Mechanism, kinetics, and environmental assessment of CTDE during OH-oxidation in the presence of NO and O2

Yu-Qi Yang¹, Wei Zhang¹, Ming-Shuai Deng¹, xiumei pan², Feng-Yang Bai¹, and Lei tan³

¹Shenyang Normal University
²Northeast Normal University
³SAIC Motor Corp Ltd

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Abstract

The transformation mechanism and kinetics of 2-chloro-1,1,2-trifluoroethyl-difluoromethyl-ether (CTDE, CHF₂OCF₂CHFCI) triggered by OH radicals were researched by DFT methods and canonical variational transition state theory. The computational rate constant including small-curvature tunneling correction was in commendable agreement with the experimental data. Two hydrogen abstraction channels to form the alkyl radicals of C·F₂OCF₂CHFCI and CHF₂OCF₂·FCl were observed, and the formation of CHF₂OCF₂·FCl was more favorable than C·F₂OCF₂CHFCI in kinetics and thermodynamics. Subsequent evolution of CHF₂OCF₂·FCl in the presence of NO and O₂ indicated that the organic nitrate (CHF₂OCF₂CONO₂FCl) was the stable product. The dechlorinate of alkoxo radical (CHF₂OCF₂C(O·)FCl) was the most favorable degradation channel and the estimated ozone depletion potential for CTDE relative to CFC-11 was 0.0204, which could lead to a consequence of ozone depletion. Computed atmospheric lifetime for CTDE was 3.69 years by considering the combined contributions from OH radicals and Cl atoms. The total radiative forcing and global warming potential of CTDE were respectively 0.547 W m⁻² ppbv and 628.58 (100 years) at 298 K, suggesting that the contribution of CTDE to the greenhouse effect is moderate.

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