Electrolyte Chemistry Analysis Capabilities *in Industrial Process Simulators*

Conversations with OLI Experts on Science of Electrolyte Chemistry
Issue 5.0

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Key Questions for the OLI Expert:

- **Can you provide some context on industrial process simulation software products – what do they do and how are they different from OLI?**
  In principle, each of the industrial process simulators - including OLI Flowsheet - do the same thing. They attempt to either simulate or design a process to gain insight and operational parameters. Most of the other process simulation products use equations of state or limited local activity models for the components in the simulation. They lack the in-depth activity predictions for electrolytes and water that OLI has in its simulations.

- **Why are electrolytes and water chemistry-based calculations important to these industrial process simulation software products?**

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Electrolytes and water are funny things. We know more about methane thermodynamically than we do of some simple salts in water. How electrolytes behave in water can dramatically affect a process. A case in point is the use of ethylene glycol to prevent the formation of gas hydrates in natural gas transmission lines. When a gas reservoir is produced, water accompanies the natural gas. This water has electrolytes in the form of dissolved salts. An odd thing about natural gas transmission lines is that the methane molecule can coordinate water molecules around it to form a clathrate. These are like icebergs in the gas line and can damage process equipment. Operators will add ethylene glycol (also known as MEG) to prevent the clathrates from forming. However, adding the MEG can change the solubility (lowering it for the most part) of many salts. So, you can have conditions where you have accidently increased solid fouling (scaling) in the process of preventing clathrate formation. This is why it is important to know both hydrocarbon chemistry and water chemistry.

- **How do products like Aspen Plus/ Hysys, Unisim, PRO/II, etc. handle electrolytes and water chemistry calculations? What alternatives do they have to OLI and what types of reactions and phenomena are they designed to predict?**
  I would like to speak just about Aspen Plus. The Aspen Plus model has an activity model for electrolytes. As I recall it is either the Chen model or Chen-NRTL model. This is a very good model and can be used to model electrolytes. However the database is rather limited with respect to the OLI database and user data regression must frequently be done. In the case of the "Hysys" products which I also include Honeywell Unisim Design and KBC Petro-Sim also have some activity models. In the case of Aspen Hysys they can also use the Chen models. However, traditionally activity models in those products assume a "Free Water" assumption that there is no interaction of the water with other species.

- **What makes the OLI software unique when it comes to electrolytes and water chemistry applications?**
  OLI has spent the past 50 years modeling electrolytes in water. We have regressed thousands of data systems with a rigorous model so the user is not required to be a data expert. We also have developed the heuristics to solve highly non-linear equations as well as phase separations.

- **What is OLI's strategy when it comes to working with industrial process simulation software? How has OLI enabled this strategy with its technology integration?**
  Aside from OLI's own software, an interface program is provided to the end-user after the process simulators have programmed their side of the interface. We try to be simulator neutral and provide the same thermodynamic data back to each simulation product regardless of the manufacturer.

- **What are some of the unique characteristics of the OLI Alliance Engine integration with Aspen, Honeywell, Aveva, KBC and PSE software?**
  For Aspen Plus, ProII and gProms, the chemistry under consideration is generated outside of the host program. An interface file is then required to be accessed by the host program. For Aspen Hysys and Honeywell Unisim Design the OLI chemistry is created inside the host program without an external program. In fact, both Hysys and Unisim Design developed this interface without OLI's help. KBC Petro-Sim is slightly different in that the OLI chemistry is currently accessed by an external program as in Aspen Plus but the external program is called from within the host program. Once the OLI chemistry has been created, by whatever mechanism, the end-user is now in a comfortable space. Everything they already know about the host program is still true, there are no exceptions to OLI other than how our data is reported.

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