Research topics

Molecular Modelling of Refinery Processes

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Abstract

A new method for characterising refinery streams in terms of their chemistry has been developed. By relating these new chemical models to the bulk properties required by refinery operators, this has allowed modelling of refinery units to be accomplished on a much more fundamental basis. By including more information on the chemistry in the models of the units, we can make refinery optimisation much more effective and we can start to manage the flow of different chemicals species through the refinery.

Project description

Because of the complexity of crude oil and refinery products, we characterise their properties using bulk properties such as boiling point curves, octane number, cetane number, API gravity, sulphur content, pour point, etc. We cannot identify most of the chemical species present in most streams in the refinery. Because of this, we resort to empirical models for the modeling of the refinery units. In distillation we usually have to resort to characterising the streams being distilled in terms of pseudo-components. These are derived from boiling point curves and bear no relation to the actual chemical make-up of the streams. The models that we use for reaction are different from those that we use for separation, leading to a situation where effective integration between units throughout the refinery is not possible because we do not take a fundamental account of the chemistry. Increasingly, constraints are placed against individual chemical species (e.g. benzene). The flow or such species around the refinery needs to be managed in an effective way so as maximise the overall profitability. Also, some of the streams from the refinery will be used for petrochemicals production. The flow of certain chemicals species through the refinery to petrochemicals production will have a critical influence on the profitability of the overall operation for petrochemicals production.

A new method for characterising refinery streams in terms of their chemistry has been developed. This takes account of different chemical families and the carbon number within each family. By relating these new chemical models to the bulk properties required by refinery operators, this has allowed modelling of refinery units to be accomplished on a much more fundamental basis.

The first benefit is that it allows more fundamental models to be built for critical operations such as hydrotreating and hydrocracking. These units have a fundamental role in satisfying the new regulations for low sulphur fuels. Chemical modelling has been used to identify the main constraints on hydrotreating and hydrocracking processes. Some common process configurations make inefficient use of hydrogen, and performance can be improved significantly.

However, the benefits of better modeling of individual units runs far deeper than the performance of the individual units. By including more information on the chemistry in the models of the units, we can make refinery optimisation much more effective. We can start to manage the flow of different chemicals species through the refinery, rather than leaving this largely to chance. This is particularly important when we consider the interface between petroleum refining and petrochemicals production.