Challenges and opportunities using Statistical Mechanics modeling in the industrial world

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Mathematical and computer skills, an inquisitive mind, imagination, intuition and the ability to work independently are important traits developed and exercised in Physical Sciences (and Mathematics) studies. Physicist and mathematicians are trained to deal with various physical challenges that they will find in the professional world, even though they may not be conscious of this. Indeed, in most industries and many companies, there are activities firmly based in scientific knowledge, and, therefore, there is a need for physicists and mathematician with the right skills. However, it is also important to be prepared to deal with these problems in an environment very different than the academic where one it is usually trained.

After a general introduction I will use, as an illustration, the application of a Statistical Mechanical based equation of state (Statistical Associating Fluid Theory – SAFT) to problems found in the chemical and oil industries. The equation was developed in an academic institution (Cornell University), in an industrial-supported project (with ExxonMobile) and it is well suited as an example of the need for accurate models, and the physics behind it, in the industrial world. In fact, it is the adequate coarse grain level behind SAFT what has made it a successful modeling tool in both, academia and industry.

It is well known that most industrial processes require a detailed knowledge of the thermodynamic properties, including phase and interfacial behavior and transport properties of their working fluids. Although the preferred method for obtaining these data would be the experimental one, there are several difficulties associated to it, mainly due to the great amount of data required to have a reliable database for multicomponent mixtures over a wide range of thermodynamic conditions. Theoretical approaches can be used as an alternative in this case; however, the intrinsic non-ideal behavior of these mixtures and the limited range of available experimental data pose a challenge to any theoretical method aimed at quantitative predictions of thermodynamic properties for these complex fluids, especially when the process works near the critical region, or for multicomponent systems. Due to their classical formulation most equations of state are unable to accurately describe the density (and concentration) fluctuations appearing as the critical region is approached. This problem has been tackled in recent years with great success thanks to the combination of renormalization group theories, such as the phase cell-space approximation, with accurate theoretical based equations of state, including different versions of SAFT. An additional advantage of these methods is that, as they are built from Statistical Mechanics, they can systematically been extended to other regions of the phase diagram or for other properties, with the same degree of accuracy.

We will first provide an overview on how having the right physics with the adequate level of approximations can lead to an accurate modeling tool for engineering purposes. However, and in spite of its great success, there are still challenges for SAFT being used as a standard modeling method in industry. This applies to SAFT and several other thermodynamic models. Some of these challenges and the opportunities coming with them will also be addressed here.