Integrating shortcut algorithms into flowsheet simulators by means of the CAPE-OPEN standard

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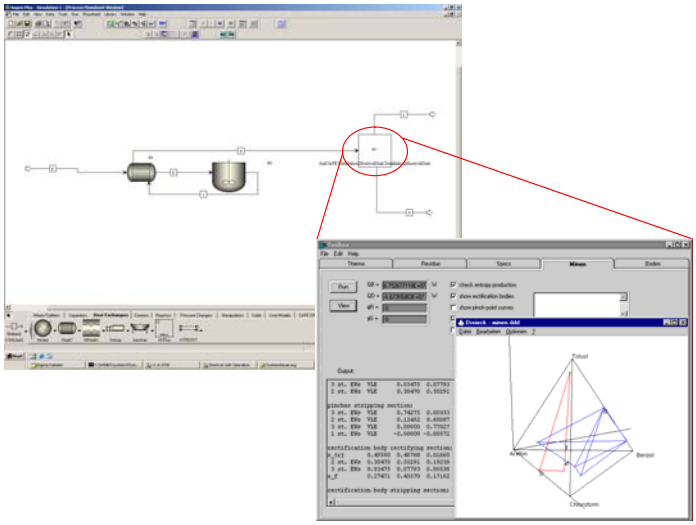
In many practical cases, process synthesis is carried out by using a simulator as an important tool, although specialized methods and tools for process synthesis are available. Hence, an integration of synthesis support into state-of-the-art flowhseet simulators is a desirable step to combine the benefits of the two worlds.

Within a simulation, a separation step can be represented by a simple splitter with fixed splitfactors. This splitter does however not take into account the thermodynamic behavior of the processing material (azeotropes and separation boundaries) and does neither permit insight into the feasibility of a separation nor into the consumption of ressources like energy or entrainer feed. Detailed distillation column models (like RadFrac in AspenPlus) on the other hand provide detailed insight but require information (like reflux ratio, number of trays and a feed tray) which is not known in early design stages.

Shortcut models rely on an approximation and combine the advantages of the approaches mentioned above. They permit the assessment of a separation step (e.g. with respect to feasibility and energy consumption) based on a simple specification of the desired products. Thus, detailed design information of an apparatus is not needed.

In this contribution we demonstrate, how such a shortcut model which was developed at Lehrstuhl für Prozesstechnik [1], RWTH Aachen, can be integrated into state-of-the-art flowsheeting tools (such as AspenPlus or Hysys) by means of the CAPE-OPEN standard for unit operations. This algorithm allows the assessment of single distillation steps regarding feasibility and minimum energy demand also in cases of non-ideal thermodynamic behavior using e.g. NRTL or UNIQUAC models. The use of this shortcut in a flowsheeting tool will allow engineers to quickly assess complex separation sequences behavior including recycles as they occur in azeotrope distillation, for example.



Based on an analysis of the software architecture of the existing prototype (written in C and Visual Basic) and an explanation of the CAPE-OPEN reference acrchitecture, a migration path will be explained. The new .NET framework technology as well as C++ have been used as a technical basis for the migration. Experiences regarding the implementation of the CAPE-OPEN unit are presented with respect to testing and performance optimization.

The use of the unit operation module developed will finally be demonstrated using practical examples.

[1] Bausa, J.: Näherungsverfahren für den konzeptionellen Entwurf und die thermodynamische Analyse von destillativen Trennprozessen. Erschienen in: Fortschritt-Berichte VDI: Reihe 3, Nr. 692. VDI-Verlag, Düsseldorf, 2001. ISBN 3-18-369203-1.