Property Prediction for Emulsion based Chemical Product Design

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Property Prediction for Emulsion based Chemical Product Design

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1. INTRODUCTION

- Chemical industry is shifting from commodities towards higher value added products
- Higher value products gain their value from a molecular or micro-structure
- Product design aims to find a product exhibiting a set of desirable or specified behaviour
- Chemical product design is getting more and more important
- Modeling of emulsions becomes relevant
- Large availability of properties is required
- Predictive property models are needed

2. PURE COMPONENT PROPERTIES

- For all components
  - Predictive models for the main properties required by a methodology for product design (viscosity, density, surface tension, solubility parameters, etc.) have been already developed
- For surfactants only
  - Predictive models for the peculiar properties of surfactants (critical micelle concentration, cloud point, hydrophilic-lipophilic balance or equivalent, Krafft temperature, etc.) are missing

3. CLOUD POINT – Original M&G GC method

- Original M&G GC method
  - 39 experimental values
  - Non-ionic surfactants, 1% w/w
  - 1st order group definition: 4 groups
  - 2nd order group definition: 1 group
  - 3rd order group definition: 0 groups
  - $R^2 = 0.85$

4. CRITICAL MICELLE CONCENTRATION – Extended M&G GC method

- Extended M&G GC method
  - 158 experimental values
  - Non-ionic surfactants, 25°C
  - 1st order group definition: 34 groups
  - 2nd order group definition: 13 groups
  - 3rd order group definition: 0 groups
  - $R^2 = 0.91$

5. MIXTURE PROPERTIES

- Predictive models for mixture properties (viscosity, density, surface tension, solubility parameters, etc.) when considering separately the continuous and the dispersed phases have already been developed
- Predictive models for mixture properties when considering the two phases together have already been partly developed (density, cost, safety and toxicity parameters, Hansen and Hildebrand solubility parameters, evaporation time)
- Predictive models for mixture properties when considering the two phases together are missing (i.e. emulsion structure, viscosity, interfacial tension)

6. WATER-SURFACTANT PHASE BEHAVIOR

- The phase diagram between water and C12EO6 is considered
- Key-points of the diagram have been identified and defined
- By measuring or predicting a few key-points, it is possible to identify “safe areas”

7. CONCLUSIONS

- M&G GC methods are suitable to predict peculiar properties of non-ionic surfactants
- The addition of new dedicated third order groups can give considerable improvements
- A new third order group definition will be determined analyzing all the surfactant properties simultaneously
- Water-surfactant phase behavior has been reduced of complexity, by defining two safe areas, identified by 6 data-points

- New surfactant properties need to be considered, including ionic surfactants
- Dedicated models for interfacial tension and viscosity need to be developed
- Stability and production will be considered

MAIN REFERENCES