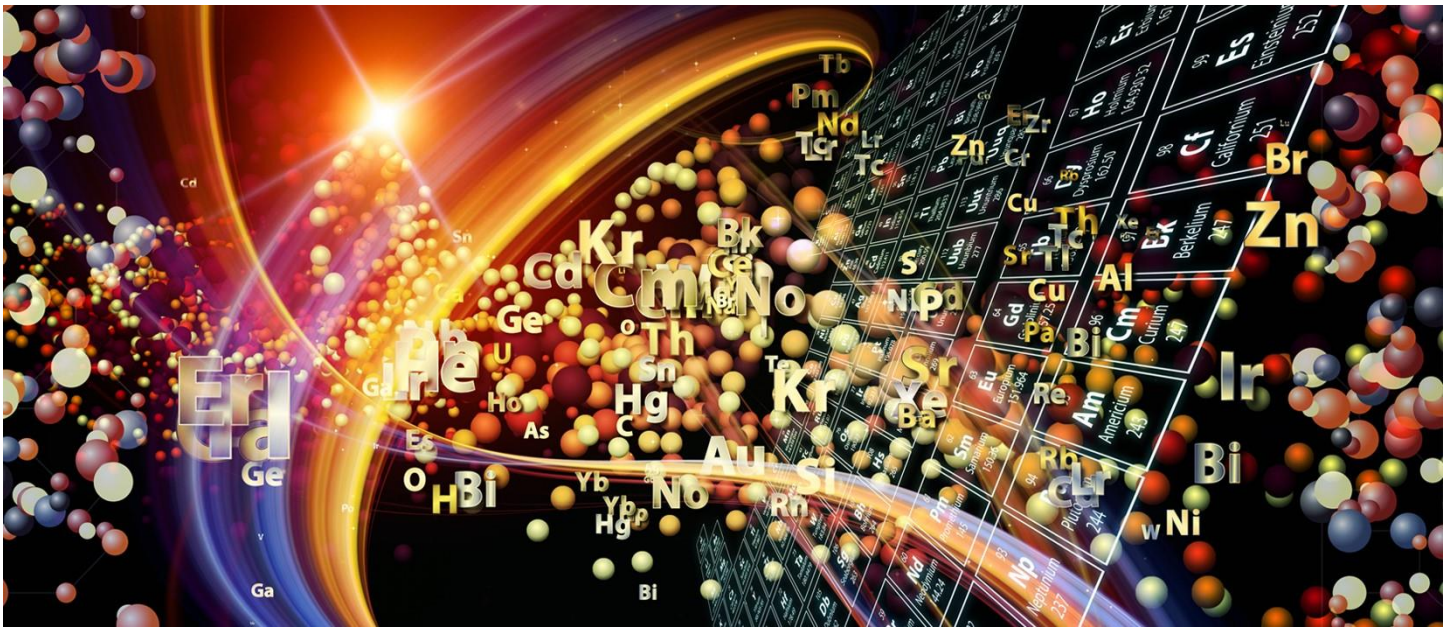
think simulation | getting the chemistry right



Modeling the HF alkylation chemistry

An OLI Joint Industry Proposal (JIP) preview

Corrosion in the HF alkylation process

The HF alkylation process for refining converts alkene hydrocarbons into alkylates for producing a premium high octane blending stock, using hydrofluoric acid (HF) as the catalyst. The fractionation can include an isostripper, a de-propanizer, and an HF stripper, along with associated pre-heating, condensing and acid recycling operations. The HF catalyst can become 'rich', that is, it can contain water; during the alkylation process the water rich HF can become entrained in droplets in the hydrocarbon streams. Corrosion from this water rich HF is a problem for this process.

Water rich HF corrosion is associated with the phase changes of the process. This could be the water rich HF condensing out of a hydrocarbon stream, where the first drops of condensate are highly concentrated with HF, or the water rich HF could vaporize as it is heated. One best practice for mitigating the water rich HF corrosion from these phase changes is to set an integrity operating window (IOW) that will avoid any phase changes outside the heat exchangers in the process. If an IOW is used, it is typically set by experience.[1]

Current modeling challenge

Ideally, the IOW for a given HF alkylation process would be fine-tuned by using process simulation. Rigorous process simulation could predict the thermodynamic phase change temperature and pressure of the streams in the unit. The temperature and pressure could then be tightly controlled to avoid the phase changes outside the heat exchangers.

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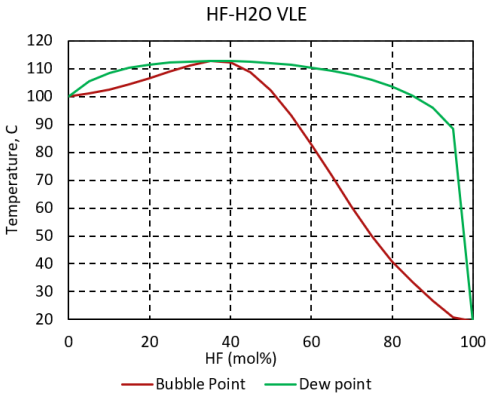
[1] Gysbers, A. (2018) "HF/Water/Hydrocarbon Modelling, Presentation, NACE CTW STG34 (206X)

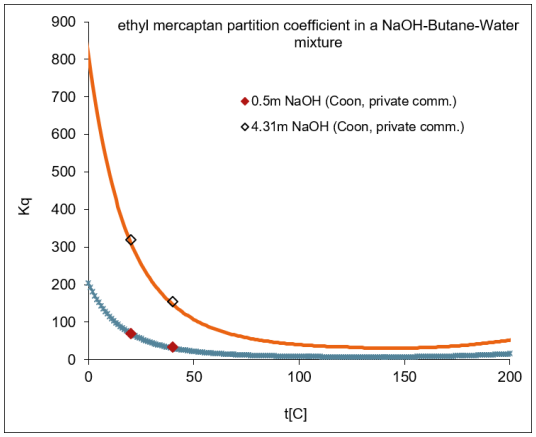
The modeling challenge is that current simulators designed to primarily model refining hydrocarbon processes cannot accurately predict the electrolyte HF changes. On the other hand, current simulators that model primarily electrolyte processes, can also model hydrocarbons. However, to do so requires the molecule-molecule interactions between the hydrocarbons and the HF for accurate modeling.

Many significant benefits will be realized once an accurate thermodynamic model is available for this process. Benefits would include measurable improvements such as longer equipment life, process optimization in terms of running the process for optimal yield and heating / cooling savings, and resource savings in terms of increased productivity of corrosion engineers and less corrosion consulting time.

OLI Systems framework

The OLI electrolyte thermodynamic framework is a robust and proven model that accurately predicts the behavior of electrolytes in any process. Given the requisite underlying binary and ternary data, this model has been successfully applied to systems where electrolytes are primary. In refining this include modeling the amine behavior for the CDU overheads, sour water strippers, sulfur recovery, gas sweetening, etc.





In addition, when the necessary binary and higher order interactions needed for ionic modeling are defined, OLI successfully models mixed hydrocarbon and electrolyte systems as well.

One such mixed electrolyte and hydrocarbon system is the Merox process. In the Merox process converts mercaptans to hydrocarbon disulfides. The OLI model accurately reproduces the mercaptan partitioning between hydrocarbons and caustic water liquids.

Proposed Joint Industry Project (JIP)

OLI proposes a JIP to provide corrosion engineers with ionic modeling capabilities for the HF alkylation process, to facilitate the development of accurate IOWs for the minimization of water rich HF corrosion. This project has two primary objectives: to develop the necessary interaction parameters for the HF alkylation process, and to develop templates in the OLI software for chemistry analysis and process analysis of the HF alkylation process

FOR MORE INFORMATION

Please let Pat McKenzie, pat.mckenzie@olisystems.com know of your interest
Pat will send the JIP proposal (available shortly) with complete information: project description, timing, funding, & benefits.

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