Getting started with Simulis® Thermodynamics

Use Case 12: Use within MATLAB®

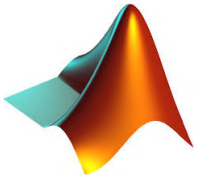
Software & Services In Process Simulation

We guide You to efficiency

ProSim

Introduction

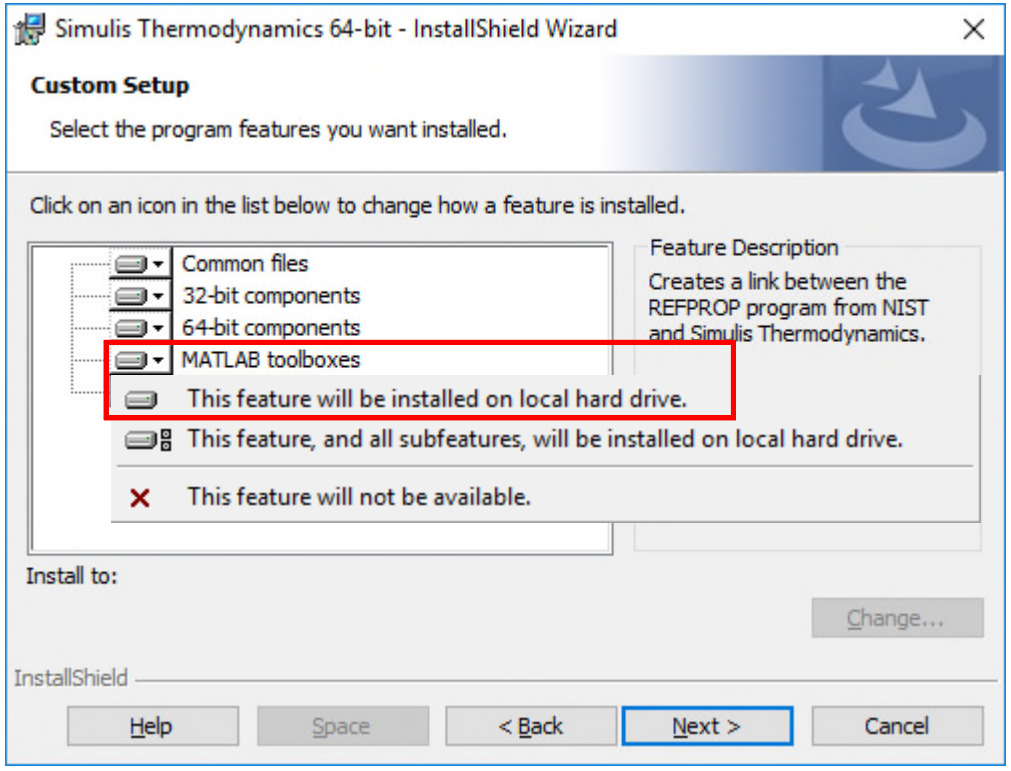
This document presents the operation of Simulis Thermodynamics in MATLAB



- Installation
- Examples
- Helps

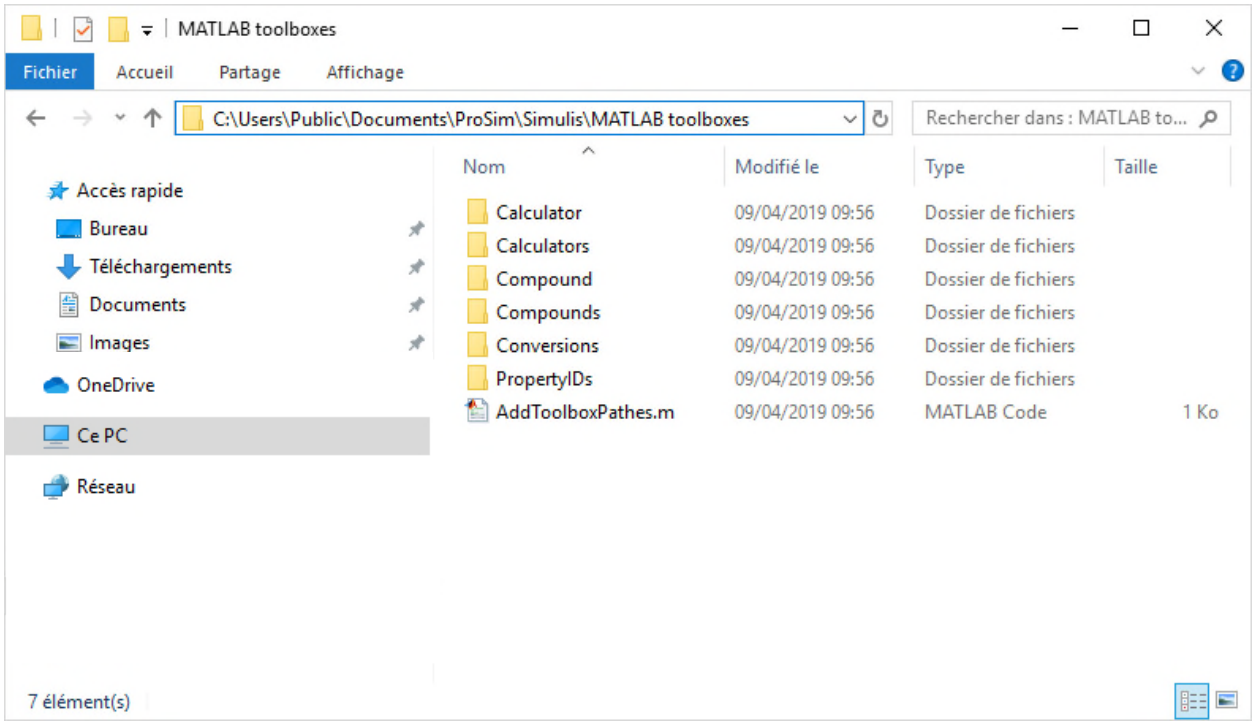
SIMULIS® THERMODYNAMICS & MATLAB

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



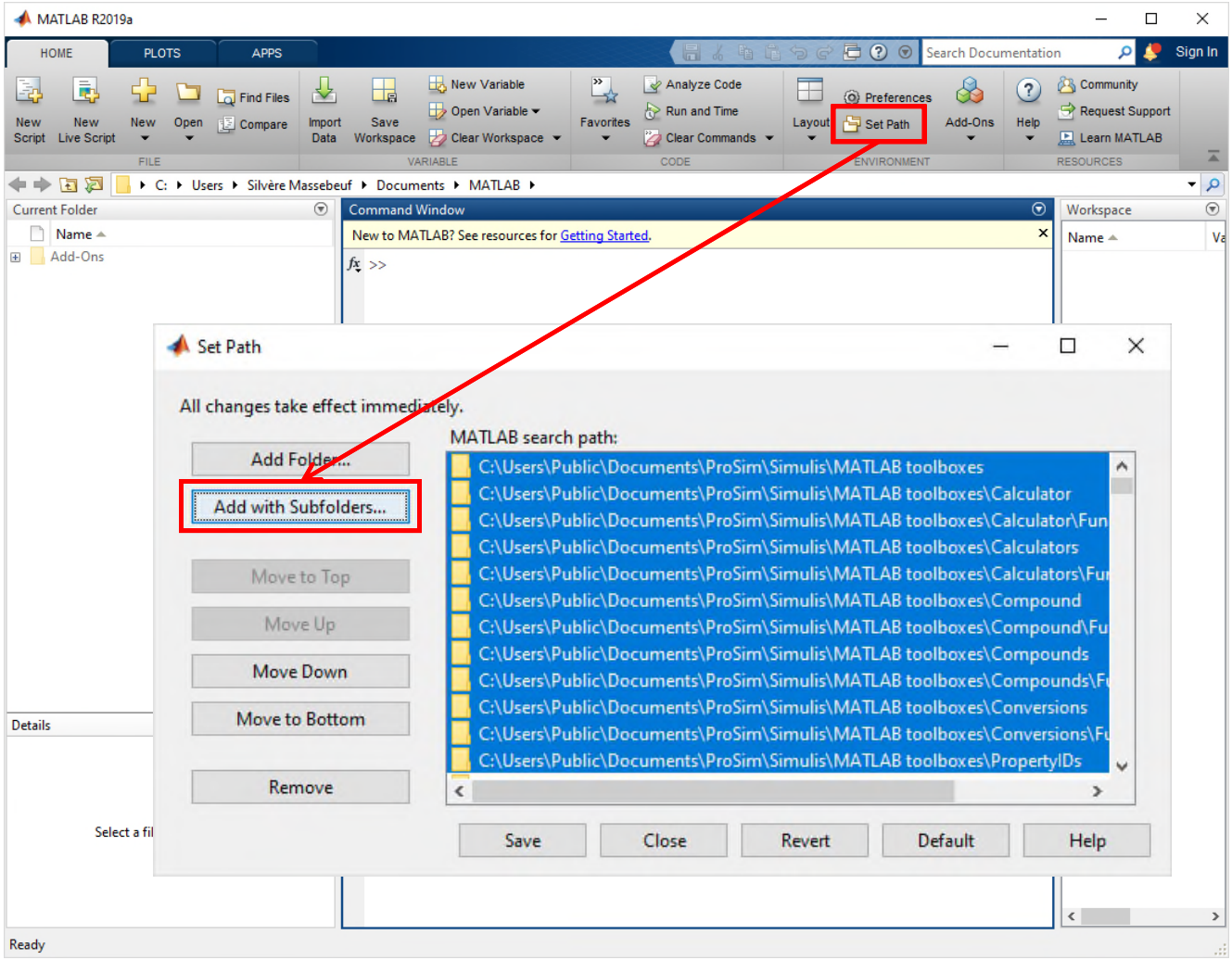
SIMULIS® THERMODYNAMICS & MATLAB

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



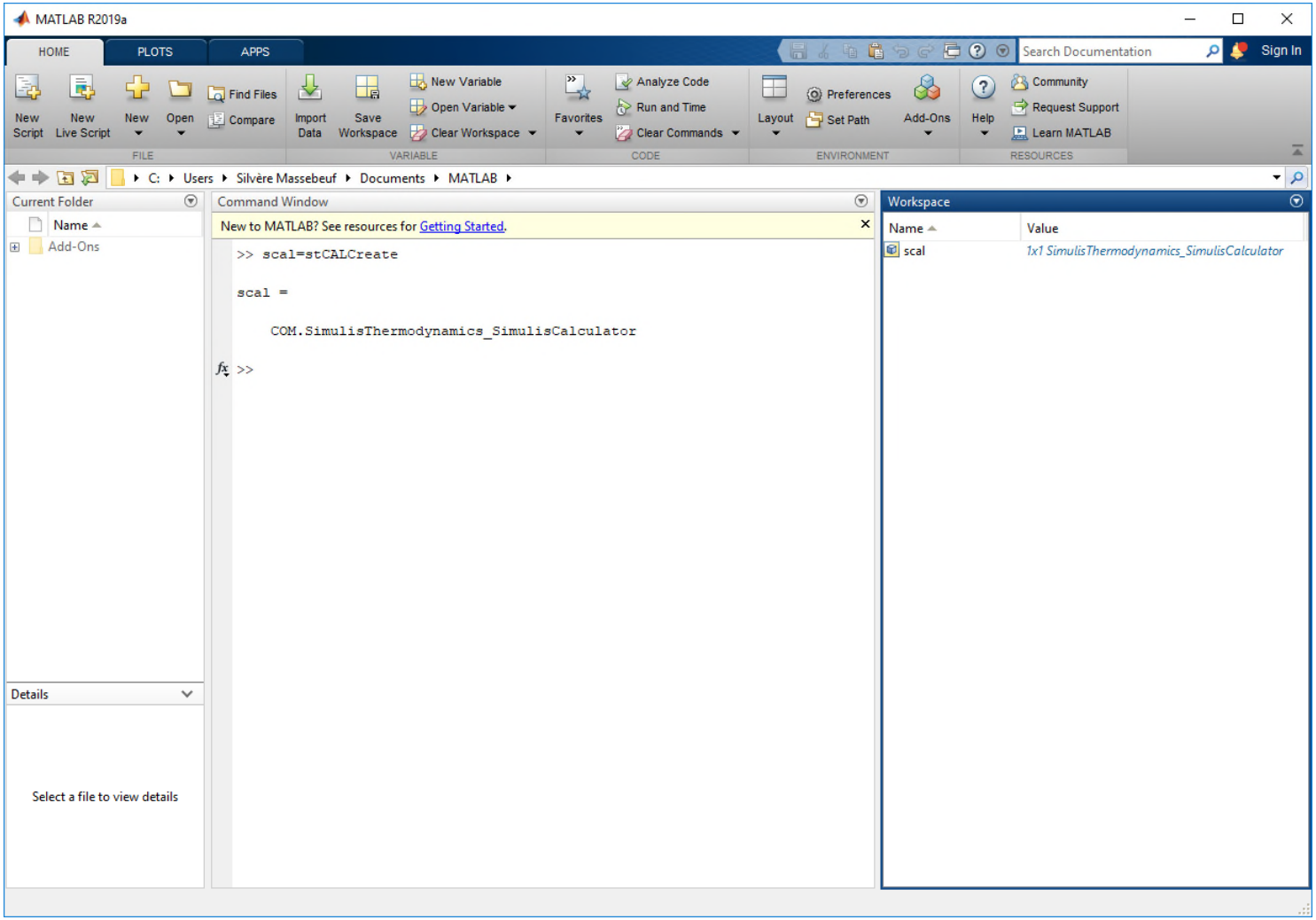
SIMULIS® THERMODYNAMICS & MATLAB

- Installation:
  - Add this MATLAB search path



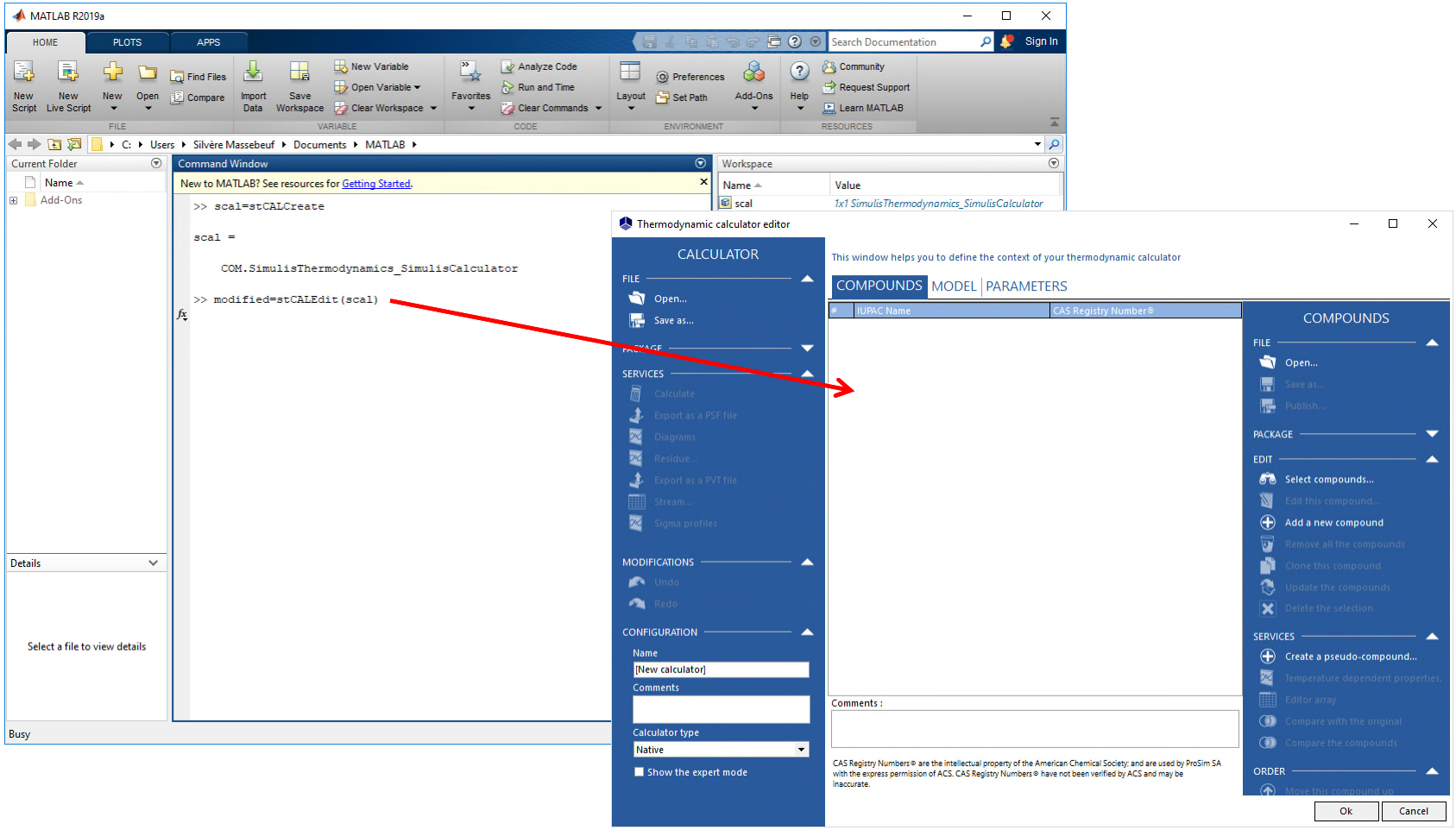
SIMULIS® THERMODYNAMICS & MATLAB

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



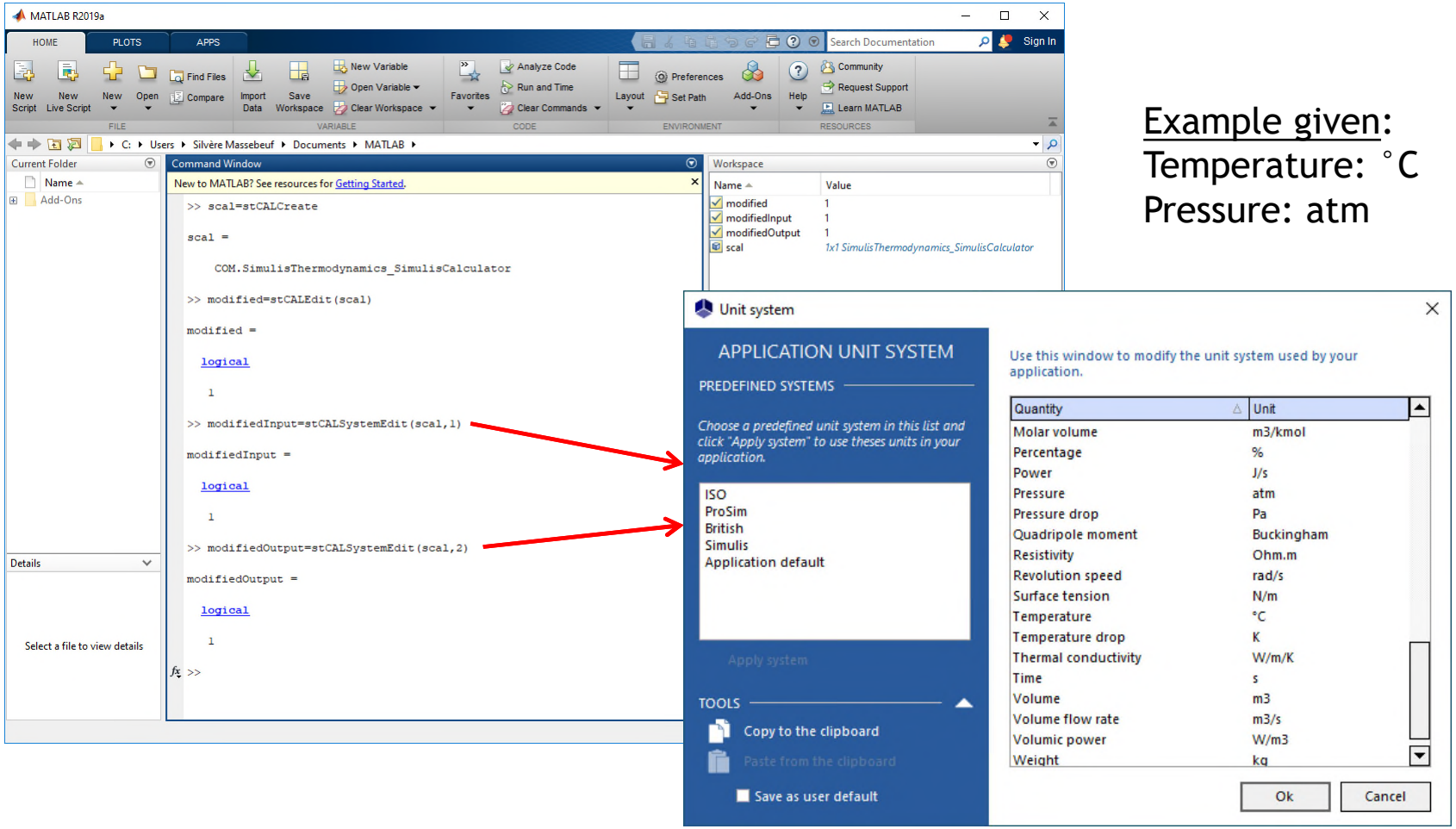
SIMULIS® THERMODYNAMICS & MATLAB

- Edit the Simulis calculator object
(define components and thermodynamic model):
  - modified=*stCALEdit*(scal)



SIMULIS® THERMODYNAMICS & MATLAB

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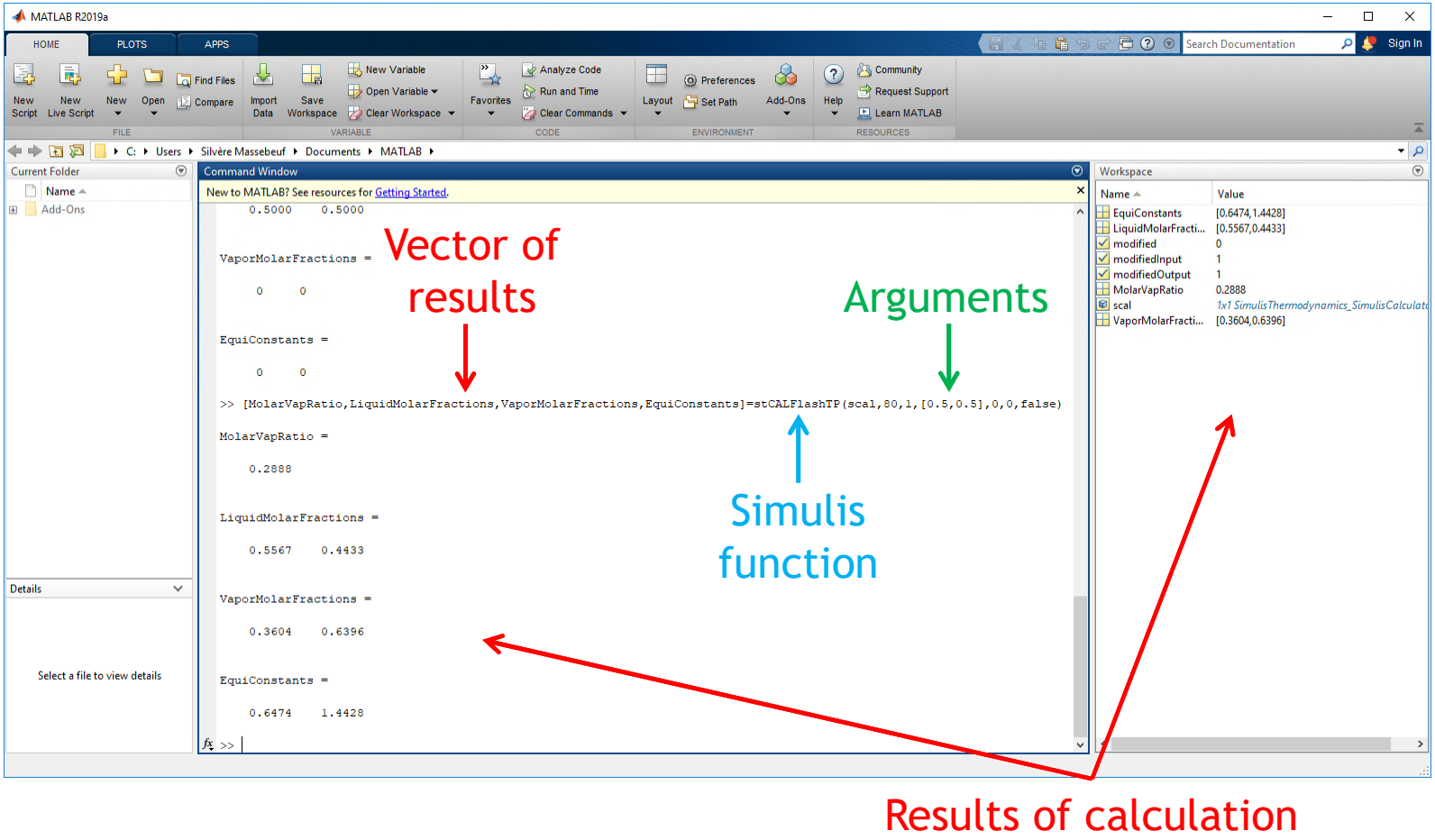
- Calculation of a flash at given temperature and pressure (e. g.: equimolar water-ethanol system at 80 °C and 1 atm):
  - [MolarVapRatio,LiquidMolarFractions,VaporMolarFractions,EquiConstants] =*stCALFlashTP(*scal,80,1,[0.5,0.5],0,0,false*)*



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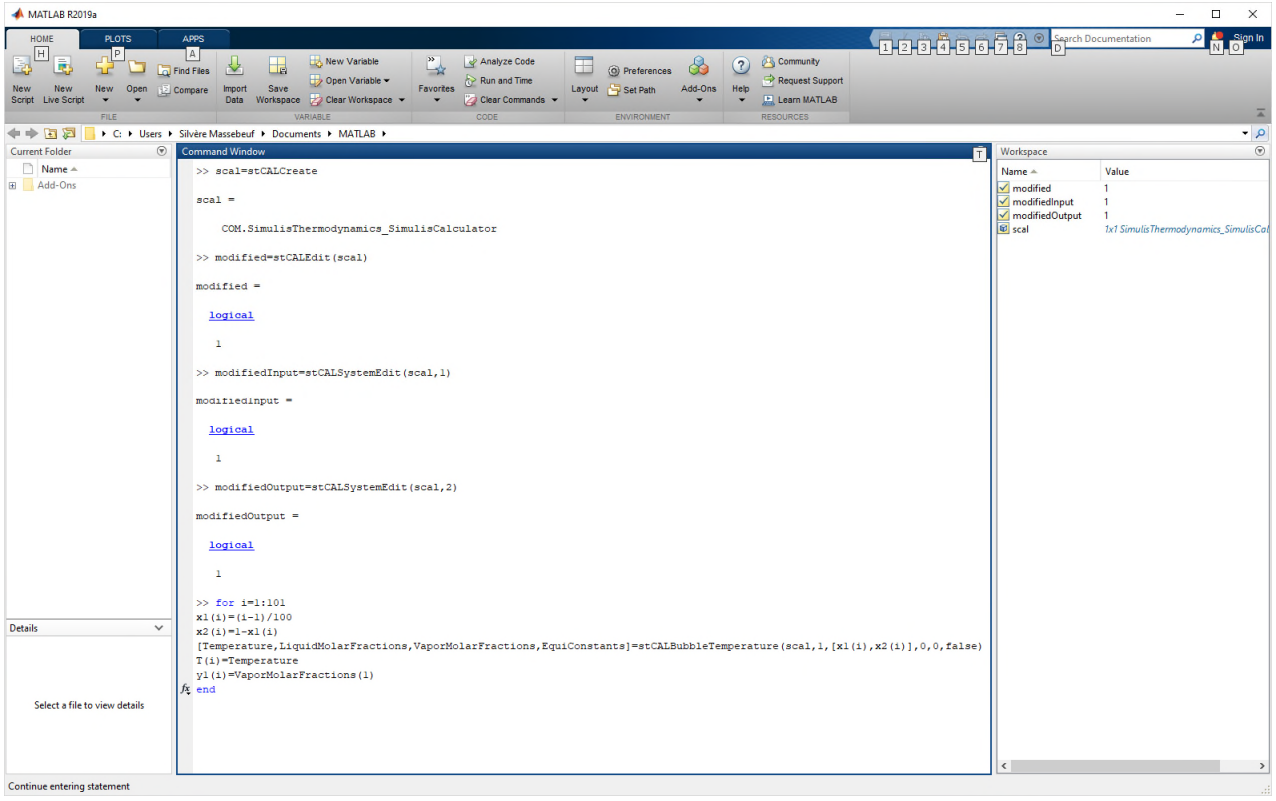
- Plot of equilibrium curves at atmospheric pressure:
  - for i=1:101

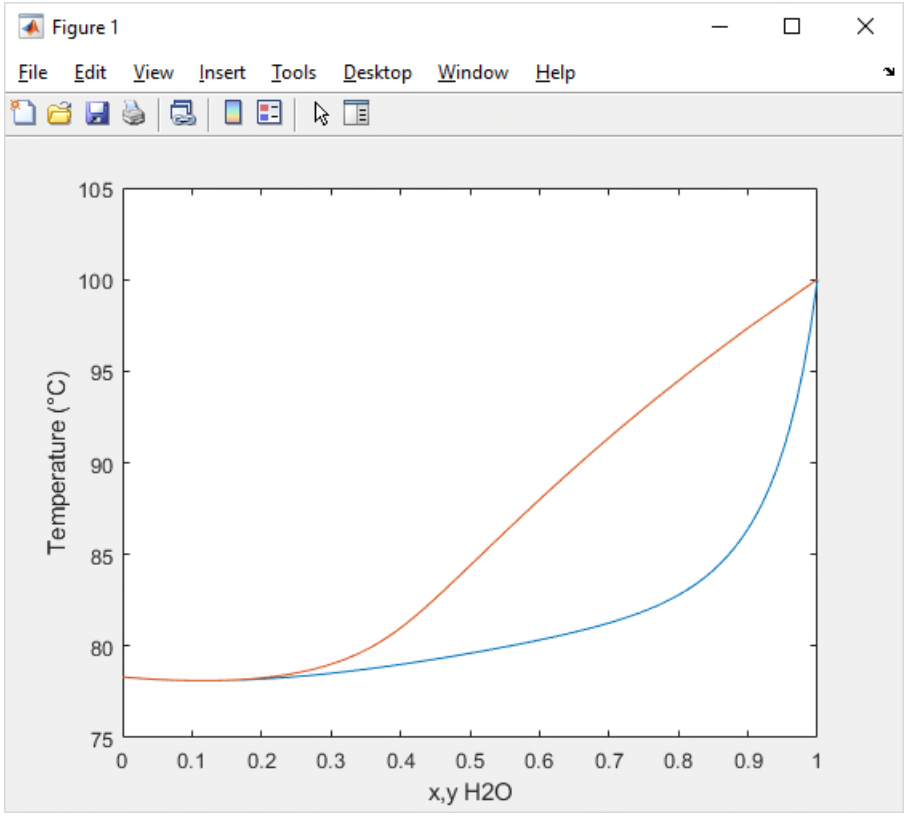
```
x1(i)=(i-1)/100
x2(i)=1-x1(i)
[Temperature,LiquidMolarFractions,VaporMolarFractions,EquiConstants]
=stCALBubbleTemperature(scal,1,[x1(i),x2(i)],0,0,false)
T(i)=Temperature
y1(i)=VaporMolarFractions(1)
```

  end



SIMULIS® THERMODYNAMICS & MATLAB

- Plot of equilibrium curves at atmospheric pressure:
  - plot(x1,T,y1,T)
    xlabel('x,y H2O')
    ylabel('Temperature (°C) ')



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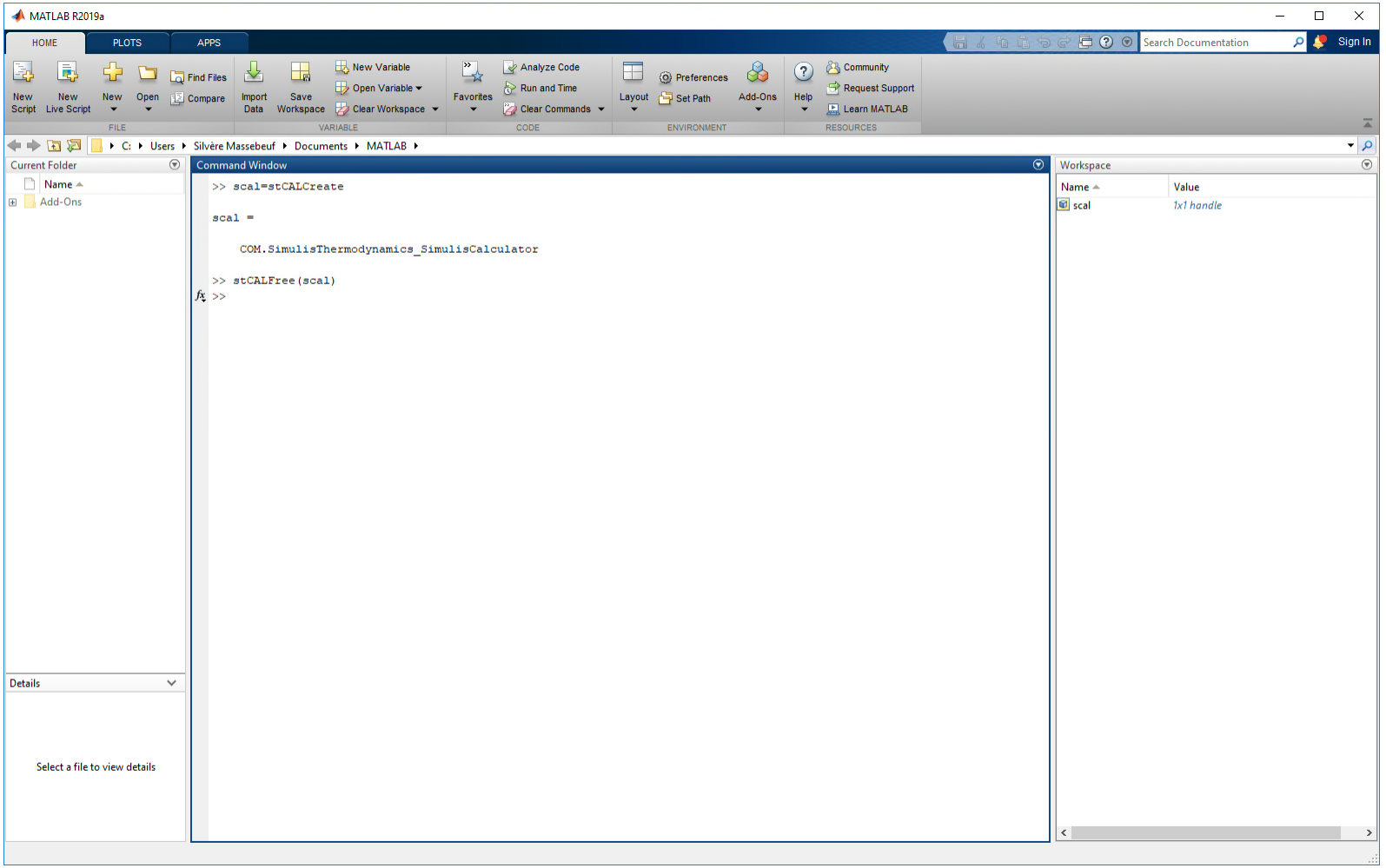
- Free a Simulis object:
  - *stCALFree(*scal*)*



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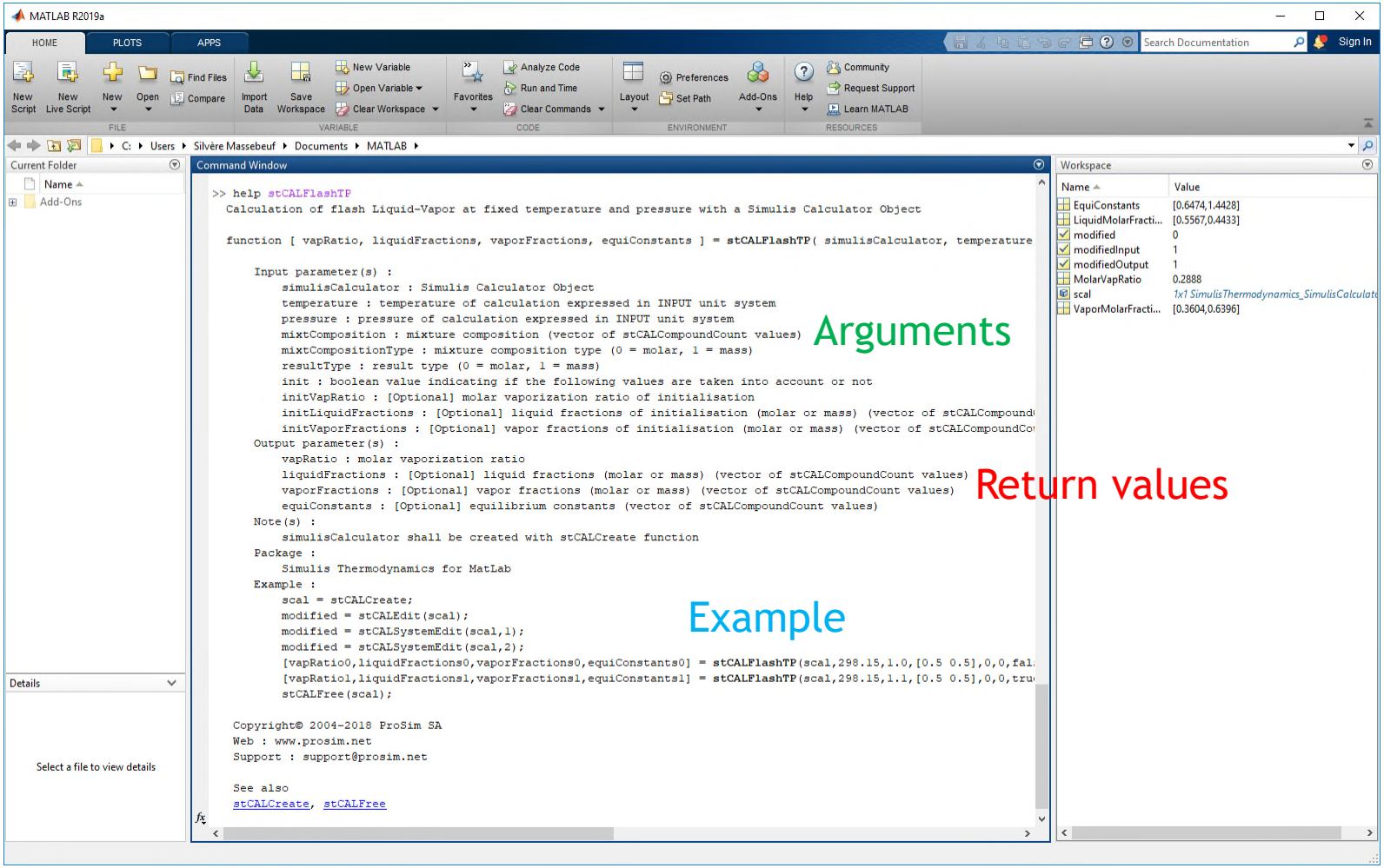
- Access to the help of the functions:
  - help *stCALFlashTP*



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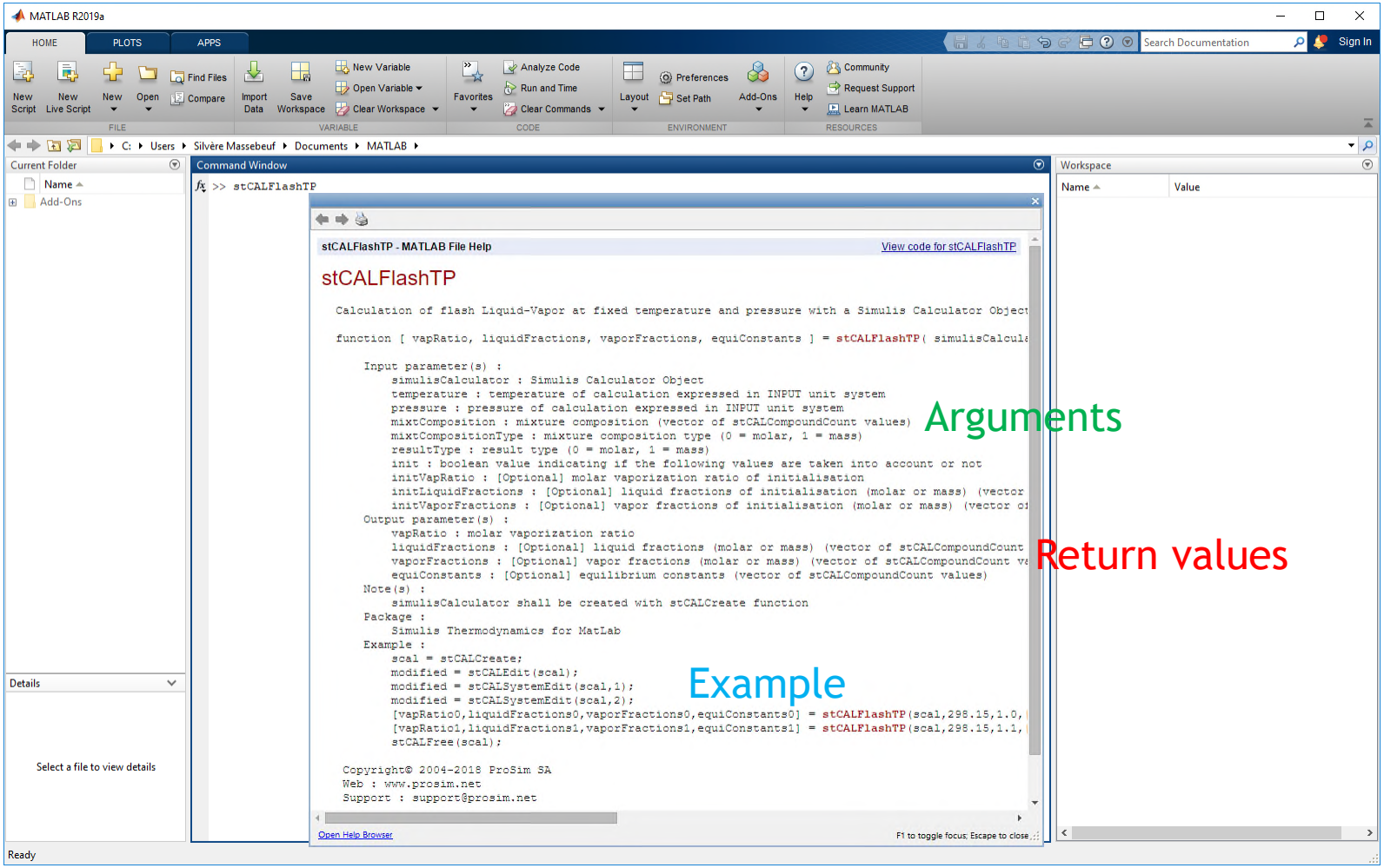
- Access to the help of the functions:
  - *stCALFlashTP* then F1



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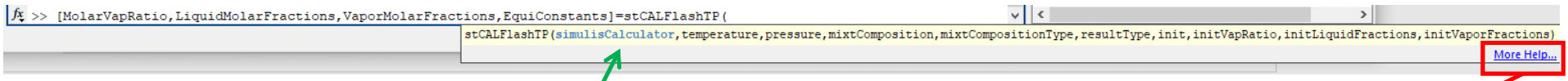
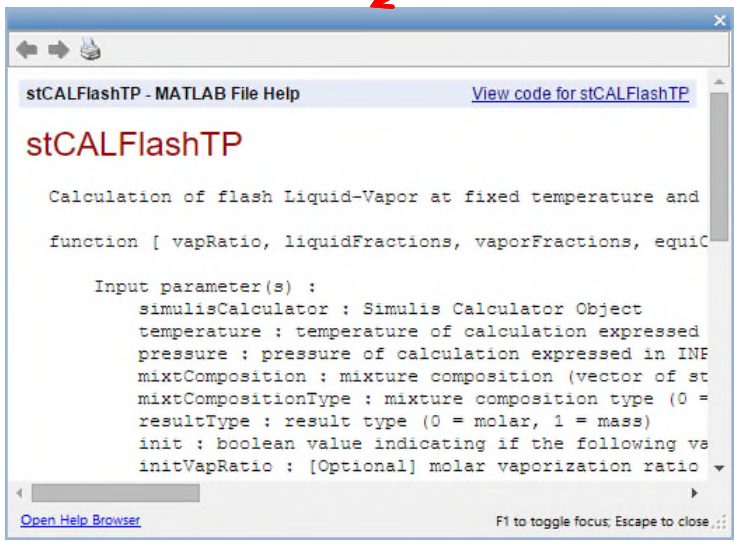
- Access to the help of the functions:
  - Interactive help *stCALFlashTP(*



Arguments



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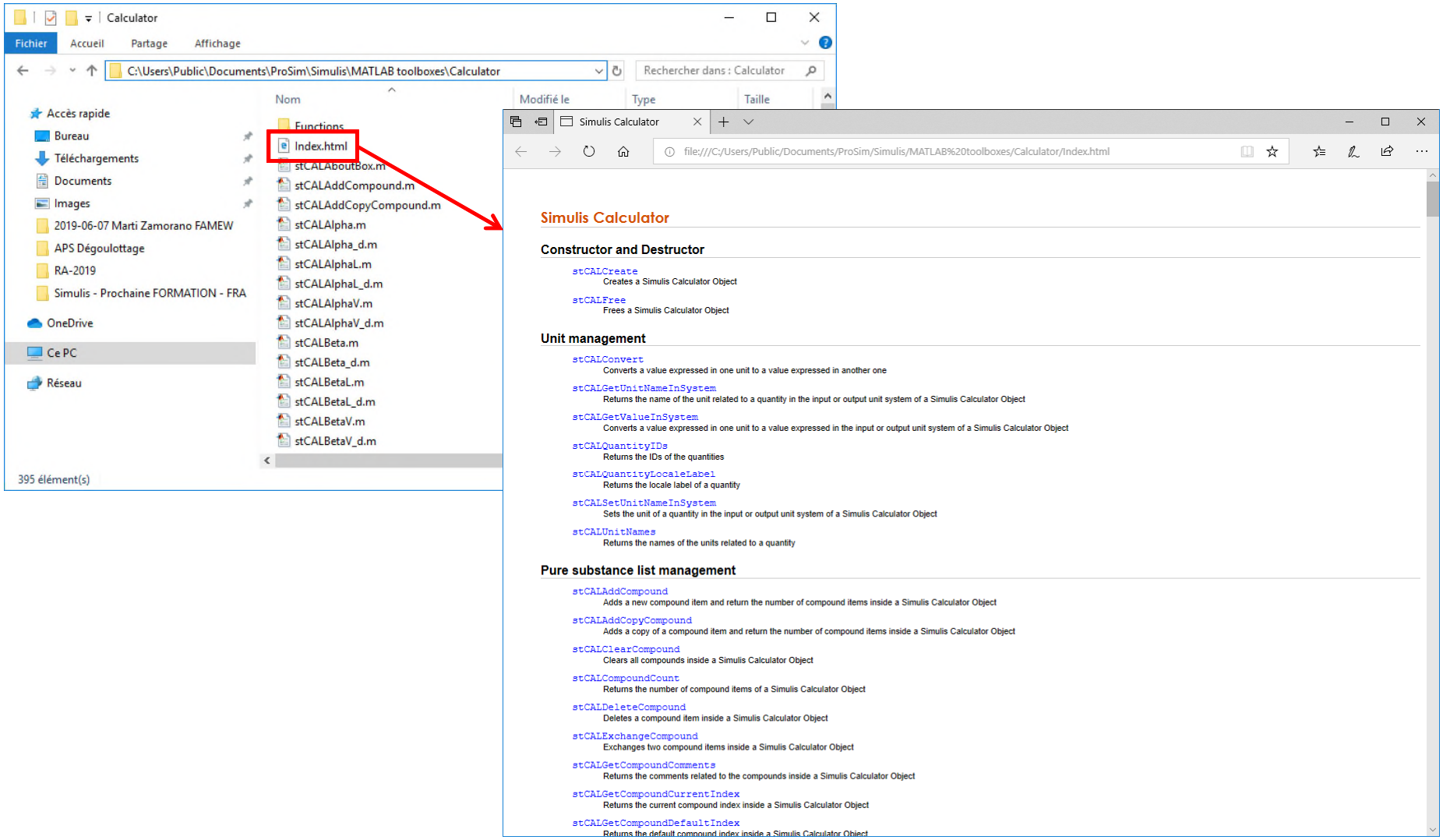
- Access to the help of the functions:
  - Directly from the installation directory with *Index.html*



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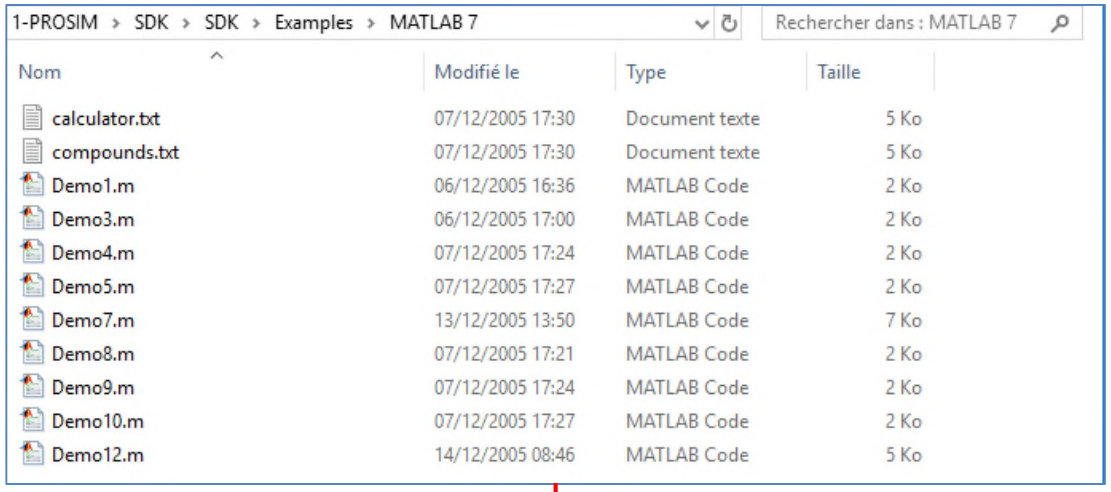
- Other examples are available in the SDK (Software Development Kit):



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

ProSim

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