



VABILO NA PREGLOV KOLOKVIJ / INVITATION TO THE PREGL COLLOQUIUM

Predavanje je tudi vključeno v program doktorskega študija Kemijske znanosti (FKKT, UL) /

This lecture is also a part of the doctoral study program Chemical Sciences (University of Ljubljana, Faculty of Chemistry and Chemical Technology)

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**Velika predavalnica Kemijskega inštituta / Lecture Hall at the
National Institute of Chemistry; Hajdrihova 19, Ljubljana**

Steam-cracking: an evergreen of the chemical process industry

Steam cracking can be described by considering a limited number of elementary reaction families not only for fossil but also for renewable feedstocks. Group contribution methods can be applied to calculate the corresponding kinetic parameters. The group contributions follow from a database obtained by high level *ab initio* calculations involving representative molecules and reactions. Based on this single-event microkinetic (SEMK) methodology a reasonable agreement with pilot and industrial data was obtained for ethane steam cracking.

SEMK requires the characterization of a feedstock in terms of types of molecules. Either fossil or renewable feedstocks typically consist of a considerable amount of types of molecules. So-called molecular reconstruction methods use macroscopic properties such as density and boiling point trajectory to obtain a characterization of the feedstock in the terms required. Of course they are based on a training set. The latter can be obtained by a GCxGC analysis of typical feeds.

Process optimization and innovation not only involves feed stocks and reactor technology but should also account for up-or downstream units like the Transfer Line Exchanger (TLE), the convection section and the interaction between the furnace and the reactor coils.

Vljudno vabljeni! / Kindly invited!

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