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Thermolib

The Key to Thermal Management in Simulink®

Introduction and Applications in the Process Industry

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Introduction

Introduction

Thermolib is ...

... modeling thermodynamic systems in Simulink.

... simulation for control.

... Model-Based Design.

... completion of physical modeling toolchain – engineering thermodynamics.

EUtech Scientific Engineering GmbH is a MathWorks Connections Partner.

Introduction

Industries

Introduction

Fields of Application

- Thermodynamic processes (cooling/heating circuits)
- Thermal Power Plants
- Process Industries
- µ-CHPs Systems
- Fuel Cells
- Heat-engines
- HVAC systems

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Features & Benefits

Features & Benefits

Key Features

- Based on the fundamental principles of engineering thermodynamics
- Thermodynamic state and state change calculations including real gas modeling
- Component blocks including heat exchangers, reactors, pumps, turbines, and valves
- Equilibrium and reaction chemistry
- Customizable and extendable thermophysical database and IAPWS-IF97 water and steam properties
- MATLAB command-line functions for thermodynamic calculations and plots

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Benefits of Thermolib

- Customer can concentrate on his core business
  - Consistent basic thermodynamic already implemented
  - Ready-to-use components
- Intuitive process design
  - Flow sheet orientated
- Cost and project time reduction
  - Model Based Design allows earlier error detection
- Risk free safety analysis
- Continuous development and support
  - Compatible with latest MATLAB® version
  - Support via on-site assistance, training, web sessions, e-mail, phone

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Examples – Process Industry

Please note: Demo models marked with * are not included in the scope of supply of the Thermolib-Basic License.

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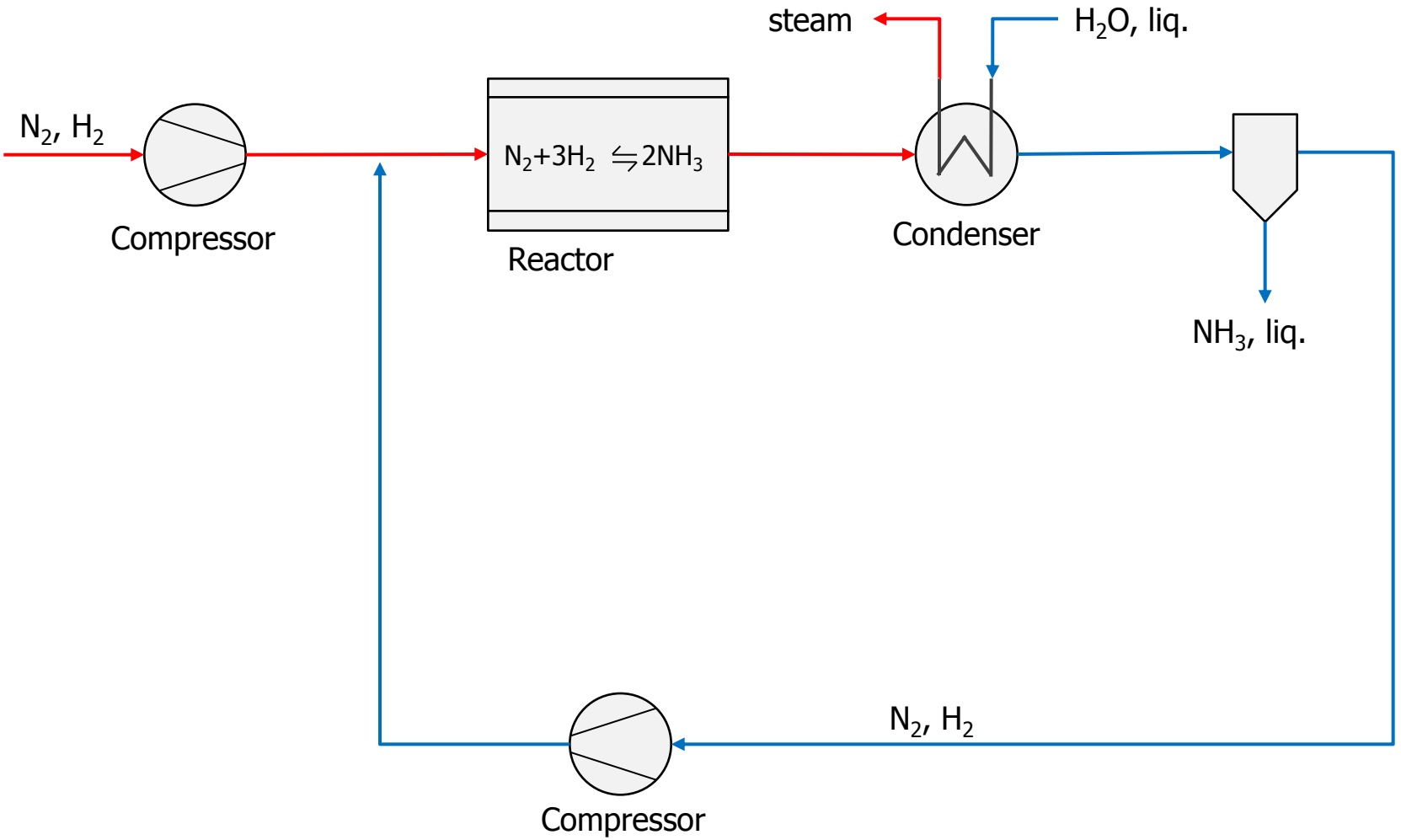
Example – Ammonia Production

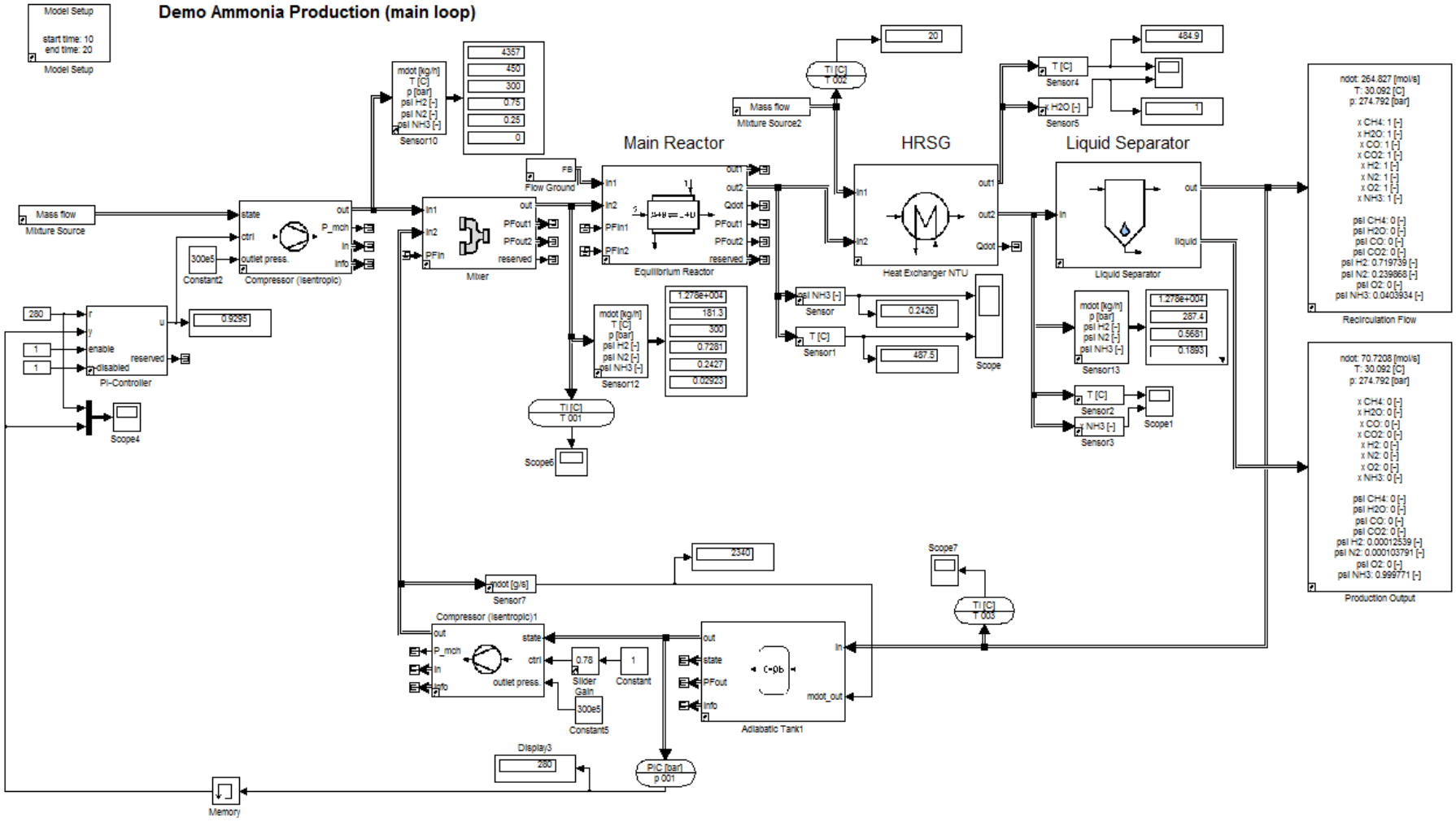
Example - Ammonia Production

Flow scheme – Main loop



Example - Ammonia Production

Simulink Model with Thermolib blocks



DemoAmmoniaProduction.mdl*

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Example – Chemical Reaction Modeling

Example – Chemical Reaction Modeling

Easy to configure

1. Parameterize your reactions:

   $CH_4 + H_2O \leftrightarrow CO + 3\,H_2$

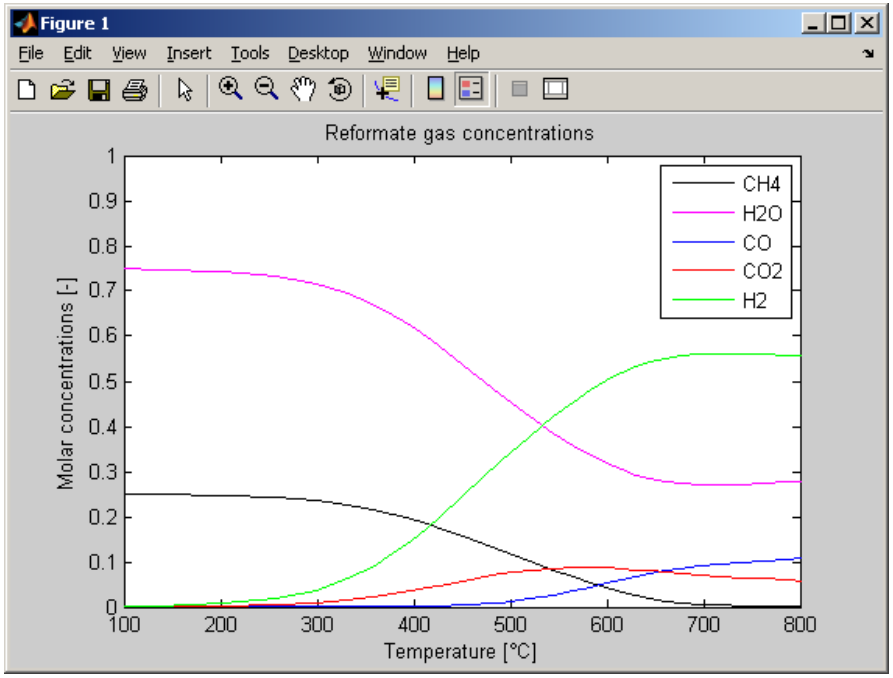
   $CO + H_2O \leftrightarrow CO_2 + H_2$

2. ThermoLib maintains chemical equilibrium at the outputs and correct heat transfer in Simulink®

$$\ln\left[\frac{\left(\frac{y_{CO}\,p_{CO}}{p_0}\right)\cdot\left(\frac{y_{H_2}\,p_{H_2}}{p_0}\right)^3}{\left(\frac{y_{CH_4}\,p_{CH_4}}{p_0}\right)\cdot\left(\frac{y_{H_2O}\,p_{H_2O}}{p_0}\right)}\right] = -\frac{\Delta G^0}{\bar{R}T}$$

$$\ln\left[\frac{\left(\frac{y_{CO_2}\,p_{CO_2}}{p_0}\right)\cdot\left(\frac{y_{H_2}\,p_{H_2}}{p_0}\right)}{\left(\frac{y_{CO}\,p_{CO}}{p_0}\right)\cdot\left(\frac{y_{H_2O}\,p_{H_2O}}{p_0}\right)}\right] = -\frac{\Delta G^0}{\bar{R}T}$$

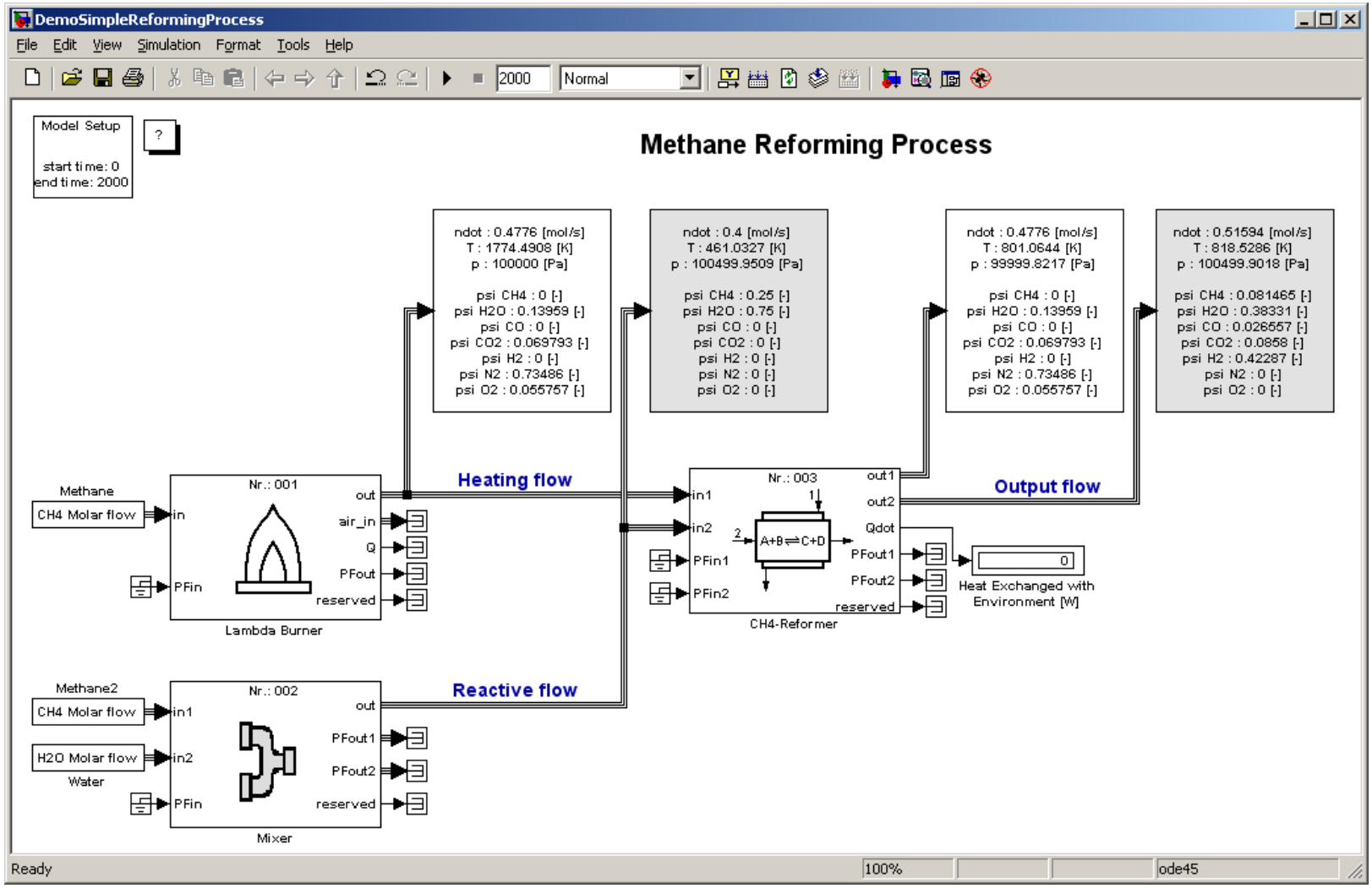
Simulation Results



Steady state molar fractions at different temperatures

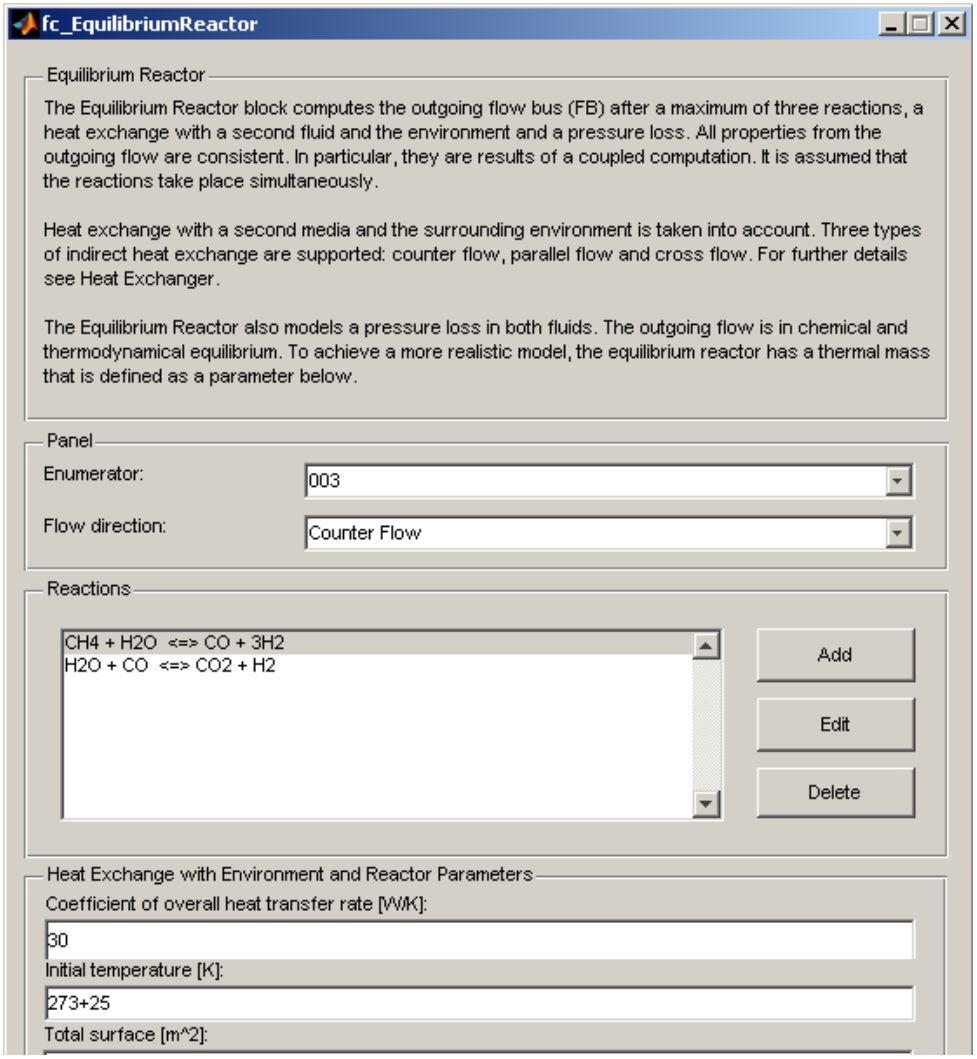
Example – Methane Reforming Process

Simulink Model with Thermolib blocks



Example – Methane Reforming Process

Easy Definition of Chemical Reactions



Example – Methane Reforming Process

Thermodynamic Balancing

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	**Modelname**	DemoSimpleReformingProcess												
2	**date**	29-May-2009 07:55:16												
3														
4	**Balance Space Name**	**Port Name**	**Port Direction**	CH4 [g]	H2O [g]	CO [g]	CO2 [g]	H2 [g]	N2 [g]	O2 [g]	H [mol]	C [mol]	O [mol]	N [mol]
5	**TotalBalance**			3612,282	-6721,59	-656,437	-8877,99	-155,663	0	12799,6	0	0	0	0
6	**Lambda Burner**													
7		Input flow	in	200	0	0	0	0	0	0	800	200	0	0
8		Input Air	in	0	0	0	0	0	1654,576	439,824	0	0	879,648	3309,152
9		Output Gas	out	0	400	0	200	0	1654,576	39,824	800	200	879,648	3309,152
10														
11	**Mixer**													
12		Input flow 1	in	200	0	0	0	0	0	0	800	200	0	0
13		Input flow 2	in	0	27,2	0	0	0	0	0	54,4	0	27,2	0
14		Output flow	out	200	27,2	0	0	0	0	0	854,4	200	27,2	0
15														
16	**Equilibrium Reactor**													
17		Input heating	in	0	400	0	200	0	1654,576	39,824	800	200	879,648	3309,152
18		Input reacting	in	200	27,2	0	0	0	0	0	854,4	200	27,2	0
19		Output heatir	out	0	400	0	200	0	1654,576	39,824	800	200	879,648	3309,152
20		Output reacti	out	174,8375	0,310976	23,43582	1,726596	77,21384	0	0	854,3996	199,9999	27,19999	0
21														
22	**Balance**			403,6821	484,4058	-656,437	-75,9875	-155,663	0	0	0	0	0	0
23														

Example – Methane Reforming Process

Thermodynamic Balancing

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	Modelname	DemoSimpleReformingProcess												
2	date	29-May-2009 07:55:16												
3														
4	Balance Space Name													
5	TotalBalance													
6	Lambda Burner													
7														
8														
9														
10														
11	Mixer													
12														
13														
14														
15														
16	Equilibrium Rea													
17														
18														
19														
20														
21														
22	Balance													
23														

BalanceTest.txt - Notepad

File Edit Format View Help

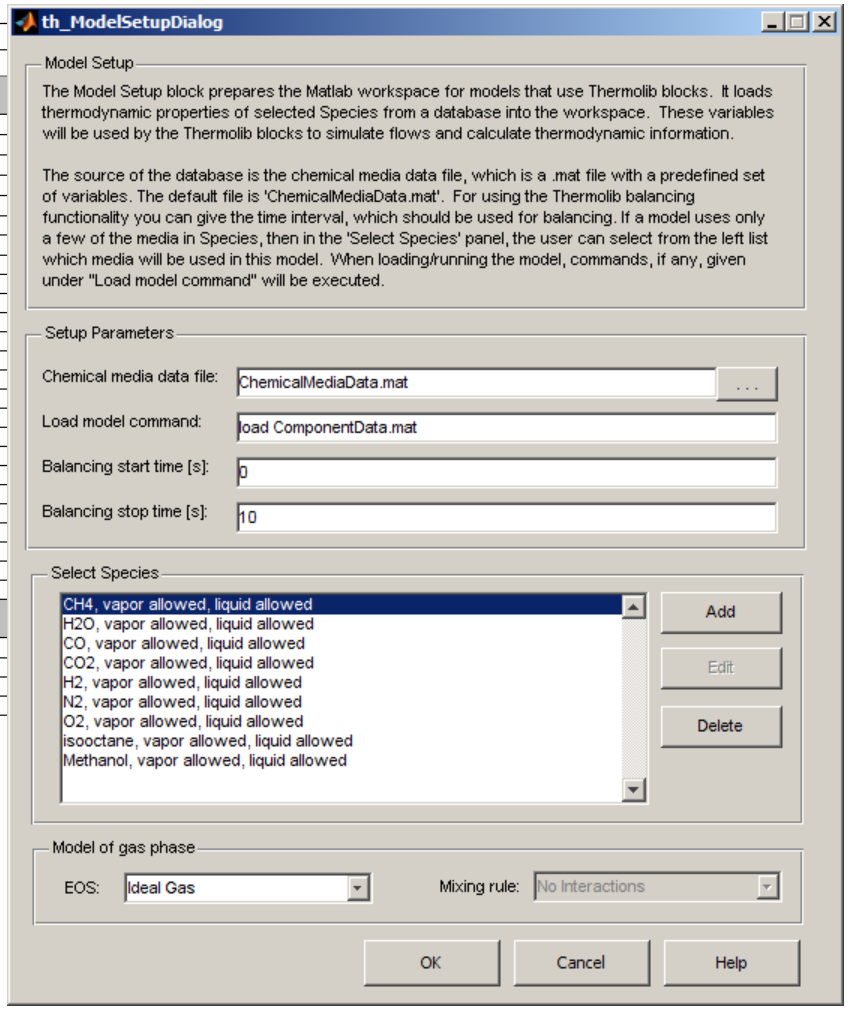
```
Modelname               DemoSimpleReformingProcess
date                    29-May-2009 07:55:16

Balance Space Name      Port Name               Port Direction          CH4 [g]             H2O [g]             CO [
TotalBalance                                                            3612.282            -6721.594           -656
Lambda Burner
                        Input flow              in                      200.000             0.000               0.00
                        Input Air               in                      0.000               0.000               0.00
                        Output Gas              out                     0.000               400.000             0.00

Mixer
                        Input flow 1            in                      200.000             0.000               0.00
                        Input flow 2            in                      0.000               27.200              0.00
                        Output flow             out                     200.000             27.200              0.00

Equilibrium Reactor
                        Input heating flow      in                      0.000               400.000             0.00
                        Input reacting flow     in                      200.000             27.200              0.00
                        Output heating flow     out                     0.000               400.000             0.00
                        Output reacting flow    out                     174.837             0.311               23.4

Balance                                                                 403.682             484.406             -656

Modelname               DemoSimpleReformingProcess
date                    29-May-2009 07:55:16

Balance Space Name      Port Name               Port Direction          [J]
TotalBalance                                                            -5259246.225
Lambda Burner
                        Qdot                    in                      -4605906.097
Mixer
Equilibrium Reactor
                        Heat loss               in                      0.000
                        Energy Thermal Mass     stored_start            653340.128
                        Energy Thermal Mass     stored_end              653340.128
Balance                                                                 -653340.128
```

Example – Methane Reforming Process

Chemical Media Data

Chemical Media Data

	Species	CH4	H2O	H2O-IF97	
	formula				
	full_name	methane	water	water IAPWS-IF97	
Chemical media data					
Molar Mass *[kg/kmol]*	M	16,043	18,015	18,015	
Liquid density *[g/m³]*	rho_liq	422620,0	1,00E+06	1,00E+06	
Antonie equation_ A *[-]*	Antoine_A	3,9895	5,111	4,5396014	
Antonie equation_ B *[-]*	Antoine_B	443,028	1685	846,3	
Antonie equation_ C *[-]*	Antoine_C	-0,49	-43,22	-288,7	
Reference temperaure for evap. properties *[K]*	T_fg_ref	111,6	298	298	
Evaporation enthalpy *[Joule/mole]*	hm_fg	8183	43961,4	43961,4	
Evaporation entropy *[Joule/mole-K]*	sm_fg	73,36664655	118,7557231	-1507,731428	
Critical Temperatur *[K]*	T_c	190,600	647,300	647,300	
Critical Pressure *[Pa]*	p_c	4,60E+06	2,21E+07	2,21E+07	
Critical Volume *[m³/mol]*	vm_c	9,90E-05	5,60E-05	5,60E-05	
Acentric Factor *[-]*	omega	0,288	0,344	0,344	
Red. De-Broglie-Wavel. *[-]*	lambda_R	999,000	999,000	999,000	
Critical Real-Factor *[-]*	Zc	0,288	0,229	0,229	
Linear Molecule *[-]*	linear	1	0	0	
Dipole Moment *[Debye]*	mue	0,0	1,8	1,8	
Boiling Temperature *[K]*	Ts	111,7	373,2	373,2	
Inner Rotation *[-]*	c_mir	999,0	-3,0	-3,0	
Number of C atoms *[-]*	C_atoms	1	0	0	
Number of H atoms *[-]*	H_atoms	4	2	2	
Number of O atoms *[-]*	O_atoms	0	1	1	
Number of N atoms *[-]*	N_atoms	0	0	0	
Number of F atoms *[-]*	F_atoms	0	0	0	
Number of Cl atoms *[-]*	Cl_atoms	0	0	0	
Heat capacity of liquid (Cp = A + B*T +C*T^2 + D*T^3)					
A-element *[J/mol*K]*	Cp_liq_A	60	5,081069E+01	5,081069E+01	
B-element *[J/mol*K^2]*	Cp_liq_B	0,000	2,129361E-01	2,129361E-01	
C-element *[J/mol*K^3]*	Cp_liq_C	0,000	-6,309691E-04	-6,309691E-04	
D-element *[J/mol*K^4]*	Cp_liq_D	0,000	6,483055E-07	6,483055E-07	



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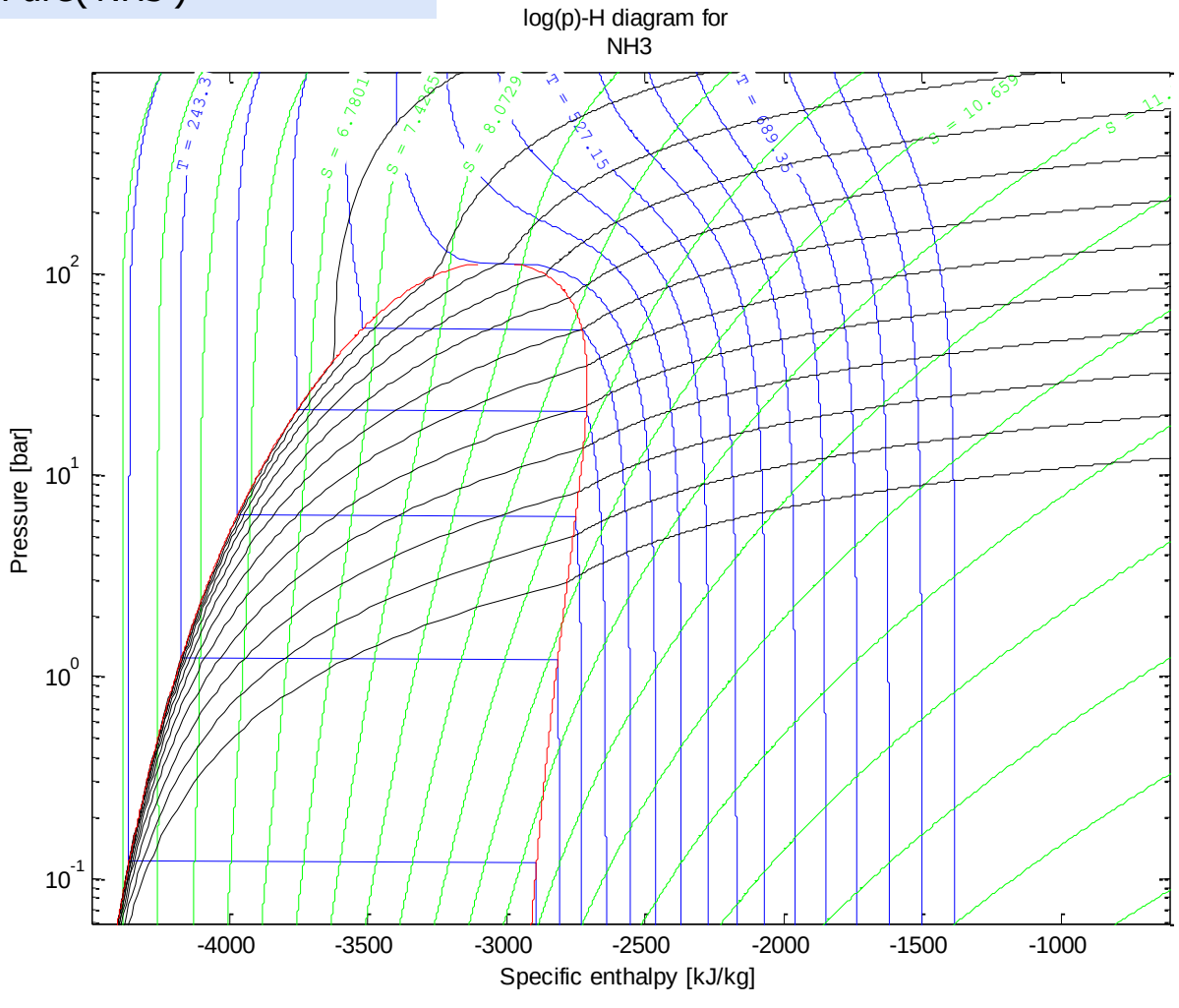
Example – Species Diagrams

Example – Species Diagrams

Species Diagrams

```
>>th_PlotLogPHPure('NH3')
```



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Example – Command Line Functions

Command Line Functions

Compression of Air

Defining the initial state:

```
initial_state = th_TpState(
    'ndot',1000/28.85,
    'T',300,
    'p',1e5,
    'psi',[0.21; 0.79],
    'species',{'O2','N2'},
    'MediaData',SMediaData);

initial_state =

     ndot: 34.6620
        T: 300
        p: 100000
     Hdot: 1.8711e+003
     Sdot: 6.8945e+003
     Gdot: -2.0665e+006
    Cpdot: 1.0115e+003
        x: [2x1 double]
      psi: [2x1 double]
```

A massflow of 1kg/s of Air (21% O2, 79% N2) At 300K and 1bar

Result is a struct containing the defined state

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Compression of Air

Calculate isentropic compression first:

```
isentropic_compression = th_SpState(
    'ndot',1000/28.85,
    'Sdot',initial_state.Sdot,
    'p',10e5,
    'psi',[0.21; 0.79],
    'species',{'O2','N2'},
    'MediaData',SMediaData);
```

Isentropic State Change

Compression by 9 bar

Calculate final state with isentropic efficiency

```
final_state = th_HpState(
    'ndot',1000/28.85,
    'Hdot',initial_state.Hdot + (isentropic_compression.Hdot -
       initial_state.Hdot) / 0.85,
    'p',10e5,
    'T_initial', isentropic_compression.T,
    'psi',[0.21; 0.79],
    'species',{'O2','N2'},
    'MediaData',SMediaData);
```

Final enthalpy calculation with isentropic efficiency of 85%

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Summary

Summary

Thermolib allows you to...

- Concentrate on your core business
- Enjoy the intuitive process design
- Reduce your costs and project time
- Benefit from continuous development and support

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www.thermolib.de