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# Comparison and Reduction of the Chemical Kinetic Mechanisms Proposed for Thermal Partial Oxidation of Methane (TPOX) in Porous Media

Friday, 4 June 2021 09:40 (1 hour)

The effectiveness and reducibility of the methane combustion kinetic mechanisms were examined for the TPOX process in a porous medium. To this end, TPOX was successfully simulated using ANSYS CHEMKIN-Pro through a reactor network model composed of perfectly stirred and honeycomb-monolith reactors. The efficacy of six chemical kinetic mechanisms was compared for the equivalence ratios (ERs) ranging from 2.4 to 2.6 with a constant thermal load of 1540 kW/m2. This comparison revealed that Konnov was the most successful mechanism in the prediction of the H2 and CO mole fractions. This mechanism along with the GRI-3.0 and USC-Mech 2.0 mechanisms were then reduced by the direct relation graph with error propagation (DRGEPSA) followed by the full species sensitivity analysis (FSSA). This approach reduced the number of species from 119 to 29 for the Konnov mechanism, from 53 to 23 for the GRI 3.0 mechanism, and from 111 to 34 for the USC-Mech 2.0 mechanism.

## **Time Block Preference**

Time Block A (09:00-12:00 CET)

## References

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#### Session Classification: Poster +

Track Classification: (MS1) Porous Media for a Green World: Energy & Climate