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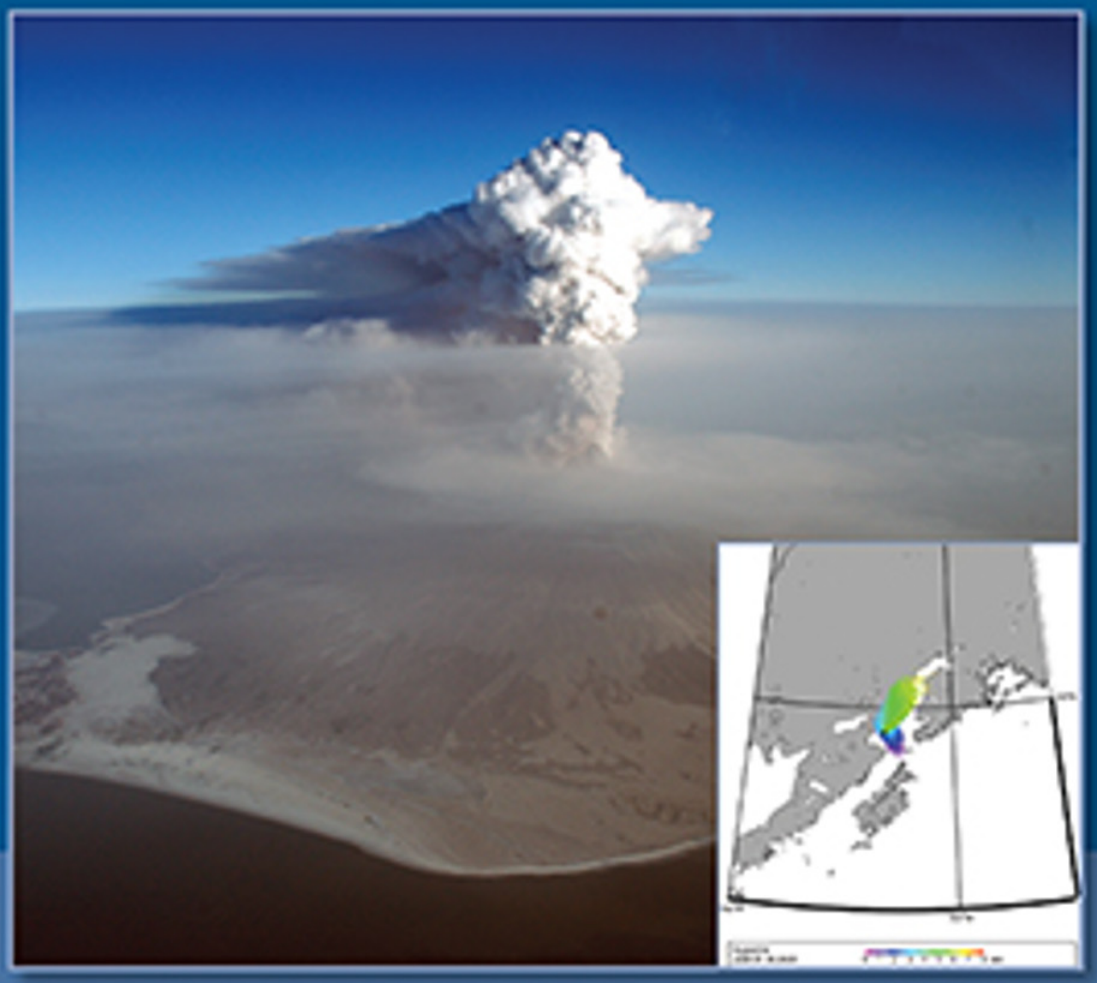
Lagrangian Modeling of the Atmosphere



John Lin, Dominik Brunner, Christoph Gerbig,
Andreas Stohl, Ashok Luhar, and Peter Webley
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Lagrangian Modeling of the Atmosphere

John Lin
Dominik Brunner
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Editors

American Geophysical Union
Washington, DC

Published under the aegis of the AGU Books Board

Kenneth R. Minschwaner, Chair; Gray E. Bebout, Kenneth H. Brink, Jiasong Fang, Ralf R. Haese, Yonggang Liu, W. Berry Lyons, Laurent Montési, Nancy N. Rabalais, Todd C. Rasmussen, A. Surjalal Sharma, David E. Siskind, Rigobert Tibi, and Peter E. van Keken, members.

Library of Congress Cataloging-in-Publication Data

Lagrangian modeling of the atmosphere / John Lin, Dominik Brunner, Christoph Gerbig, Andreas Stohl, Ashok Luhar, and Peter Webley, editors.
pages cm. – (Geophysical monograph, ISSN 0065-8448 ; 200)
Includes bibliographical references and index.
ISBN 978-0-87590-490-0 (alk. paper)
1. Atmosphere–Mathematical models. 2. Lagrangian functions. I. Lin, John, 1975- editor of compilation.
QC874.3.L34 2012
551.501'51539–dc23

2012041203

ISBN: 978-0-87590-490-0
ISSN: 0065-8448

Cover Image: Ash plume from Augustine Volcano on 30 January 2006 during its eruptive stage. Photograph of the plume at 13:09 AKST (22:09 UTC). Photograph credit: Game McGimsey. Image courtesy of Alaska Volcano Observatory/United States Geological Survey. (inset) PUFF volcanic ash Lagrangian Dispersion Particle Model (LDPM) at 22:09 UTC with ash particles indicated by altitude above sea level. Graph courtesy of Peter Webley, Geophysical Institute, University of Alaska Fairbanks.

Printed in the United States of America.

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PREFACE

Lagrangian modeling, particularly in the form of mean wind trajectories, has a long tradition in the atmospheric sciences as well as other fields of geosciences, such as oceanography. However, it has experienced explosive growth in the past few decades, thanks to theoretical advances converging with expanded computational power and increased bandwidth, which enables researchers to access three-dimensional meteorological fields from numerical weather prediction centers with which to drive the models.

As a result, Lagrangian models are playing an increasingly important role in different areas of research. Some examples include hydrometeorology, air quality, greenhouse gases, and emergency responses to volcanic eruptions and nuclear releases.

The AGU Chapman Conference "Advances in Lagrangian Modeling of the Atmosphere" was a unique opportunity for a diverse range of atmospheric researchers engaged in Lagrangian modeling, including theoreticians, developers, users, and observationalists, to congregate in the same room over 5 days in October 2011, surrounded by the beautiful scenery of Grindelwald, Switzerland.

The monograph you are holding was inspired by this Chapman Conference, as the presentations and discussions made abundantly clear the growing sophistication of Lagrangian modeling and the myriad ways in which Lagrangian approaches have been applied to yield insights into a variety of geophysical phenomena. Furthermore, participants recognized the lack of a comprehensive volume summarizing advances in Lagrangian modeling that would help a researcher starting in this field to quickly get up to speed. The few existing books on Lagrangian modeling are more focused on a single technical area or a specific application.

We hope this volume captures many of the advances in this important field and the excitement that was palpable among participants at the meeting. The reader can learn about the theoretical advances and outstanding problems, as well as the many applications in different fields written by their respective experts. It is our wish that this monograph can help graduate students and new researchers "see the forest," while providing enough description of individual "trees."

We owe an explanation to our oceanography colleagues. The decision was made during the planning of the Chapman Conference and the monograph to not focus on oceanic applications. This decision was due not to a lack of appreciation for the importance of Lagrangian approaches in oceanography but due to the simple realization that the number of papers would be overwhelming for a single meeting or book. In other words, to do justice to the important applications of Lagrangian models to the oceans, a separate monograph is necessary! That being said, some papers in the current volume explicitly tie together the ocean and the atmosphere through a Lagrangian perspective.

We would like to especially acknowledge the efforts of our fellow editors: Ashok Luhar, Andreas Stohl, and Peter Webley. We are grateful to the invaluable help from Carole Delemont and Stephan Henne during the conference. Financial support for the conference came from the European Science Foundation's TTORCH Research Networking Programme, the Swiss Academy of Sciences, the Center for Climate Systems Modeling at Swiss Federal Institute of Technology Zurich (ETH Zurich), and the International Foundation High Altitude Research Stations Jungfraujoch and Gornergrat.

Last, but definitely not least, for making this monograph possible, thanks go to AGU Meetings Department staff during the lead-up to the Chapman Conference and to Books Department staff during the preparation of the book.

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Lagrangian Modeling of the Atmosphere
Geophysical Monograph Series 200

10.1029/2012GM001355

Lagrangian Modeling of the Atmosphre: An Introduction

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Trajectory-based ("Lagrangian") atmospheric transport and dispersion modeling has gained in popularity and sophistication over the previous several decades. The objectives of this paper are twofold: (1) to provide a primer in Lagrangian modeling for readers of this AGU monograph and (2) to set the stage for the more technical and specialized papers that make up the rest of this monograph. Different types of Lagrangian modeling approaches (mean trajectory, box, Gaussian plume, and stochastic particle) are introduced; in addition, the advantages and disadvantages of Lagrangian models are discussed. Finally, linkages are made between the fundamentals of Lagrangian modeling and the content of this monograph.

1. INTRODUCTION

We spend our entire lives bathed in the atmosphere, yet most of us look right through it as if it were not even there. We are reminded of its importance, when we are hit by a cool breeze, soaked by a thunderstorm, choked by smoke, or gasp for breath in exhaustion. We breathe in and out molecules that make up the atmosphere, mostly nitrogen (N_2) and oxygen (O_2), with small quantities of argon (Ar), water (H_2O), carbon dioxide (CO_2), and other trace species. As these molecules move, interact, and modify radiant energy, the atmosphere gives rise to the bewildering array of phenomena that we are familiar with: wind, clouds, rainfall, and thunderstorms.

The state of the atmosphere dictates the physical conditions in which society is built, so the pursuit for a deeper understanding of the atmosphere has significant societal implications, in addition to scientific interest [*Crutzen and Ramanathan*, 2000]. This endeavor takes on added urgency, since humans are now understood to affect the atmosphere in numerous ways [*Intergovernmental Panel on Climate Change*, 2007], whether increasing the amount of greenhouse gases, altering the climate, or degrading air quality.

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Geophysical Monograph Series 200

10.1029/2012GM001376

A central requirement for understanding the atmosphere is the capacity to model its flow. There are two basic types of reference frames when thinking about the fluid: Lagrangian and Eulerian. Put simply, a Lagrangian perspective follows an "air parcel" (see section 2.1) around, as if one receives information from imaginary sensors, which monitor a fluid parcel's state as it moves (Figure 1a). This is contrasted with the Eulerian perspective, which is fixed in location and observes changes in fluid properties as the parcels are transported past the location (Figure 1b). The Lagrangian and Eulerian perspectives present complementary information. The Eulerian framework yields changes at a fixed location, which is natural for typical ground-based measurements or when stationary grid cells are adopted in modeling. The Lagrangian perspective follows the air parcel and so is intimately connected to the underlying flow.

The Lagrangian and Eulerian perspectives can be formally interchanged, as often discussed in textbooks on dynamic meteorology [*Holton*, 1992] and geophysical fluid dynamics [*Marshall and Plumb*, 2007]. If ψ represents any state variable associated with the air parcel (i.e., velocity, temperature, humidity, or pollutant concentration) and S is a generic source term, then the change in ψ in the Lagrangian reference frame can be written as:

$$\frac{D\psi}{Dt} = S, \tag{1a}$$

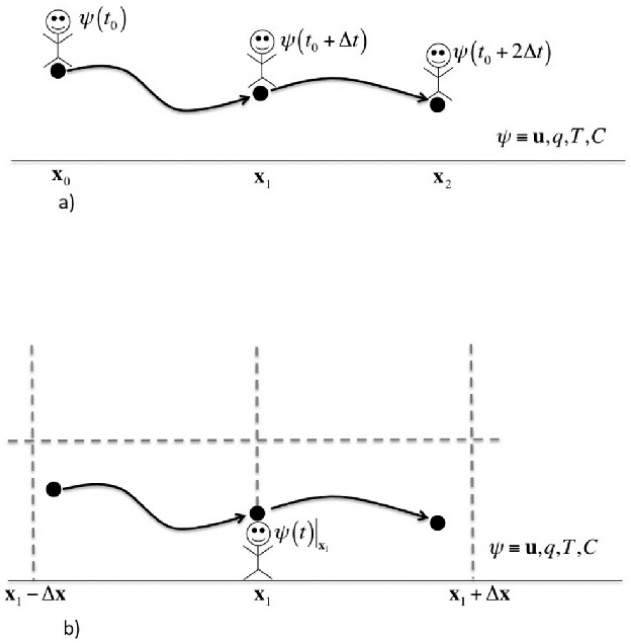

Figure 1. Comparison between the (a) Lagrangian and (b) Eulerian perspectives. In the Lagrangian perspective, the observer tracks the state variable(s) ψ of the air parcel as it moves in the atmosphere, while in the Eulerian perspective the observer remains stationary at fixed grid points and tracks the changes in ψ as the air parcel moves by. Note that the air parcel is often found in between grid locations (position is subgrid scale).

where D(. . .)/Dt represents the rate of change following the air parcel and is a special derivative given several names: the Lagrangian, total, substantial, or material derivative. For instance, if ψ is the temperature, then S denotes the sources/sinks such as diabatic heating or radiative cooling. In the case when ψ represents the velocity **u**, S stands for forces due to pressure gradients or rotation (such as Coriolis).

The Lagrangian perspective in equation (1a) can be transformed to the Eulerian reference frame with the nonlinear advection term $\mathbf{u} \cdot \nabla\psi$:

$$\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla\psi = S, \tag{1b}$$

where $\partial(\ldots)/\partial t$ represents the rate of change at a fixed position, and ∇ is the spatial gradient operator at the same position.

Since following an air parcel's position, **x**, traces out its trajectory, Lagrangian modeling is often referred to as "trajectory modeling." Using the definition D**x**/Dt = **u**, the velocity **u** can be integrated over time to yield the position of the air parcel, **x**, at various time steps. The reader is encouraged to read the detailed review on trajectory modeling by *Stohl* [1998], which focused especially on sources of error that affect the accuracy of the trajectories.

Integrating the equation D**x**/Dt = **u**, the following is the simplest first-order ("zero acceleration") solution [*Stohl*, 1998]:

$$\mathbf{x}(t_0 + \Delta t) = \mathbf{x}(t_0) + \mathbf{u}(t_0) \cdot \Delta t + \ldots, \tag{2}$$

where ". . ." indicates higher-order terms. Stated simply, Lagrangian modeling consists of determining the trajectory, **x**(t), and the values of different ψ at the different locations **x** and times t. The specific ψ of interest depends on the application at hand (see section 5): for instance, ψ = q (specific humidity) when tracking sources of moisture, whereas ψ = C (trace gas concentration) when tracking greenhouse gases.

Owing to the versatility and numerous advantages of Lagrangian models that will be discussed later, it has been applied to study a large variety of atmospheric phenomena and has grown in popularity and prominence over the previous two decades, with over a hundred papers currently published in the scientific literature every year (Figure 2).

In this introductory paper, the different types of Lagrangian models (section 2) are presented. Advantages and disadvantages of Lagrangian modeling versus its Eulerian counterpart follow in section 3. The particular importance of the underlying driver wind fields is also examined (section 4). Finally, the reader is introduced to the applications of Lagrangian models found within the contents of this monograph (section 5).

2. TYPES OF LAGRANGIAN ATMOSPHERIC MODELS

Different types of Lagrangian models are distinguished by their representations of air parcels. To illustrate the differences between models, let us begin by examining what exactly is an air parcel.

2.1. What Is an Air Parcel?

An air parcel is a concept often employed in atmospheric science. It is a "chunk" of the atmosphere that is large enough to encompass enough molecules to possess well-defined properties such as density, temperature, humidity, and pollutant concentration. On the other hand, it is small enough such that the parcel can be thought of as occupying an infinitesimal location in space. It is similar to the point mass or frictionless billiard ball commonly encountered by students in introductory physics.

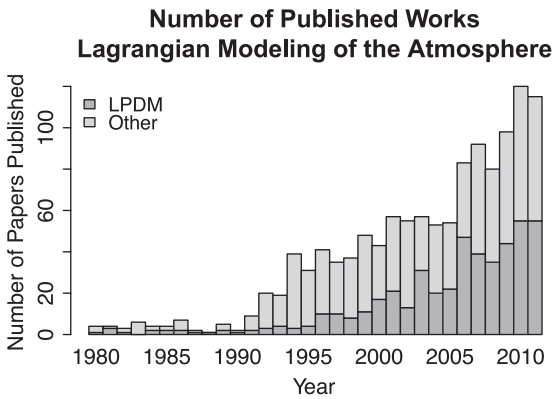

Figure 2. Estimates of the number of papers published per year relating to Lagrangian modeling of the atmosphere, between the years 1980 and 2011. "LPDM" papers refer to the number of published works applying or directly contributing to the development of Lagrangian particle dispersion models. "Other" papers show the number of works published on other topics such as mean trajectory modeling, Lagrangian box modeling, Gaussian puff modeling, and Lagrangian coherent structures. The literature search was carried out using Thomson Reuters's Web of Knowledge (http://apps.webofknowledge.com). While the retrieved papers from the search were manually checked to ensure no spurious papers were included, the possibility remains that a small number of papers may have been omitted. This figure, therefore, represents a lower bound on the number of works published.

The boundaries of an air parcel are fuzzy [*Bohren and Albrecht*, 1998], and a material surface originally encompassing the initial molecules constantly deforms due to molecular and turbulent diffusion, thereby losing their identities. The fact that individual parcels may lose their identities leads to treatment of many parcels in aggregate: as a box or a puff. Alternatively, numerous parcels can be handled more explicitly: as an ensemble of particles.

2.2. Mean Trajectories, Boxes, Puffs, and Particles

The mean trajectory modeling approach assumes that an air parcel retains its identity, and a single line is sufficient to describe its motion (Figure 3a). As indicated above, however, in order for the parcel to preserve its identity, both molecular and turbulent diffusion have to be neglected. The effect of molecular diffusion is small relative to turbulent diffusion throughout the atmosphere, except within a thin layer of a few centimeters near the ground surface [*Stull*, 1988]. Thus, the absence of turbulence is the main simplification to be considered in mean trajectories, whose name is based on the fact that the air parcel trajectory is derived by solely considering the mean velocity component $\overline{\mathbf{u}}$ and neglecting the turbulent, stochastic component $\mathbf{u}'$ in the Reynolds decomposition of $\mathbf{u}$ [*Reynolds*, 1895]:

$$\mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}'. \tag{3}$$

By neglecting turbulence, mean trajectories are the simplest representation and, thus, adopted for the longest time among all of the types of Lagrangian models. *Wiin-Nielsen* [1959] and *Danielsen* [1961] provide early examples of mean trajectory models. Such models would be more valid in atmospheric regimes where the flow is laminar or simply less turbulent (e.g., in the stratosphere). However, mean trajectories are poor indicators of average transport within the planetary boundary layer (PBL), where turbulence is strong [*Stohl and Wotawa*, 1993]. In this region of the atmosphere, an air parcel loses its identity as turbulent mixing and wind shear cause the

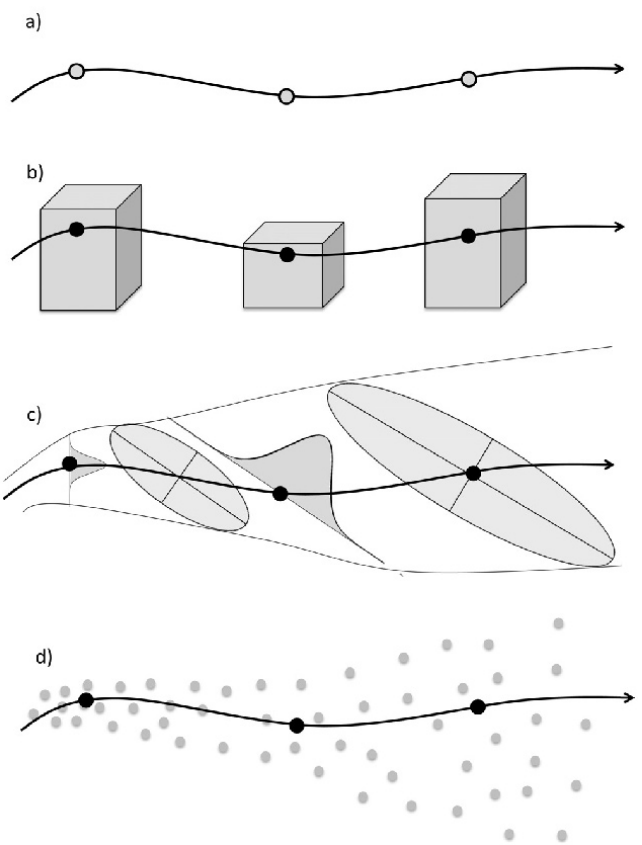

Figure 3. Schematic illustrating four types of Lagrangian models: (a) mean trajectories; (b) box models; (c) Gaussian puffs; and (d) Lagrangian particle dispersion models (LPDMs). The gray points or volumes represent air parcels, whether individual ones or in aggregate. Each black circle refers to the center of mass of air parcels at each time step. See main text for details.

molecules originally found within the air parcel to be dispersed, and a single trajectory no longer suffices.

Lagrangian box models (Figure 3b) treat numerous parcels in aggregate, as boxes whose volumes are described by the extent of mixing. Movement of the box is simulated by either single or multiple mean wind trajectories, initialized at different locations. Often the box is an atmospheric column whose top is matched to the top of the PBL [*Eliassen et al.*, 1982], in order to capture the effect of strong mixing within the PBL. Examples of Lagrangian box models include the single trajectory-based ELMO-2 model [*Strong et al.*, 2010] and the multiple trajectory-based CiTTYCAT model [*Pugh et al.*, 2012], both of which are applied to simulate atmospheric chemistry. While the multiple trajectory box approach better represents the effects on dispersion of flow deformation than a single trajectory method, the fact that the simulations are still based on mean wind trajectories translates into difficulties in modeling interactions between $\mathbf{u}'$ and wind shear that determine atmospheric dispersion in the lower troposphere. Furthermore, strong wind shear distorts the box and introduces large uncertainties to this approach [*Seaman*, 2000].

Puff models (Figure 3c) attempt to account for the effects of turbulent dispersion by representing air parcels as puffs that grow in size. The puffs usually take on Gaussian distributions in all three dimensions, following the classical work by G.I. Taylor [*Taylor*, 1920] describing plume dispersion in stationary, homogeneous turbulence. An example of a Gaussian puff model is CALPUFF [*Scire et al.*, 2000], which has been applied widely for air quality regulatory purposes.

Puff models work best when the turbulence and mean winds remain relatively constant. Puff models have difficulties capturing the interaction between turbulence and shear in mean winds in the PBL and lower troposphere, which distort plumes into non-Gaussian shapes, potentially introducing large biases into the peak concentrations and the plume area, thereby requiring ad hoc parameterizations such as puff splitting [*Walcek*, 2002]. Moreover, when multiple puffs interact, assumptions about puff merging are necessary.

Particle models (Figure 3d), often referred to as "Lagrangian particle dispersion models" (LPDMs), represent air parcels as particles of equal mass that are transported with random velocities generated by a Markov process [*Thomson and Wilson*, this volume] as a way to simulate $\mathbf{u}'$ and thus the effects of turbulence. An ensemble of particles is simulated by LPDMs to capture the stochastic effects of turbulence. Owing to the randomness introduced in the particle motion, the numerous particles disperse even when initialized at identical starting locations.

The particles in LPDMs possess special properties: they are small enough such that they "follow all turbulent eddies of the flow without being deformed" but are "large compared to the average distance between molecules" and are "so close in density to the surrounding fluid that neither their gravitational settling nor their buoyancy is significant" [*Luhar*, this volume].

LPDMs are the most sophisticated and computationally expensive, often tracking many thousands of particles in three dimensions. Whereas a single Gaussian puff sufficed to describe a plume of pollutants, many particles need to be tracked in order to characterize the plume. However, the computational cost is often outweighed by the benefit that LPDMs can bring, since they naturally deal with turbulent dispersion and its interaction with mean wind shear without ad hoc assumptions to split puffs.

Owing to the rapid rise in the availability of computational resources, full 3-D LPDM simulations that were expensive to run just a decade ago are now routinely carried out. Figure 2 shows the increase in papers published employing the LPDM method being particularly marked in the 1990s. Some examples of widely used particle models include FLEXPART [*Stohl et al.*, 2005], HYPACT [*Walko et al.*, 2001], and STILT [*Lin et al.*, 2003]. Some models even have hybrid capabilities that combine puff and particle characteristics. These models include HYSPLIT [*Draxler and Hess*, 1997], NAME [*Jones et al.*, 2007], and TAPM [*Hurley et al.*, 2005].

Most of the Lagrangian models focusing on tropospheric applications in this monograph are LPDMs. Furthermore, important theoretical advances have been made involving proper treatment of heterogeneous turbulence profiles (i.e., the "well-mixed criterion") [*Thomson*, 1987] and handling of boundaries [*Wilson and Flesch*, 1993].

The focus of the first part in this monograph is on proper formulation of LPDMs. This part includes a historical perspective [*Thomson and Wilson*, this volume], starting from the classical work by *Taylor* [1920] and extending all the way to recent advances, almost 100 years later. This part includes a specific case of Lagrangian modeling under low wind speed conditions [*Luhar*, this volume] and a diagnosis of a potential numerical issue within LPDMs, in which $\mathbf{u}'$ adopts unphysical values ("rogue velocity") [*Wilson*, this volume]. A specific parameterization for $\mathbf{u}'$ when turbulence is highly inhomogeneous, within the PBL and at its top, is also found [*Lin and Gerbig*, this volume].

2.3. Backward-Time Lagrangian Simulations

The trajectories of air parcels can be derived in a time-reversed manner by integrating equation (2) backward in time:

$$\mathbf{x}(t_0 - \Delta t) = \mathbf{x}(t_0) - \mathbf{u}(t_0) \cdot \Delta t + \ldots \tag{4}$$

Because the simulations proceed backward in time from a location of interest (the "receptor"), time-reversed simulations are also referred to as "receptor-oriented" [*Gerbig et al.*, 2003]. Such backward-time Lagrangian simulations can be used to address different questions than their forward-time counterparts (Table 1).

An example of backward Lagrangian simulations long adopted by the atmospheric science community is the "back trajectory" approach, which makes use of backward-time mean wind trajectories [e.g., *Blifford and Gillette*, 1972; *Fox and Ludwick*, 1976; *Sykes and Hatton*, 1976]. Typically, backward-time mean wind trajectories are almost perfectly time reversible: a mean back trajectory followed by a forward run retrieves the same starting position, assuming small enough time steps are adopted to minimize the numerical truncation and interpolation errors.

As discussed in section 2.1, mean wind trajectories are applicable in regions of the atmosphere experiencing minimal turbulence. However, they are subject to significant errors in the lower troposphere, in the vicinity of surface emissions. Yet time-reversed Lagrangian modeling is necessary precisely in the lower troposphere to understand surface emissions. Toward this end, LPDM models that run backward in time have been developed and are increasingly applied over the past decade. Because LPDMs incorporate the stochastic velocity $\mathbf{u}'$, time-reversibility in LPDMs is more difficult to ensure than in mean trajectories. It has been pointed out that time reversibility of LPDM simulations requires attention to the well-mixed criterion, as well as several other physical criteria [*Lin et al.*, 2003].

The types of information yielded by backward-time LPDM simulations take on different forms. The "retroplume" [*Stohl et al.*, 2003] refers to the ensemble of Lagrangian particles transported backward in time. From "touchdown velocities" of time-reversed particles, the source region of emissions at micrometeorological scales can be determined [*Flesch et al.*, 1995; *Wilson et al.*, this volume]. The "footprint" of an atmospheric concentration is its sensitivity to a unit emission in upwind source regions and is derived from the locations and times of particles found close to the ground [*Lin et al.*, 2003].

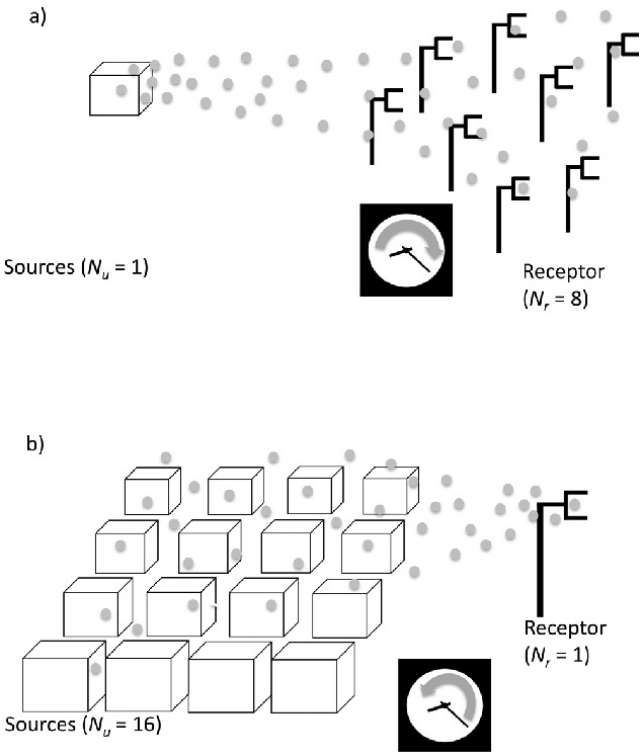

Figure 4. Contrast between instances that call for Lagrangian particle dispersion models that run (a) forward in time versus (b) backward in time. The relative computational effort necessary for backward-time versus forward-time simulations depends on the ratio between the number of receptors (N_r) in relation to the number of resolved upwind (N_u) elements. In Figure 4a, the forward-time approach is more computationally expedient because the air from a single source (N_u = 1) is observed by numerous receptors (N_r = 8). In contrast, in the case of Figure 4b, the backward-time method is more efficient because a single receptor (N_r = 1) is sampling air from 16 upwind source elements (N_u = 16).

Table 1. Some Examples of Questions That Can Be Addressed by Forward-Time Versus Backward-Time Lagrangian Simulations

Forward	Backward
Where does the air go?	Where does the air come from?
What is the downwind impact of air originating from a location of interest (source)?	What are the upwind influences on the location of interest (receptor)?
Where do tracers get transported?	Where are the source regions of tracers?
How much is the concentration of a passive tracer at downwind locations affected by a unit emission from the source?	How strong is the sensitivity of the receptor to a particular upwind source region?

If a LPDM is constructed to be time-reversible, why would a researcher carry out a backward-time rather than a forward-time simulation? The answer comes down to the number of receptors (N_r) in relation to the number of upwind (N_u) elements which are resolved [*Lin et al.*, 2003; *Seibert and Frank*, 2004]. The ratio N_r:N_u yields the relative computational effort necessary for the backward simulation versus the forward simulation (Figure 4). When $N_r << N_u$, the backward-time LPDM approach is much more computationally efficient than

its forward-time counterpart. For instance, Figure 4b shows an example in which $N_r = 1$ and $N_r << N_u$. In this case, a single backward-time simulation can reveal the upwind source region. In contrast, the forward-time approach requires many simulations starting at all N_u potential source region elements, entailing a significantly larger computational effort.

An example of a research field in which backward-time LPDM models have made widespread contributions is in inverse analyses for diagnosing emissions of trace gases from atmospheric concentrations. Here a common issue is that the number of measurement locations (N_r) is significantly smaller than the number of regions where the emissions need to be solved for (N_u). The backward LPDM runs efficiently to provide the sensitivity of receptor concentrations to upwind source regions (i.e., the Jacobian matrix) [*Seibert and Frank*, 2004] that is an essential part of the inverse analysis. The interested reader can refer to part 3 of this volume for examples of backward LPDMs applied in the context of inverse analyses. Backward-time LPDM models can also be constructed to simulate sources/sinks of water vapor [*Stohl and James*, 2004] or chemical transformations of atmospheric compounds [*Wen et al.*, 2012]. Parts 2 and 4 of this monograph contain papers applying backward-time LPDM models to water vapor and atmospheric chemistry, respectively.

3. ADVANTAGES AND DISADVANTAGES OF LAGRANGIAN MODELING

In this section, the advantages and disadvantages of Lagrangian modeling are examined.

3.1. Advantages of Lagrangian Modeling

3.1.1. Availability of trajectory information. Lagrangian simulations provide trajectory information (either forward or backward in time) that is lacking from Eulerian simulations. The knowledge of air parcel trajectories serves as powerful information to answer scientific questions, as the many papers in this monograph will illustrate.

3.1.2. Physical realism. The Lagrangian approach is a closer analog to atmospheric flows by simulating air parcels. At its essence, the atmosphere is Lagrangian: air is comprised of molecules, and atmospheric flow consists of molecules being transported. Thus, the Lagrangian approach possesses the potential to better approximate phenomena that exist in atmospheric flows such as mixing [*Konopka et al.*, this volume], transport barriers [*Sulman et al.*, this volume], turbulent eddies [*Thomson and Wilson*, this volume], and convection [*Haertel*, this volume].

3.1.3. Capability of describing nondiffusive near-field to sources. LPDMs, in particular, can capture the physics of turbulent transport in the "near-field" regime close to the sources, where turbulence is nondiffusive (or countergradient). See the work of *Thomson and Wilson* [this volume] for more details.

3.1.4. Numerical stability. Owing to the absence of the nonlinear advection term in Eulerian models (equation (1b)) and the resulting linearity of Lagrangian advection (equation (1a)), integration of the Lagrangian equations is numerically stable, even when time steps are taken, which are larger than specified by the Courant-Friedrichs-Lewy criterion [*Staniforth and Cote*, 1991; *Wohltmann and Rex*, 2009].

3.1.5. Lack of numerical diffusion. Eulerian advection is known to smear out scalar gradients due to nonphysical numerical diffusion, whose strength is larger than that of atmospheric diffusion [*Shin and Reich*, 2009; *Smolarkiewicz and Pudykiewicz*, 1992]. In contrast, Lagrangian advection is subject to minimal numerical diffusion and preserves scalar distributions where sharp gradients exist in the atmosphere, e.g., the polar vortex [*McKenna et al.*, 2002b]. This enables Lagrangian models to parameterize mixing processes that exhibit stronger fidelity to actual atmospheric mixing [*McKenna et al.*, 2002a; *Wohltmann and Rex*, 2009; *Konopka et al.,* this volume].

3.1.6. Conservation properties. The Lagrangian framework is a natural way to express conservation properties: conservation of energy, mass, and momentum follows straightforwardly when one considers the same air parcel and follows its movement. While Eulerian advection schemes may not conserve mass [*Brasseur et al.*, 1999] and may produce spurious negative mixing ratios [*Rood*, 1987], no such difficulties are encountered when one simply tags a parcel with a tracer concentration and follows it along, as is the case for Lagrangian advection [*Henne et al.*, this volume].

3.1.7. Resolving subgrid scale variability. The positions of Lagrangian air parcels are not tied to regular grid cells (Figure 1). This means that the air parcels can carry subgrid-scale information, helping to resolving the finer-scale heterogeneity not resolved by Eulerian grid cells [*Lin et al.*, 2003]. This is particularly important in the areas immediately upwind of the receptor site for backward-time models or directly downwind of a source region.

3.2. Disadvantages of Lagrangian Modeling

3.2.1. Computational cost. Lagrangian models are often computationally cheap to run in comparison to Eulerian

models, in large part because they do not solve the atmosphere's equations of motions, but instead rely on output from Eulerian models (section 4). However, depending on the specific application, the computational cost of Lagrangian models can be significant. This is particularly so for LPDMs that simulate large particle ensembles and adopt small time steps to resolve turbulent velocity fluctuations [*Thomson and Wilson*, this volume]. With the widespread availability of computational resources, however, the disadvantage associated with computational cost is being overcome. Also, for applications in which the air parcels need not interact with one another, Lagrangian simulations are "embarrassingly parallel" and can be parallelized with minimal effort, in which different parcels can be simulated using separate computational nodes. An example of such a simulation is Lagrangian modeling of a chemically inert trace gas like CO_2 [*Zeng et al.*, this volume].

3.2.2. Irregularity of "grids". The fact that Lagrangian air parcel positions are not fixed at regular intervals like grid cells in Eulerian models means that the "grid" comprised by the ensemble of trajectories would be irregular, even if the parcels were initialized at regular intervals. This requires an additional procedure of parcel insertion or merging [*McKenna et al.*, 2002a], parcel counting within regular grid cells [*Stein et al.*, 2000; *Tinarelli et al.*, this volume], kernel density estimators [*Song et al.*, 2003], or parcels representing dynamic volume [*Haertel*, this volume].

3.2.3. Inconsistencies with Eulerian driving meteorological fields. Most Lagrangian models require gridded output from another Eulerian model to simulate air parcel trajectories. See section 4 for a discussion on this point. The two models can be inconsistent with one another, especially if variables are omitted in the output or interpolated from internal model coordinates to common pressure levels. A new development in Lagrangian modeling is overcoming such inconsistencies by having the Lagrangian model simulate atmospheric dynamics, thereby bypassing the Eulerian model entirely [*Alam and Lin*, 2008; *Haertel*, this volume].

4. METEOROLOGICAL FIELDS TO DRIVE LAGRANGIAN ATMOSPHERIC MODELS

For the vast majority of Lagrangian models, equation (1a) is not solved for $\psi = \mathbf{u}$. Instead, the **u** field (along with other meteorological variables) is generated by an Eulerian model: either an operational numerical weather prediction model, a general circulation model, or a mesoscale model. The **u** field from the output is then interpolated to the air parcel location and then integrated in time to determine the trajectory (equation (2)).

The "garbage in, garbage out" principle holds for Lagrangian modeling: the quality of Lagrangian simulations can hardly be enhanced if the input meteorological fields are not improved [e.g., *Davis and Dacre*, 2009; *Kretschmer et al.*, this volume; *Webley and Steensen*, this volume]. This means that the driver meteorological fields require as much attention as the Lagrangian model itself.

Other than **u**, another important quantity provided by the driving meteorology is the mixing height: i.e., the vertical extent and intensity of mixing within the PBL. Applications in trace gas transport are strongly dependent on the mixing height [*Gerbig et al.*, 2008]; yet methods to diagnose these properties from meteorological fields are still unsatisfactory in many cases [*Seibert et al.*, 2000]. This has led to efforts to directly assimilate mixing height observations within the Lagrangian simulations [*Kretschmer et al.*, this volume].

Owing to storage limitations, the Eulerian output is often degraded in temporal (and sometimes in spatial) resolution [*Stohl et al.*, 1995] and interpolated to pressure levels [*Hoerling and Sanford*, 1993]. One symptom of the degradation in the driving meteorological fields is violation of mass conservation, which has been shown to affect simulated trajectories in a way that forward and backward LPDM simulations yield inconsistent results (nonreversibility) [*Lin et al.*, 2003]. Utilization of assimilated meteorological data from different assimilation cycles, which is required to cover transport periods longer than the forecast period, causes dynamical inconsistencies, with dramatic effects on stratosphere-troposphere exchange fluxes [*Stohl et al.*, 2004]. Owing to the same reason, spurious changes in specific humidity and equivalent potential temperature were observed along Lagrangian trajectories, indicating inconsistencies in the humidity and heat budgets [*Stohl et al.*, 2004].

To minimize inconsistencies between the Eulerian output and the Lagrangian models, efforts have been undertaken to closely couple the two kinds of models, with an eye toward conservation properties [*Brioude et al.*, 2012; *Nehrkorn et al.*, 2010].

5. APPLICATIONS OF LAGRANGIAN MODELS

This monograph includes numerous papers that take advantage of the strengths of Lagrangian models mentioned in section 3 to address geophysical questions of interest.

Part 1 of this volume focuses on the formulation of LPDMs and has already been mentioned above in section 2.1.

Part 2 examines the application of Lagrangian models to study geophysical flows. Trajectories can be used to construct "Lagrangian coherent structures" that reveal transport

pathways and mixing characteristics of geophysical flows, both in the atmosphere and the ocean [*Sulman et al.*, this volume]. The geophysical flow can be solved in a Lagrangian frame, taking advantage of its numerical strengths (section 3.1) to build Lagrangian dynamical models of both the atmosphere and the ocean [*Haertel*, this volume]. *Konopka et al.* [this volume] examine the issue of numerical diffusion in particular, showing how the strength of numerical diffusion can be controlled explicitly in Lagrangian (irregular) grids to mimic actual atmospheric diffusion. The role of geophysical flows in transporting water, the all-important ingredient of weather and climate, is investigated by *Liberato et al.* [this volume], who combine Lagrangian investigation of moisture sources and a storm-tracking methodology to study an extreme flood event in Portugal. *Orza et al.* [this volume] examine the transport pathways in Europe and their association with the North Atlantic Oscillation by adopting a back-trajectory clustering technique.

Part 3 is a compendium of several papers applying Lagrangian models to understand greenhouse gases (GHG). The target species is CO_2 in most of the papers, and one paper focuses on halocarbons [*Brunner et al.*, this volume], but the framework and discussion in this part is relevant for most other GHGs (e.g., methane (CH_4) or nitrous oxide (N_2O)). The framework involves tagging particles in LPDMs with concentrations of GHGs and comparing against measured concentrations to derive regional-scale surface fluxes as part of a formal inverse framework [*Brunner et al.*, this volume; *Kretschmer et al.*, this volume; *Oda et al.*, this volume; *Zeng et al.*, this volume]. The LPDMs are run backward in time, due to the smaller number of GHG observational sites versus the number of source elements (section 2.3). An application of backward-time Lagrangian models to determine micrometeorological (local)-scale emissions is also presented [*Wilson et al.*, this volume].

Part 4 examines species in the atmosphere, which undergo chemical transformations and deposition, unlike many GHGs, which are relatively inert in the atmosphere. An approach is to leverage the myriad advantages for simulating tracer transport in Lagrangian models and combine them with linearized chemistry [*Henne et al.*, this volume]. A related linear approach is to first simulate atmospheric transport backward in time, using a Lagrangian model, and then carry out a regression analysis to solve for coefficients controlling both the rates of chemical mechanisms as well as emission strengths [*Benmergui et al.*, this volume].

Part 5 examines the role of Lagrangian models as a central component of emergency warning systems that predict the transport and dispersion of materials that could pose immediate societal risks, which unfortunately have been amply borne out by two events in recent memory. As demonstrated by the 2010 eruption of Eyjafjallajökull in Iceland, one threat includes volcanic ash [*Denlinger et al.*, this volume; *Webley and Steenson*, this volume]. Second, the meltdown at Japan's Fukushima Daiichi nuclear power plant following the 2011 earthquake showed the continuing risk of accidental releases of radioactive species from nuclear sites [*Arnold et al.*, this volume]. This part of the volume also includes an example of a sophisticated LPDM and illustrates its application in simulating accidental releases and urban pollution dispersion [*Tinarelli et al.*, this volume].

In conclusion, the numerous applications discussed throughout this monograph underscore the fact that Lagrangian models play a critical role in helping scientists understand phenomena in the geosciences and assisting human society to grapple with several hazards, either natural or anthropogenic in origin. It is my belief that Lagrangian models will continue to grow in significance as a tool in the researcher's arsenal (Figure 2) and follow its own "upward trajectory" in sophistication and usefulness.

Acknowledgments. I am grateful to Joshua Benmergui for comments and assistance in preparing Figure 2. Valuable input from fellow editors of this monograph is also acknowledged.

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Section I
Turbulent Dispersion: Theory and Parameterization

Turbulent Dispersion: Theory and Parameterization—Overview

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The Lagrangian stochastic modeling approach for describing dispersion is based on the study of the random motion of particles as they travel in a given turbulent flow. It has its origins in the theory of Brownian motion, particularly the Langevin equation. This section concerns developments in the theory and application of this approach. A brief introduction to the theme of the present section is followed by an overview of its four chapters. They present the following: a lucid, up-to-date account of the history of Lagrangian stochastic models and the current use of the "well-mixed condition" for model derivation; an application of the approach with varying model formulations for dispersion in light winds under different atmospheric stabilities; the issue of unrealistically large magnitudes of particle velocity in numerical schemes used for solving stochastic model equations; and how to ensure the well-mixed state of particles in cases where the input flow and turbulence quantities may have sharp gradients.

The basis of the Lagrangian approach of dispersion is the study of the stochastic motion of particles (or marked fluid elements) as they travel in a given turbulent flow. The statistical theory of Brownian motion developed by Einstein, Langevin, Ornstein and Uhlenbeck, and others in the early years of the last century and summarized in a fundamental paper by *Chandrasekhar* [1943], provides a useful background to tackling the more difficult problem of turbulent dispersion. In Brownian motion, a particle of colloidal size (called a Brownian particle) undergoes random collisions in succession (~10^{21} collisions per second) with the molecules of the surrounding fluid, which is assumed to be uniform and steady (or stationary). Each collision produces a random change in the particle velocity. In addition, the Brownian particle experiences a viscous resistance in the fluid, which damps its velocity. The time scale (τ_B) at which the particle ceases to "remember" its initial velocity due to this viscous resistance is very small, typically of the order of one-hundredth of a microsecond [*Csanady*, 1973]. The quantity τ_B can also be thought of as the time scale on which the Brownian particle exchanges momentum with the fluid and is referred to as the relaxation or dissipation time. Because τ_B is very small, and the time intervals of interest are generally larger than τ_B, it can be assumed that the velocity of the particle changes with random jumps after every time interval. This suggests that the particle velocity can be modeled by a white-noise process. However, if the time intervals of interest are smaller than τ_B, a better model for Brownian motion is the Langevin equation, in which the change in particle velocity (i.e., particle acceleration) is modeled as a sum of two components: a systematic (or deterministic) part, representing the viscous resistance experienced by the particle, and a random part, which represents the change in the particle velocity due to its collision with the molecules of the surrounding fluid.

In turbulent dispersion, the motion of particles on a macroscopic scale is considered, whereby a particle undergoes random impacts in a field of turbulence (which is characterized by ambient fluid parcels, or eddies, of diverse shapes and sizes undergoing irregular movements). Particle displacements due to Brownian forces at the molecular scale continue to occur, but are statistically independent and negligibly small compared to those due to turbulent impacts (see the

Lagrangian Modeling of the Atmosphere
Geophysical Monograph Series 200
Published in 2012 by the American Geophysical Union.
10.1029/2012GM001432

work of *Csanady* [1973] for a detailed introduction to turbulent dispersion). In the case of turbulent flows, the analog of τ_B is τ_L, the Lagrangian integral time scale; the latter can be a function of time and space depending on the complexity of the turbulent flow under consideration. Typically, the magnitude of τ_L is tens of seconds to a few minutes in the atmospheric boundary layer. For these flows, we are often interested in time intervals smaller than τ_L, and therefore, the Langevin concept of particle velocity increment is taken as the starting point for constructing Lagrangian stochastic models of turbulent dispersion [see *Thomson and Wilson*, this volume, equation (1)].

Before the Langevin model was adopted as a framework for turbulent dispersion, *Taylor* [1921] published his landmark paper, presenting an analytical Lagrangian analysis of the continuous motion of particles released from a single point in homogeneous, stationary turbulence. His analysis showed that the near-field (or small-time) behavior of the root-mean-square particle displacement is proportional to travel time (t), whereas the far-field (or large-time) behavior is proportional to $\sqrt{t}$. The latter represents the diffusive phase in which the size of the plume (or puff) is larger than the size of the dominant turbulent eddies. The time of transition between the near field and far field depends on the properties of the turbulent flow as well as the initial source characteristics. Traditional eddy-diffusion (or gradient-transfer) models based on the Fickian theory of molecular diffusion are able to represent the far field, but not the near field in which the plume size is small compared to the size of the dominant turbulent eddies (hence, these eddies transport the initial plume instead of diffusing it). In contrast, the basic Langevin model for an idealized field of homogeneous and stationary turbulence reproduces the analytical forms of both near- and far-field behaviors of tracer dispersion.

The theme of the present section is Lagrangian stochastic modeling of mean dispersion in a turbulent flow. This approach normally involves releasing a large number of particles corresponding to different flow realizations with suitable initial conditions, such as a point source. The motion of each particle is treated as completely independent of that of other particles and is determined via a set of stochastic differential equations for velocity and position increments. The calculated trajectory distribution simulates the source plume and can be used to compute mean dispersion quantities, such as the average concentration, mean plume height, or plume spread. Increasing the number of particles reduces the statistical uncertainty in the dispersion calculations. With the present-day computational resources, it is feasible to release particles numbering hundreds of thousands to a few million for short-range dispersion studies. This type of modeling for mean dispersion is also referred to as one- or single-particle modeling because the motion of each particle is independent.

While *Taylor*'s [1921] analysis provided a solid foundation for understanding diffusion and developing parameterizations of diffusion coefficients in applied Gaussian models, its scope for application to complex, real-world flows was limited. The first paper in this section, by *Thomson and Wilson* [this volume], provides a lucid account of the history of Lagrangian stochastic models for turbulent dispersion, involving the differing ways in which the deterministic and random terms were constructed. These authors discuss early heuristic Lagrangian stochastic models when the Langevin framework involving a Gaussian random forcing started to be extended to nonidealized flows in the lower atmosphere. This required numerical computations as the flow complexity made derivation of any analytical solutions impossible. Models were formulated for inhomogeneous flows by varying τ_L with space, by varying both τ_L and the Eulerian velocity variance with space, by considering particle velocity scaled by its standard deviation, and by considering a skewed random forcing for application to non-Gaussian turbulence. Their applications ranged from small-scale canopy turbulence to the full convective boundary layer dominated by large-scale thermals and downdrafts. As *Thomson and Wilson* [this volume] report, some of these applications demonstrated a remarkable degree of success of the Lagrangian stochastic approach, but there were several problems, some fundamental (such as the use of a skewed random forcing, which is strictly unrealizable and may lead to negative probabilities).

In his seminal paper, *Thomson* [1987] developed a generalized Lagrangian stochastic framework by considering particle motion as a continuous Markov process in velocity-position phase space. He demonstrated that the random forcing term must be Gaussian and developed a set of rigorous criteria that a Lagrangian stochastic model needs to meet. Moreover, *Thomson* [1987] showed that if one of the criteria, the so-called well-mixed condition, is satisfied, the rest will be satisfied, too. In simple terms, the well-mixed criterion states that in a bounded region away from the source, if the distribution of particles becomes well mixed, then it should remain so for all subsequent times. It is equivalent to the second law of thermodynamics and is mathematically represented by the Fokker-Plank equation for the evolution of the probability density function of particle velocity and position. The Thomson well-mixed condition now serves as the basis for the derivation of the deterministic term of a Lagrangian stochastic model and for checking model consistency. It leads to a unique model in one dimension, and a unique 3-D model can be constructed if variables in one dimension are assumed to be independent of those in the other dimensions.

However, if there is a dimensional interdependence of variables (e.g., the velocity covariances in the neutral surface layer), the well-mixed condition does not lead to a unique solution, and different models satisfying the well-mixed criterion can yield different dispersion estimates. As pointed out by *Thomson and Wilson* [this volume], there remains room for progress on further selection criteria for the multidimensional case.

Several specialized stochastic model formulations and applications have followed the work of *Thomson* [1987] in atmospheric dispersion areas such as the atmospheric boundary layer under different stability conditions, urban and vegetation canopies, complex terrain and coastal dispersion processes, nonpassive tracers (e.g., buoyant plumes, heavy gases, and heavy particles), chemically interactive particles, concentration fluctuations (e.g., through micromixing techniques). Lagrangian stochastic models have also been developed in an inverse framework for estimating source strength based on ambient concentration measurements and for determining flux footprint of upwind sources at a measurement point. These models are also being used in operational air pollution modeling systems, sometimes in a hybrid manner (for example, through coupling with a Gaussian puff model and/or an Eulerian gradient-transfer model) for improved computational efficiency.

The second paper by *Luhar* [this volume] presents an application of the Lagrangian stochastic approach to dispersion in light winds, which are characterized by horizontal plume meandering and significant upwind diffusion. In stable atmospheric conditions, two model formulations in the horizontal plane are considered: one in which the Lagrangian velocity autocorrelation is oscillatory and the other, a more traditional one, with an exponential Lagrangian velocity autocorrelation. The turbulence is axisymmetric along the vertical direction. This is a simple case of model nonuniqueness where both models satisfy the Thomson well-mixed condition, but the first one is known to lead to significant reduction of dispersion and spiraling particle trajectories compared to the second. *Luhar* [this volume] finds that the first model performs slightly better; its use of an oscillatory velocity autocorrelation is supported by the light wind data considered. (This indicates that how well a particular model represents the flow is not fully determined by the well-mixed condition, and additional conformities are needed.) It is emphasized that regardless of which model formulation is used, the time scales and the turbulent kinetic energy must include the low-frequency meander component in the horizontal. *Luhar*'s [this volume] subsequent modeling of dispersion in the convective boundary exemplifies the increasing importance of the effects of upwind diffusion and of the time elapsed since the start of the release as the wind becomes lighter. He also quantifies the decrease in the maximum ground-level concentration and the increase in the ground area impacted by a given concentration level, with decreasing wind speed.

Lagrangian models for real-world flows employ numerical methods to calculate particle velocity. Occasionally, the magnitude of particle velocities can take unrealistically large values, sometimes even beyond the possible computational bounds. The third paper, by *Wilson* [this volume], terms these "rogue velocities" and examines if one reason for their occurrence is the use of an insufficiently small time step (Δt) in the numerical scheme. An artificial case of 1-D inhomogeneous Gaussian turbulence, in which two spatial regimes of differing constant velocity variance are joined by a linear ramp, is considered. In this, the gradient in the velocity variance is discontinuous at the two ends of the ramp region. The tracer distribution is initially well mixed, and its evolution is computed by numerically integrating the Chapman-Kolmogorov equation. For comparison, the evolution is also computed using a Lagrangian stochastic model. The selected field of Eulerian velocity statistics implies an inhomogeneity time scale (τ_D) that is an order of magnitude smaller than τ_L (it is more appropriate to term the latter as a Lagrangian decorrelation time scale in inhomogeneous turbulence). It is shown that when Δt is much smaller than both τ_D and τ_L, the particles remain well mixed. However, when $\Delta t \approx \tau_D << \tau_L$ the well-mixed condition is violated, and rogue velocities occur. In practical applications, it is generally not feasible to decrease the time step sufficiently to eliminate rogue velocities, and researchers use various fixes to deal with the problem. *Wilson* [this volume] concludes that rogue velocities may be tolerable when one is only interested in the mean concentration, but they may pose difficulties when computing higher-order moments of concentration via techniques involving the one-particle Lagrangian stochastic approach.

Lagrangian stochastic models have traditionally been driven by semiempirical parameterizations of flow and turbulence quantities, often involving similarity relationships. Such parameterizations are constantly under development based on new/better observational studies. For common flows, these are scattered among research papers and books on the atmospheric boundary layer [e.g., *Stull*, 1988], but a compilation with suggested generalized forms can be found in the work of *Rodean* [1996]. In these parameterizations, the vertical variation of flow and turbulence quantities and their gradients is continuous, and it is often assumed that the turbulent flow is horizontally homogeneous. However, Lagrangian stochastic models are increasingly being coupled to atmospheric flow models for real-world applications at a range of scales. Unlike the parameterized forms, the predicted flow and turbulence quantities are discrete in time,

spatially gridded, nonstationary, and may have sharp horizontal and vertical gradients. The last paper, by *Lin and Gerbig* [this volume], emphasizes that in such a complex flow field, the particle distribution can deviate from the well-mixed state. They consider an example case in which vertical turbulence at discrete altitudes is treated as step functions. Hence, the turbulence is homogeneous in each vertical layer, but discontinuous at the interface between two layers. *Lin and Gerbig* [this volume] devise a practical reflection/transmission algorithm for handling the particle behavior at the interface. Its application for a number of increasingly complex turbulence cases shows that it preserves the well-mixed condition. One advantage of this scheme is that because the turbulence is homogeneous within layers, the computational time step is not restricted by the relatively small value of the time scale implied by the turbulence inhomogeneity. The reflection/transmission scheme was not tested within a flow model at regional or global scale, but the scheme has potential for use in operational modeling.

The present-day Lagrangian stochastic models find their use in transport and dispersion applications ranging from micrometeorological to global scales. The success of the Lagrangian approach in addressing a wide range of dispersion processes has also led to its further development, including in areas such as source determination and nonpassive sources. Hybrid techniques, taking advantage of the capabilities of both Lagrangian and Eulerian approaches, have also been formulated to enhance computational efficiency in operational modeling systems. However, as illustrated by the papers in this section, there is always scope for further developments, including research on aspects such as theory, numerics, and parameterizations, as well as new applications including higher-order concentration statistics and formulations for operational use.

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History of Lagrangian Stochastic Models for Turbulent Dispersion

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This article briefly summarizes the historical evolution of the modern Lagrangian stochastic (LS) class of models for the calculation of fluid element (or particle) paths in turbulence. The fundamental advantages of a "first-order" LS model relative to alternative descriptions of turbulent dispersion are (1) its ability to correctly describe the concentration field even in the nondiffusive "near field" of sources and (2) its ability to rationally incorporate all available statistical information on the velocity field, even in the case that the latter is nonstationary and inhomogeneous in all directions. There are also advantages of convenience: for example, being grid free, LS models are easy to implement; and because particle paths are computed independently, they are amenable to easy parallelization. LS models are presently used to treat atmospheric transport and dispersion problems on scales ranging from the intercontinental (for which case typically they are "driven" by motion fields from numerical weather models) down to the scale of the atmospheric surface layer (meters to hundreds of meters). Papers at the Chapman Conference on Langrangian modeling, from which this chapter was derived, exhibited many interesting applications.

1. INTRODUCTION

The aim of a Lagrangian stochastic (LS) model is to compute an ensemble of random paths of marked fluid elements through a turbulent flow, based on knowledge of velocity statistics. The simplest class of LS model is the random displacement model (RDM, or zeroth-order LS model), which represents a particle trajectory by a sequence of random increments in position. The more sophisticated "generalized Langevin approach" or first-order LS model (which draws ideas from Langevin's 1908 work on Brownian motion) creates the particle path by integrating a sequence of (damped) random increments in *velocity*, such that the particle position **X** and velocity **U** together constitute a Markovian state variable. To be more specific, the general form of the first-order model is

$$\mathrm{d}U_i = a_i\ \mathrm{d}t + b_{ij}\ \mathrm{d}\xi_j, \tag{1}$$

$$\mathrm{d}X_i = U_i\ \mathrm{d}t \tag{2}$$

where t is time, $a_i = a_i(\mathbf{X}, \mathbf{U}, t)$ is the systematic part of the acceleration, and b_{ij} (normally diagonal) is another coefficient scaling the random Gaussian forcing $\mathrm{d}\xi_j$. Equations (1) and (2) can be integrated numerically by replacing the infinitesimal $\mathrm{d}t$ with a finite time step Δt, whose magnitude may vary along the trajectory in proportion to a local turbulence time scale. Heuristic arguments for the validity of equation (1) as an approximation to the Navier-Stokes equations can be made

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[e.g., *van Dop et al.*, 1985], and specification of the coefficients a_i, b_{ij} is the selection problem for LS models. Many interesting and useful models are known, applying to diverse regimes of turbulence spanning from the ideal (unbounded homogeneous, isotropic turbulence) through the everyday (stratified atmospheric surface layer in a horizontally homogeneous state; convective boundary layer (CBL)) to the exotic (three-dimensionally inhomogeneous urban flow with buildings resolved).

However, this article is not intended as a thorough review of the science of modern Lagrangian models, which may be sought elsewhere [*Sawford*, 1985; *Thomson*, 1987; *Wilson and Sawford*, 1996; *Rodean*, 1996]. Rather, its intent is to capture some of the broad trends and developments that have brought us to where we now are. We give some flavor of the antecedent models and of the diverse disciplines, backgrounds, motivations, and styles of early contributors; we illustrate the range and impact of contributions driven by intuition and by rigor; and we note a chronological evolution in the specificity of the turbulence regime addressed and in the degree of connection with (or disconnection from) observations of dispersion. We restrict the focus to LS models where the particles are (conceptually) sampled independently from an ensemble of turbulent flows and so move independently (so called one-particle models), and to nonbuoyant and nonreactive ("passive") particles, in flows for which the turbulence prescription is limited to single-point statistics. Meteorological applications are emphasized.

2. EARLY DEVELOPMENT OF THE LAGRANGIAN PERSPECTIVE ON TURBULENT DISPERSION

Taylor [1921] provided an exact Lagrangian solution for the rate of spread of tracer in unbounded, stationary homogeneous turbulence. Let us take the case where particles are independently released into such a flow at $z = 0$ (here, and generally when we consider dispersion in one dimension only, we take the direction to be the vertical axis). For each realization, i.e., for each trajectory, the clock is reset ($t = 0$) upon release. Taylor showed that the rate of increase in time of the ensemble mean spread (as measured by the variance $\overline{z'^2} \equiv \sigma_z^2$ of displacement along the z axis) is given exactly by (Taylor's equation 17)

$$\frac{d\sigma_z^2}{dt} = 2\int_0^t \overline{w(t')w(t'+\xi)}\; d\xi \equiv 2\sigma_w^2 \int_0^t R_{ww}(\xi)\; d\xi, \qquad (3)$$

where $R_{ww}(\xi)$ is the Lagrangian velocity autocorrelation function, first introduced by Taylor, and σ_w^2 the velocity variance. (In terms of the eddy diffusion paradigm, the left-hand side of equation (3) is twice the eddy diffusivity). Integrating this result gives

$$\begin{aligned} \overline{z'^2} &= 2\sigma_w^2 \int_0^t \int_0^{t'} R_{ww}(\xi)\; d\xi\; dt' \\ &= 2\sigma_w^2 \int_0^t (t-\xi)\, R_{ww}(\xi)\; d\xi. \end{aligned} \qquad (4)$$

Let $\tau = \int_0^\infty R_{ww}(\xi)\; d\xi$ be the Lagrangian integral time scale. Equation (4) has asymptotic "near-field" and "far-field" limits

$$\overline{z'^2} = \begin{cases} \sigma_w^2\, t^2, & t \ll \tau \\ 2\sigma_w^2\, \tau t, & t \gg \tau \end{cases} \qquad (5)$$

corresponding to a nondiffusive regime of "memory-dominated" spread during which the release velocity is preserved ($t \ll \tau$), and a long time regime in which the turbulent convection of tracer may legitimately be *represented* as "diffusion," with effective far-field eddy diffusivity $K_\infty = \sigma_w^2 \tau$. Taylor's result proves, then, that the classic "eddy diffusion" paradigm for the evolution of the particle concentration $p = p(z,t)$ in this 1-D (z-) space, namely,

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial z}\left(-K\frac{\partial p}{\partial z}\right) = K\frac{\partial^2 p}{\partial z^2}, \qquad (6)$$

(constant eddy diffusivity K, Fickian diffusion equation) is insufficiently general. Being equivalent to the eddy diffusion treatment (not shown, but see *Monin and Yaglom* [1977, section 10.3] and *Boughton et al.* [1987]), a zeroth-order LS model (i.e., random displacement model or "random walk in position") cannot represent the near field. Conversely, the first-order LS model gives the correct small and large time behavior and, indeed, agrees exactly with Taylor's result at intermediate times in the case where R_{ww} decays exponentially. This represents the *fundamental* advantage of the (first-order) LS models over simpler models, though in practice, this capability is decisive only for a restricted range of problems involving the near field of sources (we expand on this in section 5).

Ever since its derivation, Taylor's result has served to guide turbulent dispersion modeling, and with suitable restriction as to the domain occupied by a puff or plume of dispersing tracer, it can be used in an approximate way for sources in real flows. However, its adequate extension to inhomogeneous and nonstationary turbulence, in the form of today's Lagrangian stochastic models, occurred only after newfound access to computers spurred heuristic experiments in the numerical simulation of particle trajectories and after these experiments, in turn, stimulated the development

during the 1980s of guidance in formulating the models for general flows (see section 4). Of course, there were many ingenious and illuminating developments, both theoretical and experimental, in the period between Taylor's work and the advent of (accessible) computers: for example, *Batchelor's* [1949] reexpression of Taylor's result in terms of a weighted integral

$$\overline{z'^2} = \sigma_w^2 \, t^2 \int_0^\infty S_w^{(L)}(f) \frac{\sin^2(\pi f t)}{(\pi f t)^2} \, \mathrm{d}f \tag{7}$$

of the Lagrangian velocity spectrum (f representing frequency). The transformation from equation (4) to equation (7) is straightforward (the Lagrangian spectrum and the Lagrangian autocorrelation function constituting a Fourier transform pair). The low-pass spectral filter $\sin^2(\pi\, ft)/(\pi\, ft)^2$ expresses the (intuitive) fact that for small travel times t, all eddies contribute to spread, while, with increasing t, increasingly only "slow" (small f) eddies dominate.

As already noted, and as testified by its prominence in textbooks [e.g. *Sutton*, 1953; *Pasquill and Smith*, 1983], Taylor's Lagrangian paradigm proved preeminent, either explicitly or indirectly, in subsequent efforts to deepen the theoretical framework and provide useable real-world dispersion models, one example of the latter being *Sutton's* [1953, equation 8.31] model for dispersion from a continuous ground-level point source in the atmospheric surface layer [see also *Monin and Yaglom*, 1977, section 10.5]. For several decades one of the influences of Taylor's work could be found in theoretical papers that attempted to interrelate Eulerian and Lagrangian statistics in idealized flow regimes, for "the relation between Lagrangian and Eulerian correlation functions is basic to the understanding of turbulent diffusion" [*Weinstock*, 1976]. Summing up a symposium at Oxford University, *Sutton* [1959, p. 438] stated:

> It is most appropriate that, with Sir Geoffrey Taylor in our midst, so much of the work has been founded on his famous paper of 1921 on the random walk. I have given up counting the number of times that celebrated equation connecting the Lagrangian correlation coefficient with the standard deviation of the particles has been written out on the blackboard.

Many influential scientists (including S. Corrsin, J. L. Lumley, R. H. Kraichnan, J. R. Philip, and P. G. Saffman) participated in this prolonged effort to relate Lagrangian to Eulerian statistical properties, and following a widely cited contribution by *Hay and Pasquill* [1959] delivered at the above-mentioned symposium, namely, a practicable method for short-range air pollution calculations involving the ratio β of Lagrangian to Eulerian integral time scales, a particular focus was the provision of theoretical values for that ratio [e.g., *Corrsin*, 1963; *Philip*, 1967; *Smith*, 1968]. It is interesting to remark that a modern LS model, if it respects the well-mixed condition [*Thomson*, 1987] for a given regime of flow having a specific (postulated) Eulerian velocity pdf, must "produce" the long sought for Lagrangian statistics, though in numerical rather than analytic form, and with the time scales determined using turbulence phenomenological relations (e.g., a parameterization of the energy dissipation rate) and hinging on the specified value of a dimensionless constant "C_0" (that we define and discuss later). Thus, the LS model can be said to "solve" the problem of relating Lagrangian to Eulerian statistics, albeit in a restricted sense: for the LS approach achieves this outcome by virtue of adopting the (plausible, but nonrigorous) Markovian framework that (possibly) these scientists might have considered a too sweeping simplification.

Taylor's result may easily be obtained by an analysis of *Langevin's* [1908] equation, which had been developed to describe Brownian motion and represents "the first example of a stochastic differential equation" [*Lemons*, 2002; *Gardiner*, 2004]; indeed, as a precursor to his main result, Taylor himself gave an alternative analysis breaking a trajectory into a sequence of discrete steps whose magnitudes were correlated from one to the next. Representing Lagrangian variables in upper case, and translating Langevin's coefficients into a notation appropriate to our ends, Langevin's equation may be written

$$\mathrm{d}W = -\frac{W}{\tau}\mathrm{d}t + \sqrt{\frac{2\sigma_w^2}{\tau}}\,\mathrm{d}\xi, \tag{8}$$

where $\mathrm{d}\xi$ represents an uncorrelated sequence of Gaussian random numbers having vanishing mean and variance $\mathrm{d}t$. Increments in velocity over intervals $\mathrm{d}t$ comprise a deterministic component (usually, as here, having the effect of damping the excursions in W on a time scale τ) and a purely random component. In stationary homogeneous turbulence, equation (8) reproduces Taylor's result for the special case of an exponential correlation function.

In modern parlance, a *generalized* Langevin equation is taken as the framework for developing Lagrangian models and typically is written

$$\mathrm{d}U_i = a_i(\mathbf{X}, \mathbf{U}, t)\,\mathrm{d}t + b_{ij}(\mathbf{X}, \mathbf{U}, t)\,\mathrm{d}\xi_j, \tag{9}$$

where the random forcing $\mathrm{d}\xi_i$ is Gaussian, with $\overline{\mathrm{d}\xi_i} = 0$ and $\overline{\mathrm{d}\xi_i \mathrm{d}\xi_j} = \mathrm{d}t\ \delta_{ij}$. The selection problem for first-order LS models amounts to the prescription of the systematic part of the acceleration a_i and the scaling coefficient b_{ij}, and we return to this later.

For the comprehensibility of what is to follow, this is an appropriate point to introduce the Fokker-Planck (FP) equation corresponding to equation (9). Let $p(\mathbf{x},\mathbf{u},t)$ represent the