

Contents

ABSTRACT	i
Principal Symbols	iii
1 INTRODUCTION AND MOTIVATION	1
2 PHYSICAL DESCRIPTION OF RECCM MODEL	5
2.1 Background about development of REMO	5
2.2 Model domain and coordinates	5
2.3 Governing equations in REMO	7
2.4 Continuity Equation of Chemical Species	11
2.4.1 Horizontal transport and vertical advection	12
2.4.2 Turbulent diffusion and dry deposition	13
2.4.3 Redistribution by convective up- and downdrafts	14
3 CHEMISTRY MODULE	15
3.1 Chemistry Mechanisms RACM and ReLACS	15
3.2 Equations for Chemical Transformation	16
3.3 ODE Solver for chemical kinetic integration	18
3.3.1 Importance of ODE solver for multiple processes	18
3.3.2 Introduction to the α -QSS method	19
3.3.3 Application of α -QSS method and Validation of Box Model	21
3.3.4 Accuracy and efficiency analysis	28
3.4 Photolysis rates and application of Fast- J2	34
4 EMISSIONS and BOUNDARY CONDITIONS	38
4.1 Emissions	38
4.1.1 Description of Data sources	38
4.1.2 Grid Data Transformation	38
4.1.3 VOC Speciation	43
4.1.4 Temporal Disaggregation	43
4.1.5 The Treatment of Emissions in the Model	46
4.2 Initial and Boundary Conditions	47
4.2.1 Initial conditions	47
4.2.2 Boundary conditions	49
5 MODEL APPLICATION: Simulation of the Annual Ozone Cycle for 1999	52
5.1 Model setup	52
5.2 Models Results and Comparisons	53

Contents

5.2.1	Observation data for comparisons	53
5.2.2	Overview of model results in 1999	59
5.2.3	Regional pattern of ozone	59
5.2.4	Early spring ozone in 1999	67
5.2.5	High ozone smog episode in summer 1999	70
5.3	Quantitative Model Evaluation	70
6	SUMMARY, CONCLUSIONS AND FUTURE RESEARCH	89
6.1	Summary and Conclusions	89
6.2	Model limitations and suggestions for future research	90
	List of figure captions	91
	References	97
	Appendix A: RACM and ReLACS Species List	106
	Appendix B: Chemical Reactions in ReLACS	109
	Acknowledgements	112