**BENZENE HYDROGENATION**

Hydrogenation of benzene is an industrially relevant process. It lowers the aromatic content in fuels to meet international requirements for air pollution, and increases the cetane number which results in higher quality diesel fuels.

**AIM**

Propose a methodology to construct Single-Event Microkinetic (SEMK) simplified models to describe metal catalyzed reactions via global rate expressions.

Hydrogenation of benzene is considered to test the ideas proposed in this work.

**JUSTIFICATION**

When modeling metal catalysis process the total amount of different reaction paths and elementary steps is considerably high. Thus, a methodology that accomplishes to lump reactions for the entire catalytic cycle looks like a worth effort matter of research.

**SEMK MODEL FOR BENZENE HYDROGENATION**

The single-event rate coefficient for hydrogenation of benzene (Bera, T., et al, 2011)

\[ k = n_e \cdot \tilde{k}_{(m,n)} \]

Saturation degree of the reactant carbon

\[ n=2 \]

\[ m=0,1 \text{ or } 2 \]

Number of unsaturated nearest carbons to the reactant carbon

**ONLY 3 REACTION FAMILIES**

\[ r_L^g \rightarrow L_h = L C \cdot k_{L} \cdot C_{L} \]

\[ L C_{L_g} \rightarrow L_h = \frac{N \cdot K_{ref}}{K_{L_s}} \]

**“REDUCTION OF REACTIONS PATHS”**

Traditional ReLumping in acid catalysis


\[ T(e_g-\eta_b) = \sum_{L} (L C) \cdot k_{L} \cdot C_{L} \]

However, for metal catalysis:

- Complex reaction networks instead of complex pool of compounds
- Several non quasi equilibrated steps

**Proposal for Metal Catalysis**

\[ R_{CIH} = f(k_{(0,2)} \cdot L C_{0,2}, k_{(1,2)} \cdot L C_{1,2}, L C_{2}) \]

The product formation might be represented as the linear combination of reaction families. Concept under revision.

**SURFACE CONCENTRATIONS**

The formation rate \( R_j \) for the 13 intermediate surface concentrations \( \mathbf{j} \):

\[ R_j = \sum_{j} \left[ (n_{j_1} \cdot \tilde{k}_{\text{hyd}(\eta_{j_2})} C_{j_1} - n_{j_1} \cdot \tilde{k}_{\text{des}(\eta_{j_2})} C_{j_2}) \right] \]

\[ - \sum_{j} \left[ (n_{j_1} \cdot \tilde{k}_{\text{hyd}(\eta_{j_2})} C_{j_1} - n_{j_1} \cdot \tilde{k}_{\text{des}(\eta_{j_2})} C_{j_2}) \right] \]

E.g. 1,2,4-Trihydro-Benzene when assuming PSSA

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