Getting started with Simulis® Thermodynamics

Use Case 2: Create, dispatch and install a Simulis Thermodynamic Package

Software & Services In Process Simulation

We guide You to efficiency

ProSim

Introduction

A Thermodynamic Package gathers all information on a thermodynamic model (compounds, thermodynamic profile, binaries interaction coefficients…). It can be used in Simulis Thermodynamics or, through the CAPE-OPEN interfaces, in other applications (Aspen Plus, Pro/II, gPROMS,….)

This document presents the different steps to follow in order to create a Simulis Thermodynamic Package and then to dispatch this package to other users. This document also shows how to install and edit a Thermodynamic Package.

The steps are the following:

- Step 1: Creating a Simulis Thermodynamic Package
- Step 2: Creating the set up file for dispatch
- Step 3: Installing a Simulis Thermodynamic Package
- Step 4: Using a Simulis Thermodynamic Package

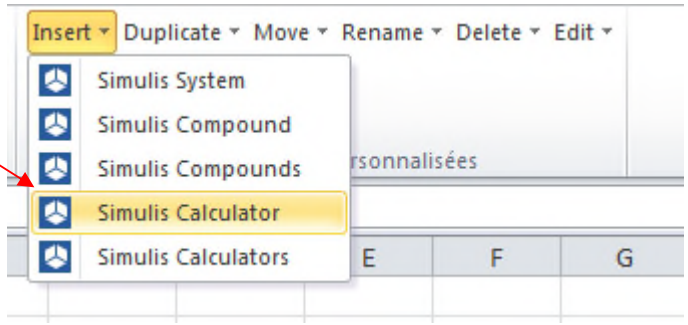
Before studying this chapter, it is recommended to consult "Getting Started with Simulis Thermodynamic: Use Case 1" that explains how to create a thermodynamic model and a function if Simulis Thermodynamics is used in Excel.

Step 1: Creating a Simulis Thermodynamic Package

ACCESS THE THERMODYNAMIC CALCULATOR EDITOR:

- **<u>If you are using Simulis Thermodynamics in Excel</u>:**

Create the calculator object in a spreadsheet



- **<u>If you are using Simulis Thermodynamics within another ProSim environment</u> (ProSimPlus, BatchReactor, BatchColumn etc…):**

Click on the thermodynamic icon to open the calculator editor:

or

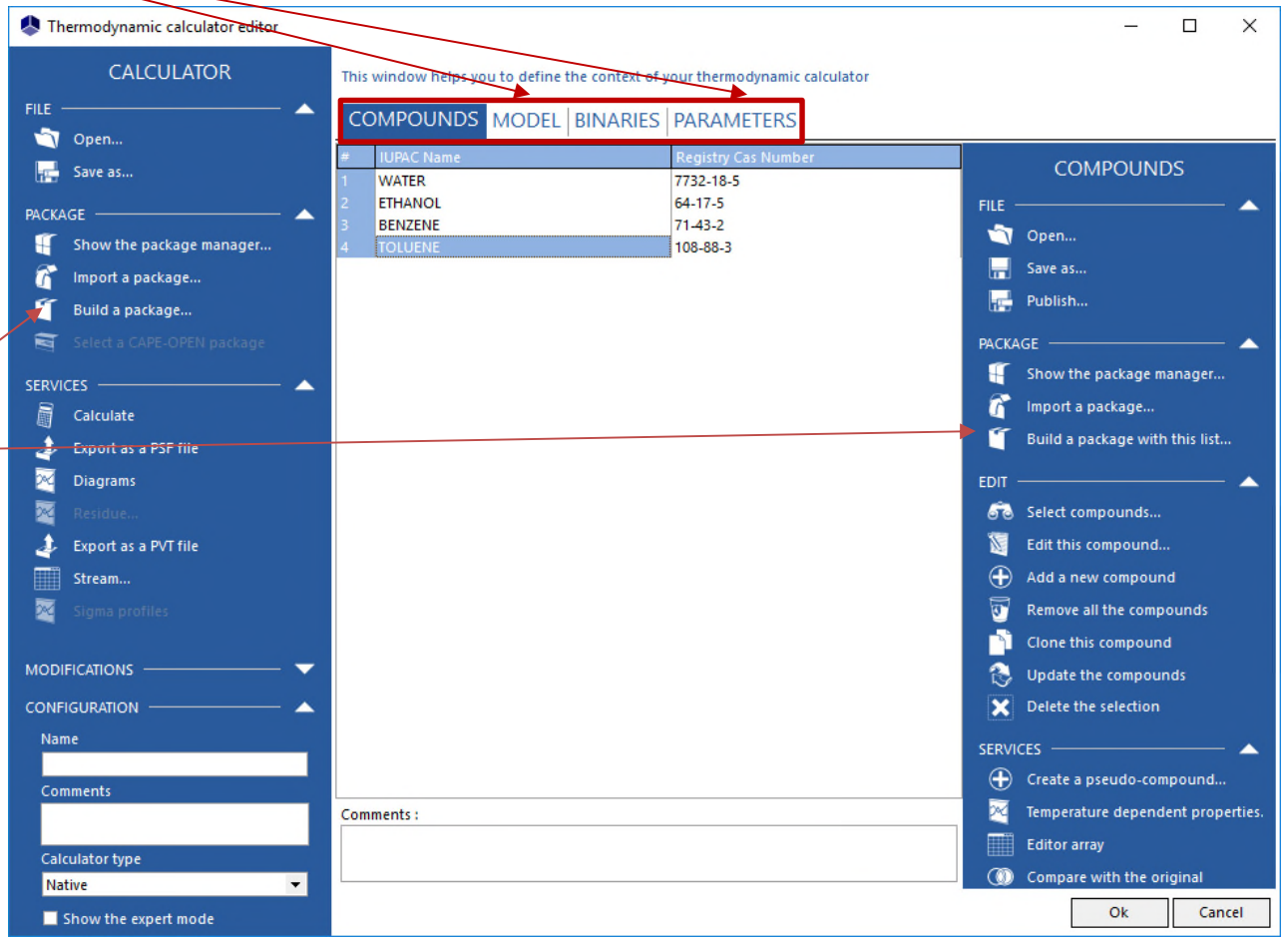
Simulis Thermodynamics is a « software component » that you can integrate into different applications: ProSim software, Excel, Matlab, your own software, etc…

Step 1: Creating a Simulis Thermodynamic Package

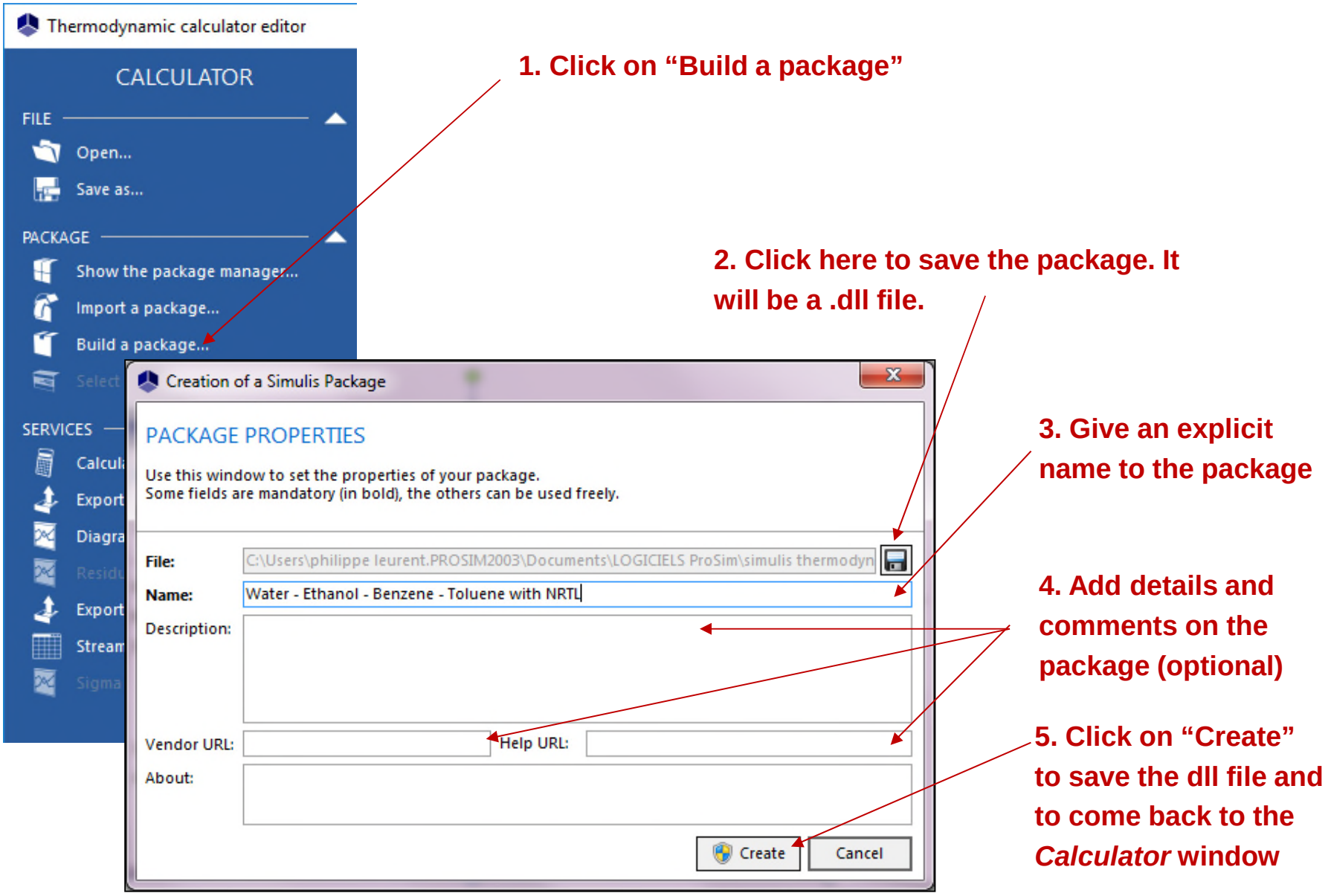
Build your thermodynamic model with the compounds, the thermodynamic profile and the binaries interaction coefficients

(Refer to "Getting Started with Simulis Thermodynamic – Use case 1" for details on this operation)

You can build two types of package: A *thermodynamic package* that includes the whole thermodynamic system, or a *compounds package* that only includes the compounds



Step 1: Creating a Simulis Thermodynamic Package



1. Click on “Build a package”

2. Click here to save the package. It will be a .dll file.

3. Give an explicit name to the package

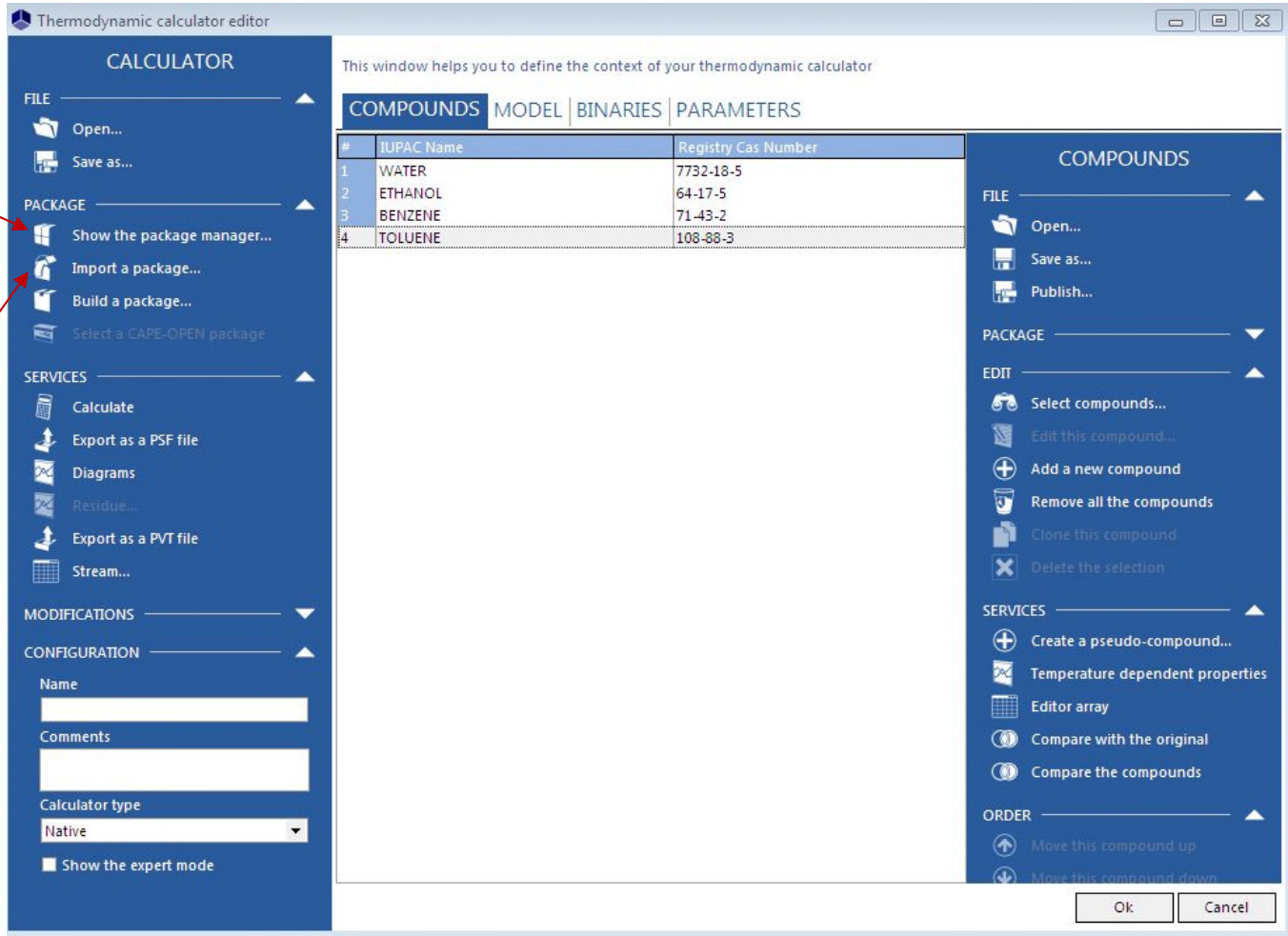
4. Add details and comments on the package (optional)

5. Click on “Create” to save the dll file and to come back to the *Calculator* window

Step 2: Creating the set up file for dispatch

The package manager allows you to edit, delete, or dispatch the package

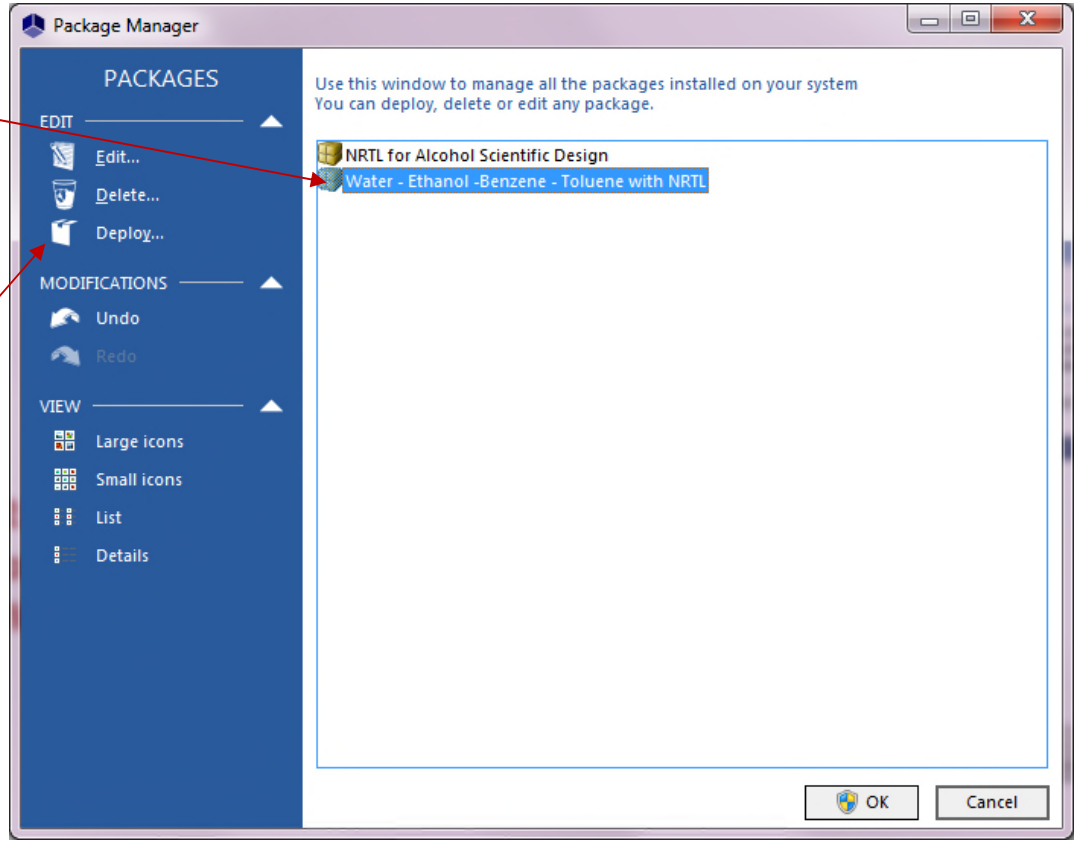
Import a package allows you to open a package previously created



Step 2: Creating the set up file for dispatch

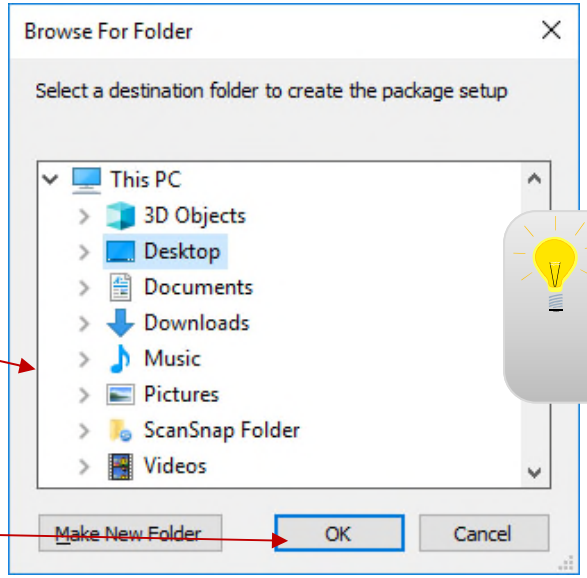
1. Select the package

2. Click on *"Deploy"* to create an installation file (.exe)



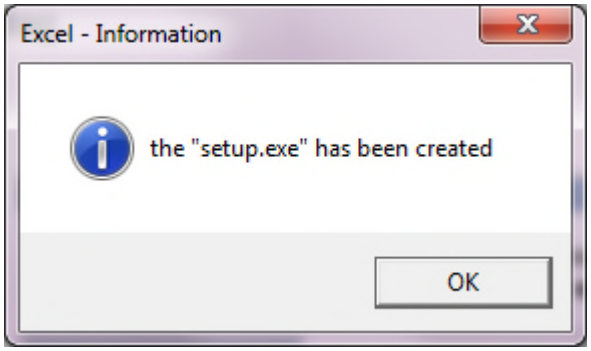
Step 2: Creating the set up file for dispatch

1. Save the .exe file in the folder of your choice



The thermodynamic packages created with Simulis Thermodynamics are automatically CAPE-OPEN compliant

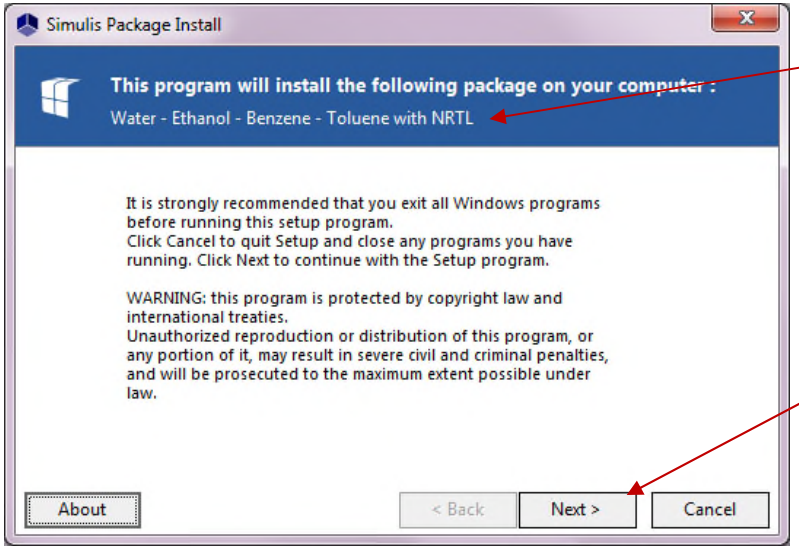
2. Validate your choice



Your executable file has been created under the name “install_[dll name].exe”. This file can now be dispatched to other users.

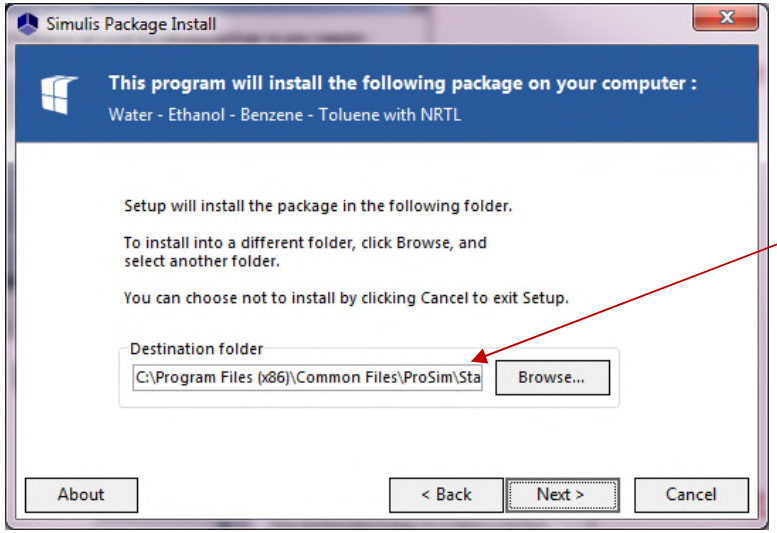
Step 3: Installing a Simulis Thermodynamic Package

1. Double click on the .exe file you received or created to start the installation and open the package information window

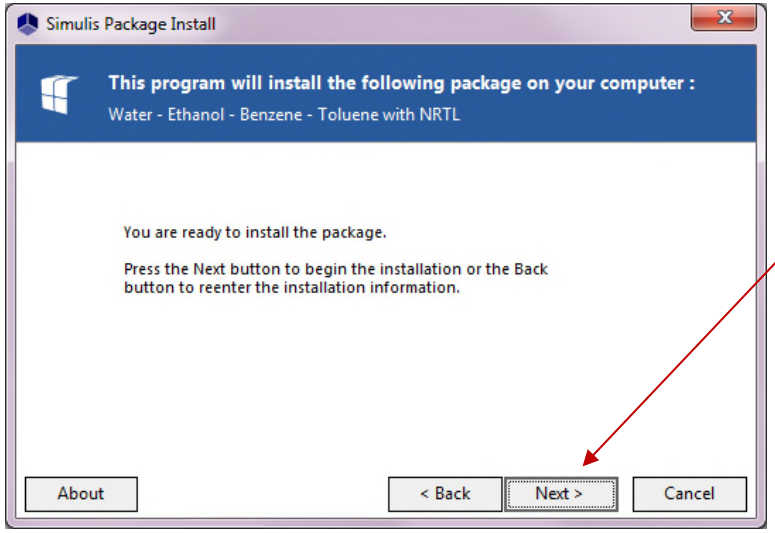


2. Check the name of the package and click on “Next”

Step 3: Installing a Simulis Thermodynamic Package

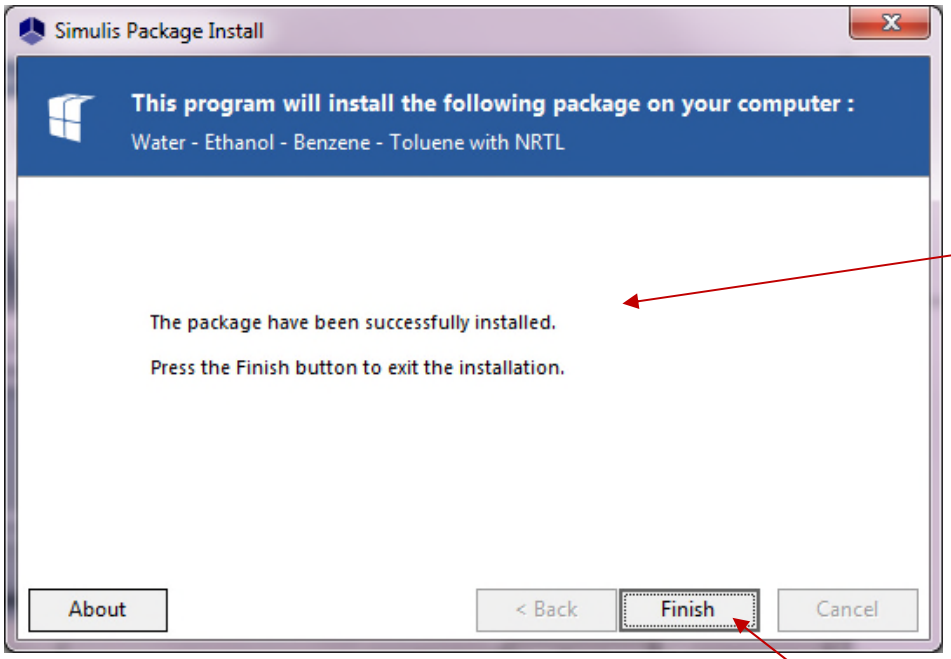


1. Select the destination folder



2. The Simulis Thermodynamic Package is ready to be installed. Click on “Next” to complete the operation.

Step 3: Installing a Simulis Thermodynamic Package



1. Installation is confirmed

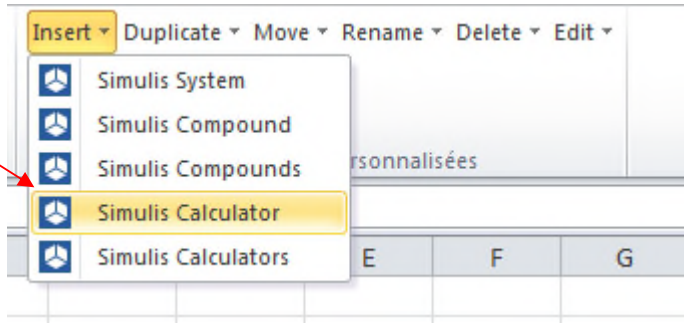
2. You can exit the installation process

Step 4: Using a Simulis Thermodynamic Package

ACCESS THE THERMODYNAMIC CALCULATOR EDITOR:

- **<u>If you are using Simulis Thermodynamics in Excel</u>:**

Create the calculator object in a spreadsheet



- **<u>If you are using Simulis Thermodynamics within another ProSim environment</u> (ProSimPlus, BatchReactor, BatchColumn etc…):**

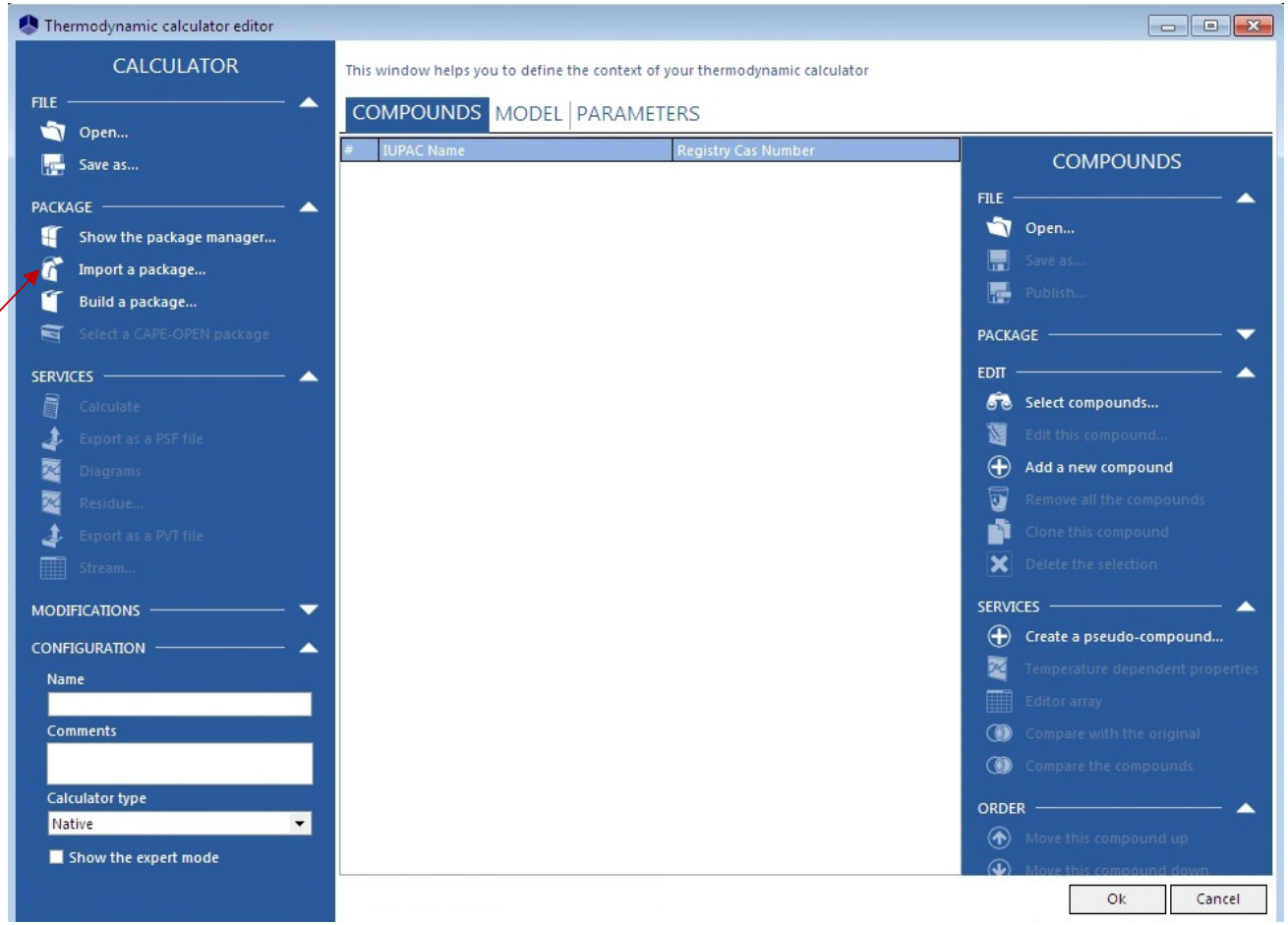
Click on the thermodynamic icon to open the calculator editor:

or

Simulis Thermodynamics is a « software component » that you can integrate into different applications: ProSim software, Excel, Matlab, your own software, etc…

Step 4: Using a Simulis Thermodynamic Package

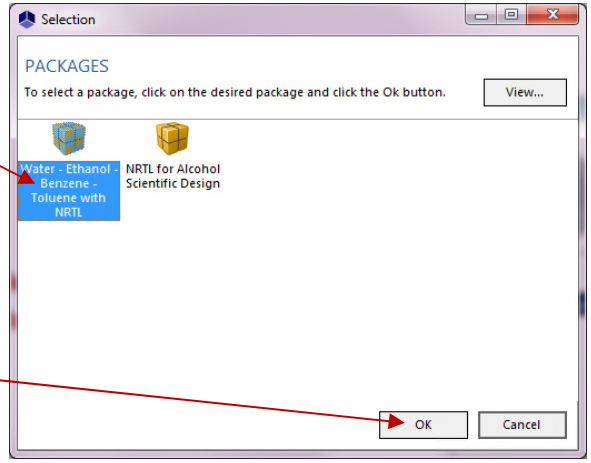
Import the Simulis Thermodynamic Package

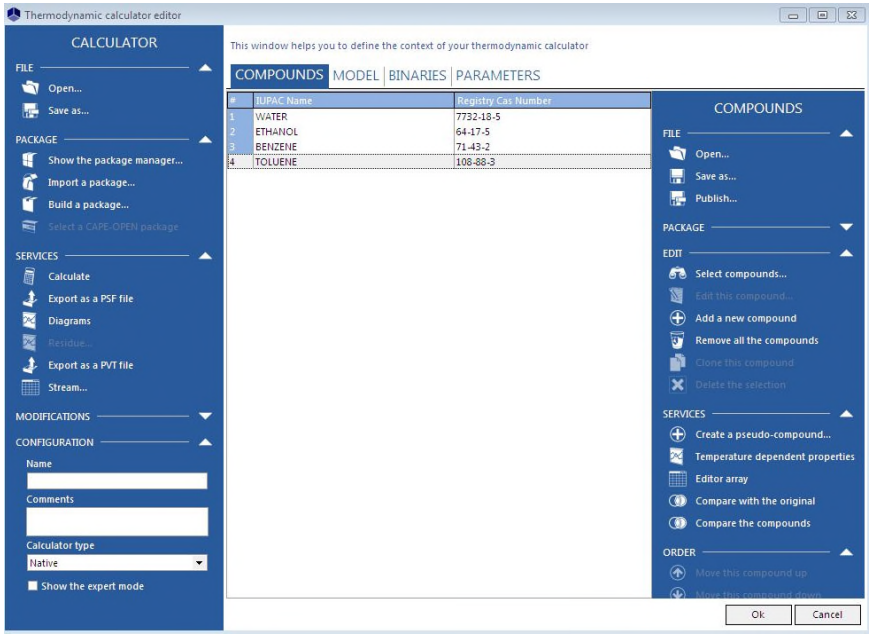


Step 4: Using a Simulis Thermodynamic Package

1. Select the package you wish to use

2. Click on "*OK*" to validate





The Thermodynamic Package is installed in the *Simulis Calculator*.
You can use all the information however you can not modify the data in the package. To modify them, you need to create a different package.

ProSim

Software & Services In Process Simulation

ProSim SA
51, rue Ampère
Immeuble Stratège A
F-31670 Labège
France

☎: +33 (0) 5 62 88 24 30

www.prosim.net

info@prosim.net

ProSim, Inc.
325 Chestnut Street, Suite 800
Philadelphia, PA 19106
U.S.A.

☎: +1 215 600 3759