

Reactions to COCO

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Abstract:

COCO's reaction package CORN has until previous releases only served for obtaining reaction chemistry and stoichiometry. The current release of COCO's unit operation package COUSCOUS has: fixed conversion reactor, equilibrium reactor, stirred tank reactor. Full usage is therefore made from the reaction package's ability to not only supply reaction chemistry, but also equilibrium constants, heats of reaction and reaction kinetics.

Reaction packages are not widely supported at this point. However, using reaction packages has advantages of being able to configure one set of reactions and use this throughout the entire simulation. Taking the reaction configuration away from the reactor unit operation configuration allows for ease of exchanging one reactor for another as well as using multiple reactors in one simulation. Reaction packages can be re-used between simulations, like thermo property packages. An overview will be presented of the work flow of bringing together reaction packages, thermo material objects and unit operations, and the level of implementation that is required by a PME to make things work.

It will be demonstrated how to operate reactors within the COFE flowsheeting environment.

Heat of reaction deserves some special attention, as recently property enthalpyF has been added to the thermo standard. EnthalpyF is guaranteed to include the heats of formation, whereas property Enthalpy is not guaranteed to have heats of formation in- or excluded.

Compound identification will also be highlighted.

It will be shown that COCO adopts some assumptions about the reaction package interface that are in contrast with the current chemical reaction interface standard specification. Suggestions will be presented on how to enhance the chemical reaction standard specification, as well as a look into the future of development of thermo and reaction standards. Developers of PMEs will be encouraged to provide support for reaction packages, as CAPE-OPEN reactor unit operations that depend on them are generally unable to obtain access to a reaction package other than via the PME, much like thermodynamic property packages are accessed via a material object that is implemented by the PME.

Cocosimulator.org's compliancy testing programme currently supplies testing for unit operation sockets and plugs, and thermo sockets and plugs. Reaction package sockets and plugs testing programmes have not yet been devised, awaiting wider support of reaction package implementations.