Inverse Problems in Atmospheric Constituent Transport

The critical role of trace gases in global atmospheric change makes an improved understanding of these gases imperative. Measurements of the distributions of these gases in space and time provide important information, but the interpretation of this information often involves ill-conditioned model inversions. Various techniques have therefore been developed in order to analyse these problems.

Inverse Problems in Atmospheric Constituent Transport is the first book to give comprehensive coverage of the work on this topic. The trace-gas-inversion problem is presented in general terms and the various approaches are unified by treating the inversion problem as one of statistical estimation. Later chapters demonstrate the application of these methods to studies of carbon dioxide, methane, halocarbons and other gases implicated in global climate change. Finally, the emerging field of down-scaling global inversion techniques to estimate fluxes on sub-continental scales is introduced.

This book is aimed at graduate students and researchers embarking upon studies of global atmospheric change and biogeochemical cycles in particular and, more generally, earth-systems science. Established researchers will also find it an invaluable resource due to its extensive referencing and the conceptual linking of the various techniques.

Cambridge Atmospheric and Space Science Series
Editors: A. J. Dessler, J. T. Houghton, and M. J. Rycroft

This series of upper-level texts and research monographs covers the physics and chemistry of the various regions of the earth's atmosphere, from the troposphere and stratosphere, up through the ionosphere and magnetosphere and out to the interplanetary medium.

Ian Enting is a senior principal research scientist at CSIRO Atmospheric Research, Aspendale, Victoria, Australia. He is head of the greenhouse-gas-modelling team and specialises in diagnostic modelling in general and ill-conditioned inverse problems in particular. This work has resulted in numerous research papers and several chapters in books. He was also a lead author for the *Radiative Forcing Report* and the *Second Assessment Report* of the Intergovernmental Panel on Climate Change (IPCC).

Cambridge Atmospheric and Space Science Series

EDITORS

Alexander J. Dessler

John T. Houghton

Michael J. Rycroft

TITLES IN PRINT IN THE SERIES

M. H. Rees
Physics and chemistry of the upper atmosphere

R. Daley
Atmospheric data analysis

J. R. Garratt
The atmospheric boundary layer

J. K. Hargreaves
The solar–terrestrial environment

S. Sazhin
Whistler-mode waves in a hot plasma

S. P. Gary
Theory of space plasma microinstabilities

M. Walt
Introduction to geomagnetically trapped radiation

T. I. Gombosi
Gaskinetic theory

B. A. Kagan
Ocean–atmosphere interaction and climate modelling

I. N. James
Introduction to circulating atmospheres

J. C. King and J. Turner
Antarctic meteorology and climatology

J. F. Lemaire and K. I. Gringauz
The Earth's plasmasphere

D. Hastings and H. Garrett
Spacecraft–environment interactions

T. E. Cravens
Physics of solar system plasmas

J. Green
Atmospheric dynamics

G. E. Thomas and K. Stamnes
Radiative transfer in the atmosphere and ocean

T. I. Gombosi
Physics of space environment

R. W. Schunk and A. F. Nagy
Ionospheres: Physics, plasma physics, and chemistry

R. Hunsucker and J. Hargreaves
The high-latitude ionosphere and its effects on radio propagation

I. Enting
Inverse problems in atmospheric constituent transport

Inverse Problems in Atmospheric Constituent Transport

I. G. Enting

CAMBRIDGE
UNIVERSITY PRESS

PUBLISHED BY THE PRESS SYNDICATE OF THE UNIVERSITY OF CAMBRIDGE
The Pitt Building, Trumpington Street, Cambridge, United Kingdom

CAMBRIDGE UNIVERSITY PRESS
The Edinburgh Building, Cambridge CB2 2RU, UK
40 West 20th Street, New York, NY 10011-4211, USA
477 Williamstown Road, Port Melbourne, VIC 3207, Australia
Ruiz de Alarcón 13, 28014 Madrid, Spain
Dock House, The Waterfront, Cape Town 8001, South Africa

http://www.cambridge.org

First published 2002

Printed in the United Kingdom at the University Press, Cambridge

Typefaces Times 10.25 / 13.5 pt and Joanna *System* LaTeX 2_ε [TB]

A catalogue record for this book is available from the British Library

Library of Congress Cataloguing in Publication data

Enting, I. G.
Inverse problems in atmospheric constituent transport / I. G. Enting.
p. cm.
Includes bibliographical references and index.
ISBN 0 521 81210 0
1. Atmospheric diffusion – Mathematical models. 2. Dynamic meteorology – Mathematical models.
3. Inverse problems (Differential equations) I. Title.

QC880.4.A8 E68 2002
628.5′3′015118 – dc21 2001052977

ISBN 0 521 81210 0 hardback

Contents

Preface

My first contact with ill-conditioned inverse problems was while flying to the 1977 Australian Applied Mathematics Conference at Terrigal, NSW. By chance, I was seated next to Bob Anderssen, who showed me his recent report [8] on regularisation expressed in terms of Fredholm integrals.

Ill-conditioned problems have now dominated the largest part of my scientific career. However, back in 1977, my (private) reaction to Bob's work was 'why would any reasonable person want to work on such perversely difficult problems?'. The answer, 'that this is the form in which we get most of our information about the real world', completely escaped me. In any case, my idealised modelling of phase transitions in lattice systems was seemingly only loosely related to the real world – even my percolation modelling of bubble trapping [125] lay many years in the future.

Two jobs later, I had left mathematical physics as a career and was working for CSIRO modelling the carbon cycle. In particular, I was trying to calibrate our model. My attempts at finding a best-fit parameter set were thrashing around in some poorly defined subspace, when a vague memory stirred. It took me about two days to find Bob's report again and start to realise what I was up against and what I should do about it.

One important point is that what Bob gave me was a technical report. This genre is much-maligned as 'grey-literature'. It can, however, have the advantage of telling 'the truth' and 'the whole truth', even if the lack of anonymous peer review means occasional failures of 'nothing but the truth'. As well as giving important details, technical reports can and do contain things such as motivation and false leads that for reasons of space, style and tradition are fiercely suppressed in the peer-reviewed scientific journals of today. Sir Peter Medawar has discussed this situation in his article 'Is the scientific paper a fraud?' [314].

This starting point meant that much of my initial influence came from seismology. In particular Jackson's paper [224] 'Interpretation of inaccurate, insufficient and inconsistent data' provided me with a concise introduction to the key mathematical concepts. This influence continued, with our network-design calculations [400] based directly on an example from seismology [194]. At times I have used the analogy of a seismologist, confined to the earth's surface and looking down, compared with an atmospheric chemist confined to the earth's surface (by budget constraints) and looking up. Other influences on my thinking on inverse problems have been Twomey [488], Wunsch [521] and, most importantly, Tarantola [471].

In studying biogeochemical cycles, much of the excitement and much of the frustration comes from the apparent need to know about everything: meteorology, oceanography, chemistry, biology, statistics, applied mathematics and many subfields of these major disciplines. In a small way, even my work on the lattice statistics of percolation became relevant when I came to study the trapping of air bubbles in polar ice [125].

This book aims to capture some of this diversity and pull together the techniques and applications of inversions of distributions of atmospheric trace gases. The emphasis is on the inversion calculations as techniques for producing statistical estimates. Breakout boxes cover some of the tangential matters that could not be easily included with any pretence of a linear ordering in the book.

The book is intended for graduate students and beginning researchers in global biogeochemical cycles. My hope is that researchers and students in the more general and growing area of earth-systems science will also find it useful. My expectation is that inverse calculations will play an important role in validating earth-system models by allowing the specification of interactions between earth-system components in terms of boundary conditions based on observations.

The use of this book for a course on the topic of tracer inversion depends on the time available and the background of the students.

- The minimal course would be the early parts of Chapter 3 on estimation, Chapter 10 on Green's functions (probably omitting adjoint techniques), Chapter 11 and then applications from one or more of Chapters 14, 15 and 16. Essentially, this was the content of my tutorial lecture for the Heraklion conference [133] from which this book has grown.
- For an expanded course, I would add Chapters 8 and 13. Chapter 7 could form an important part of integrating this book into a more general course on earth-system modelling.
- Chapter 12 is a potential mathematical framework for student projects that go beyond applying tested techniques to new problems. Chapter 9 would be part of the basis for such extensions and Chapter 17 (and to a lesser extent Chapter 18) shows some areas of application where such extensions may be possible. Depending on the problem, such work may draw on Chapters 4 and 6.

- Chapters 2 and 5 are background that is included to give some semblance of completeness. The coverage emphasises those aspects of most relevance to tracer inversions. I would expect that courses covering these areas would use other textbooks.
- Variations and extensions to a course could be based on the related topics that are introduced in some of the breakout boxes.
- The book includes a small number of exercises at the ends of the chapters. Mostly, these are mathematical derivations that illustrate or extend matters covered in the text. This is because these are the questions for which it is possible to provide answers and regarding which there is no need to make assumptions about what computer software is available. The exercises are confined to the chapters that cover the principles. Some of them are data-oriented and could be used, given appropriate data sets, in several different areas of application. Additional exercises can be constructed by applying some of the illustrative analyses used in the figures to new data sets.

Beyond the influence from seismology, my work has been shaped by many factors. The Applied Mathematics Conferences of the Australian Mathematics Society have influenced me far beyond my initial contact with Bob Anderssen. Because of the small number of scientists working in any one field in Australia, the Applied Mathematics Conferences emphasise communication across fields. This exposed me to a diverse range of mathematical techniques, which I found extremely beneficial when starting work in the relatively new field of atmospheric composition. In a very different way, the diversity fostered by the American Geophysical Union with its emphasis on breaking down barriers between aspects of earth and planetary science has, through its publications and meetings, been a continuing source of inspiration.

An important part of my work environment over 1993–2000 was the Cooperative Research Centre for Southern Hemisphere Meteorology (CRCSHM). The CRCSHM was funded through the Australian Government's Cooperative Research Centre programme as a seven-year initiative bringing together contributions from the CSIRO (divisions of Atmospheric Research and Applied Physics) (later Telecommunications and Industrial Physics), the Australian Bureau of Meteorology, the Mathematics Department of Monash University and Cray Research, Australia (later Silicon Graphics). Throughout its seven-year life, the CRCSHM provided an environment that fostered high-quality research and a vibrant graduate programme. In particular this reflects the efforts of the directors, David Karoly and Graeme Stephens. One of my aims in writing this book is to create a concrete reminder of what we achieved at the CRCSHM.

The cooperative nature of the CSIRO and CRCSHM working environments means that many of the concepts described here have involved shared or parallel development. There are two important cases where I have taken ideas about communication directly from unpublished ideas of my colleagues. First, there is Roger Francey's idea of presenting our understanding of the atmospheric carbon budget in terms of the last few decades' sequence of new concepts (see Section 14.1). Secondly, there is Peter Rayner's emphasis of the complementary nature of synthesis versus mass-balance inversions. Both involve spatial interpolation of data: synthesis does it in the source space and mass-balance does it in the concentration space.

Several colleagues have kindly provided either diagrams of their results or the data from which to produce examples and diagrams. Detailed acknowledgements are given in Appendix E, but the assistance from Rachel Law has been invaluable.

Examples that are based on our initial synthesis inversions [145] have mostly been recalculated for this book (based on the specifications in Box 10.1), but these calculations derive from the initial work by Cathy Trudinger.

Valuable collaboration has come from other present and former colleagues at the CSIRO and CRCSHM, particularly Jim Mansbridge, Cathy Trudinger, Reter Rayner and Rachel Law. Liz Davy and her team in the library have good-naturedly tolerated my fractal return rate and aided me in tracking down obscure references. At the CSIRO, the chief, Graeme Pearman, and my programme and project leaders, Ian Galbally and Paul Steele, have provided encouragement and support, as did Keith Ryan at the CRCSHM. From my first day at the CSIRO, Roger Francey has been a source of wisdom, support and scientific vision.

Beyond the CSIRO, Gary Newsam, George Kuczera and, most importantly, Tony Guttmann, have given me ongoing contact with broader areas of applied mathematics.

Because of the global nature of greenhouse-gas problems, I have had the pleasure of working with scientists from many parts of the world as collaborators; and as co-authors in the case of Martin Heimann, Pieter Tans, Inez Fung, Keith Lassey, Thomas Kaminski and Tom Wigley. My participation in the IPCC assessment process gave me the privilege of participating in a unique exercise in communicating science in response to urgent policy needs and I thank my co-authors for their part in what we achieved together and for all that I learnt from this. My fellow participants in the IGBP–GAIM TransCom project have been a continuing source of ideas and inspiration.

While it often seems that biogeochemical modelling requires its practitioners to know about virtually everything, of course none of us can really do so. It is inevitable that many of the specialist fields have been dealt with in a manner that the relevant experts will find unsatisfactory. In a field lacking clear-cut boundaries some incompleteness is inevitable. I hope that the number of outright errors is small.

One area of possible criticism, for which I expect to remain totally unrepentant, is my adoption of a Bayesian approach. This is a contentious issue [79]. While critics scoff at the possibility of prior knowledge, proponents such as Jeffreys [231] argue that it is only the Bayesian approach that answers the questions that working scientists really ask. Tarantola [471] simply regards the Bayesian approach (somewhat generalised) as reflecting the normal process of natural science, continually building on past knowledge, albeit critically re-examined.

Bard [22] suggests that there are three cases in which the use of a prior distribution is not controversial:

(i) assigning $p_{\text{prior}}(\mathbf{x}) = 0$ to physically impossible values of $\mathbf{x}$;
(ii) if $\mathbf{x}$ truly is a random variable then its distribution function should be used as $p_{\text{prior}}(\mathbf{x})$; and
(iii) when $p_{\text{prior}}(\mathbf{x})$ represents the results from earlier experiments.

The aim in this book is to try to bring the use of Bayesian estimation into the compass of case (iii). This may, of course, include (i) or (ii) as special cases identified on the basis of earlier experiments. In the context of this book, this is simply a recognition that the use of atmospheric-transport modelling to study trace gases does not occur in isolation from other areas of science.

References (in square brackets) are listed in chronological order of publication or, sometimes, in order of importance.

While the errors, omissions and obscurities in this book must remain my responsibility, I have been helped in reducing their number by several colleagues who have kindly read various chapters: Rachel Law, Cathy Trudinger, Paul Fraser, Ying-Ping Wang, Peter Rayner, Simon Bentley, Roger Francey, Ian Galbally, Mick Meyer and Colin Allison. John Garratt kindly gave me the benefit of his editorial experience by reading the full text.

The skill and support of the editorial and production team at Cambridge University Press has made the task of going from typescript to finished book refreshingly hassle-free.

The idea for writing a book like this has been bouncing around my head for several years. The real impetus came from writing my overview of synthesis inversion [133] for the *Workshop on Inverse Problems in Biogeochemistry*, held in Heraklion in 1998 – thanks to Martin Heimann and his fellow organisers, it was a great meeting.

My task in writing this book has been supported by the CSIRO and particularly by the CRCSHM. However, the effort has extended far beyond my normal work-time, which has meant a great reduction in time with my family. I thank them for their forbearance.