Reactive kinetics of carbon dioxide loaded aqueous blend of 2-amino-2-ethyl-1,3-propanediol and piperazine using a pressure drop method

In this study, a new pressure drop method has been used to investigate the kinetics of carbon dioxide reaction with aqueous blend of 2-amino-2-ethyl-1,3-propanediol (AEPD) with piperazine (PZ). The blending of a small amount of PZ with AEPD has a significant effect on the observed rate constant, \( k_{\text{obs}} \). It was observed that \( k_{\text{obs}} \) values of the blend increased more than twice than the summation of \( k_{\text{obs}} \) values of individual alkanolamines. The reaction kinetics in this study were modeled by assuming a termolecular mechanism. The addition of 0.1 mol/L of PZ to 1 mol/L AEPD exhibited an observed rate constant, \( k_{\text{obs}} \) of 8824.1 s\(^{-1}\), which is comparable to other alkanolamine mixtures. Hence, PZ/AEPD mixtures can be potentially used for rapid carbon dioxide capture.
Experimental and Kinetic Modeling Study of C2H2 Oxidation at High Pressure

A detailed chemical kinetic model for oxidation of acetylene at intermediate temperatures and high pressure has been developed and evaluated experimentally. The rate coefficients for the reactions of C2H2 with HO2 and O2 were investigated, based on the recent analysis of the potential energy diagram for C2H3 + O2 by Goldsmith et al. and on new ab initio calculations, respectively. The C2H2 + HO2 reaction involves nine pressure- and temperature-dependent product channels, with formation of triplet CHCHO being dominant under most conditions. The barrier to reaction for C2H2 + O2 was found to be more than 50 kcal mol\(^{-1}\) and predictions of the initiation temperature were not sensitive to this reaction. Experiments were conducted with C2H2/O2 mixtures highly diluted in N2 in a high-pressure flow reactor at 600–900 K and 60 bar, varying the reaction stoichiometry from very lean to fuel-rich conditions. Model predictions were generally in satisfactory agreement with the experimental data. Under the investigated conditions, the oxidation pathways for C2H2 are more complex than those prevailing at higher temperatures and lower pressures. Acetylene is mostly consumed by recombination with H to form vinyl (reducing conditions) or with OH to form a CHCHOH adduct (stoichiometric to lean conditions). Both C2H3 and CHCHOH then react primarily with O2. The CHCHOH + O2 reaction leads to formation of significant amounts of glyoxal (OCHCHO) and formic acid (HOCHO), and the oxidation chemistry of these intermediates is important for the overall reaction.

General information
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Technical University of Denmark, University of North Texas, Brown University
Pages: 724-738
Publication date: 2016
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 48
Issue number: 11
ISSN (Print): 0538-8066
Ratings:
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.47 SJR 0.392 SNIP 0.827
Web of Science (2016): Impact factor 1.386
Web of Science (2016): Indexed yes
Original language: English
DOIs:
10.1002/kin.21028
Source: FindIt
Source-ID: 2342425014
Research output: Contribution to journal › Journal article – Annual report year: 2016 › Research › peer-review

Formation of NO from N2/O2 mixtures in a flow reactor: Toward an accurate prediction of thermal NO

We have conducted flow reactor experiments for NO formation from N2/O2 mixtures at high temperatures and atmospheric pressure, controlling accurately temperature and reaction time. Under these conditions, atomic oxygen...
equilibrates rapidly with $O_2$. The experimental results were interpreted by a detailed chemical model to determine the rate constant for the reaction $N_2 + O \rightarrow NO + N$ (R1). We obtain $k_1 = 1.4 \times 10^{14} \exp(-38,300/T)$ cm$^3$ mol$^{-1}$ s$^{-1}$ at 1700-1800 K, with an error limit of ±30%. This value is 25% below the recommendation of Baulch et al. for $k_1$, while it corresponds to a value $k_{1b}$ of the reverse reaction 25% above the Baulch et al. evaluation. Combination of our results with literature values leads to a recommended rate constant for $k_{1b}$ of $9.4 \times 10^{12} T^{0.14}$ cm$^3$ mol$^{-1}$ s$^{-1}$ over 250-3000 K. This value, which reconciles the differences between the forward and reverse rate constant, is recommended for use in kinetic modeling.

**General information**
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, University of Zaragoza
Contributors: Abian, M., Alzueta, M. U., Glarborg, P.
Number of pages: 15
Pages: 518-532
Publication date: 2015
Peer-reviewed: Yes

**Publication information**
Journal: International Journal of Chemical Kinetics
Volume: 47
Issue number: 8
ISSN (Print): 0538-8066
Ratings:
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.01 SJR 1.007 SNIP 1.007
Web of Science (2015): Impact factor 1.736
Web of Science (2015): Indexed yes
Original language: English
Electronic versions:
Formation_of_NO_from_N2_O2_mixtures_in_a_flow_reactor_postprint.pdf. Embargo ended: 06/06/2016
DOIs:
10.1002/kin.20929
Source: FindIt
Source-ID: 275272785
Research output: Contribution to journal > Journal article – Annual report year: 2015 > Research > peer-review

**Experimental and Kinetic Modeling Study of Methanol Ignition and Oxidation at High Pressure**
A detailed chemical kinetic model for oxidation of CH$_3$OH at high pressure and intermediate temperatures has been developed and validated experimentally. Ab initio calculations and Rice–Ramsperger–Kassel–Marcus/transition state theory (RRKM/TST) analysis were used to obtain rate coefficients for CH$_2$OH $\rightarrow$ CH$_2$O+H, CH$_3$O$\rightarrow$ CH$_2$O+H, CH$_3$O$\rightarrow$ CH$_2$OH, and CH$_3$O+O$_2$ $\rightarrow$ CH$_2$O+HO$_2$. The experiments, involving CH$_3$OH/O$_2$ mixtures diluted in N$_2$, were carried out in a high-pressure flow reactor at 600–900 K and 20–100 bar, varying the reaction stoichiometry from very lean to fuel-rich conditions. Under the conditions studied, the onset temperature for methanol oxidation was not dependent on the stoichiometry, whereas increasing pressure shifted the ignition temperature toward lower values. Model predictions of the present experimental results, as well as rapid compression machine data from the literature, were generally satisfactory. The governing reaction pathways have been outlined based on calculations with the kinetic model. Unlike what has been observed for unsaturated hydrocarbons, the oxidation pathways for CH$_3$OH under the investigated conditions were very similar to those prevailing at higher temperatures and lower pressures. At the high pressures, the modeling predictions for onset of reaction were particularly sensitive to the CH$_3$OH + HO$_2$ $\rightarrow$ CH$_2$OH +H$_2$O$_2$ reaction.

**General information**
Publication status: Published
Organisations: Department of Management Engineering, UNEP Risø Centre, Department of Chemical and Biochemical Engineering, CHEC Research Centre, University of Zaragoza, DNV GL USA, University of North Texas
Contributors: Aranda, V., Christensen, J. M., Alzueta, M., Glarborg, P., Gersen, S., Gao, Y., Marshall, P.
Pages: 283-294
Publication date: 2013
Peer-reviewed: Yes

**Publication information**
Journal: International Journal of Chemical Kinetics
Volume: 45
Issue number: 5
ISSN (Print): 0538-8066
Oxidation of Reduced Sulfur Species: Carbonyl Sulfide
A detailed chemical kinetic model for oxidation of carbonyl sulfide (OCS) has been developed, based on a critical evaluation of data from the literature. The mechanism has been validated against experimental results from batch reactors, flow reactors, and shock tubes. The model predicts satisfactorily oxidation of OCS over a wide range of stoichiometric air–fuel ratios (0.5 ≤λ≤7.3), temperatures (450–1700 K), and pressures (0.02–3.0 atm) under dry conditions. The governing reaction mechanisms are outlined based on calculations with the kinetic model. The oxidation rate of OCS is controlled by the competition between chain-branching and -propagating steps; modeling predictions are particularly sensitive to the branching fraction for the OCS + O reaction to form CO + SO or CO2 + S.

General information
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Contributors: Glarborg, P., Marshall, P.
Pages: 429-439
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 45
Issue number: 7
ISSN (Print): 0538-8066
Ratings:
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.47 SJR 0.619 SNIP 0.927
Web of Science (2013): Impact factor 1.566
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Original language: English
Electronic versions:
manus.pdf
DOIs:
10.1002/kin.20764
Source: dtu
Source-ID: n::oai:DTIC-ART:wiley/384660077::27754
Research output: Contribution to journal › Journal article – Annual report year: 2013 › Research › peer-review

Reduced chemical kinetic mechanisms for NOx emission prediction in biomass combustion
Because of the complex composition of biomass, the chemical mechanism contains many different species and therefore a large number of reactions. Although biomass gas-phase combustion is fairly well researched and understood, the proposed mechanisms are still complex and need very long computational time and powerful hardware resources. A reduction of the mechanism for biomass volatile oxidation has therefore been performed to avoid these difficulties. The selected detailed mechanism in this study contains 81 species and 703 elementary reactions. Necessity analysis is used to determine which species and reactions are of less importance for the predictability of the final result and, hence, can be discarded. For validation, numerical results using the derived reduced mechanism are compared with the results obtained with the original detailed mechanism. The reduced mechanism contains much fewer reactions and chemical species, that is, 35 species and 198 reactions, corresponding to 72% reduction in the number of reactions and, therefore, improving the computational time considerably. Yet, the model based on the reduced mechanism predicts correctly concentrations of NOx and CO that are essentially identical to those of the complete mechanism in the range of reaction conditions of interest, especially for the medium-temperature range. The reduced mechanism failed to predict the concentrations in the
high- and low-temperature range. Therefore, two more reduced mechanisms are also proposed for the high- and low-temperature range with 26 and 52 species, respectively. The modeling conditions are selected in a way to mimic values in the range of temperature 700–1400°C, excess air ratio 0.8–3.3, and four different residence times: 1, 0.1, 0.01, and 0.001 s, since these variables are the main affecting parameters on NOx emission. © 2012 Wiley Periodicals, Inc. Int J Chem Kinet 44: 219–231, 2012

**General information**
Publication status: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Norwegian University of Science and Technology, SINTEF
Contributors: Houshfar, E., Skreiberg, Ø., Glarborg, P., Løvås, T.
Pages: 219-231
Publication date: 2012
Peer-reviewed: Yes

**Publication information**
Journal: International Journal of Chemical Kinetics
Volume: 44
Issue number: 4
ISSN (Print): 0538-8066
Ratings:
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.08 SJR 0.378 SNIP 0.734
Web of Science (2012): Impact factor 1.187
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Original language: English
DOIs: 10.1002/kin.20716
Source: orbit
Source-ID: 319011
Research output: Contribution to journal › Journal article – Annual report year: 2012 › Research › peer-review

**Experimental Measurements and Kinetic Modeling of CH4/O2 and CH4/C2H6/O2 Conversion at High Pressure**

**General information**
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, Experimental Surface and Nanomaterials Physics, Department of Physics, CHEC Research Centre
Contributors: Rasmussen, C. L., Jakobsen, J. G., Glarborg, P.
Pages: 778-807
Publication date: 2008
Peer-reviewed: Yes

**Publication information**
Journal: International Journal of Chemical Kinetics
Volume: 40
Issue number: 12
ISSN (Print): 0538-8066
Ratings:
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.446 SNIP 0.961
Web of Science (2008): Indexed yes
Original language: English
DOIs: 10.1002/kin.20352
Source: orbit
Source-ID: 233484
Research output: Contribution to journal › Journal article – Annual report year: 2008 › Research › peer-review

**Experimental Measurements and Kinetic Modeling of CO/H2/O2/NOx Conversion at High Pressure**

**General information**
Methanol oxidation in a flow reactor: Implications for the branching ratio of the CH3OH+OH reaction
The oxidation of methanol in a flow reactor has been studied experimentally under diluted, fuel-lean conditions at 650-1350 K, over a wide range of O2 concentrations (1%-16%), and with and without the presence of nitric oxide. The reaction is initiated above 900 K, with the oxidation rate decreasing slightly with the increasing O2 concentration. Addition of NO results in a mutually promoted oxidation of CH3OH and NO in the 750-1100 K range. The experimental results are interpreted in terms of a revised chemical kinetic model. Owing to the high sensitivity of the mutual sensitization of CH3OH and NO oxidation to the partitioning of CH3O and CH2OH, the CH3OH + OH branching fraction could be estimated as alpha = 0.10 +/- 0.05 at 990 K. Combined with low-temperature measurements, this value implies a branching fraction that is largely independent of temperature. It is in good agreement with recent theoretical estimates, but considerably lower than values employed in previous modeling studies. Modeling predictions with the present chemical kinetic model is in quantitative agreement with experimental results below 1100 K, but at higher temperatures and high O2 concentration the model underpredicts the oxidation rate.

Experimental and Kinetic Modeling Study of the Effect of NO and SO2 on the Oxidation of CO-H2 Mixtures
The oxidation of methanol in a flow reactor has been studied experimentally under diluted, fuel-lean conditions at 650-1350 K, over a wide range of O2 concentrations (1%-16%), and with and without the presence of nitric oxide. The reaction is initiated above 900 K, with the oxidation rate decreasing slightly with the increasing O2 concentration. Addition of NO results in a mutually promoted oxidation of CH3OH and NO in the 750-1100 K range. The experimental results are interpreted in terms of a revised chemical kinetic model. Owing to the high sensitivity of the mutual sensitization of CH3OH and NO oxidation to the partitioning of CH3O and CH2OH, the CH3OH + OH branching fraction could be estimated as alpha = 0.10 +/- 0.05 at 990 K. Combined with low-temperature measurements, this value implies a branching fraction that is largely independent of temperature. It is in good agreement with recent theoretical estimates, but considerably lower than values employed in previous modeling studies. Modeling predictions with the present chemical kinetic model is in quantitative agreement with experimental results below 1100 K, but at higher temperatures and high O2 concentration the model underpredicts the oxidation rate.
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Contributors: Dagaut, P., Lecomte, F., Mieritz, J., Glarborg, P.
Pages: 564-575
Publication date: 2003
Peer-reviewed: Yes

**Publication information**
Journal: International Journal of Chemical Kinetics
Volume: 35
Issue number: 11
ISSN (Print): 0538-8066
Ratings:
Scopus rating (2003): SJR 0.711 SNIP 0.936
Web of Science (2003): Indexed yes
Original language: English
Source: orbit
Source-ID: 41134
Research output: Contribution to journal › Journal article – Annual report year: 2003 › Research › peer-review

**Rate constants and activation energies for ozonolysis of isoprene methacrolein and methyl-vinyl-ketone in aqueous solution: Significance to the in-cloud ozonation of isoprene**

**General information**
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Pedersen, T., Sehested, K.
Pages: 182-190
Publication date: 2001
Peer-reviewed: Yes

**Publication information**
Journal: International Journal of Chemical Kinetics
Volume: 33
ISSN (Print): 0538-8066
Ratings:
Scopus rating (2001): SJR 0.61 SNIP 1.166
Web of Science (2001): Indexed yes
Original language: English
Source: orbit
Source-ID: 302269
Research output: Contribution to journal › Journal article – Annual report year: 2001 › Research › peer-review

**Experimental and Kinetic Modeling Study of the Oxidation of Benzene**

**General information**
Publication status: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Contributors: Alzueta, M., Glarborg, P., Dam-Johansen, K.
Pages: 498-522
Publication date: 2000
Peer-reviewed: Yes

**Publication information**
Journal: International Journal of Chemical Kinetics
Volume: 32
Issue number: 8
ISSN (Print): 0538-8066
Ratings:
Scopus rating (2000): SJR 0.796 SNIP 0.931
Web of Science (2000): Indexed yes
Original language: English
DOIs:
Modeling the Thermal De-NOx Process: Closing in on a Final Solution

General information
Publication status: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Contributors: Miller, J. A., Glarborg, P.
Pages: 757-765
Publication date: 1999
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 31
Issue number: 11
ISSN (Print): 0538-8066
Ratings:
Scopus rating (1999): SJR 0.519 SNIP 0.798
Original language: English

Bibliographical note
CHEC paper 9922

Nitromethane Dissociation: Implications for the CH₃+NO₂ Reaction

General information
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering
Contributors: Glarborg, P., Bendtsen, A. B., Miller, J. A.
Pages: 591-602
Publication date: 1999
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 31
Issue number: 9
ISSN (Print): 0538-8066
Ratings:
Scopus rating (1999): SJR 0.519 SNIP 0.798
Original language: English

Bibliographical note
CHEC paper 9917

Absolute rate constants for F⁺CH₃CHO and CH₃CO⁺O₂⁻, relative rate study of CH₃CO⁺No, and the product distribution of the F⁺CH₃CHO reaction

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Sehested, J., Christensen, L., Nielsen, O., Wallington, T.
Pages: 913-921
Publication date: 1998
Peer-reviewed: Yes
Atmospheric chemistry of acetone: Kinetic study of the CH₃C(O)CH₂O₂⁻NO/NO₂ reactions and decomposition of CH₃C(O)CH₂O₂NO₂

Oxidation of manganese(II) by ozone and reduction of manganese(III) by hydrogen peroxide in acidic solution

Parabenzoquinone Pyrolysis and Oxidation in a Flow Reactor
Reactions of the ferryl ion with some compounds found in cloud water

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Jacobsen, F., Holcman, J., Sehested, K.
Pages: 215-221
Publication date: 1998
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 30
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 298863
Research output: Contribution to journal » Journal article – Annual report year: 1998 » Research » peer-review

The CH3+NO Rate Coefficient at High Temperatures: Theoretical Analysis and Comparison with Experiment.

General information
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, Sandia National Laboratories
Contributors: Miller, J., Melius, C., Glarborg, P.
Pages: 223-228
Publication date: 1998
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 30
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 170327
Research output: Contribution to journal » Journal article – Annual report year: 1998 » Research » peer-review

Absolute rate constants for the self reactions of HO2, CF3CFHO2, and CF3O2 radicals and the cross reactions of HO2 with FO2, HO2 with CF3CFHO2, and HO2 with CF3O2 at 295 K

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Sehested, J., Møgelberg, T., Fagerström, K., Mahmoud, G., Wallington, T.
Pages: 673-682
Publication date: 1997
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 29
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 296837
Research output: Contribution to journal » Journal article – Annual report year: 1997 » Research » peer-review
Activation parameters of ferryl ion reactions in aqueous acid solutions

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Jacobsen, F., Holcman, J., Sehested, K.
Pages: 17-24
Publication date: 1997
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 29
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 297356
Research output: Contribution to journal › Journal article – Annual report year: 1997 › Research › peer-review

Atmospheric chemistry of HFC-134a: Kinetics of the decomposition of the alkoxy radical CF₃CFHO

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Møgelberg, T., Sehested, J., Wallington, T., Nielsen, O.
Pages: 209-217
Publication date: 1997
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 29
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 297248
Research output: Contribution to journal › Journal article – Annual report year: 1997 › Research › peer-review

Oxidation of dimethyl ether: Absolute rate constants for the self reaction of CH₃OCH₂ radicals, the reaction of CH₃OCH₂ radicals with O₂, and the thermal decomposition of CH₃OCH₂ radicals

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Sehested, J., Sehested, K., Platz, J., Egsgaard, H., Nielsen, O.
Pages: 627-636
Publication date: 1997
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 29
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 296874
Research output: Contribution to journal › Journal article – Annual report year: 1997 › Research › peer-review

The temperature dependence of the exchange reaction between oxygen atoms and dioxygen molecules studied by means of isotopes and spectroscopy

General information
Atmospheric chemistry of Di-tert-Butyl ether: Rates and products of the reactions with chlorine atoms, hydroxyl radicals, and nitrate radicals

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
 Contributors: Langer, S., Ljungström, E., Wängberg, I., Wallington, T., Hurley, M., Nielsen, O.
Pages: 299-306
Publication date: 1996
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 28
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 294350
Research output: Contribution to journal › Journal article – Annual report year: 1996 › Research › peer-review

Impact of SO2 and NO on CO Oxidation under Post-Flame Conditions
An experimental and theoretical study of the effect of SO2 on moist CO oxidation with and without NO present was carried out under plug-flow conditions. The H/S/O thermochemistry and reaction subset was revised and a chemical kinetic model established that provide a good description of the effect of SO2 and NO on CO oxidation as well as the SO2/SO3 ratio in the products.

General information
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, New Jersey Institute of Technology
Contributors: Glarborg, P., Kubel, D., Dam-Johansen, K., Chiang, H., Bozzelli, J. W.
Pages: 773-790
Publication date: 1996
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 28
Issue number: 10
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 167907
Research output: Contribution to journal › Journal article – Annual report year: 1996 › Research › peer-review

Kinetics and mechanism of the reaction of CF3 radicals with NO2
Atmospheric chemistry of FC(O)x radicals: Kinetic and mechanistic study of the FC(O)O2 + NO2 reaction

The reaction of ammonia with nitrogen dioxide in a flow reactor: Implications for the NH2 + NO2 reaction

The NH3/NO2 system has been investigated experimentally in an isothermal flow reactor in the temperature range 850-1350 K. The Experimental data were interpreted in terms of a detailed reaction mechanism. The flow reactor results, supported by a theoretical analysis of the NH2-NO2 complex, suggest that the NH2 + NO2 reaction has two major product channels, both proceeding without activation barriers:

R20: \( \text{NH}_2 \rightleftharpoons \text{N}_2\text{O} + \text{H}_2\text{O} \)

R21: \( \text{H}_2\text{NO} + \text{NO} \)

Our findings indicate that the \( \text{N}_2\text{O} + \text{H}_2\text{O} \) channel is dominant at low temperatures while \( \text{H}_2\text{NO} + \text{NO} \) dominates at high temperatures. The rate constant for reaction (R21) is estimated to be \( 3.5 \times 10^{12} \text{ cm}^3/\text{mol-s} \) in the temperature range studied with an uncertainty of a factor of 3.

The reaction of ammonia with nitrogen dioxide in a flow reactor: Implications for the NH2 + NO2 reaction

The NH3/NO2 system has been investigated experimentally in an isothermal flow reactor in the temperature range 850-1350 K. The Experimental data were interpreted in terms of a detailed reaction mechanism. The flow reactor results, supported by a theoretical analysis of the NH2-NO2 complex, suggest that the NH2 + NO2 reaction has two major product channels, both proceeding without activation barriers:

R20: \( \text{NH}_2 \rightleftharpoons \text{N}_2\text{O} + \text{H}_2\text{O} \)

R21: \( \text{H}_2\text{NO} + \text{NO} \)

Our findings indicate that the \( \text{N}_2\text{O} + \text{H}_2\text{O} \) channel is dominant at low temperatures while \( \text{H}_2\text{NO} + \text{NO} \) dominates at high temperatures. The rate constant for reaction (R21) is estimated to be \( 3.5 \times 10^{12} \text{ cm}^3/\text{mol-s} \) in the temperature range studied with an uncertainty of a factor of 3.
**A spectrokinetic study of CH₂I and CH₂IO₂ radicals**

**General information**
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Sehested, J., Ellermann, T., Nielsen, O.
Pages: 259-272
Publication date: 1994
Peer-reviewed: Yes

**Publication information**
Journal: International Journal of Chemical Kinetics
Volume: 26
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 292698
Research output: Contribution to journal › Journal article – Annual report year: 1994 › Research › peer-review

**Modeling the thermal DENOx process in flow reactors. Surface effects and Nitrous Oxide formation**
We have investigated the impact of surface reactions such as NH₃ decomposition and radical adsorption on quartz flow reactor data for Thermal DeNOₓ using a model that accounts for surface chemistry as well as molecular transport. Our calculations support experimental observations that surface effects are not important for experiments carried out in low surface to volume quartz reactors. The reaction mechanism for Thermal DeNOₓ has been revised in order to reflect recent experimental results. Among the important changes are a smaller chain branching ratio for the NH₂ + NO reaction and a shorter NNH lifetime than previously used in modeling. The revised mechanism has been tested against a range of experimental flow reactor data for Thermal DeNOₓ with reasonable results. The formation of N₂O in Thermal DeNOₓ has been modelled and calculations show good agreement with experimental data. The important reactions in formation and destruction of N₂O have been identified. Our calculations indicate that N₂O is formed primarily from the reaction between NH and NO, although the NH₂ + NO₂ reaction possibly contributes at lower temperatures. At higher temperatures N₂O concentrations are limited by thermal dissociation of N₂O and by reaction with radicals, primarily OH. © 1994 John Wiley & Sons, Inc.

**General information**
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST), Sandia National Laboratories CA, Sandia National Laboratories NM
Corresponding author: Glarborg, P.
Contributors: Glarborg, P., Dam‐Johansen, K., Miller, J. A., Kee, R. J., Coltrin, M. E.
Pages: 421-436
Publication date: 1994
Peer-reviewed: Yes

**Publication information**
Journal: International Journal of Chemical Kinetics
Volume: 26
Issue number: 4
ISSN (Print): 0538-8066
Original language: English
DOIs: 10.1002/kin.550260405
Source: Scopus
Source-ID: 0028406373
Research output: Contribution to journal › Journal article – Annual report year: 1994 › Research › peer-review

**Spectrokinetic study of SF₅ and SF₅O₂ radicals and the reaction of SF₅O₂ with NO**

**General information**
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Sehested, J., Ellermann, T., Nielsen, O., Wallington, T.
Pages: 615-629
Publication date: 1994
UV absorption spectrum of CF₃CFClO₂ and kinetics of the self reaction of CF₃CFCI and CF₃CFClO₂ and the reactions of CF₃CFClO₂ with NO and NO₂

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Sehested, J.
Pages: 1023-1039
Publication date: 1994
Peer-reviewed: Yes

A kinetic study of reaction of fluorine atoms with CH₃F, CH₂Cl, CH₃Br, CF₂H₂, CO, CF₃H, CF₃CHCl₂, CF₃CH₂F, CHF₂, CHF₂CH₂H, CHF₂CO, CF₂ClCH₃, CHF₂CH₃, and CF₃CF₂H at 295 ± 2 K

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Wallington, T., Hurley, M., Jichun Shi, Maricq, M., Sehested, J., Nielsen, O., Ellermann, T.
Pages: 651-665
Publication date: 1993
Peer-reviewed: Yes

UV absorption spectrum, and kinetics and mechanism of the self reaction of CF₃CF₂O₂ radicals in the gas phase at 295 K

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Sehested, J., Ellermann, T., Nielsen, O., Wallington, T., Hurley, M.
Pages: 701-717
Publication date: 1993
Peer-reviewed: Yes
Pulse radiolysis and Fourier transform infrared study of neopentyl peroxy radicals in the gas phase at 297 K

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Wallington, T., Andino, J., Potts, A., Nielsen, O.
Pages: 649-663
Publication date: 1992
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 24
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 290172
Research output: Contribution to journal › Journal article – Annual report year: 1992 › Research › peer-review

UV absorption spectra, kinetics, and mechanisms of the self reaction of CF₃O₂ radicals in the gas phase at 295 K

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Nielsen, O., Ellermann, T., Sehested, J., Bartkiewicz, E., Wallington, T., Hurley, M.
Pages: 1009-1021
Publication date: 1992
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 24
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 289995
Research output: Contribution to journal › Journal article – Annual report year: 1992 › Research › peer-review

Rate constants for the gas-phase reactions of OH radicals and Cl atoms with n-alkyl nitrites at atmospheric pressure and 298 K

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Nielsen, O., Sidebottom, H., Donlon, M., Treacy, J.
Pages: 1095-1109
Publication date: 1991
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 23
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 289034
Research output: Contribution to journal › Journal article – Annual report year: 1991 › Research › peer-review
UV absorption spectra and kinetics of the self reaction of CFCl₂CH₂O₂ and CF₂ClCH₂O₂ radicals in the gas phase at 298 K

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Wallington, T., Nielsen, O.
Pages: 785-798
Publication date: 1991
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 23
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 289239
Research output: Contribution to journal - Journal article – Annual report year: 1991 - Research - peer-review

Absolute and relative rate constants for the reactions of hydroxyl radicals and chlorine atoms with a series of aliphatic alcohols and ethers at 298 K

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Nelson, L., Rattigan, O., Neavyn, R., Sidebottom, H., Treacy, J., Nielsen, O.
Pages: 1111-1126
Publication date: 1990
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 22
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 288700
Research output: Contribution to journal - Journal article – Annual report year: 1990 - Research - peer-review

Kinetics and mechanism for the oxidation of 1,1,1-trichloroethane

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Nelson, L., Shanahan, I., Sidebottom, H., Treacy, J., Nielsen, O.
Pages: 577-590
Publication date: 1990
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 22
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 288716
Research output: Contribution to journal - Journal article – Annual report year: 1990 - Research - peer-review

Rate constants for the reactions of OH radicals and Cl atoms with diethyl sulfide, Di-n-propyl sulfide, and Di-n-butyl sulfide

General information
An Absolute and Relative Rate Study of the Reaction of OH Radicals with Dimethyl Sulfide

General information
Publication status: Published
Organisations: Risø National Laboratory for Sustainable Energy
Contributors: Nielsen, O., Sidebottom, H., Nelson, L., Rattigan, O., Treacy, J., O'Farrell, D.
Pages: 1101-1112
Publication date: 1989
Peer-reviewed: Yes

Publication information
Journal: International Journal of Chemical Kinetics
Volume: 21
ISSN (Print): 0538-8066
Original language: English
Source: orbit
Source-ID: 288200
Research output: Contribution to journal › Journal article – Annual report year: 1989 › Research › peer-review