HF alkylation project meeting

25 March 2019

Project overview

- ✓ Objective
- ✓ Modeling plan
- ✓ Simulation plan
- ✓ Timing

Popular questions

- ✓ Feasibility of ASOs
- ✓ Sulfolane
- ✓ Member data
- ✓ Simulation vs actual
- ✓ OLI licenses
- ✓ Late joins

Open mic

What's on your mind?

Project objective

To give engineers ionic modeling capabilities for the HF Alkylation process

- ✓ To facilitate development of accurate Integrity Operating Windows (IOWs)
- ✓ To minimize phase-change-driven water rich HF corrosion
- ✓ For process optimization
- ✓ For safer operation of HF Alkylation units

By using a two step plan

1. Modeling
Developing necessary thermodynamic simulation parameters

2. Simulation
Developing case studies and case templates for member companies

Modeling plan

Model phase equilibria in HF – hydrocarbon mixtures

Model secondary components: acid soluble oils and fluorinated hydrocarbons

Deploy chemistry simulation parameters in software

Validate results where possible based on case studies

Phase equilibria in HF – hydrocarbon mixtures

- Literature review has been completed

Hydrocarbon	T Range, C	Data Type	Reference
Octane	25 - 65	Solubility of HF in hydrocarbon	Simons (1931)
Benzene	20 - 75		
Propane	0 - 40	Mutual solubility of HF and hydrocarbon	Butler et al. (1946)
Butane	5 - 40		
Isobutane	0 - 50		
Pentane	-25 - 40	Mutual solubility of HF and hydrocarbon	Marcus et al. (1970)
Hexane	-25 - 40		
Heptane	-25 - 40		
Propane	30 - 90	Mutual solubility of HF and hydrocarbon	Chen et al. (1994)
Butane	30 - 90		
Isobutane	30 - 90		
Butene-1	30 - 90		
Benzene	30 - 90		
Propane	20, 30	VLE PTx data	Kang (1999)

Simons J. H., "The Solubility of Hydrogen Fluoride in Benzene and in Octane", Journal of the American Chemical Society, 53, (1), 83-87, 1931.
Butler E. B., Miles C. B., Kuhn Jr. C. S., "Hydrogen Fluoride Paraffin Systems. Significance of Liquid Phase Equilibria in the Hydrogen Fluoride Alkylation Process", Industrial and Engineering Chemistry, 38, (2), 147-155, 1946.
Marcus Y., Shamir J., Soriano J., "Mutual Solubility of Anhydrous Hydrogen Fluoride and Aliphatic Hydrocarbons", Journal of Physical Chemistry, 74, (1), 133-139, 1970.
Chen X., Lee C., Wu Z., "The Measurement of Mutual Solubility Data for Hydrogen Fluoride Systems", AIChE DIPPR Data Series, (2), 28-33, 1994.
Kang Y. W., "Phase Equilibria for the Binary Mixtures Containing Hydrogen Fluoride and Non-Polar Compound", Fluid Phase Equilibria, 154, (1), 139-151, 1999.

Phase equilibria in HF – hydrocarbon mixtures

The amount of literature data is rather small
(compared to other hydrocarbon systems)

→ Good news: it is sufficient to establish a thermodynamic model

- Modeling scope
  - Vapor-liquid and liquid-liquid equilibria (VLE and LLE)
    for discrete HF – hydrocarbon mixtures
  - Develop a generalized correlation for HF
    with paraffins and olefins to fill gaps in experimental data
  - Prediction of phase equilibria and speciation
    in HF – H_2O – hydrocarbon mixtures

Modeling secondary components

- Fluorocarbons
  - Phase equilibria for C1-C4 fluorocarbons with HF, H_2O and hydrocarbons
  - Generalized correlations for C1-C4 fluorocarbons with hydrocarbons
- Acid soluble oils
  - Developing an estimate for the properties of ASO and their phase equilibria with HF and water
- Verification during the JIP simulation segment - case studies
  - Model will be tested by members on case studies
    results will be reviewed by OLI
    where members have known information they can share
    with possible adjustment to parameters

Simulation plan

3 members case studies will form the basis of case templates for other members

Both chemistry studies (OLI Studio) and process studies (OLI Flowsheet: ESP) will be made

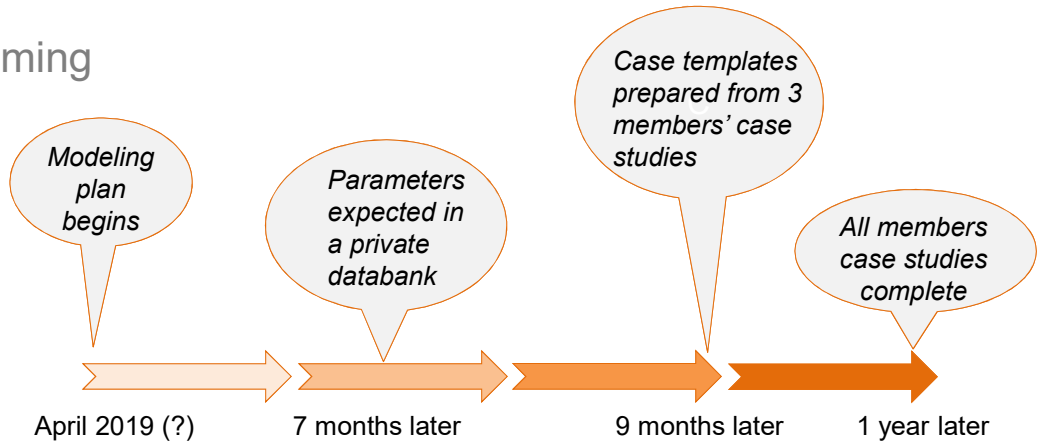
Web training on case templates

Individual guidance for case development for each member on their own unit

Possible revision of simulation parameters in model

Validate results where possible based on case studies

Timing



Notes

- ✓ **Start depends on 7 SIGNED contracts**
- ✓ Case studies and case templates will be partial, not entire simulations
- ✓ Verification, possible model revisions based on case studies

Frequently asked questions about this JIP

Can OLI realistically model all **ASOs**?

What about **sulfolane,** is this part of the project scope?

My **company IP on HF** - do you need it? Do I have to get permission to share it?

Will the simulation match my process? How will I know?

I don't have an **OLI license,** do I need one?

My company wants to join, doubtful it will be in April – are there **late joins**?

When will these parameters be made public to other **OLI clients?**

Your question!

ASOs

Can OLI realistically model all ASOs?

- ✓ Two categories of secondary components
  - ✓ Fluorinated HC
  - ✓ ASOs
- ✓ Fluorinated HC, same approach as are using for HF – HC
  - ✓ Some data, some correlations
- ✓ ASOs needs a literature review and an estimate approach
  - ✓ Almost certain there will be no high-quality experimental data
  - ✓ We will rely on estimations

Sulfolane

Will sulfolane be part of this project?

- ✓ Unfortunately, we will not be including sulfolane
- ✓ However, we are considering a companion project
- ✓ Important component in refining
- ✓ Others (beyond HF Alkylation) will be interested in this component

→ Let us know you are interested!

Member IP on HF alkylation

Will I need to contribute my company's IP on HF alkylation?

- ✓ No!
- ✓ When you setup case studies, you can compare the simulation to your data
- ✓ You may choose to investigate a particular case under NDA with OLI
- ✓ Model verification will be better for simulations versus actual comparisons

Simulation versus plant data

Will the simulation match my actual process?

- ✓ **The simulation target is thermodynamic for calculating IOWs**
  - ✓ It will show feasibility / infeasibility
    (e.g. above this T, no formation is possible)
- ✓ Possible kinetic effects in some process places / incomplete mixing etc.
- ✓ Comparison of simulation versus actual will yield insights
  - ✓ We may recommend a study of kinetics
  - ✓ We may re-investigate the thermodynamic parameters

OLI licenses

I don't have an OLI license, how can I use the simulation capability

- ✓ 4-month licenses to OLI Studio and OLI Flowsheet: ESP are given
- ✓ Ample time for a chemistry and process study
  - ✓ Training planned
  - ✓ Technical Advisors will be leading / assisting your case formulations
- ✓ Ample time to determine whether a future OLI license will make sense
- ✓ If you decide to lease the software
  - ✓ Only the base lease cost will be charged
  - ✓ HF license fee for 2 years waived

HF data made public

When will the HF alkylation parameters be put into the OLI public databank?

- ✓ They will not be made public
- ✓ A refinery license will be required in addition to the base license
- ✓ The refinery license will be waived for JIP members for 2 years following the JIP

Late joins

I will not make the April contract-signed deadline – will there be late joins?

- ✓ Yes, late joins will be allowed
- ✓ We will accept a contract under review in April as qualifying for full benefits
- ✓ The refinery license benefit will be reduced by 1 year for 2019 late joins

Please return your contracts for an April start!