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STRUCTURE-PROPERTY MODELLING IN THE OIL INDUSTRY

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The oil industry involves numerous scientific domains each applied to various operations such as extraction, refining, synthesis of chemicals... Numerical simulation tools are now widely used during these operations, and IFP Energies nouvelles (IFPEN) recently investigated the use of Quantitative Structure Property Relationship (QSPR) to predict properties of petrochemicals, materials... The purpose hereafter is to present some recent works perfomed at IFPEN with a focus on the QSPR modelling of mixtures: surfactants, alternative fuels, and adsorption of gases in nanoporous materials.

In its duration, the process of crude oil extraction can be composed of three stages, with the third being the enhanced oil recovery (EOR). The chemical EOR consists in the injection of alkaline/surfactant/polymer (ASP), and the formulation of ASP combinations is a challenging and time consuming task considering that each potentially eligible reservoir exhibits its own conditions. The optimal salinity is one of the key properties to consider during the selection of surfactants' formulation, and we proposed QSPR based models to assist the formulation [1-2].

Property predictions for alternative fuels can be used to assist the formulation of biofuels. We developed QSPR models to predict some fuels' specifications (physical properties such as cetane number, flash point, enthalpy of combustion, melting point, density and viscosity) for families of compounds similar to those found in biofuels: hydrocarbons and oxygenated compounds [3-4]. First, QSPR based models of pure compound properties were developed. Then, the case of mixtures has been examinated and two types of approaches were investigated: (i) the direct application of machine learning methods to mixture property data; (ii) the use of the previously developed pure compound property models in combination with theoretically based mixing rules.

The compatibility of materials with fuels' components is of major concern especially as the fuel composition varies within a year and with the consideration of oxygenated compounds in the pool of renewable molecules. Machine learning approaches have been used to model the sorption of neat compounds and up to quinary mixtures of some hydrocarbons, alcohols and ethers, in a semicrystalline poly(ethylene) [5]. QSPR based models were further tested for surrogate gasolines, and predictions were in excellent agreement with experimental sorption values.

In the adsorption field, promising porous materials have already been identified for carbone dioxide (CO_2) capture applications, among them Zeolitic Imidazolate Frameworks (ZIF). The design of new nanoporous materials could be highly accelerated using QSPR models [6]. However, the development of relevant descriptors for such materials remains a challenge.

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