Oxygen-containing contaminants and steam cracking: Understanding their impact using COILSIM1D

Abstract:

Depleting oil reserves and increasing environmental concerns have enhanced the interest in alternative and renewable feedstocks for the production of base chemicals. Consequently, significant efforts are being carried out aiming at the fundamental understanding and the development of micro kinetic models of the thermal degradation of oxygen containing renewable feeds and oxygen-containing contaminants, which can be of interest as feedstocks for olefin production via steam cracking. Unfortunately, these oxygen-containing species can affect the product distribution, and therefore accurately describing the thermal decomposition of these components is of high importance. Besides the yields of high valuable chemicals (small olefins), it is necessary to predict the yields of the small oxygen containing components, e.g. methanol and aldehydes, which affect the operation of the process: They can lead to problems in the upstream separation train, such as off-spec products, and are known to lead to gums formation.

This paper focusses on the (co)-cracking of renewable feeds or feeds with a considerable amount of oxygen-containing contaminants. COILSIM1D is a well-known tool for accurate yield prediction of industrial steam crackers. Recently, its microkinetic model has been extended to account for various common oxygen-containing compounds. The fundamental model of COILSIM1D explicitly accounts for the elementary steps and the corresponding kinetic and thermodynamic parameters are derived from high level ab-initio calculations. Therefore, the model has a broad validity range in terms of feeds and operating conditions. To illustrate this, a case study of steam cracking of oxygen containing species in a hydrocarbon mixture matrix will be presented. Particular attention will be paid to the small pyrolysis products which are important contaminants of the upstream separation section. The results of the COILSIM1D simulations are compared with experimental data for validation purposes.