Ab initio calculations and kinetic modeling of thermal conversion of methyl chloride: implications for gasification of biomass - DTU Orbit (14/12/2018)

Ab initio calculations and kinetic modeling of thermal conversion of methyl chloride: implications for gasification of biomass

Limitations in current hot gas cleaning methods for chlorine species from biomass gasification may be a challenge for end use such as gas turbines, engines, and fuel cells, all requiring very low levels of chlorine. During devolatilization of biomass, chlorine is released partly as methyl chloride. In the present work, the thermal conversion of CH₃Cl under gasification conditions was investigated. A detailed chemical kinetic model for pyrolysis and oxidation of methyl chloride was developed and validated against selected experimental data from the literature. Key reactions of CH₂Cl with O₂ and C₂H₄ for which data are scarce were studied by ab initio methods. The model was used to analyze the fate of methyl chloride in gasification processes. The results indicate that CH₃Cl emissions will be negligible for most gasification technologies, but could be a concern for fluidized bed gasifiers, in particular in low-temperature gasification. The present work illustrates how ab initio theory and chemical kinetic modeling can help to resolve emission issues for thermal processes in industrial scale.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Technical University of Denmark, Polytechnic University of Milan, University of North Texas
Pages: 10741-10752
Publication date: 2018
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 20
Issue number: 16
ISSN (Print): 1463-9076
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.04 SJR 1.686 SNIP 1.089
Web of Science (2017): Impact factor 3.906
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.113
Web of Science (2016): Impact factor 4.123
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.45 SJR 1.725 SNIP 1.205
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.29 SJR 1.771 SNIP 1.239
Web of Science (2014): Impact factor 4.493
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.05 SJR 1.72 SNIP 1.207
Web of Science (2013): Impact factor 4.198
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.67 SJR 1.921 SNIP 1.177
Web of Science (2012): Impact factor 3.829
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2