

# Thermolib

The Key to Thermal Management in Simulink®

Introduction and Applications in the Process Industry

Release 5.3



Thermolib

- Introduction
- Features & Benefits
- Examples – Process Industry
  - Ammonia Production
  - Chemical Reaction Modeling
  - Species Diagrams
  - Command Line Functions
- Summary

**Thermolib**

# 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.



## Industries



## Fields of Application

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



**Thermolib**

## **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

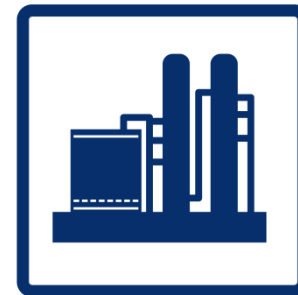


### Benefits of Thermolib

- 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<sup>®</sup> version
  - Support via on-site assistance, training, web sessions, e-mail, phone

**Thermolib**

## Examples – Process Industry



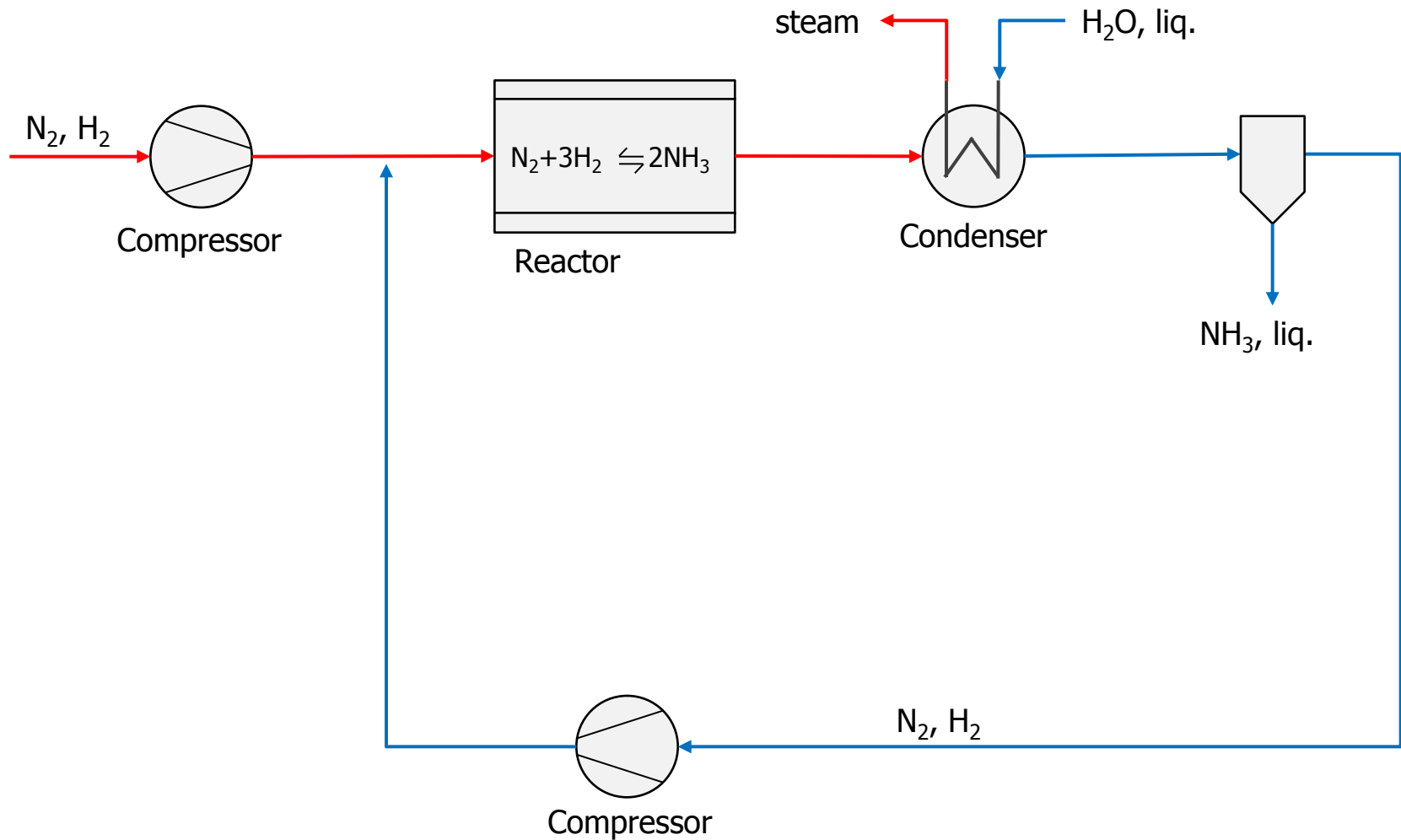
Please note: Demo models marked with \* are not included in the scope of supply of the Thermolib-Basic License.

**Thermolib**

## Example – Ammonia Production

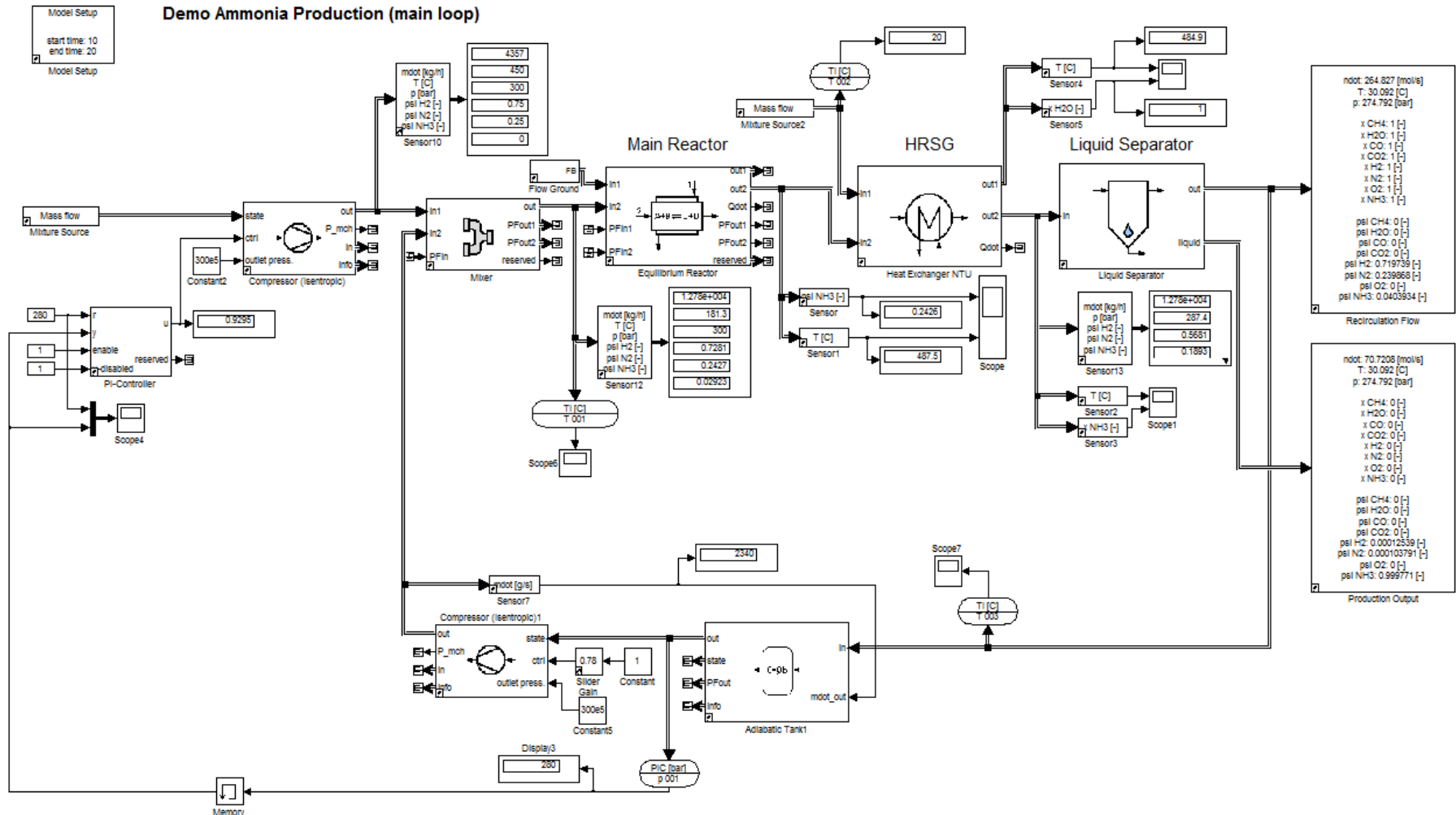
# Example - Ammonia Production

## Flow scheme – Main loop



# Example - Ammonia Production

## Simulink Model with Thermolib blocks



DemoAmmoniaProduction.mdl\*

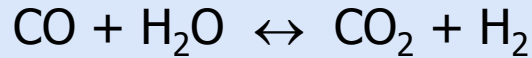
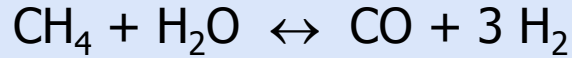
**Thermolib**

## Example – Chemical Reaction Modeling

# Example – Chemical Reaction Modeling

## Easy to configure

1. Parameterize your reactions:

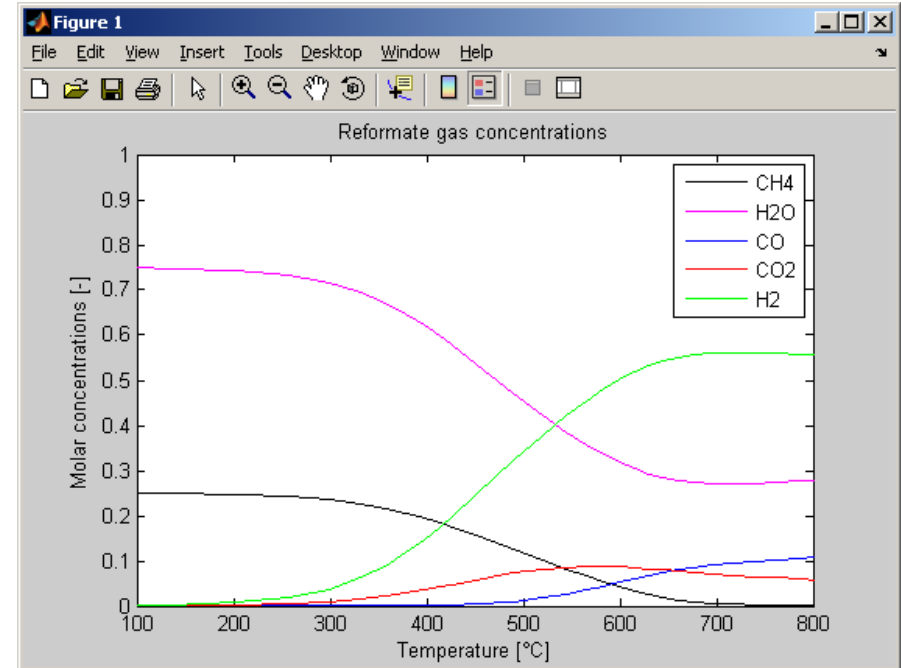


2. ThermoLib maintains chemical equilibrium at the outputs and correct heat transfer in Simulink®

$$\ln \left[ \frac{\left( \frac{y_{\text{CO}} P_{\text{CO}}}{p_0} \right) \cdot \left( \frac{y_{\text{H}_2} P_{\text{H}_2}}{p_0} \right)^3}{\left( \frac{y_{\text{CH}_4} P_{\text{CH}_4}}{p_0} \right) \cdot \left( \frac{y_{\text{H}_2\text{O}} P_{\text{H}_2\text{O}}}{p_0} \right)} \right] = - \frac{\Delta G^0}{RT}$$

$$\ln \left[ \frac{\left( \frac{y_{\text{CO}_2} P_{\text{CO}_2}}{p_0} \right) \cdot \left( \frac{y_{\text{H}_2} P_{\text{H}_2}}{p_0} \right)}{\left( \frac{y_{\text{CO}} P_{\text{CO}}}{p_0} \right) \cdot \left( \frac{y_{\text{H}_2\text{O}} P_{\text{H}_2\text{O}}}{p_0} \right)} \right] = - \frac{\Delta G^0}{RT}$$

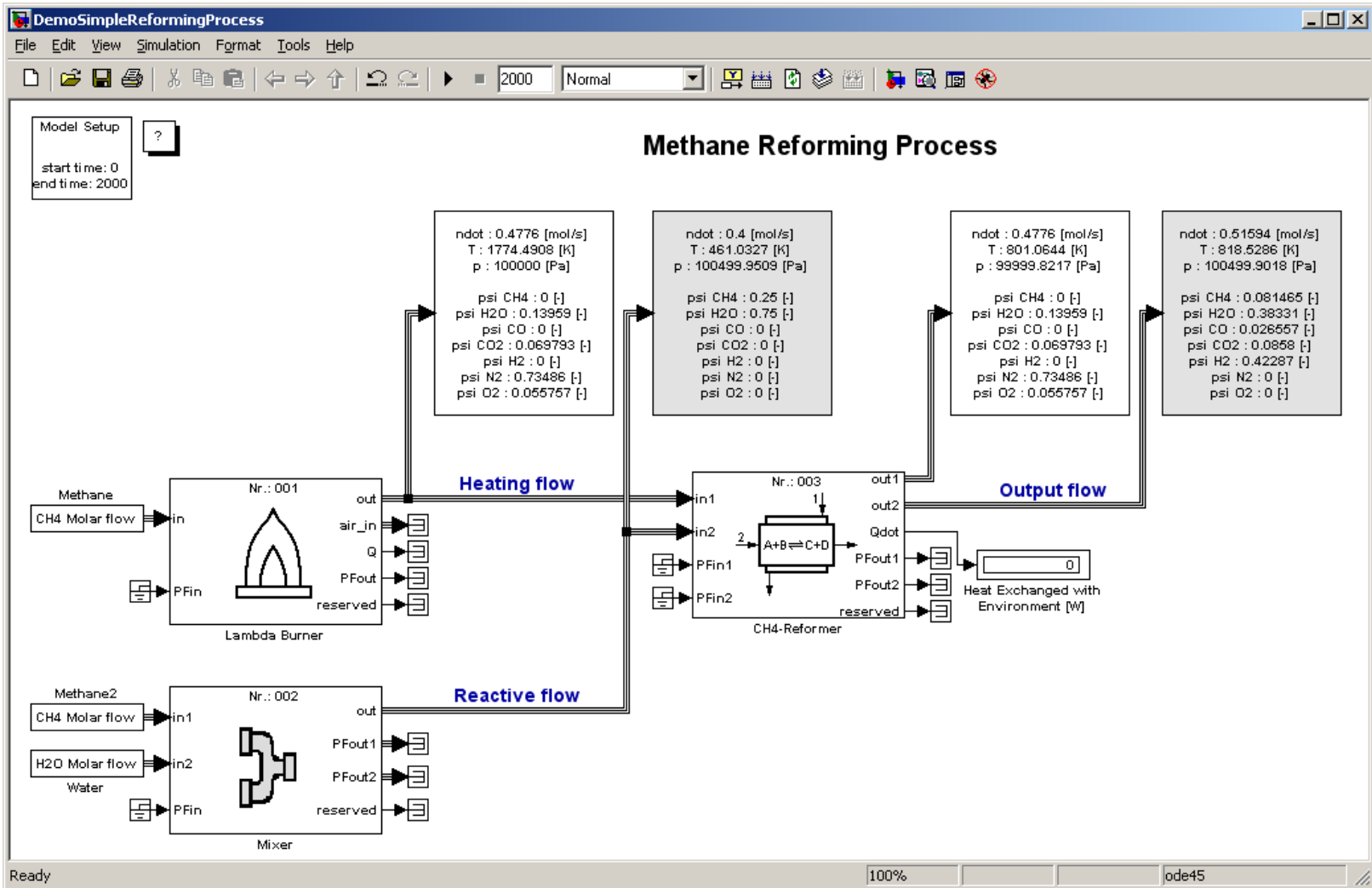
## Simulation Results



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

**fc\_EquilibriumReactor**

Equilibrium Reactor

The Equilibrium Reactor block computes the outgoing flow bus (FB) after a maximum of three reactions, a heat exchange with a second fluid and the environment and a pressure loss. All properties from the outgoing flow are consistent. In particular, they are results of a coupled computation. It is assumed that the reactions take place simultaneously.

Heat exchange with a second media and the surrounding environment is taken into account. Three types of indirect heat exchange are supported: counter flow, parallel flow and cross flow. For further details see Heat Exchanger.

The Equilibrium Reactor also models a pressure loss in both fluids. The outgoing flow is in chemical and thermodynamical equilibrium. To achieve a more realistic model, the equilibrium reactor has a thermal mass that is defined as a parameter below.

Panel

Enumerator:

Flow direction:

Reactions

Heat Exchange with Environment and Reactor Parameters

Coefficient of overall heat transfer rate [W/K]:

Initial temperature [K]:

Total surface [m<sup>2</sup>]:

# 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 heating out		0	400	0	200	0	1654,576	39,824	800	200	879,648	3309,152
20		Output reacting 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																																																																																														
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# Example – Methane Reforming Process

## Chemical Media Data

Chemical Media Data				
Species	CH4	H2O	H2O-IF97	
formula				
full_name	methane	water	water IAPWS-IF97	
<b>Chemical media data</b>				
Molar Mass [kg/kmol]	M	16,043	18,015	18,015
Liquid density [g/m <sup>3</sup> ]	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 temperature 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 [m <sup>3</sup> /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
<b>Heat capacity of liquid (Cp = A + B*T + C*T^2 + D*T^3)</b>				
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

### th\_ModelSetupDialog

**Model Setup**

The Model Setup block prepares the Matlab workspace for models that use Thermolib blocks. It loads thermodynamic properties of selected Species from a database into the workspace. These variables will be used by the Thermolib blocks to simulate flows and calculate thermodynamic information.

The source of the database is the chemical media data file, which is a .mat file with a predefined set of variables. The default file is 'ChemicalMediaData.mat'. For using the Thermolib balancing functionality you can give the time interval, which should be used for balancing. If a model uses only a few of the media in Species, then in the 'Select Species' panel, the user can select from the left list which media will be used in this model. When loading/running the model, commands, if any, given under "Load model command" will be executed.

**Setup Parameters**

Chemical media data file:  ...

Load model command:

Balancing start time [s]:

Balancing stop time [s]:

**Select Species**

- CH4, vapor allowed, liquid allowed
- H2O, vapor allowed, liquid allowed
- CO, vapor allowed, liquid allowed
- CO2, vapor allowed, liquid allowed
- H2, vapor allowed, liquid allowed
- N2, vapor allowed, liquid allowed
- O2, vapor allowed, liquid allowed
- isooctane, vapor allowed, liquid allowed
- Methanol, vapor allowed, liquid allowed

**Model of gas phase**

EOS:       Mixing rule:

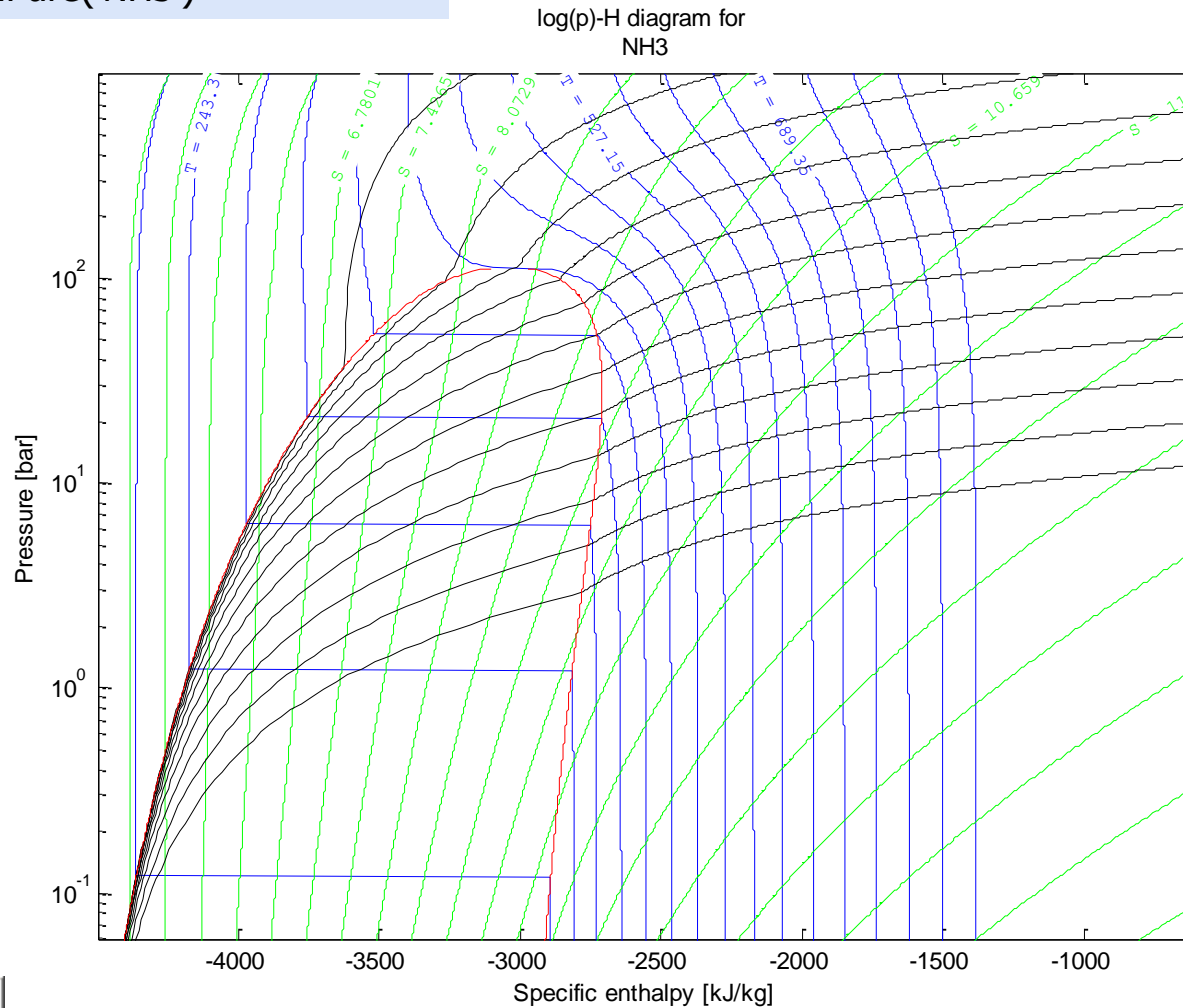
**Thermolib**

## Example – Species Diagrams

# Example – Species Diagrams

## Species Diagrams

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



**Thermolib**

## Example – 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);
```

A massflow of 1kg/s of  
Air (21% O<sub>2</sub>, 79% N<sub>2</sub>)  
At 300K and 1bar

```
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]
```

Result is a struct  
containing the defined  
state



## Compression of Air

Calculate isentropic compression first:

```
isentropic_compression = th_SpState(  
    'ndot', 1000/28.85,  
    'Sdot', initial_state.Sdot, ← Isentropic State Change  
    'p', 10e5, ← Compression by 9 bar  
    'psi', [0.21; 0.79],  
    'species', {'O2', 'N2'},  
    'MediaData', SMediaData);
```

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, ← Final enthalpy calculation with  
    'p', 10e5, isentropic efficiency of 85%  
    'T_initial', isentropic_compression.T,  
    'psi', [0.21; 0.79],  
    'species', {'O2', 'N2'},  
    'MediaData', SMediaData);
```

**Thermolib**

## 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

**[www.thermolib.de](http://www.thermolib.de)**