

Getting started with Simulis® Thermodynamics

Use Case 12: Use within MATLAB®

Software & Services In Process Simulation

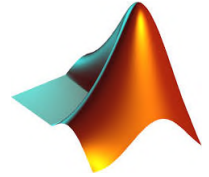
We guide You to efficiency



ProSim

Introduction

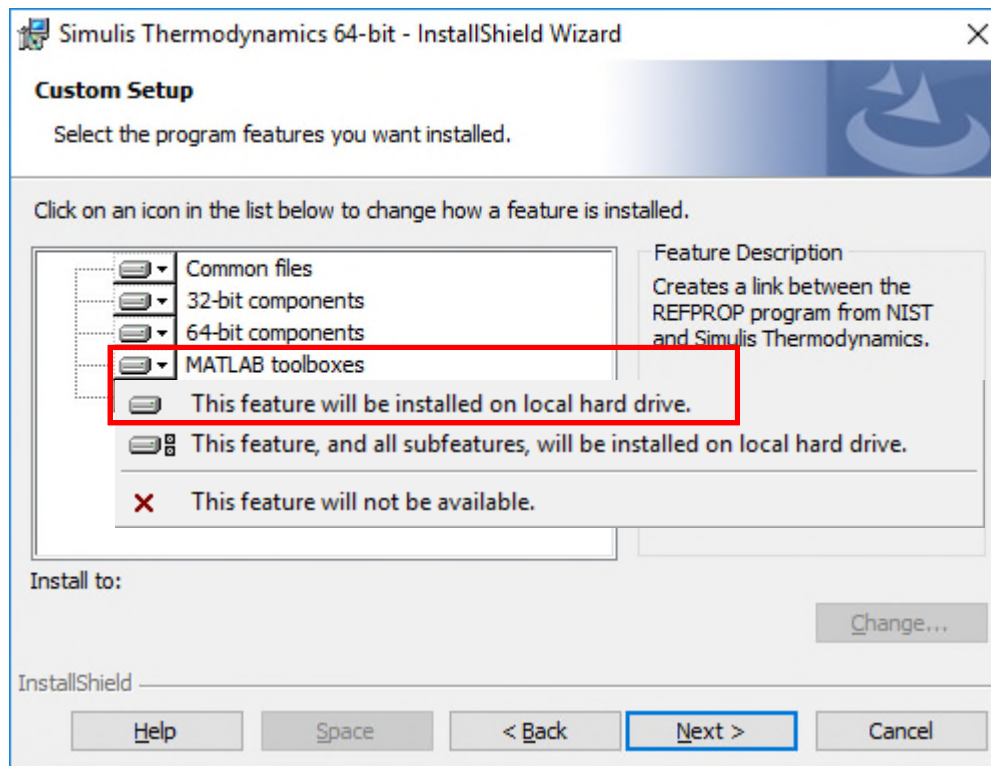
This document presents the operation of Simulis Thermodynamics in MATLAB



- Installation
- Examples
- Helps

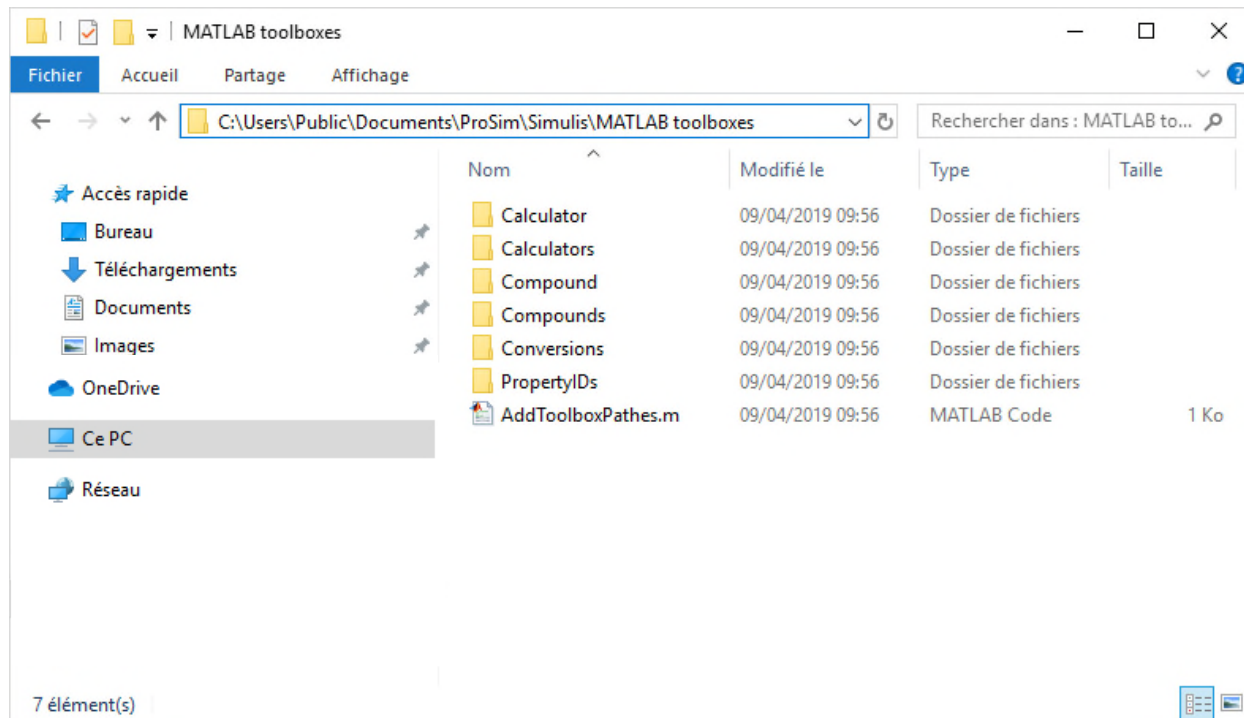
SIMULIS® THERMODYNAMICS & MATLAB

- Installation:
 - Select "MATLAB toolboxes" to be installed when installing Simulis Thermodynamics



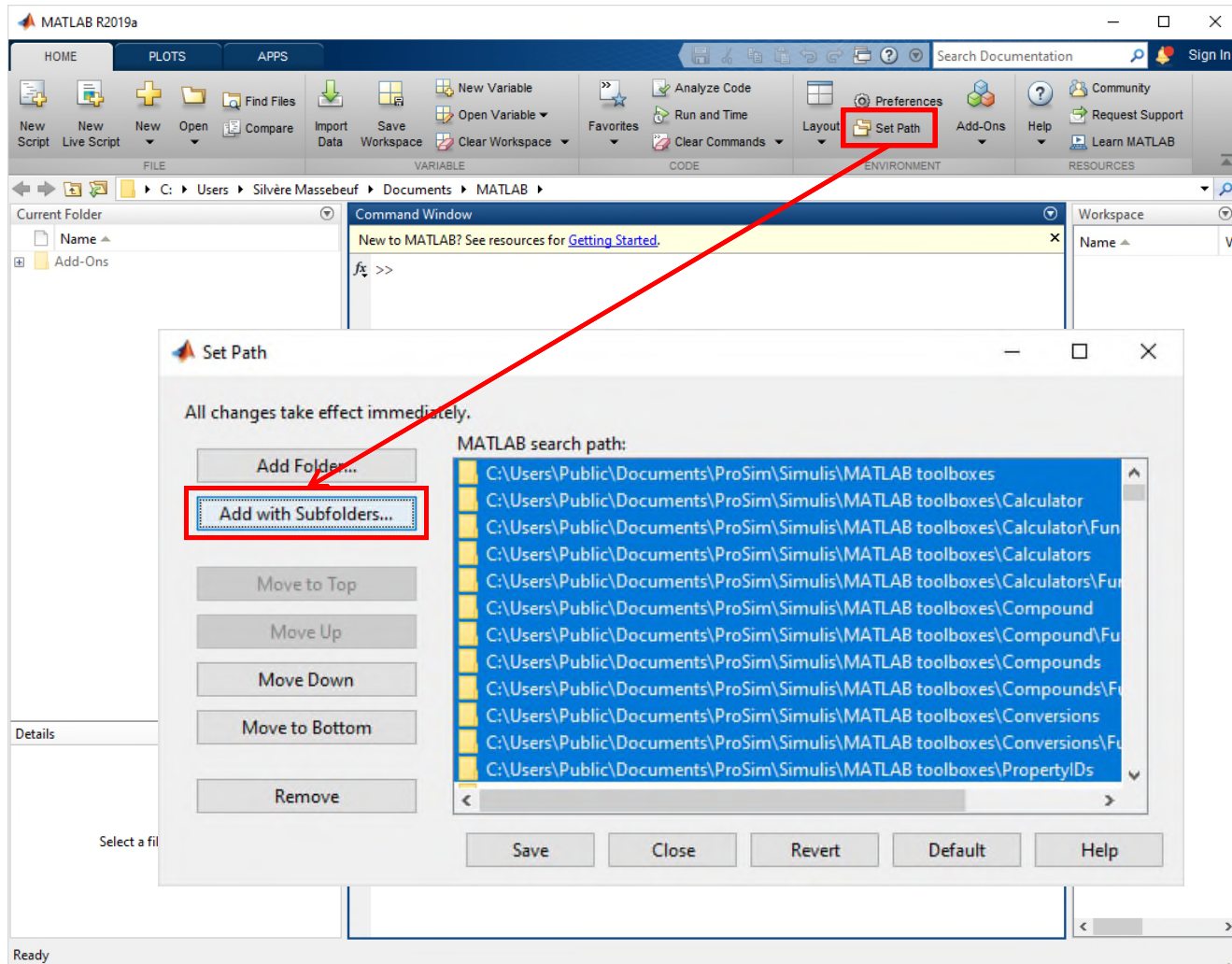
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- Installation:
 - Check in the installation directory:
C:\Users\Public\Documents\ProSim\Simulis\MATLAB toolboxes



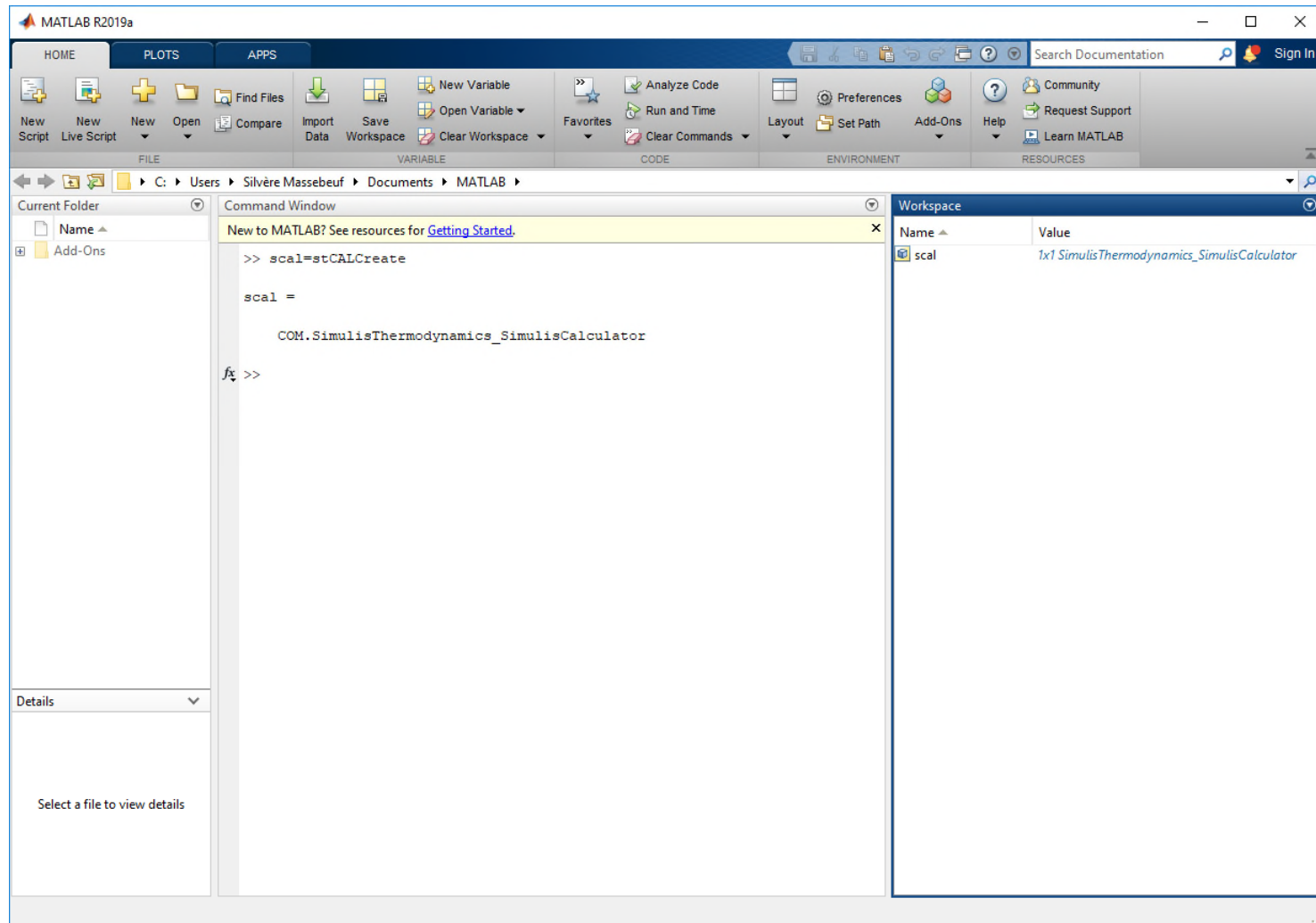
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- Installation:
 - Add this MATLAB search path



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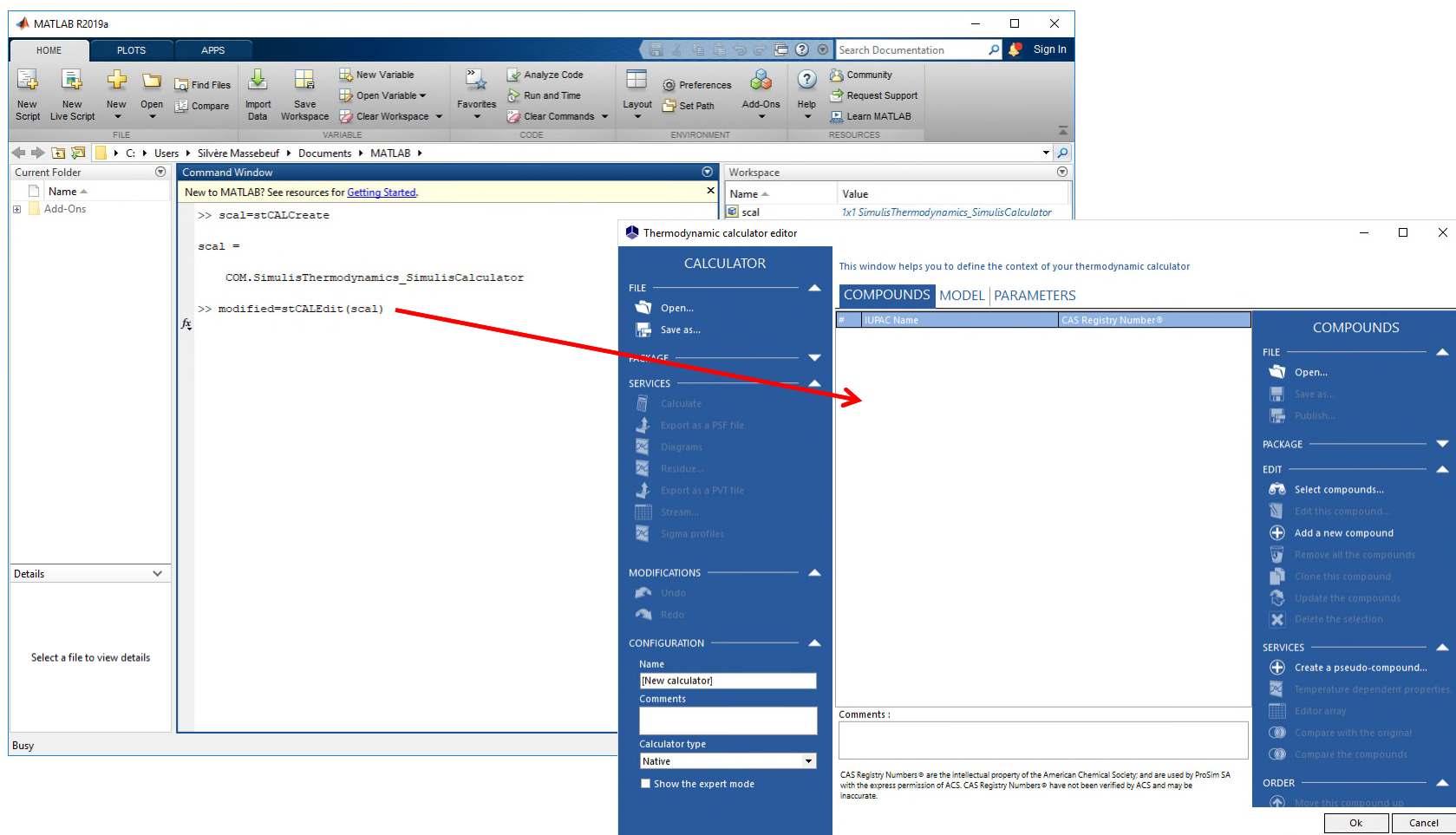
- Create a Simulis calculator object:
 - `scal=stCALCreate`



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- Edit the Simulis calculator object
(define components and thermodynamic model):

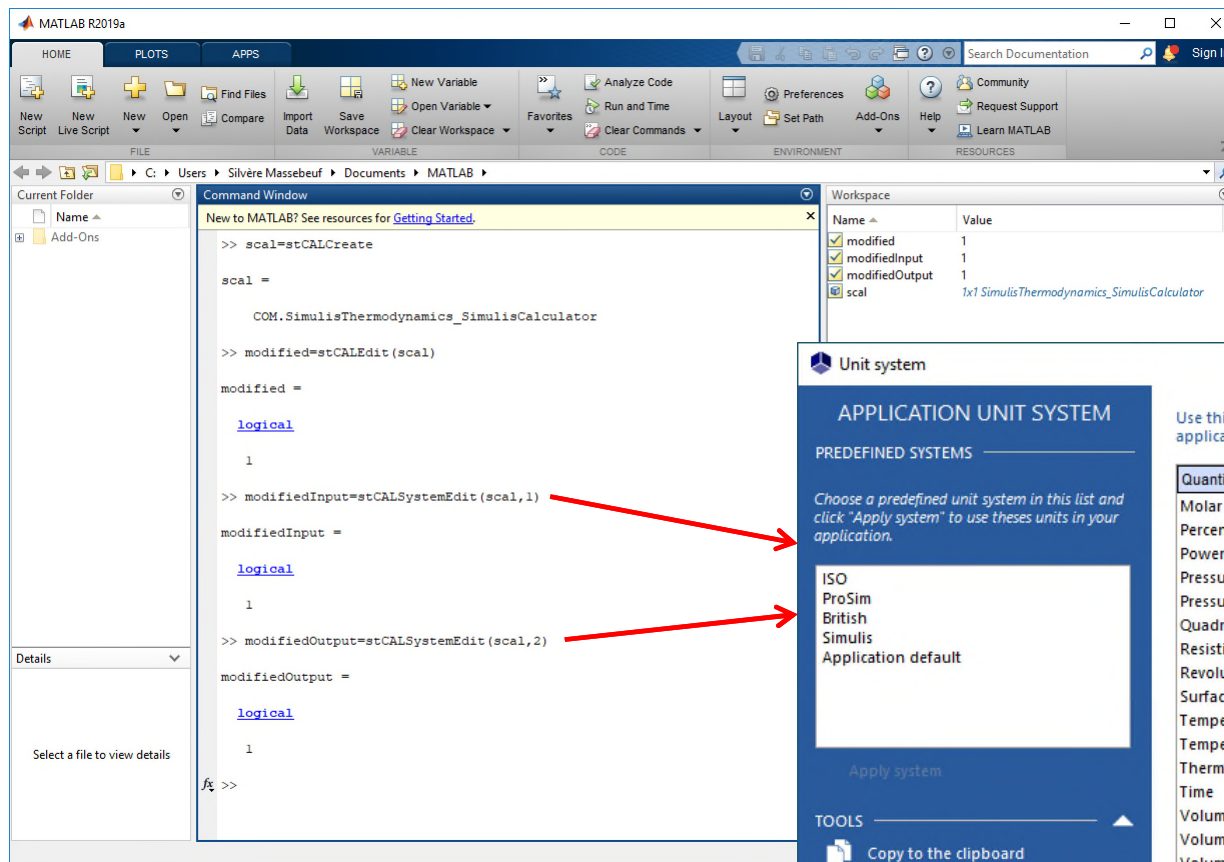
- **modified**=stCALEdit(scal)



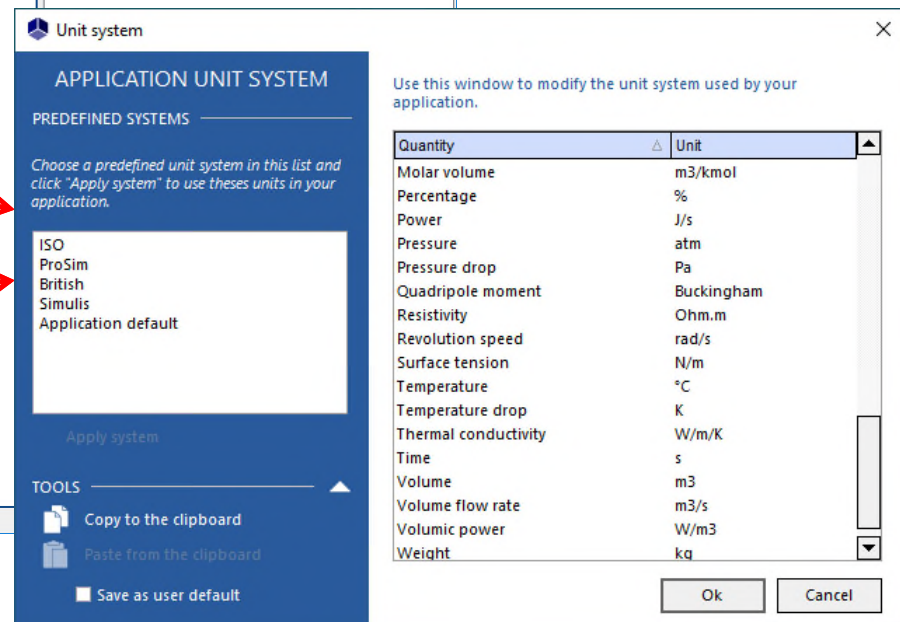
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Unit systems of the Simulis calculator object (input and output):

- **modifiedInput**=stCALSystemEdit(scal,1)
- **modifiedOutput**=stCALSystemEdit(scal,2)

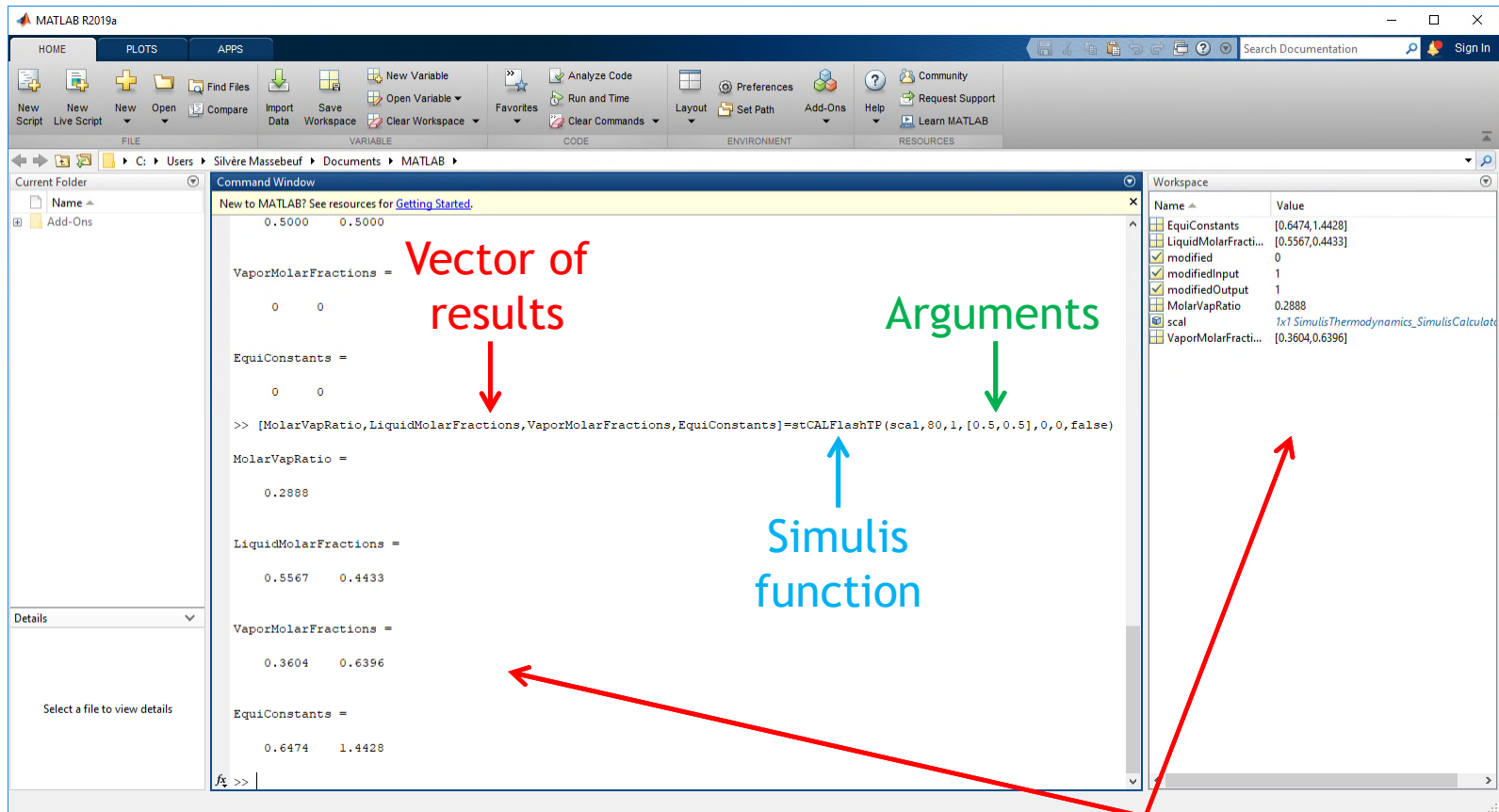


Example given:
Temperature: °C
Pressure: atm



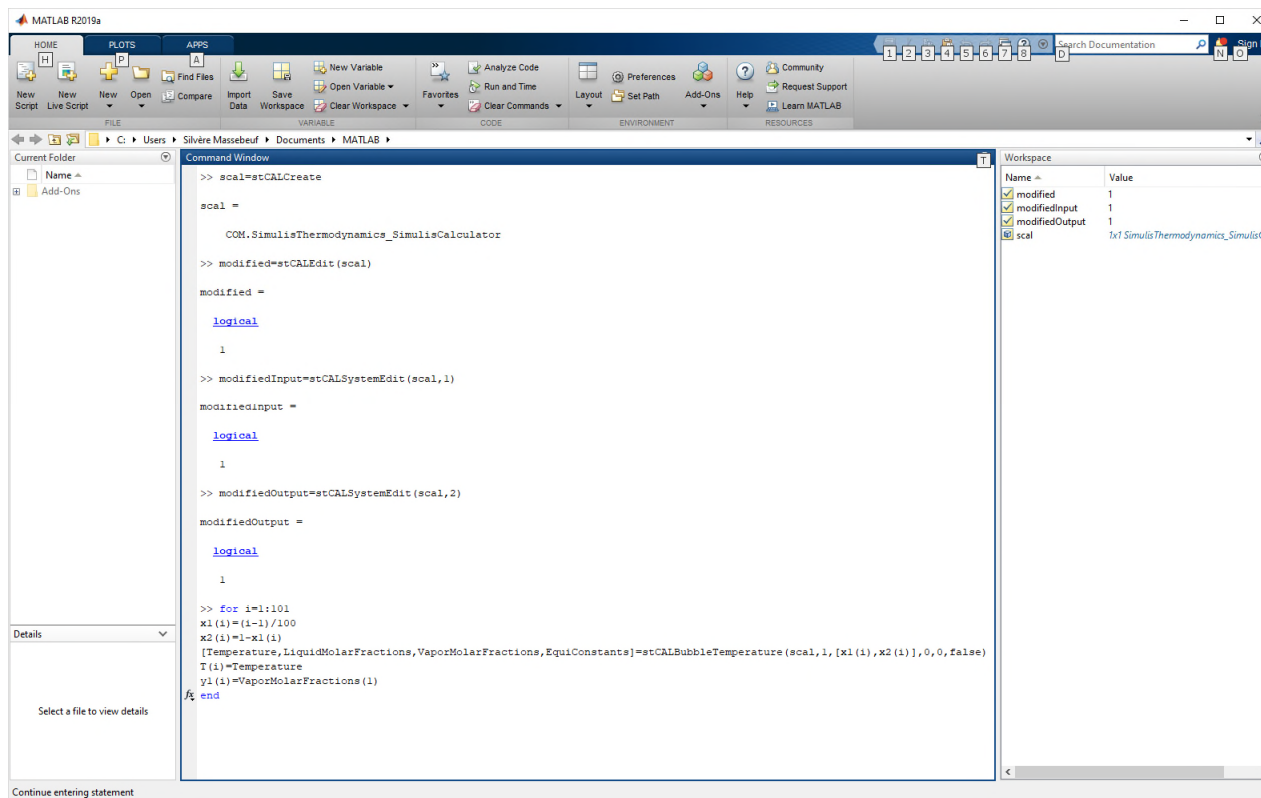
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- Calculation of a flash at given temperature and pressure (e. g.: equimolar water-ethanol system at 80 °C and 1 atm):
 - **[MolarVapRatio, LiquidMolarFractions, VaporMolarFractions, EquiConstants]**
=stCALFlashTP(scal, 80, 1, [0.5, 0.5], 0, 0, false)



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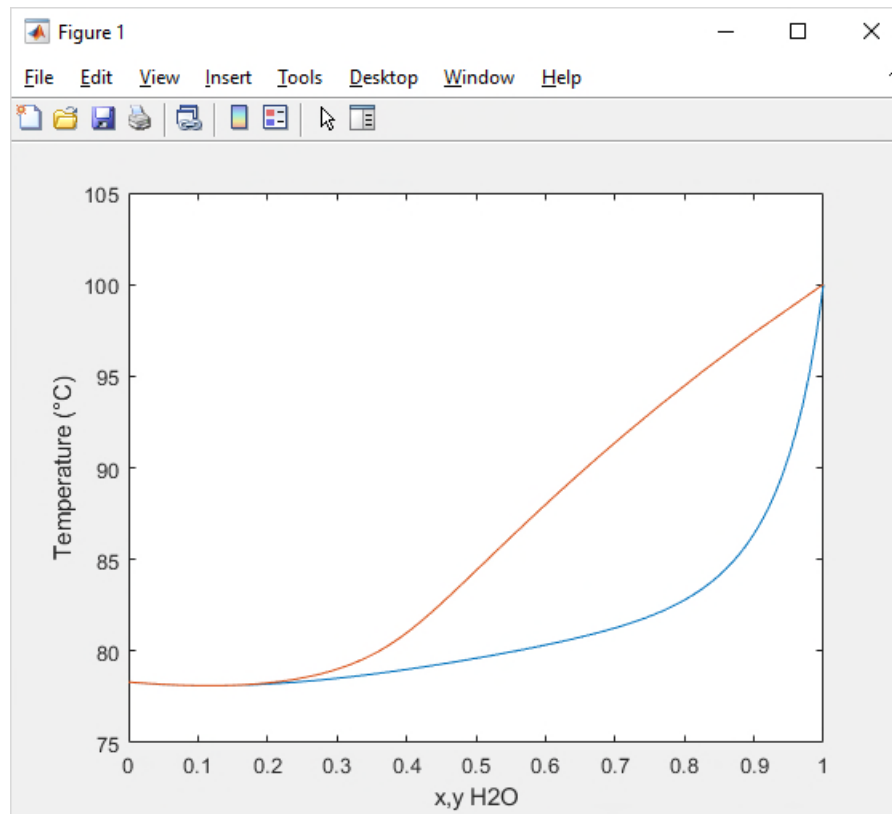
- Plot of equilibrium curves at atmospheric pressure:
 - for i=1:101
 - $x_1(i) = (i-1)/100$
 - $x_2(i) = 1 - x_1(i)$
 - [Temperature, LiquidMolarFractions, VaporMolarFractions, EquiConstants]
 - =stCALBubbleTemperature(scal, 1, [x1(i), x2(i)], 0, 0, false)
 - T(i)=Temperature
 - y1(i)=VaporMolarFractions(1)
 - end



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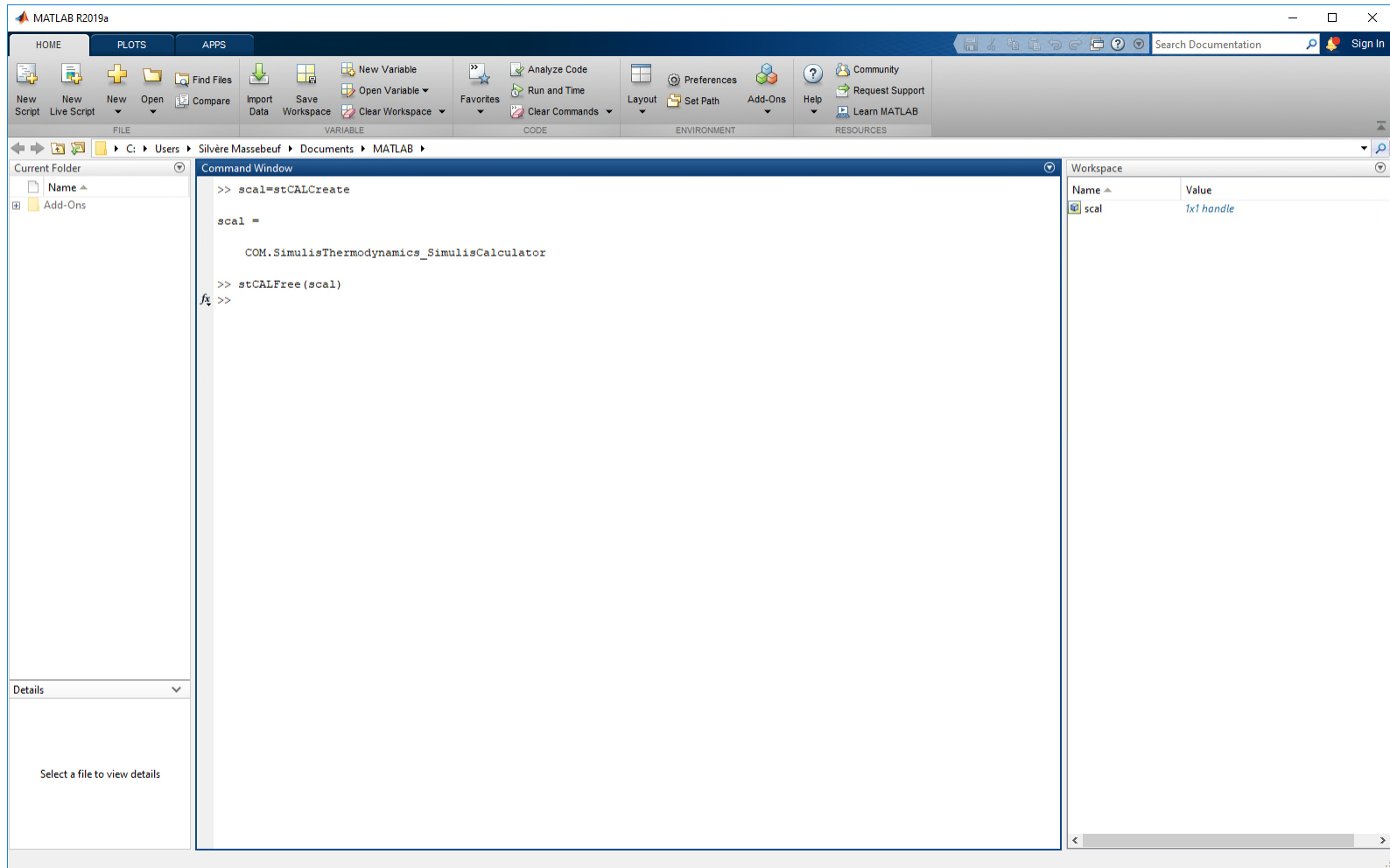
- Plot of equilibrium curves at atmospheric pressure:

- `plot(x1,T,y1,T)`
`xlabel('x,y H2O')`
`ylabel('Temperature (°C)')`



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- Free a Simulis object:
 - `stCALFree(scal)`



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■ Access to the help of the functions:

- **help** *stCALFlashTP*

The screenshot shows the MATLAB R2019a interface. The Command Window displays the help for the `stCALFlashTP` function. The Workspace window shows the return values of the function.

Arguments

Return values

Example

```
>> help stCALFlashTP
Calculation of flash Liquid-Vapor at fixed temperature and pressure with a Simulis Calculator Object

function [ vapRatio, liquidFractions, vaporFractions, equiConstants ] = stCALFlashTP( simulisCalculator, temperature

Input parameter(s) :
simulisCalculator : Simulis Calculator Object
temperature : temperature of calculation expressed in INPUT unit system
pressure : pressure of calculation expressed in INPUT unit system
mixtComposition : mixture composition (vector of stCALCompoundCount values)
mixtCompositionType : mixture composition type (0 = molar, 1 = mass)
resultType : result type (0 = molar, 1 = mass)
init : boolean value indicating if the following values are taken into account or not
initVapRatio : [Optional] molar vaporization ratio of initialisation
initLiquidFractions : [Optional] liquid fractions of initialisation (molar or mass) (vector of stCALCompoundCount values)
initVaporFractions : [Optional] vapor fractions of initialisation (molar or mass) (vector of stCALCompoundCount values)

Output parameter(s) :
vapRatio : molar vaporization ratio
liquidFractions : [Optional] liquid fractions (molar or mass) (vector of stCALCompoundCount values)
vaporFractions : [Optional] vapor fractions (molar or mass) (vector of stCALCompoundCount values)
equiConstants : [Optional] equilibrium constants (vector of stCALCompoundCount values)

Note(s) :
simulisCalculator shall be created with stCALCreate function

Package :
Simulis Thermodynamics for MatLab

Example :
scal = stCALCreate;
modified = stCALEdit(scal);
modified = stCALSystemEdit(scal,1);
modified = stCALSystemEdit(scal,2);
[vapRatio0,liquidFractions0,vaporFractions0,equiConstants0] = stCALFlashTP(scal,298.15,1.0,[0.5 0.5],0,0,fal
[vapRatio1,liquidFractions1,vaporFractions1,equiConstants1] = stCALFlashTP(scal,298.15,1.1,[0.5 0.5],0,0,tru
stCALFree(scal);

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See also
stCALCreate, stCALFree
```

Name	Value
EquiConstants	[0.6474,1.4428]
LiquidMolarFracti...	[0.5567,0.4433]
modified	0
modifiedInput	1
modifiedOutput	1
MolarVapRatio	0.2888
scal	1x1 SimulisThermodynamics_SimulisCalculate
VaporMolarFracti...	[0.3604,0.6396]

SIMULIS® THERMODYNAMICS & MATLAB

■ Access to the help of the functions:

- *stCALFlashTP* then **F1**

The screenshot shows the MATLAB R2019a environment. The Command Window is active, displaying the help for the `stCALFlashTP` function. The help text includes the function signature, input parameters, output parameters, and an example usage.

stCALFlashTP - MATLAB File Help

stCALFlashTP

Calculation of flash Liquid-Vapor at fixed temperature and pressure with a Simulis Calculator Object

function [vapRatio, liquidFractions, vaporFractions, equiConstants] = **stCALFlashTP**(simulisCalcula

Input parameter(s) :

- simulisCalculator : Simulis Calculator Object
- temperature : temperature of calculation expressed in INPUT unit system
- pressure : pressure of calculation expressed in INPUT unit system
- mixtComposition : mixture composition (vector of stCALCompoundCount values)
- mixtCompositionType : mixture composition type (0 = molar, 1 = mass)
- resultType : result type (0 = molar, 1 = mass)
- init : boolean value indicating if the following values are taken into account or not
- initVapRatio : [Optional] molar vaporization ratio of initialisation
- initLiquidFractions : [Optional] liquid fractions of initialisation (molar or mass) (vector of stCALCompoundCount values)
- initVaporFractions : [Optional] vapor fractions of initialisation (molar or mass) (vector of stCALCompoundCount values)

Output parameter(s) :

- vapRatio : molar vaporization ratio
- liquidFractions : [Optional] liquid fractions (molar or mass) (vector of stCALCompoundCount values)
- vaporFractions : [Optional] vapor fractions (molar or mass) (vector of stCALCompoundCount values)
- equiConstants : [Optional] equilibrium constants (vector of stCALCompoundCount values)

Note(s) :

- simulisCalculator shall be created with stCALCreate function

Package :

- Simulis Thermodynamics for MatLab

Example :

```
scal = stCALCreate;
modified = stCALEdit(scal);
modified = stCALSystemEdit(scal,1);
modified = stCALSystemEdit(scal,2);
[vapRatio0,liquidFractions0,vaporFractions0,equiConstants0] = stCALFlashTP(scal,298.15,1.0,
[vapRatio1,liquidFractions1,vaporFractions1,equiConstants1] = stCALFlashTP(scal,298.15,1.1,
stCALFree(scal);
```

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Arguments (green text pointing to input parameters)

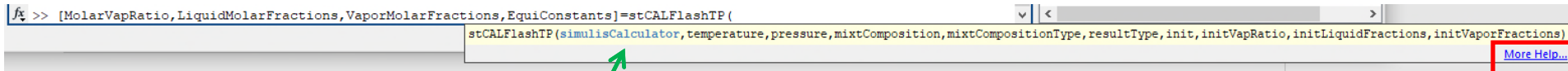
Return values (red text pointing to output parameters)

Example (blue text pointing to the example code)

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- Access to the help of the functions:

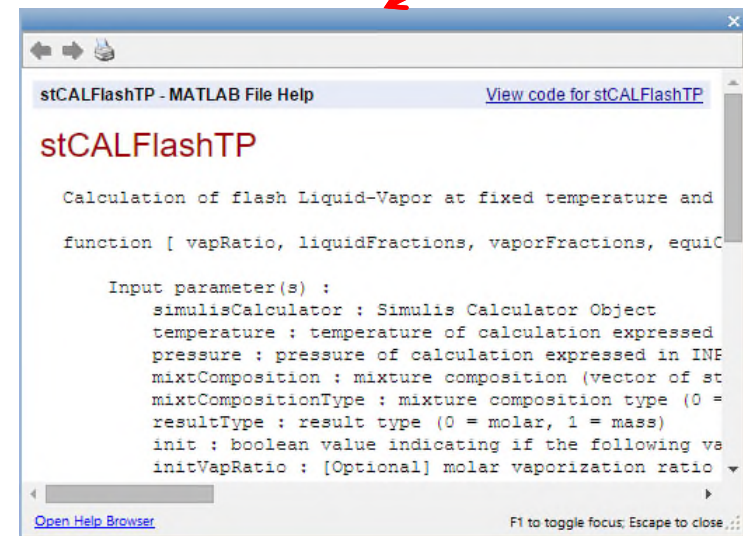
- Interactive help *stCALFlashTP*(



```

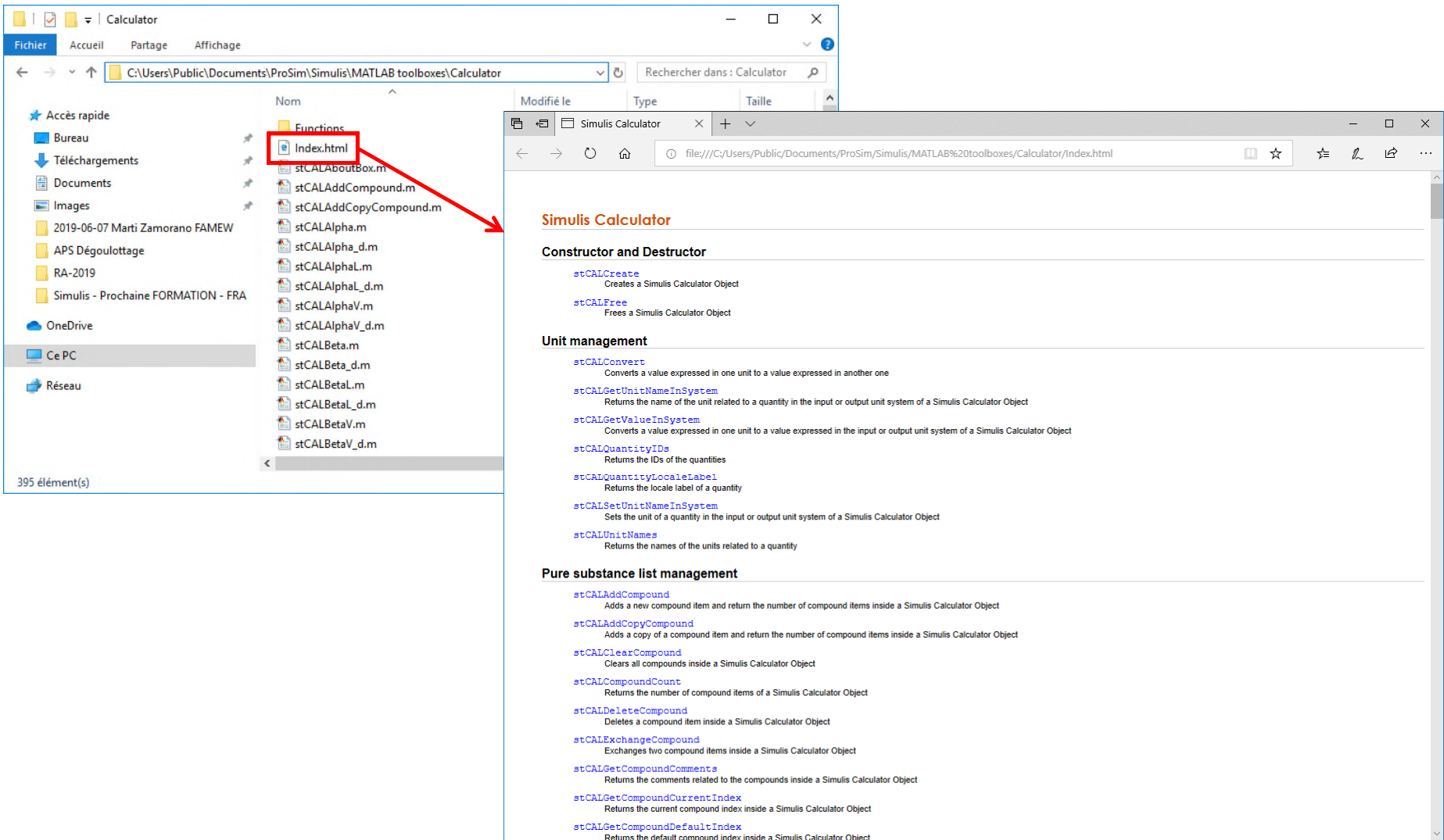
>> [MolarVapRatio,LiquidMolarFractions,VaporMolarFractions,EquiConstants]=stCALFlashTP(
stCALFlashTP(simulisCalculator,temperature,pressure,mixtComposition,mixtCompositionType,resultType,init,initVapRatio,initLiquidFractions,initVaporFractions)
More Help...
  
```

Arguments



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- Access to the help of the functions:
 - Directly from the installation directory with *Index.html*



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- Other examples are available in the SDK (Software Development Kit):

1-PROSIM > SDK > SDK > Examples > MATLAB 7				Rechercher dans : MATLAB 7
Nom	Modifié le	Type	Taille	
calculator.txt	07/12/2005 17:30	Document texte	5 Ko	
compounds.txt	07/12/2005 17:30	Document texte	5 Ko	
Demo1.m	06/12/2005 16:36	MATLAB Code	2 Ko	
Demo3.m	06/12/2005 17:00	MATLAB Code	2 Ko	
Demo4.m	07/12/2005 17:24	MATLAB Code	2 Ko	
Demo5.m	07/12/2005 17:27	MATLAB Code	2 Ko	
Demo7.m	13/12/2005 13:50	MATLAB Code	7 Ko	
Demo8.m	07/12/2005 17:21	MATLAB Code	2 Ko	
Demo9.m	07/12/2005 17:24	MATLAB Code	2 Ko	
Demo10.m	07/12/2005 17:27	MATLAB Code	2 Ko	
Demo12.m	14/12/2005 08:46	MATLAB Code	5 Ko	

Demo1	Example of conversions	System
Demo3	Example of edition of a Compounds Object	Compounds
Demo4	Edit and Save a Compounds Object	Compounds
Demo5	Load and Edit a Compounds Object	Compounds
Demo7	Get property values of a Compounds Object	Compounds
Demo8	Example of edition of a Calculator Object	Calculator
Demo9	Edit and Save a Calculator Object	Calculator
Demo10	Load and Edit a Calculator Object	Calculator
Demo12	Edition and use of a Calculator Object	Calculator



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Software & Services In Process Simulation

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