

# Démarrer avec Simulis<sup>®</sup> Thermodynamics

Cas 12 : Utilisation dans MATLAB<sup>®</sup>

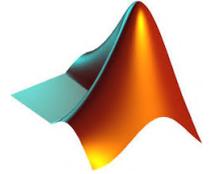
Software & Services In Process Simulation

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ProSim

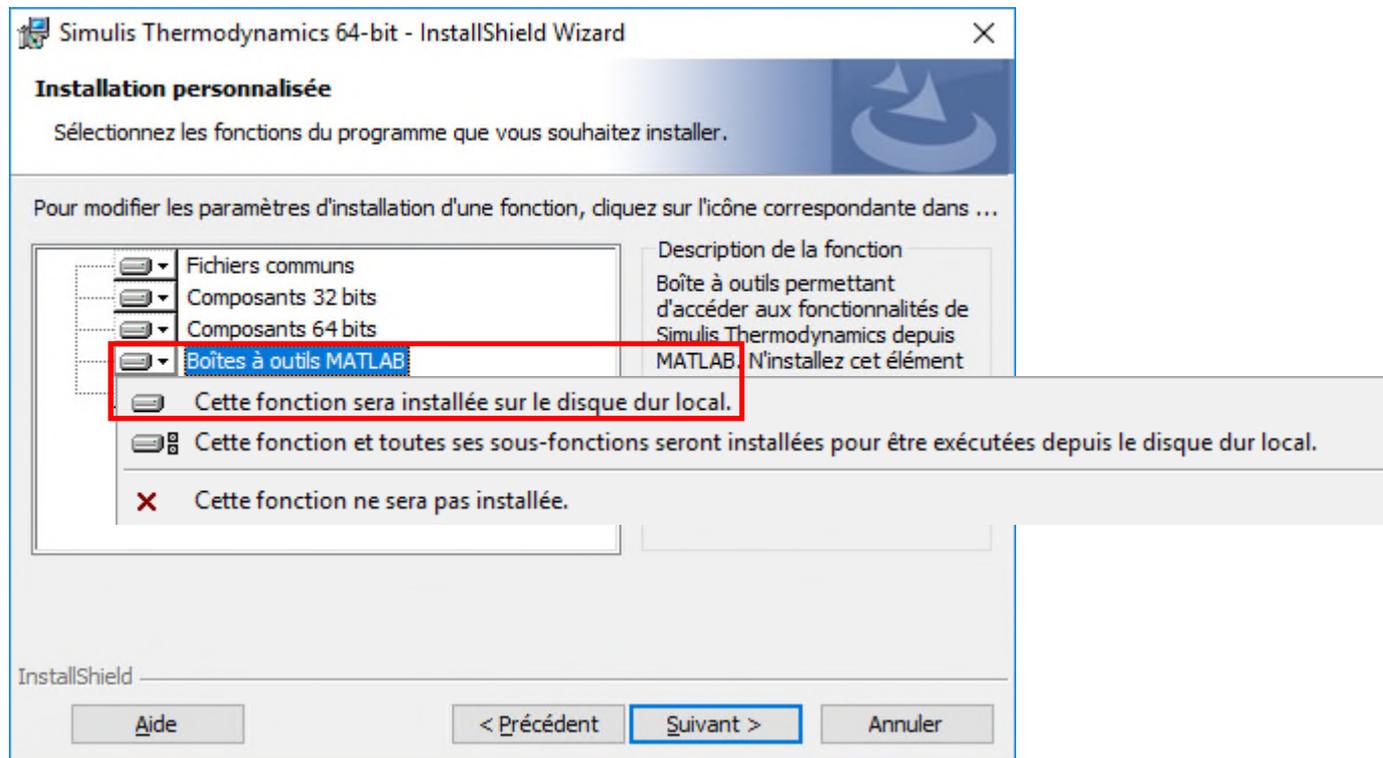
Ce document présente le fonctionnement de Simulis Thermodynamics dans MATLAB



- Installation
- Exemples d'utilisation
- Aides

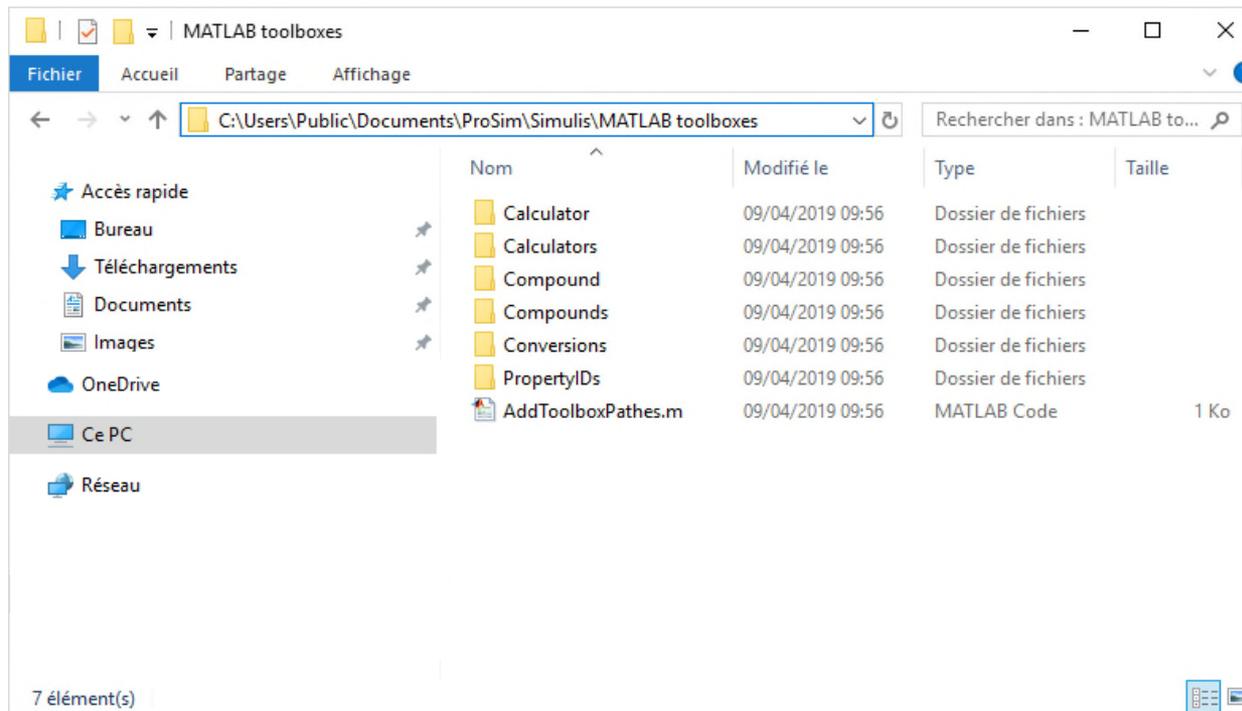
# SIMULIS® THERMODYNAMICS & MATLAB

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



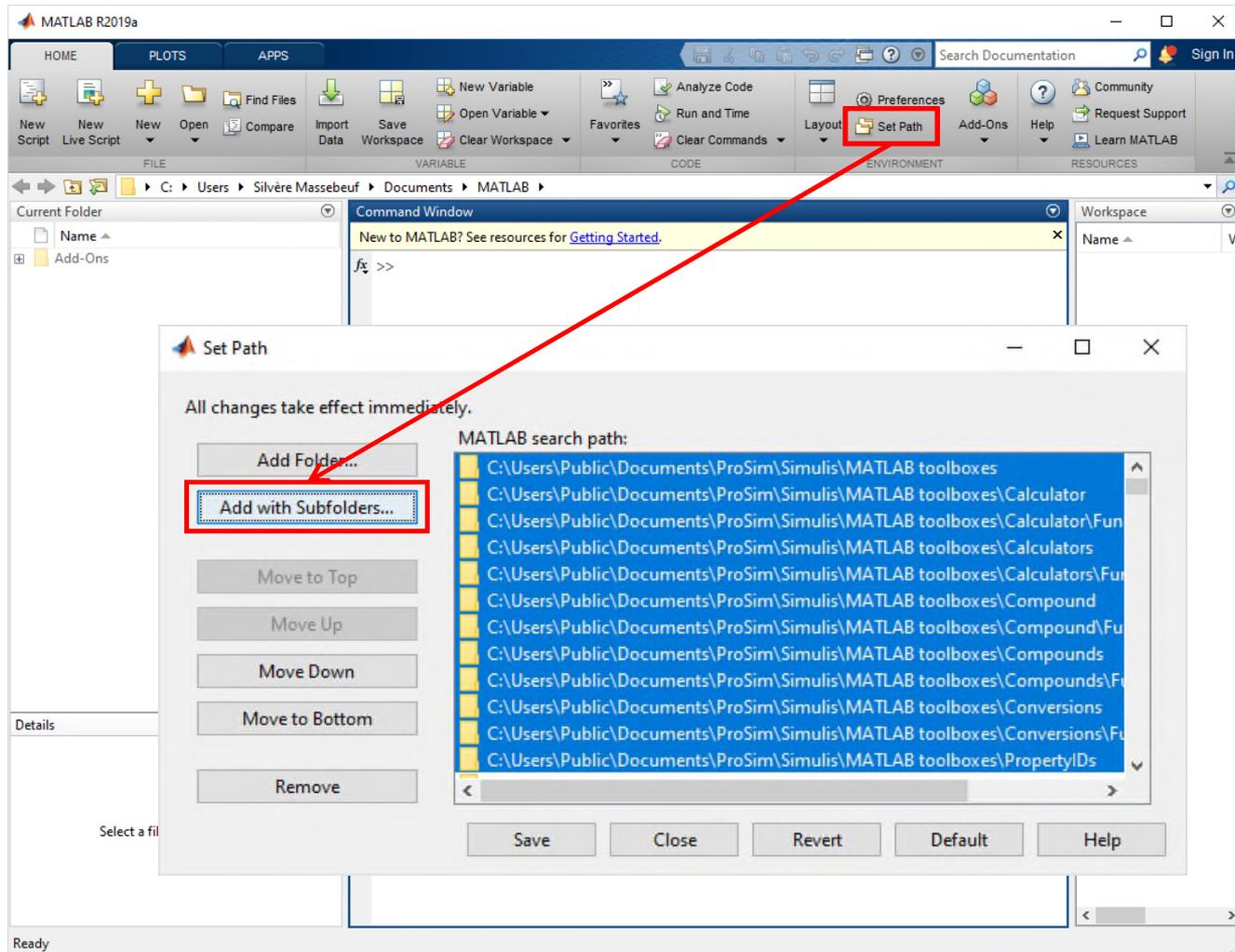
# SIMULIS® THERMODYNAMICS & MATLAB

- Installation :
  - Vérification dans le répertoire d'installation :  
C:\Users\Public\Documents\ProSim\Simulis\MATLAB toolboxes



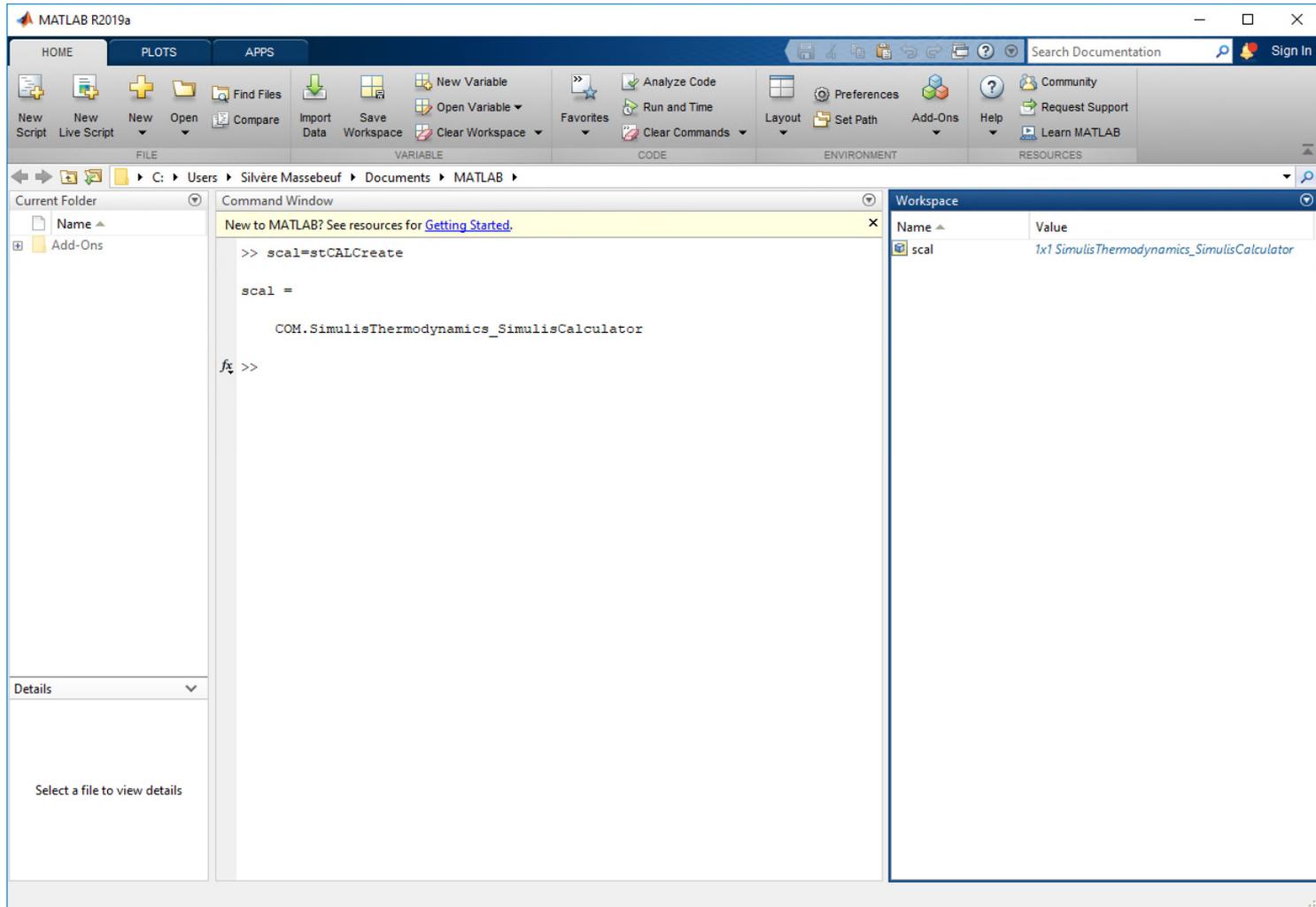
# SIMULIS® THERMODYNAMICS & MATLAB

- Installation :
  - Ajouter ce chemin de recherche MATLAB



# SIMULIS® THERMODYNAMICS & MATLAB

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



# SIMULIS® THERMODYNAMICS & MATLAB

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

The screenshot displays the MATLAB R2019a environment. In the Command Window, the following code is entered:

```
>> scal=stCALCreate
scal =
    COM.SimulisThermodynamics_SimulisCalculator
>> modified=stCALEdit(scal)
```

A red arrow points from the last line of code to the 'Editeur de calculator thermodynamique' dialog box. The dialog box is titled 'Editeur de calculator thermodynamique' and contains the following sections:

- CALCULATOR**
  - FICHIER: Ouvrir..., Enregistrer sous...
  - PACKAGE: (dropdown)
  - SERVICES: Calculer, Générer un fichier PSF, Diagrammes, Résidu..., Générer un fichier PVT, Courant..., Sigma profiles
  - MODIFICATIONS: Défaire, Refaire
  - CONFIGURATION: Nom: [Nouveau calculator], Commentaires: (text area), Type de calculator: Natif (dropdown),  Montrer le mode expert
- CONSTITUANTS** (active tab)
  - Table with columns: Nom IUPAC, CAS Registry Number®
  - Buttons: Sélectionner les constituants..., Editer ce constituant..., Ajouter un nouveau constituant, Supprimer tous les constituants, Cloner ce constituant, Mettre à jour les constituants, Supprimer la sélection
  - SERVICES: Créer un pseudo-constituant..., Propriétés dépendantes de T..., Editeur tableau, Comparer à l'original, Comparer les constituants
  - ORDRE: Déplacer ce constituant vers le haut

At the bottom of the dialog box, there is a text area for 'Commentaires :', 'OK' and 'Annuler' buttons, and a small disclaimer: 'Les CAS Registry Numbers® sont la propriété intellectuelle de American Chemical Society et sont utilisés par ProSim SA avec l'autorisation expresse d'ACS. Les CAS Registry Numbers® n'ont pas été vérifiés par ACS et peuvent être inactifs.'

# SIMULIS® THERMODYNAMICS & MATLAB

- Systèmes d'unités de l'objet Simulis calculator (entrée et sortie) :
  - **modifiedInput**=*stCALSystemEdit*(scal,1)
  - **modifiedOutput**=*stCALSystemEdit*(scal,2)

```

MATLAB R2019a
HOME PLOTS APPS
New Script New Live Script New Open Find Files Import Data Save Workspace Open Variable Clear Workspace Favorites Run and Time Analyze Code Preferences Community
FILE VARIABLE CODE ENVIRONMENT RESOURCES
C:\Users\SilvèreMassebeuf\Documents\MATLAB
Current Folder
Name
Add-Ons
Command Window
New to MATLAB? See resources for Getting Started.
>> scal=stCALCreate

scal =

COM.SimulisThermodynamics_SimulisCalculator

>> modified=stCAEdit (scal)

modified =

logical

1

>> modifiedInput=stCALSystemEdit (scal,1)

modifiedInput =

logical

1

>> modifiedOutput=stCALSystemEdit (scal,2)

modifiedOutput =

logical

1

fx >>
  
```

Par exemple :  
Température : °C  
Pression : atm

Système d'unités

UNITÉS DE L'APPLICATION

SYSTÈMES PRÉDÉFINIS

Choisissez un système d'unités prédéfini dans cette liste et cliquez sur "Appliquer le système" pour utiliser ses unités dans votre application.

- ISO
- ProSim
- Anglais
- Simulis
- Système de l'application

Appliquer le système

OUTILS

- Copier dans le presse-papier
- Coller depuis le presse-papier
- Utiliser ce système par défaut

Utilisez cette fenêtre pour modifier le système d'unités utilisé par votre application.

Grandeur	Unité
Masse molaire	kg/mol
Masse volumique	kg/m3
Molalité	mol/kg
Moment dipolaire	D
Moment quadripolaire	Buckingham
Pourcentage	%
Pression	atm
Puissance	J/s
Puissance volumique	W/m3
Quantité de matière	mol
Quantité de matière volumique	mol/m3
Résistance électrique	Ohm
Résistivité	Ohm.m
Surface	m2
Temps	s
Température	°C
Tension superficielle	N/m

Ok Annuler

# SIMULIS® THERMODYNAMICS & MATLAB

- 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)**

The screenshot shows the MATLAB Command Window with the following content:

```

New to MATLAB? See resources for Getting Started.
0.5000    0.5000

VaporMolarFractions = Vecteur
                      résultats
                      ↓
0     0

EquiConstants =
0     0

>> [MolarVapRatio, LiquidMolarFractions, VaporMolarFractions, EquiConstants]=stCALFlashTP(scal, 80, 1, [0.5, 0.5], 0, 0, false)
MolarVapRatio =
0.2888

LiquidMolarFractions =
0.5567    0.4433

VaporMolarFractions =
0.3604    0.6396

EquiConstants =
0.6474    1.4428
  
```

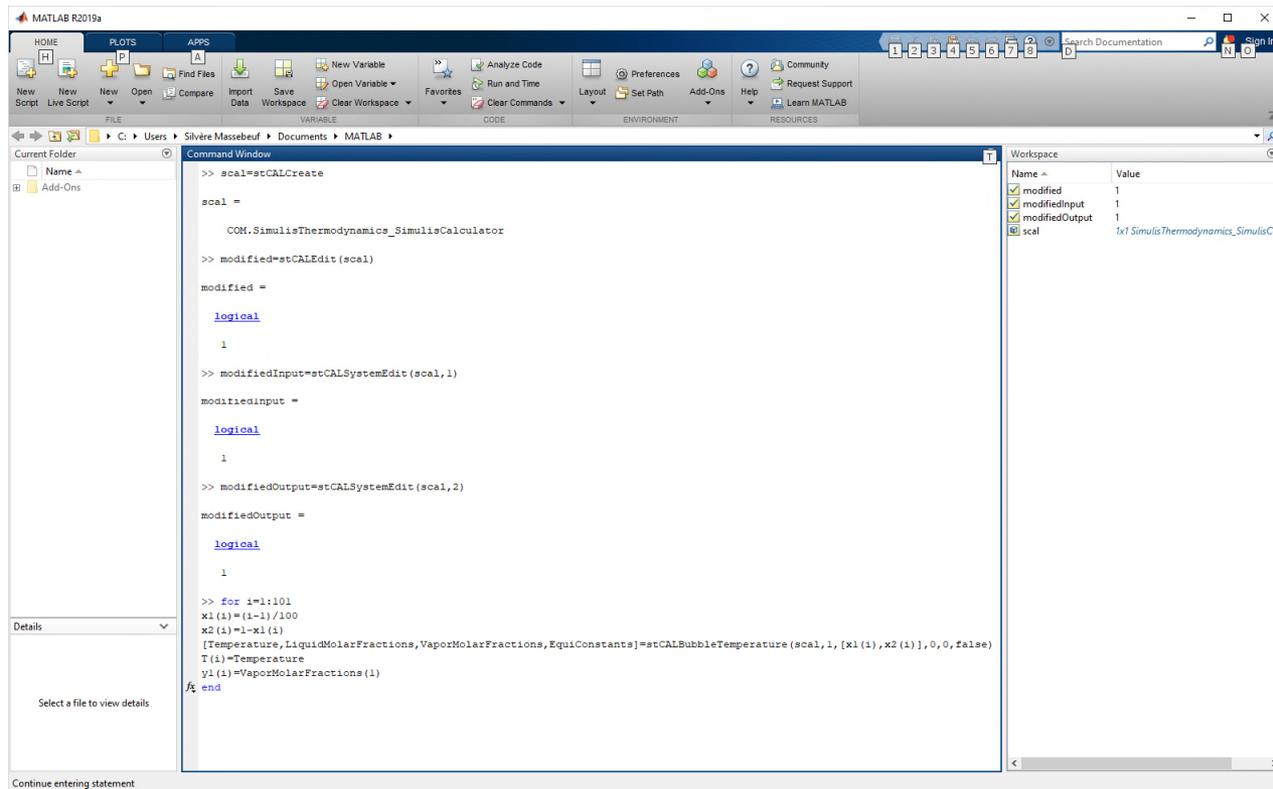
The Workspace window on the right shows the following variables and their values:

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

Résultats de calcul

# SIMULIS® THERMODYNAMICS & MATLAB

- 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



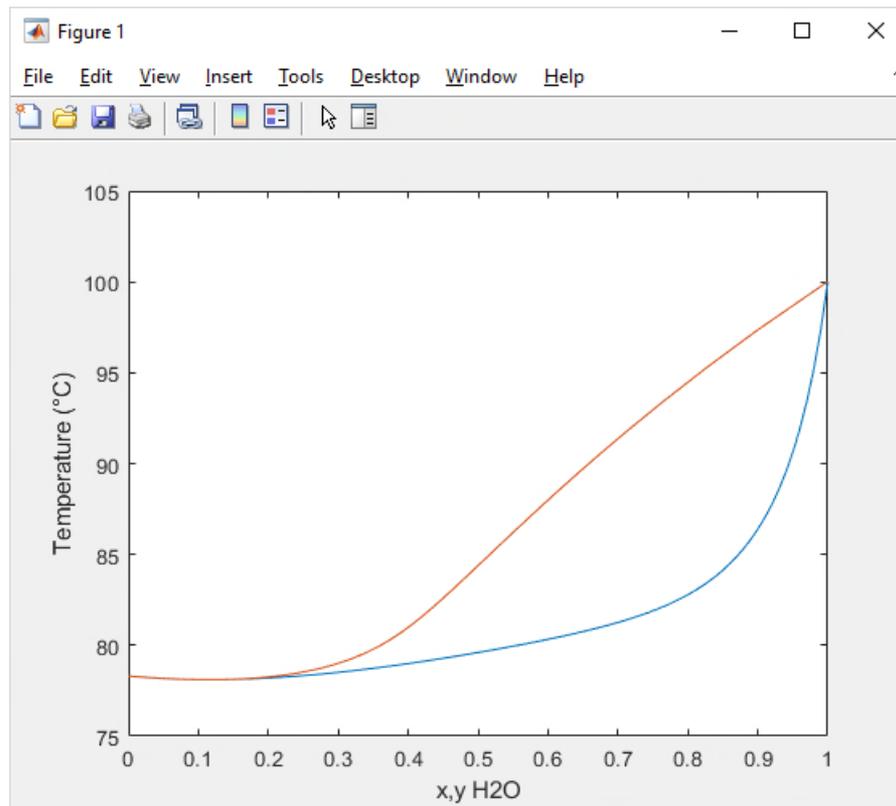
```

MATLAB R2019a
HOME PLOTS APPS
New Script Live Script New Open Compare Import Save Open Variable Favorites Analyze Code Run and Time Layout Set Path Add-Ons Help Community
FILE VARIABLE CODE ENVIRONMENT RESOURCES
C:\Users\Silvère Massebeuf\Documents\MATLAB
Current Folder
Name
Add-Ons
Details
Select a file to view details
Command Window
>> scal=stCALCreate
scal =
    COM.SimulisThermodynamics_SimulisCalculator
>> modified=stCALEdit(scal)
modified =
    logical
    1
>> modifiedInput=stCALSystemEdit(scal,1)
modifiedInput =
    logical
    1
>> modifiedOutput=stCALSystemEdit(scal,2)
modifiedOutput =
    logical
    1
>> 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
Workspace
Name Value
modified 1
modifiedInput 1
modifiedOutput 1
scal Tx1 SimulisThermodynamics_SimulisCa

```

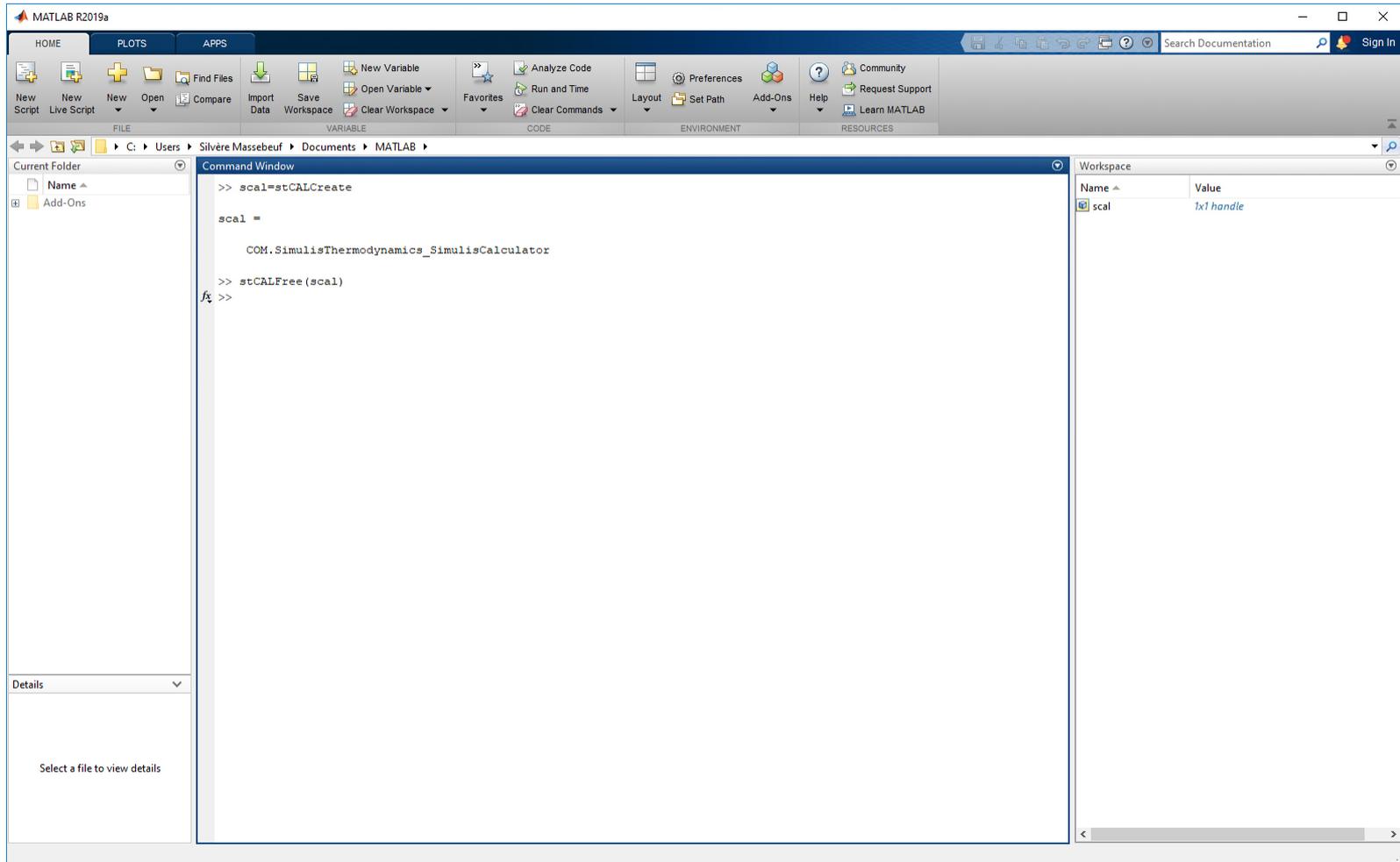
# SIMULIS® THERMODYNAMICS & MATLAB

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



# SIMULIS® THERMODYNAMICS & MATLAB

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



# SIMULIS® THERMODYNAMICS & MATLAB

## ■ Accès à l'aide des fonctions :

- **help** *stCALFlashTP*

The screenshot shows the MATLAB R2019a interface. The Command Window displays the help documentation for the `stCALFlashTP` function. The documentation includes the function signature, input parameters, output parameters, and an example of usage. The Workspace window shows the variables created during the execution of the example.

**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 stCALCompoundCo
initVaporFractions : [Optional] vapor fractions of initialisation (molar or mass) (vector of stCALCompoundCo

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);

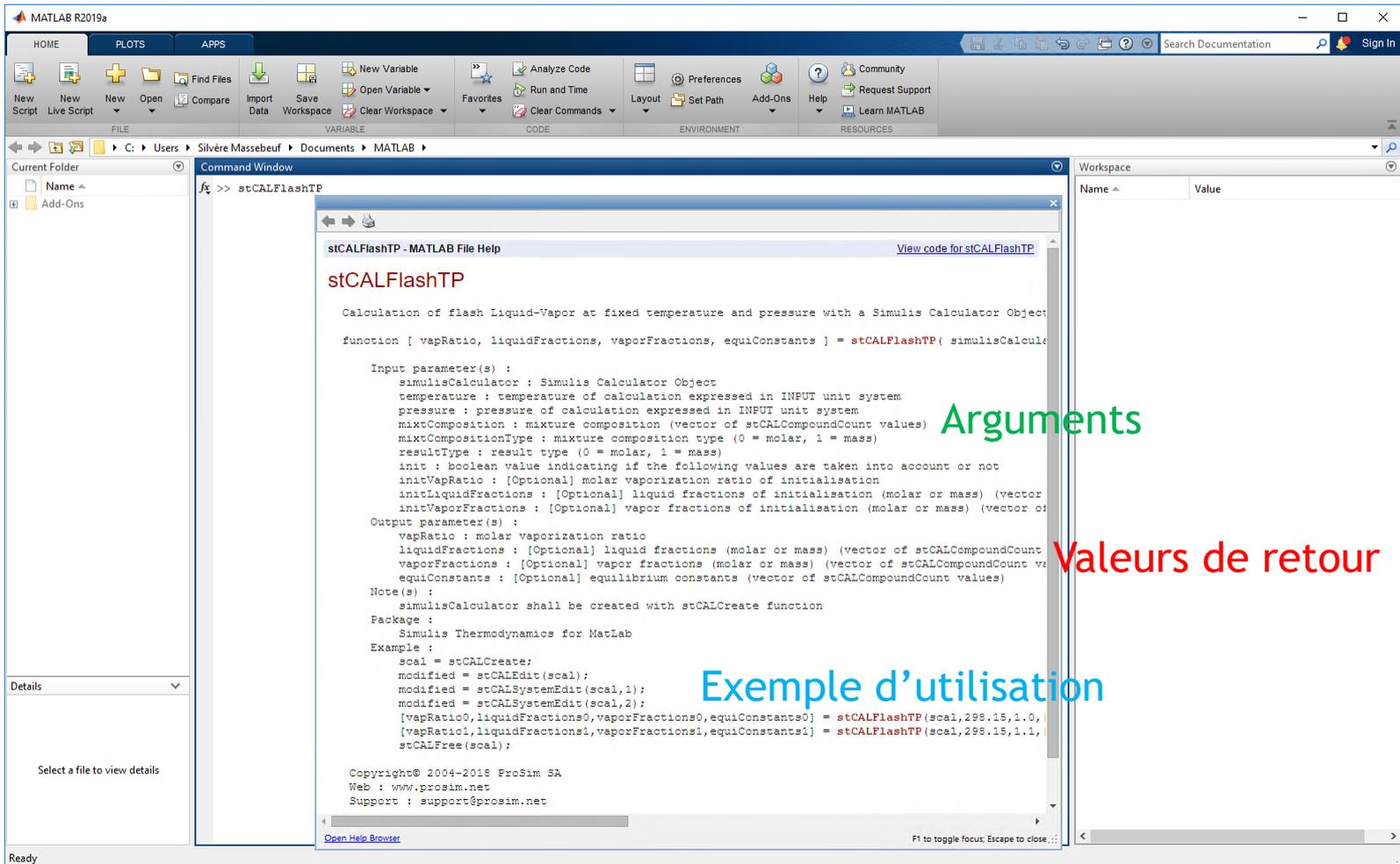
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Web : www.prosim.net
Support : support@prosim.net

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_SimulisCalcula...
VaporMolarFracti...	[0.3604,0.6396]

# SIMULIS® THERMODYNAMICS & MATLAB

- Accès à l'aide des fonctions :
  - *stCALFlashTP* puis **F1**



The screenshot shows the MATLAB R2019a interface. The Command Window contains the command `stCALFlashTP`. The Help window displays the following information:

**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
- initVaporFractions : [Optional] vapor fractions of initialisation (molar or mass) (vector of

Output parameter(s) :

- vapRatio : molar vaporization ratio
- liquidFractions : [Optional] liquid fractions (molar or mass) (vector of stCALCompoundCount
- vaporFractions : [Optional] vapor fractions (molar or mass) (vector of stCALCompoundCount ve
- 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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Support : support@prosim.net

Annotations in the image:

- 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

```
stCALFlashTP - MATLAB File Help View code for stCALFlashTP

stCALFlashTP

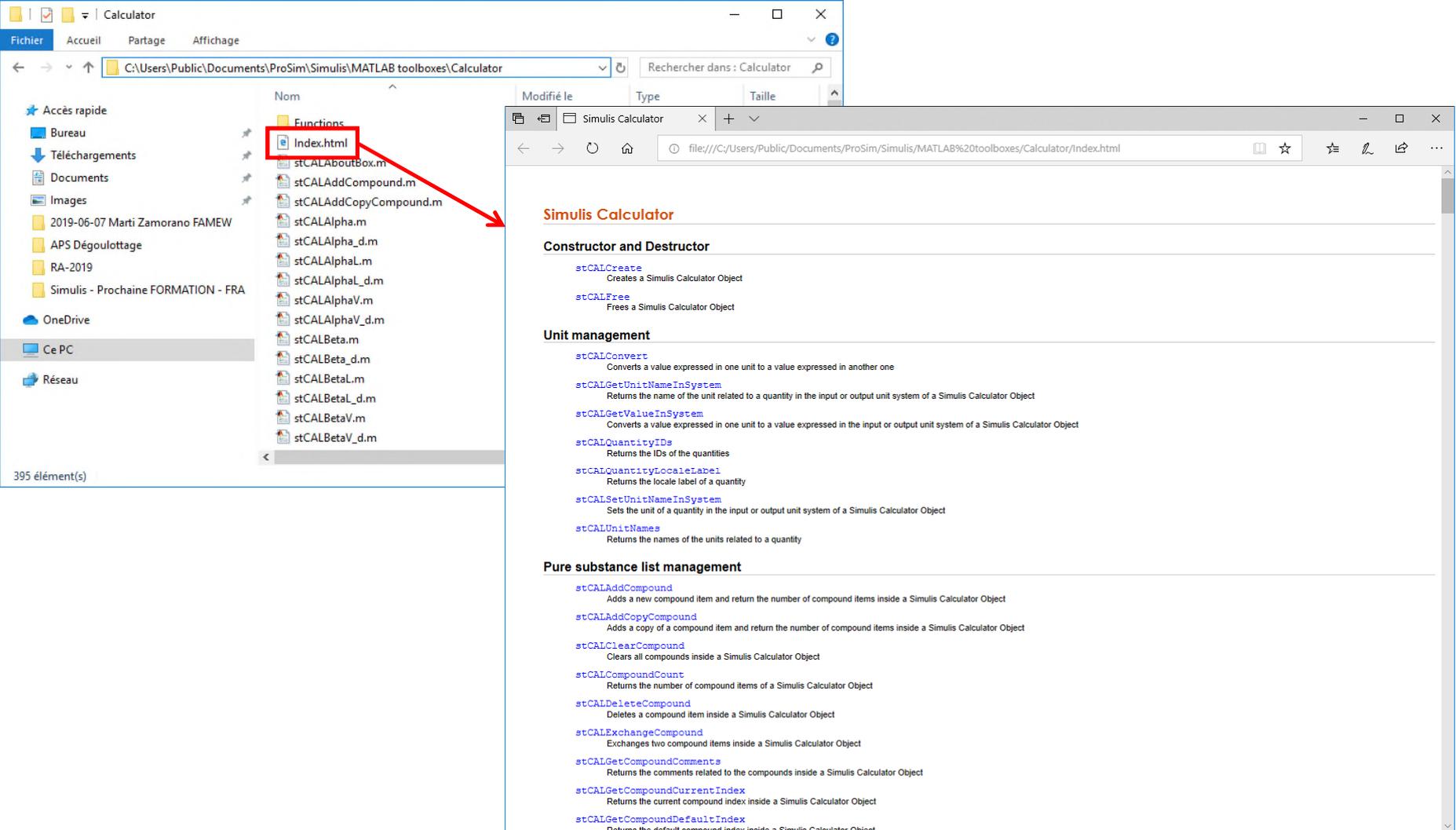
Calculation of flash Liquid-Vapor at fixed temperature and
function [ vapRatio, liquidFractions, vaporFractions, equiC

Input parameter(s) :
  simulisCalculator : Simulis Calculator Object
  temperature       : temperature of calculation expressed
  pressure          : pressure of calculation expressed in INE
  mixtComposition   : mixture composition (vector of st
  mixtCompositionType : mixture composition type (0 =
  resultType        : result type (0 = molar, 1 = mass)
  init              : boolean value indicating if the following va
  initVapRatio      : [Optional] molar vaporization ratio

Open Help Browser F1 to toggle focus, Escape to close...
```

# SIMULIS® THERMODYNAMICS & MATLAB

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



The image displays two windows illustrating the access to the Simulis Calculator help files. On the left, a Windows File Explorer window shows the directory `C:\Users\Public\Documents\ProSim\Simulis\MATLAB toolboxes\Calculator`. A red box highlights the `Index.html` file, with a red arrow pointing to the browser window on the right. The browser window shows the content of `Index.html`, which is titled "Simulis Calculator" and lists various functions under different categories:

- Constructor and Destructor**
  - `stCALCreate`: Creates a Simulis Calculator Object
  - `stCALFree`: Frees a Simulis Calculator Object
- Unit management**
  - `stCALConvert`: Converts a value expressed in one unit to a value expressed in another one
  - `stCALGetUnitNameInSystem`: Returns the name of the unit related to a quantity in the input or output unit system of a Simulis Calculator Object
  - `stCALGetValueInSystem`: Converts a value expressed in one unit to a value expressed in the input or output unit system of a Simulis Calculator Object
  - `stCALQuantityIDs`: Returns the IDs of the quantities
  - `stCALQuantityLocaleLabel`: Returns the locale label of a quantity
  - `stCALSetUnitNameInSystem`: Sets the unit of a quantity in the input or output unit system of a Simulis Calculator Object
  - `stCALUnitNames`: Returns the names of the units related to a quantity
- Pure substance list management**
  - `stCALAddCompound`: Adds a new compound item and return the number of compound items inside a Simulis Calculator Object
  - `stCALAddCopyCompound`: Adds a copy of a compound item and return the number of compound items inside a Simulis Calculator Object
  - `stCALClearCompound`: Clears all compounds inside a Simulis Calculator Object
  - `stCALCompoundCount`: Returns the number of compound items of a Simulis Calculator Object
  - `stCALDeleteCompound`: Deletes a compound item inside a Simulis Calculator Object
  - `stCALExchangeCompound`: Exchanges two compound items inside a Simulis Calculator Object
  - `stCALGetCompoundComments`: Returns the comments related to the compounds inside a Simulis Calculator Object
  - `stCALGetCompoundCurrentIndex`: Returns the current compound index inside a Simulis Calculator Object
  - `stCALGetCompoundDefaultIndex`: Returns the default compound index inside a Simulis Calculator Object

# SIMULIS® THERMODYNAMICS & MATLAB

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

1-PROSIM > SDK > SDK > Exemples > 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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# ProSim

Software & Services In Process Simulation

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