

## Modeling of Atmospheric Chemistry

Mathematical modeling of atmospheric composition is a formidable scientific and computational challenge. This comprehensive presentation of the modeling methods used in atmospheric chemistry focuses on both theory and practice, from the fundamental principles behind models, through to their applications in interpreting observations. An encyclopedic coverage of methods used in atmospheric modeling, including their advantages and disadvantages, makes this a one-stop resource with a large scope. Particular emphasis is given to the mathematical formulation of chemical, radiative, and aerosol processes; advection and turbulent transport; emission and deposition processes; as well as major chapters on model evaluation and inverse modeling. The modeling of atmospheric chemistry is an intrinsically interdisciplinary endeavor, bringing together meteorology, radiative transfer, physical chemistry, and biogeochemistry. This book is therefore of value to a broad readership. Introductory chapters and a review of the relevant mathematics make the book instantly accessible to graduate students and researchers in the atmospheric sciences.

**Guy P. Brasseur** is a Senior Scientist and former Director at the Max Planck Institute for Meteorology in Hamburg, Germany, and a Distinguished Scholar at the National Center for Atmospheric Research in Boulder, USA. He received his doctor's degree at the University of Brussels and has conducted research in Belgium, the USA, and Germany. He was Professor at the Universities of Brussels and Hamburg. His scientific interests include questions related to atmospheric chemistry and air pollution, biogeochemical cycles, climate change, and upper atmosphere chemistry and dynamics. He has chaired several international research programs, and is associated with national academies in Hamburg, Germany, Brussels, Belgium, and Oslo, Norway.

**Daniel J. Jacob** is the Vasco McCoy Family Professor of Atmospheric Chemistry and Environmental Engineering at Harvard University. He received his PhD from Caltech in 1985 and joined the Harvard faculty in 1987. His research covers a wide range of topics in atmospheric composition, with focus on model development and applications to interpretation of observations. Among his professional honors are the NASA Distinguished Public Service Medal (2003), the AGU Macelwane Medal (1994), and the Packard Fellowship for Science and Engineering (1989). Jacob has published over 350 research papers and trained over 80 PhD students and postdocs in atmospheric chemistry modeling over the course of his career.

“This exceptional volume by two pioneers in the field covers every essential aspect of atmospheric modeling.”

- John Seinfeld, *California Institute of Technology*

“An impressive and comprehensive description of the theoretical underpinning and practical application of atmospheric chemistry modeling. Soon to be a classic reference for graduate students and researchers in the field.”

- Colette L. Heald, *Massachusetts Institute of Technology*

“Brasseur and Jacob, both world leaders in modeling atmospheric chemistry, have written a thoroughly engaging textbook. The breadth and depth of the material covered in the book is impressive, but a major strength of the book is the ability of the authors to present often complex information in an accessible way. I have no doubt that this book will help educate future generations of scientists and be a reference point for researchers worldwide. It will certainly become a well-thumbed volume on my bookshelf.

- Paul Palmer, *University of Edinburgh*

“This excellent book provides a comprehensive introduction and reference to modeling of atmospheric chemistry from two of the pioneering authorities in the field. From the historical motivations through to modern-day approaches, the atmospheric physical, chemical and radiative components of the model framework are described. What makes this book particularly relevant and timely is the discussion of the methods for integrating observations and models that are at the forefront of current scientific advancement.”

- David P. Edwards, *National Center for Atmospheric Research*

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Frontmatter  
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# Modeling of Atmospheric Chemistry

GUY P. BRASSEUR

Max Planck Institute for Meteorology and  
National Center for Atmospheric Research

DANIEL J. JACOB

Harvard University



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## Preface

Modern science dealing with complex dynamical systems increasingly makes use of mathematical models to formalize the description of interactive processes and predict responses to perturbations. Models have become fundamental tools in many disciplines of natural sciences, engineering, and social sciences. They describe the essential aspects of a system using mathematical concepts and languages and they can in this manner provide powerful approximations of reality. They are used to analyze observations, understand relationships, test hypotheses, and project future evolution. Disagreements between models and observations often lead to important advances in theoretical understanding. Models also play a critical role in the development of policy options and in decision-making.

In atmospheric science, mathematical models have long been central tools for weather prediction and climate research. They are now also used extensively to describe the chemistry of the atmosphere. The corresponding model equations describe the factors controlling atmospheric concentrations of chemical species as a function of emissions, transport, chemistry, and deposition. Chemical species are often coupled through intricate mechanisms, and the corresponding differential equations are then also coupled. Simulation of aerosol particles needs to account in addition for microphysical processes governing particle size and composition, as well as interactions with the hydrological cycle through cloud formation. The difficulty of modeling atmospheric composition is compounded by the need to resolve a continuum of temporal and spatial scales stretching over many orders of magnitude from microseconds to many years, from local to global, and involving coupling of transport and chemistry on all scales.

Mathematical modeling of atmospheric chemistry is thus a formidable scientific and computational challenge. It integrates elements of meteorology, radiative transfer, physical chemistry, and biogeochemistry. Solving the large systems of coupled nonlinear partial differential equations that characterize the atmospheric evolution of chemical species requires advanced numerical algorithms and pushes the limits of supercomputing resources.

The purpose of this book is to provide insight into the methods used in models of atmospheric chemistry. The book is designed for graduate students and professionals in atmospheric chemistry, but also more broadly for researchers interested in atmospheric models, numerical methods, and optimization theory.

The book is divided into three parts. The first part presents background material. Chapter 1 introduces the reader to the concept of model and provides a historical perspective on the development of atmospheric and climate models, leading to the development of atmospheric chemistry models. It reviews the

different types of atmospheric chemistry models and highlights their role as components of observing systems.

Fundamentals of atmospheric dynamics and chemistry are presented in Chapters 2 and 3. Chapter 2 describes the vertical structure of the atmosphere, defines key parameters that characterize the dry and the wet atmosphere, and introduces the concept of static stability and geostrophic balance. It goes on to describe the general circulation of the atmosphere. Chapter 3 provides a summary survey of the chemical processes relevant to the atmosphere as well as the microphysical processes controlling the evolution of aerosol particles. Chapter 4 presents the fundamental mathematical equations on which atmospheric models are based and gives an introduction to the numerical methods used to solve these equations.

The second part of this book focuses on the formulation of model processes and reviews the numerical algorithms used to solve the model equations. Chapter 5 covers the formulation of radiative transfer, chemical kinetics, and aerosol microphysics. Chapter 6 reviews numerical methods to solve the stiff systems of nonlinear ordinary differential equations that describe atmospheric chemistry mechanisms. Chapter 7 presents numerical algorithms used to solve the advection equation describing transport by resolved winds. The formulation of small-scale (parameterized) transport processes including turbulent mixing, organized convection, plumes, and boundary layer dynamics is addressed in Chapter 8. Chapter 9 reviews formulations of emissions to the atmosphere, deposition to the surface, and two-way coupling between the atmosphere and surface reservoirs.

The third part of this book deals with the role of models as components of the atmospheric observing system. Chapter 10 focuses on model evaluation and presents different metrics for this purpose. It illustrates the importance of models for the interpretation of observational data. Chapter 11 covers fundamental concepts of inverse modeling and data assimilation. It shows how chemical transport models can be integrated with atmospheric observations through optimization theory to provide best estimates of the chemical state of the system and of the driving variables.

At the end of the volume, the reader will find several appendices with numerical values of physical constants and other quantities, unit conversions, and a list of important chemical reactions with corresponding rate constants. Some basic mathematical definitions and relations are also provided.

Over the years, both of us have benefited from numerous discussions with our colleagues, students, and postdoctoral fellows. Several of them have contributed to this book by reviewing chapters, making suggestions, and providing scientific material. We are deeply indebted to them. We would like to thank in particular Helen Amos, Alexander Archibald, Jerome Barre, Mary Barth, Cathy Clerbaux, Jim Crawford, Louisa Emmons, Rolando Garcia, Paul Ginoux, Claire Granier, Alex Guenther, Colette Heald, Jan Kazil, Patrick Kim, Douglas Kinnison, Monika Kopacz, Jean-François Lamarque, Peter Lauritzen, Sasha Madronich, Daniel Marsh, Iain Murray, Vincent-Henri Peuch, Philip Rasch, Brian Ridley, Anne Smith, Piotr Smolarkiewicz, Alex Turner, Xuexi Tie, Stacy Walters, Kevin Wecht, Christine Wiedinmyer, Lin Zhang, and Peter Zoogman. We would like also to acknowledge Sebastian Eastham, Emilie Ehretsmann, Natasha Goss, Lu Hu, Rajesh Kumar, Eloise

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Symbols

The symbols used in the different chapters of this book are listed below with their corresponding units in the MKSA system. When no units are given, the quantity is either dimensionless or has no intrinsic dimensions. Appendix B gives further information on units, prefixes, and conversion factors. In some cases, when no confusion exists, the same symbols are used to characterize different variables. Scalars are represented as italics (alphabet letters) or as regular font (Greek and other symbols). Vectors and matrices are represented by lowercase and uppercase bold fonts, respectively.

<b>A</b>	
<i>a</i>	Earth’s radius [m]
<i>A</i>	Surface area density of atmospheric particles [m <sup>2</sup> m <sup>-3</sup> ]
<b>A</b>	Averaging kernel matrix
<b>B</b>	
<i>B</i>	Blackbody radiative emission flux [W m <sup>-2</sup> ]
<i>B<sub>λ</sub></i>	Spectral density of blackbody emission flux (Planck function) [W m <sup>-2</sup> nm <sup>-1</sup> ]
<b>C</b>	
<i>c</i>	One-dimensional constant flow velocity [m s <sup>-1</sup> ]
<i>c</i>	Speed of light in vacuum [m s <sup>-1</sup> ]
<i>c*</i>	Phase velocity of a wave [m s <sup>-1</sup> ]
<i>c<sub>g</sub>*</i>	Group velocity of a wave [m s <sup>-1</sup> ]
<i>c<sub>p</sub></i>	Specific heat at constant pressure [J K <sup>-1</sup> kg <sup>-1</sup> ]
<i>c<sub>v</sub></i>	Specific heat at constant volume [J K <sup>-1</sup> kg <sup>-1</sup> ]
<i>C<sub>c</sub></i>	Slip correction factor
<i>C<sub>D</sub></i>	Drag coefficient
<i>C<sub>i</sub></i>	Mole fraction or molar mixing ratio of species <i>i</i>
<i>CRMSE</i>	Centered root-mean-square-error
<b>D</b>	
<i>d</i>	Displacement height [m]
<i>D</i>	Divergence of the flow [s <sup>-1</sup> ]
<i>Da</i>	Damköhler number
<i>D<sub>d</sub></i>	Detrainment rate associated with downdrafts in convective systems [kg m <sup>-3</sup> s <sup>-1</sup> ]
<i>D<sub>i</sub></i>	Molecular diffusion coefficient for species <i>i</i> [m <sup>2</sup> s <sup>-1</sup> ]
<i>D<sub>p</sub></i>	Particle diameter [m]



xvii	Symbols
$D_u$	Detrainment rate associated with updrafts in convective systems [ $\text{kg m}^{-3} \text{s}^{-1}$ ]
$DOFS$	Degrees of freedom for signal
<b>E</b>	
$e$	Water vapor partial pressure [Pa]
$e_s$	Saturation water vapor pressure [Pa]
<b>e</b>	Eigenvector
$E$	Emission flux [ $\text{kg m}^{-2} \text{s}^{-1}$ ]
<b>E</b>	Eliassen–Palm Flux [components $E_\phi$ and $E_z$ in $\text{kg s}^{-2}$ ]
<b>E</b>	Matrix of eigenvectors arranged by columns
$E(k)$	Spectral distribution of turbulent energy for a given wavenumber $k$ [ $\text{m}^3 \text{s}^{-2}$ ]
$E_a$	Activation energy [ $\text{J mol}^{-1}$ ]
$E_d$	Entrainment rate associated with downdraft in convective systems [ $\text{kg m}^{-3} \text{s}^{-1}$ ]
$E_u$	Entrainment rate associated with updraft in convective systems [ $\text{kg m}^{-3} \text{s}^{-1}$ ]
<b>F</b>	
$f$	Coriolis factor [ $\text{s}^{-1}$ ]
$f_A$	Fractional area of a model grid cell experiencing precipitation
$f_A$	Fractional area of land suitable for saltation
$f_{i,I}$	Fraction of soluble compound $i$ partitioned in ice water
$f_{i,L}$	Fraction of soluble compound $i$ partitioned in liquid water
$F$	Mass flux [ $\text{kg m}^{-2} \text{s}^{-1}$ ]
$F$	Radiative flux [ $\text{W m}^{-2}$ ]
$\mathcal{F}$	Air mass factor
<b>F</b>	Force vector with its three components $F_x$ , $F_y$ , and $F_z$ [N]
<b>F</b>	Forward model
$F_{D,i}$	Deposition flux of species $i$ [ $\text{kg m}^{-2} \text{s}^{-1}$ ]
$F_\lambda$	Spectral density of the radiative flux [ $\text{W m}^{-2} \text{nm}^{-1}$ ]
<b>G</b>	
<b>g</b>	Vector of gravitational acceleration [ $\text{m s}^{-2}$ ]
$g$	Amplitude of gravitational acceleration [ $\text{m s}^{-2}$ ]
$g$	Amplification function in numerical methods
$g$	Asymmetry factor
$g$	Gain factor
$G$	Green function
$G$	Gravity wave drag [ $\text{m s}^{-2}$ ]
<b>G</b>	Gain matrix
$G_m$	Grade of model $m$
<b>H</b>	
$h$	Mixing depth [m]
$H$	Atmospheric scale height [m]
$\mathcal{H}$	Effective (constant) scale height [m]
$H_i$	Dimensionless Henry’s law constant for species $i$

**I**

- i** Unit vector in the zonal ( $x$ ) direction  
*I* Light intensity [ $\text{W m}^{-2}$ ]  
**I** Identity matrix  
*I<sub>AB</sub>* Segregation ratio for chemical compounds A and B  
*I<sub>i</sub>* Condensation growth rate of species  $i$  [ $\text{m}^3 \text{s}^{-1}$ ]

**J**

- j** Unit vector in the meridional ( $y$ ) direction  
*j* Radiative source term [ $\text{Wm}^{-2} \text{sr}^{-1} \text{nm}^{-1} \text{m}^{-1}$ ]  
*J* Radiative source function [ $\text{Wm}^{-2} \text{sr}^{-1} \text{nm}^{-1}$ ]  
*J* Photodissociation (photolysis) frequency [ $\text{s}^{-1}$ ]  
*J* Cost function  
**J** Jacobian matrix  
*J<sub>i,j</sub>* Coagulation rate between particles  $i$  and  $j$  [ $\text{m}^{-3} \text{s}^{-1}$ ]  
*J<sub>0</sub>* Nucleation rate [ $\text{m}^{-3} \text{s}^{-1}$ ]

**K**

- k** Unit vector in the vertical ( $z$ ) direction  
*k* Wavenumber [ $\text{m}^{-1}$ ]  
*k* Boltzmann's constant ( $1.38 \times 10^{-23} \text{J K}^{-1}$ )  
*k* von Karman's constant (0.35)  
*k* Chemical rate constant [first order:  $\text{s}^{-1}$ ; second order:  $\text{cm}^3 \text{s}^{-1}$ ; third order:  $\text{cm}^6 \text{s}^{-2}$ ]  
*k<sub>ext</sub>* Mass extinction cross-section [ $\text{m}^2 \text{kg}^{-1}$ ]  
*k<sub>G,i</sub>* Conductance for vertical transfer of species  $i$  in the gas phase [ $\text{m s}^{-1}$ ]  
*k<sub>W,i</sub>* Conductance for vertical transfer of species  $i$  in the water phase [ $\text{m s}^{-1}$ ]  
*K* Eddy diffusion coefficient [ $\text{m}^2 \text{s}^{-1}$ ]  
*K* Equilibrium constant  
*K* Henry's law constant [ $\text{M atm}^{-1}$ ]  
*K\** Effective Henry's law constant [ $\text{M atm}^{-1}$ ]  
**K** Eddy diffusion tensor  
**K** Jacobian matrix (Chapter 11)  
*K<sub>a</sub>* Acid dissociation constant  
*K<sub>m</sub>* Eddy viscosity coefficient [ $\text{m}^2 \text{s}^{-1}$ ]  
*Kn* Knudsen number  
*K<sub>i</sub>* Air-sea exchange velocity for species  $i$  [ $\text{m s}^{-1}$ ]  
*K<sub>0</sub>* Eddy diffusivity of heat [ $\text{m}^2 \text{s}^{-1}$ ]

**L**

- l* Mixing length [ $\text{m}$ ]  
 $\mathcal{L}_i$  Loss rate constant or loss coefficient of species  $i$  [ $\text{s}^{-1}$ ]  
*L* Characteristic length [ $\text{m}$ ]  
*L* Liquid water content [ $\text{kg water/kg air}$ ]  
*L* Monin–Obukhov length [ $\text{m}$ ]

xix	Symbols
$L$	Lagrange function
$L_i$	Loss rate of species $i$ [ $\text{m}^{-3} \text{s}^{-1}$ ]
$L_{vap}$	Latent heat of vaporization of liquid water [ $\text{J kg}^{-1}$ ]
$L_\lambda$	Spectral density of the radiance at wavelength $\lambda$ [ $\text{W m}^{-2} \text{sr}^{-1} \text{nm}^{-1}$ ]
<b>M</b>	
$m$	Mean molecular mass of air ( $4.81 \times 10^{-26} \text{ kg}$ )
$m$	Refraction index
$m$	Wavenumber
$M_a$	Molar mass of air ( $28.97 \times 10^{-3} \text{ kg mol}^{-1}$ )
$M_d$	Mean vertical downdraft convective flux of air [ $\text{kg m}^{-2} \text{s}^{-1}$ ]
$M_e$	Mean subsidence flux compensating for convective fluxes [ $\text{kg m}^{-2} \text{s}^{-1}$ ]
$M_i$	Molar mass of species $i$ [ $\text{kg mol}^{-1}$ ]
$M_k$	Moment of order $k$ for a given aerosol distribution
$M_u$	Mean vertical updraft convective flux of air [ $\text{kg m}^{-2} \text{s}^{-1}$ ]
$M_w$	Molar mass of water ( $18.01 \times 10^{-3} \text{ kg mol}^{-1}$ )
$MAD$	Mean absolute deviation
$MAE$	Mean absolute error
$MFB$	Mean fractional bias
$MFE$	Mean fractional error
$MNAE$	Mean normalized absolute error
$MNB$	Mean normalized bias
<b>N</b>	
$\mathbf{n}$	Unit outward vector normal to a surface
$n_a$	Number density for air [ $\text{m}^{-3}$ ]
$n_i$	Number density for species $i$ [ $\text{m}^{-3}$ ]
$n_N$	Particle number size distribution function [ $\text{m}^{-4}$ ]
$n_S$	Particle surface distribution function [ $\text{m}^2 \text{m}^{-4}$ ]
$n_V$	Particle volume distribution function [ $\text{m}^3 \text{m}^{-4}$ ]
$\mathcal{N}_A$	Avogadro number ( $6.022 \times 10^{23}$ molecules per mole)
$NMB$	Normalized mean bias
<b>P</b>	
$p$	Pressure [Pa]
$p_d$	Pressure of dry air [Pa]
$p_i$	Production rate of species $i$ [ $\text{kg m}^{-3} \text{s}^{-1}$ ]
$p_s$	Surface pressure [Pa]
$P$	Phase function for scattered radiation
$P$	Ertel potential vorticity [ $\text{m}^2 \text{s}^{-2} \text{K kg}^{-1}$ ]
$P$	Probability density function
$\mathcal{P}$	Steric factor
$Pe$	Péclet number
$P_i$	Production rate of species $i$ [ $\text{m}^{-3} \text{s}^{-1}$ ]
$P_l^m$	Associated Legendre polynomial
$Pr$	Prandtl number

**Q**

$q$	Specific humidity [kg water vapor/kg of air]
$q$	Diabatic heating expressed in K day <sup>-1</sup>
$q$	Actinic flux [photons m <sup>-2</sup> s <sup>-1</sup> ]
$q_k$	Water concentration in hydrometeor of type $k$
$q_\lambda$	Photon flux density [photons m <sup>-2</sup> s <sup>-1</sup> nm <sup>-1</sup> ]
$Q$	Diabatic heating rate [J kg <sup>-1</sup> s <sup>-1</sup> or W m <sup>-3</sup> ]
$Q_{abs}$	Absorption efficiency
$Q_{ext}$	Extinction efficiency
$Q_s$	Saltation flux [kg m <sup>-1</sup> s <sup>-1</sup> ]
$Q_{scat}$	Scattering efficiency

**R**

$r$	Geometric distance from the center of the Earth
$\mathbf{r}$	Position vector
$r$	Particle radius [m]
$r_w$	Mass mixing ratio of water vapor [kg kg <sup>-1</sup> ]
$r$	Pearson correlation coefficient
$R$	Gas constant for air [J K <sup>-1</sup> kg <sup>-1</sup> ]
$\mathcal{R}$	Universal gas constant (8.3143 J K <sup>-1</sup> mol <sup>-1</sup> )
$R^2$	Coefficient of determination
$R_A$	Aerodynamic resistance [s m <sup>-1</sup> ]
$R_{B,i}$	Boundary resistance for species $i$ [s m <sup>-1</sup> ]
$R_{C,i}$	Surface resistance for species $i$ [s m <sup>-1</sup> ]
$R_d$	Gas constant for dry air (287 J K <sup>-1</sup> kg <sup>-1</sup> )
$Re$	Reynolds number
$RH$	Relative humidity [percent]
$Ri$	Richardson number
$R_i$	Total resistance to dry deposition of species $i$ [s m <sup>-1</sup> ]
$RMSE$	Root mean square error
$R_w$	Gas constant for water vapor (461.5 J K <sup>-1</sup> kg <sup>-1</sup> )

**S**

$s_i$	Source rate of species $i$ (in mass) [kg m <sup>-3</sup> s <sup>-1</sup> ]
$S$	Solar energy flux [W m <sup>-2</sup> ] or solar constant (approx. 1368 W m <sup>-2</sup> )
$\mathbf{S}$	Error covariance matrix
$\mathbf{S}'$	Error correlation matrix
$\mathbf{S}_a$	Aggregation error covariance matrix
$\mathbf{S}_A$	Prior error covariance matrix
$\mathbf{S}_I$	Instrument error covariance matrix
$\mathbf{S}_M$	Forward model error covariance matrix
$\mathbf{S}_O$	Observational error covariance matrix
$\mathbf{S}_R$	Representation error covariance matrix
$\hat{\mathbf{S}}$	Posterior error covariance matrix
$Sc_i$	Schmidt number for species $i$

xxi	Symbols
<b>T</b>	
$t$	Time [s]
$t$	Student's variable for the $t$ -test
$T$	Transmission of radiation
$T$	Absolute temperature [K]
$T_E$	Effective temperature of the Earth [K]
$TKE$	Turbulent kinetic energy [m <sup>2</sup> s <sup>-1</sup> ]
$T_s$	Effective temperature of the Sun
$T_v$	Virtual temperature [K]
<b>U</b>	
$u$	Zonal component of wind velocity [m s <sup>-1</sup> ]
$u$	Path length [kg m <sup>-2</sup> ]
$u^*$	Friction velocity [m s <sup>-1</sup> ]
$u^*$	Residual zonal wind velocity [m s <sup>-1</sup> ]
$u^A$	Anti-diffusion velocity [m s <sup>-1</sup> ]
$u_g$	Zonal component of the geostrophic wind [m s <sup>-1</sup> ]
$u_{10}$	Wind velocity 10 m above the surface [m s <sup>-1</sup> ]
<b>V</b>	
$v$	Meridional component of wind velocity [m s <sup>-1</sup> ]
$v^*$	Residual meridional wind velocity [m s <sup>-1</sup> ]
$\mathbf{v}$	Wind velocity vector in Earth's rotating frame [m s <sup>-1</sup> ]
$v_g$	Meridional component of the geostrophic wind [m s <sup>-1</sup> ]
$v_i$	Mean thermal velocity [m s <sup>-1</sup> ]
$V$	Molar volume [m <sup>3</sup> mol <sup>-1</sup> ]
$V$	Aerosol volume density [m <sup>3</sup> m <sup>-3</sup> ]
$\mathbf{V}$	Wind velocity in inertial frame [m s <sup>-1</sup> ]
$V_T$	Translational Earth's rotation velocity [m s <sup>-1</sup> ]
<b>W</b>	
$w$	Vertical component of wind velocity [m s <sup>-1</sup> ]
$w^*$	Residual vertical wind velocity [m s <sup>-1</sup> ]
$w^*$	Convective velocity scale [m s <sup>-1</sup> ]
$w_{D,i}$	Surface deposition velocity of species $i$ [m s <sup>-1</sup> ]
$w_s$	Terminal settling velocity [m s <sup>-1</sup> ]
<b>X</b>	
$x$	Geometric distance in the zonal direction [m]
$\mathbf{x}$	State vector (often refers to the true value)
$\hat{\mathbf{x}}$	Optimal estimate of state vector
$\mathbf{x}_A$	Prior estimate of state vector
<b>Y</b>	
$y$	Geometric distance in the meridional direction [m]
$\mathbf{y}$	Observation vector

<b>Z</b>	
$z$	Geometric altitude [m]
$z_{0,m}$	Aerodynamic roughness length [m]
$Z$	Log pressure altitude [m]
$Z$	Potential vorticity [ $\text{s}^{-1} \text{m}^{-1}$ ]
$Z_{AB}$	Collision frequency for molecules A and B [ $\text{s}^{-1}$ ]
<b><math>\alpha</math></b>	
$\alpha$	Albedo
$\alpha$	Aerosol particle size parameter
$\alpha$	Mass accommodation coefficient
$\alpha$	Courant number
$\alpha_T$	Thermal diffusion factor
<b><math>\beta</math></b>	
$\beta$	Fourier number
$\beta_{ext}$	Aerosol extinction coefficient [ $\text{m}^{-1}$ ]
$\beta_{abs}$	Aerosol absorption coefficient [ $\text{m}^{-1}$ ]
$\beta_{scat}$	Aerosol scattering coefficient [ $\text{m}^{-1}$ ]
$\beta_{i,j}$	Coagulation coefficient for particles $i$ and $j$ [ $\text{m}^3 \text{s}^{-1}$ ]
<b><math>\gamma</math></b>	
$\gamma$	Reactive uptake coefficient for heterogeneous chemical process
$\gamma$	Regularization factor
$\gamma_c$	Coefficient for non-local turbulent transfer
$\Gamma$	Actual atmospheric lapse rate [ $\text{K m}^{-1}$ ]
$\Gamma$	Mean age of air [s]
$\Gamma_d$	Dry adiabatic lapse rate [ $\text{K m}^{-1}$ ]
$\Gamma_w$	Wet adiabatic lapse rate [ $\text{K m}^{-1}$ ]
$\Gamma_{\varpi}$	Aggregation matrix
<b><math>\delta</math></b>	
$\delta$	Dirac function
$\Delta H$	Enthalpy of dissolution [ $\text{J mol}^{-1}$ ]
<b><math>\epsilon</math></b>	
$\epsilon_A$	Quantum efficiency (or yield) for the photolysis of molecule A
$\epsilon_O$	Observational error vector
$\epsilon_a$	Aggregation error vector
$\epsilon_A$	Prior estimate error vector
$\epsilon_I$	Instrument error vector
$\epsilon_M$	Forward model error vector
$\epsilon_R$	Representation error vector
<b><math>\zeta</math></b>	
$\zeta$	Relative vorticity of the flow [ $\text{s}^{-1}$ ]

xxiii	Symbols
$\eta$	
$\eta$	Step mountain coordinate (eta coordinate)
$\theta$	
$\theta$	Zenithal direction [radians]
$\theta$	Potential temperature [K]
$\theta_v$	Virtual potential temperature [K]
$\lambda$	
$\lambda$	Longitude [radians]
$\lambda$	Wavelength [m]
$\lambda$	Mean free path of air molecules [m]
$\lambda$	Lyapunov exponent [s <sup>-1</sup> ]
$\lambda_i$	Eigenvalue associated with eigenvector $\mathbf{e}_i$
$\Lambda$	Leaf area index (LAI) [m <sup>2</sup> m <sup>-2</sup> ]
$\mu$	
$\mu$	Cosine of zenithal direction ( $\theta$ )
$\mu$	Molecular dynamic viscosity coefficient [Pa s or kg m <sup>-1</sup> s <sup>-1</sup> ]
$\mu_i$	Mass mixing ratio of species $i$ [kg kg <sup>-1</sup> ]
$\mu_w$	Mass mixing ratio of water vapor [kg kg <sup>-1</sup> ]
$\nu$	
$\nu$	Kinematic viscosity [m <sup>2</sup> s <sup>-1</sup> ]
$\nu$	Asselin-filter parameter
$\nu$	Frequency [Hz]
$\nu_{ion}$	Ion-neutral collision frequency [s <sup>-1</sup> ]
$\pi$	
$\pi$	3.14159
$\rho$	
$\rho_a$	Mass density of air [kg m <sup>-3</sup> ]
$\rho_d$	Mass density of dry air [kg m <sup>-3</sup> ]
$\rho_i$	Mass density of species $i$ [kg m <sup>-3</sup> ]
$\rho_p$	Mass density of particles or drops [kg m <sup>-3</sup> ]
$\rho_w$	Mass density of water vapor [kg m <sup>-3</sup> ]
$\sigma$	
$\sigma$	Stefan-Boltzmann constant (5.67 × 10 <sup>-8</sup> W m <sup>-2</sup> K <sup>-4</sup> )
$\sigma$	Standard deviation
$\sigma$	Normalized pressure coordinate (sigma coordinate)
$\tilde{\sigma}$	Pseudo density in isentropic coordinates
$\sigma_A$	Absorption cross-section for molecule A [m <sup>2</sup> ]

$\tau$	
$\tau$	Optical depth
$\tau$	Lifetime [s]
$\tau$	Stress tensor
$\tau_{i,j}$	Element of the stress tensor
$\varphi$	
$\varphi$	Latitude [radians]
$\varphi$	Azimuthal direction
$\phi$	Radial basis function
$\Phi$	Geopotential [ $\text{m}^2 \text{s}^{-2}$ ]
$\Phi_\infty$	Solar flux at the top of the atmosphere [ $\text{W m}^{-2}$ ]
$\Phi_k$	Basis function in the spectral element method
$\Phi_\lambda$	Spectral density of solar flux [ $\text{W m}^{-2} \text{nm}^{-1}$ ]
$\chi$	
$\chi$	Solar zenith angle
$\chi$	Velocity potential
$\psi$	
$\Psi$	Generic mathematical function or variable
$\Psi$	Streamfunction of the flow
$\Psi$	Montgomery function (isentropic coordinate system) [ $\text{J kg}^{-1}$ or $\text{m}^2 \text{s}^{-2}$ ]
$\omega$	
$\omega$	“Vertical” velocity in the pressure coordinate system [ $\text{Pa s}^{-1}$ ]
$\omega$	Single scattering albedo
$\Omega$	Angular Earth rotation period ( $7.292 \times 10^{-5} \text{ rad s}^{-1}$ )
$\Omega$	Column concentration [ $\text{molecules m}^{-2}$ ]
$\Omega_s$	Slant column concentration [ $\text{molecules m}^{-2}$ ]