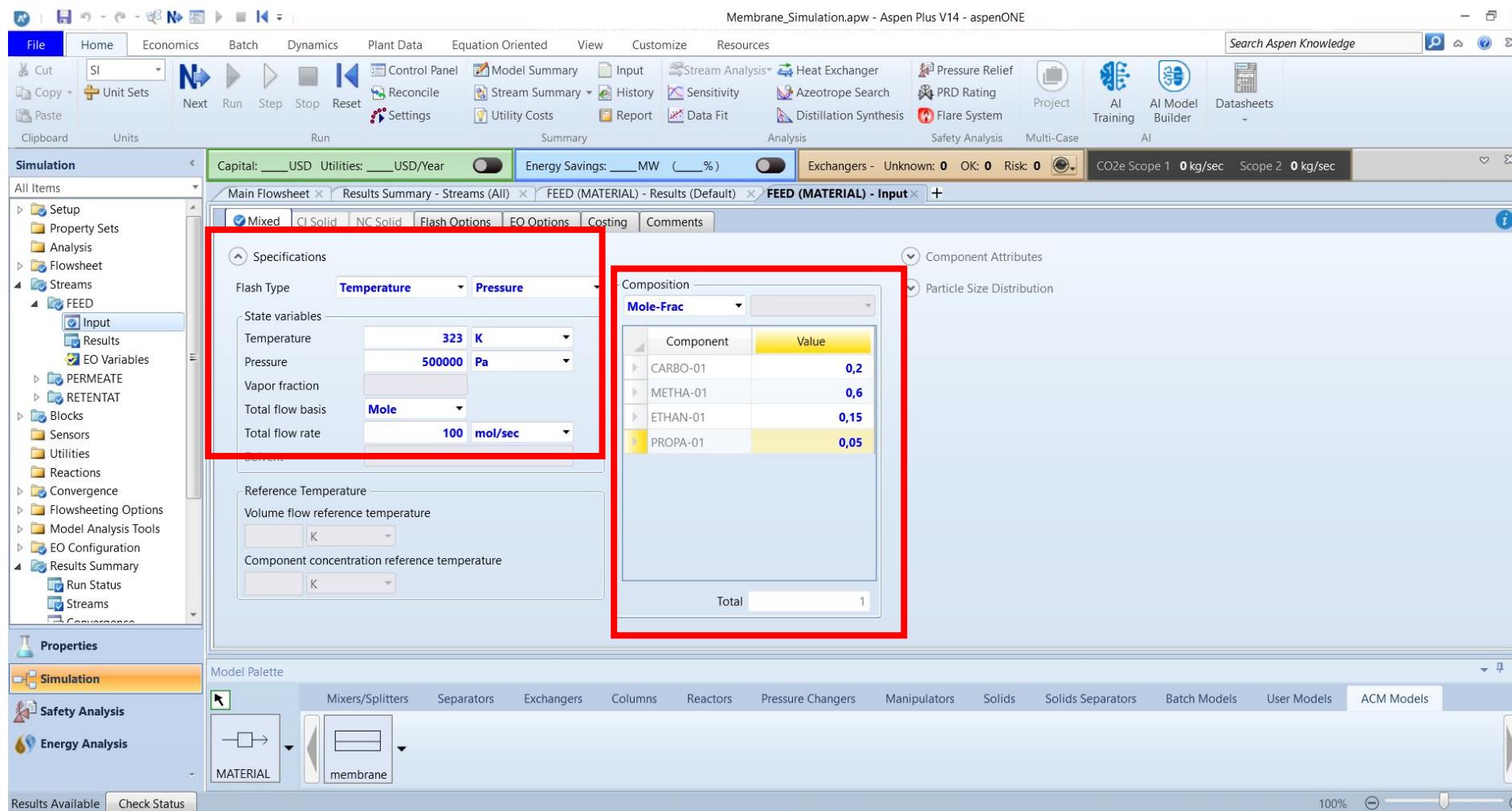
# Utilizando em Aspen Plus o modelo criado

Conectar as correntes de entrada e saída



# Utilizando em Aspen Plus o modelo criado

Especificar as condições da corrente de entrada



# Utilizando em Aspen Plus o modelo criado

## Especificar os parâmetros do modelo de membrana

The screenshot shows the Aspen Plus V14 interface with the project 'Membrane\_Simulation.apw' open. The 'Simulation' tab is selected in the ribbon. On the left, the 'Blocks' tree view shows the 'B1' block expanded, with 'Variables' selected. The main workspace displays a table titled 'AllVariables' under the 'B1 (membrane) - Variables' tab. The table lists various parameters and their properties. A red box highlights the first six rows of the table, which correspond to membrane properties: L, A, P\_RATIO, K(CARBO-01), K(METHA-01), and K(ETHAN-01). The 'Properties' panel on the left shows 'Simulation' selected. The 'Model Palette' at the bottom includes icons for Mixers/Splitters, Separators, Columns, Reactors, Pressure Changers, Manipulators, Solids, Solids Separators, Batch Models, User Models, and ACM Models. The 'mATERIAL' icon is highlighted.

Variable	Value	Units	Physical Type	Specification	Lower Bound	Upper Bound
L	0,003	METER	LENGTH	Constant	0	5e+06
A	10	SQM	AREA	Constant	0	1e+06
P_RATIO	0,8	*	UNTYPED	Constant	0	1
K(CARBO-01)	4,6e-08	*	UNTYPED	Constant	-1e+30	1e+30
K(METHA-01)	1,8e-08	*	UNTYPED	Constant	-1e+30	1e+30
K(ETHAN-01)	6,1e-09	*	UNTYPED	Constant	-1e+30	1e+30
K(PROPA-01)	8,2e-10	*	UNTYPED	Constant	-1e+30	1e+30
J(CARBO-01)	1,53333e-05	KMOL/SQM-S	FLUX-MOLE	Calculated	-10000	10000
J(METHA-01)	6e-06	KMOL/SQM-S	FLUX-MOLE	Calculated	-10000	10000
J(ETHAN-01)	2,03333e-06	KMOL/SQM-S	FLUX-MOLE	Calculated	-10000	10000
J(PROPA-01)	2,73333e-07	KMOL/SQM-S	FLUX-MOLE	Calculated	-10000	10000
INLET.F	0,1	KMOL/SEC	MOLE-FLOW	Constant	0	2,77778e+06
INLET.Z(CARBO-01)	0,2	FRACTION	CONTENTS	Constant	0	1
INLET.Z(METHA-01)	0,6	FRACTION	CONTENTS	Constant	0	1
INLET.Z(ETHAN-01)	0,15	FRACTION	CONTENTS	Constant	0	1

# Utilizando em Aspen Plus o modelo criado

Conferir que os graus de liberdade estão zerados e rodar a simulação

The screenshot shows the Aspen Plus V14 software interface with the following details:

- Title Bar:** Membrane\_Simulation.apw - Aspen Plus V14 - aspenONE
- Toolbar:** Includes icons for Rotate, Flip Horizontal, Flip Vertical, Reconnect, Break, Insert, Align, 3D Icons, Temperature, Mass Flow Rate, Pressure, Mole Flow Rate, Vapor Fraction, Volume Flow Rate, GLOBAL, Show All, Lock Flowsheet, View Parent, Export, View Child, Move Selection, Import, and a Search bar.
- Flowsheet Tab:** Selected tab.
- Simulation Panel:** Capital: \_\_\_\_ USD, Utilities: \_\_\_\_ USD/Year, Energy Savings: \_\_\_\_ MW (\_\_\_\_%), Exchangers - Unknown: 0, OK: 0, Risk: 0, CO2e Scope 1, Scope 2.
- Left Sidebar:** Simulation (Setup, Property Sets, Analysis, Flowsheet, Streams, Blocks, Sensors, Utilities, Reactions, Convergence, Flowsheeting Options, Model Analysis Tools, EO Configuration, Results Summary, Run Status, Streams, Convergence, Operating Costs, CO2 Emissions, Models, Equipment, Datasheets, Dynamic Configuration).
- Properties Panel:** Simulation (selected), Safety Analysis, Energy Analysis.
- Model Palette:** Mixers/Splitters, Separators, Exchangers, Columns, Reactors, Pressure Changers, Manipulators, Solids, Solids Separators, Batch Models, User Models, ACM Models. The "membrane" icon is highlighted.
- Bottom Bar:** Required Input Complete (button with red border), Check Status, and a progress bar at 194%.

The main Flowsheet window displays a process flow for a membrane separation unit (B1). The flow starts with a "FEED" stream entering the unit from the left. From the bottom of the unit, a "PERMEATE" stream exits downwards, and a "RETENTAT" stream exits to the right. The unit is represented by a large rectangular box labeled "B1".

# Dúvidas?



# Recados importantes

- Próxima aula: Reator de Van der Vusse em EMSO
- Os slides desta aula estarão disponíveis no Classroom da disciplina.

“Ensinar não é transferir conhecimento, mas criar as possibilidades para a sua própria produção ou a sua construção.”

Paulo Freire