Interoperability between Modelling Tools (MoT) and Process Simulators (ProSim) through Cape-Open Standards

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The objective of this presentation is to highlight the application of computer-aided modelling tools for the generation and use of modelling objects in CAPE-OPEN compliant process simulators. This presentation will highlight the use of external modelling objects for unit operation models as well as thermodynamic property models. What we need are the following: a process simulator with a CAPE-OPEN socket (ProSimPlus), a CAPE-OPEN unit/thermo wrapper (link) that is able to receive an external model object from an external source and the model object representing any thermodynamic model. In addition, a computer-aided modelling tool called ICAS-MoT, is used to generate new model objects (unit operation and/or thermo). The advantage of using ICAS-MoT is that it is able to transfer the model equations representing any new unit operation/thermo into a COM-object with a well defined interface without the user having to write any programming code. It also orders the equations into a lower-tridiagonal form (if feasible) and provides a list of the model equations and the variables classified as unknown (to be calculated), known (to be specified), parameters fixed by the problem (data for the thermo-model, etc.). The generated model object calculates the unknown property variables, using its own built-in solver for the model equations (algebraic equations, differential-algebraic equations, partial differential-algebraic equations). The presentation will highlight the application of an uncommon unit operation: a short-path evaporation model normally used for the recovery of temperature sensitive chemical products in the pharmaceutical, food and aroma industries. Here, the model for the short-path evaporator is generated and tested in ICAS-MoT and then its equivalent COM-object is created. This COM-object is then wrapped by a specific unit-wrapper and plugged into the CAPE-OPEN socket of ProSimPlus (CAPE-OPEN compliant process simulator). Note that the short-path evaporator is a steady state model represented by a set of partial differential equations (with respect to height and width). It is discretized in width and integrated with respect to height to obtain the steady state profiles of the compositions and temperatures. The calculations involving binary and multicomponent mixtures will be highlighted. Details of the integration of an external thermo-model (PC-SAFT EOS) will also be provided. In principle, any process simulator with a CAPE-OPEN socket could be used.