Modeling of EDC Thermal Cracking

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EDC (ethylene dichloride) thermal cracking reactions were modeled with radical reaction schemes. The modeling study was performed with respect to 100 reversible elementary reactions with 47 species – 26 molecules and 21 radicals. We developed a general modeling framework for a gas phase reaction using gPROMS with MS Excel interface. Kinetic schemes such as radical reactions, thermal decomposition of molecules, radical chain reactions, and pure molecular reactions were included. Some of activation energies were estimated by PW91/DNP and compared with the values from other sources. In this study, we could reconfirm that the addition of CCl4 promotes the generation of Cl radical, an important key player in the progression of the reactions as reported in various articles. Well known coke precursors such as chloroprene and acetylene are produced as major by-products. Modeling results were compared with the industrial data. The reaction model can be used to predict cracking yield and by-product formation. Developed modeling framework can be easily modified for other reaction modeling applications and reactor designs.