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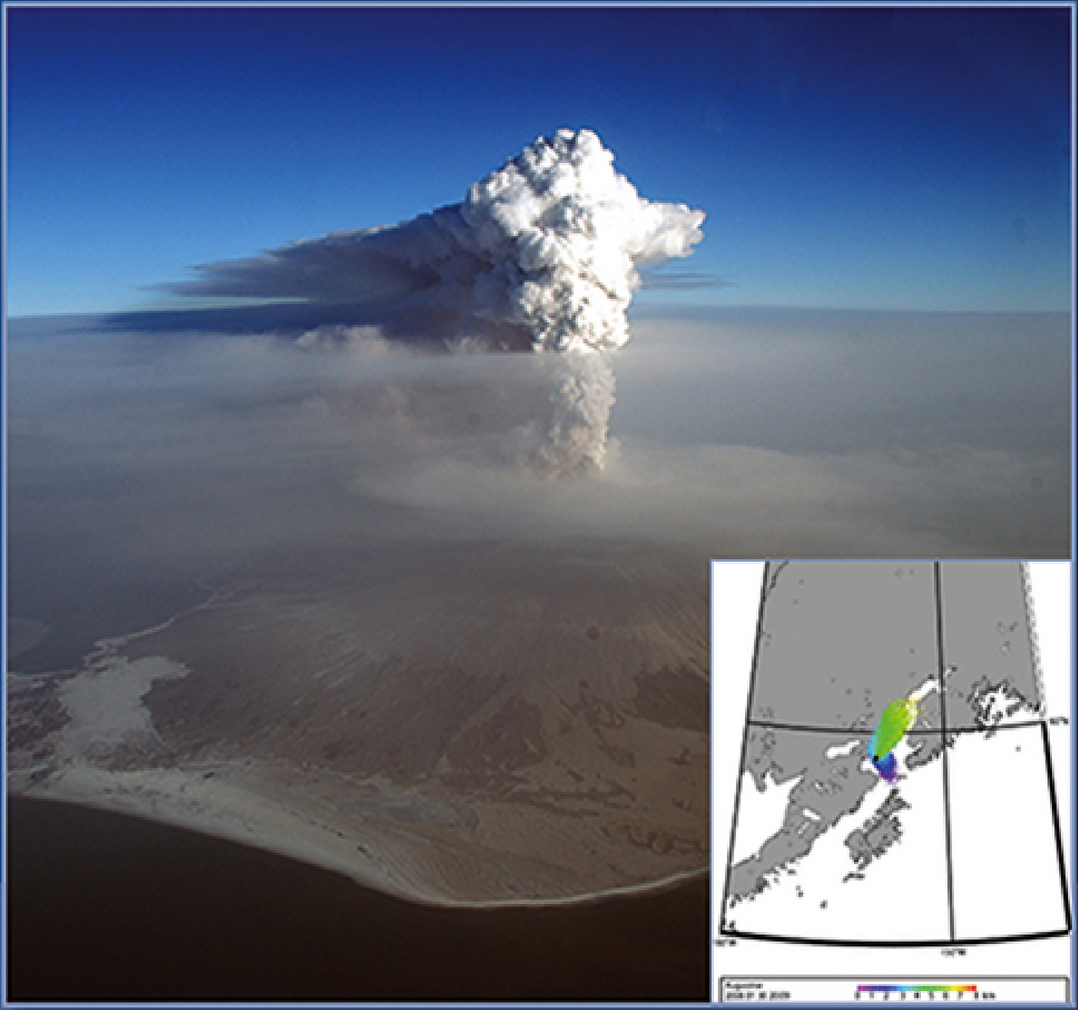
Lagrangian Modeling of the Atmosphere



John Lin, Dominik Brunner, Christoph Gerbig,
Andreas Stohl, Ashok Luhar, and Peter Webley
Editors

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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.

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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 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.

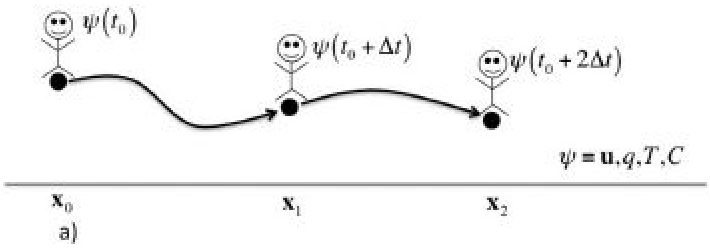
A central requirement for understanding the atmosphere is the capacity to model its flow. There are two basic types of reference frames when thinking about the fluid: Lagrangian and Eulerian. Put simply, a Lagrangian perspective follows an “air parcel” (see section 2.1) around, as if one receives information 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.

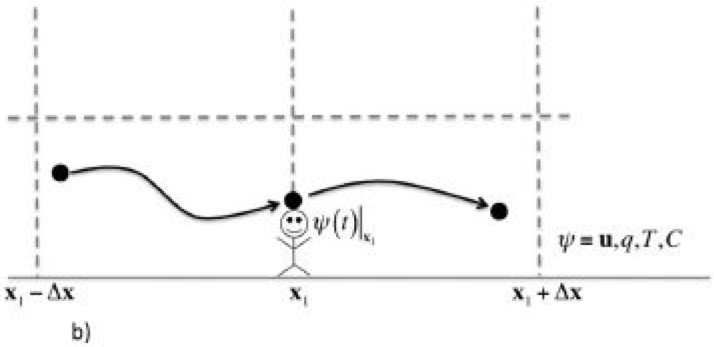
The Lagrangian and Eulerian perspectives can be formally interchanged, as often discussed in textbooks on dynamic meteorology [*Holton*, 1992] and geophysical fluid dynamics [*Marshall and Plumb*, 2007]. If ψ represents any state variable associated with the air parcel (i.e., velocity, temperature, humidity,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

$$\frac{D\psi}{Dt} = S, \quad (1a)$$

where D(…)/D*t* 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).

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).





The Lagrangian perspective in equation (1a) can be transformed to the Eulerian reference frame with the nonlinear advection term **u** · ∇ψ:

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

where ∂(…)/∂*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**/D*t* = **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**/D*t* = **u**, the following is the simplest first-order ("zero acceleration") solution [*Stohl*, 1998]:

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

where "…" indicates higher-order terms. Stated simply, Lagrangian modeling consists of determining the trajectory, $\mathbf{x}(t)$, and the values of different ψ at the different locations $\mathbf{x}$ and times t. The specific ψ of interest depends on the application at hand (see section 5): for instance, $\psi = q$ (specific humidity) when tracking sources of moisture, whereas $\psi = C$ (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).

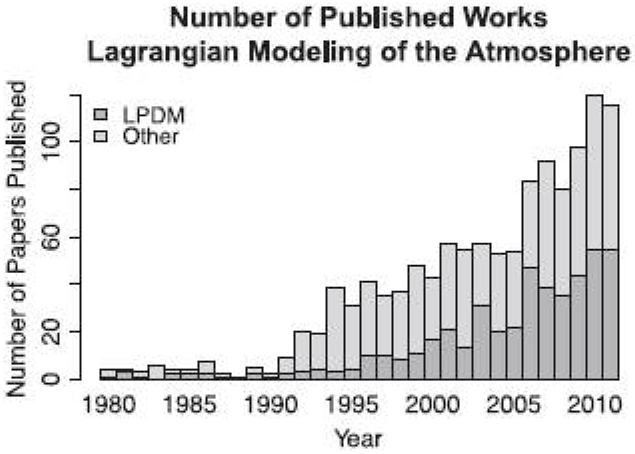
2. TYPES OF LAGRANGIAN ATMOSPHERIC MODELS

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.

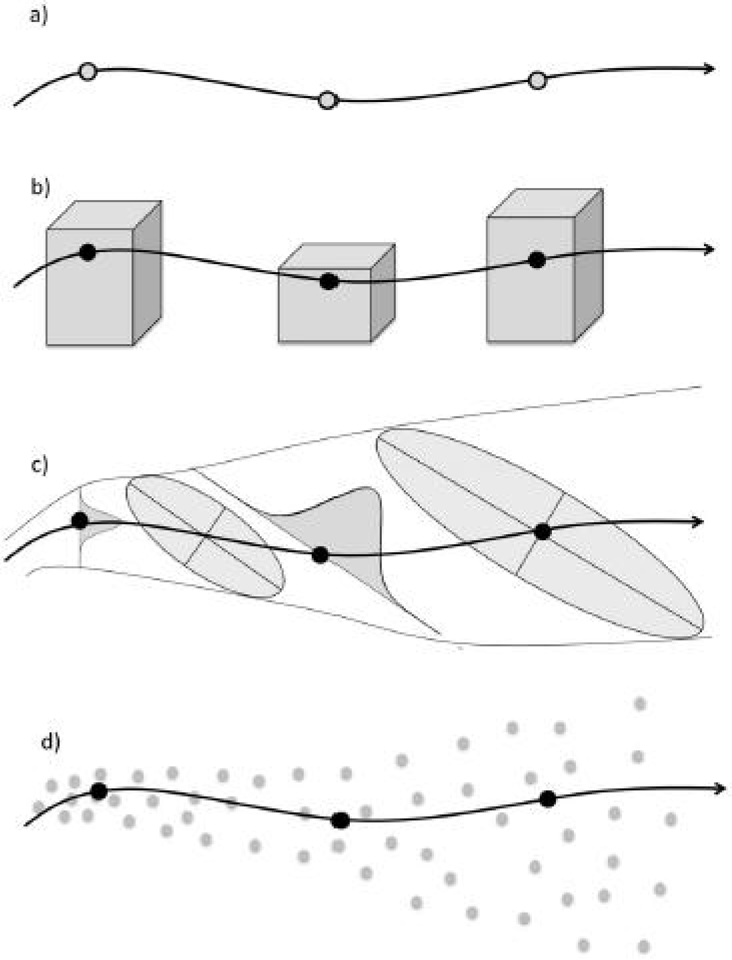
2.2. Mean Trajectories, Boxes, Puffs, and Particles

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 $\bar{\mathbf{u}}$ and neglecting the turbulent, stochastic component **u**′ in the Reynolds decomposition of **u** [*Reynolds*, 1895]:

$$\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'. \quad (3)$$

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

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.



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