

Executing a gPROMS model within PRO/II using the gPROMS CAPE-OPEN Unit Object (gO:CAPE-OPEN) by Mark MATZOPOULOS, Process Systems Enterprise Ltd.

The gPROMS CAPE-OPEN Unit Object (**gO:CAPE-OPEN**) plug has recently been successfully tested and demonstrated executing a gPROMS model within SimSci Esscor's PRO/II steady-state flowsheeting package. PSE would like to thank SimSci-Esscor for their assistance in this project.

gO:CAPE-OPEN is one of the gPROMS Objects, the family of products that enable gPROMS models to execute within a variety of engineering software environments such as Computational Fluid Dynamic packages and the Mathworks MATLAB[®] and Simulink[®] environments.

gO:CAPE-OPEN allows a gPROMS model of a unit operation to run inside any CAPE-OPEN compliant process simulator. It has been successfully tested in the past on a large-scale application that involved executing a 50,000 equation rate-based gPROMS distillation column model within Aspen Technology's Aspen Plus.

gPROMS facilities for CAPE-OPEN Units

The full set of capabilities of gPROMS related to CAPE-OPEN comprises three major components:

- **gO:CAPE-OPEN** itself, a software wrapper that executes the gPROMS model within the target environment.
- **CAPE-OPEN Thermodynamics**, a software socket within gPROMS that allows gPROMS models to make use of any CAPE-OPEN compliant physical properties packages.
- **Export to CAPE-OPEN facilities** in the gPROMS ModelBuilder. These allow the user to specify all the information required to execute the model in the target environment, then to export it at the push of a button – no programming is required

gO:CAPE-OPEN in fact wrappers all the solution software required to solve the gPROMS Integro-Partial Differential Algebraic (IPDAE) set of equations and execute it within the target environment. This means that any model that runs in gPROMS will execute identically in, for example, PRO/II. Thus models can contain any of the features for which gPROMS is typically used, such as distributions with respect to space or particle size, detailed rate-based heat and mass transfer relationships, or complex reaction kinetics.

Benefits of using gPROMS models within CAPE-OPEN simulators

There are a number of advantages in building and executing models in gPROMS prior to using them within flowsheeting simulators. The primary advantage is the ability to deploy gPROMS' custom modelling capabilities which allow the construction of models of virtually any level of complexity – steady-state or dynamic – and easy validation against laboratory, pilot plant or operating data.

Typical applications of gPROMS custom modelling are the construction of high-accuracy first-principles models of reactors, complex separation units (including, for example, “HIDiC” heat-integrated distillation columns), crystallisers, etc. Once these models have fulfilled their primary purpose – typically detailed unit design – they can add further value in process and control design, and even in online operations. The approach helps to ensure consistency throughout the design and operations space.

This article describes how a model is prepared in gPROMS, exported, and executed within PRO/II.

Preparing and executing a gPROMS model within PRO/II

Any gPROMS model can be exported for execution by gO:CAPE-OPEN within a CAPE-OPEN compliant simulator. The model can use its own physical properties, or call the physical properties package of the target simulation environment via the gPROMS CAPE-OPEN properties socket. All you need to do to run a gPROMS model in PRO/II is to perform five simple steps:

1. Configure the gPROMS model for use in a flowsheeting simulator
2. Export the gPROMS model
3. Insert the gPROMS model as a unit within PRO/II
4. Configure the gPROMS unit within PRO/II
5. Execute the model in PRO/II and examine the results.

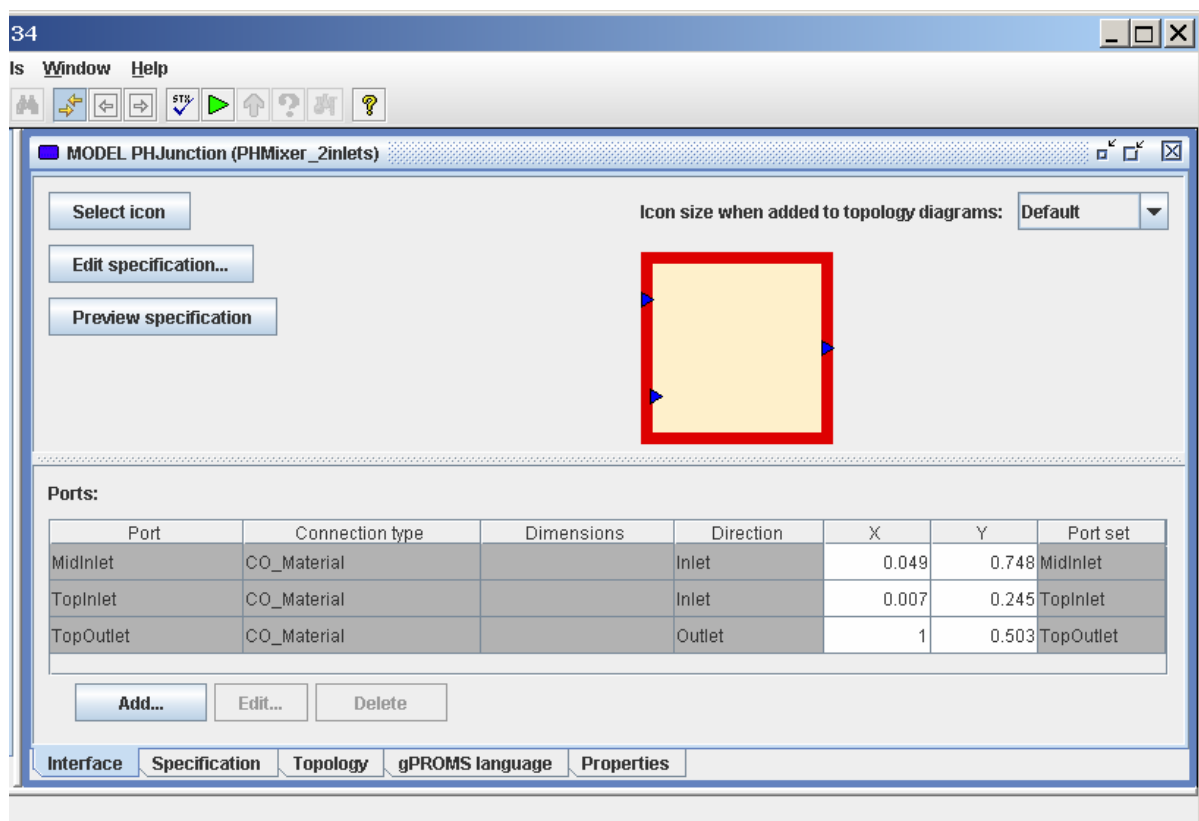
The following example takes a simple mixer model written in gPROMS, for the sake of illustration, and uses it to replace a mixer in a PRO/II flowsheet.

1. Use the gPROMS ModelBuilder to configure the gPROMS model for use in a flowsheeting simulator

Preparing the gPROMS model requires the following steps:

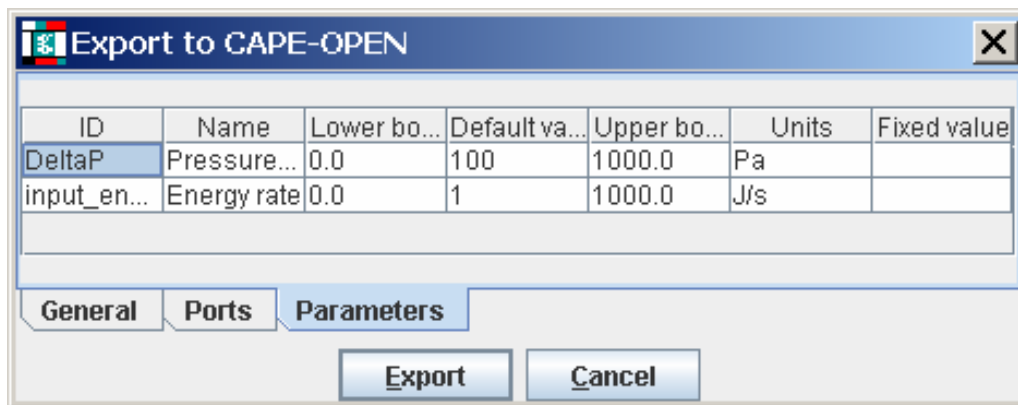
Ensure that the streams conform to the CAPE-OPEN stream structure. In order to link the gPROMS model correctly within the CAPE-OPEN flowsheeting package, the streams used in the model must conform to the standard CAPE-OPEN definition.

gPROMS is supplied with a "CAPE-OPEN_Unit" library that contains a CO Material stream type definition. To make your model CAPE-OPEN compliant, simply define inlet and outlet ports (with connection type "CO_Material") using the standard gPROMS port definition mechanism (below).



Define the unit parameters. Select the **Export to CAPE-OPEN ...** dialogue from the **Tools** menu. The Parameters tab allows you to define the parameters of the unit operation that the PRO/II user will need to set before executing the unit within PRO/II.

gPROMS v3.0 allows a model to have any number of parameters in its public interface. The ones to be made visible via the CAPE-OPEN interface are a subset of these parameters; they may also be given default values.



In the example, two input unit parameters are required:

- Energy rate, with a default of 1 J/s.
- Pressure drop, which has a default value of 100 Pa.

Similarly, we could add one or more output parameters – for example, important performance indicators that are computed by the model.

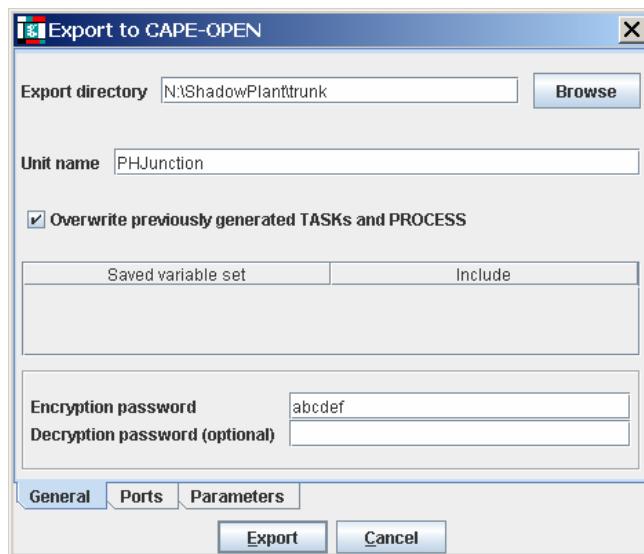
Test the model fully. It is of course essential to ensure that the model is fully tested over the entire range of operation it is likely to encounter in the flowsheeting simulator. You can do this easily by using the gPROMS TASK language to set up a comprehensive test that will step automatically through a large number of combinations of input variable values selected either systematically (e.g. using a uniform grid of values) or by sampling random variable distributions.

2. Use the gPROMS ModelBuilder to export the gPROMS model

Once the information above has been defined, exporting is a simple matter that just requires specification of a:

- destination directory
- a unit name
- an encryption password.

In the gPROMS ModelBuilder, this is done by selecting the model in the gPROMS Project directory tree, then selecting the **Export to CAPE-OPEN...** dialogue from the **Tools** menu. The dialogue box is shown below.

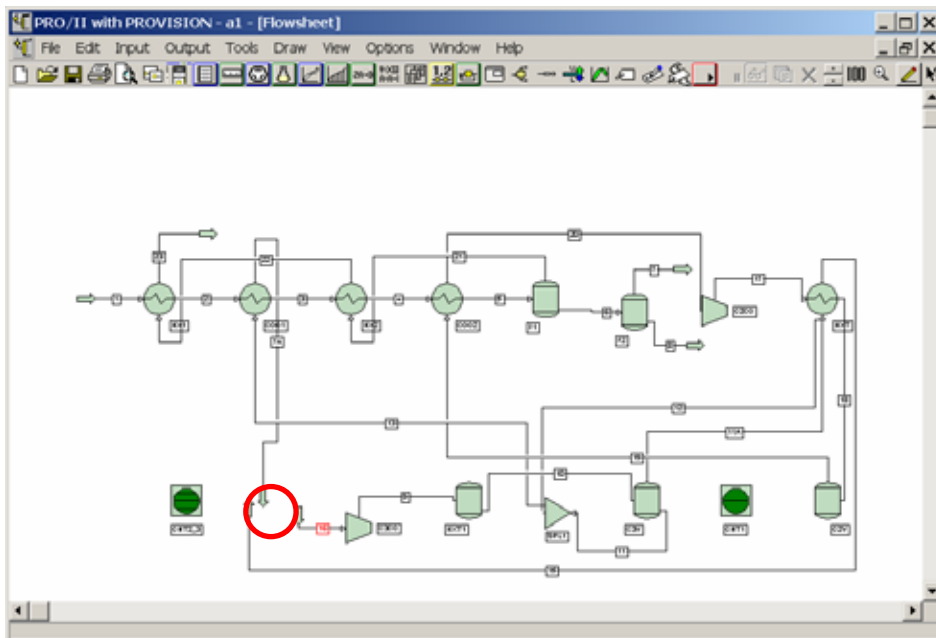


The exported file is encrypted in order to protect the intellectual property that may be embedded within the model and to prevent unauthorised changes being made to it.

The export operation creates a gPROMS CAPE-OPEN (gCO) file. This contains all the information required for running the model within a CAPE-OPEN compliant simulator using the gO:CAPE-OPEN software, as described below.

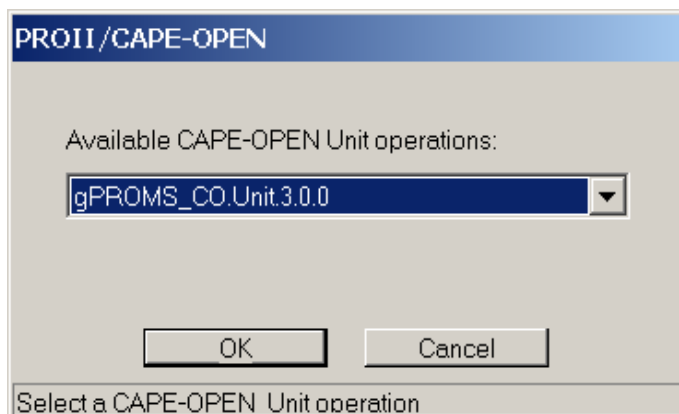
3. Insert the gPROMS model as a unit within PRO/II using gO:CAPEOPEN

For demonstration purposes, one of the standard example flowsheets provided with PRO/II (below) is used.



One of the “native” PRO/II mixers will be deleted (red circle) and substituted with a gPROMS mixer model prepared for use in steps 1 and 2 above. The gPROMS CAPE-OPEN mixer model is inserted in the following steps:

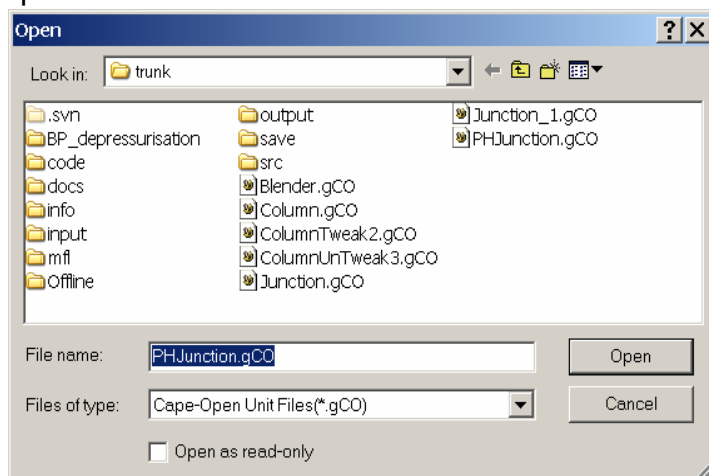
Select the gPROMS_CO unit. From within PRO/II, call up the CAPE-OPEN PFD palette. This displays the **PRO/II CAPE-OPEN** dialogue box shown here.



Select the gO:CAPEOPEN v3.0 unit from the list of available CAPE-OPEN units.

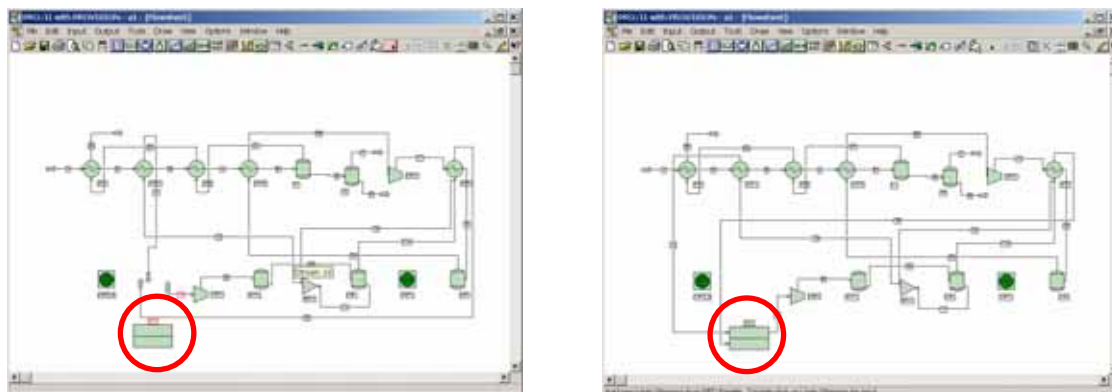
Select the required gCO file. Selecting the gO:CAPEOPEN unit signals your intention to insert an instance of a gPROMS-based model in the PRO/II flowsheet. You now have to specify which such model you want to use – remember that you may have already exported any number of such models from the gPROMS ModelBuilder. An **Open** dialogue shows you the list of gPROMS CAPE-OPEN (gCO) models available.

Select the file PHJunction.CO from the list. This is in fact the gCO file that was created by the Export in step 2.



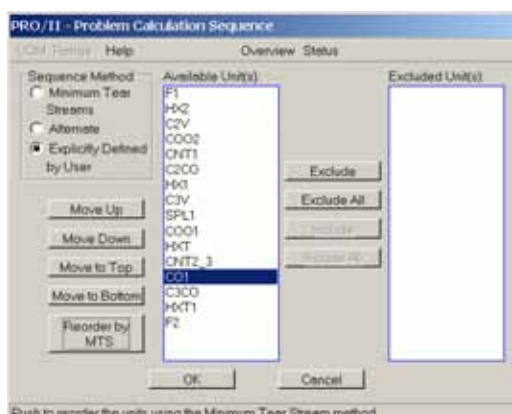
Connect the unit. When you select a unit, it appears in the PRO/II flowsheet just like any standard PRO/II unit.

Use the PRO/II connection tools to connect the unit into the flowsheet in the same way that the original mixer was connected (below):



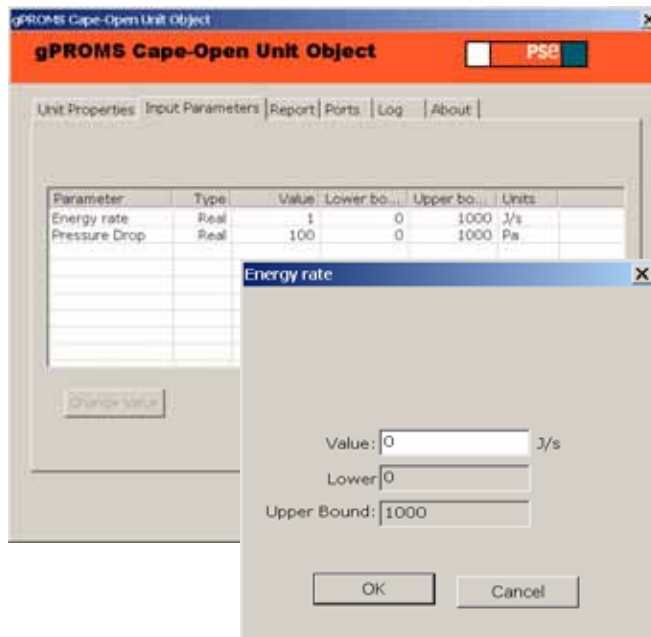
Define its position in the calculation sequence. Now select **Input>Calculation Sequence** to call up the PRO/II Problem Calculation Sequence dialogue.

Specify the position of the gPROMS mixer unit in the calculation sequence. This step is only necessary with some flowsheets, particularly those such as this which have complex recycles.



4. Configure the gPROMS unit within PRO/II

Now that the gPROMS mixer is in the PRO/II flowsheet, you can set the unit parameter information to the required values. Double-click on the gPROMS mixer unit in the PRO/II flowsheet, and then select the **Input Parameters** tab. This displays the dialogue on the right. Here you can see the values for energy rate and pressure drop as defined in step 2. Highlight the energy rate field, click on the Change Parameter button and set the value to zero. Do the same for the pressure drop, in order to emulate the behaviour of the original PRO/II mixer.



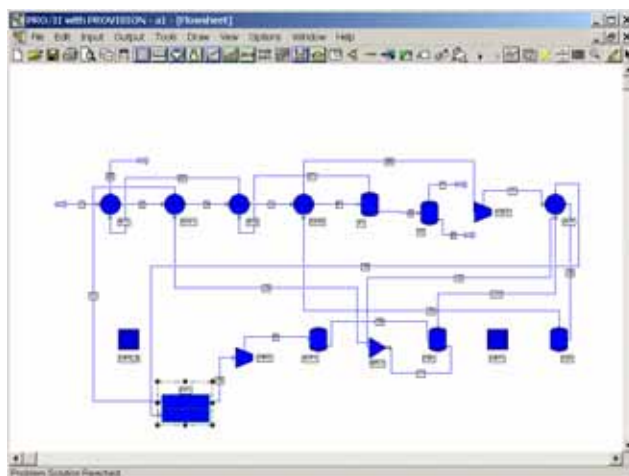
5. Execute the model in PRO/II and examine the results

You are now ready to run the PRO/II flowsheet just as you would any standard flowsheet. Perform the execution and wait for the units to turn blue, indicating successful solution.

Once the flowsheet has solved, the results for the gPROMS mixer unit can be viewed in three different ways:

- The streams into and out of the unit can be seen in the standard PRO/II stream tables.
- Unit information appears in the standard PRO/II unit tables.
- You can call up the gO:CAPE-OPEN display for the unit, as shown here.

The “Ports” tab in the gO:CAPE-OPEN dialog shows the properties of all streams attached to this unit. Other information pertaining to the unit is shown in the Report tab.



Property	Units	MidInlet	TopInlet	TopOutlet
TotalFlow	[mol/s]	2.2891	6.51444	8.80354
Temperat...	[K]	233.15	321.368	300.127
Pressure	[Pa]	111270	76796.4	76796.4
Enthalpy	[J/mol]	14364.7	20715.2	19063.9
Fraction	[mol/...]			
C1		0	0	0
C2		0	0	0
C3		1	1	1
IC4		0	0	0
NC4		0	0	0
IC5		0	0	0
NCS		0	0	0
NC6		0	0	0

At this stage you have successfully executed a gPROMS model within PRO/II. Although this was a simple model, the same steps apply for a model of any complexity.

PSE CAPE-OPEN commitment and developments

PSE is strongly committed to furthering the principles and application of CAPE-OPEN. Some of the CAPE-OPEN implementations completed by PSE are:

- The gPROMS CAPE-OPEN Physical Properties Socket, successfully demonstrated with Aspen Properties, Infochem Multiflash and ProSim SIMULIS.
- The gPROMS Object for CAPE-OPEN (PSE product gO:CAPE-OPEN), which is the subject of this article. gO:CAPE-OPEN has been executed with Aspen Plus for a 50,000 equation rate-based distillation column, and now with PRO/II.

In other developments currently underway, PSE is:

- assisting Honeywell in implementing CAPE-OPEN functionality within Honeywell simulation products.
- implementing a CAPE-OPEN unit socket within gPROMS, and is working closely with Fluent to implement the Vision 21 controller as the first test case.

PSE has also successfully advocated the adoption of CAPE-OPEN standards in the Virtual Plant Demonstration Model (VPDM), a UK publicly-funded power industry R&D project aimed at integrating power generation equipment models from different vendors within Process Modelling Environment (PME) frameworks. CAPE-OPEN has been adopted as the standard, with gPROMS is the primary integrating PME. As part of the project, a CAPE-OPEN wrapper for legacy FORTRAN models making use of text-based input and output has been developed.

PSE has also continued to adhere to the less widely adopted CAPE-OPEN solver standards in its internal architecture, and this is now promising to bear fruit by allowing the easy adoption of a newly developed academic code (IPOPT from Carnegie-Mellon University) as an optimisation solver. We are hopeful this will be the first of many such benefits.