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Development of a CAPE-Open Simulation Component for a GAMS-modeled Process Unit

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Abstract

In this paper, a method to incorporate a GAMS-modeled process unit in HYSYS is presented. The design and implementation of a user-friendly GAMS-compatible module that supports the CAPE-Open (CO) interface were carried out. More specifically, a CO-compatible simulation component for a reactive distillation column was developed. HYSYS was used in order to test the developed component, which became an available extension on the list of operation units. One of CO wizards that targets the mechanical generation of the Operation Unit (OU) Package was used. This wizard generates a Visual Basic project containing the source code of the OU and the installation package. In particular, the calculation routine and the Graphical Unit Interface (GUI) were implemented. The GAMS model was modified in order to read input values from a GDX file. An Excel file, which contains the user-defined parameters and the incoming stream properties, was created in the GUI written in Visual Basic programming language. Afterwards, the GDX file was created from the Excel file using the GDXXRW utility of GAMS. We have attained the technical know-how about the method to incorporate a user-defined item of equipment that was both previously modeled and simulated via GAMS. The reactive distillation column module embedded in HYSYS profits from its complete property-package, which is lacking in GAMS, in order to carry out the accurate computation of the chemical and equilibrium properties.

Keywords: CAPE-Open, Reactive Distillation, GAMS, Simulation., object-oriented

1. Introduction

In the area of process engineering, there are a lot of useful models made with common software (GAMS [1], Fortran [2]) that can be turned into a plug-in for the popular applications (Aspen [3], HYSYS [4]) in order to deal with the existing variety comfortably. The present trends involve making the software available worldwide. These ideas of user-friendliness comprise one main objective of the Cape Open (CO) project [5]. In this work we carried out the design and implementation of a user-friendly GAMS-compatible module that supports the CAPE-Open interface. A CO-compatible simulation component for a reactive distillation column was developed so that it satisfied the definitions and guidelines established by the standard. Conceptually speaking, reactive distillation [6] is the simultaneous implementation of chemical reaction and distillation in a counter-current column. Due to this combination of processes, the resulting mathematical model for the equipment is a large complex nonlinear equations system. Reactive distillation is applied worldwide in many plants in order to carry out different chemical processes. Some examples are: alkylation of aromatics and aliphatics, hydroisomerizations, hydrolyses, dimerization, decomposition of ethers to high purity olefins and oxidative dehydrogenations.

The commercial process simulator called HYSYS was used in order to test the developed component. The distillation column module embedded in HYSYS has two main advantages. In the first place, we have attained the technical know-how about the method to incorporate a user-defined item of equipment that was both previously modeled and simulated via GAMS. Thus, any GAMS model becomes compatible with HYSYS by following the proposed steps. Secondly, we have the possibility of profiting from the complete HYSYS property-package, which is lacking in GAMS, in order to carry out the accurate computation of the chemical and equilibrium properties. In this way, we can avoid the inclusion of the corresponding equations, correlations, and data (critical pressure, acentric factor, etc) in the GAMS mathematical model.

2. The CAPE-Open project

In order to obtain better results when solving a specific problem, it should be possible to access more than one vendor simulator and to in-house software containing company specific methods or data. The main projects working on this area are: IK CAPE, CAPE-OPEN and GLOBAL CAPE-OPEN [7].

Implementation of CO standard is the main activity of the CO Laboratories Network (CO-LaN). It is an internationally recognized, user-driven organization that facilitates the implementation of CO standard interfaces in commercial software to make open simulation a practical reality [5]. CO-Lan missions are to expose user priorities for the CO standard to software vendors, ensure the standard exploitation and dissemination, provide training and migration facilities; and supply compliance testers and interoperability tests.

2.1. Scope of the CAPE-OPEN project

The specific focus of the CAPE-OPEN project has been on general tools for process modeling and their use for steady-state and dynamic simulation [8]. The project has recognized two types of such tools, modular and equation oriented ones.

In an architecture for modular process modeling tools there exists a modular Process Modeling Executive (PME) which is responsible for constructing the model and carrying out all necessary computations to solve it. For this purpose it communicates with other modules that describe individual unit operations. Each module needs to communicate with property packages to compute the physical properties that occur within the unit operation model. As each unit operation module needs to solve the equations of the mathematical model associated, they may also perform specialized algorithms or call external numerical solvers.

An important characteristic of modular process modeling tools is the need for the executive to organize and coordinate the computations carried out by the individual unit operation modules.

The basic structure in an architecture for an equation oriented process package is almost the same as the one presented. The main difference is that the unit operation modules do not need to solve their own equations. Instead, they pass the information to the

Executive which assembles them into a large set of equations and solves it by interacting with one or more numerical solvers.

The ultimate vision of CAPE-OPEN is to allow complex process modeling tasks and model-based applications to be performed successfully and cost-effectively using collaborative software components coming from several sources and possibly being executed on different computer hardware.

An example for this is shown in Fig. 1. Here, the PME is supplied by one vendor, whereas the Process Modeling Components (PMC) come from different suppliers.

This analysis leads to the identification of the following classes candidates to standardization:

- Thermo: provides physical properties services.
- Unit Operation Modules.
- Numerics: provides numerical solvers and services.
- Flowsheet analysis tools.

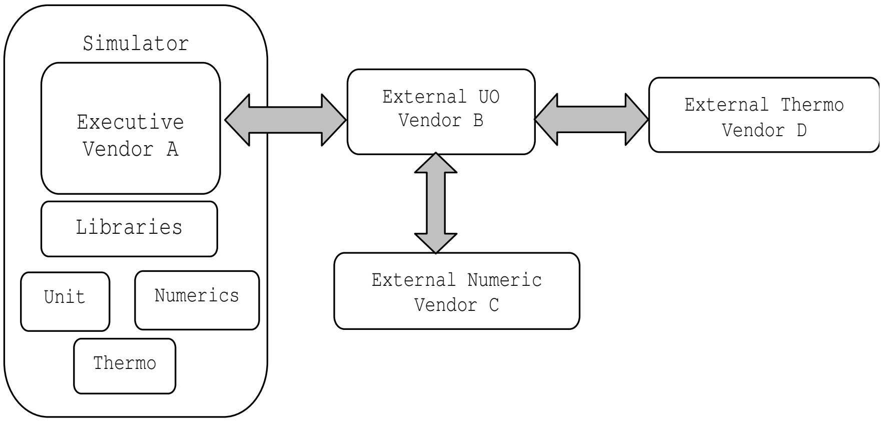

Figure 1. Integration of different CO tools.

The interfaces mentioned above could be implemented in various different ways, for example as a simple subroutine call in standard procedural languages such as FORTRAN or C [8]. However, CAPE-OPEN has chosen to adopt a component software and object-orientated approach which views each PMC as a separate object. Communication between objects is handled by middleware such as the Object Management Group's (OMG) CORBA [9] and Microsoft's COM [10]. Using these technologies each software object is able to interact with others based on a formal interface definition expressed in standard languages. The communicating objects can be running as part of the same process, or in different processes on the same or different computer hardware connected in a network, thus providing local/remote transparency.

Each interface in CO involves a set of methods and arguments which are expressed in CORBA Interface Definition Language (IDL) and COM IDL. Developers of CAPE-OPEN compliant components will need to incorporate the same declarations in their applications and to use IDL compilers to generate the corresponding instructions in source language. The wrapping code generated in this manner can then be linked with the rest of the components. Legacy code, such as FORTRAN models, can also be used by encapsulation within CAPE-OPEN compliant wrappers.

The definition of interfaces throughout the project was done following a development process based on the Unified Modeling Language (UML) object-orientated notation for all formal models of the interfaces, including the user requirements, producing use cases, sequence diagrams, state transition diagrams, class diagrams and, finally, interface diagrams which accompany the corresponding middleware implementation [8]. The project is using UML because it is the current best practice in software engineering.

3. Our approach: Steps on how to embed software

3.1. Software Embedment

In order to obtain a CAPE-Open compliant module of the reactive distillation column we used the CO Unit Operation Wizard developed by the CO Project [11]. This wizard generates a Visual Basic project containing the source code of the Operation Unit (OU) and the installation package to install it in other machines. In particular, the calculation routine and the Graphical Unit Interface are not generated. It is the developer's responsibility to provide this code. The OU generated will be compatible with the 0-9-3 version of the CO standard.

In the first place, the distillation column model was developed and tested in the General Algebraic Modeling System (GAMS), a high-level modeling system for mathematical programming and optimization. As the wizard-generated code was written in Visual Basic, a code migration was required to integrate pieces of code that have been implemented in different programming languages.

The original GAMS code was modified, in order to obtain simulation data from an external source. For this propose the GDX (GAMS Data Exchange) was used [12]. A GDX file is a file that stores the values of one or more GAMS symbols such as sets, parameters, variables and equations. This facility provides a utility called GDXXRW that allows reading and writing data of an Excel spreadsheet.

The OU code generated creates an Excel spreadsheet with all the necessary input data and then calls GDXXRW before running the GAMS model. Once the model is solved, the output data is written into another Excel spreadsheet so it can be read from OU Visual Basic code (Fig. 2).

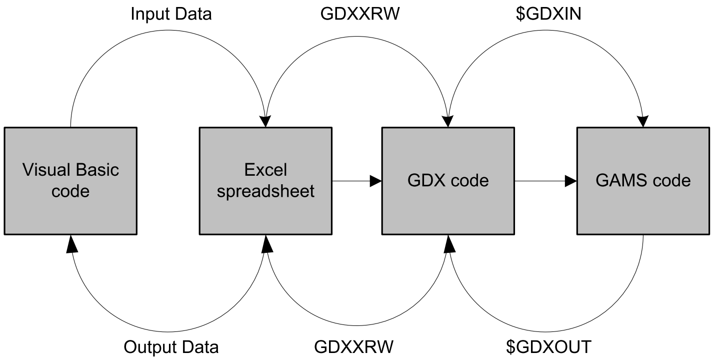

Figure 2: Resulting bridging approach.

In summary, the HYSYS OU, which was naturally programmed in Visual Basic, calls GAMS, where the OU mathematical model should be previously introduced. It is important to note that GAMS solves that model, and sends the results back to HYSYS. These results may be employed by HYSYS as the entry to any other equipment entries in order to continue with the complete simulation of the process plant.

3.2. Steps on how to embed existing software

In order to develop a CO Operation Unit from an existing GAMS model, some small modifications should be done in the original GAMS code. For instance, all the user defined data must be provided from an external file. Our approach for data input consists in creating an Excel file (i.e. datain.xls) with all the user defined data and then creating a GDX file (i.e. datain.gdx) using the GDXXRW tool.
GAMS code includes the following:

```
$GDXIN datain.gdx (load the GDX file)
SET VAR1 (*)  (define a variable)
$LOAD VAR1 (load the value from the external file)
```

Once the GAMS code has been tested in GAMS IDE, we developed a CO Operation Unit using the Wizard tool provided by CO Project.
The Visual Basic code generated by the wizard was modified in order to create the Excel file with input data and to call GAMS IDE. Visual Basic code includes the following:

```
x = CreateProcessA(0&, "gams.exe model.gms", 0&, 0&, 1&,
NORMAL_PRIORITY_CLASS, 0&, 0&, NameStart, NameOfProc)
(call to model.gms)
x = WaitForSingleObject(NameOfProc.hProcess, INFINITE)
x = CloseHandle(NameOfProc.hProcess)
```

Once the Visual Basic code was tested, the OU was installed in Hysys and it became available as an External Unit.

4. Case study

4.1. The reactive distillation module

To take advantage of the existing software, we concentrated on a complex model for a reactive column that had been built and tested in advance [13].
Reactive distillation is a hybrid operation that combines two key tasks in chemical engineering, i.e. reaction and separation processes. Considering the next reversible reaction scheme:

$$C1 + C2 \leftrightarrow C3 + C4$$

where the boiling points of the components follow the sequence C1, C3, C4 and C2, the traditional flow-sheet for this process consists of -a reactor and a sequence of distillation columns (Fig. 3a). Components C1 and C2 are fed to the reactor, where the equilibrium reaction takes place in the presence of a catalyst. distillation train is required to produce C3 and C4, which are obtained as pure products. An alternative for this process is the use of a reactive distillation column .
The reactive distillation column, see Fig. 3b, integrates reaction and separation and offers the possibility to overcome restrictions given by chemical and phase equilibrium. It consists of a reactive section in the middle with non-reactive rectifying and stripping sections at the top and bottom. The task of the rectifying section is to recover reactant C2 from the product stream C3. In the stripping section, the reactant C1 is stripped from the product stream C4. In the reactive section the products are separated, driving the equilibrium to the right and preventing any undesired side reactions between the reactants with any of the products. For a properly designed column, virtually 100% conversion can be achieved.

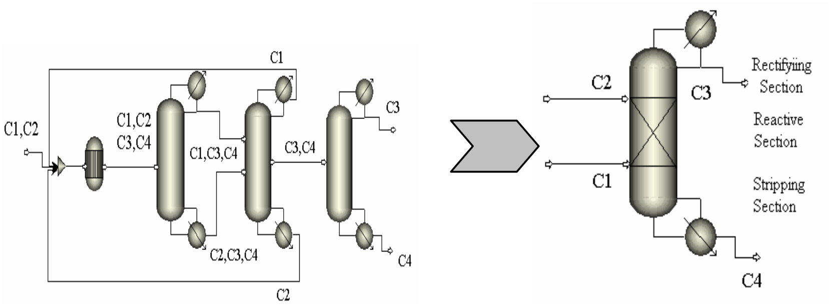

Figure 3 a) Conventional process b) Reactive distillation

The CO-compliant OU was successfully installed and it became available in HYSYS as an extension to the Unit Operations list. Results obtained under the HYSYS interface were similar to those we had obtained in previous studies, where the reactive distillation module was modeled in GAMS.

5. Conclusions

The proposal for software embedding described in this paper is useful for the industry, where HYSYS has become widespread. For simulation purposes, HYSYS provides a lot of general models. In contrast, there are some dedicated, accurate, specific models in any plant, which the process engineers need to include in their simulation. Thanks to our methodology, the engineers can easily take advantage of their accurate models, which surely demanded hard efforts for their development.

We have developed a method to incorporate a user-defined process unit that was both previously modeled and simulated via GAMS. In this way, it is possible to make any GAMS model compatible with HYSYS. Moreover, there is access to the complete HYSYS property-package, which is lacking in GAMS. This facility enables to carry out the accurate computation of the chemical and equilibrium properties. It is advantageous because the cumbersome procedure of adding thermodynamic equations, correlations and property data in the GAMS mathematical model can be avoided.

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