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

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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:

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 If you are using Simulis Thermodynamics within another ProSim environment (ProSimPlus, BatchReactor, BatchColumn etc...):

Click on the thermodynamic icon to open the calculator editor:

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

Step 1: Creating a Simulis Thermodynamic Package

Build your thermodynamic model with the compounds, the Thermodynamic calculator editor X thermodynamic profile CALCULATOR This window helps you to define the context of your thermodynamic calculator and the binaries COMPOUNDS MODEL BINARIES PARAMETERS 🗂 Open... interaction coefficients COMPOUNDS Save as... WATER 7732-18-5 ETHANOL 64-17-5 (Refer to "Getting Started with Simulis PACKAGE BENZENE 71-43-2 Open... Thermodynamic – Use case 1" for Show the package manager... 108-88-3 Save as... details on this operation) n Import a package... Publish... Build a package... PACKAGE Show the package manager... SERVICES R Import a package... 冒 Calculate You can build two Build a package with this list... 🔔 Export as a PSF file R Diagrams FDIT types of package: A Select compounds... thermodynamic £ Export as a PVT file \mathbb{N} Edit this compound... æ Add a new compound Stream... package that × Remove all the compounds Clone this compound includes the whole MODIFICATIONS 2 Update the compounds thermodynamic Delete the selection CONFIGURATION Name SERVICES system, or a Create a pseudo-compound... Comments compounds package 24 Temperature dependent properties. Comments : Editor array Calculator type that only includes the Compare with the original Native • Ok Cancel compounds Show the expert mode

Step 1: Creating a Simulis Thermodynamic Package

🔕 Thermodynamic calculator editor



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

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Step 2: Creating the set up file for dispatch



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



Step 2: Creating the set up file for dispatch



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



Step 3: Installing a Simulis Thermodynamic Package



You are ready to install the package. Press the Next button to begin the installation or the Back button to reenter the installation information. About < Back Next > Cancel

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

1. Select the destination folder

X

Step 3: Installing a Simulis Thermodynamic Package



Step 4: Using a Simulis Thermodynamic Package

ACCESS THE THERMODYNAMIC CALCULATOR EDITOR:

If you are using Simulis Thermodynamics in Excel:							
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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



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.

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