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A review of the concepts for deriving the equations of change from the classical kinetic theory of gases: Single-component, multicomponent, and reactive gases

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ABSTRACT

This paper examines the mathematical operations performed developing the macroscopic equations of change for total mass, species mass, momentum and energy starting from the microscopic Boltzmann equation. In the standard literature on kinetic theory of gases, two formulations of the Boltzmann equation are presented. That is, the Boltzmann equation can be formulated both in terms of the molecular velocity and in terms of the peculiar velocity. In these two formulations of the Boltzmann equation two different coordinate systems are employed. Consequently, two different sets of moment equations can be derived from the Boltzmann equation being generalized frameworks for deducing the equations of change. Dependent on the choice of the generalized property, the equations of change for mass, momentum, and energy can be derived from the moment equations. The convenience of using two different velocities, coordinate systems and generalized property definitions is not sufficient elucidated in the literature. Hence, this paper outlines the use of the molecular and peculiar velocities in these frameworks for deriving the equations of change for mass, species mass, momentum and energy. Moreover, for completeness, the equations of change for single-component gases, multicomponent non-reacting gases, and multicomponent reacting gases are derived. Thus, this paper presents a rigorous examination of the various approaches for deriving the equations of change within the framework of the Boltzmann equation.

Contents

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1. Introduction

There are two main frameworks for deriving the transport equations for mass, species mass, momentum, and energy. The two frameworks are continuum mechanics and statistical mechanics. In this paper, the focus is placed on kinetic theory of gases; a particular branch of statistical mechanics. Fig. 1 gives an overview of the possible approaches for deriving equations of change for mass, species mass, momentum, and energy.

For a thorough understanding of transport phenomena in multicomponent mixtures the kinetic theory is considered a useful analysis tool. Moreover, the classical kinetic theory of gases is also used as basis deriving models for dispersed multiphase flows as well as dispersed multiphase reactive flows.

A possible concept for describing the behavior of a large number of particles can be found in statistical mechanics. Statistical methods aim at predicting the most probable behavior of a large collection of particles without being concerned with the precise states of the individual particles. The most probable state of the ensemble of particles is considered when calculating the macroscopic properties. Following the work by Boltzmann [2], the statistical unit is the molecule and the statistical ensemble is a large number of molecules.

In kinetic theory of gases, the gas is described in terms of a time dependent distribution function which contains information of the spatial distribution of the molecules as well as the molecular velocity distribution. Moments of the distribution function represent macroscopic (ensemble) mean quantities like mass density, gas velocity, internal energy, kinetic energy flux, and pressure tensor. The Boltzmann equation is an integro-differential equation which describes the evolution of the distribution function in the phase space (which is composed of the physical and velocity spaces) and time. It is possible to derive the equations of change for mass, species mass, momentum and energy starting out from the Boltzmann equation. That is, particular moments of the distribution function can be obtained multiplying the Boltzmann equation by a quantity ψ (representing successively molecular mass, momentum, and energy), and thereafter integrating the equation over the whole velocity space.

In the standard literature on kinetic theory of gases (e.g. [3,4]), two formulations of the Boltzmann equation are presented. The conventional formulation presents the Boltzmann equation with the molecular velocity **c** as the velocity coordinate. An alternative is to formulate the Boltzmann equation using the peculiar velocity **C** as the velocity coordinate. It follows that two different sets of generalized moment equations from the Boltzmann equation can be derived and utilized deducing the generalized equations of change. Dependent on the framework, the generalized property may be defined in terms of the molecular velocity, $\psi = \psi(\mathbf{c})$, and/or in terms of the peculiar velocity, $\psi = \psi(\mathbf{C})$ (Fig. 2). In particular, the choice of framework influences on the manipulation complexity required in order to derive the transport equations for the different energy forms (i.e. total energy, kinetic energy, and internal energy). Moreover, the formulation in **C** might be considered more convenient