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Kinetic Theories for the Coagulation and Sedimentation of Particles

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The coagulation and sedimentation of particles is central to many environmental and industrial processes. Kinetic descriptions of this process can be divided into two approaches. Population balance equation (PBE) theory accounts for mass transfer between particle size classes by coagulation and loss of particle mass by sedimentation. Its practical application is limited by the fact that the rate constants, or kernels, for coagulation between all combinations of cluster sizes are unknown, and only a few solutions are available for simplified forms of the coagulation kernel. A second approach involves the use of simple rate expressions for the loss of particle mass with time, where the order of the reaction is determined by the mathematical properties of the coagulation kernel and the sedimentation term. Two different theories (similarity theory, ST, and the quasi-steady-state hypothesis, QSSH) give conflicting estimates for the order of the reaction. In this paper, we derive a PBE solution for the choice of a constant kernel and a particle removal rate that increases linearly with cluster volume. The kinetics of mass removal predicted by this solution are then compared directly to generalized forms of ST and QSSH which we also derive. We find that the PBE solution does not rigorously conform to either ST or QSSH, although the predictions of ST may be close enough for practical applications. This paper presents the first rigorous comparison of PBE, ST, and QSSH descriptions of particle coagulation and sedimentation. © 2001 Academic Press

Key Words: coagulation and sedimentation; similarity theory; quasi-steady-state hypothesis; population balance equation.

1. INTRODUCTION

The unsteady coagulation and sedimentation of fluidborne particles is at the core of many problems in science and engineering. Here we define sedimentation in the broadest possible sense as any process that leads to the size-dependent removal of particle mass from a system. Examples include the generation and settling of particulate pollutants in the air column over urban areas (1), the downward flux of phytoplankton from the surface of the ocean (2), the formation of protoplanetary disks in turbulent solar nebula (3), the removal of colloidal contaminants from water during water treatment (4), and the cohesiveness of bottom sediments formed by the coagulation and sedimentation of fine particles in near-shore environments (5), to name a few. A detailed analysis of particle coagulation and sedimentation is complicated by a number of factors:

(i) The collision rate between particle clusters and their sedimentation rate depends on the number of particles that constitute the individual clusters, or their size.

(ii) The time evolution of any cluster size is coupled to all other cluster sizes through an infinite set of nonlinear differential equations.

(iii) Many of the physical and surface-chemical forces that develop between clusters on close approach are poorly understood.

(iv) Even if these forces were well understood, their influence on the coagulation rate between any two clusters is an *N-body* problem in physics for which the analytical challenges are formidable.

In this paper, we generalize several older theories of the kinetics of particle coagulation and sedimentation. These generalized theories are then tested against a solution of the population balance equations that describe the coagulation and sedimentation of particles in a homogeneous fluid. The solution is for a special case where the reactivity between clusters is independent of cluster volume (constant kernel) and the sedimentation rate increases linearly with cluster volume.

The paper is organized as follows. The population balance equations describing particle coagulation and sedimentation are presented in Section 2. Several approaches for analyzing the equation when sedimentation is negligible are reviewed, including von Smoluchowski's solution (Section 3), the dynamic scaling theory proposed by Friedlander (Section 4), and the generalized dynamic scaling theory developed by van Dongen and Ernst (Section 5). Previously published theories for the unsteady coagulation and sedimentation of particles are generalized in Section 6, and these generalized theories are tested against our mathematical solution in Sections 7 and 8. The main conclusions and implications of this study are discussed in Section 9.

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