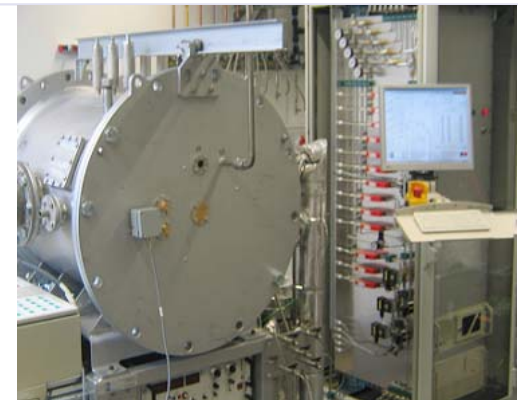
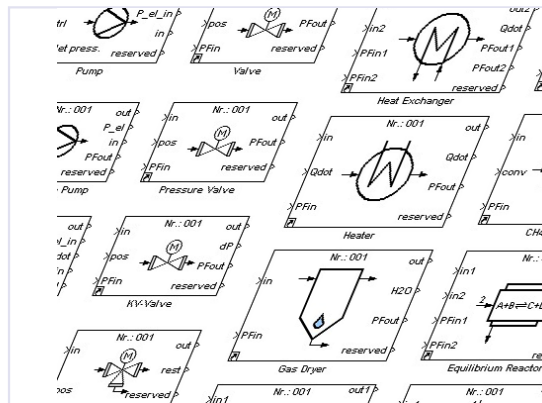


# Thermolib

Thermodynamic systems library

Introduction and Applications

Release 5.0



5.0.0.2/5.0c

## Introduction

### Thermolib ...

- ... is a Simulink® library for modeling and simulation of thermodynamic **systems**.
- ... focuses on modeling and simulation at the **systems level**  
**=> simulation for control.**
- ... provides seamless integration with The MathWorks tools used for Model-Based Design and rapid control prototyping.
- ... fills a gap in The MathWorks products suite – engineering thermodynamic modeling.

EUtech Scientific Engineering GmbH is member in  
The MathWorks Connections program.



# Content

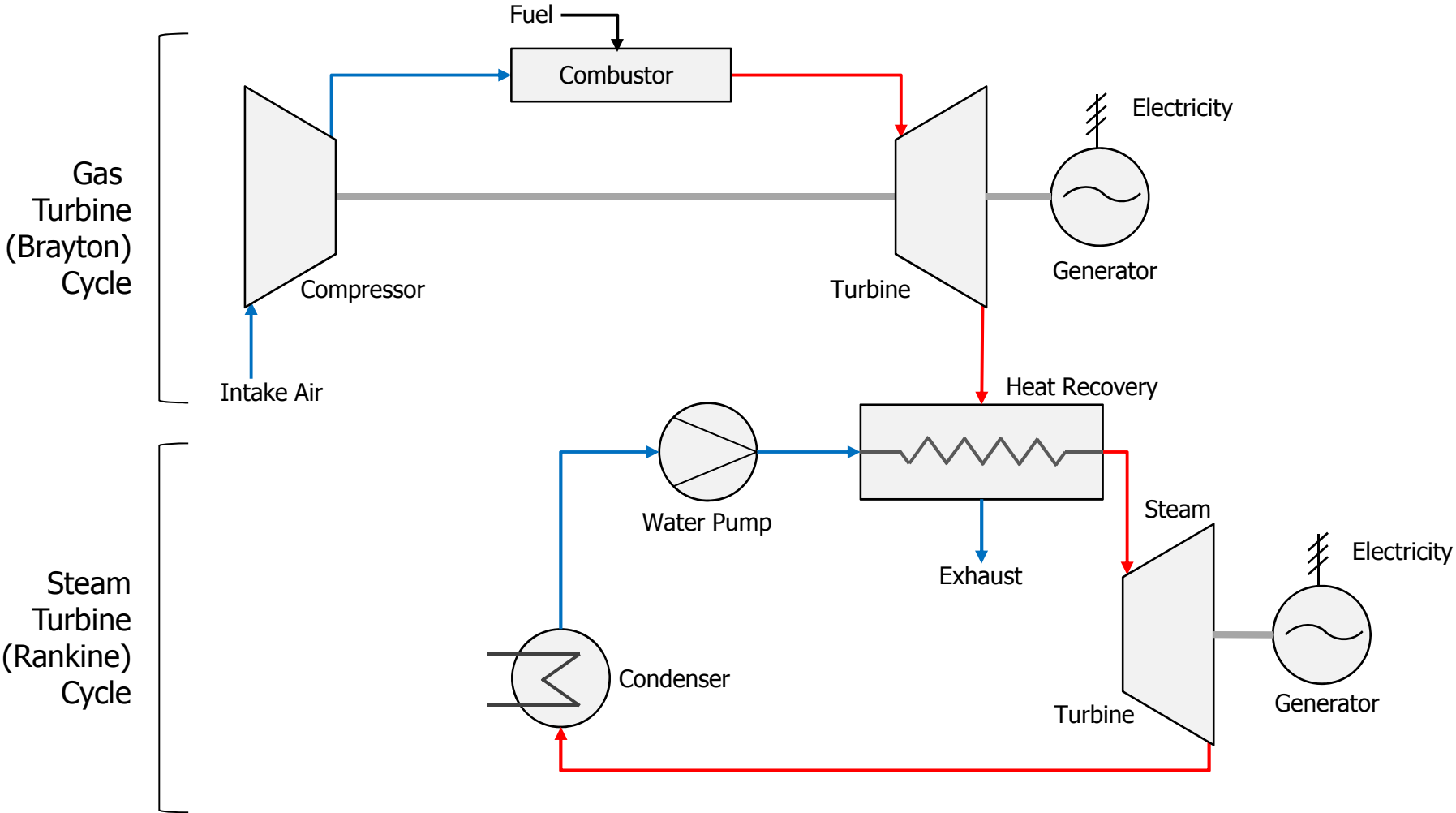
- Examples
  - Power Plants (Combined Cycle, Forced Circulation, Solar Thermal)
  - Fuel Cell Vehicle
  - Ammonia Production
  - Heating Installation
  - Air Conditioning
  - Reforming Process
- Architecture
  - Special features
  - Command line functions
- How does Thermolib integrate into The MathWorks tool chain?
- Summary

# Systems that can be modeled ...

# Example – Combined Cycle Power Plant

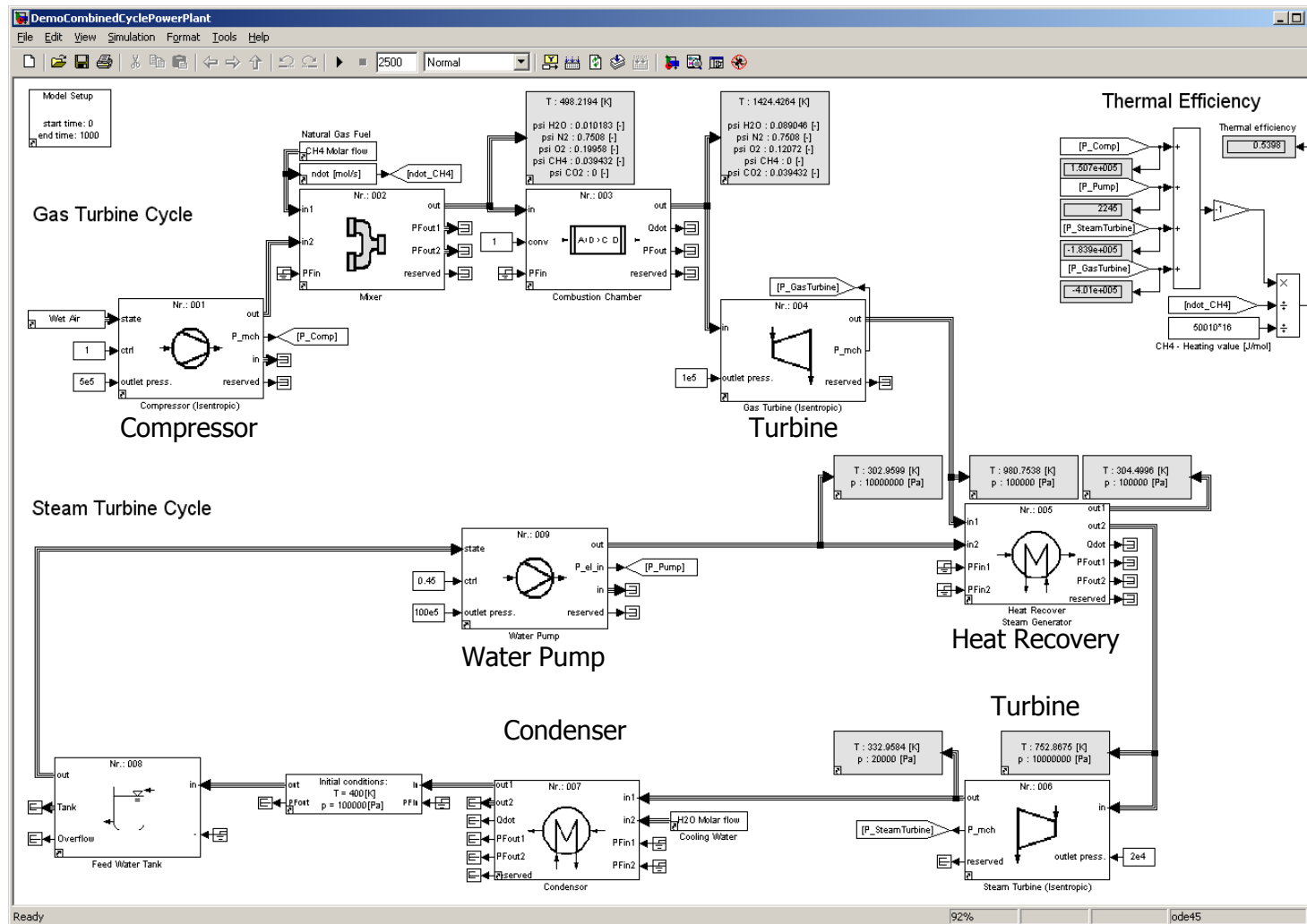
# Example – Combined Cycle Power Plant

## Flow scheme



# Example – Combined cycle power plant

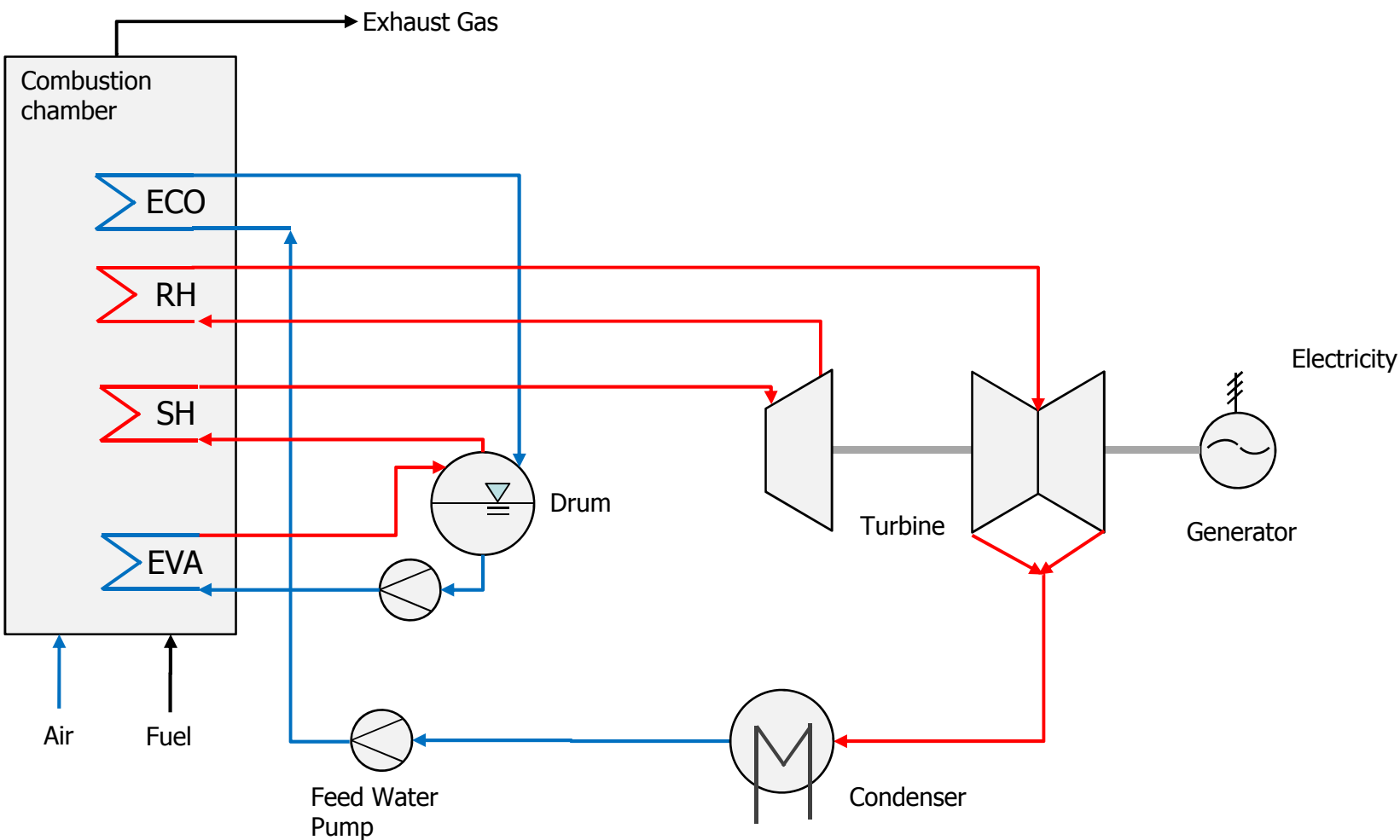
## Simulink Model with Thermolib blocks



# Example – Forced Circulation Boiler

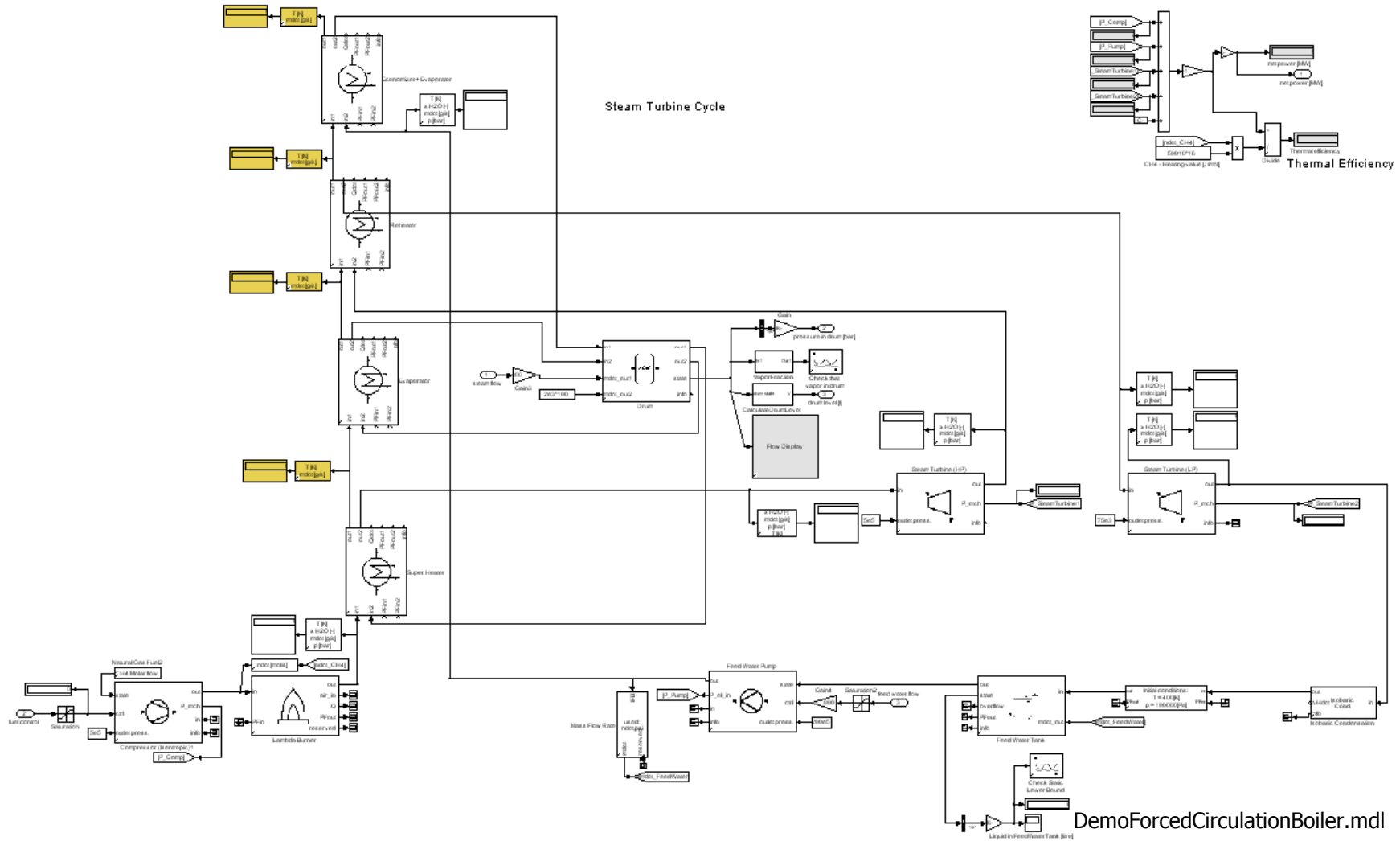
# Example – Forced Circulation Boiler

## Flow scheme



# Example – Forced Circulation Boiler

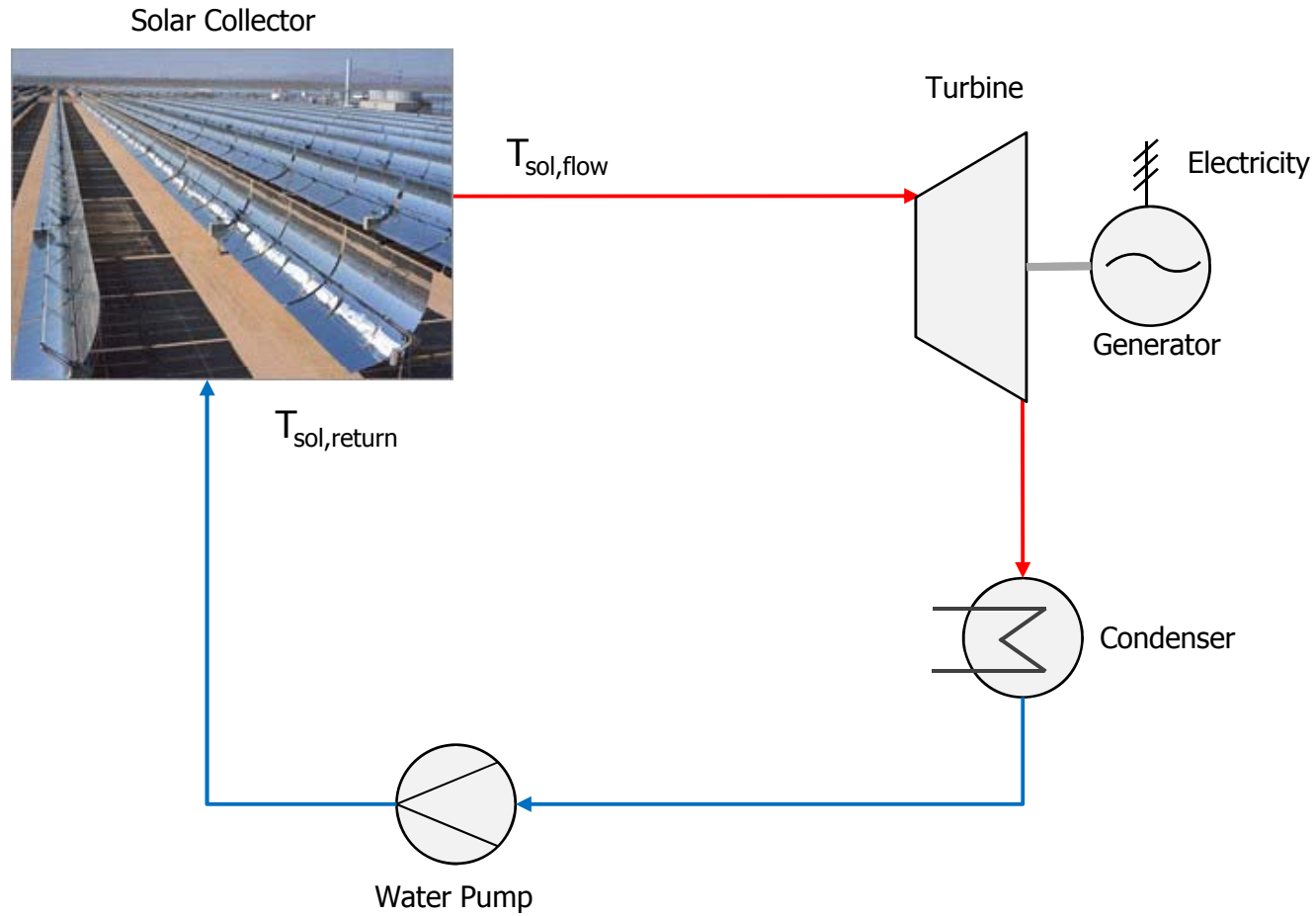
## Simulink implementation using Thermolib



# Example – Solar Thermal Plant

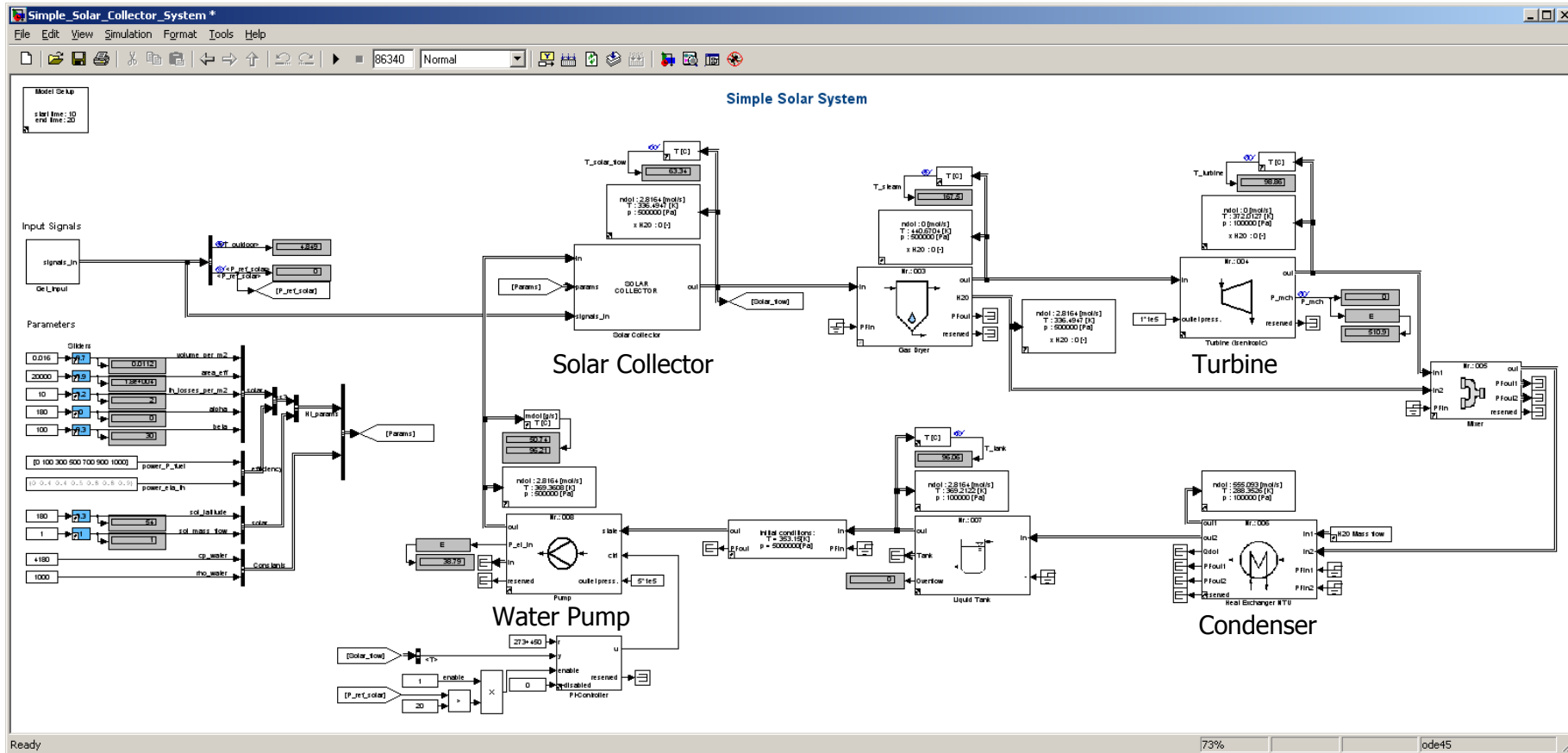
# Example – Solar Thermal Plant

## Flow scheme



# Example – Solar Thermal Plant

## Simulink Model with Thermolib blocks



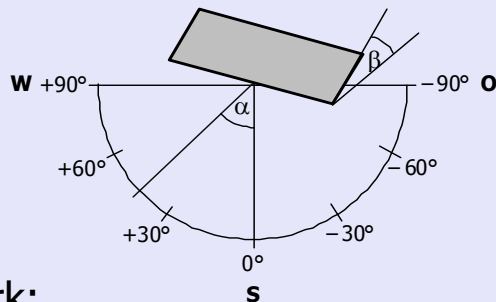
DemoSimpleSolarCollectorSystem.mdl



## Example – Solar Thermal Plant

### Configuration

1. Effective area of solar collectors: 18,000 square meters.
2. Slope  $\beta = 30^\circ$
3. Oriented  $36^\circ$  west of south

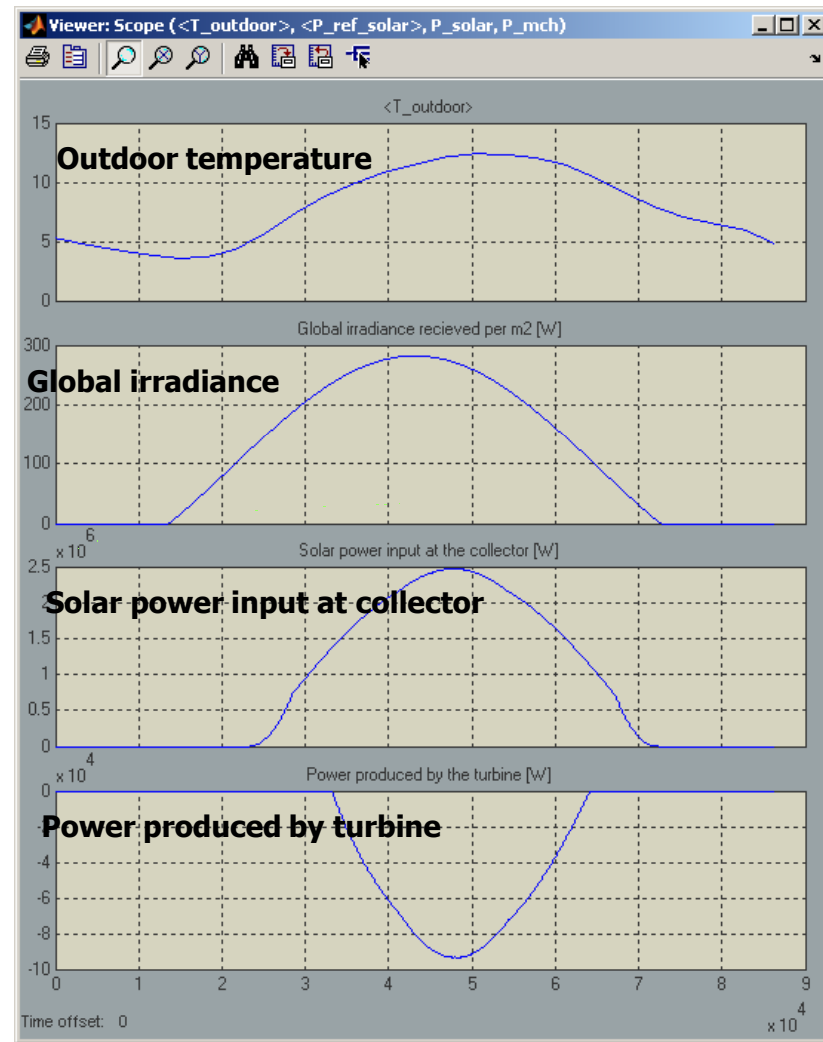


Remark:

The position and the west orientation is just to show the effects in this example (see lag of turbine power against irradiance).

A real world plant would adjust position to geographical location and could optionally use active tracking of current sun position to maximize input power.

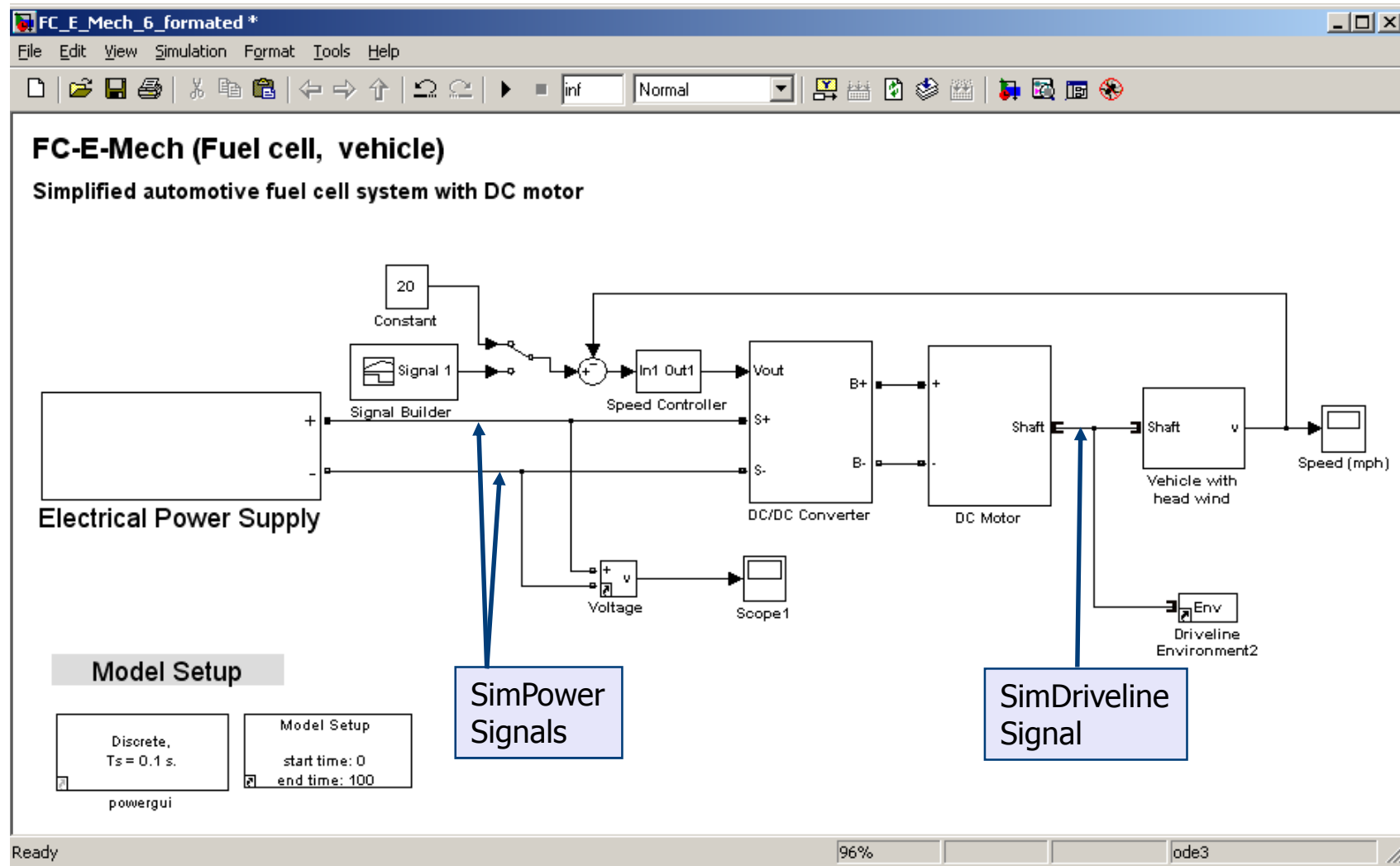
### Simulation Results



# Example – Fuel Cell Vehicle

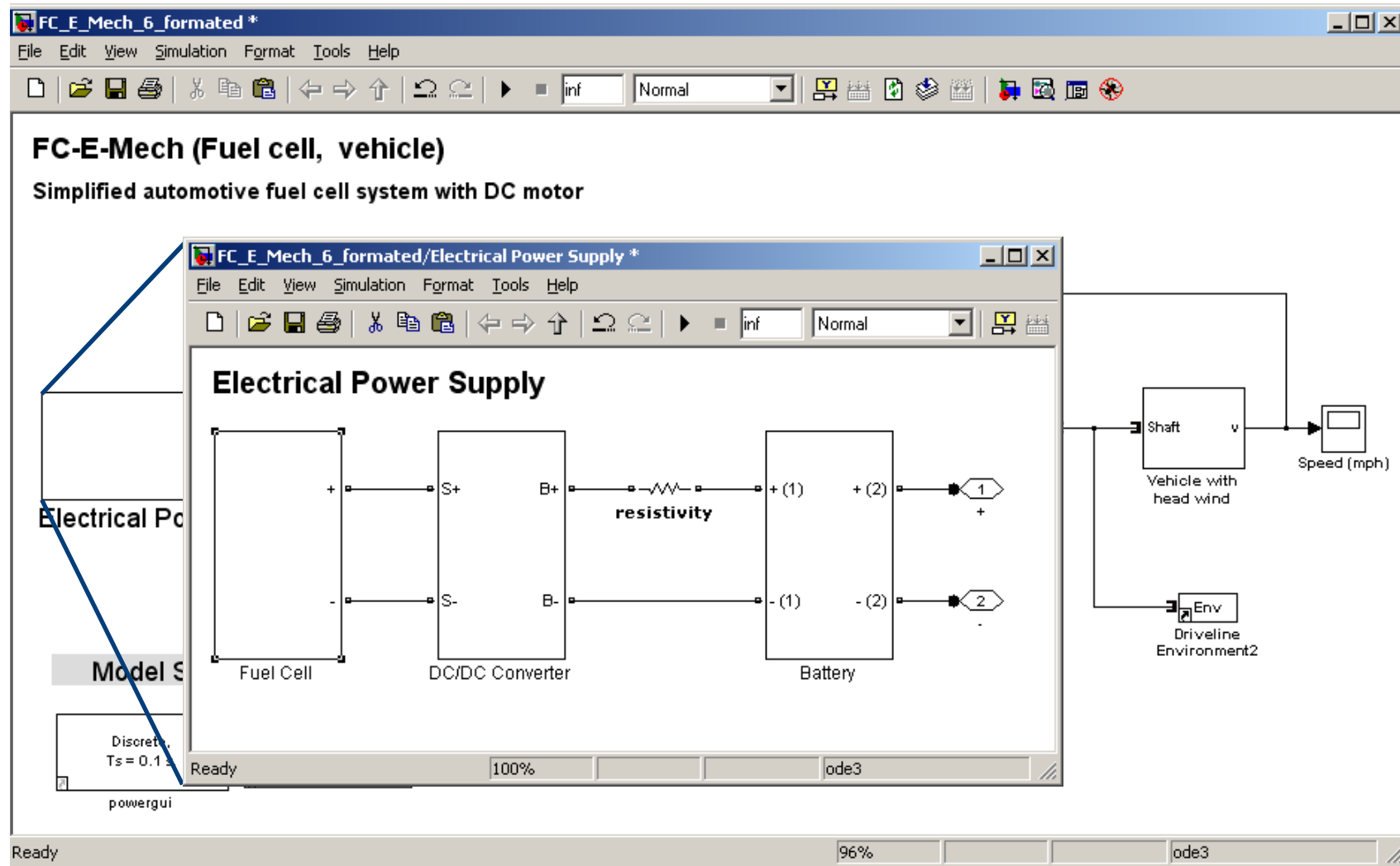
# Example – Fuel Cell Vehicle

## Overview



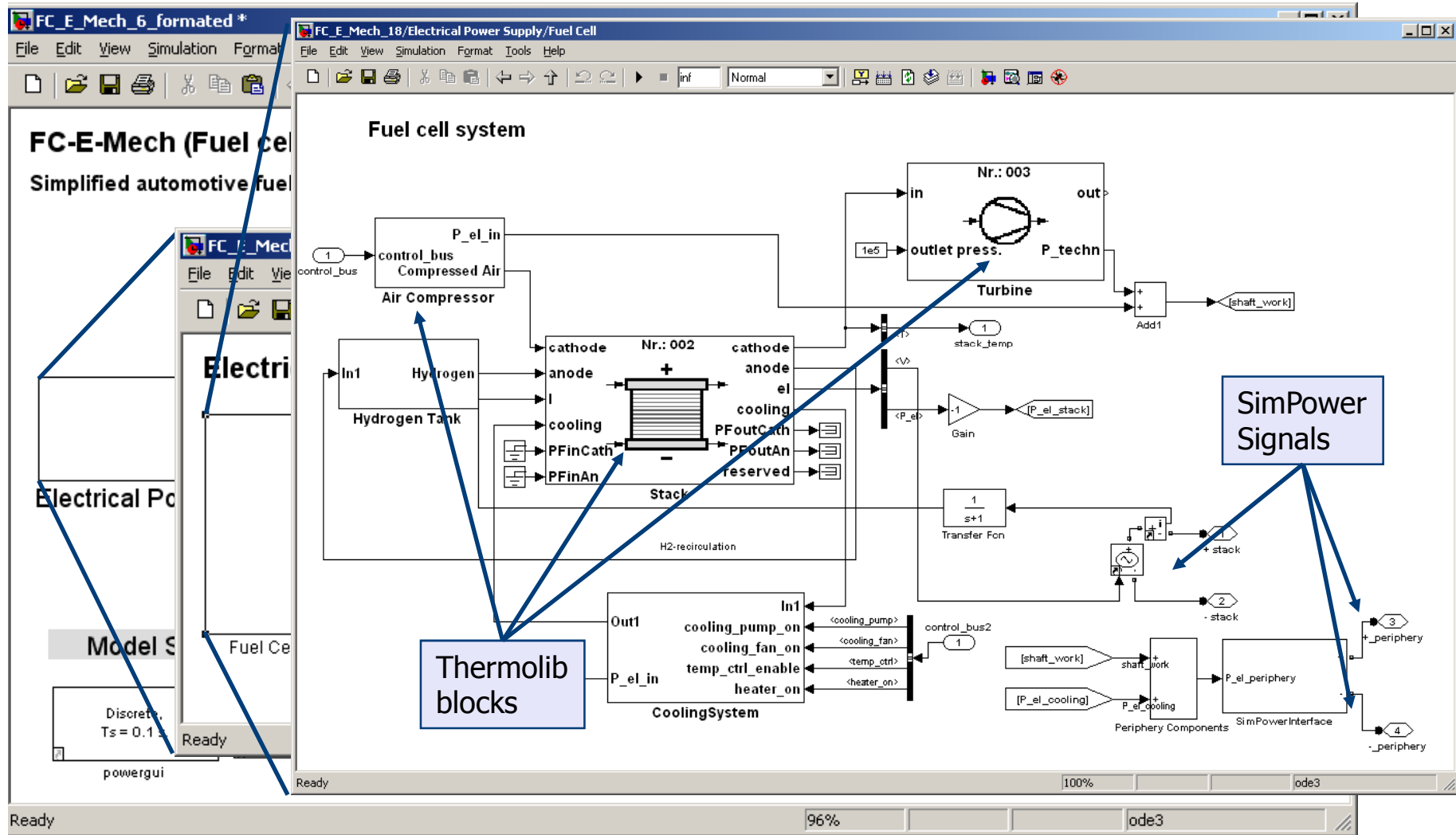
# Example – Fuel Cell Vehicle

## Electrical Power Supply



# Example – Fuel Cell Vehicle

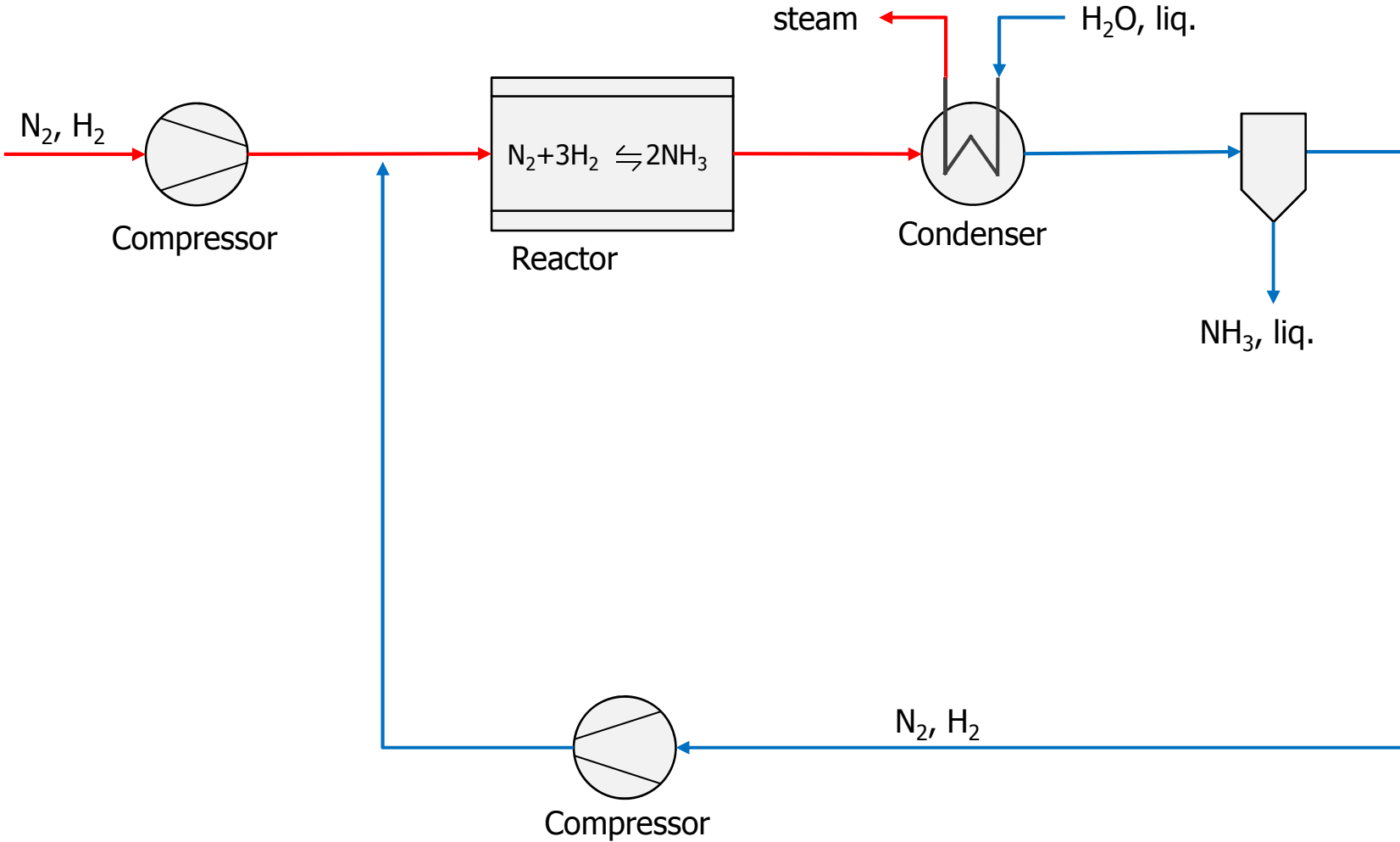
## Fuel Cell modeled with Thermolib



# Example – Ammonia Production

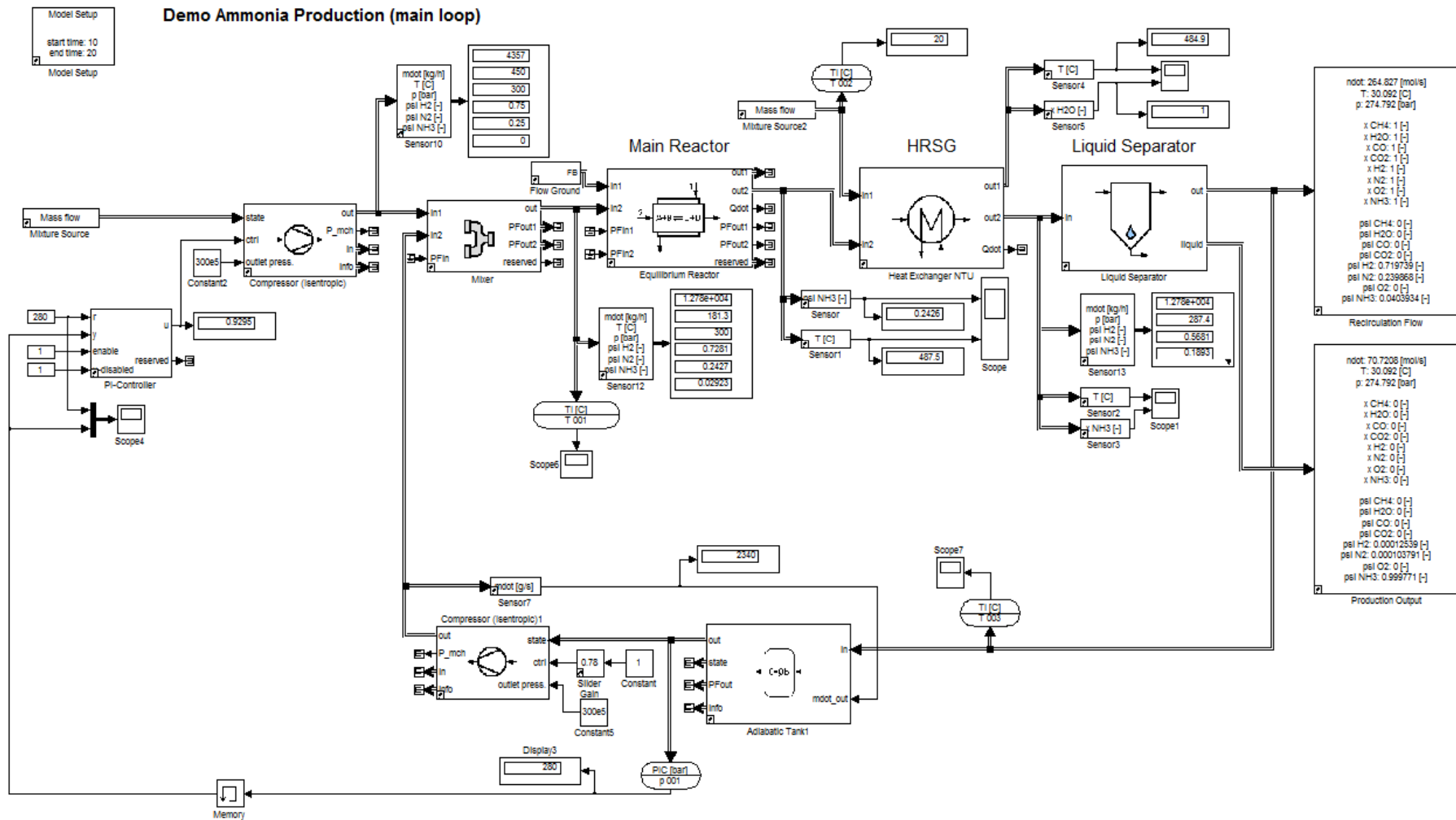
# Example - Ammonia Production

## Flow scheme – Main loop



# Example - Ammonia Production

## Flow scheme

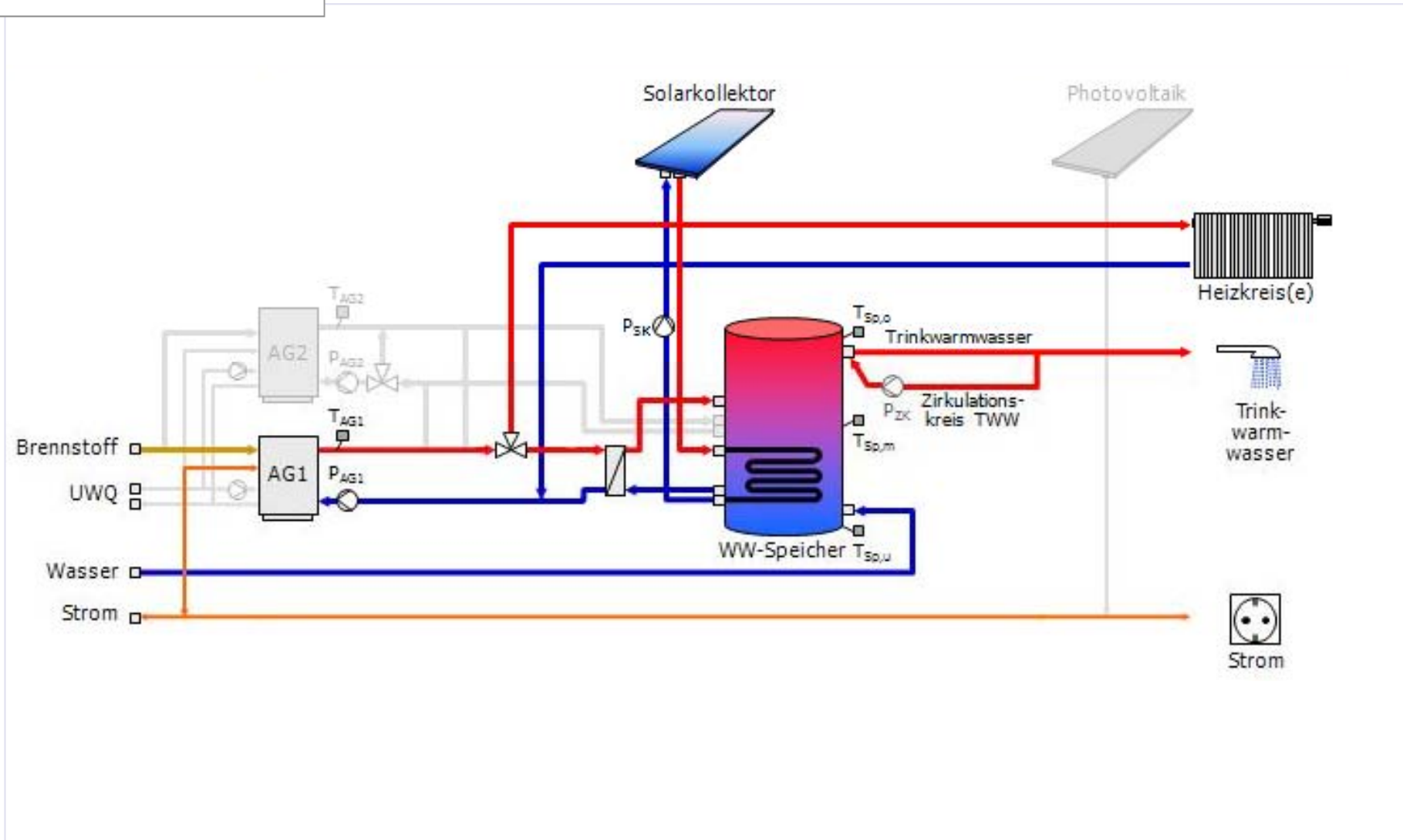


DemoAmmoniaProduction.mdl

# Example – Heating Installation

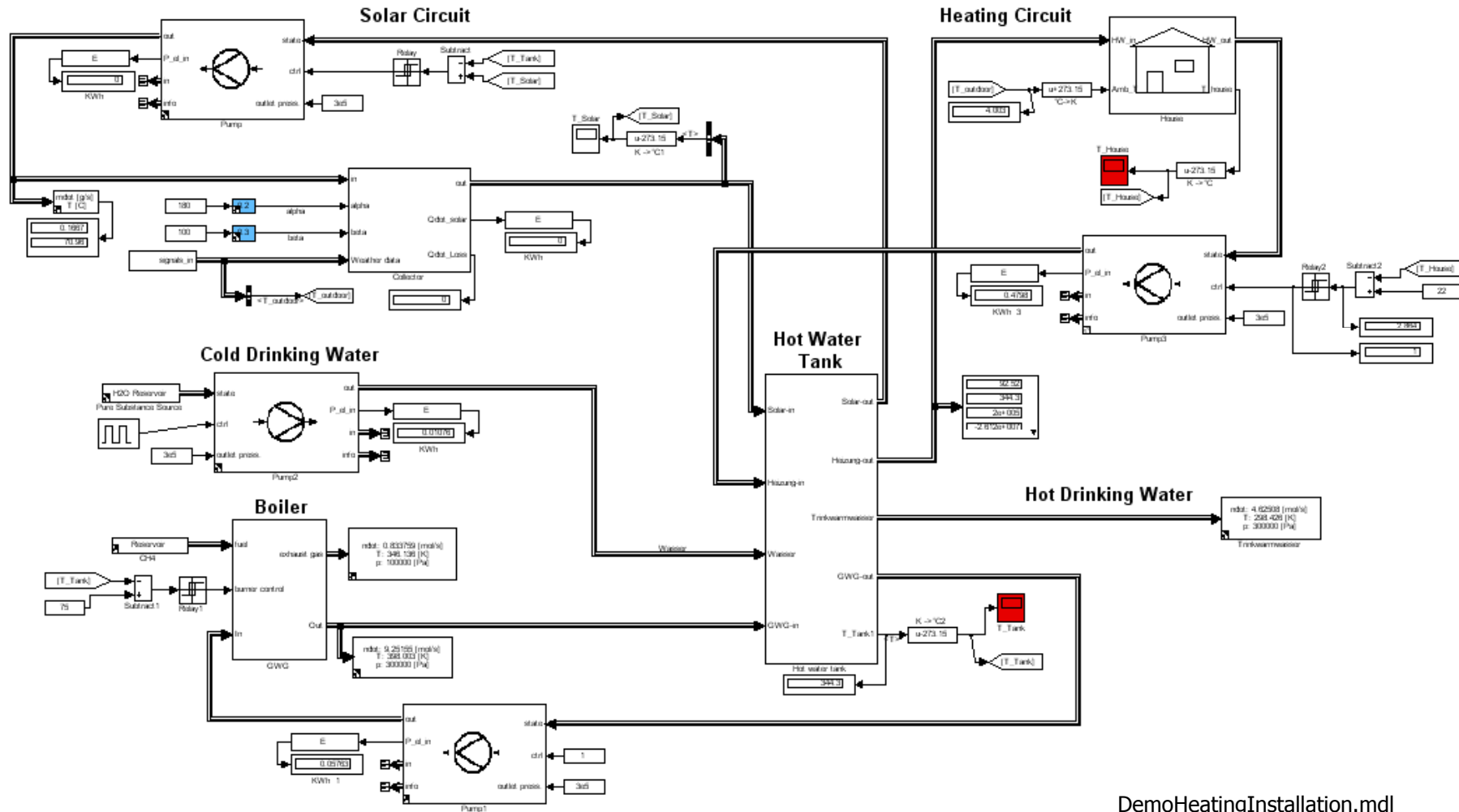
# Example – Heating Installation

## Flow scheme



# Example – Heating Installation

## Simulink Model with Thermolib blocks

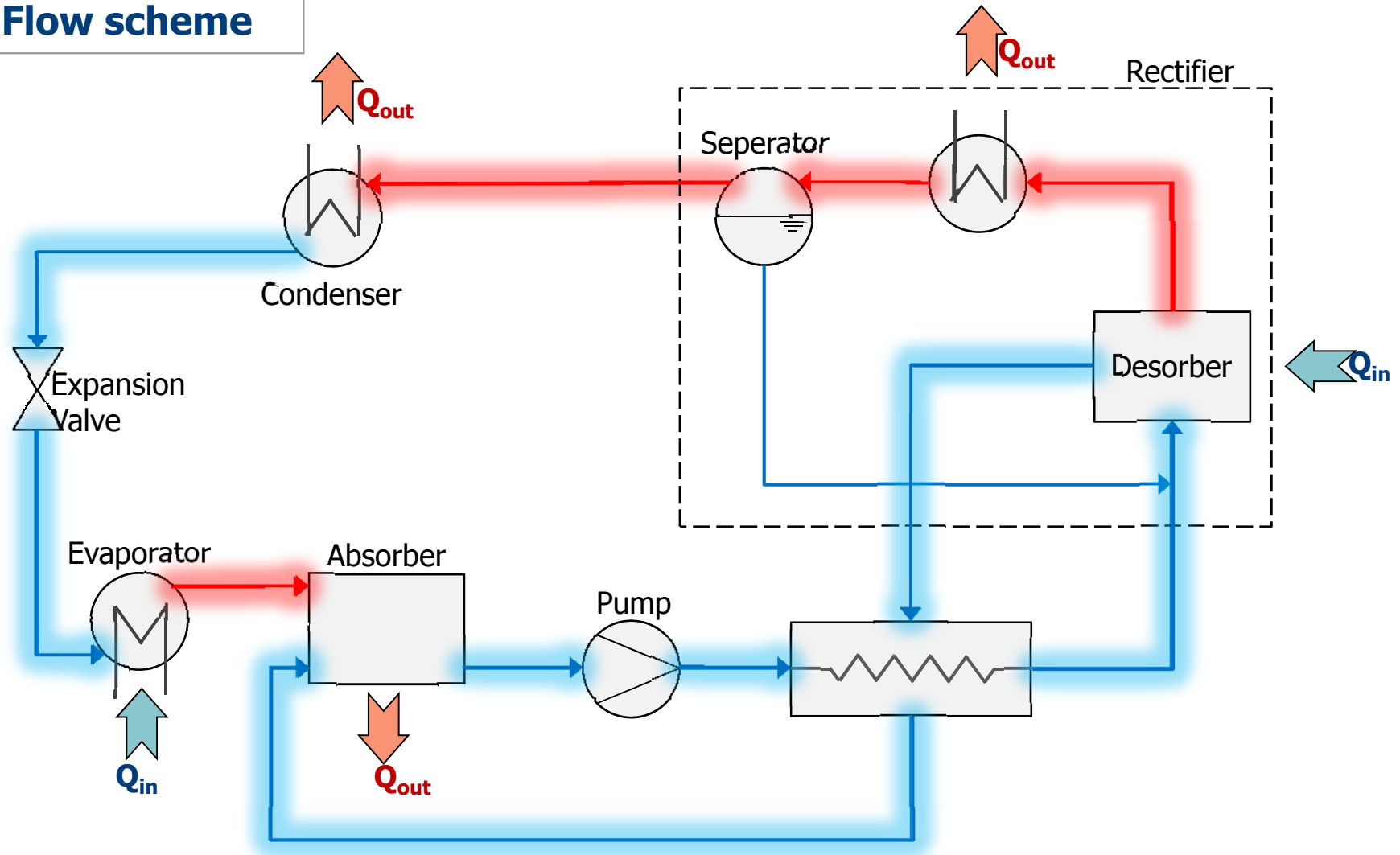


DemoHeatingInstallation.mdl

# Example – Absorption Heat Pump

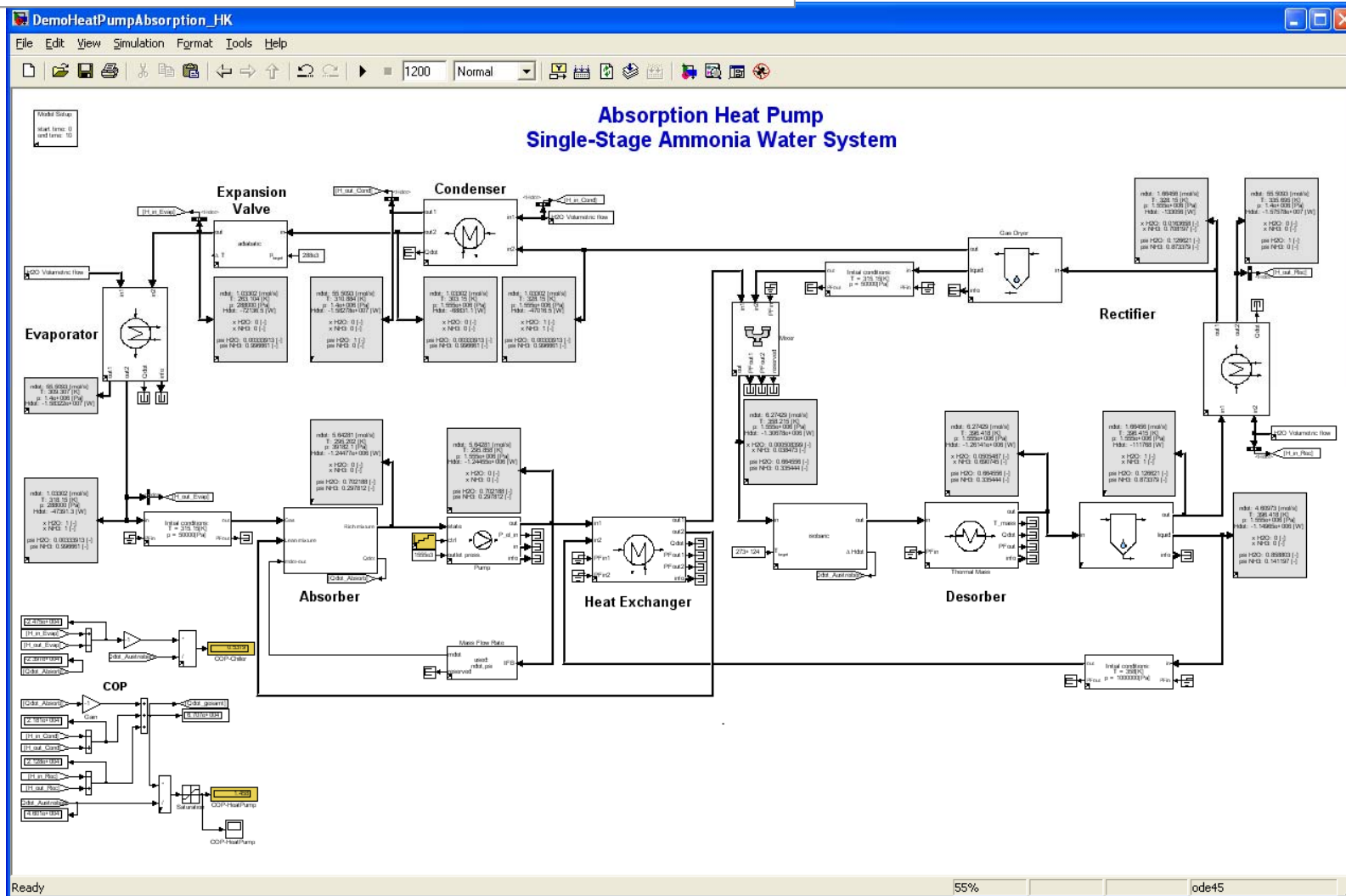
# Example – Absorption Heat Pump

## Flow scheme



# Example – Absorption Heat Pump

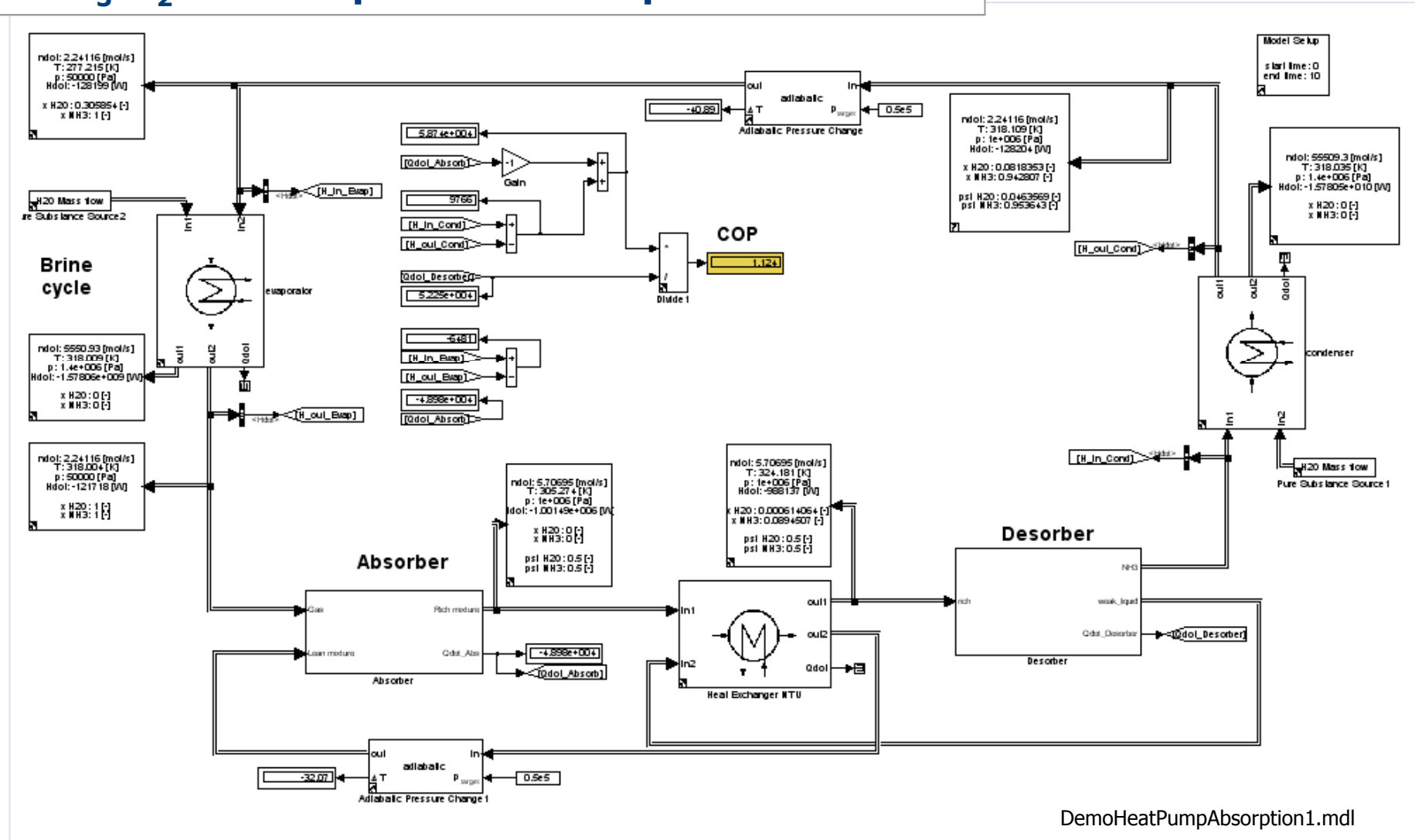
## Simulink Model with Thermolib blocks



DemoHeatPumpAbsorption2.mdl

# Example – Heat Pump

## NH<sub>3</sub>-H<sub>2</sub>O – Absorption Heat Pump with Thermolib

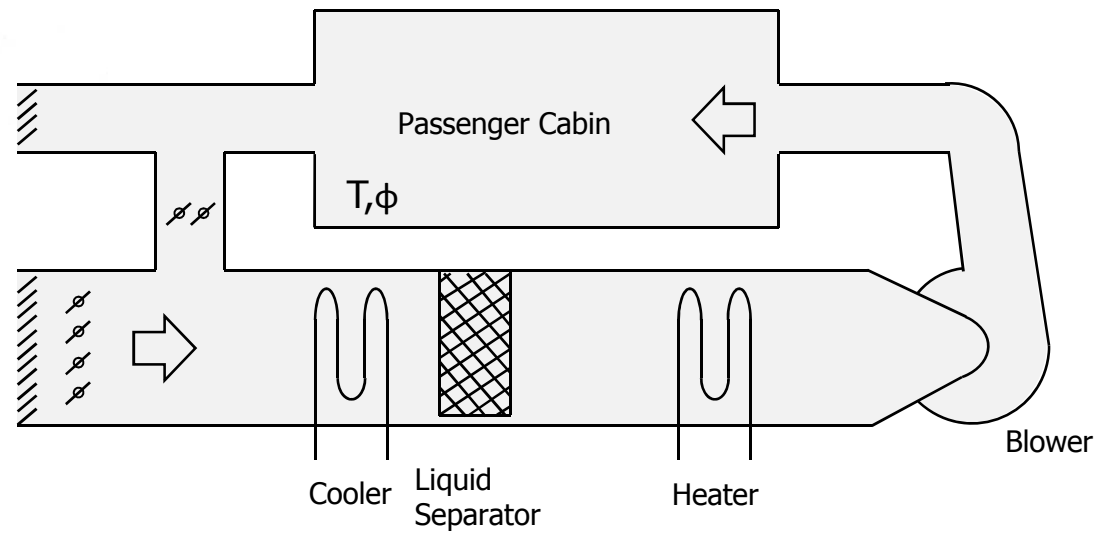
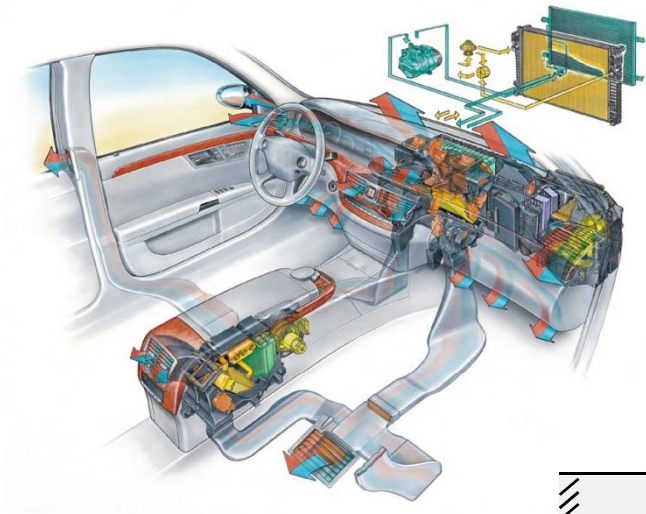


DemoHeatPumpAbsorption1.mdl

# Example – Air Conditioning

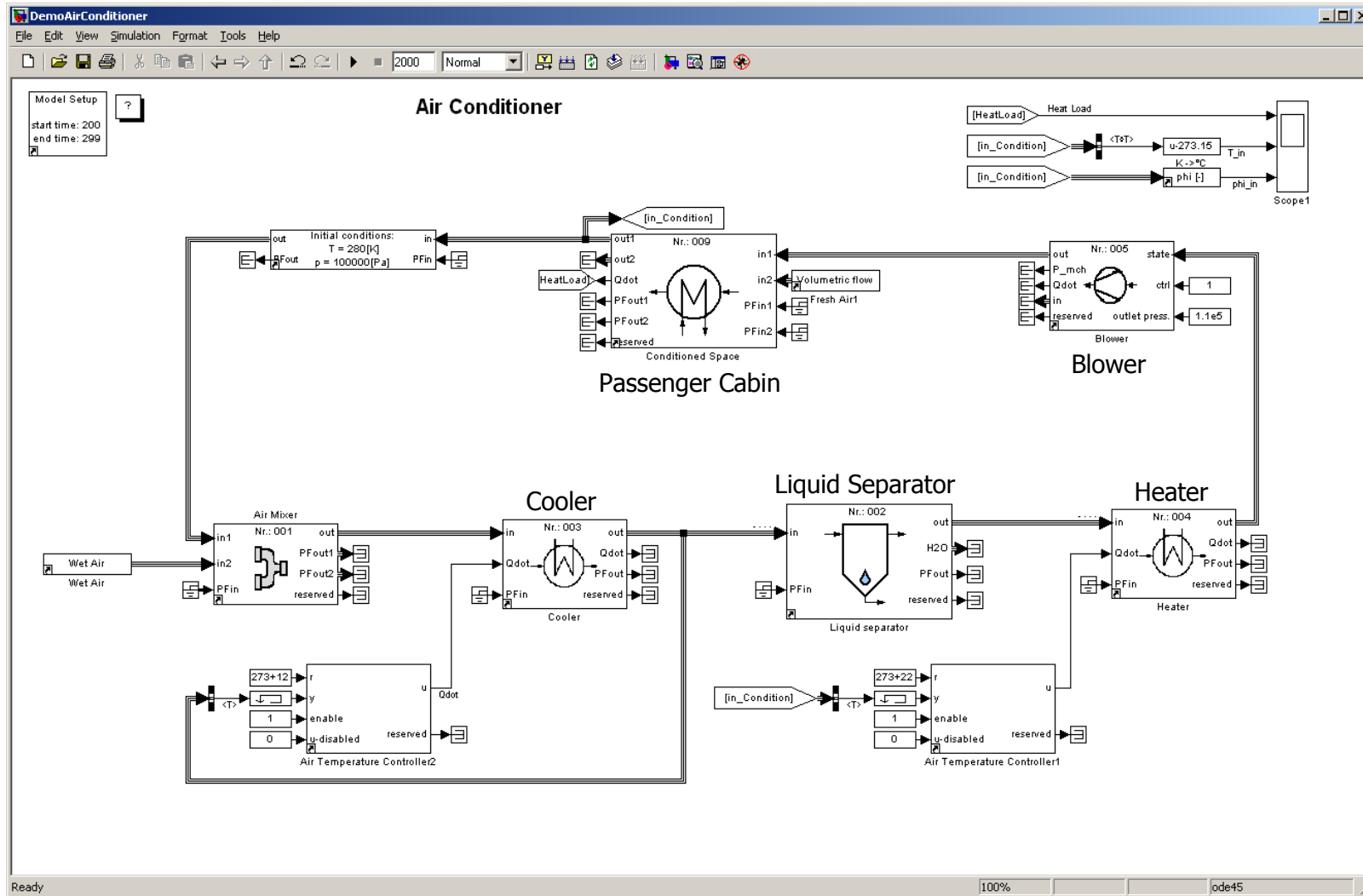
# Example – Air Conditioning Example

## Flow Scheme



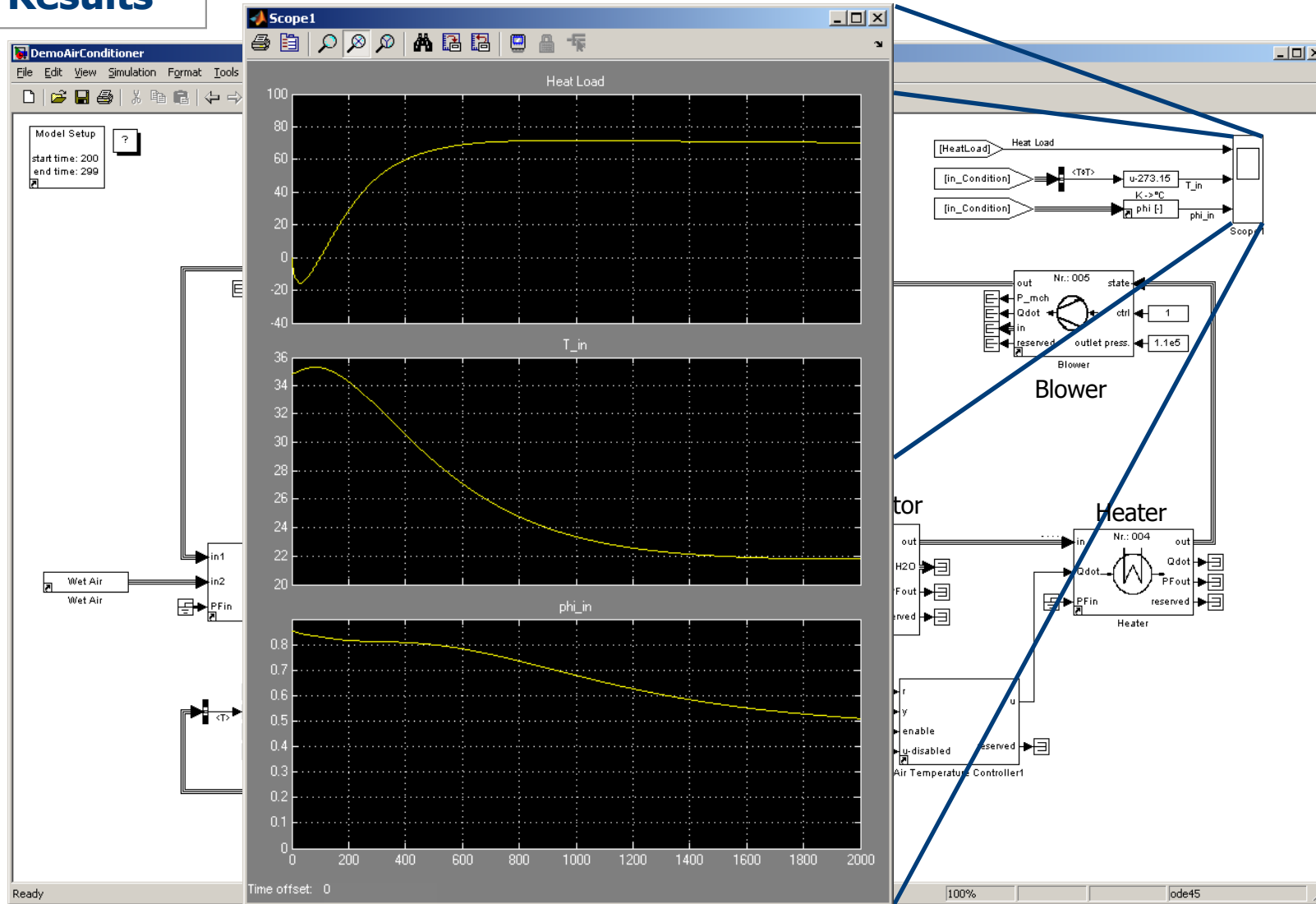
# Example – Air Conditioning Example

## Simulink Model with Thermolib blocks



# Example – Air Conditioning Example

## Results



# Example – Chemical Reaction Modeling

## Easy to configure

1. Parameterize your reactions:  

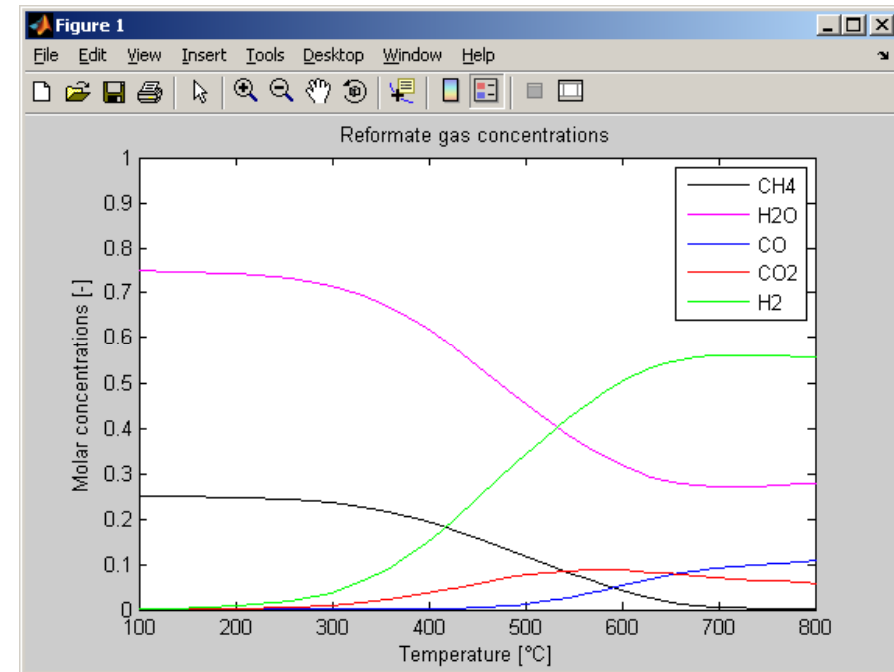
$$\text{CH}_4 + \text{H}_2\text{O} \leftrightarrow \text{CO} + 3 \text{H}_2$$

$$\text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2$$
2. ThermoLib maintains chemical equilibrium at the outputs and correct heat transfer in Simulink®

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

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

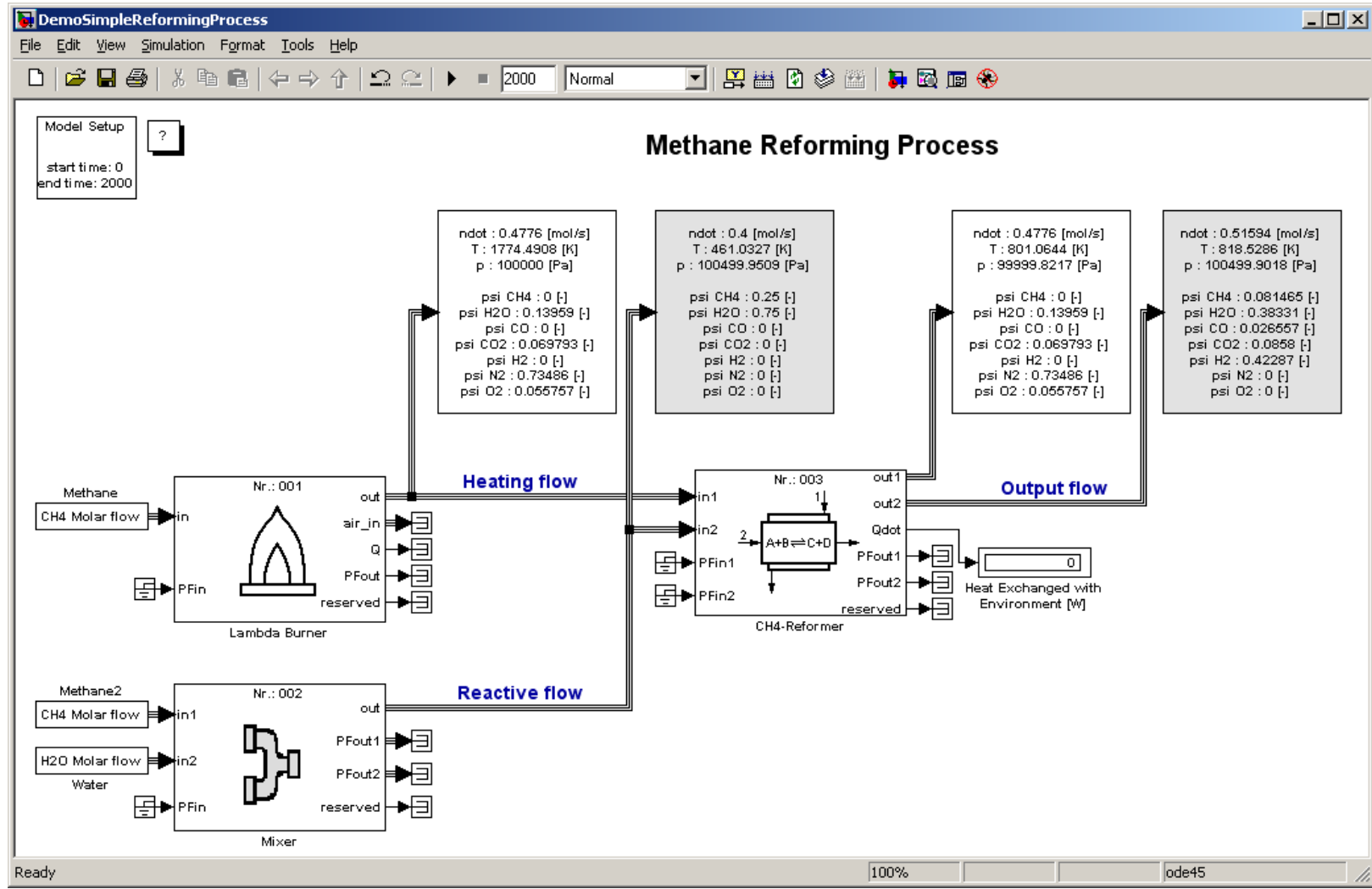
## Simulation Results



Steady state molar fractions at different temperatures

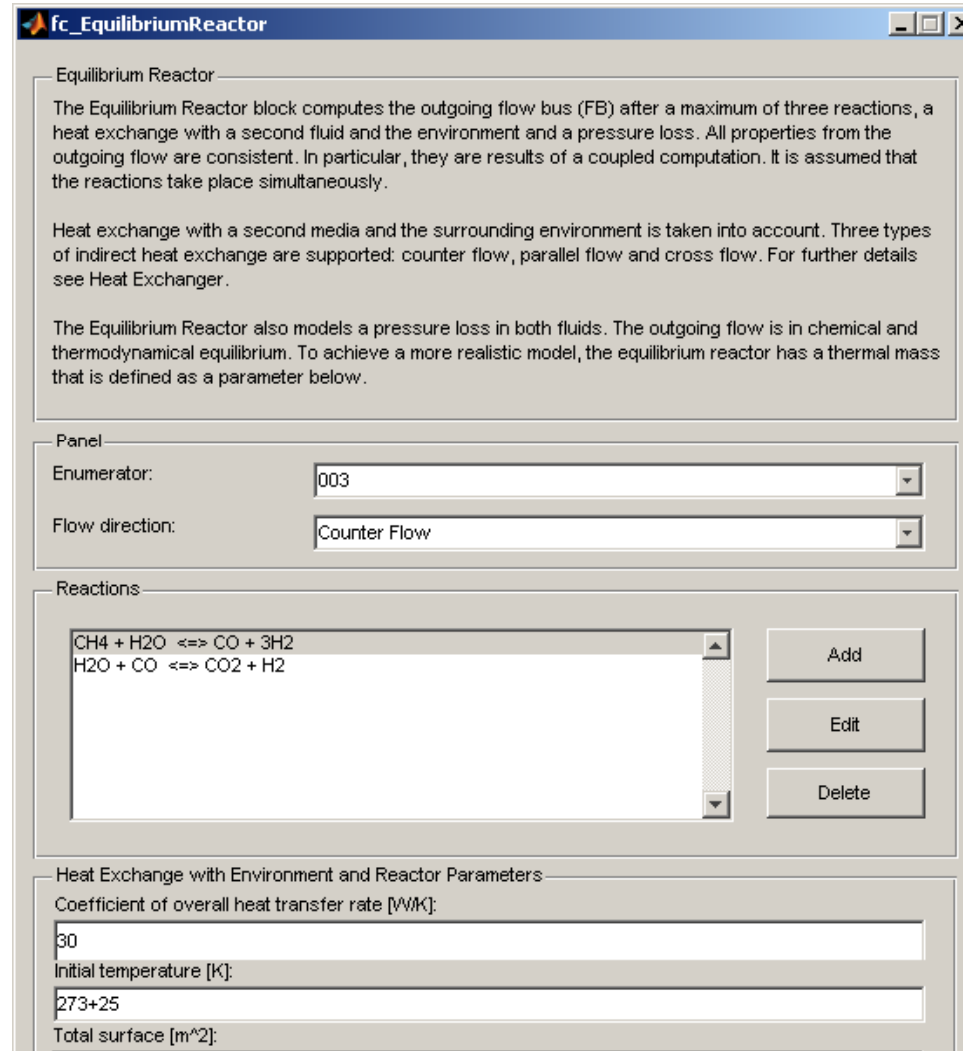
# Example – Methane Reforming Process

## 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: 003

Flow direction: Counter Flow

Reactions

CH4 + H2O  $\rightleftharpoons$  CO + 3H2  
H2O + CO  $\rightleftharpoons$  CO2 + H2

Add  
Edit  
Delete

Heat Exchange with Environment and Reactor Parameters

Coefficient of overall heat transfer rate [WK]: 30

Initial temperature [K]: 273+25

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	<b>ModelName</b>	DemoSimpleReformingProcess												
2	<b>date</b>	29-May-2009 07:55:16												
3														
4	<b>Balance Space Name</b>	<b>Port Name</b>	<b>Port Direction</b>	<b>CH4 [g]</b>	<b>H2O [g]</b>	<b>CO [g]</b>	<b>CO2 [g]</b>	<b>H2 [g]</b>	<b>N2 [g]</b>	<b>O2 [g]</b>	<b>H [mol]</b>	<b>C [mol]</b>	<b>O [mol]</b>	<b>N [mol]</b>
5	<b>TotalBalance</b>			3612,282	-6721,59	-656,437	-8877,99	-155,663	0	12799,6	0	0	0	0
6	<b>Lambda Burner</b>													
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	<b>Mixer</b>													
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	<b>Equilibrium Reactor</b>													
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	<b>Balance</b>			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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2	<b>date</b>	29-May-2009 07:55:16																																																				
3		<div style="border: 1px solid black; padding: 5px;"> <p><b>BalanceTest.txt - Notepad</b></p> <p>File Edit Format View Help</p> <pre> Modelname      DemoSimpleReformingProcess date           29-May-2009 07:55:16  Balance Space Name      Port Name      Port Direction      CH4 [g]      H2O [g]      CO [g] TotalBalance Lambda Burner   Input flow            in              200.000            0.000        0.000   Input Air              in              0.000              0.000        0.000   Output Gas            out             0.000              400.000      0.000  Mixer   Input flow 1          in              200.000            0.000        0.000   Input flow 2          in              0.000              27.200       0.000   Output flow           out             200.000            27.200       0.000  Equilibrium Reactor   Input heating flow    in              0.000              400.000      0.000   Input reacting flow   in              200.000            0.000        0.000   Output heating flow   out             0.000              400.000      0.000   Output reacting flow  out             174.837            0.311        23.4  Balance   CH4 [g]              403.682   H2O [g]              484.406   CO [g]               -656.000  Modelname      DemoSimpleReformingProcess date           29-May-2009 07:55:16  Balance Space Name      Port Name      Port Direction      [J] TotalBalance 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   Energy Thermal Mass stored_end    -653340.128                     </pre> </div>																																																				
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	Heat loss	in	0.000																																																			
	Energy Thermal Mass stored_start		653340.128																																																			
	Energy Thermal Mass stored_end		653340.128																																																			
Balance			-653340.128																																																			
21																																																						
22																																																						
23																																																						

# 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 [-]	Antonie_A	3,9895	5,111	4,5396014
Antonie equation_B [-]	Antonie_B	443,028	1685	846,3
Antonie equation_C [-]	Antonie_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

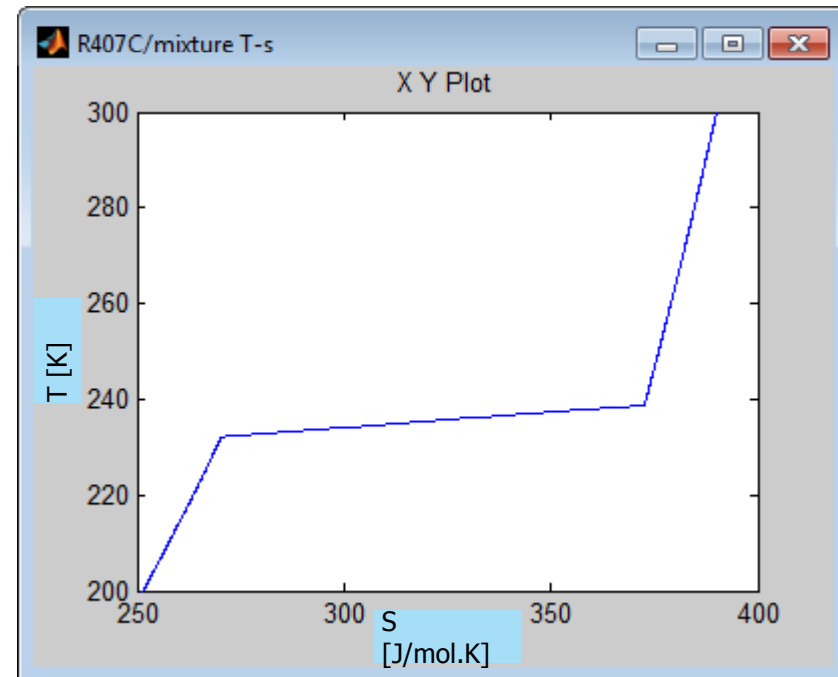
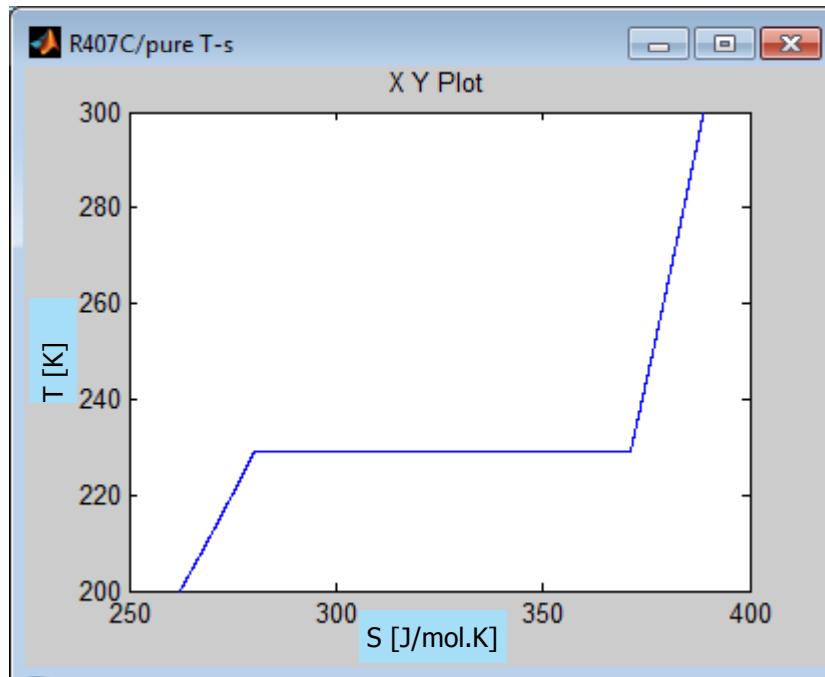
- CH4, vapor allowed, liquid allowed
- H2O, vapor allowed, liquid allowed
- CO, vapor allowed, liquid allowed
- CO2, vapor allowed, liquid allowed
- H2, vapor allowed, liquid allowed
- N2, vapor allowed, liquid allowed
- O2, vapor allowed, liquid allowed
- isooctane, vapor allowed, liquid allowed
- Methanol,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

Model of gas phase

EOS:       Mixing rule:

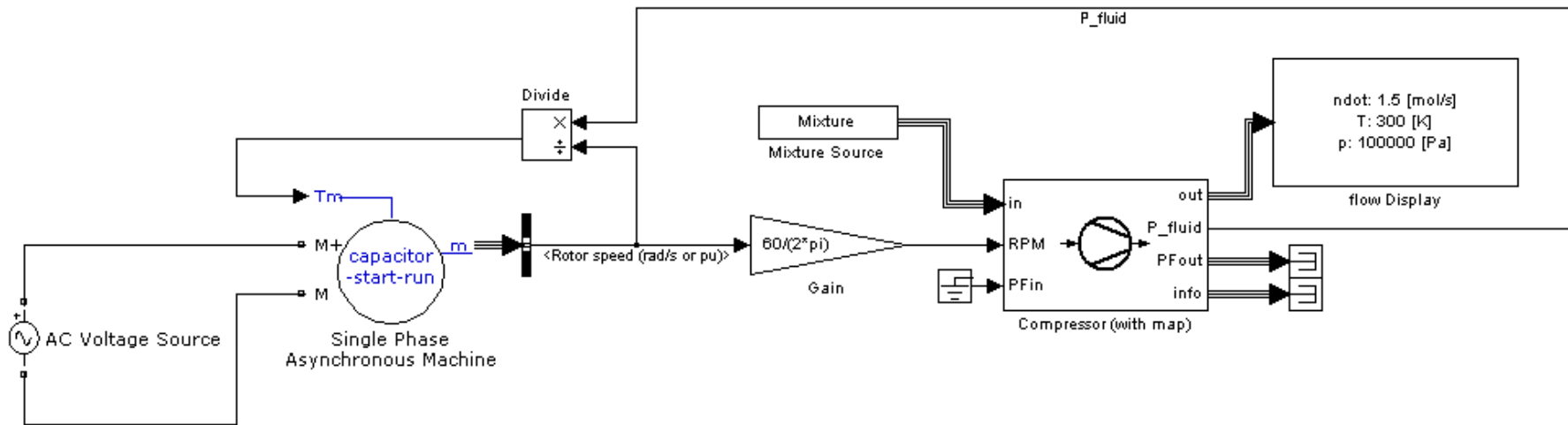
## Mixture Evaporation

- Thermolib allows multi-component vapor-liquid-equilibrium calculations / flash calculations
- Typical refrigerants in HVAC-systems are mixtures!
- Example R407c is a mixture of R134a, R125, R32
- DemoTempGlideR407c.mdl demonstrates the difference



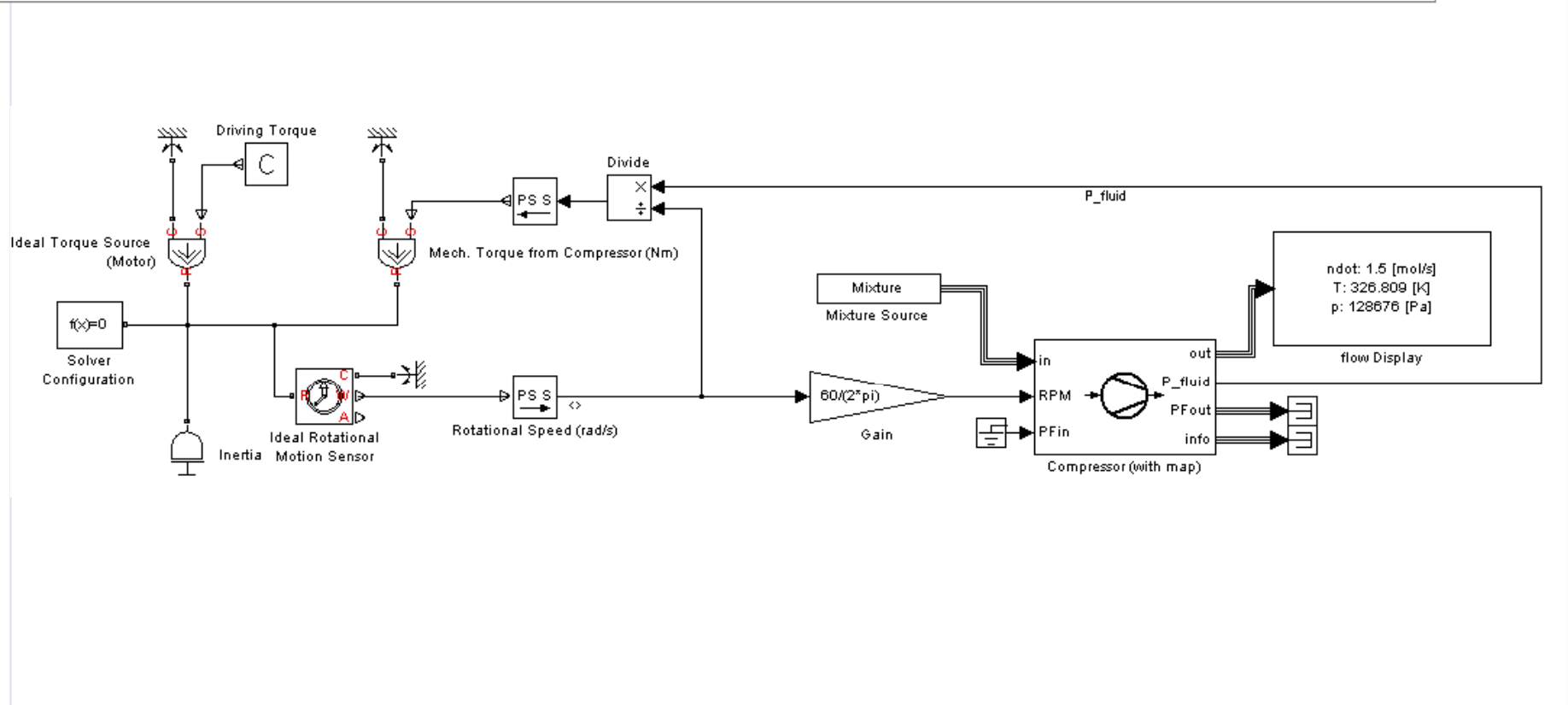
# Interfacing Thermolib with SimScape & SimPowerSystems

## Thermolib Compressor driven by SimPower Machine



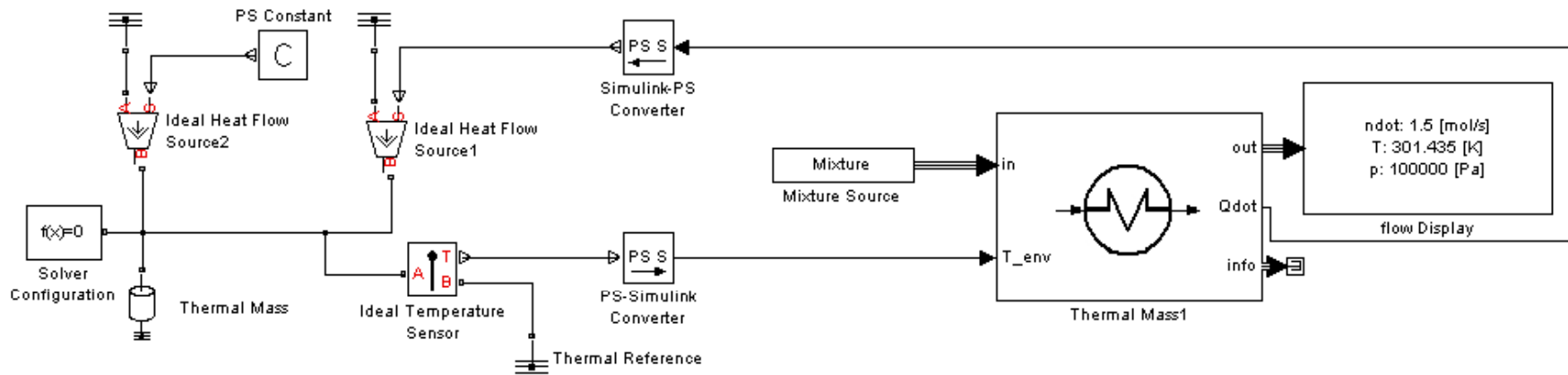
- Simple interface via mechanical torque ( $T_m$ ) and rotor speed ( $w$ )
- Time scales need attention  
(in SimPowerSystems typically milliseconds, while in Thermolib seconds)

## Thermolib Compressor driven by SimScape Rotational Elements



- Simple interface via mechanical torque ( $T_m$ ) and rotor speed ( $\omega$ )

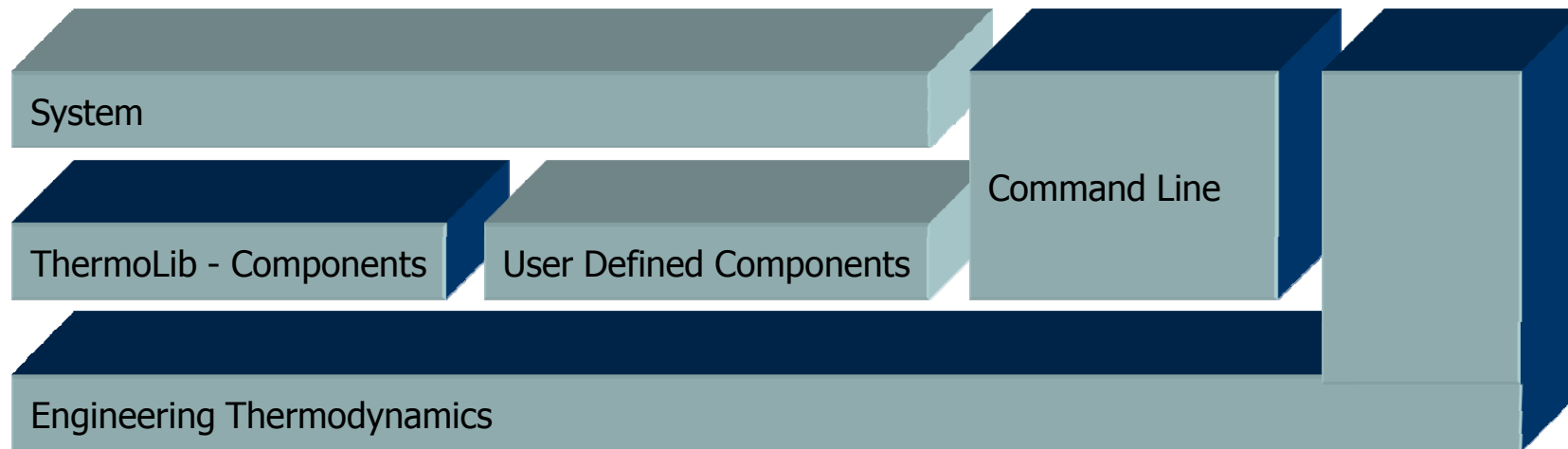
## Thermolib thermal mass and thermal foundation domain



- Simple interface via heat flow and temperature

# Architecture ...

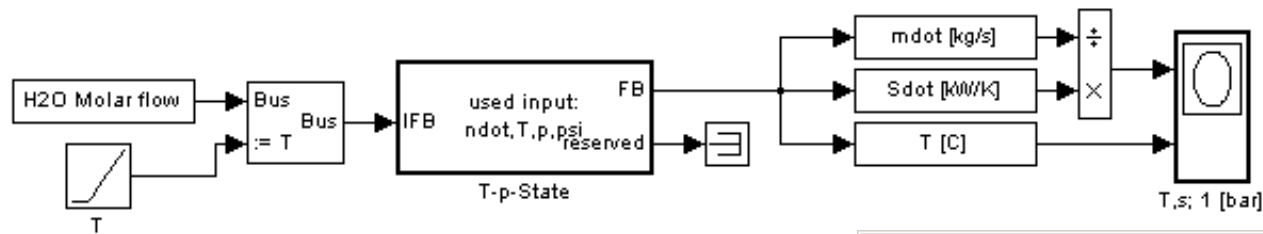
## Architecture



## Key features

- High flexibility by systematic use of engineering thermodynamics
- Easy set up of new components => fast adaption to new processes
- EUtech offers development of customized blocks

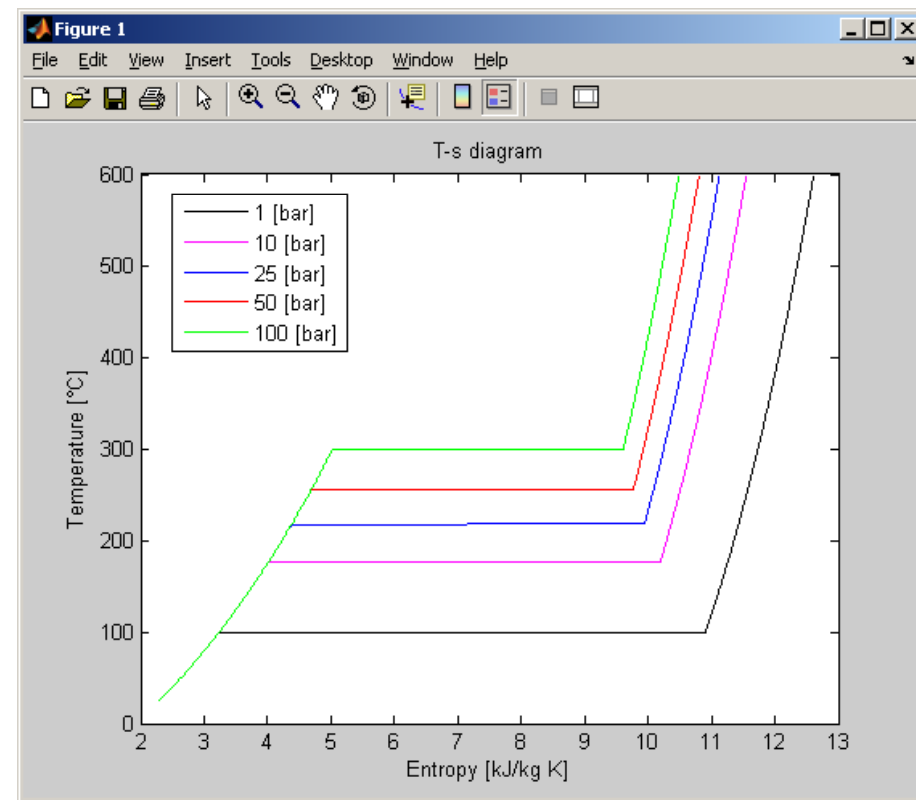
## Example: Isobaric evaporation



## Key features

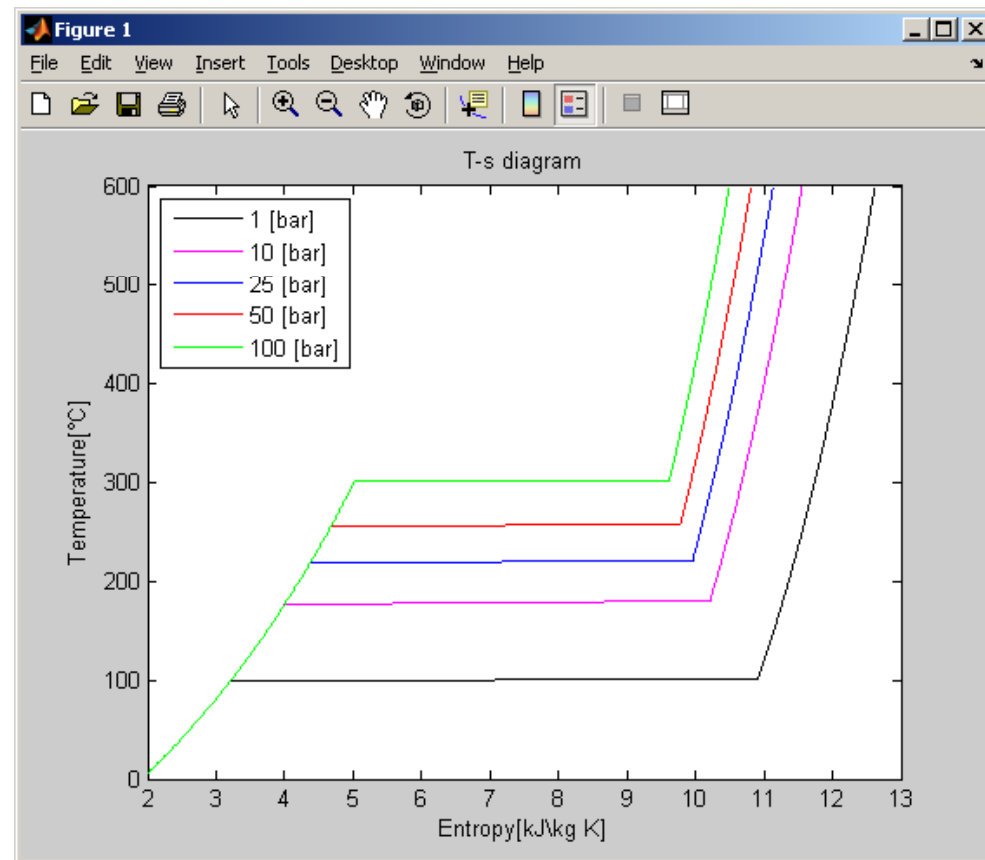
User accessible fundamental thermodynamic functionality

- build new components
- thermodynamic calculations
- ...



## Command Line

- `[hdot,b,c,d,e]=th_TpState('species',{'H2O'},'T',T,'p',p,'psi',[1],...  
'ndot',[1],'MediaData',SMediaData);`



### Available Thermolib Add-on-Products

- Thermolib-IF97
  - Enables high precision water calculations according to the International Association for Properties of Water and Steam with industrial formulation of 1997 (IAPWS-IF97)
  - Common standard for power plant calculations
- Thermolib-RTWE
  - Thermolib real time workshop extensions
  - Provides .tlc files and static linked libraries to compile Thermolib models into standalone applications with the following targets:
    - Generic Real Time target, S-function target, Rapid Simulation target, xPC-target
  - (currently not yet available, but coming within 2010).
- Planned 2011: Thermolib-DIPPR801
  - Access to standard DIPPR 801 species database to enable simulations with more than 2000 species (<http://dippr.byu.edu/>)

## New features in Release 5.0

- Real gas behavior using Peng-Robinson equation of state.
- Precise water calculations using IAPWS-IF97 standard available as Add-on (Thermolib IF97).
- RTW-extension available to generate with standalone executable models using the Real-Time Workshop targets
- Thermolib can handle now general flash calculations.
- ChemicalMediaData now contain several new refrigerants (R125, R32, ...)
- Viscosity and thermal conductivity data available (Reynolds number calculations)
- A general Tank block – outputs configurable “top” or “bottom”
- A new Li-Ion cell block models for battery thermal management simulations
- Licensing scheme based on software activation available

## Summary

### Key features

With Thermolib thermodynamic systems can be easily modeled.

- Based on fundamental engineering thermodynamic principles
- Focused on modeling for control (system level; dynamics)
- More than 40 thermodynamic components blocks
- Handles system hydraulics with pressure feedback
- Extensive thermodynamic balancing
- Customizable database of thermodynamic species
- Completely based on standard Simulink®
- Fully integrates with The MathWorks tool-chain
- Real-time capabilities (Rapid Control prototyping, HiL)

## Summary

### Field of Application

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

Further information at [www.thermolib.de](http://www.thermolib.de)

**Questions?**

**Contact: [thermolib@eutech.de](mailto:thermolib@eutech.de)**