

## Computational chemical engineering modeling applied to energy and reactor design

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Chemical engineering is the combination of physical, chemical, biological ...operations on an energy or chemical plant. For process design, we have to carry out optimisations based on a multiple of parameters all the more so since the needs of processes in industry change very rapidly. These industries have to integrate new constraints linked to the energy cost and the environmental impact coupled with a need for more and more technical product.

Chemical engineering will play a key role to maintain the efficiency of the industry in a global market in which the processes offer become more and more technological and has to take into account :

- higher system integration to minimised energy consumption by coupling different process steps (ie : coupling of endothermal and exothermal steps, reaction and separation....),
- better optimisation of units design,
- higher product selectivity to avoid or limit by-product,
- production of new products.

To achieve these new developments the approach cover a large domain of technical disciplines and also a multiscale approach in time and length. This new complexity require to increase the relative weight of modeling and scientific calculation in the process development.

For exemple, CFD calculation is currently used for the development of reactor technologies and reactor internal, but most of the time it is difficult to couple hydrodynamic modelisation and reaction modelisation. A lot of improvement are expected by coupling these two approaches.

The molecular modelisation has also a large potential in process development and has to be coupled with more classical approach. For process integration, the thermodynamic optimisation is very useful mainly for developing new processes (pinch technology).

The modeling tools have to be used in all the steps of process development taking into account a multiscale approach and without forgetting the measurement technologies needed for model validation.