A void-based description of compaction and segregation in flowing granular materials

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Guided by the kinematical treatment of vacancies in theories for solid-state diffusion, we develop a theory for compaction and segregation in flowing granular materials. This theory leads to a partial differential equation for the macroscopic motion of the material coupled to a system of partial differential equations for the volume fractions of the individual particle types. When segregation is ignored, so that the focus is compaction, the latter system is replaced by a scalar partial differential equation that closely resembles equations arising in theories of traffic flow. To illustrate the manner in which the theory describes compaction and segregation, we present three explicit solutions. In particular, for an arbitrary loosely packed mixture of small and large particles in a fixed container under the influence of gravity, we show that a layer of large particles forms at the free surface and grows with time, while a closely packed mixture of large and small particles forms and grows from the base of the container; the final solution, attained in finite time, consists of a layer of closely packed large particles above a closely packed mixed state. At the mundane level of everyday experience, this solution at least qualitatively explains why in a container of mixed nuts, Brazil nuts are generally found at the top.

1. Introduction

A granular material is a collection of solid particles together with an interstitial fluid such as air or water. Granular materials consist not of identical particles, but, rather, of various particle types that may differ in size, shape, density, resilience, and roughness. When a polydisperse granular material flows in the presence of gravity, its constituents tend to segregate. Consider, for example, a horizontal cylinder filled partially with a granular material involving particles of two types. If the cylinder is rotated slowly about its axis, an axial separation occurs, involving a series of alternating bands containing only particles of one or the other type (Donald & Roseman 1962; Campbell & Bauer 1966). Further, by altering the cylinder rotation speed, this separation can be reversed to create a state in which the two particle types are well-mixed (Hill & Kakalios 1994).

While segregation may occur in any granular material consisting of particles with disparate properties, differences in particle size are thought to be dominant (Brown 1939; Williams 1963, 1976; Bridgewater 1976). In particular, contrary to what experience with conventional fluids might lead one to expect, experiments conducted with horizontally vibrated binary mixtures of small and large particles show that the large particles rise

upward against gravity even when the density of a large particle exceeds markedly that of a small particle (Harwood 1977).

While mineral processing technologies exploit the tendency for granular materials to segregate, industrial mixing technologies must counteract this tendency. Though vital to the chemical, pharmaceutical, powder metallurgy, glass, ceramic, paint, food, and construction industries, separation and mixing technologies are presently limited by a reliance upon empirically-based heuristics (Ottino & Khakhar 2000). An enhanced understanding of the mechanisms underlying segregation is therefore likely to lead to significant advances in a broad spectrum of industrial enterprises.

At present, molecular dynamics appears to be the method of choice for numerical simulations of segregation-by-particle-type (Haff & Werner 1986; Ohtsuki et al. 1993; Baumann et al. 1994; Ristow 1994; Dury & Ristow 1997). However, even with the most advanced computing resources currently available, the inherent memory demands of this method make it infeasible for systems of more than 10^6 particles. Thus, to simulate geophysical and industrial flows, which generally entail extremely large numbers of particles, an alternative approach would be useful.

One such alternative would be provided by a continuum theory involving evolution equations appropriately analogous to those arising in the Navier–Stokes theory. Indeed, when faced with the challenge of modeling granular materials involving great numbers of particles, the advantage of a continuum theory is clear: in such a theory, each point in the region occupied by the medium corresponds to a great number of particles. Insofar as monodisperse granular materials are concerned, continuum-level theories have been exploited to considerable advantage (Savage 1984; Hutter & Rajagopal 1994; Wang & Hutter 2001). Avenues to such a framework are provided by the kinetic theory (Jenkins & Mancini 1989; Arnarson & Willits 1998; Jenkins 1998; Arnarson & Jenkins 2000) and by mixture theory (Aranson et al. 1999; Khakhar et al. 1999).

Here, we take an alternative approach that emphasizes the essential role of voids in the segregation process (Rosato et al. 1986, 1987; Savage & Lun 1988; Fitt & Wilmott 1992). In so doing, we are guided by the treatment of vacancies in theories of solid-state diffusion (Ågren 1982; Cahn & Larché 1983; Larché & Cahn 1983; Mullins & Sekereka 1985; Fried & Gurtin 1999). In these theories, vacancies are viewed as an 'atomic species,' are endowed with chemical potential, and may diffuse through the crystal lattice. This allows for an efficient bookkeeping whereby vacancies enter the basic laws in a physically relevant manner. The analogy between the role of vacancies in solid-state diffusion and of voids in granular flow has been recognized earlier by Litwiniszyn (1963), Mullins (1972), and Caram & Hong (1992) in works concerning monodisperse granular materials.

Because our approach is nonstandard, the main purpose of this work is to develop a kinematical foundation for the treatment of voids and to formulate the basic physical laws within a setting that allows for segregation via the diffusion of different particle types. We focus on media in which rigid particles of one or more discrete types are represented, ignore all forms of inertia, and restrict attention to flows in which the particles remain in close contact. Insofar as constitutive equations are concerned, we emphasize the development of equations that describe the relative diffusion between particles and between particles and voids, leaving aside the detailed discussion of constitutive equations for the extra stress.

The final governing equations of our theory include a partial differential equation for the macroscopic motion of the material coupled to a system of partial differential equations for the volume fractions of the individual particle types. When segregation is ignored, so that the focus is compaction, the system of equations for the volume fractions is replaced by a scalar partial differential equation that closely resembles equations

arising in theories of traffic flow. For what we call a 'simple granular material,' the system of equations for the volume fractions is hyperbolic. A simple granular material is a cohesionless medium consisting of particles that differ only by size and for which: (*i*) the particulate mobilities depend separably on the particulate volume fractions and the invariants of the aggregate strain rate; (*ii*) the particulate mobilities and the extra stress depend on the particulate volume fractions only through their sum — the void fraction. Hence, shocks are possible in a cohesionless medium. We develop the general conditions governing particulate shocks and discuss their specialization to *compactification* and *segregation* shocks. We also discuss the conditions that hold at free surfaces and at solid boundaries.

To illustrate the manner in which our theory describes compaction and segregation, we focus on simple granular materials. Within this setting, we present three explicit solutions. First, for loosely packed particles of a single type in a fixed container under the influence of gravity, we show that a closely packed layer of particles forms and grows from the base of the container resulting in a final solution, attained in finite time consisting of closely packed particles. Next, for an arbitrary loosely packed mixture of small and large particles in a fixed container under the influence of gravity, we show that a layer of large particles forms at the free surface and grows with time, while a closely packed mixture of large and small particles forms and grows from the base of the container; the final solution, attained in finite time, consists of a layer of closely packed large particles above a closely packed mixed state. Finally, we show that, under very special conditions, our theory allows for the desegration of a layer of small particles above a mixture of small and large particles but that, once mixed, the medium segregates to leave a layer of large particles above.

2. Volume-based kinematics. Conservation of volume

2.1. *Volume fractions for particles and voids*

Consider a mixture of rigid particles and voids. We view the mixture as a continuum and, with the aim of developing local field equations, focus attention on a fixed control volume $\mathcal{R}$ through which this mixture is flowing. We write $\boldsymbol{x}$ for an arbitrary point of $\mathcal{R}$, $\boldsymbol{n}(\boldsymbol{x})$ for the outward unit normal on $\partial\mathcal{R}$, and t for any arbitrary instant of time.

We assume that the particles are of K discrete types and denote by $\varphi_k(\boldsymbol{x},t)$ the *volume fraction of particles of type* $k=1,2,\dots,K$ and by $\varphi^{\mathrm{v}}(\boldsymbol{x},t)$ the *volume fraction of voids*. Consistent with the requirement that all volume be accounted for by particles and voids, we assume that

$$\sum_{k=1}^{K}\varphi_k+\varphi^{\mathrm{v}}=1. \tag{2.1}$$

We also insist that the volume fractions take values between 0 and 1, so that $0\le\varphi_k\le 1$ for each $k=1,2,\dots,K$ and $0\le\varphi^{\mathrm{v}}\le 1$, which, in combination with (2.1), yields the constraint

$$\sum_{k=1}^{K}\varphi_k\le 1. \tag{2.2}$$

We write $\boldsymbol{v}_k(\boldsymbol{x},t)$ for the *velocity of particles of type* k and $\boldsymbol{v}^{\mathrm{v}}(\boldsymbol{x},t)$ for the *velocity of*

voids, take the *volume-weighted velocity*

$$\boldsymbol{v} = \sum_{k=1}^{K} \varphi_k \boldsymbol{v}_k + \varphi^{\mathrm{v}} \boldsymbol{v}^{\mathrm{v}} \tag{2.3}$$

as the relevant velocity field for the mixture, and describe the motion of particles and voids relative to the mixture through the *relative velocities* $\boldsymbol{u}_k(\boldsymbol{x},t)$ and $\boldsymbol{u}^{\mathrm{v}}(\boldsymbol{x},t)$ defined via

$$\boldsymbol{u}_k = \boldsymbol{v}_k - \boldsymbol{v} \qquad \text{and} \qquad \boldsymbol{u}^{\mathrm{v}} = \boldsymbol{v}^{\mathrm{v}} - \boldsymbol{v}. \tag{2.4}$$

We write $\partial/\partial t$ for the *spatial time-derivative* (with respect to t holding $\boldsymbol{x}$ fixed) and use grad and div to denote the spatial gradient and spatial divergence (with respect to $\boldsymbol{x}$ holding t fixed). We consider the mixture as a continuum that convects with the volume-weighted velocity $\boldsymbol{v}$; consistent with this, we write $\mathrm{D}/\mathrm{D}t$ for the *material time-derivative*, so that

$$\frac{\mathrm{D}g}{\mathrm{D}t} = \frac{\partial g}{\partial t} + \boldsymbol{v} \cdot (\operatorname{grad} g) \tag{2.5}$$

for a scalar field $g(\boldsymbol{x},t)$ and similarly for a vector field.

Since the particles are rigid, the volume occupied by each particle type and the volume occupied by voids must be preserved throughout the motion. The integrals

$$\int\limits_{\mathcal{R}} \varphi_k \,\mathrm{d}V \qquad \text{and} \qquad -\int\limits_{\partial\mathcal{R}} \varphi_k \,\boldsymbol{v}_k \cdot \boldsymbol{n} \,\mathrm{d}A$$

represent the volume of particles of type k in $\mathcal{R}$ and the volume of particles of that type entering $\mathcal{R}$ across $\partial\mathcal{R}$, per unit time, and analogous statements hold for voids. Conservation of volume is therefore the requirement that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{R}} \varphi_k \,\mathrm{d}V = -\int\limits_{\partial\mathcal{R}} \varphi_k \boldsymbol{v}_k \cdot \boldsymbol{n} \,\mathrm{d}A \qquad \text{and} \qquad \frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{R}} \varphi^{\mathrm{v}} \,\mathrm{d}V = -\int\limits_{\partial\mathcal{R}} \varphi^{\mathrm{v}} \boldsymbol{v}^{\mathrm{v}} \cdot \boldsymbol{n} \,\mathrm{d}A \tag{2.6}$$

for all control volumes $\mathcal{R}$; since $\mathcal{R}$ is fixed,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{R}} g(\boldsymbol{x},t) \,\mathrm{d}V_{\boldsymbol{x}} = \int\limits_{\mathcal{R}} \frac{\partial g(\boldsymbol{x},t)}{\partial t} \,\mathrm{d}V_{\boldsymbol{x}} \tag{2.7}$$

for any field $g(\boldsymbol{x},t)$, and we are led to the local balances

$$\frac{\partial \varphi_k}{\partial t} = -\operatorname{div}(\varphi_k \boldsymbol{v}_k) \qquad \text{and} \qquad \frac{\partial \varphi^{\mathrm{v}}}{\partial t} = -\operatorname{div}(\varphi^{\mathrm{v}} \boldsymbol{v}^{\mathrm{v}}). \tag{2.8}$$

Summing these relations over all constituents (voids and particles) we find, with the aid of (2.1) and (2.3), that the mixture is locally volume-preserving; viz.,

$$\operatorname{div} \boldsymbol{v} = 0, \tag{2.9}$$

which manifests our use of voids to provide an accounting for all volume. By (2.7), (2.9), and the divergence theorem,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{R}} g \,\mathrm{d}V + \int\limits_{\partial\mathcal{R}} g\boldsymbol{v} \cdot \boldsymbol{n} \,\mathrm{d}A = \int\limits_{\mathcal{R}} \frac{\mathrm{D}g}{\mathrm{D}t} \,\mathrm{d}V. \tag{2.10}$$

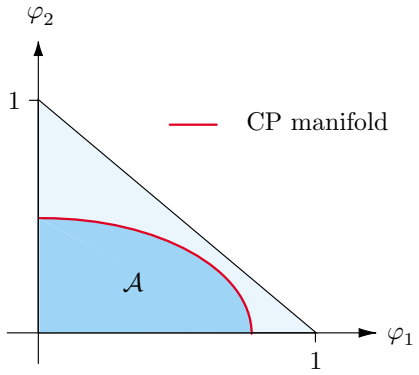

FIGURE 1. Schematic of the packing domain $\mathcal{A}$ and the closely-packed manifold for the special case of two particle types.

Using (2.9), (2.4), and (2.5), we may rewrite (2.8) in the alternative form

$$\frac{\mathrm{D}\varphi_k}{\mathrm{D}t} = -\mathrm{div}\,(\varphi_k \boldsymbol{u}_k) \qquad \text{and} \qquad \frac{\mathrm{D}\varphi^{\mathrm{v}}}{\mathrm{D}t} = -\mathrm{div}\,(\varphi^{\mathrm{v}} \boldsymbol{u}^{\mathrm{v}}). \tag{2.11}$$

The field

$$\boldsymbol{\jmath}_k = \varphi_k \boldsymbol{u}_k \tag{2.12}$$

represents the *volume flux of particles of type k*, and their introduction allows us to rewrite $(2.11)_1$ as

$$\frac{\mathrm{D}\varphi_k}{\mathrm{D}t} = -\mathrm{div}\,\boldsymbol{\jmath}_k. \tag{2.13}$$

2.2. *Packings*

We refer to lists

$$\vec{\varphi} = (\varphi_1, \varphi_2, \ldots, \varphi_K),$$

as *packings* and consistently use the abbreviation

$$\mathrm{CP} = \text{closely packed}.$$

We assume that each packing $\vec{\varphi}$ belongs to a closed subset $\mathcal{A}$ of the unit cube $[0,1] \times [0,1] \times \cdots \times [0,1]$ in R^K; $\mathcal{A}$ is called the *packing domain*. The set of all packings that are CP, called the CP *manifold*, is then a smooth subsurface of $\partial\mathcal{A}$. It is beyond our present scope to describe in detail the properties of the packing domain and the CP manifold; Figure 1 gives a schematic of these sets for the special case of two particle types.

3. Mass-based kinematics. Conservation of mass

Restricting attention momentarily to particles, we denote by m_k the mass density of a single particle of type k and define the mass density $\rho_k(\boldsymbol{x}, t)$ of particles of type k, per unit mixture-volume, by

$$\rho_k = m_k \varphi_k. \tag{3.1}$$

Then

$$\rho = \sum_{k=1}^{K} \rho_k \tag{3.2}$$

represents the *mixture density* $\rho(\boldsymbol{x},t)$,

$$c_k = \frac{\rho_k}{\rho} \tag{3.3}$$

gives the *mass concentration* $c_k(\boldsymbol{x},t)$ of particles of type k,

$$\boldsymbol{v}^{\mathrm{p}} = \sum_{k=1}^{K} c_k \boldsymbol{v}_k \tag{3.4}$$

determines the *mass-weighted velocity* $\boldsymbol{v}^{\mathrm{p}}(\boldsymbol{x},t)$, and

$$\boldsymbol{u}^{\mathrm{p}} = \boldsymbol{v}^{\mathrm{p}} - \boldsymbol{v} = \sum_{k=1}^{K} c_k \boldsymbol{u}_k \tag{3.5}$$

characterizes the *net relative-velocity* $\boldsymbol{u}^{\mathrm{p}}(\boldsymbol{x},t)$.

Multiplying $(2.11)_1$ by m_k we arrive at the mass balance

$$\frac{\mathrm{D}\rho_k}{\mathrm{D}t} = -\mathrm{div}\,(\rho_k \boldsymbol{u}_k), \tag{3.6}$$

for particles of type k. When summed over all particulate species, (3.6) yields the net mass-balance

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\mathrm{div}\,(\rho \boldsymbol{u}^{\mathrm{p}}), \tag{3.7}$$

showing that, although the mixture itself is locally volume-preserving, density changes are not excluded. Using (2.5) with $g = \rho$, (3.5), and (2.9), we observe that (3.7) can be rewritten as

$$\frac{\partial\rho}{\partial t} = -\mathrm{div}\,(\rho \boldsymbol{v}^{\mathrm{p}}). \tag{3.8}$$

4. Force and moment balances

We assume that inertia is negligible and write $\boldsymbol{T}(\boldsymbol{x},t)$ for the *stress*, carrying dimensions of force per unit mixture-area, and $\boldsymbol{f}(\boldsymbol{x},t)$ for the *specific body-force*, carrying dimensions of force per unit mass, so that $\rho\boldsymbol{f}$ represents the body force, per unit mixture-volume.

The balance laws for forces and moments require that

$$\int\limits_{\partial\mathcal{R}} \boldsymbol{T}\boldsymbol{n}\,\mathrm{d}A + \int\limits_{\mathcal{R}} \rho\boldsymbol{f}\,\mathrm{d}V = \boldsymbol{0} \tag{4.1}$$

and

$$\int\limits_{\partial\mathcal{R}} (\boldsymbol{x}-\boldsymbol{0}) \times \boldsymbol{T}\boldsymbol{n}\,\mathrm{d}A + \int\limits_{\mathcal{R}} (\boldsymbol{x}-\boldsymbol{0}) \times \rho\boldsymbol{f}\,\mathrm{d}V = \boldsymbol{0} \tag{4.2}$$

for each control volume $\mathcal{R}$, whereby the standard local relations

$$\mathrm{div}\boldsymbol{T} + \rho\boldsymbol{f} = \boldsymbol{0} \qquad \text{and} \qquad \boldsymbol{T} = \boldsymbol{T}^{\top} \tag{4.3}$$

hold.

For convenience, we decompose $\boldsymbol{T}$ in the form

$$\boldsymbol{T} = \boldsymbol{S} - p\boldsymbol{1}, \qquad p = -\tfrac{1}{3}\mathrm{tr}\boldsymbol{T}, \tag{4.4}$$

with $\boldsymbol{S}(\boldsymbol{x},t)$ the *extra stress* and $p(\boldsymbol{x},t)$ the *pressure*; the relations (4.3) then become

$$\operatorname{div}\boldsymbol{S}+\rho\boldsymbol{f}=\operatorname{grad}p \qquad \text{and} \qquad \boldsymbol{S}=\boldsymbol{S}^{\top}. \tag{4.5}$$

Finally, note that, trivially, the body force admits the decomposition

$$\rho\boldsymbol{f}=\sum_{k=1}^{K}\rho_k\boldsymbol{f}. \tag{4.6}$$

5. Energetics

5.1. *Energetics associated with the field* $\boldsymbol{f}$

Basic to our theory is the view that $\boldsymbol{f}$ is a *background field* that interacts with massy quantities moving through space. Thus

$$\int_{\mathcal{R}}\rho\boldsymbol{f}\,\mathrm{d}V \qquad \text{and} \qquad \int_{\mathcal{R}}\rho_k\boldsymbol{f}\,\mathrm{d}V$$

represent respective net forces exerted by the field $\boldsymbol{f}$ on the mixture in $\mathcal{R}$ and on particles of type k in $\mathcal{R}$. We assume that the body force $\rho_k\boldsymbol{f}$ acting on particles of type k expends power over the particle velocity $\boldsymbol{v}_k$; thus the total power expended by the body force, per unit mixture-volume, is, by (3.4),

$$\sum_{k=1}^{K}\rho_k\boldsymbol{f}\cdot\boldsymbol{v}_k=\rho\boldsymbol{f}\cdot\boldsymbol{v}^{\mathrm{p}}.$$

Given any control volume $\mathcal{R}$, the integral

$$\int_{\mathcal{R}}\rho\boldsymbol{f}\cdot\boldsymbol{v}^{\mathrm{p}}\,\mathrm{d}V$$

then represents the net working of the body force on that portion of the mixture in $\mathcal{R}$.

We assume that $\boldsymbol{f}$ is time-independent and conservative with *potential energy* $\Psi(\boldsymbol{x})$, per unit mass:

$$\boldsymbol{f}=-\operatorname{grad}\Psi. \tag{5.1}$$

In many, if not most, applications of interest the field $\boldsymbol{f}$ will be gravitational and hence of the form $\boldsymbol{f}=\boldsymbol{g}$, with $\boldsymbol{g}$ the (constant) gravitational acceleration, so that, ignoring an inconsequential constant,

$$\Psi(\boldsymbol{x})=-\boldsymbol{g}\cdot\boldsymbol{x}.$$

Our general results, however, are independent of the particular choice of $\boldsymbol{f}$.

Given a control volume $\mathcal{R}$, it follows from (3.8) and (5.1) that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{R}}\rho\Psi\,\mathrm{d}V&=\int_{\mathcal{R}}\frac{\partial\rho}{\partial t}\Psi\,\mathrm{d}V\\&=-\int_{\mathcal{R}}\Psi\operatorname{div}(\rho\boldsymbol{v}^{\mathrm{p}})\,\mathrm{d}V\\&=-\int_{\partial\mathcal{R}}\rho\Psi\boldsymbol{v}^{\mathrm{p}}\cdot\boldsymbol{n}\,\mathrm{d}A-\int_{\mathcal{R}}\rho\boldsymbol{f}\cdot\boldsymbol{v}^{\mathrm{p}}\,\mathrm{d}V,\end{aligned}$$

and we have the identity:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{R}}\rho\Psi\,\mathrm{d}V+\int\limits_{\partial\mathcal{R}}\rho\Psi\boldsymbol{v}^{\mathrm{p}}\cdot\boldsymbol{n}\,\mathrm{d}A=-\int\limits_{\mathcal{R}}\rho\boldsymbol{f}\cdot\boldsymbol{v}^{\mathrm{p}}\,\mathrm{d}V. \tag{5.2}$$

The left side of (5.2) represents the potential energy produced within $\mathcal{R}$, per unit time, as it expresses, for $\mathcal{R}$, the temporal change in potential energy plus the rate at which potential energy is carried out across $\partial\mathcal{R}$ by particle flow. The identity (5.2) therefore shows that the action of the body force on the mixture may be expressed alternatively as a production of potential energy or as an expenditure of power.

By (3.3) and (3.5), the left side of (5.2) may be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{R}}\rho\Psi\,\mathrm{d}V+\int\limits_{\partial\mathcal{R}}\rho\Psi\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}A+\sum_{k=1}^{K}\int\limits_{\partial\mathcal{R}}\rho_k\Psi\boldsymbol{u}_k\cdot\boldsymbol{n}\,\mathrm{d}A$$

and therefore, by (2.12) and (3.1), we may express (5.2) equivalently as

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{R}}\rho\Psi\,\mathrm{d}V+\int\limits_{\partial\mathcal{R}}\rho\Psi\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}A=-\sum_{k=1}^{K}\int\limits_{\partial\mathcal{R}}(m_k\Psi)\boldsymbol{\jmath}_k\cdot\boldsymbol{n}\,\mathrm{d}A-\sum_{k=1}^{K}\int\limits_{\mathcal{R}}\rho_k\boldsymbol{f}\cdot\boldsymbol{v}_k\,\mathrm{d}V. \tag{5.3}$$

The left side of (5.3) represents the temporal change in the potential energy of the *convected* control volume that occupies the *fixed* region $\mathcal{R}$ at the current time. The first term on the right represents the potential energy carried out of this convected control volume across its boundary by the diffusion of particles relative to the mixture, an identification that establishes $m_k\Psi$ as the *chemical potential of particles of type* k in the field $\boldsymbol{f}$.

5.2. *Energy imbalance*

In our purely mechanical setting, the first and second laws of thermodynamics are replaced by an energy imbalance asserting that the energy in a control volume $\mathcal{R}$ increases at a rate no greater than the net rate at which work is performed on $\mathcal{R}$ plus the rate at which energy flows into $\mathcal{R}$ across $\partial\mathcal{R}$. We allow for a *free-energy density* ψ for the mixture as a whole and a *chemical potential* μ_k for each particle type k. Thus, since we neglect inertia, the *energy imbalance* is the requirement that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{R}}(\psi+\rho\Psi)\,\mathrm{d}V+\int\limits_{\partial\mathcal{R}}(\psi+\rho\Psi)\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}A&\\ \leq-\sum_{k=1}^{K}\int\limits_{\partial\mathcal{R}}(\mu_k+m_k\Psi)\,\boldsymbol{\jmath}_k\cdot\boldsymbol{n}\,\mathrm{d}A+\int\limits_{\partial\mathcal{R}}\boldsymbol{T}\boldsymbol{n}\cdot\boldsymbol{v}\,\mathrm{d}A,&\end{aligned} \tag{5.4}$$

or equivalently, by (5.3), that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{R}}\psi\,\mathrm{d}V+\int\limits_{\partial\mathcal{R}}\psi\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}A\leq-\sum_{k=1}^{K}\int\limits_{\partial\mathcal{R}}\mu_k\,\boldsymbol{\jmath}_k\cdot\boldsymbol{n}\,\mathrm{d}A+\int\limits_{\partial\mathcal{R}}\boldsymbol{T}\boldsymbol{n}\cdot\boldsymbol{v}\,\mathrm{d}A+\int\limits_{\mathcal{R}}\rho\boldsymbol{f}\cdot\boldsymbol{v}^{\mathrm{p}}\,\mathrm{d}V. \tag{5.5}$$

5.3. *Local dissipation inequality*

We now localize the energy imbalance (5.5). By the force balance $(4.3)_1$, the decomposition (4.4) of $\boldsymbol{T}$, the moment balance $(4.5)_2$, and the relation $\operatorname{div}\boldsymbol{v}=0$,

$$\int\limits_{\partial\mathcal{R}}\boldsymbol{T}\boldsymbol{n}\cdot\boldsymbol{v}\,\mathrm{d}A+\int\limits_{\mathcal{R}}\rho\boldsymbol{f}\cdot\boldsymbol{v}\,\mathrm{d}V=\int\limits_{\mathcal{R}}\boldsymbol{T}\cdot\operatorname{grad}\boldsymbol{v}\,\mathrm{d}A=\int\limits_{\mathcal{R}}\boldsymbol{S}\cdot\boldsymbol{D}\,\mathrm{d}V,\tag{5.6}$$

with

$$\boldsymbol{D}=\tfrac{1}{2}\big(\operatorname{grad}\boldsymbol{v}+(\operatorname{grad}\boldsymbol{v})^{\top}\big)\tag{5.7}$$

the *strain-rate*. Using the definition (3.5), we therefore arrive at the *power balance*

$$\int\limits_{\partial\mathcal{R}}\boldsymbol{T}\boldsymbol{n}\cdot\boldsymbol{v}\,\mathrm{d}A+\int\limits_{\mathcal{R}}\rho\boldsymbol{f}\cdot\boldsymbol{v}^{\mathrm{p}}\,\mathrm{d}V=\int\limits_{\mathcal{R}}(\boldsymbol{S}\cdot\boldsymbol{D}+\rho\boldsymbol{f}\cdot\boldsymbol{u}^{\mathrm{p}})\,\mathrm{d}V.\tag{5.8}$$

The left side of this balance represents power expended *externally* on the mixture in $\mathcal{R}$ by tractions exerted across $\partial\mathcal{R}$ and by the field $\boldsymbol{f}$, while the right side represents power expended *internally* via the stress power $\boldsymbol{S}\cdot\boldsymbol{D}$, which is classical, and a nonstandard term $\rho\boldsymbol{f}\cdot\boldsymbol{u}^{\mathrm{p}}$ that represents an interaction between *particles* and the particle-void *mixture*; particles do not convect with the mixture and hence interact internally with the mixture through the background field $\boldsymbol{f}$.

Finally, applying (2.10) with $g=\psi$, (5.8), and the divergence theorem to (5.5),

$$\int\limits_{\mathcal{R}}\frac{\mathrm{D}\psi}{\mathrm{D}t}\,\mathrm{d}V\leq\sum_{k=1}^{K}\int\limits_{\mathcal{R}}\big(\boldsymbol{S}\cdot\boldsymbol{D}+\rho\boldsymbol{f}\cdot\boldsymbol{u}^{\mathrm{p}}-\operatorname{div}(\mu_k\boldsymbol{\jmath}_k)\big)\,\mathrm{d}V,$$

and, since $\rho\boldsymbol{f}\cdot\boldsymbol{u}^{\mathrm{p}}=m_k\boldsymbol{\jmath}_k\cdot\boldsymbol{f}$ and $\boldsymbol{\jmath}_k=\varphi_k\boldsymbol{u}_k$, we may use (2.13) to conclude that

$$\boldsymbol{S}\cdot\boldsymbol{D}+\sum_{k=1}^{K}\boldsymbol{\jmath}_k\cdot(m_k\boldsymbol{f}-\operatorname{grad}\mu_k)\geq\frac{\mathrm{D}\psi}{\mathrm{D}t}-\sum_{k=1}^{K}\mu_k\frac{\mathrm{D}\varphi_k}{\mathrm{D}t}.\tag{5.9}$$

We regard this *dissipation inequality* as a restriction on possible constitutive equations.

6. Constitutive equations

Our goal is not a general set of constitutive equations, but instead a fairly simple set that exhibits compaction and segregation.

6.1. *Free energy and chemical potentials. Residual inequality*

We assume that the free-energy density is a function

$$\psi=\hat{\psi}(\vec{\varphi})$$

of the particulate volume fractions, and that the particulate chemical potentials are given by the classical expression

$$\mu_k=\frac{\partial\hat{\psi}(\vec{\varphi})}{\partial\varphi_k}.\tag{6.1}$$

We consider two special cases of the theory: (*i*) a *cohesionless material* in which $\psi\equiv 0$ (so that all particulate chemical potentials μ_k vanish); (*ii*) a *cohesive material* in which ψ does not vanish identically.

Returning to the general theory, (6.1) reduces (5.9) to the residual inequality

$$\boldsymbol{S}\cdot\boldsymbol{D}+\sum_{k=1}^{K}\boldsymbol{\jmath}_k\cdot(m_k\boldsymbol{f}-\operatorname{grad}\mu_k)\geq 0. \tag{6.2}$$

In fact, we restrict attention to constitutive equations consistent with the more stringent requirement that the *diffusive dissipation*† and the *stress power* be separately nonnegative:

$$\boldsymbol{S}\cdot\boldsymbol{D}\geq 0 \qquad \text{and} \qquad \sum_{k=1}^{K}\boldsymbol{\jmath}_k\cdot(m_k\boldsymbol{f}-\operatorname{grad}\mu_k)\geq 0. \tag{6.3}$$

Trivially, $(6.3)_2$ may be written in an alternative form,

$$\sum_{k=1}^{K}\boldsymbol{\jmath}_k\cdot\operatorname{grad}(m_k\Psi+\mu_k)\leq 0, \tag{6.4}$$

asserting that, in the absence of other particles, particles of type k diffuse down the gradient of the *net* chemical potential $m_k\Psi+\mu_k$.

6.2. *Particulate volume fluxes*

It is convenient to write $\imath_{\boldsymbol{D}}$ for the list

$$\imath_{\boldsymbol{D}}=(|\boldsymbol{D}|,\det\boldsymbol{D}) \tag{6.5}$$

of invariants of the strain-rate $\boldsymbol{D}$. We suppose that the relative velocities $\boldsymbol{u}_k$ of the particulate species are characterized by *velocity moduli* $U_{kj}(\vec{\varphi},\imath_{\boldsymbol{D}})$ through constitutive relations of the form

$$\boldsymbol{u}_k=\sum_{j=1}^{K}U_{kj}(\vec{\varphi},\imath_{\boldsymbol{D}})(m_k\boldsymbol{f}-\operatorname{grad}\mu_j), \tag{6.6}$$

$k=1,2,\dots,K$. If we define *flux moduli* through

$$J_{kj}(\vec{\varphi},\imath_{\boldsymbol{D}})=\varphi_k U_{kj}(\vec{\varphi},\imath_{\boldsymbol{D}}),$$

then we can rewrite the constitutive relations (6.6) in the form

$$\boldsymbol{\jmath}_k=\sum_{j=1}^{K}J_{kj}(\vec{\varphi},\imath_{\boldsymbol{D}})(m_k\boldsymbol{f}-\operatorname{grad}\mu_j). \tag{6.7}$$

We assume that the $K\times K$ matrix with entries J_{kj} is positive semi-definite to ensure that $(6.3)_2$ is satisfied.

Since particle diffusion should be impossible at all closely packed states, we require that

$$U_{kj}(\vec{\varphi},\imath_{\boldsymbol{D}})=0 \qquad \text{for all } \vec{\varphi} \text{ that are CP}, \tag{6.8}$$

$j,k=1,2,\dots,K$; then, trivially, $J_{kj}(\vec{\varphi},\imath_{\boldsymbol{D}})=0$ for $\vec{\varphi}$ CP. (One might expect that packings that are not CP should not diffuse without sufficient agitation, and for that reason one might assume that the mixture is undergoing a background agitation of sufficiently small amplitude that its presence is not mentioned explicitly in the underlying theory or

† We use the terms 'diffusion' and 'diffusive' when discussing the relative motion of particles, even though the equations that govern cohesionless materials are generally *hyperbolic*.

should allow for the possibility that, for each $\vec{\varphi}$, the moduli $U_{kj}(\vec{\varphi}, \imath_{\boldsymbol{D}})$ vanish for some set of values of $\imath_{\boldsymbol{D}}$. We will not explicitly address this issue.)

For a *cohesionless material* the chemical potentials vanish identically and we may, without loss in generality, take

$$U_{kj} = 0 \quad \text{for} \quad k \neq j \qquad \text{and write} \qquad U_k = U_{kk}$$

(and similarly for the flux mobilities); (6.6) and (6.7) then become

$$\boldsymbol{u}_k = m_k U_k(\vec{\varphi}, \imath_{\boldsymbol{D}})\boldsymbol{f} \qquad \text{and} \qquad \boldsymbol{\jmath}_k = m_k J_k(\vec{\varphi}, \imath_{\boldsymbol{D}})\boldsymbol{f}. \tag{6.9}$$

6.3. *Extra stress*

Invariance under changes of observer requires the extra stress $\boldsymbol{S}$ be an isotropic function of $\boldsymbol{D}$ and $\vec{\varphi}$ consistent with $(6.3)_1$. If this function is well-defined at $\boldsymbol{D} = \boldsymbol{0}$, it follows that $\boldsymbol{S} = \boldsymbol{0}$ when $\boldsymbol{D} = \boldsymbol{0}$ independent of $\vec{\varphi}$. A particularly simple example of this type is the generalized Newtonian relation

$$\boldsymbol{S} = 2\eta(\vec{\varphi}, |\boldsymbol{D}|)\boldsymbol{D} \tag{6.10}$$

with *viscosity* consistent with $\eta(\vec{\varphi}, |\boldsymbol{D}|) \geq 0$.

More generally, we can consider a relation which is not defined at $\boldsymbol{D} = \boldsymbol{0}$. In this case, $\boldsymbol{S}$ is indeterminate when $\boldsymbol{D} = \boldsymbol{0}$, but objectvity requires that the set of attainable extra stresses be invariant. An example of this type is the generalized Bingham relation

$$\begin{cases} |\boldsymbol{S}| \leq s(\vec{\varphi}) & \text{when } \boldsymbol{D} = \boldsymbol{0}, \\ \boldsymbol{S} = s(\vec{\varphi})\dfrac{\boldsymbol{D}}{|\boldsymbol{D}|} + 2\eta(\vec{\varphi}, |\boldsymbol{D}|)\boldsymbol{D} & \text{when } \boldsymbol{D} \neq \boldsymbol{0}, \end{cases} \tag{6.11}$$

with *yield stress* $s(\vec{\varphi}) > 0$ and *viscosity* $\eta(\vec{\varphi}, |\boldsymbol{D}|) \geq 0$, which might potentially describe plug flows.

Both (6.10) and (6.11) are capable of encompassing the quadratic dependence of shear stress on shear strain-rate that has been observed for granular materials (Bagnold 1954; Shahinpoor & Lin 1982). However, because they cannot account for the normal stress differences that typically arise in granular materials, these choice represent severe idealizations. More generally, we would find acceptable any expression for $\boldsymbol{S}$ that encompasses the observed non-Newtonian characteristics of granular materials and that satisfies $\boldsymbol{S} \cdot \boldsymbol{D} \geq 0$. A thorough discussion of such relations is beyond the scope of this paper, especially since little is known about the effect of particle size distributions on flow.† The subsequent discussion will be independent of the particular constitutive equation chosen for $\boldsymbol{S}$.

6.4. *Simple granular materials*

We now describe a class of materials that hopefully characterizes at least qualitatively the tendency of granular materials to segregate by size. These materials, called *simple granular materials*, are defined by the following set of constitutive assumptions:

(G1) The material is *cohesionless:*

$$\psi \equiv 0.$$

(G2) Particles differ only by size:

$$m_1 = m_2 = \cdots = m_K = m. \tag{6.12}$$

† See the review articles of Hutter & Rajagopal (1994) and Wang & Hutter (2001) for discussions of constitutive equations for the stress in a monodisperse granular medium.

(G3) The packing domain $\mathcal{A}$ is the set of all packings $\vec{\varphi}$ such that the *total particulate volume fraction*

$$\varphi^{\mathrm{p}} = \sum_{k=1}^{K} \varphi_k \tag{6.13}$$

satisfies

$$\varphi^{\mathrm{p}} \leq \overset{*}{\varphi}, \tag{6.14}$$

where $\overset{*}{\varphi}$ is a constitutive constant consistent with $0 < \overset{*}{\varphi} < 1$. (By definition, packings $\vec{\varphi}$ automatically satisfy $\varphi_k \geq 0$, $k = 1, 2, \ldots, K$.) The CP manifold is then the set of all packings $\vec{\varphi}$ such that

$$\varphi^{\mathrm{p}} = \overset{*}{\varphi},$$

so that the total particulate volume fraction has the same value at all CP states, as does the void fraction $\varphi^{\mathrm{v}} = 1 - \varphi^{\mathrm{p}}$, which has the value

$$\overset{*}{\varphi}^{\mathrm{v}} = 1 - \overset{*}{\varphi}. \tag{6.15}$$

(G4) The constitutive relations for the velocity moduli have the simple form

$$U_k(\vec{\varphi}, \imath_{\boldsymbol{D}}) = \frac{1}{m} \alpha_k(\imath_{\boldsymbol{D}}) h(\varphi^{\mathrm{p}}), \tag{6.16}$$

with $\alpha_k(\imath_{\boldsymbol{D}}) \geq 0$ and

$$h(\varphi^{\mathrm{p}}) > 0 \ \text{ for } \ 0 < \varphi^{\mathrm{p}} < \overset{*}{\varphi}, \qquad h(\varphi^{\mathrm{p}}) = 0 \ \text{ for } \ \varphi^{\mathrm{p}} \geq \overset{*}{\varphi}, \tag{6.17}$$

so that $(6.3)_2$ is satisfied and so that the relative velocities vanish when the packing is CP. The corresponding flux moduli are given by

$$J_k(\vec{\varphi}, \imath_{\boldsymbol{D}}) = \frac{1}{m} \varphi_k \alpha_k(\imath_{\boldsymbol{D}}) h(\varphi^{\mathrm{p}}). \tag{6.18}$$

We refer to h as the *compaction function* and to the α_k as the *effective mobilities*. The only constitutive moduli that differentiate between particle types are then the effective mobilities $\alpha_k(\imath_{\boldsymbol{D}})$. We assume that these mobilities are nonzero (even when $\boldsymbol{D} = \boldsymbol{0}$); without loss in generality, we may then assume that

$$\alpha_1(\imath_{\boldsymbol{D}}) > \alpha_2(\imath_{\boldsymbol{D}}) > \cdots > \alpha_K(\imath_{\boldsymbol{D}}) > 0 \tag{6.19}$$

for all $\boldsymbol{D}$, so that, for $\vec{\varphi}$ not CP,

$$U_1(\vec{\varphi}, \imath_{\boldsymbol{D}}) > U_2(\vec{\varphi}, \imath_{\boldsymbol{D}}) > \cdots > U_K(\vec{\varphi}, \imath_{\boldsymbol{D}}) > 0 \tag{6.20}$$

for all $\boldsymbol{D}$.

(G5) The constitutive equation for the extra stress depends on $\vec{\varphi}$ through φ^{p}, so that, for example, (6.10) would specialize to

$$\boldsymbol{S} = 2\eta(\varphi^{\mathrm{p}}, \imath_{\boldsymbol{D}}) \boldsymbol{D}.$$

7. Governing equations

7.1. *Basic evolution equations*

Our theory yields evolution equations for $\boldsymbol{v}$, p, and the particulate fields φ_k and $\boldsymbol{u}_k$. These consist of the constraint equation

$$\operatorname{div} \boldsymbol{v} = 0, \tag{7.1}$$

the force balance

$$\operatorname{div} \boldsymbol{S} + \sum_{k=1}^{K} m_k \varphi_k \boldsymbol{f} = \operatorname{grad} p \tag{7.2}$$

supplemented by a constitutive relation for $\boldsymbol{S}$, and the (constitutively augmented) particulate volume balances

$$\frac{\mathrm{D}\varphi_k}{\mathrm{D}t} = -\sum_{j=1}^{K} \operatorname{div}\big(J_{kj}(\vec{\varphi}, \imath_{\boldsymbol{D}})(m_k \boldsymbol{f} - \operatorname{grad} \mu_j)\big) \qquad \text{with} \qquad \mu_k = \frac{\partial \hat{\psi}(\vec{\varphi})}{\partial \varphi_k}, \tag{7.3}$$

$k = 1, 2, \dots, K$. (Cf. (2.13), (3.1), (3.2), (4.5), (6.7).) For a cohesive material, the presence of the chemical potentials complicates these equations.

If the material is cohesionless the chemical potentials vanish and we may use (6.9) in place of (6.7) for the fluxes; the result is

$$\frac{\mathrm{D}\varphi_k}{\mathrm{D}t} = -m_k \operatorname{div}\big(\varphi_k U_k(\vec{\varphi}, \imath_{\boldsymbol{D}})\boldsymbol{f}\big). \tag{7.4}$$

Unless further restrictions are placed on the mobilities, this system — as a system of first-order partial differential equations for $\vec{\varphi}$, given the field $\boldsymbol{v}$ — is without type and hence intricate with respect to the choice of natural boundary conditions. A second difficulty arises in the requirement that $\vec{\varphi}$ is constrained to lie in a closed set, the packing domain, which in the case of a simple granular material has the form (6.14).

The special case of one particle type ($K = 1$) is useful in the study of pure compaction; here, omitting subscripts, there is a single volume balance

$$\frac{\mathrm{D}\varphi}{\mathrm{D}t} = -\operatorname{div}\big(\varphi U(\varphi, \imath_{\boldsymbol{D}})(m\boldsymbol{f} - \hat{\psi}'(\varphi)\operatorname{grad}\varphi)\big). \tag{7.5}$$

For a cohesionless material this balance has the form

$$\frac{\mathrm{D}\varphi}{\mathrm{D}t} = -m \operatorname{div}\big(\varphi U(\varphi, \imath_{\boldsymbol{D}})\boldsymbol{f}\big) \tag{7.6}$$

and represents a *hyperbolic* partial differential equation for φ, given the field $\boldsymbol{v}$, in contrast to the parabolic nature of such equations in more standard theories of diffusion.

7.2. *Volume balances for simple granular materials*

If the material is simple, then the flux is given by (6.18) and the system of volume balances takes the form

$$\frac{\mathrm{D}\varphi_k}{\mathrm{D}t} = -\operatorname{div}\big(\varphi_k \alpha_k(\imath_{\boldsymbol{D}}) h(\varphi^{\mathrm{p}})\boldsymbol{f}\big), \qquad \varphi^{\mathrm{p}} = \sum_{k=1}^{K} \varphi_k, \tag{7.7}$$

with volume fractions subject to the constraint

$$\varphi_k \geq 0, \quad k = 1, 2, \dots, K, \qquad \varphi^{\mathrm{p}} \leq \overset{*}{\varphi}. \tag{7.8}$$

Less succinctly, (7.7) may be written in the form

$$\frac{\mathrm{D}\varphi_k}{\mathrm{D}t} = -\alpha_k(\imath_{\boldsymbol{D}}) \sum_{j=1}^{K} \big(\delta_{jk} h(\varphi^{\mathrm{p}}) + \varphi_k h'(\varphi^{\mathrm{p}})\big)\boldsymbol{f} \cdot \operatorname{grad}\varphi_j + \Phi_k(\vec{\varphi}, \boldsymbol{D}, \operatorname{grad}\boldsymbol{D}), \tag{7.9}$$

with δ_{jk} the Kronecker delta. Let

$$M_{kj}(\vec{\varphi}) = \delta_{jk} h(\varphi^{\mathrm{p}}) + \varphi_k h'(\varphi^{\mathrm{p}}).$$

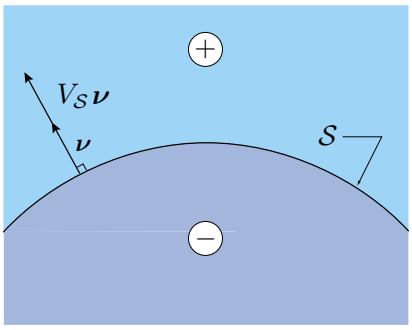

FIGURE 2. Schematic of shock surface $\mathcal{S}$ with orientation $\boldsymbol{\nu}$ and scalar normal velocity $V_{\mathcal{S}}$ across which the volume fractions are discontinuous.

Then for $\vec{\varphi}$ in the interior of the constraint set defined by (7.8), $M_{kj}(\vec{\varphi}) = \varphi_k B_{kj}(\vec{\varphi})$ with $B_{kj} = B_{jk}$. The $K \times K$ coefficient matrix with entries $\alpha_k(\imath_{\boldsymbol{D}})M_{kj}(\vec{\varphi})$ therefore has K (not necessarily distinct) eigenvalues for each such choice of $\vec{\varphi}$. Thus for $\alpha_k(\imath_{\boldsymbol{D}})M_{kj}(\vec{\varphi})$ and $\Phi_k(\vec{\varphi}, \boldsymbol{D}, \operatorname{grad}\boldsymbol{D})$ "frozen" at fixed values of their arguments, the resulting *linear system* for $\vec{\varphi}$ may be rewritten in diagonal form; in this sense the system (7.9) is *hyperbolic*.

8. Particulate shocks in cohesionless materials

We assume throughout this section that the material is cohesionless.

8.1. *Particulate shocks*

The force balance, although coupled to the volume balances, is the basic evolution equation for the velocity field $\boldsymbol{v}$ and we expect that, as in more standard theories of Newtonian and non-Newtonian fluids, this equation should lead to behavior in which $\boldsymbol{v}$ *is continuous* — an expectation we now take as a basic assumption. On the other hand, as we have seen, for a cohesionless material the volume balances can be hyperbolic; with this in mind, we now discuss possible jump conditions at a surface across which the particulate volume fractions and relative velocities suffer jump discontinuities. We refer to such surfaces as *particulate shocks*. Here it is important to note that if the constitutive equation for the extra stress $\boldsymbol{S}$ involves the volume fractions $\vec{\varphi}$, as in (6.10), then one would expect jump discontinuities in $\boldsymbol{S}$ and $\boldsymbol{D}$.

Consider a particulate shock $\mathcal{S}$, let $\boldsymbol{\nu}$ denote a continuous unit normal field for $\mathcal{S}$, and let $V_{\mathcal{S}}$ denote the (scalar normal) velocity of $\mathcal{S}$ in the direction of $\boldsymbol{\nu}$, so that

$$V = V_{\mathcal{S}} - \boldsymbol{v} \cdot \boldsymbol{\nu} \tag{8.1}$$

represents the velocity of the shock relative to the mixture. Further, given a field g, let g^+ denote the limit of g, on $\mathcal{S}$, taken from the region into which $\boldsymbol{\nu}$ points (the $(+)$ side of $\mathcal{S}$), let g^- denote the corresponding limit from the other side of $\mathcal{S}$ (the $(-)$ side), and let $[\![g]\!] = g^+ - g^-$.

Choose a control volume $\mathcal{R}$ that contains $\mathcal{S}$. Then, localizing the integral statement (4.1) for balance of forces at a point on $\mathcal{S}$, we find (for $\rho\boldsymbol{f}$ integrable) that

$$[\![\boldsymbol{S}]\!]\boldsymbol{\nu} - [\![p]\!]\boldsymbol{\nu} = \boldsymbol{0}.$$

Similarly, localizing the volume balance $(2.6)_1$ for particles of type k, we obtain $[\![\varphi_k]\!]V_{\mathcal{S}} = [\![\varphi_k \boldsymbol{v}_k]\!] \cdot \boldsymbol{\nu}$, or equivalently, by $(2.4)_1$ and (8.1),

$$[\![\varphi_k]\!]V = [\![\varphi_k \boldsymbol{u}_k]\!] \cdot \boldsymbol{\nu}.$$

Thus, by (6.9),

$$[\![\varphi_k]\!]V = m_k[\![\varphi_k U_k(\vec{\varphi}, \imath_{\boldsymbol{D}})]\!]\boldsymbol{f}\cdot\boldsymbol{\nu}, \qquad k = 1, 2, \ldots, K. \tag{8.2}$$

If $\boldsymbol{f}\cdot\boldsymbol{\nu} = 0$, then, granted at least one the particulate volume fraction is discontinuous at $\mathcal{S}$, then $V = 0$ and *the shock convects with the mixture.*

We henceforth assume that

$$\boldsymbol{f}\cdot\boldsymbol{\nu} \neq 0.$$

We find it convenient to write

$$U_k^{\pm} = U_k(\vec{\varphi}^{\pm}, \imath_{\boldsymbol{D}}^{\pm}),$$

and for a simple granular material,

$$\alpha_k^{\pm} = \alpha_k(\imath_{\boldsymbol{D}^{\pm}}) \quad \text{and} \quad h_k^{\pm} = h_k(\varphi^{p\pm}).$$

8.2. *Compactification shocks*

We say that a packing on, say, the (+)-side, is *compatible* with a packing on the (−)-side if (8.2) is satisfied for some choice of V. For example, any two CP packings are compatible, and $V = 0$ is always the corresponding velocity (cf. (6.8)).

We now determine the class of CP packings compatible with a prescribed LP packing, where we use the abbreviation

$$\text{LP} = \text{not CP}.$$

Such CP packings are said to *compactify* the LP material. More specifically, we say that a shock $\mathcal{S}$ *compactifies* LP *material on its* (+)*-side* if:

- the particles on the (+)-side are LP;
- the (−)-side consists of exactly the same particle types as the (+) side;
- the (−)-side is CP.

Given such a *compactification shock* $\mathcal{S}$, we may, without loss of generality, relabel the particle types present on its two sides by the integers $1, 2, \ldots, A$, with $A \leq K$, so that

$$\varphi^{\text{P}+} = \varphi_1^+ + \varphi_2^+ + \cdots + \varphi_A^+ \qquad \text{and} \qquad \varphi^{\text{P}-} = \varphi_1^- + \varphi_2^- + \cdots + \varphi_A^- = \overset{*}{\varphi}. \tag{8.3}$$

Thus, by (6.8), $U_k^- = 0$ for $k = 1, 2, \ldots, A$ and (8.2) yields

$$(\varphi_k^+ - \varphi_k^-)V = R_k^+\,\boldsymbol{f}\cdot\boldsymbol{\nu} \tag{8.4}$$

with

$$R_k^+ = m_k\varphi_k^+ U_k^+ > 0.$$

Summing over all particle types we find, with the aid of (8.3), that

$$V = -\frac{(R_1^+ + R_2^+ + \cdots + R_A^+)}{(\overset{*}{\varphi} - \varphi^{p+})}\,\boldsymbol{f}\cdot\boldsymbol{\nu}, \tag{8.5}$$

so that the sign of V is opposite to that of $\boldsymbol{f}\cdot\boldsymbol{\nu}$. (Note that if $\boldsymbol{f}$ is gravitational and points "down," and if the CP particles lie "below" the other particles, so that $\boldsymbol{\nu}$ points "up," then the shock moves upward compacting the material above it.)

Using (8.5), we may eliminate V from (8.2); the result is an equation

$$\varphi_k^- = \varphi_k^+ + \frac{R_k^+(\overset{*}{\varphi} - \varphi^{p+})}{R_1^+ + R_2^+ + \cdots + R_A^+} \tag{8.6}$$

giving each of the volume fractions on the (−)-side, which is CP, in terms of the volume fractions on the (+)-side, which is LP. Thus *there is exactly one* LP *packing compatible with a prescribed* CP *packing:* the particulate volume fractions of the LP packing are given

by (8.6) and the velocity of the shock by (8.5). Note that the process of compactification strictly raises the volume fraction of each of the particle types involved, with *relative compaction*

$$\kappa_k = \frac{\varphi_k^-}{\varphi_k^+} - 1 \tag{8.7}$$

proportional to $m_k U_k^+$. Since $\overset{*}{\varphi} - \varphi^{\mathrm{p}+} = \varphi^{\mathrm{v}+} - (1 - \overset{*}{\varphi})$, the relative compaction increases linearly with the volume fraction of voids on the loosely packed side of the shock.

For a simple granular material, $R_k^+ = m\varphi_k^+ U_k^+ = \varphi_k^+ \alpha_k^+ h^+$ (cf. (6.16)) and

$$\left.\begin{aligned} V &= -\frac{(\varphi_1^+\alpha_1^+ + \varphi_2^+\alpha_2^+ + \cdots + \varphi_A^+\alpha_A^+)h^+}{\overset{*}{\varphi} - \varphi^{\mathrm{p}+}}\, \boldsymbol{f}\cdot\boldsymbol{\nu}, \\ \kappa_k &= \frac{\varphi_k^+\alpha_k^+(\overset{*}{\varphi} - \varphi^{\mathrm{p}+})}{\varphi_1^+\alpha_1^+ + \varphi_2^+\alpha_2^+ + \cdots + \varphi_A^+\alpha_A^+}. \end{aligned}\right\} \tag{8.8}$$

When φ_k^+ has the same value φ^+ for all particle types k present at the shock,

$$\left.\begin{aligned} V &= -\frac{(\alpha_1^+ + \alpha_2^+ + \cdots + \alpha_A^+)\varphi^+ h^+}{\overset{*}{\varphi} - \varphi^{\mathrm{p}+}}\, \boldsymbol{f}\cdot\boldsymbol{\nu}, \\ \kappa_k &= \frac{\alpha_k^+(\overset{*}{\varphi} - \varphi^{\mathrm{p}+})}{\alpha_1^+ + \alpha_2^+ + \cdots + \alpha_A^+}, \end{aligned}\right\} \tag{8.9}$$

and the relative compactions of any two particle types are in direct ratio to their effective mobilities.

8.3. *Shocks separating particles of a single type from a mixture*

We, here, consider an important class of shocks that separate particles of a single type from a mixture. A shock $\mathcal{S}$ *separates particles of type* k if particles of that type are present on just one side of $\mathcal{S}$, say the $(-)$ side:

$$\varphi_k^- > 0 \quad \text{and} \quad \varphi_k^+ = 0. \tag{8.10}$$

In this case, (8.2) yields an explit expression for the relative velocity of the shock:

$$V = m_k U_k^-\, \boldsymbol{f}\cdot\boldsymbol{\nu}. \tag{8.11}$$

In particular, if $\mathcal{S}$ separates particles of a given type and if the side of $\mathcal{S}$ on which that type is present is CP, then $\mathcal{S}$ convects with the mixture. Further, by (8.11), if a single shock separates particles of more than one type — with the sides on which the separeted types are present allowed to vary from type to type — then the mass-weighted velocity-moduli of the separated types must coincide at the shock.

Consider a *simple granular material* and let $\mathcal{S}$ be a shock that separate particles of a single type from a mixture. Assume that

$$V \neq 0 \quad \text{and} \quad [\![\boldsymbol{D}]\!] = \boldsymbol{0}.$$

Then, by (6.12) and (6.20), $\mathcal{S}$ *can separate at most one particle type* s, and, for $\varphi_s^+ = 0$,

$$V = \alpha_s h^-\, \boldsymbol{f}\cdot\boldsymbol{\nu}, \tag{8.12}$$

where we suppress the argument $\imath_{\boldsymbol{D}}$, since $\alpha_s(\imath_{\boldsymbol{D}})$ is continuous across the shock. For a shock of this type, one may ask what packings on the $(+)$-side are compatible with a

given packing on the (−)-side. We now answer this question for the special case $K = 2$ of two particle types, with

$$[\![\varphi_1]\!] \neq 0, \qquad \varphi_2^+ = 0, \qquad \varphi_2^- > 0,$$

and a compaction function of the special form

$$h(\varphi^p) = \overset{*}{\varphi} - \varphi^{\mathrm{p}}. \tag{8.13}$$

Thus,

$$h^+ = \overset{*}{\varphi} - \varphi_1^+ \quad \text{and} \quad h^- = \overset{*}{\varphi} - \varphi_1^- - \varphi_2^- = \overset{*}{\varphi} - \varphi^{\mathrm{p}-},$$

and (8.2) yields

$$\left.\begin{aligned} V &= \alpha_1 h^- \boldsymbol{f}\cdot\boldsymbol{\nu}, \\ V(\varphi_1^+ - \varphi_1^-) &= \alpha_2(\varphi_1^+(\overset{*}{\varphi} - \varphi_1^+) - \varphi_1^- h^-)\boldsymbol{f}\cdot\boldsymbol{\nu}. \end{aligned}\right\} \tag{8.14}$$

Eliminating V between $(8.14)_1$ and $(8.14)_2$, we get a quadratic equation for φ_1^+, which is the unknown volume fraction of the (+)-side packing. Defining

$$\delta = \frac{\alpha_2}{\alpha_1} - 1, \tag{8.15}$$

the two solutions of this quadratic equation are determined by

$$\varphi_1^+ = \frac{1}{2}\left(\varphi^{\mathrm{p}-} - \delta(\overset{*}{\varphi} - \varphi^{\mathrm{p}-}) \pm \sqrt{(\varphi^{\mathrm{p}-} - \delta(\overset{*}{\varphi} - \varphi^{\mathrm{p}-}))^2 + 4\delta(\overset{*}{\varphi} - \varphi^{\mathrm{p}-})\varphi_1^-}\right). \tag{8.16}$$

For (8.16) to yield a volume fraction, we must have

$$0 < \varphi_1^+ < \overset{*}{\varphi}. \tag{8.17}$$

In the case $\delta > 0$, only the root taking the plus-sign has $\varphi_1^+ > 0$ and a straightforward calculation shows that this root obeys $\varphi_1^+ < \varphi^{\mathrm{p}-}$ and, thus, yields a unique volume fraction. In the case $-1 < \delta < 0$, both roots have $\varphi_1^+ > 0$ and straightforward algebraic manipulations show that the root taking the plus-sign obeys $\varphi^{\mathrm{p}-} < \varphi_1^+ < \overset{*}{\varphi}$ and that the root taking the minus-sign obeys $0 < \varphi_1^+ < \varphi_1^-$. Thus, both roots yield volume fractions.

9. Boundary conditions associated with the particulate balances

9.1. *Particulate free surfaces*

A (particulate) *free surface* is an evolving surface $\mathcal{S}$ that separates a region containing a mixture of particles and voids from a region of pure voids.† Letting $\boldsymbol{\nu}$ denote a continuous unit normal field for $\mathcal{S}$ directed into the region of pure voids, the argument leading to (8.11) yields a free-boundary condition

$$m_k U_k = \frac{V}{\boldsymbol{f}\cdot\boldsymbol{\nu}} \tag{9.1}$$

for any particle type k present at the free surface. In particular, by (6.12) and (6.20), *at most one particle type can be present at the free surface of a simple granular material*. If that particle type is CP then the free surface convects with the mixture.

† In problems involving the transport of granular material by a fluid a particulate free surface would be an interface between the region containing grains and that containing pure fluid.

9.2. *Solid boundaries*

Consider a solid boundary $\mathcal{S}$ with orientation $\boldsymbol{\nu}$ directed outward from the mixture. Then $V_{\mathcal{S}} = \boldsymbol{v}\cdot\boldsymbol{\nu} = \boldsymbol{v}_k\cdot\boldsymbol{\nu}$ for each particle type k; hence $\boldsymbol{u}_k\cdot\boldsymbol{\nu} = 0$ and

$$\varphi_k U_k \boldsymbol{f}\cdot\boldsymbol{\nu} = 0, \tag{9.2}$$

so that, for $\boldsymbol{f}\cdot\boldsymbol{\nu} \neq 0$,

$$\varphi_k = 0 \qquad \text{or} \qquad U_k = 0 \tag{9.3}$$

for each particle type k. Thus, by (6.12) and (6.20), *for a simple granular material, particles present at a solid boundary must be* CP.

10. Compaction and segretation by gravity in a cohesionless material: some simple solutions

10.1. *Problem setting*

We suppose that the body force is purely gravitational, viz.,

$$\boldsymbol{f} = \boldsymbol{g}, \tag{10.1}$$

with $\boldsymbol{g}$ the gravitational acceleration. We let z denote the Cartesian coordinate in the direction $\boldsymbol{e} = -\boldsymbol{g}/|\boldsymbol{g}|$ and seek solutions of the evolution equations for which the mixture fields $\boldsymbol{v}$ and p and the particulate fields φ_k and $\boldsymbol{u}_k$ are functions of z and t, with

$$\boldsymbol{v} = v\boldsymbol{e} \qquad \text{and} \qquad \boldsymbol{u}_k = u_k\boldsymbol{e}.$$

Then, since $\operatorname{div}\boldsymbol{v} = 0$, v must be constant and we may, without loss in generality, assume that

$$v \equiv 0.$$

Thus, $\boldsymbol{D} = \boldsymbol{0}$ and, as per our discussion in § 6.3, the extra stress $\boldsymbol{S}$ either vanishes or is indeterminate. For the indeterminate case, we take $\boldsymbol{S} = S\boldsymbol{e}\otimes\boldsymbol{e}$. Force balance requires that

$$\frac{\partial(p-S)}{\partial z} = -\sum_{k=1}^{K} m_k\varphi_k|\boldsymbol{g}| \tag{10.2}$$

which, given the volume fractions φ_k, determines the difference $p-S$ between the pressure and the extra stress. Equation (10.2) holds with $S = 0$ when the constitutive relation for $\boldsymbol{S}$ is well-defined at $\boldsymbol{D} = \boldsymbol{0}$.

We assume that the material is cohesionless; the particulate volume balances (7.4) then take the form

$$\frac{\partial\varphi_k}{\partial t} = w_k\,\frac{\partial}{\partial z}\Big(\varphi_k U_k(\vec{\varphi})\Big) \tag{10.3}$$

for each particle type k, with

$$w_k = m_k|\boldsymbol{g}|. \tag{10.4}$$

(We omit the argument $\boldsymbol{D} = \boldsymbol{0}$.) Regarding the shock conditions, we choose $\boldsymbol{\nu} = \boldsymbol{e}$, so that

$$\boldsymbol{f}\cdot\boldsymbol{\nu} = -|\boldsymbol{g}|, \qquad m_k\boldsymbol{f}\cdot\boldsymbol{\nu} = -w_k.$$

We limit our discussion to evolution in a *fixed container* that occupies the interval

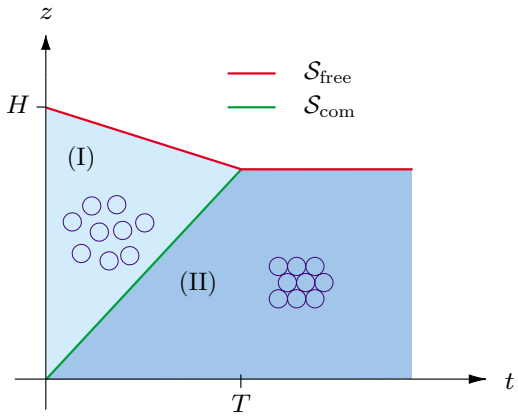

FIGURE 3. Compaction, by gravity, of particles of a single type in a fixed container. Up until time T, the solution at any t consists of constant states separated by a shock. The states are denoted by roman numerals: (I) consists of loosely packed particles; (II) of closely packed particles. $\mathcal{S}_{\text{free}}$ and $\mathcal{S}_{\text{com}}$ denote the free surface and the compaction shock.

$0 \le z \le H$, with $z = 0$ an impermeable base and $z = H$ the initial free surface. We assume that initially each volume fraction φ_k has a prescribed *constant* value:

$$\varphi_k(z,0) = \mathring{\varphi}_k, \qquad 0 \le z \le H,$$

for $k = 1, 2, \dots, K$, with the initial packing LP, so that, in the special case of a simple granular material,

$$\mathring{\varphi}^p = \mathring{\varphi}_1^+ + \mathring{\varphi}_2^+ + \cdots + \mathring{\varphi}_K^+ < \overset{*}{\varphi}.$$

We shall consider solutions $\vec{\varphi}(z,t)$ that consist of *constant states separated by shocks*; i.e., fields $\vec{\varphi}(z,t)$ that are constant in any open set in the (z,t)-plane not intersected by a shock. Any such field $\vec{\varphi}(z,t)$ satisfies the volume balances (10.3) identically away from all shocks, thus to show that such a field $\vec{\varphi}(z,t)$ is a solution we need only verify: that its values lie in the packing domain; that the relevant jump conditions are satisfied across all shocks; that the boundary condition (9.3) is satisfied at the base $z = 0$; and that (9.1) is satisfied at the free boundary defined by the uppermost point of the particulate aggregate.

10.2. *Gravity-driven compaction of a single particle species*

To demonstrate the process of compaction, we consider a single particle type $K = 1$ and assume that its velocity modulus satisfies

$$U(\varphi) > 0, \quad 0 < \varphi < \overset{*}{\varphi}, \qquad U(\varphi) = 0, \quad \overset{*}{\varphi} \le \varphi < 1.$$

with $\overset{*}{\varphi}$ the CP volume fraction.

As a candidate for a solution we consider the field $\varphi(z,t)$ characterized in Figure 3. This candidate is the union of:

- a uniform LP state (I) in which $\varphi \equiv \mathring{\varphi}$; this state is bounded by a free surface $\mathcal{S}_{\text{free}}$ and a compaction shock $\mathcal{S}_{\text{com}}$;
- a uniform CP state (II) bounded by the container base and the compaction shock $\mathcal{S}_{\text{com}}$; at the time T, $\mathcal{S}_{\text{com}}$ and $\mathcal{S}_{\text{free}}$ meet and all of the material is CP; from then on $\mathcal{S}_{\text{free}}$ is horizontal.

To verify that this candidate is a solution, we write V_{free} for the velocity of $\mathcal{S}_{\text{free}}$ and

$V_{\rm com}$ for the velocity of $\mathcal{S}_{\rm com}$. We have only to show that the following conditions are satisfied:

(i) the solid-boundary condition (cf. $(9.3)_2$)

$$U(\varphi) = 0 \qquad \text{at} \quad z = 0 \tag{10.5}$$

for $t > 0$;

(ii) the jump condition (cf. (9.1))

$$[\![\varphi]\!] V_{\rm com} = -w\,[\![\varphi U(\varphi)]\!] \qquad \text{on} \quad \mathcal{S}_{\rm com} \tag{10.6}$$

for $0 < t < T$;

(iii) the free-surface conditions (9.1)

$$V_{\rm free} = -w\,U(\varphi) \qquad \text{on} \quad \mathcal{S}_{\rm free} \tag{10.7}$$

for $0 < t < T$ and

$$V_{\rm free} = 0 \qquad \text{on} \quad \mathcal{S}_{\rm free} \tag{10.8}$$

for $t \geq T$.

The first of (10.5) is immediate, since $\varphi(0,t) = \overset{*}{\varphi}$ and $U(\overset{*}{\varphi}) = 0$; (10.6) gives the velocity

$$V_{\rm com} = w\,\frac{\varphi_0 U(\varphi_0)}{\overset{*}{\varphi} - \varphi_0} \qquad \text{on} \quad \mathcal{S}_{\rm com},$$

while (10.7) gives the velocity

$$V_{\rm free} = -w\,U(\varphi_0) \qquad \text{on} \quad \mathcal{S}_{\rm free}.$$

Since these formulas give $V_{\rm com} > 0$ and $V_{\rm free} < 0$, there is a time T at which $\mathcal{S}_{\rm com}$ and $\mathcal{S}_{\rm free}$ meet. For $t > T$ the material is CP and $U(\overset{*}{\varphi}) = 0$; this yields (10.8).

10.3. *Gravity-driven compaction and segregation*

As in § 8.3 we consider a simple granular material involving two particle types: large particles labelled b and small particles labelled s. We assume that the smaller particles are more mobile than the larger ones and we restrict attention to the compaction function

$$h(\varphi^p) = \overset{*}{\varphi} - \varphi^p.$$

Our candidate solution is shown in Figure 4; it is the union of:

- a uniform LP state (I) consisting only of large particles; this state is bounded by a free surface $\mathcal{S}_{\rm free}$ and a segregation shock $\mathcal{S}_{\rm seg}$;
- a mixed uniform LP state (II) in which $\varphi_b \equiv \overset{\circ}{\varphi}_b$, $\varphi_s \equiv \overset{\circ}{\varphi}_s$; this state is bounded by $\mathcal{S}_{\rm seg}$ and a compaction shock $\mathcal{S}_{\rm com}$; at the time T_1 these shocks meet; from then on $\mathcal{S}_{\rm seg}$ is horizontal;
- a mixed uniform CP state (III) that is bounded by the container base and the compaction shock $\mathcal{S}_{\rm com}$ until the time T_1; after T_1 this state is bounded by the base and $\mathcal{S}_{\rm seg}$.
- a uniform CP state (IV) consisting only of large particles; until the time T_2 this state is bounded by a compaction shock $\mathcal{S}_{\rm com}$ and the segregation shock $\mathcal{S}_{\rm seg}$; at T_2 the shock $\mathcal{S}_{\rm com}$ meets $\mathcal{S}_{\rm free}$; from then on the material is CP and $\mathcal{S}_{\rm free}$ is horizontal.

To verify that this candidate is a solution, we write $V_{\rm free}$ for the velocity of $\mathcal{S}_{\rm free}$ and $V_{\rm com}$ for the velocity of $\mathcal{S}_{\rm com}$. We have only to show that the following conditions are satisfied:

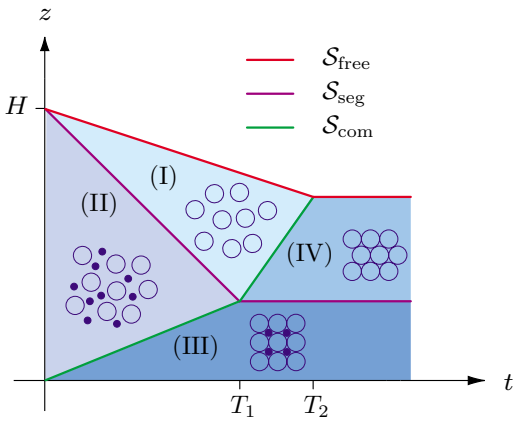

FIGURE 4. Compaction and segregation, by gravity, of a granular aggregate of large and small particles in a fixed container. The solution at any t consists of constant states separated by shocks. The states are denoted by roman numerals: (I) and (II) consist of loosely packed particles; (III) and (IV) of closely packed particles. $\mathcal{S}_{\rm free}$ denotes the free surface while $\mathcal{S}_{\rm seg}$ and $\mathcal{S}_{\rm com}$ denote the segregation and compaction shocks.

(*i*) the solid-boundary condition (cf. $(9.3)_2$)

$$U(\varphi^{\rm p}) = 0 \qquad \text{at} \quad z = 0 \tag{10.9}$$

for $t > 0$;

(*ii*) the jump conditions (cf. (9.1))

$$[\![\varphi_k]\!] V_{\rm com} = -w\alpha_k [\![\varphi_k h(\varphi)]\!] \qquad \text{on} \quad \mathcal{S}_{\rm com} \tag{10.10}$$

and

$$[\![\varphi_k]\!] V_{\rm seg} = -w\alpha_k [\![\varphi_k h(\varphi)]\!] \qquad \text{on} \quad \mathcal{S}_{\rm seg} \tag{10.11}$$

for $0 < t < T_1$, $k = s, b$;

(*iii*) the interface condition (cf. (9.1))

$$V_{\rm seg} = 0 \qquad \text{on} \quad \mathcal{S}_{\rm seg} \tag{10.12}$$

for $t \geq T_1$;

(*iv*) the jump conditions (cf. (9.1))

$$[\![\varphi_k]\!] V_{\rm com} = -w\alpha_k [\![\varphi_k h(\varphi^{\rm p})]\!] \qquad \text{on} \quad \mathcal{S}_{\rm com} \tag{10.13}$$

for $T_1 < t < T_2$, $k = s, b$;

(*V*) the free-surface conditions (9.1)

$$V_{\rm free} = -w\mathring{\varphi}_b h(^{\rm p}) \qquad \text{on} \quad \mathcal{S}_{\rm free} \tag{10.14}$$

for $0 < t < T_2$ and

$$V_{\rm free} = 0 \qquad \text{on} \quad \mathcal{S}_{\rm free} \tag{10.15}$$

for $t \geq T_2$.

The first of (10.5) is immediate, since $\varphi^{\rm p}(0,t) = \overset{*}{\varphi}$ and $h(\overset{*}{\varphi}) = 0$; (10.10) gives the velocity

$$V_{\rm com} = w(\alpha_b \mathring{\varphi}_b + \alpha_s \mathring{\varphi}_s) \qquad \text{on} \quad \mathcal{S}_{\rm com},$$

while (10.11) gives the velocity

$$V_{\rm seg} = -w\alpha_s(\overset{*}{\varphi} - \mathring{\varphi}_b - \mathring{\varphi}_s) \qquad \text{on} \quad \mathcal{S}_{\rm seg}.$$

Since these formulas give $V_{\rm com} > 0$ and $V_{\rm seg} < 0$, there is a time T_1 at which $\mathcal{S}_{\rm com}$ and $\mathcal{S}_{\rm seg}$ meet. For $t < T_1$ the material below $S_{\rm com}$ is CP and $h(\overset{*}{\varphi}) = 0$; this yields (10.12) and determines uniquely the volume fractions (cf. (8.6))

$$\varphi_b^{\rm III} = \mathring{\varphi}_b + \frac{\alpha_b\mathring{\varphi}_b(\overset{*}{\varphi} - \mathring{\varphi}_b - \mathring{\varphi}_s)}{(\alpha_b\mathring{\varphi}_b + \alpha_s\mathring{\varphi}_s)} \qquad \text{and} \qquad \varphi_s^{\rm III} = \mathring{\varphi}_s + \frac{\alpha_s\mathring{\varphi}_s(\overset{*}{\varphi} - \mathring{\varphi}_b - \mathring{\varphi}_s)}{(\alpha_b\mathring{\varphi}_b + \alpha_s\mathring{\varphi}_s)}$$

in (III). Next, (10.13) gives the velocity

$$V_{\rm com} = w\alpha_b\varphi_b^{\rm I}$$

while (10.14) gives the velocity

$$V_{\rm free} = -w\alpha_b(\overset{*}{\varphi} - \varphi_b^{\rm I}).$$

To determine $\varphi_b^{\rm I}$, we employ the results of § 8.3 across $\mathcal{S}_{\rm seg}$ between $t = 0$ and $t = T_1$. Since the large particles are above, b and s identitified, respectively, with 1 and 2. Hence, we obtain

$$\varphi_b^{\rm I} = \frac{1}{2}\left(\mathring{\varphi}^{\rm p^-} - \delta(\overset{*}{\varphi} - \mathring{\varphi}^{\rm p^-}) + \sqrt{(\mathring{\varphi}^{\rm p^-} - \delta(\overset{*}{\varphi} - \mathring{\varphi}^{\rm p^-}))^2 + 4\delta(\overset{*}{\varphi} - \mathring{\varphi}^{\rm p^-})\mathring{\varphi}_b^-}\right),$$

with

$$\delta = \frac{\alpha_s}{\alpha_b} - 1 > 0.$$

Since these formulas give $V_{\rm com} > 0$ and $V_{\rm free} < 0$, there is a time $T_2 > T_1$ at which $\mathcal{S}_{\rm com}$ and $\mathcal{S}_{\rm free}$ meet. For $t > T_2$ the volume fraction of slow particles in (IV) is CP and $h(\overset{*}{\varphi}) = 0$; this yields (10.15).

10.4. *Gravity-driven desegregation of a more mobile species*

The problems considered in §§ 10.2–10.3 illustrate the manner in which our theory describes the compaction and segregation of cohesionless granular mixtures under the influence of gravity. In addition to these generic results, our theory also predicts that, for a *special* class of initial conditions, gravity may drive a layer of small particles resting on a mixture of small and large particles to desegregate. We emphasize that, subsequent to such a process, segregation of the type discussed in § 10.3 occurs. Thus, for these special initial conditions, desegregation is a necessary precursor to segregation.

As before, we use b and s to denote the species of large and small particles. We continue to assume that the smaller particles are more mobile than the larger particles, so that $\alpha_s > \alpha_b$, and to restrict attention to the compaction function $h(\varphi^p) = \overset{*}{\varphi} - \varphi^p$. To focus on the phenomenon in question, we consider a layer of small particles of height H resting on a mixture of small and large particles occupying the semi-infinite interval $(-\infty, 0)$. We denote by $\mathring{\varphi}_s^+$ the volume fraction of the small particles in the layer and by $\mathring{\varphi}_b^-$ and $\mathring{\varphi}_s^-$ the volume fractions of small and large particles in the mixture below.

We identify, until further notice, s and b with species 1 and 2 in § 8.3. Then

$$-1 < \delta = \frac{\alpha_b}{\alpha_s} - 1 < 0$$

and, provided that $\mathring{\varphi}_s^+$ is related to $\mathring{\varphi}_b^-$ and $\mathring{\varphi}_s^-$ by either of the two solutions (cf. (8.16))

$$\mathring{\varphi}_s^+ = \frac{1}{2}\left(\mathring{\varphi}^{\rm p^-} - \delta(\overset{*}{\varphi} - \mathring{\varphi}^{\rm p^-}) \pm \sqrt{(\mathring{\varphi}^{\rm p^-} - \delta(\overset{*}{\varphi} - \mathring{\varphi}^{\rm p^-}))^2 + 4\delta(\overset{*}{\varphi} - \mathring{\varphi}^{\rm p^-})\mathring{\varphi}_s^-}\right),$$

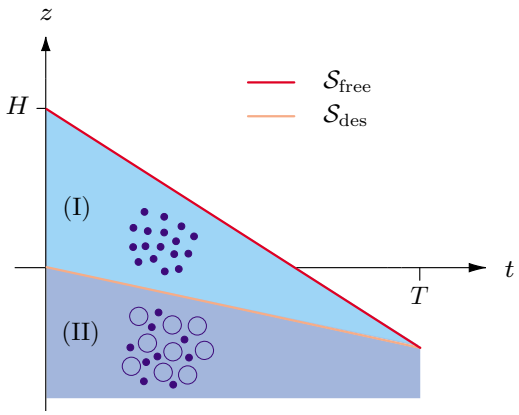

FIGURE 5. Desegregation, by gravity, of a granular aggregate that initially consists of a layer of small particles over a semi-infinite layer of large and small particles. Up until time T the solution involves constant states separated by shocks. The states are denoted by roman numerals: (I) consists of loosely packed small particles; (II) of loosely packed large and small particles. $\mathcal{S}_{\rm free}$ denotes the free surface and $\mathcal{S}_{\rm des}$ denotes the desegregation shock. With the disappearance, at time T, of the initial layer of small particles, a segregation shock forms at the free surface and a layer of large particles with volume fraction determined by the proportions of small and large particles in (II) develops.

it follows that there exists a free surface $\mathcal{S}_{\rm free}$ and a shock $\mathcal{S}_{\rm des}$ with velocities

$$V_{\rm free} = -w\alpha_s(\overset{*}{\varphi} - \mathring{\varphi}_s^+) \qquad \text{and} \qquad V_{\rm des} = -w\alpha_b(\overset{*}{\varphi} - \mathring{\varphi}^{\rm p-})$$

emanating, respectively, from the free surface and from the interface that initially separates the layer of small particles from the mixture below.

Using these formulas, we find that $V_* > V_{\rm free}$. Thus, there exists a time T at which the shocks $\mathcal{S}_{\rm free}$ and $\mathcal{S}_{\rm des}$ will meet and $\mathcal{S}_{\rm des}$ is a *desegregation* shock. The results of § 10.3 show that, at time T, a segregation shock will issue downward from the free surface at the intersection of $\mathcal{S}_{\rm free}$ and $\mathcal{S}_{\rm des}$. Hence, subsequent to time T, the medium segregates, developing a layer of large particles adjacent to the free surface.

Suppose that the volume fractions $\mathring{\varphi}_b^-$ and $\mathring{\varphi}_s^-$ are given. The different signs in the expression for $\mathring{\varphi}_s^+$ then correspond to two different states for which desegregation may occur. For $\mathring{\varphi}_s^+$ determined by the plus-sign, $\mathring{\varphi}_s^+ > \mathring{\varphi}^{\rm p-}$ and the layer of small particles above is more closely packed than the mixture. Thus, it is not surprising that small particles diffuse into the mixture. For $\mathring{\varphi}_s^+$ determined by the minus-sign, $\mathring{\varphi}_s^+ < \mathring{\varphi}_s^- < \mathring{\varphi}^{\rm p-}$. Although the mixture is more closely packed than the layer, diffusion still occurs in this case.

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