Direct Non-Oxidative Methane Conversion by Dielectric Barrier Discharge – a Modeling Study

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***Abstract*—Methane's relative abundance and clean burning process makes it a very attractive fuel. However, its potential for the production of H2, ethylene or liquid hydrocarbon fuels has not been fully utilized, since the C-H bond of methane is thermodynamically stable and its dissociation requires 4.5 eV energy input. Thus, thermal-catalytic dry reforming is very energy consuming, and have side products of COx which will result in catalyst coking. Therefore, the direct conversion of methane by non-thermal plasma is an alternative approach, and draws more and more interest. While this reaction has been previously studied by plasma methods, it has rarely been looked at simultaneously by experimental and modeling techniques.**

In this work, we use a combined experimental and simulation method to study direct plasma conversion of methane. A microkinetic modeling for methane conversion by DBD plasma is developed, solving 352 elementary reactions, involving 36 species including neutrals, ions and radicals. Among them, the rate constants of those electron impact reactions are obtained from solving Boltzmann equation. Our DBD plasma model takes consideration of both spatial and temporal dependencies of the filamentary behavior of this non-thermal plasma. The plasma model parameters are based on filament features from experimental measurement without approximation. The simulations show that as the volume is increased, the conversion is dominated by the plasma power, rather than the volume or power density. And increasing flow rate will result in decrease of conversion. These trends have been validated with our in house experimental measurement. The modeling results also show that the product distribution and selectivity is a function of the extent of conversion, regardless of other operating conditions.