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A reduced and optimized kinetic mechanism for coke oven gas as a clean alternative vehicle fuel

Key words: Coke oven gas (COG); Kinetic mechanism; Sensitivity analysis; Particle swarm optimization (PSO); Spark-ignition (SI) engine; Computational fluid dynamics (CFD) simulation

Method

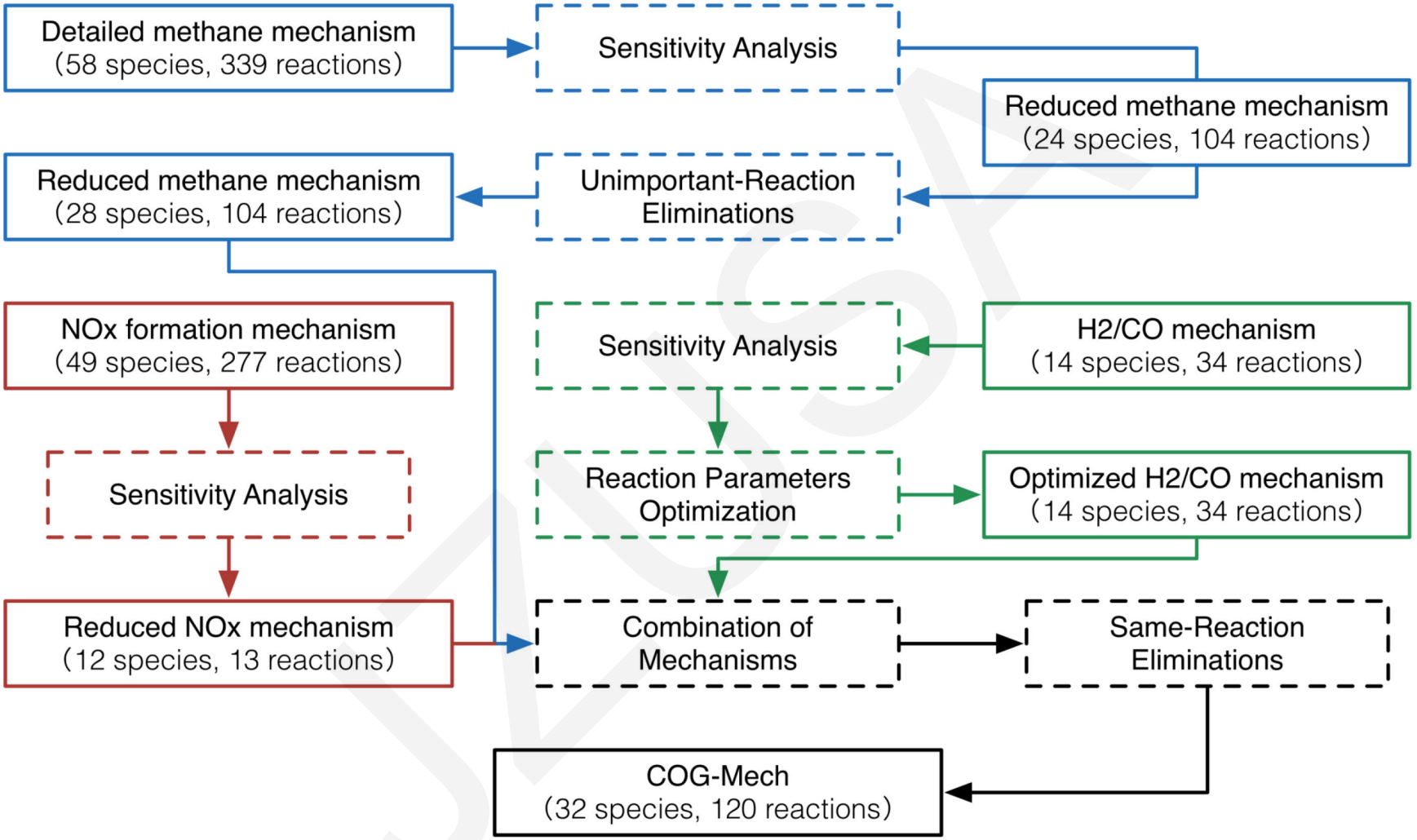


Figure 1. Construction Process of COG Mechanism

Method

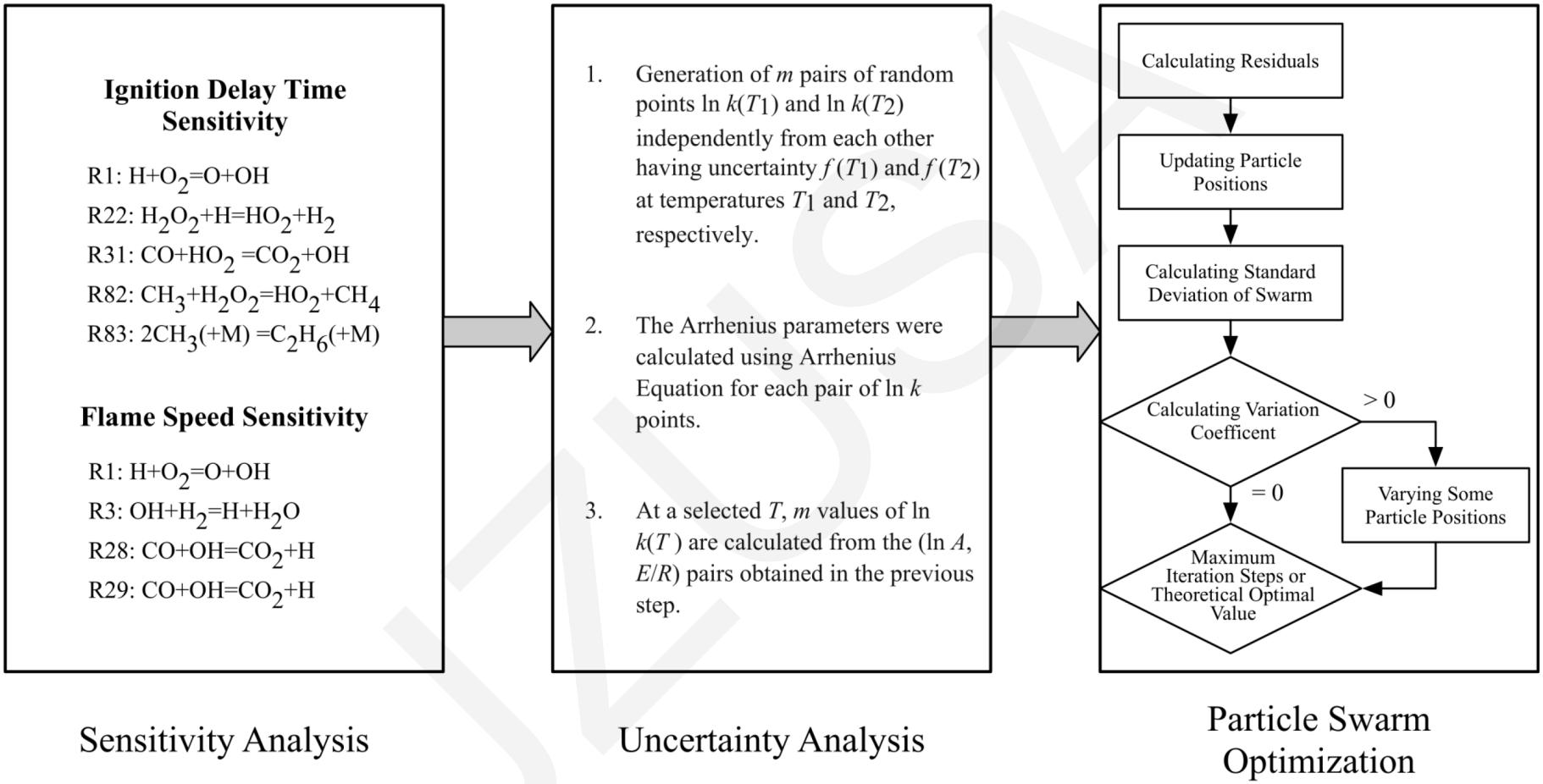


Figure 2. Optimization Process of COG Mechanism

Results and Conclusions

- Based on a detailed methane mechanism, an H_2/CO combustion model, and a NO_x formation mechanism, a COG Mechanism including 33 species and 120 reactions was constructed.
- Based on sensitivity analysis, uncertainty analysis and particle swarm optimization, the COG Mechanism was optimized.
- Based on the models established with CHEMKIN code, the fundamental combustion characteristics simulated with COG Mechanism were investigated. The results from shock-tube experiments were used to validate the ignition delay times, and COG Mechanism showed a significantly higher accuracy. The premixed flame data measured with different methods were used for the validation of laminar flame speeds, and COG Mechanism showed good agreement with the experimental data, while some small differences existed.
- Based on the engine test bench, the in-cylinder pressure and NO_x emission measured by combustion analyzer and FTIR spectrometer were used to validate the applicability of kinetic mechanism in engine simulations, and a 3D in-cylinder model coupled with COG Mechanism was established with the open source software KIVA-CHEMKIN. The simulated in-cylinder pressure and NO_x emission showed good agreement with the experimental data.