Supporting information

The Merit of Pressure Dependent Kinetic Modelling in Steam Cracking

Jeroen Aerssens¹, Florence Vermeire¹, Syam Ukkandanth Arravindikashan¹, Ruben

Van de Vijver¹, Kevin M. Van Geem^{1,*}

¹ Laboratory for Chemical Technology (LCT), Ghent University, Technologiepark 125, B-9052 Ghent, Belgium

* Corresponding author: <u>Kevin.VanGeem@UGent.be</u>, Technologiepark 125, B-9052 Gent, Belgium;

1. Experimental bench scale steam cracker setup



Figure 1: Schematic overview of the bench scale steam cracker.

2. Experimental results

The experimental data acquired for the steam cracking of ethane and propane on a bench scale steam cracker (tubular reactor) is provided as a separate Excel spreadsheet. Detailed temperature profiles are also available in this spreadsheet.

3. PCA using Quantis



Below one can find the data quality assessment that was performed in Quantis. Run reference numbers are referenced in the experimental data.

Figure 2: Data quality assessment of ethane steam cracking results: a) H balance of the experiments after carbon normalization b) PCA of carbon normalized yields of all GC injections.



Figure 3: Data quality assessment of propane steam cracking results: a) H balance of the experiments after carbon normalization balance b) PCA of carbon normalized yields of all GC injections.

4. Kinetic model

The kinetic model in CHEMKIN format developed for the pyrolysis of ethane and propane is provided as a separate text file. This model corresponds to the P dep. case. Other cases can be reconstructed by disabling the P dependent parameters (TROE or PLOG format, at the end of this file) and enabling the high pressure limit that is provided.