



# Investigation of current and future anthropogenic chemical regimes in simulation chamber experiments

Michelle Färber

Energie & Umwelt / Energy & Environment

Band / Volume 657

ISBN 978-3-95806-809-4

Forschungszentrum Jülich GmbH  
Institute of Climate and Energy Systems (ICE)  
Troposphäre (ICE-3)

# **Investigation of current and future anthropogenic chemical regimes in simulation chamber experiments**

Michelle Färber

Schriften des Forschungszentrums Jülich  
Reihe Energie & Umwelt / Energy & Environment

Band / Volume 657

---

ISSN 1866-1793

ISBN 978-3-95806-809-4

# Contents

<b>1</b>	<b>Introduction</b>	<b>3</b>
1.1	Anthropogenic emissions in urban areas	5
1.2	Tropospheric daytime and nighttime chemistry	7
1.3	Atmospheric radical measurement by laser-induced fluorescence	16
1.4	Objectives of this thesis	19
<b>2</b>	<b>Investigation of chamber effects and gas-phase product yields in different simulation chambers</b>	<b>23</b>
2.1	Introduction	24
2.2	Methods	26
2.2.1	Properties of the simulation chambers	26
2.2.2	Instrumentation	27
2.2.3	Experimental conditions and procedures	28
2.2.4	Analysis of the experiments	29
2.3	Results and discussion	33
2.3.1	Observations in the experiments	33
2.3.2	Chamber-specific features and observations in the experiments	34
2.3.3	Comparison of results from the simulation chambers	47
2.4	Summary and conclusions	51
<b>3</b>	<b>Daytime and nighttime radical chemistry in urban environments</b>	<b>53</b>
3.1	Methodology	53
3.1.1	Studying air quality in the atmospheric simulation chamber SAPHIR	53
3.1.2	Detection system for OH, HO <sub>2</sub> , and RO <sub>2</sub> radicals at the atmospheric simulation chamber SAPHIR	55
3.2	Photooxidation of anthropogenic VOCs and the impact of the alkoxy chemistry on the ozone production	64
3.2.1	Introduction	66
3.2.2	Methodology	68
3.2.3	Model-measurement comparison	78
3.3	Nighttime oxidation chemistry of anthropogenic VOCs and the role of the formation of alkyl peroxy nitrates	81
3.3.1	Introduction	82
3.3.2	Introduction	83
3.3.3	Methodology	85
3.3.4	Results	88
3.3.5	Discussion	90
3.3.6	Summary & Conclusions	91
3.3.7	References	92
<b>4</b>	<b>Conclusions</b>	<b>95</b>
	<b>Bibliography</b>	<b>99</b>

<b>List of Figures</b> . . . . .	<b>115</b>
<b>List of Tables</b> . . . . .	<b>119</b>
<b>Acknowledgments</b> . . . . .	<b>121</b>
<b>A Appendix</b> . . . . .	<b>123</b>
A.1 Supplementary materials to Chapter 2 . . . . .	123
A.1.1 Detailed information about the participating simulation chambers . . . . .	123
A.1.2 List of experimental conditions for each experiment . . . . .	126
A.1.3 Correction of time series of gas-phase products for the calculation of product yields . . . . .	129
A.1.4 Further experiments analysed in the multi-chamber study . . . . .	130
A.1.5 Relation between consumed $\alpha$ -pinene and formed gas-phase products . . . . .	153
A.2 Supplementary materials to Section 3.2 . . . . .	159
A.2.1 OH reaction schemes of compounds investigated in this work . . . . .	162
A.2.2 Model-measurement comparisons . . . . .	168
A.2.3 Overview of modelled and measured observables . . . . .	175
A.2.4 Alkoxy chemistry following C96O2 . . . . .	176
A.2.5 References . . . . .	177
A.3 Supplementary materials to Section 3.3 . . . . .	187
A.3.1 Investigation of the ozonolysis of trans-2-hexene . . . . .	189
A.3.2 Estimation of the NO <sub>3</sub> interference in the RO <sub>x</sub> system . . . . .	194
A.3.3 Modified CH <sub>3</sub> CH(NO <sub>3</sub> )CH(CH <sub>3</sub> )O decomposition rate . . . . .	198
A.3.4 Instrumental details . . . . .	200
A.3.5 Contribution of NO <sub>3</sub> and O <sub>3</sub> to the oxidation of cis-2-butene and trans- 2-hexene . . . . .	201
A.3.6 Comparison of modelled and measured acetaldehyde from the oxidation of cis-2-butene by NO <sub>3</sub> . . . . .	202
A.3.7 Nighttime oxidation of trans-2-hexene at different temperatures . . . . .	203
A.3.8 References . . . . .	209
<b>B Anhänge gemäß Prüfungsordnung</b> . . . . .	<b>211</b>
B.1 Own contributions to publications and manuscripts . . . . .	211
B.2 Erklärung zur Dissertation . . . . .	213

Energie & Umwelt / Energy & Environment  
Band / Volume 657  
ISBN 978-3-95806-809-4