

Démarrer avec Simulis® Thermodynamics

Cas 12 : Utilisation dans MATLAB®

Software & Services In Process Simulation

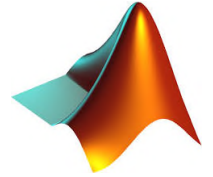
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ProSim

Introduction

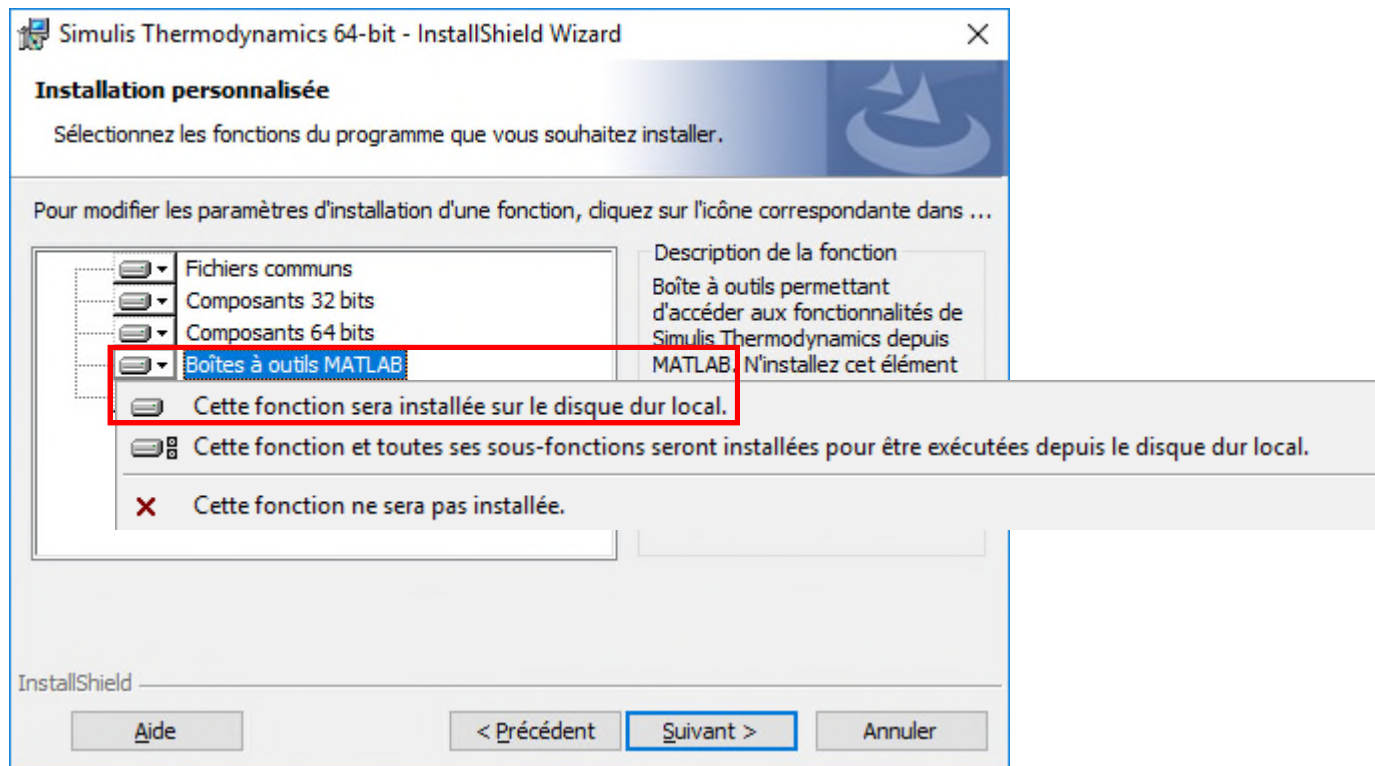
Ce document présente le fonctionnement de Simulis Thermodynamics dans MATLAB



- Installation
- Exemples d'utilisation
- Aides

SIMULIS® THERMODYNAMICS & MATLAB

- Installation :
 - Sélectionner « Boîtes à outils MATLAB » à installer durant l'installation de Simulis Thermodynamics

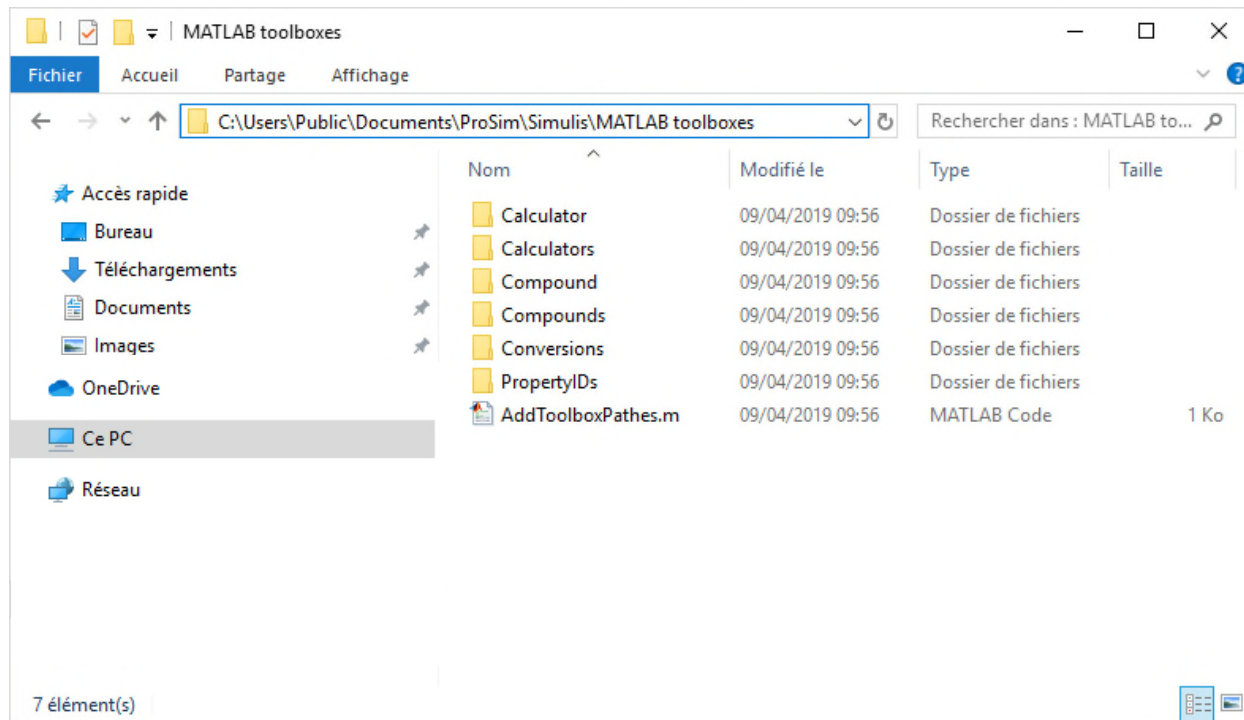


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■ Installation :

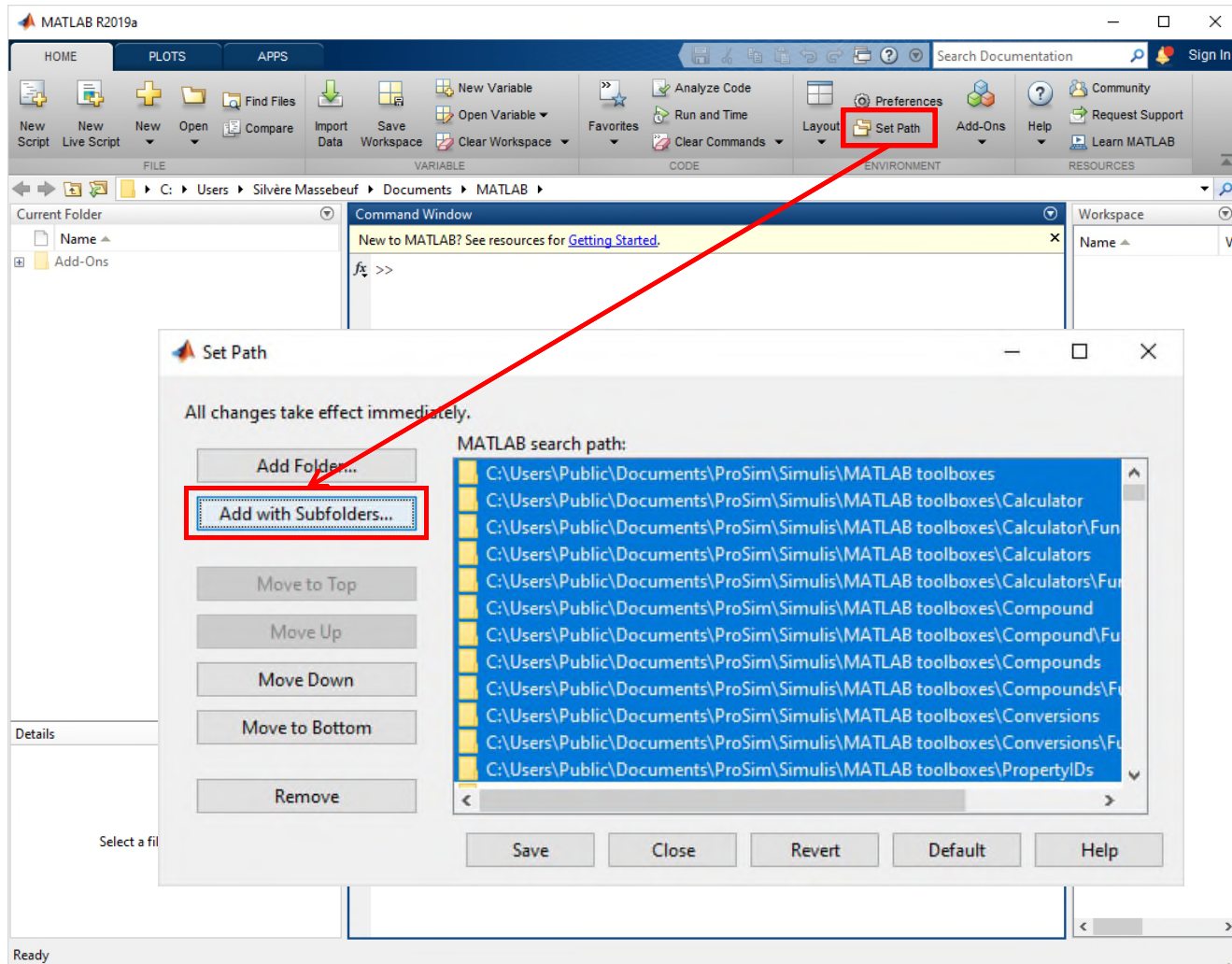
- Vérification dans le répertoire d'installation :

C:\Users\Public\Documents\ProSim\Simulis\MATLAB toolboxes



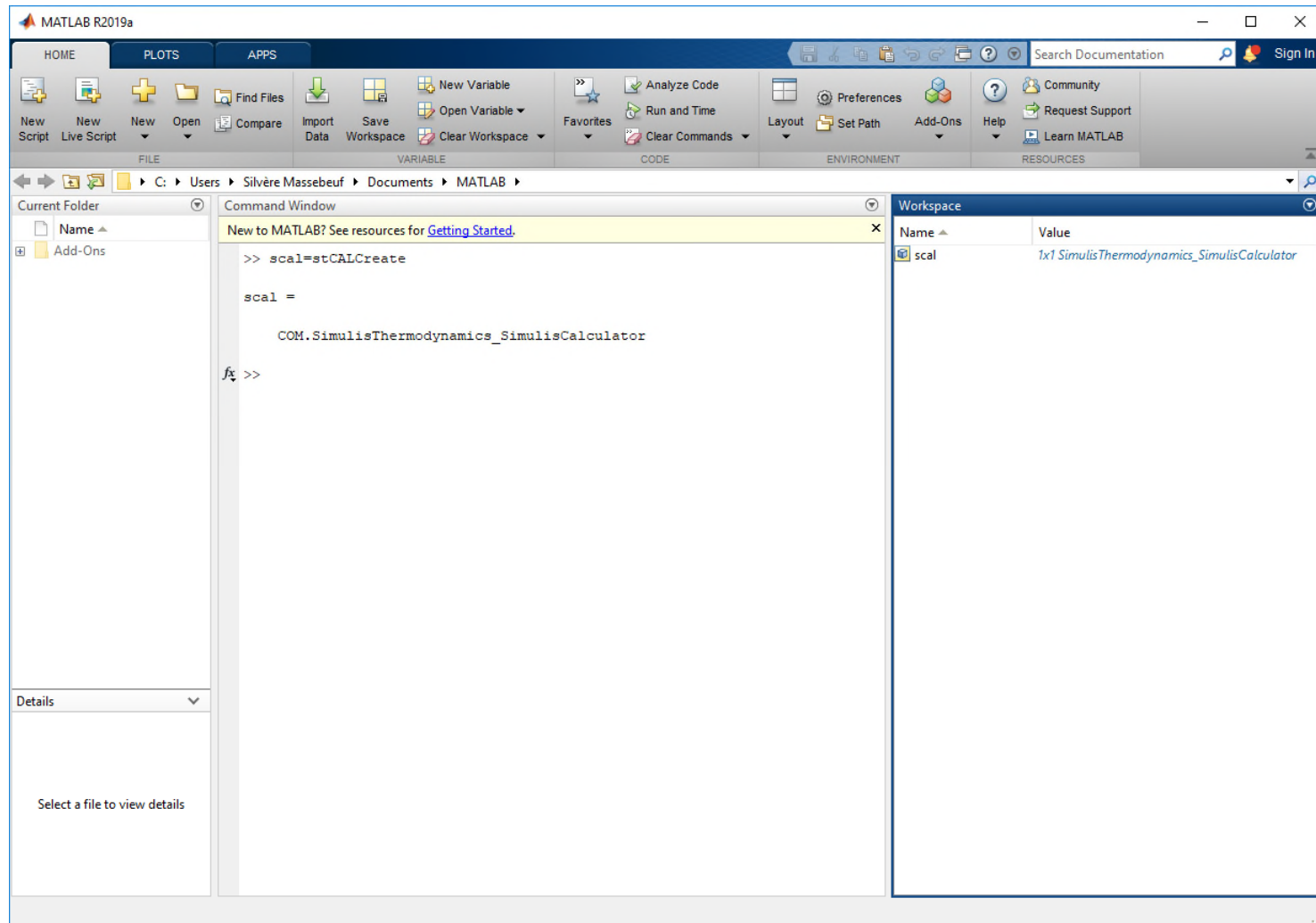
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- Installation :
 - Ajouter ce chemin de recherche MATLAB



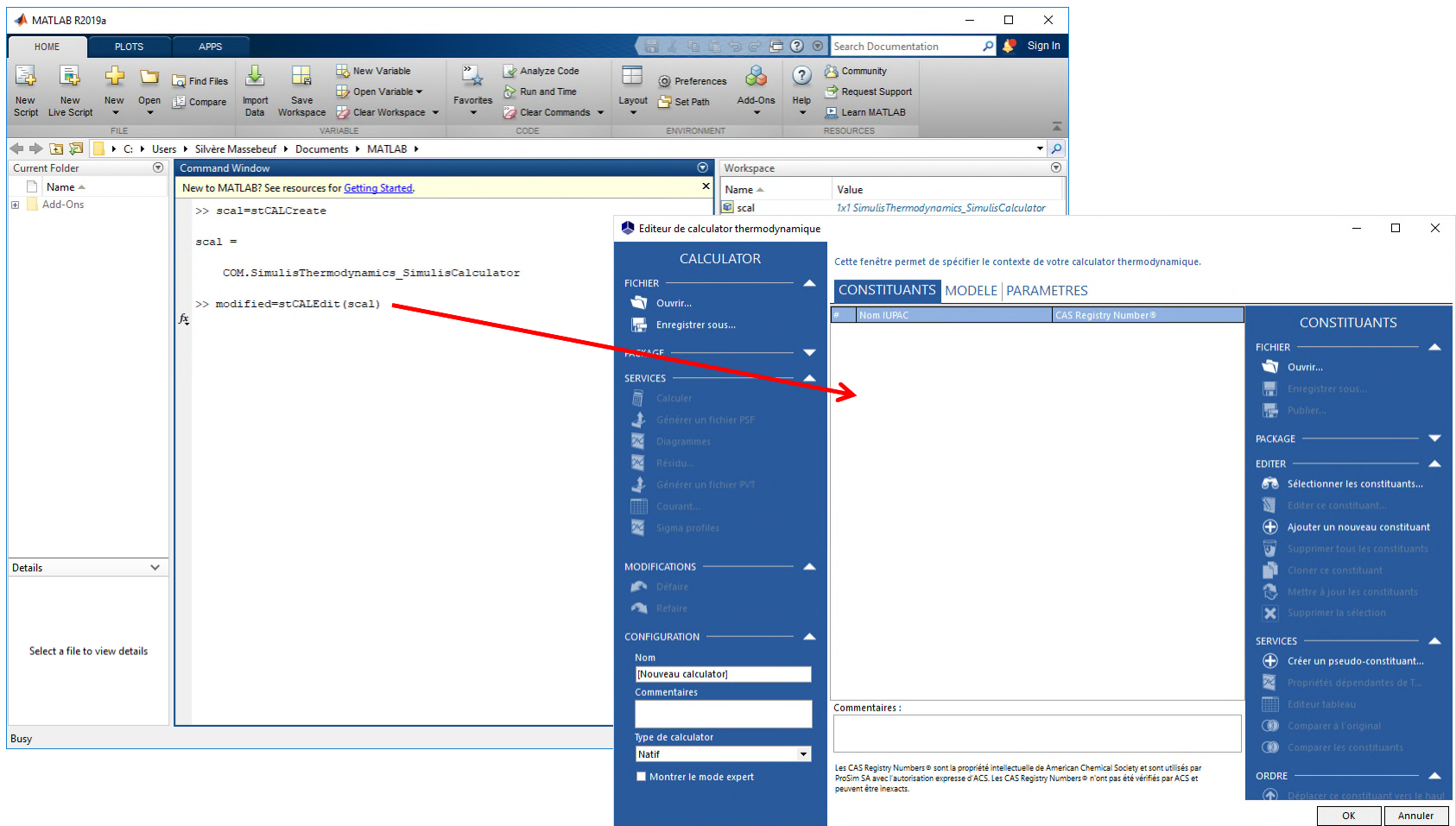
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- Création d'un objet Simulis calculator :
 - `scal=stCALCreate`



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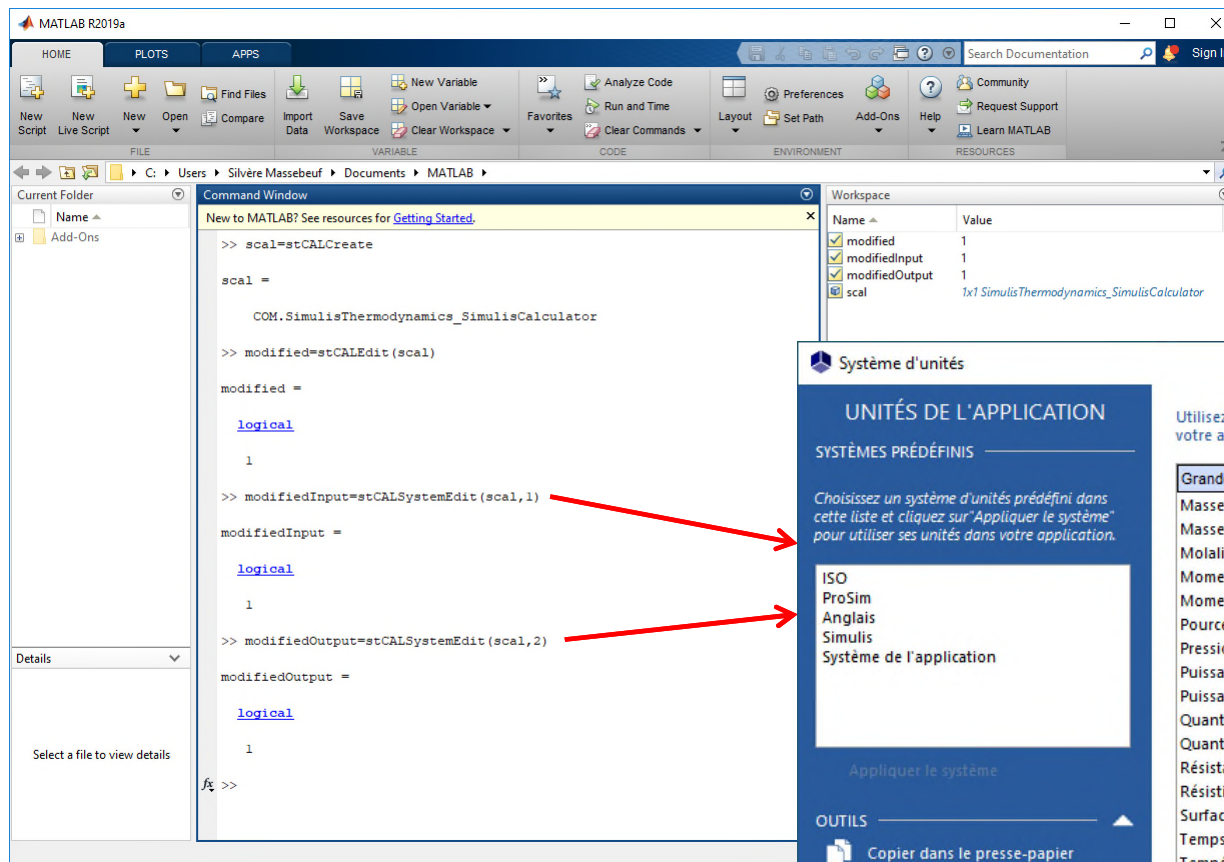
- Edition de l'objet Simulis calculator
(définition des constituants et du modèle thermodynamique) :
 - **modified**=stCALEdit(scal)



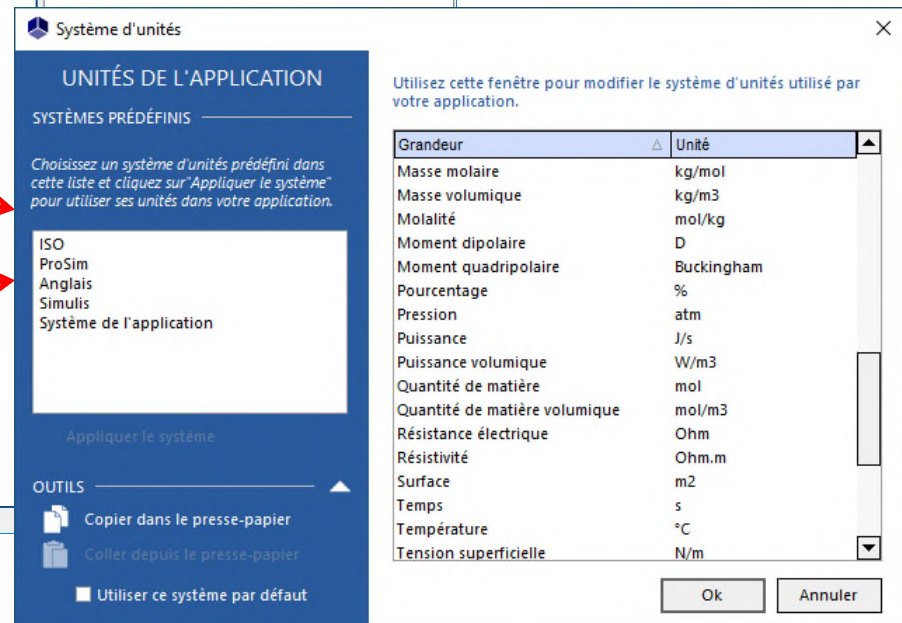
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- Systèmes d'unités de l'objet Simulis calculator (entrée et sortie) :

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

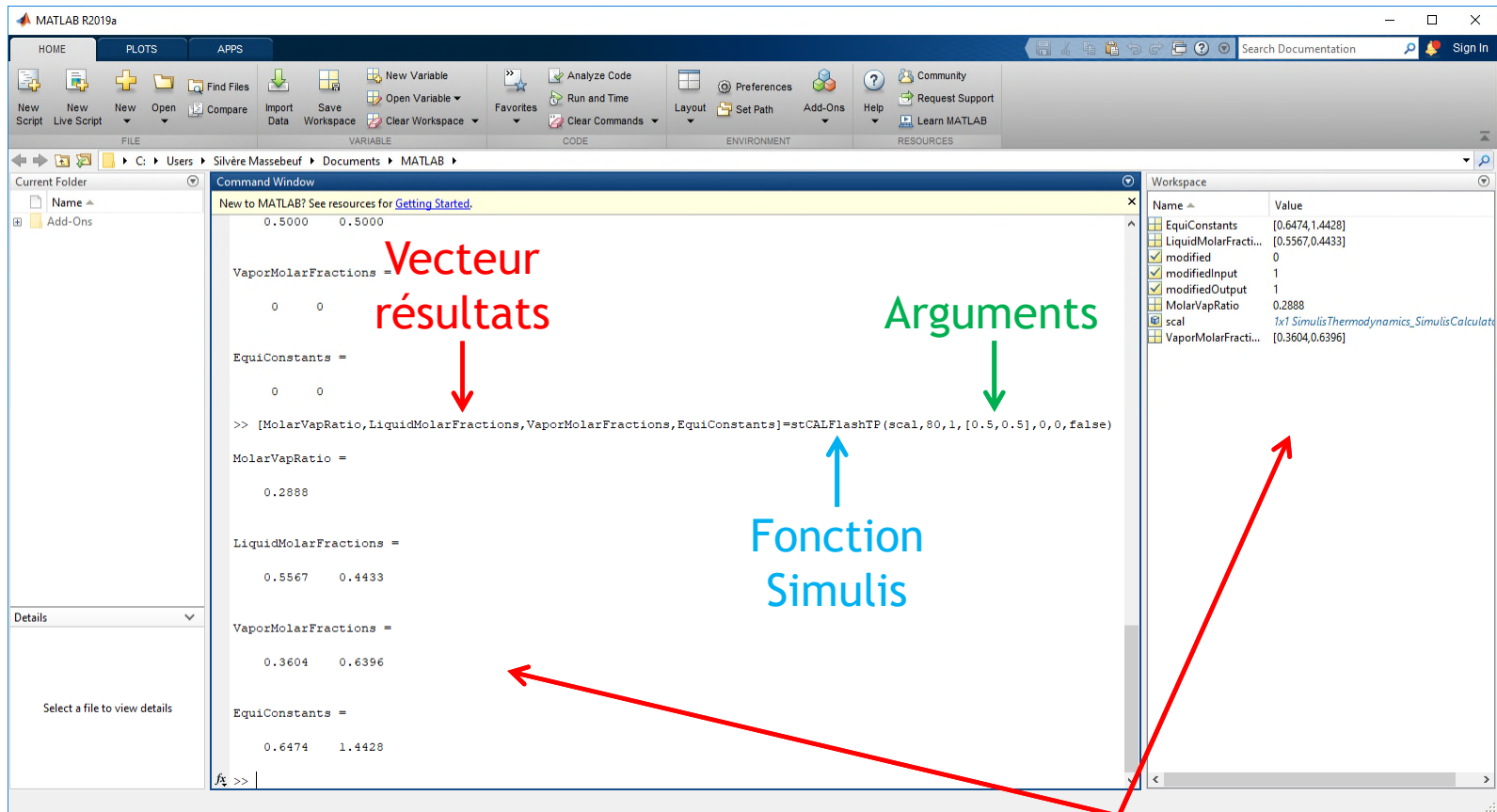


Par exemple :
Température : °C
Pression : atm



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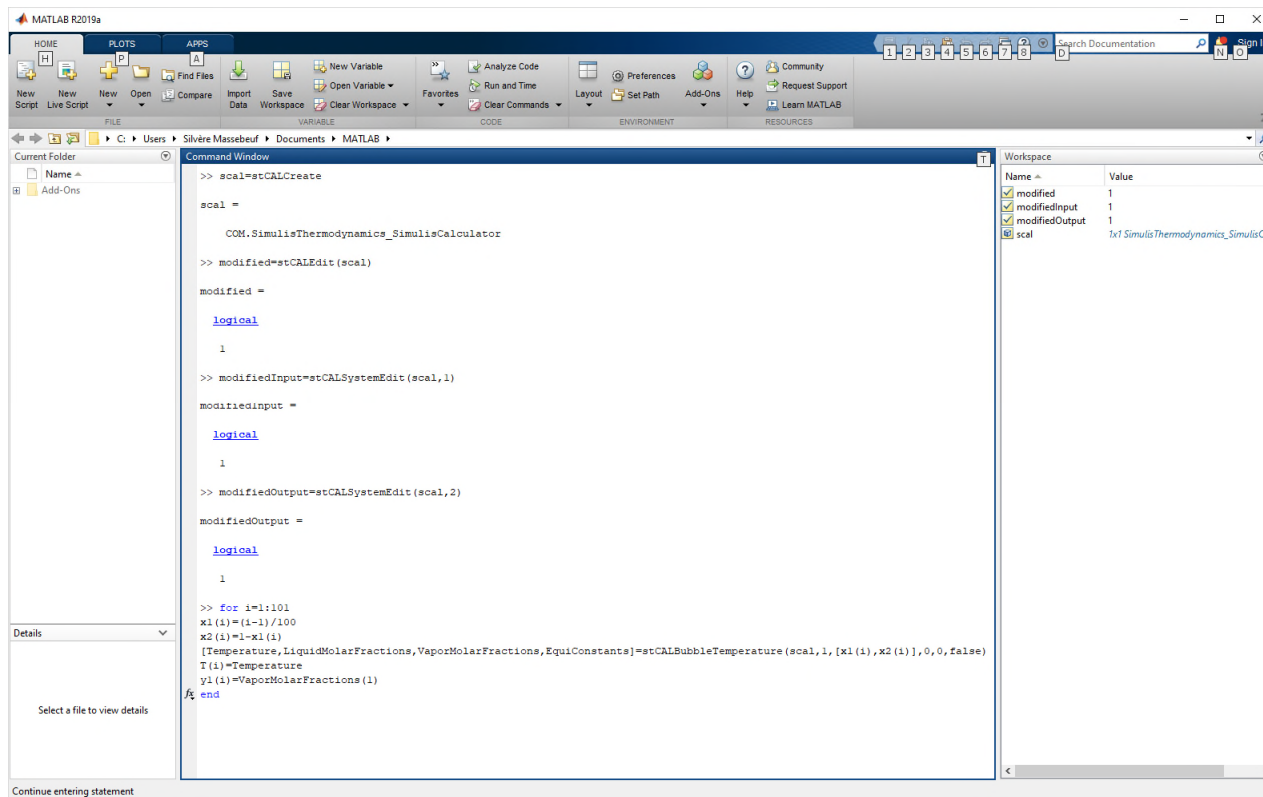
- Calcul d'un flash à température et pression données
(ex. : système eau-éthanol équimolaire à 80 °C et 1 atm) :
 - **[MolarVapRatio, LiquidMolarFractions, VaporMolarFractions, EquiConstants]**
=stCALFlashTP(scal, 80, 1, [0.5, 0.5], 0, 0, false)



Résultats de calcul

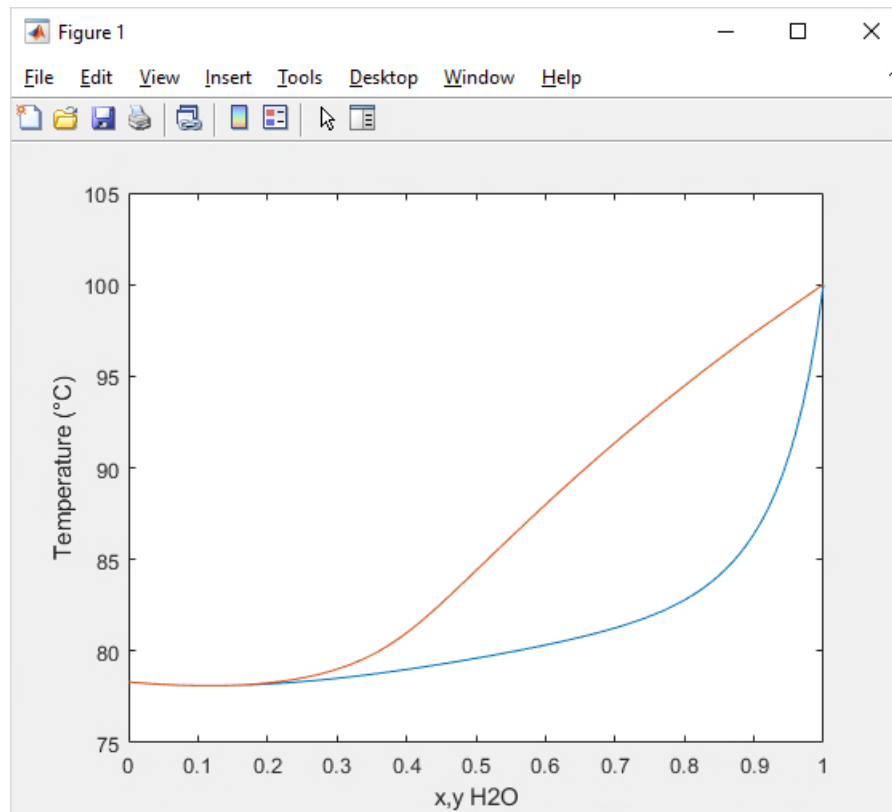
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- Tracé de courbes d'équilibre à pression atmosphérique :
 - `for i=1:101`
 - `x1(i)=(i-1)/100`
 - `x2(i)=1-x1(i)`
 - `[Temperature,LiquidMolarFractions,VaporMolarFractions,EquiConstants]`
 - `=stCALBubbleTemperature(scal,1,[x1(i),x2(i)],0,0,false)`
 - `T(i)=Temperature`
 - `y1(i)=VaporMolarFractions(1)`
 - `end`



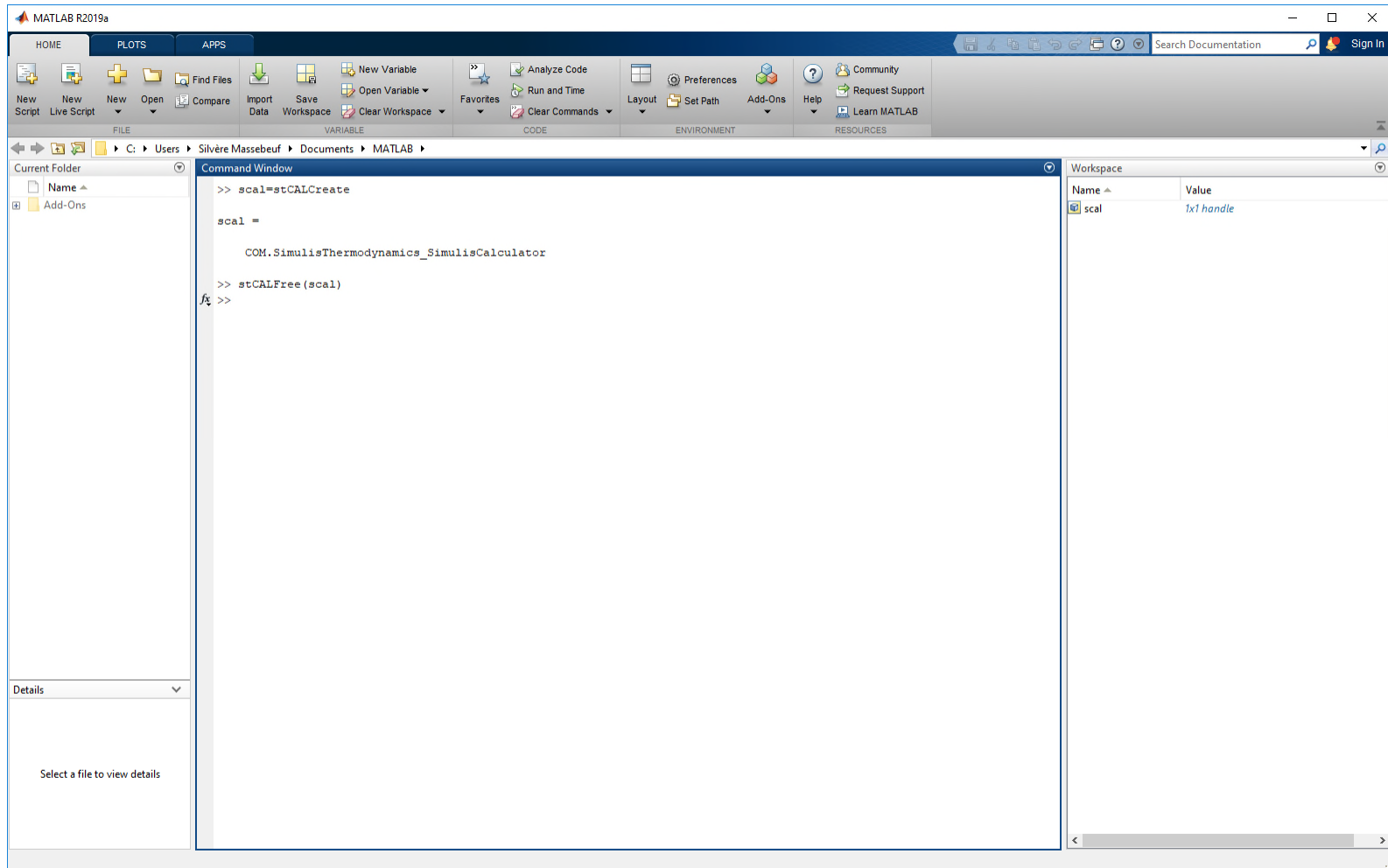
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- Tracé de courbes d'équilibre à pression atmosphérique :
 - `plot(x1,T,y1,T)`
`xlabel('x,y H2O')`
`ylabel('Temperature (°C)')`



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- Libérer l'objet Simulis :
 - *stCALFree(scal)*



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■ Accès à l'aide des fonctions :

- **help** *stCALFlashTP*

The screenshot shows the MATLAB R2019a interface with the Command Window displaying the help documentation for the `stCALFlashTP` function. The Workspace window shows the values of the output variables.

Arguments

Valeurs de retour

Exemple d'utilisation

```
>> 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,false);
[vapRatio1,liquidFractions1,vaporFractions1,equiConstants1] = stCALFlashTP(scal,298.15,1.1,[0.5 0.5],0,0,true);
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

■ Accès à l'aide des fonctions :

- *stCALFlashTP* puis **F1**

The screenshot shows the MATLAB R2019a environment with the help window for the `stCALFlashTP` function open. The Command Window contains the following text:

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);
```

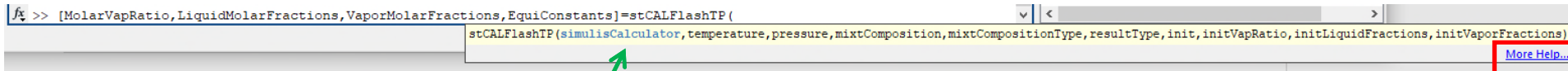
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Annotations on the screenshot:

- Arguments** (green text) points to the input parameters section.
- Valeurs de retour** (red text) points to the output parameters section.
- Exemple d'utilisation** (blue text) points to the example code block.

SIMULIS® THERMODYNAMICS & MATLAB

- Accès à l'aide des fonctions :
 - Aide interactive *stCALFlashTP*(

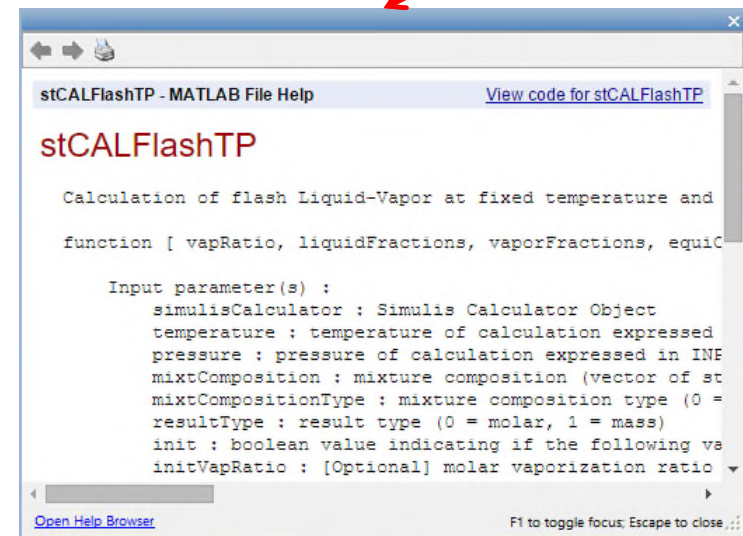


```

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

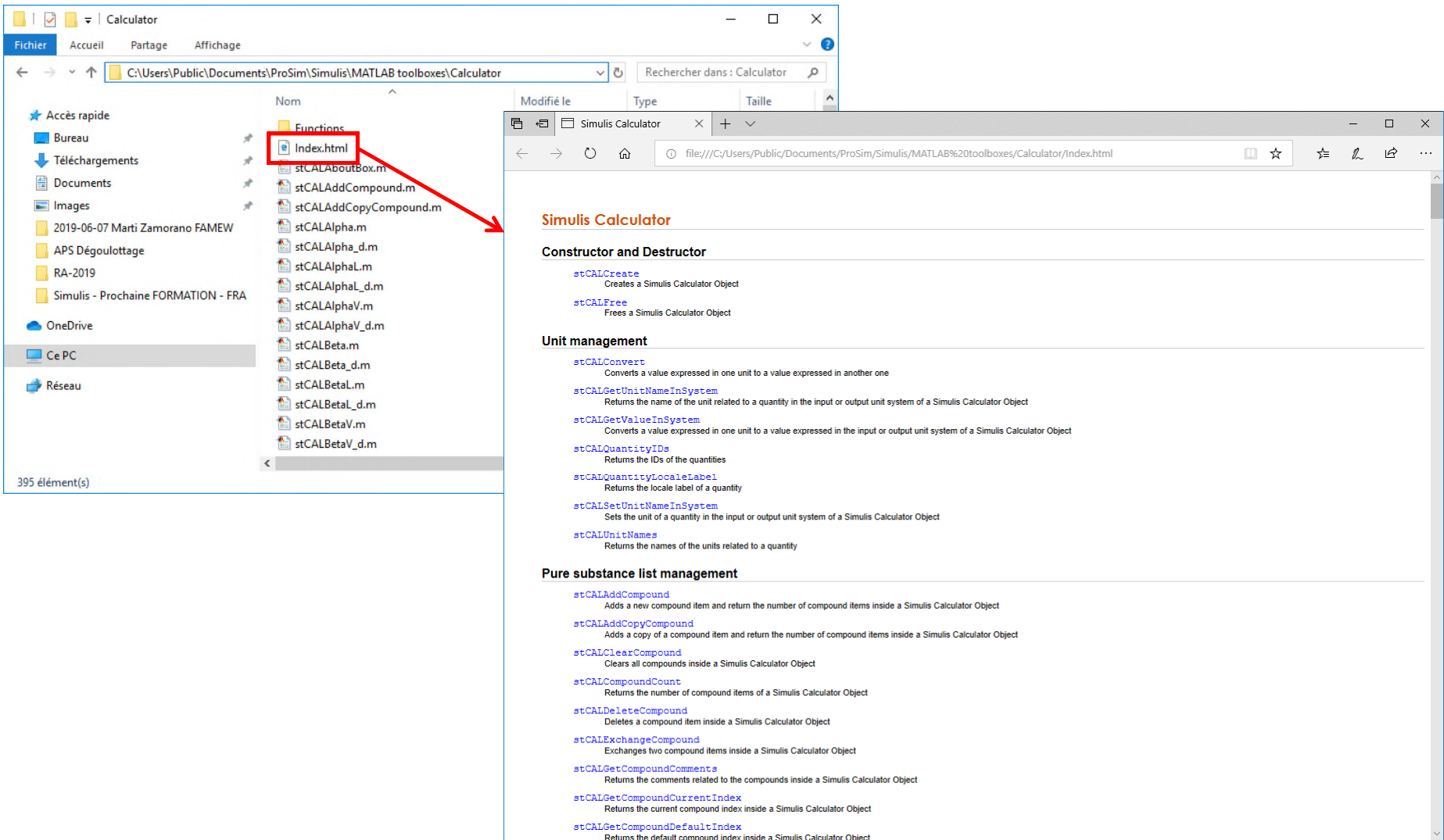
```

Arguments



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- Accès à l'aide de toutes les fonctions :
 - Directement depuis le répertoire d'installation via l'*Index.html*



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- Autres exemples disponibles dans le SDK (Software Development Kit) :

1-PROSIM > SDK > SDK > Exemples > 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	Exemple de conversions	System
Demo3	Exemple d'édition d'un objet Compounds	Compounds
Demo4	Editer et sauvegarder un objet Compounds	Compounds
Demo5	Charger et éditer un objet Compounds	Compounds
Demo7	Récupérer une propriété d'un objet Compounds	Compounds
Demo8	Exemple d'édition d'un objet Calculator	Calculator
Demo9	Editer et sauvegarder un objet Calculator	Calculator
Demo10	Charger et éditer un objet Calculator	Calculator
Demo12	Editer et utiliser un objet Calculator	Calculator



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Software & Services In Process Simulation

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