CO-ChemSep

Nonequilibrium Modelling: the CAPE OPEN Way

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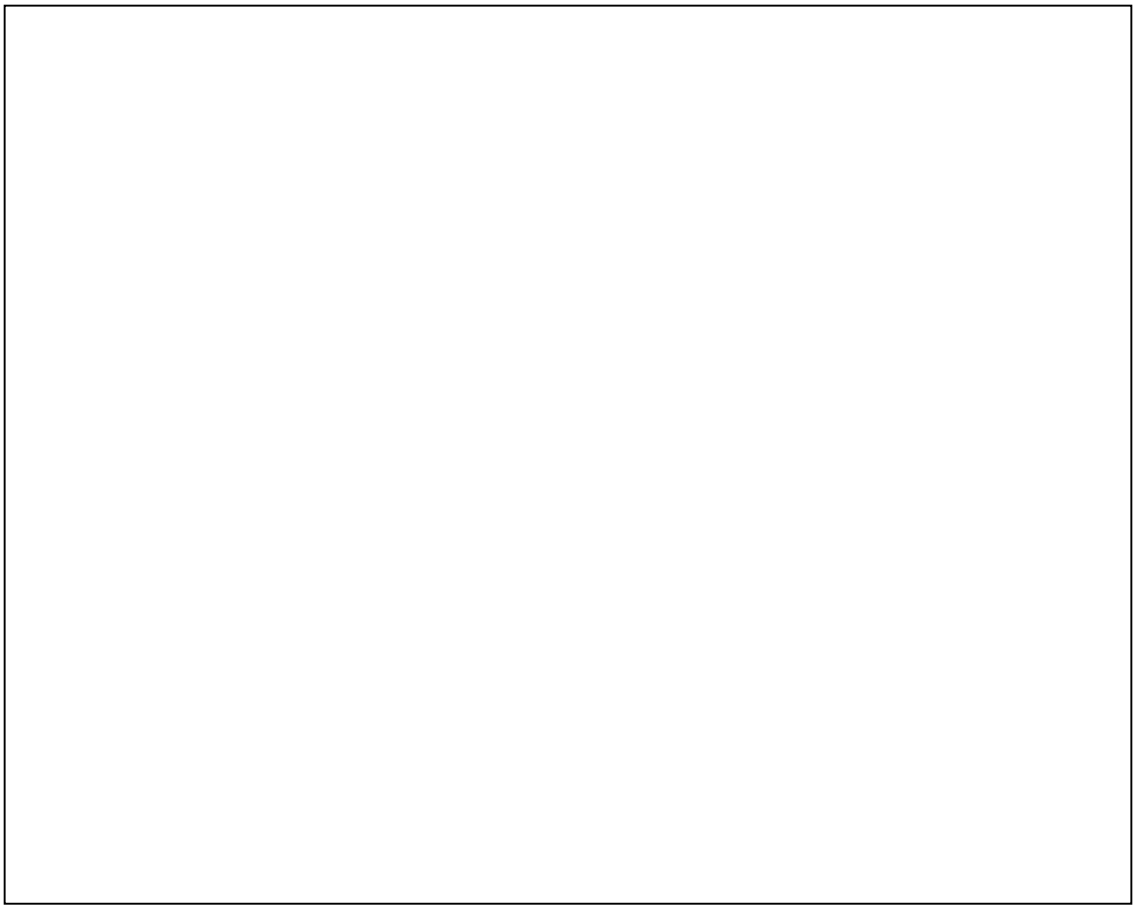


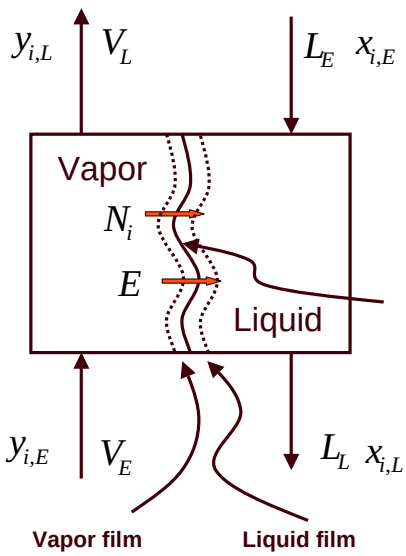
What is ChemSep?

- Just another distillation column simulator.
- Features the original nonequilibrium column model.
- Widely used in academia.
- Few commercial users
  – despite considerable interest.

ChemSep™ is a software system for modeling distillation, absorption, and extraction operations. **ChemSep** was designed to be easy to use by students with little or no experience of engineering software, while having sufficient flexibility and power to appeal to expert users and engineers in industry.

ChemSep is one of the few column simulation packages that feature a nonequilibrium column model. The model has been described in detail elsewhere (see, for example, Taylor and Krishna (*Multicomponent mass transfer*, John Wiley, New York, 1993) and Kooijman and Taylor (*The ChemSep Book*, Books on Demand, Norderstedt, Germany, 2001; available from www.cache.org) .

The first version of the program was released to a very limited student audience in 1998. The program has been much further developed and totally re-written since then and now the program is used in dozens of academic institutions in all parts of the world. Quite literally, thousands of students have learned to simulate distillation operations using **ChemSep**. However, **ChemSep** has not been widely used in industry despite considerable interest. We will return to this issue later in the presentation.



Nonequilibrium Stage Model

Nearly everybody has one!

Aspen Tech
Simulation Sciences ESSCOR
Chemstations
PSE
and many more…

All inspired by the model in ChemSep!

ChemSep includes perhaps the most detailed and comprehensive nonequilibrium model developed to date. A schematic diagram of the nonequilibrium model is shown above. A complete column is modeled as a sequence of such stages.

Numerical solution of the model equations provides the engineer with all of the quantities normally associated with the conventional equilibrium stage model (temperatures, flow rates, mole fractions). However, a nonequilibrium model can also provide considerable additional information such as mass transfer rates, efficiencies. McCabe-Thiele diagrams also can be constructed and are just as useful for a nonequilibrium model as they are for binary distillation problems; the only difference is that they have to be drawn using the results of a simulation. Last, but most definitely not least, the nonequilibrium model has been endowed with a design mode; the program actually provides a design of the equipment type that you have chosen to use for the simulation (sieve tray column, column with wire mesh structured packing, for example). This is important because it allows the program to simulate columns that do not yet exist (i.e. for preliminary design purposes).

There are several commercial implementations of nonequilibrium models, all inspired by the model in **ChemSep** (although **ChemSep** was not the first such model to be made commercially available).

Model Issues:

1. **Mass transfer coefficients and interfacial areas**
   (48 models in ChemSep)
2. **Hold up and pressure drop**
   (24 models in ChemSep)
3. **Flow models**

ChemSep contains a very extensive collection of correlations for mass transfer coefficients, pressure drop, and holdup. All three are needed in a consistent model. We believe that our collection of these models, while it could be improved, is significantly larger than the collections available in any other package. Knowing which correlations to use and when is very important to this kind of modeling.

Mass transfer coefficients: **ChemSeo** contains no less than **48 different models** including: AIChE model, Chan Fair, Zuiderweg, Hughmark, Harris, Onda et al., Bravo-Fair, and Bravo-Rocha-Fair.

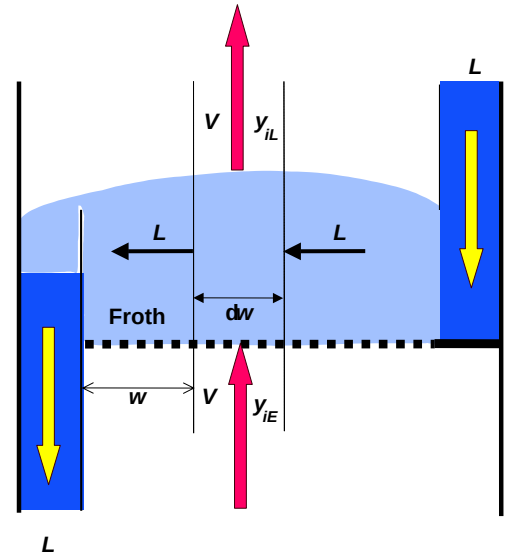
Pressure Drop Models: **ChemSep** has **18 different models** including: Ludwig, Leva GPDC, Billet-Schultes, Bravo-Rocha-Fair, Stichlmair-Bravo-Fair, and Bravo-Rocha-Fair.

Holdup: **ChemSep** includes **16 different models** including: Billet-Schultes, Bravo-Roch-Fair, Stichlmair-Rocha-Fair, and Bravo-Rocha-Fair.

We have developed a way for users to add their own mass transfer coefficient models using DLLs. **ChemSep** users have used this method successfully to implement correlations for what might be considered non-standard equipment designs. This approach is appealing for a variety of reasons, one of which is that the user does not have to deal with the entire source code. We have also developed a procedure for automating the creation of code for mass (and heat) transfer coefficients.

Flow Modeling is Critical!

- **Mixed flow**
- **Plug flow**
- **Dispersion flow**



Modeling the flow patterns is critical to the accurate prediction of real column performance. Most nonequilibrium models including ChemSep include the two limiting cases of completely mixed flow and plug flow. Real column performance typically lies between these two extremes. Dispersion models typically are used to represent departures from these ideal flow patterns. By varying the Peclet number from zero to infinity one can model flow regimes between the extremes of mixed flow and plug flow. Dispersion models have long been available for binary systems but it is not so simple to implement a dispersion flow model for multicomponent systems. To the best of our knowledge ChemSep is the only rate-based column model to include a dispersion flow model based on the ideas of Kooijman and Taylor (Modelling Mass Transfer in Multicomponent Distillation, *Chem. Eng. J*. **57**, 177-188, 1995).

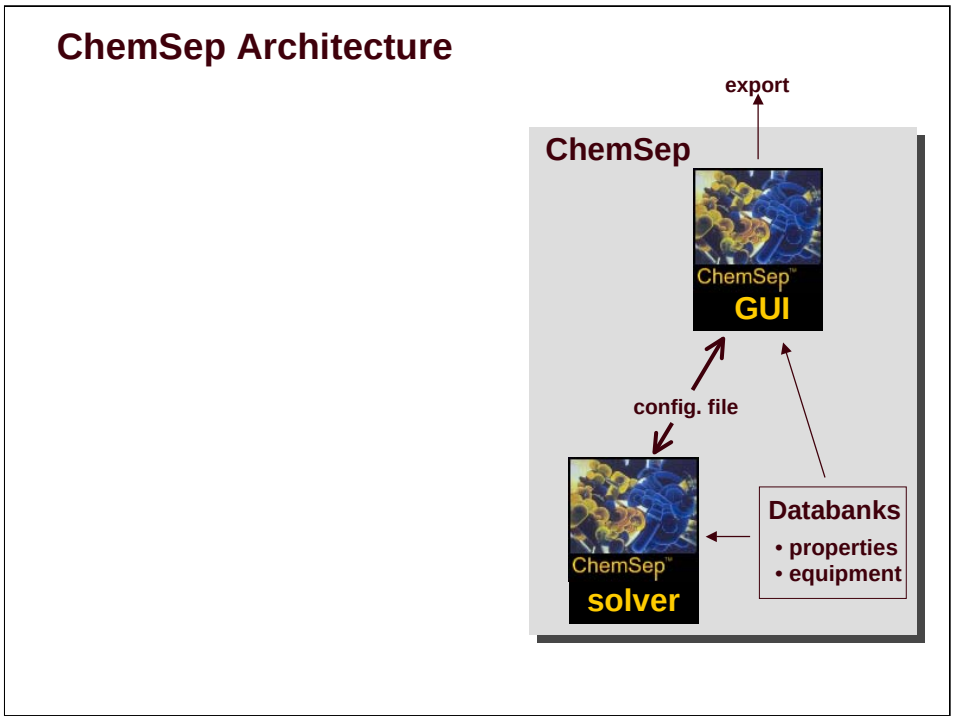
CO ChemSep: Why?

- **Little commercial use**
  – despite considerable interest.

  (because it did not function with flowsheet simulators).

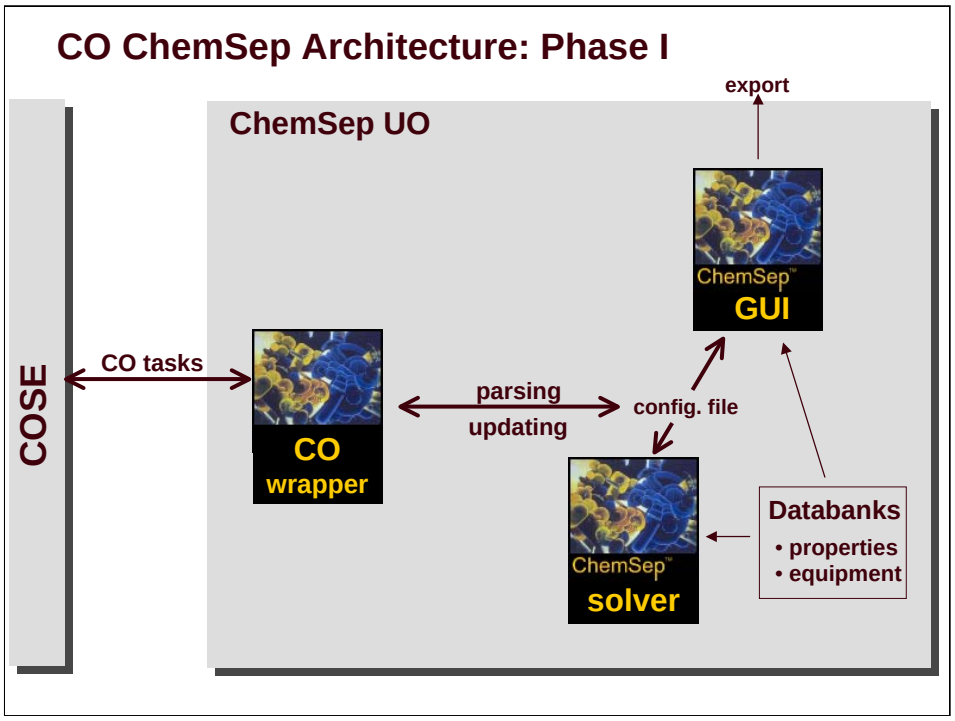
- **CAPE OPEN provides a way to make ChemSep function with any CO process simulator.**

Despite considerable interest for many years, **ChemSep** has not been widely used in industry. The primary reason for the lack of commercial users is that **ChemSep** does not function well with major commercial flowsheet simulation programs. The main requirement for an industrial user is for **ChemSep** to use the thermodynamic models available in the flowsheet simulator. The protocols developed under the CAPE OPEN movement have made it possible to link make **ChemSep** function as a user model in any CAPE OPEN compliant process simulation system. This includes the ability to use the thermodynamic property packages of the favored simulation system, but ANY CAPE OPEN compliant thermodynamics package could be used with **ChemSep**.



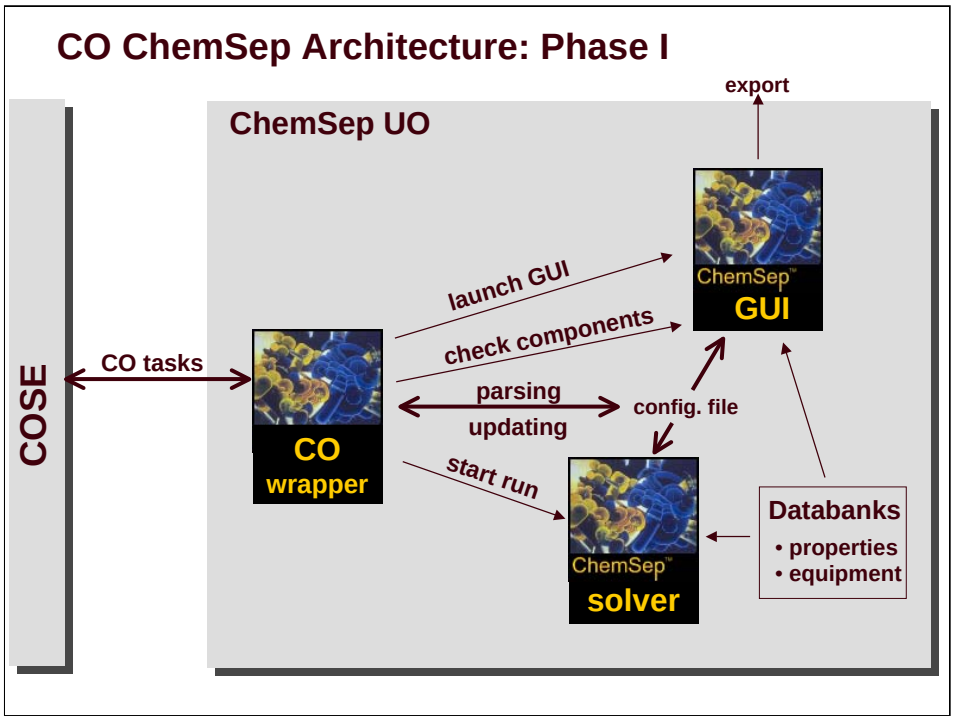
The basic architecture of the standalone version of **ChemSep** is shown above. New in Release 5.0 is a graphical user interface for Windows that retains much of the look and feel of the classic **ChemSep** interface. Problem solving is even easier with the new version however; new features make navigation within the interface much faster and the novice is taken through the problem solving process in a natural way. Input may include simple algebraic calculations as well as units. **ChemSep** checks your input, lets you know when each phase of problem setup is complete, and flags potential sources of difficulty before running a simulation.

The GUI communicates with the model solver by writing an input/output file (in plain text). The solver is a standalone program that takes its input from the file written by the GUI and to which the solver adds the results of the simulation. Both GUI and solver read from the physical properties databank. The GUI reads equipment design data from equipment databanks; this information is passed to the solver in the configuration file.



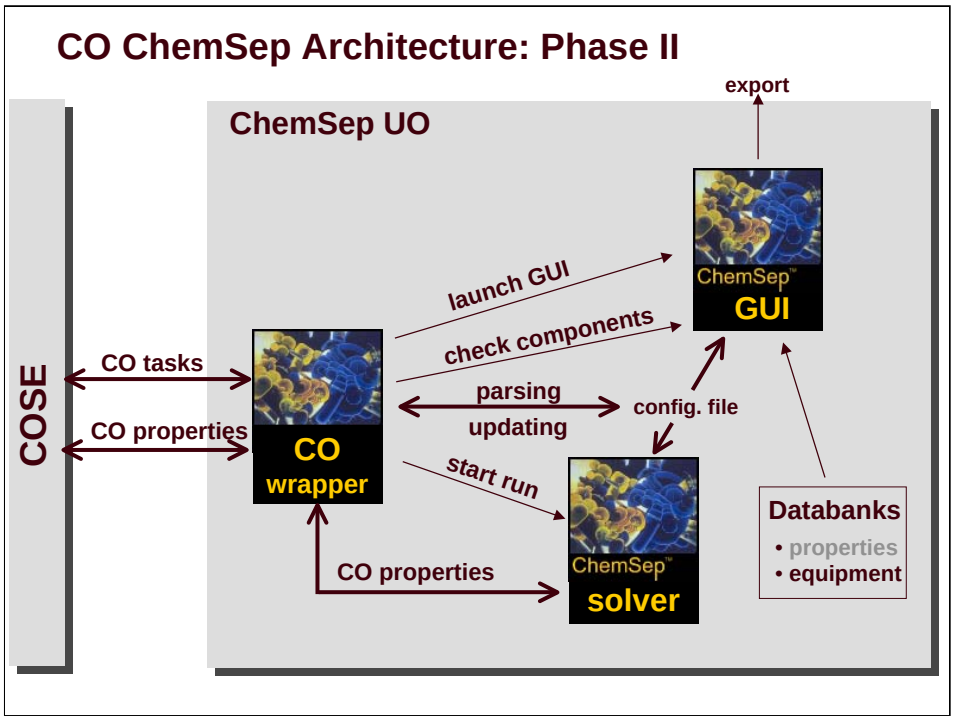
In phase I of our development of a CAPE OPEN compliant version of ChemSep (Putnam, R., M.S. Thesis, Clarkson University, 2004) we used a wrapper as the interface between **ChemSep** and the CAPE OPEN simulator executive (COSE) as illustrated schematically above. In this version **ChemSep** did not "know" that it was being called from another computer program and the user worked with the GUI in much the same way as he/she would if using the standalone version.

The creation of the wrapper was greatly assisted by the Unit Operation wizards available from CO-LAN. The wizard writes a skeleton wrapper in the Visual Basic programming language. A great deal of code must be added in order to create a functional wrapper, but the wizard was a considerable help to this phase of our work.



Some of the tasks required of the wrapper are shown here. The wrapper communicates directly with the COSE. It also interacts with the GUI. Unlike standalone ChemSep the solver is executed by the wrapper and not by the GUI. The GUI is used to create the input/output file that remains the way that information on components, column design, property models, and equipment design is passed to the solver. The solver (and GUI) read the ChemSep pure component data bank.

While this version functioned well within CO compliant flowsheet simulators, the main drawback was that it made absolutely no use of any CO compliant thermodynamics packages and relied instead on the (extensive) collection of property models already available in **ChemSep**. This serious limitation of **CO ChemSep** was addressed in Phase II and described next.

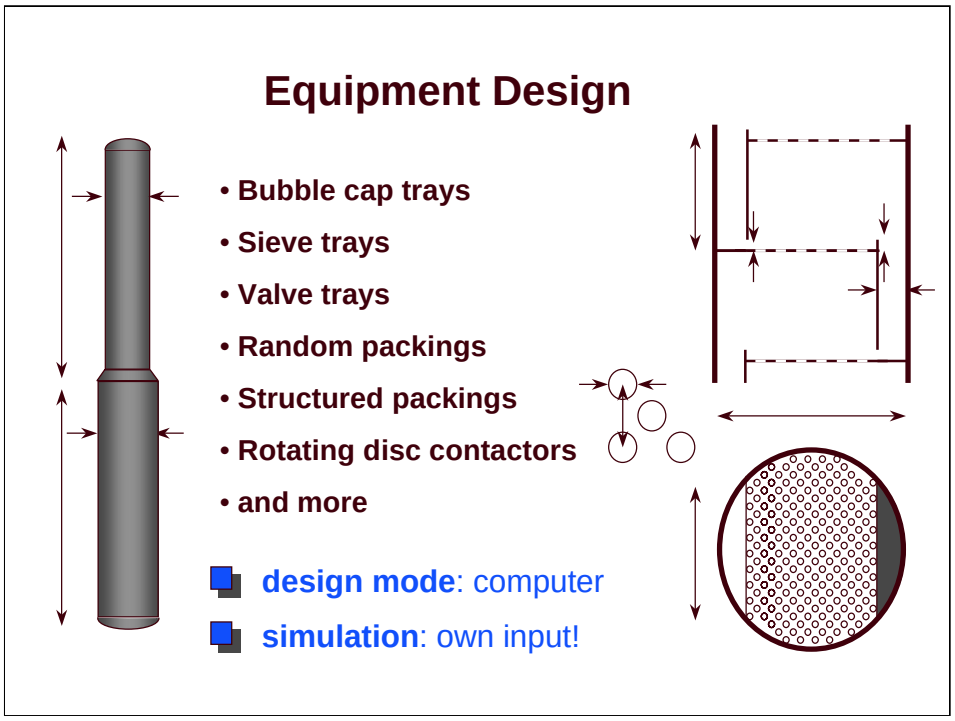


In phase II we wished to create a CO version of **ChemSep** that would be able to obtain thermodynamic and physical properties from the COSE (or other CO package). This required modifying the Fortran code of the model/solver to make calls to the wrapper, which would make a call to the COSE for thermodynamic and/or physical properties. The link between the solver and the **ChemSep** pure component databank now is entirely broken. The GUI remains able to read the pure component databank but it does not make much use of the data.

The Phase II wrapper was created entirely from scratch in C++.

Two more concerns:

1. Equipment design
2. Physical Properties



The estimation of mass transfer coefficients and interfacial areas from empirical correlations nearly always requires us to know something about the column design. At the very least we need to know the diameter and type of internal (although usually we need to know more than that since most empirical correlations for mass transfer coefficients have some dependency on equipment design parameters – weir height of trays for example). This need for more or less complete equipment design details suggests that nonequilibrium models cannot be used in preliminary process design (before any actual equipment design has been carried out). This is not true, however. Column design methods are available in the literature as well in most process simulation programs and it is straightforward to carry out equipment sizing calculations at the same time as the stage equations are being solved. This does not add significantly to the difficulty of the calculation, while providing the very significant advantage of allowing nonequilibrium or rate-based models to be used at all stages of process simulation:

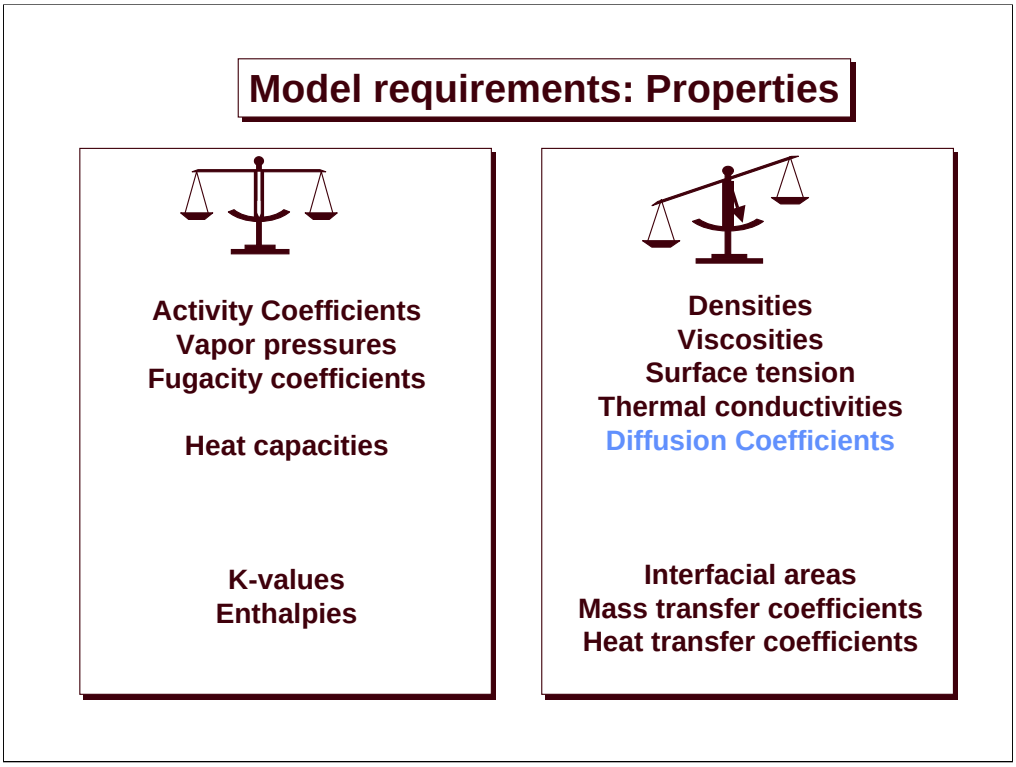
•preliminary design

•detailed plant design and simulation

•troubleshooting

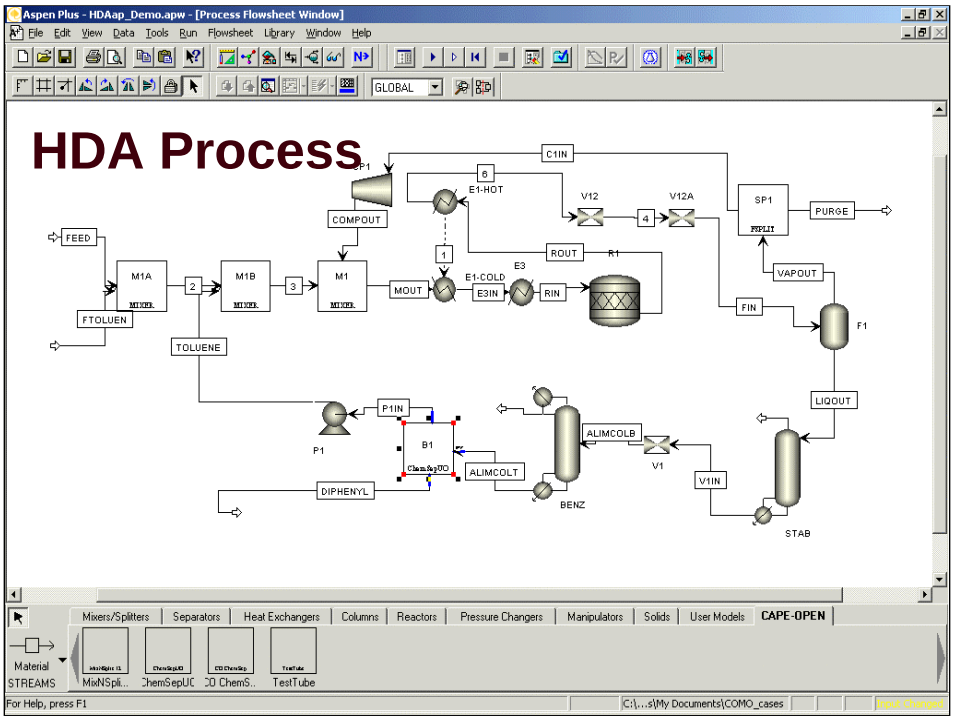
•retrofitting.

In fact, the last two of these are where nonequilibrium models can be particularly valuable, even to the point of helping identify what particular equipment design detail might be responsible for a column failing to deliver what it was designed to produce.



Physical property requirements for the equilibrium model are shown in the left panel above, the additional properties required by a nonequilibrium model appear on the right. It is obvious that nonequilibrium models are rather more demanding of physical property data than are equilibrium stage models. The only physical properties needed for an equilibrium stage simulation are those needed to calculate K-values and enthalpies and those same properties are needed for nonequilibrium models as well.

Mass transfer coefficients and interfacial areas must be computed from empirical correlations, or theoretical models. There are a great many correlations for mass transfer coefficients in the literature. These coefficients depend on the column design as well as on its method of operation, as well as on the physical properties listed in the panel on the right above. These properties can be obtained from the many models included in **ChemSep** or from a CO property package. It should be noted that most COSEs do not provide many options for estimating diffusion coefficients. Thus, in general we estimate diffusion coefficients from models available in **ChemSep**.



In this illustration, we see the well known HDA process as implemented in Aspen Plus. The HDA process contains a number of units that could be modeled using **CO ChemSep**. This includes the flash unit (far right., center), and three distillation columns (lower half). In this illustration the third column has been modeled using **ChemSep**.

A more complete tour of **CO ChemSep** in the HDA process is available separately.

CO ChemSep: Issues

- Using CAPE Open thermo greatly increases run time.
- Most simulation packages do not provide binary Maxwell-Stefan diffusion coefficients.
- SMILES and UNIFAC structures should be CO property constants.

As a result of our work on a CAPE OPEN compliant version of **ChemSep** we find that using thermodynamics packages from an external CO package results in a significant increase in run time. This is because the CO package we are using does not provide correct values of the partial derivatives of the thermodynamic properties. Thus, all partial derivatives are estimated numerically. This greatly increases the number of physical properties calculations with consequent increase in the computational cost.

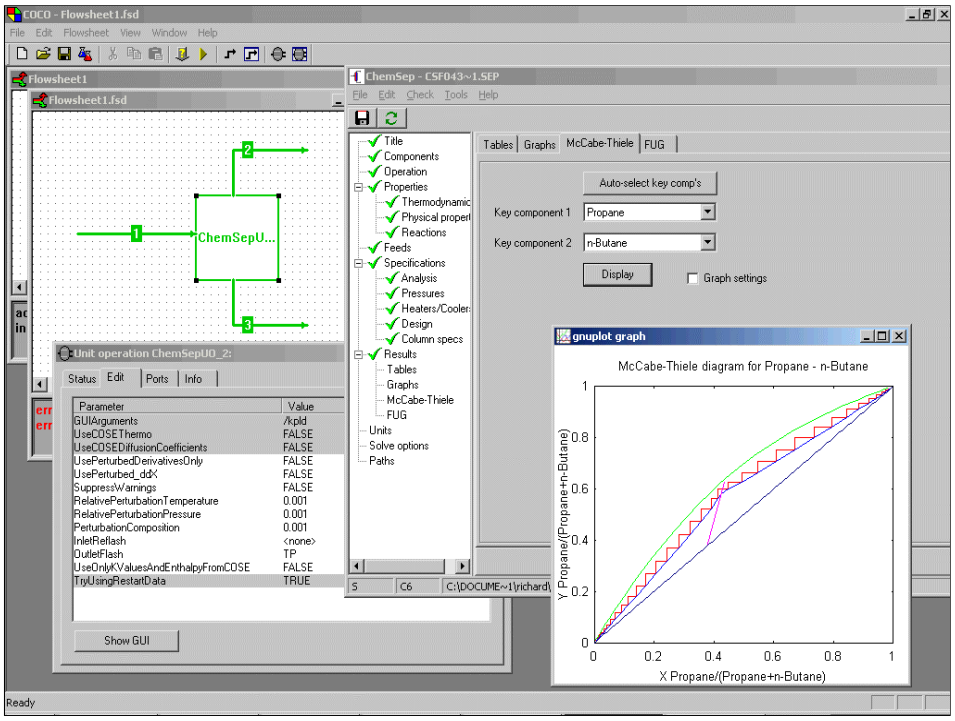
As noted earlier, most simulation packages do not provide many options for the estimation of binary Maxwell-Stefan diffusion coefficients. These are needed in rate-based simulations. **ChemSep** provides many estimation methods, but it makes sense to encapsulate these methods as an independent CO properties package.

We recommend that SMILES (a method for representing molecular structures) and UNIFAC structures

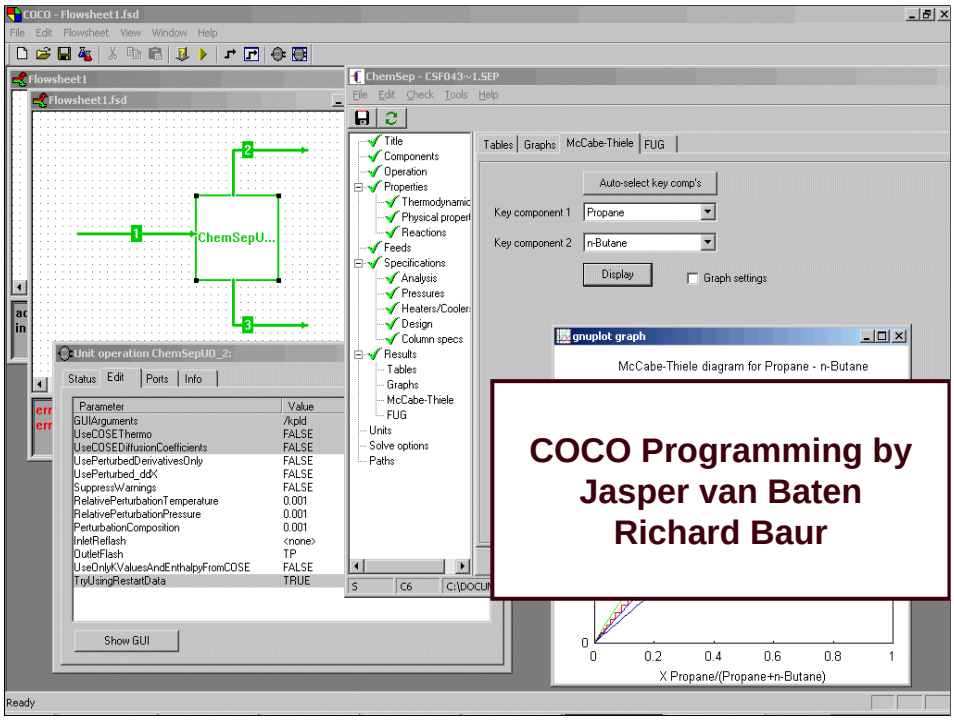
What is ChemSep Now?

- More than just a distillation column simulator.
- Features the original nonequilibrium column model.
- Functions with your favorite process flowsheet simulator
  - as long as it is CAPE OPEN compliant.
- Tested with Aspen Plus, HYSYS, COCO(?).

ChemSep now is more than a standalone column simulation program featuring the rate-based model that has served as the inspiration for all of the rate-based models now commercially available. ChemSep now works with any flowsheet simulation program that is fully CAPE OPEN compliant. CO ChemSep has been tested with Aspen Plus, HYSYS and COCO.



COCO is a CAPE OPEN compliant flowsheet simulation executive built from the ground up (in C++). COCO contains no unit operation models, no thermodynamics packages, and no solvers. Those must be available from other CAPE OPEN compliant packages such as ChemSep. Here we see COCO running a simple distillation column with ChemSep. The ChemSep window is shown on top of the COCO window. The McCabe-Thiele diagram is plotted by GNUplot called from the ChemSep GUI.



COCO was written in C++ by Jasper van Baten and Richard Baur.

What's next for CO ChemSep?

- Three-phase nonequilibrium model
- Flow models
- Reactive distillation

www.chemsep.org

Following completion of the CO version of ChemSep we plan to create a CO version of our nonequilibrium model for three-phase distillation. We are also working on improved flow models and on a CO version of our family of nonequilibrium models for reactive distillation.