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**Theoretical and numerical analysis of hydrostatics and low-Mach
number flows of two-phase granular mixtures**

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To my parents and Nina

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Abstract

In this PhD Thesis we are concerned with the theoretical and numerical analysis of hydrostatics and low-Mach number flows of two-phase granular mixtures. Our research is based on a particular continuum model which in the Thesis is referred to as the *two-phase flow model of reference*. However, both the analytical and the numerical results that we develop are applicable to other models for granular flows, due to similarities between them.

In the first part, we generalize the concept of low-Mach number approximation to multi-phase flows and apply it to the two-phase flow model of reference. In our approach the governing system of equations is first non-dimensionalized with values that correspond to a reference thermodynamic state of the phase with the smaller speed of sound. By doing so, the Mach number based on this reference state emerges as a perturbation parameter of the equations at hand. Subsequently, we expand each variable in power series of this parameter and apply singular perturbation techniques to derive the low-Mach number equations. The structure of the low-Mach number equations for two special cases of particular interest, namely, constant density flows and the equilibrium limit is also discussed and analyzed. The first part concludes with some proposals for experimental validation of the equations.

In the second part, we analyze the equilibrium limit of the two-phase flow model of reference, and develop an algorithm for its numerical approximation. At equilibrium, this model reduces to a system of equations that describes the hydrostatics of two-phase granular mixtures. This is a strongly coupled, overdetermined system of nonlinear elliptic partial differential equations with respect to the pressure and the volume fraction of the granular phase. First we carry a perturbation analysis based on standard hydrostatic-type scaling arguments which reduces the complexity of the coupling of the equations. The perturbed system is then supplemented by an appropriate compatibility condition which arises from the properties of the gradient operator. Further, based on the Helmholtz

decomposition and Ladyzhenskaya's decomposition theorem, we develop a projection-type, Successive-Over-Relaxation numerical method. We also prove that this method is both stable and consistent hence convergent. The second part concludes with the presentation of representative numerical results.

In the third part, we present an existence theory for the equilibrium limit of the two-phase flow model of reference. First, we conduct an integrability analysis of the system in hand, which leads to its transformation to a singular nonlinear elliptic partial differential equation (PDE) with natural growth. By applying weak convergence methods and by using suitably chosen nonlinear test-functions, we show that the transformed elliptic PDE admits weak solutions, in the sense of distributions. Subsequently we proceed to establish an existence theory for the original system.

In the fourth part, we develop a numerical method for the calculation of constant density flows of two-phase granular mixtures, as predicted by the two-phase flow model of reference. The proposed algorithm employs a predictor-corrector time-marching scheme combined with a projection method for the computation of the pressures of the two phases. A Poisson equation and a second-order elliptic equation are solved at both the predictor and the corrector stages for the pressures of the granular and the fluid phase, respectively. The algorithm is also coupled with an interface detection and treatment scheme based on a local regularization method. The efficiency and robustness of the proposed algorithm are tested in numerical simulations of an unsteady, two-dimensional shear flow for a mixture of sand with water.

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Nomenclature

List of symbols

s	Subscript denoting granular phase.
f	Subscript denoting fluid phase.
$^{\wedge}$	Superscript denoting a dimensional parameter.
η	Entropy.
e	Internal energy.
ψ	Helmholtz free energy.
ρ	Density
T	Temperature.
p	Pressure.
ϕ	Volume fraction.
β	Configuration pressure.
$\mathbf{h}$	Configuration stress vector.
Γ	Configuration stress coefficient.
$\mathbf{u}$	Velocity vector.
$\mathbf{g}$	Gravity vector.
δ	Interfasial force coefficient.
h	Interfasial heat transfer coefficient.
μ	Shear viscosity coefficient.
ζ	Bulk viscosity coefficient.
κ	Thermal conductivity coefficient.

c_p	Specific heat under constant pressure.
c_v	Specific heat under constant volume.
R	Difference between specific heats $c_p - c_v$.
P_∞	Correction pressure for the stiffened gas state equation.
γ	Heat-capacity ratio.
k_1, k_2	Material dependent constants.
d_p	Grain diameter.
Re	Reynolds number.
Pr	Prandtl number.
M	Mach number.
c	Speed of sound.
C_D	Interfacial drag coefficient.

Mathematical notation

$\mathbf{n}$	Unit outward normal vector.
$\ \cdot \ _X$	Norm of the function space X .
$\ \cdot \ _{\max}$	Maximum norm of a function (or vector) f .
$\ \cdot \ _\infty$	Maximum absolute row-sum norm of a matrix.
L^p	Lebesgue space of p -integrable functions.
$L^{p,m}$	Lebesgue space of p -integrable, m -dimensional vector-fields.
L^p_{loc}	Lebesgue space of locally p -integrable functions.
L^∞	Space of all essentially bounded functions.
$W^{k,p}$	Sobolev space of L^p -functions with L^p -weak derivatives up to order k .
H^k	Sobolev space $W^{k,2}$ with $p = 2$.
$W^{k,p}_{loc}(\Omega), H^k_{loc}(\Omega)$	Sobolev spaces with functions and weak derivatives locally integrable.
$X(T : Y)$	Bochner space of the Banach spaces X, Y over the domain T .
C^k	Space of functions with continuous classical derivatives up to order k .
C_c^∞	Space of compactly supported smooth functions.
H^1_0	Closure of compactly supported smooth functions in H^1 .

Chapter 1

Introduction

1.1 An introduction to granular materials

Granular materials are defined as conglomerates of discrete macroscopic particles (grains). The typical size of these particles encompasses a wide range of scales from the lower limit of $1\ \mu\text{m}$ to several kilometers, (Duran 2000). Well-known examples include sand, coal, coffee, rice, sugar, fertilizers, cereals, cornstarch, talk-powder, rocks, boulders, asteroids, *etc.*

Granular materials have properties reminiscent of both solids, liquids and gases. However, there are important differences with each of these forms of matter that render the behavior of granular materials unique. For example, granular materials support shear stresses at equilibrium, they compact, they tend to clog when driven through area constrictions, they can produce arches and avalanches, they tend to cluster and clump, *etc.*, (Hutter & Rajagopal 1994, Wang & Hutter 2001). Because of these reasons, it has been suggested that granular materials should be considered as a *new state of matter*, (Jaeger & Nagel 1992).

In this respect, four fundamental characteristics that contribute to the unconventional behavior of granular materials are identified.

- i) The typical size of the particles is large enough that thermal fluctuations are negligible compared to the energy scale required to move the particles, (Jaeger *et al.* 1996*a*).
- ii) In the course of interactions between the particles there is energy dissipation. This is because of static friction and the fact that the collisions between the particles are inelastic, (Goldhirsch 2003).
- iii) Granular materials are typically immersed in a carrier fluid thus forming a heterogeneous two-phase immiscible mixture, *e.g.* sand-water, sugar-air, *etc.* In the

presence of gravity, a realistic representation of granular flows cannot be obtained if the carrier fluid is neglected, (Meruane *et al.* 2010).

- iv) Granular materials have micro-structure (structure at the grain level). Therefore, there is no clear scale separation between the diameter of the grains and the characteristic length of the flow, (Tan & Goldhirsch 1998).

It is important to remark that the above list of characteristics may not be exhaustive. According to Campbell (2006), the complete set of the granular materials' characteristics that govern their flows, is not yet identified.

1.2 Applications of granular materials

Two-phase flows of granular materials are ubiquitous in industrial and technological applications. They play a prominent role in mining, construction, process industries, pharmaceutical and food industries, power plants, propulsion, *etc.* In fact, granular materials are the second most employed material in industry, the first one being water, (Richard *et al.* 2005). In other words, the worldwide annual production of granular materials is vast. For illustration purposes, we mention that the worldwide annual production of construction aggregates alone is over 16 billion tons, (Langer *et al.* 2004).

Besides their industrial applicability, granular materials are encountered in several natural phenomena and geophysical processes, such as sedimentation transport in coasts and rivers, desert sand pile motions, volcanic explosions, move of tectonic plates and others. Therefore, their study is deemed important for the description and prediction of natural hazards like pyroclastic flows, landslide, rock avalanches, *etc.*

Because of their wide applicability, intense research efforts have been devoted to the study of two-phase flows of granular materials; see, for example, Campbell (1990), Hutter & Rajagopal (1994), De Gennes (1999), Ottino & Khakhar (2000), Wang & Hutter (2001), Goldhirsch (2003), Aranson & Tsimring (2006), Campbell (2006), Forterre & Pouliquen (2008) and the references therein. However, despite the long reference list and more than five decades of theoretical and experimental investigations, our knowledge of these flows is unsatisfactory. This has dramatic consequences for industrial applications. More specifically, many industrial plants operate nearly 40% below their designed efficiency due to problems encountered in the transport of granular materials from one part of the factory floor to another, (Jaeger *et al.* 1996b).

Further, our insufficient understanding of these flows has impeded the development of efficient methodologies for the treatment of disruptive phenomena that occur during the handling of granular materials, *e.g.* formation of plugs, grain segregation, *etc.* To this extent, many of the existing methodologies in the construction industry date back in the nineteenth century, (Duran 2000). Similarly, De Gennes (1999) mentions that

the manipulation of powders, which concerns a large part of food and pharmaceutical industries, involves various clumsy and/or dangerous operations.

Summing up, we deduce that even small advances in our understanding of the behavior of granular materials are expected to have a large economic impact.

1.3 Modelling of two-phase flows of granular materials

Early mathematical models of two-phase flows of granular materials suffered from a closure problem and more precisely from an underdeterminacy in the governing equations; see, for example, Atkin & Craine (1976) for a tentative review. In order to overcome this problem, the authors of these models employed additional assumptions as a remedy. For example, Gough & Zwarts (1979) assumed that the granular phase is incompressible but it still follows an equation of state. Wallis (1969) assumed that the pressures of the carrier fluid and the granular phase are equal. Also, Krier & Gokhale (1978) assumed a contribution from the configuration changes of the granular material, in their definition of the pressure of the granular phase. However, all these assumptions are restrictive and quite often unjustifiable from the physical point of view. For example, the assumption of pressure equilibrium between the two phases results in an ill-posed problem, (Stuhmiller 1977). Moreover, some of the early models are thermodynamically incorrect, *i.e.* they second (entropy) law of thermodynamics. Also, some other models employ expressions for the thermodynamic potentials of the granular material that do not take into account its microstructure. An example of the latter case, is the mathematical model of Baer & Nunziato (1986) for compressible granular flows whose deficiencies and inconsistencies were pointed out by Powers *et al.* (1990), Bdzil *et al.* (1999) and Papalexandris (2004). Finally, some of the early models ignore the volume occupied by the granular phase and were, therefore, applicable only to very dilute mixtures, (Miura & Glass 1982, Loth *et al.* 1997). As a consequence, the applicability of these early models to the flows of interest is quite limited.

In the recent past, several more elaborate and more sophisticated mathematical models have been proposed. Typically, their derivation has been based either on an averaging or on a mixture-theory approach. Both approaches have advantages and drawbacks associated with them; for a self-contained presentation and description see Gidaspow (1994) and Drew & Passman (1999).

The averaging approach employs aspects from kinetic theories and is based on modifying the equations of motion of a single constituent to account for the presence of the other constituents and then averaging these equations over time and space. In particular, space averaging is performed over a representative volume which must be large with respect to the particle diameters and small with respect to the size of the conglomerate, (Jenkins

& Savage 1983, Jenkins & Richman 1985, Goldshtein & Shapiro 1995). In fact, under the assumption that the system is ergodic, the ensemble averages can be set equal to time averages. Examples of mathematical models that have been derived in this manner are the ones of Ding & Gidaspow (1990), Huilin *et al.* (2000; 2001; 2003*b*), Serero *et al.* (2006) and Kumaran (2008).

The main advantage of the averaging approach, is that it is a “first principle” approach and, therefore, requires a few initial postulates. However, the inelastic collisions between grains are often modelled in a rudimentary way. Further, the typical number of grains is much smaller than Avogadro’s number. To this extend, in some cases, a few thousands or even hundreds of particles can justify statistical approaches, (Aranson & Tsimring 2006). In general, however, the small number of particles renders fluctuations of greater relative magnitude than in molecular gases. Also, the statistics may be dominated by rare events. Finally, averaging theories rely on the validity of the *molecular chaos hypothesis*, *i.e.* the assumption that the velocities and positions of colliding particles are correlation-free, (Serero *et al.* 2006). This may be justified for dilute mixtures but it is unlikely to hold for moderate and high concentrations of the granular material, (Soto *et al.* 2001).

Immiscible mixture theories treat the system as a multi-component continuum. More precisely, the mixture is assumed to consist of two separate, identifiable and coexisting continua that are in non-equilibrium with each other. Each phase is assigned its own set of thermodynamic variables and velocity vector and satisfies separately conservation of mass, momentum and energy. The challenging part is then to derive constitutive expressions for the irreversible phenomena that take place, such as, viscosity, heat transfer, phase interactions, *etc.* This can be achieved by adopting a non-equilibrium thermodynamic formalism and taking advantage of the constraints that are imposed by the entropy inequality law. Mathematical models based on the mixture theory approach have been derived in Goodman & Cowin (1972), Passman *et al.* (1986), Svendsen & Hutter (1995), Bdzil *et al.* (1999), Massoudi & Mehrabadi (2001), Gavriluk & Saurel (2002*a*), Ván (2004), Papalexandris (2004) and Wang & Hutter (2006).

This approach has the advantage that it provides a set of governing equations in a straightforward and elegant way. However, it has scale-related limitations stemming from the continuum hypothesis. In particular, the diameter of the grains has to be at least two orders of magnitude smaller than the size of the flow domain; see, for example, Drew & Passman (1999). Further, all limitations and drawbacks of the thermodynamic formalism used for the derivation of the mathematical model carry over to the model itself.

1.4 Motivations and objectives of this PhD Thesis

For the development of a comprehensive continuum theory for the flows of interest, the derivation of mathematical models should be supplemented with their mathematical analysis and the development of algorithms for their numerical treatment. In fact, the acquisition of numerical results and their comparison with experiments is essential for the validation of the theory.

Mathematical results for continuum models of two-phase flows of granular materials are scarce and are valid only for very special types of flows. For example, Hutter *et al.* (1986) studied the dependence of the existence of solutions on boundary conditions for steady-state flows over inclined planes. Also, Rajagopal *et al.* (1992) investigated the existence and uniqueness of solutions to the same flow problem. For such flows, however, the governing equations reduce to a system of nonlinear ODEs, for which an existence theory is available. On the other hand, existence and regularity results for mathematical models derived via the mixture theory approach, in dimensions larger than one, are currently not available in the literature.

A similar pattern is observed in the literature of the algorithm development and simulation of granular flows. Numerical results for two-phase flows of granular materials in a general setting (transient, multi-dimensional flows in a complicated geometry) have been obtained only for dilute mixtures; see, for example, Lun (2000), Huilin *et al.* (2003a), Huanpenga *et al.* (2004), Benavides & van Wachem (2008), Levy & Sayed (2008), Bisi *et al.* (2012) and others. For dense granular mixtures, numerical results are available for very special cases, *i.e.* steady-state, one-dimensional flows in planar geometry; see Passman *et al.* (1986), Wang & Hutter (1999a;b), Massoudi & Phuoc (2005).

The objective of this Thesis is to advance the theoretical and numerical analysis of two-phase flows of dense granular mixtures. Our studies are based on the mathematical model of Papalexandris (2004) which, henceforth, will be referred to as the “*two-phase flow model of reference*”. However, it is important to underline that both the theoretical results that we derive and the numerical methods that we develop are applicable to other constitutive models for the mixtures of interest. This is because there are several similarities between the various models and many of them share the same structure.

In the first part of the Thesis we generalize the concept of low-Mach number approximation to multi-phase flows. Subsequently, we apply it to the two-phase flow model of reference and derive the low-Mach number equations for two-phase flows of granular materials. A formal methodology for the systematic reduction of compressible multi-phase flow models to their incompressible limit currently does not exist.

In the second and third part of the Thesis we present a numerical and theoretical analysis of the equilibrium limit of the two-phase flow model of reference, respectively. Our existence theory and numerical results give a positive answer to the open question of the well-posedness of continuum models for granular materials at equilibrium.

In the fourth part of the Thesis we propose a numerical method for the calculation of incompressible, unsteady flows of fluid-saturated granular materials in the case where both constituents have constant density. This is a predictor-corrector algorithm that combines a projection method for the pressure of each phase and an interface-tracking scheme. Subsequently, we employ this algorithm to investigate numerically an unsteady, two-dimensional shear flow for a reference mixture of sand and water. This is the first numerical study for unsteady, multi-dimensional granular flows.

Chapter 2

Low-Mach number asymptotics for two-phase flows of granular materials

2.1 Introduction

According to the well known incompressibility criterion, a flow is said to be incompressible if both the velocity variations and the reference velocity, *i.e* the average velocity over space and time, are small with respect to the speed of sound, (Gallavotti 2002). In particular, a fluid flow is incompressible if the square of the Mach number remains much smaller than unity. According to this criterion, compressibility effects are absent from flows in which density variations result from temperature variations only. Such flows are usually referred to as low-Mach number or dilatational flows and are encountered in numerous technological applications and natural phenomena.

On the other hand, the Mach number appears explicitly in the non-dimensionalized energy balance equation for simple fluids. More specifically, it appears as a multiplying factor in the expression for the work performed by the surface forces that act on the fluid. Therefore, it arises naturally as a perturbation parameter for low-Mach number flows. This, in turn, suggests the application of singular perturbation techniques to derive a simplified version of the balance equations when the Mach number is small. The resulting system is usually referred to as the *low-Mach number equations*. This singular perturbation analysis has the following advantages.

1. It identifies terms whose magnitude remains sufficiently small and, therefore, can be neglected. More specifically, it removes all terms associated with compressibility effects. As a consequence, the momentum and energy equations essentially decouple

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from each other. Thus, the resulting system is much simpler than the unperturbed, compressible one.

2. As the Mach number approaches zero, the fluid velocity becomes increasingly smaller than the sound speed and, therefore, the time-step required for the numerical integration of the (compressible) equations becomes very small, due to the constraint imposed by the Courant-Friedrichs-Lewy (CFL) condition. Special acceleration techniques such as preconditioning, multigrid, and residual smoothing can only partially alleviate this problem. However, the low-Mach number equations are not subject to such constraints, due to the removal of all terms associated with compressibility effects. Therefore, they can be integrated with much larger time-steps, which results in dramatic computational savings.
3. In the low-Mach number regime, the accuracy and efficiency of standard numerical methods for compressible flows are being reduced considerably, (Volpe 1993), independently of their performance in other regimes, e.g. in the transonic or the supersonic regime. This deterioration is likely due to the fact that the zero-Mach number limit of the unperturbed, compressible equations is singular. On the other hand, the low-Mach number equations are not singular in the limit as the Mach number goes to zero, because they result from singular perturbation expansion. This, in turn, simplifies considerably the design of time-accurate and efficient algorithms for their numerical treatment.

The price that must be paid for the use of the low-Mach number approximation is the complete loss of acoustic effects. Indeed, terms that describe these effects are of higher order and, therefore, are neglected from the low-Mach number equations. Nonetheless, for many flows of interest, this is usually a small price to pay when compared to the computational gain resulting from the low-Mach number approximation.

In the past, several authors contributed to the development of algorithms for the low-Mach number equations of simple fluids. For example, Chenoweth & Paolucci (1986) developed a predictor-corrector type algorithm and studied natural convection in enclosed domains, whereas Herczynski & Kassoy (1991) studied the same problem in absence of gravity via semi-analytical techniques based on Laplace transform, in one dimension. Further, Majda & Sethian (1985) presented an algorithm for low-Mach number flows with combustion based on random vortex techniques. Also, for the same type of flows, Cook & Riley (1996) proposed an algorithm based on sixth-order compact differences and a fifth-order compact boundary scheme, and Najm *et al.* (1998) proposed an additive semi-implicit projection method. More recently, Lessani & Papalexandris (2006) designed and implemented an algorithm for low-Mach number flows with strong temperature gradients, with or without combustion, based on a predictor-corrector time integration scheme and a projection method for the momentum equation. A detailed list and a comprehensive

description of various numerical methods for low-Mach number flows can be found in the recent article of Knikker (2011). Comparisons of the efficiency and robustness of these methods can also be found in that article.

Alongside algorithm development and numerical analysis, considerable research efforts have been devoted to the mathematical analysis of the low-Mach number equations for simple fluids. For example, Klainerman & Majda (1981) developed a general theoretical framework for the study of singular limits of quasilinear hyperbolic systems. As an application, the authors proved the convergence of strong (classical) solutions of the isentropic compressible Navier-Stokes to strong solutions of the incompressible ones, provided that strong solutions for the compressible equations exist and that the initial data are subject to scaling constraints so as to balance the acoustic components, *i.e* they are “nearly incompressible”. In other words, for isentropic flows, the low-Mach number expansion is convergent. This result has subsequently been generalized to other types of flows. The most general case, *i.e* the Navier-Stokes-Fourier equations, has been studied by Alazard (2006) and Feireisl & Novotný (2007). More specifically, Alazard (2006) proved the short-time convergence of the low-Mach number expansion for classical solutions, albeit for “nearly incompressible” initial data. Finally, Feireisl & Novotný (2007) proved the large-time convergence of the low-Mach number expansion for weak solutions, under similar assumptions for the initial data.

In this Chapter we present the generalization of low-Mach number asymptotics to continuum models for multi-phase mixtures and apply it to the model of reference. To the best of our knowledge, low-Mach number asymptotics has not yet been generalized to multi-phase flow models. This can possibly be attributed to the size and complexity of these models. In fact, the number of equations in these models is much larger than in single-phase flow models. Further, they contain high-order nonlinear differential operators and relaxation terms to describe interactions between phases and phenomena due to the microstructure of the mixture. These additional terms increase significantly the complexity of the equations at hand. Nonetheless, incompressible multi-phase flows with strong temperature gradients are encountered in numerous technological applications and natural phenomena. Therefore, it would be useful to generalize the concept of the low-Mach number approximation for these flows and benefit from the afore-mentioned advantages of this approximation.

In particular, low-Mach number equations are well adapted for the study of irreversible phenomena such as diffusive processes and relaxation mechanisms in the mixtures of interest, by virtue of the decoupling between the energy and momentum balance equations. They are also convenient for the study of the interplay between these phenomena as two-phase granular mixtures are driven to an equilibrium or a stationary state. Further, they are well adapted for the study of a number of phenomena emerging in two-phase flows that are currently not well understood. Examples include the structure of boundary layers, the evolution of interfaces, the formation and evolution of zones of high particle

concentrations (compaction zones) and others.

As regards the numerical treatment of the flows of interest, the low-Mach number expansion results in equation that are much easier to study numerically than the unperturbed compressible ones. This is of particular importance because, up to now, numerical results for incompressible multi-phase flows with temperature gradients exist only for very special cases that are of little practical interest such as, for example, very dilute mixtures in which the volume occupied by the solid particles is negligible.

This Chapter is organized as follows. In the second section we describe briefly the two-phase flow model of reference. We also give the equation of state of the solid phase and discuss its implications to the modelling of the micro-structure of the mixture and to the structure of the solid energy equation. In the third section, we generalize the concept of low-Mach number asymptotics to two-phase flows, derive the low-Mach number equations for the constitutive model at hand, and discuss some important characteristics of these equations. In the fourth section we discuss the structure of the low-Mach number equations for two interesting special cases, namely, constant density flows and the equilibrium limit of two-phase granular materials. Finally, the fifth section contains some remarks about the experimental validation of the low-Mach number equations derived herein.

2.2 The two-phase flow model of reference

Let us consider a mixture of an isotropic granular material and a simple fluid occupying a domain $\Omega \subset \mathbb{R}^3$. It is assumed that the mixture is immiscible and saturated, and that there are no phase transformations and chemical reactions. According to the continuum-theory approach, the mixture is assumed to consist of two separate, identifiable continua occupying the same space: the fluid phase and the granular phase, also referred to as the solid phase.

The mass, momentum and energy equations for the fluid phase read, (Drew & Passman 1999, Papalexandris 2004),

$$\frac{D_f \hat{\rho}_f \phi_f}{D\hat{t}} + \hat{\rho}_f \phi_f \hat{\nabla} \cdot \hat{\mathbf{u}}_f = 0, \quad (2.2.1a)$$

$$\hat{\rho}_f \phi_f \frac{D_f \hat{\mathbf{u}}_f}{D\hat{t}} + \hat{\nabla}(\hat{p}_f \phi_f) = -\hat{\nabla}(\hat{p}_f^v \phi_f) + \hat{\nabla} \cdot (\phi_f \hat{\mathbf{P}}_f^v) - \hat{\mathbf{f}} + \hat{\rho}_f \phi_f \hat{\mathbf{g}}, \quad (2.2.1b)$$

$$\begin{aligned} \hat{\rho}_f \phi_f \frac{D_f \hat{e}_f}{D\hat{t}} + \hat{p}_f \phi_f \hat{\nabla} \cdot \hat{\mathbf{u}}_f = & -\hat{p}_f^v \phi_f \hat{\nabla} \cdot \hat{\mathbf{u}}_f + \phi_f \hat{\mathbf{P}}_f^v : \hat{\mathbf{V}}_f^v - \hat{\nabla} \cdot (\phi_f \hat{\mathbf{q}}_f) \\ & + \hat{\mathbf{f}} \cdot (\hat{\mathbf{u}}_f - \hat{\mathbf{u}}_s) - \hat{E}, \end{aligned} \quad (2.2.1c)$$

respectively, whereas for the solid phase they read

$$\frac{D_s \hat{\rho}_s \phi_s}{D\hat{t}} + \hat{\rho}_s \phi_s \hat{\nabla} \cdot \hat{\mathbf{u}}_s = 0, \quad (2.2.1d)$$

$$\hat{\rho}_s \phi_s \frac{D_s \hat{\mathbf{u}}_s}{D\hat{t}} + \hat{\nabla}(\hat{p}_s \phi_s) = -\hat{\nabla}(\hat{p}_s^v \phi_s) + \hat{\nabla} \cdot (\phi_s \hat{\mathbf{P}}_s^v) + \hat{\mathbf{f}} + \hat{\rho}_s \phi_s \hat{\mathbf{g}}, \quad (2.2.1e)$$

$$\hat{\rho}_s \phi_s \frac{D_s \hat{e}_s}{D\hat{t}} + \hat{p}_s \phi_s \hat{\nabla} \cdot \hat{\mathbf{u}}_s = -\hat{p}_s^v \phi_s \hat{\nabla} \cdot \hat{\mathbf{u}}_s + \phi_s \hat{\mathbf{P}}_s^v : \hat{\mathbf{V}}_s^v - \nabla \cdot (\phi_s \hat{\mathbf{q}}_s) + \hat{E}, \quad (2.2.1f)$$

respectively.

In the above equations, the subscripts “ s ” and “ f ” denote the solid and fluid phase, respectively. Further, $\hat{\rho}_i, \hat{p}_i, \hat{\mathbf{u}}_i, \phi_i$ and $\hat{e}_i$, $i = s, f$, are the density, pressure, velocity vector, volume fraction and internal energy of the phase i . Also, in the above equations, and throughout this dissertation, the hat symbol “ $\hat{}$ ” over a variable denotes that the variable is in dimensional form and the symbol “ $:$ ” stands for the component-wise (Hadamard) product of two tensors. Further, the operator $\frac{D_i}{D\hat{t}} = \frac{\partial}{\partial \hat{t}} + \hat{\mathbf{u}}_i \cdot \hat{\nabla}$ stands for the derivative along the streamlines of the phase i (material derivative).

The quantities $\hat{p}_i^v$ and $\hat{\mathbf{P}}_i^v$ result from the natural decomposition of the stress tensor $\hat{\mathbf{P}}$ into a diagonal part and a traceless deviatoric part,

$$\hat{\mathbf{P}}_i = -(\hat{p}_i + \hat{p}_i^v) \mathbf{I} + \hat{\mathbf{P}}_i^v, \quad i = s, f, \quad (2.2.2)$$

where $\hat{p}_i^v$ are the bulk viscous pressures, respectively, and $\mathbf{I}$ is the identity matrix. Further, $\hat{\mathbf{V}}_i^v$ are the traceless deviatoric parts of the deformation tensors $\hat{\mathbf{V}}_i$. In other words, $\hat{\mathbf{V}}_i = \frac{1}{2}(\hat{\nabla} \hat{\mathbf{u}}_i + (\hat{\nabla} \hat{\mathbf{u}}_i)^T)$ and $\hat{\mathbf{V}}_i^v = \hat{\mathbf{V}}_i - \frac{1}{3}(\hat{\nabla} \cdot \hat{\mathbf{u}}_i) \mathbf{I}$. Finally, $\hat{\mathbf{q}}_i$ are the heat conduction fluxes inside each phase, and $\hat{\mathbf{f}}, \hat{E}$ represent the momentum and heat exchanges between the two phases, respectively.

This system is closed with an evolution equation for the solid volume fraction, state equations for both phases, and the saturation condition,

$$\phi_s(\mathbf{x}) + \phi_f(\mathbf{x}) = 1, \quad \mathbf{x} \in \Omega. \quad (2.2.3)$$

Equations (2.2.1a)-(2.2.1f) must be supplemented with constitutive relations for all dissipative (irreversible) processes in the mixture. Papalexandris (2004) provided such constitutive relations and derived the two-phase flow model of reference by assuming that a generalized Gibbs equation holds for each phase and by taking advantage of the constraints imposed by the entropy inequality for the mixture. For the derivation of this model the following constitutive assumptions are made.

1. Each phase of the mixture is endowed with its own set of thermodynamic variables and velocity vector.

2. Each phase is in a local (equilibrium) state. Therefore, the entropy of each phase is a state variable, and its differential 1-form is exact and defined by a Gibbs equation.
3. The momentum and energy exchanges between the two phases are pure, *i.e.* their sum vanishes.
4. The principle of phase separation holds. This implies that irreversible phenomena that take place “inside” one phase depend only on thermodynamic variables of this phase.
5. Microinertia effects of the solid phase can be ignored.

In conclusion, the two phases of the mixture are treated as two separate thermodynamic subsystems that interact with each other. Nonetheless, the entire system, *i.e.* the mixture, can be open, closed or isolated, depending on the boundary conditions.

Since granular materials possess microstructure, additional variables are needed for the complete description of the thermodynamic state of the solid phase. In the two-phase flow model of reference, these additional variables are the solid volume fraction and its spatial gradient, ϕ_s and $\hat{\nabla}\phi_s$, respectively. The use of ϕ_s as a concentration parameter is standard in multi-phase flow problems. Usually it is defined through averaging over a so-called “representative volume”. According to its usual interpretation, the mixture consists of two co-existing continua. However, when applied to granular materials, this definition is unsatisfactory both from the mathematical and the physical point of view, because of the microstructure of these materials. In fact, in many granular mixtures, even the naked eye can observe the phase separation and determine if a given point in space is occupied by one phase or the other. For this reason, we consider that it is more appropriate to interpret the volume fraction as the probability to find one phase or the other in a given measurable set in space and at a given time. In other words, the volume fraction is a probability density function defined through the Radon-Nikodym theorem; (Goodman & Cowin 1972). This axiomatic definition of the volume fraction is consistent with the measure-theoretic framework of thermodynamics and has important consequences in the mathematical analysis of the governing equations.

Further, the rearrangement of grains in space leads to the development of contact forces. These forces depend on the amount of contact surface, *i.e.* the intergranular area density. However, the sum of the interphasial and the intergranular areas is equal to the total area of the grains. This, in turn, implies that these contact forces can be expressed in terms of the interphasial area density as well. On the other hand, as shown in Drew & Passman (1999), $\hat{\nabla}\phi_s$ is a natural measure of the interphasial area density. Therefore, it is introduced as the additional degree of freedom that is required for the constitutive description of these forces.

Summing up, the fluid phase is treated as a simple Newtonian fluid, hence its state variable vector is $(\hat{\rho}_f, \hat{e}_f)^T$. On the other hand, the state-variable vector for the solid

phase is $(\hat{\rho}_s, \hat{e}_s, \phi_s, \hat{\nabla}\phi_s)^T$. Therefore, the standard Gibbs relation holds for the fluid phase,

$$\hat{T}_f d\hat{\eta}_f = d\hat{e}_f - \frac{\hat{p}_f}{\hat{\rho}_f^2} d\hat{\rho}_f, \quad (2.2.4)$$

whereas a generalized Gibbs relation holds for the solid phase,

$$\hat{T}_s d\hat{\eta}_s = d\hat{e}_s - \frac{\hat{p}_s}{\hat{\rho}_s^2} d\hat{\rho}_s - \frac{\hat{\beta}_s}{\hat{\rho}_s \phi_s} d\phi_s - \frac{1}{\hat{\rho}_s \phi_s} \hat{\mathbf{h}}_s \cdot d(\hat{\nabla}\phi_s). \quad (2.2.5)$$

In these equations $\hat{\eta}_i$, $i = f, s$, is the entropy of the phase i . Further, the quantities $\hat{\beta}_s$ and $\hat{\mathbf{h}}_s$ are defined via the granular material's Helmholtz free energy $\hat{\psi}_s$ as follows

$$\hat{\beta}_s = \hat{\rho}_s \phi_s \frac{\partial \hat{\psi}_s}{\partial \phi_s}, \quad \hat{\mathbf{h}}_s = \hat{\rho}_s \phi_s \frac{\partial \hat{\psi}_s}{\partial (\hat{\nabla}\phi_s)}. \quad (2.2.6)$$

In particular, $\hat{\beta}_s$ is the *configuration pressure* and represents the normal forces that are developed between grains under compaction. The vector $\hat{\mathbf{h}}_s$ represents the afore-mentioned contact forces due to rearrangements of grains in space. As mentioned above, these forces can be expressed in terms of the interphasial area density, *i.e.* they depend on $\hat{\nabla}\phi_s$. As such, these forces are of weakly non-local character. Additionally, since rearrangements of grains in space affect the speed of propagating waves in the granular phase, we can consider that these forces are also of dispersive character. Henceforth, and in analogy with the name adopted for $\hat{\beta}_s$, $\hat{\mathbf{h}}_s$ will be referred to as the *configuration stress vector*.

The presumed isotropy of the granular material implies that the Helmholtz free energy of the solid phase $\hat{\psi}_s$ is an isotropic function, *i.e.* $\hat{\psi}_s(\dots, \hat{\nabla}\phi_s) = \hat{\psi}_s(\dots, \hat{\nabla}\phi_s \cdot \hat{\nabla}\phi_s)$. Consequently, the configuration stress vector $\hat{\mathbf{h}}_s$ can be rewritten as follows,

$$\hat{\mathbf{h}}_s = \hat{\Gamma}_s \hat{\nabla}\phi_s, \quad \text{where} \quad \hat{\Gamma}_s \equiv 2\hat{\rho}_s \phi_s \frac{\partial \hat{\psi}_s}{\partial |\hat{\nabla}\phi_s|^2}. \quad (2.2.7)$$

The coefficient $\hat{\Gamma}_s$ will be referred to as the *configuration stress coefficient*. In principle, both $\hat{\beta}_s$ and $\hat{\Gamma}_s$ are functions of all state variables of the solid phase.

It is worth mentioning that the Gibbs relation for the solid phase (2.2.5), implies that the only elastic shear stresses acting on the grains are those related to the microstructure of the granular medium, *i.e.* the stresses due to the grain distribution and configuration in space. In other words, it is assumed that elastic shear effects are negligible at length scales *smaller* than the grain diameter. Experience shows that this constitutive assumption holds for many incompressible granular flows of interest under moderate external forcing, see Bagnold (1954) and Savage (1979). Further, it has been adopted in

all previous mixture theories for granular media; see, for example, Goodman & Cowin (1972), Passman *et al.* (1986), Wang & Hutter (1999a), Wang & Hutter (2006), and others. Nonetheless, this constitutive assumption can easily be relaxed. For example, one can model the granular material as an elastic solid by adding to (2.2.5) the terms that describe the reversible work performed by (elastic) shear stresses.

The balance equations of the mixture (2.2.1a)-(2.2.1f) and the Gibbs equations (2.2.4) and (2.2.5) can be used to derive an expression for the (non-negative) entropy production in the mixture as a sum of products between thermodynamic fluxes J_i and thermodynamic forces X_k , (Groot & Mazur 1984, Lebon *et al.* 2008). By assuming linear relations between conjugate fluxes and forces ($i = k$), and by ignoring couplings between non-conjugate ones ($i \neq k$), the following constitutive expressions are derived for the thermodynamic fluxes

$$\hat{E} = \hat{h} \left(\frac{1}{\hat{T}_s} - \frac{1}{\hat{T}_f} \right), \quad (2.2.8a)$$

$$\hat{p}_f^v = -\hat{\zeta}_f \hat{\nabla} \cdot \hat{\mathbf{u}}_f, \quad (2.2.8b)$$

$$\hat{p}_s^v = \frac{\hat{\Gamma}_s}{3\phi_s} |\hat{\nabla}\phi_s|^2 - \hat{\zeta}_s \hat{\nabla} \cdot \hat{\mathbf{u}}_s, \quad (2.2.8c)$$

$$\hat{\mathbf{q}}_f = -\hat{\kappa}_f \hat{\nabla} \hat{T}_f, \quad (2.2.8d)$$

$$\hat{\mathbf{q}}_s = -\hat{\kappa}_s \hat{\nabla} \hat{T}_s, \quad (2.2.8e)$$

$$\hat{\mathbf{f}} = \hat{p}_f \hat{\nabla} \phi_s + \hat{\delta} (\hat{\mathbf{u}}_f - \hat{\mathbf{u}}_s), \quad (2.2.8f)$$

$$\hat{\mathbf{P}}_f^v = 2\hat{\mu}_f \hat{\mathbf{V}}_f^v, \quad (2.2.8g)$$

$$\hat{\mathbf{P}}_s^v = \frac{\hat{\Gamma}_s}{\phi_s} \hat{\Phi}_s^v + 2\hat{\mu}_s \hat{\mathbf{V}}_s^v, \quad (2.2.8h)$$

$$\frac{D_s \phi_s}{D \hat{t}} = \frac{1}{\hat{\mu}_c} \left(\frac{\hat{p}_s - \hat{\beta}_s}{\hat{T}_s} - \frac{\hat{p}_f}{\hat{T}_f} + \hat{\nabla} \cdot \left(\frac{\hat{\Gamma}_s}{\hat{T}_s} \hat{\nabla} \phi_s \right) \right). \quad (2.2.8i)$$

In the above equations $\hat{\zeta}_i$ is the bulk viscosity, $\hat{\mu}_i$ is the shear viscosity and $\hat{\kappa}_i$ is the thermal conductivity of the phase i . Further, $\hat{h}$ is the interfacial heat transfer coefficient, $\hat{\delta}$ is an interfacial force coefficient, and $\hat{\mu}_c$ is the dynamic compaction coefficient. Also, in the above equations, $\hat{\Phi}_s^v$ is defined as the traceless deviatoric part of $\hat{\nabla}\phi_s \otimes \hat{\nabla}\phi_s$,

$$\hat{\nabla}\phi_s \otimes \hat{\nabla}\phi_s = \frac{1}{3} |\hat{\nabla}\phi_s|^2 \mathbf{I} + \hat{\Phi}_s^v, \quad (2.2.9)$$

where the symbol “ $\otimes$ ” denotes the tensor product of two vectors. The compaction equation (2.2.8i) describes the evolution of the solid volume fraction and takes the form of

a non-linear diffusion equation along the streamlines of the granular material. In contrast to other models that have been proposed for two-phase flows of granular materials, the two-phase flow model of reference predicts that the evolution of ϕ_s also depends on the phasial temperatures, hence on the thermal non-equilibrium between the two phases. This implies that the evolution of ϕ_s is not reversible, even in the absence of configuration stresses, for as long as the two phases are not in thermal equilibrium with each other. Consequently, the solid phase entropy is not conserved along streamlines of the solid phase. As we will see below, these properties have important implications in the structure of the low-Mach equations for the mixtures of interest.

2.2.1 Equations of state

The thermodynamics of the mixtures of interest is complex, even in low-Mach number flows, because of the microstructure of granular materials and the increased number of state variables required to describe these mixtures. Further, since the governing system (2.2.1a)-(2.2.1f), (2.2.8a)-(2.2.8i) is written in terms of both the temperatures and the internal energies of the two phases, appropriate equations of state have to be specified to both phases for its closure. Therefore, the low-Mach number expansion has to be applied to the equations of state as well. For these reasons, it is useful to discuss the implications of the equations of state for each phase in the governing system and the derivation of the low-Mach number approximation.

First, it is important to make the distinction between *solid material* and *solid phase*. By the term “solid material” we denote the material that the solid particles (grains) consist of. By contrast, by the term “solid phase” or “granular material” we denote the ensemble of the grains, whose thermodynamic state vector consists of the thermodynamic vector of the solid material plus the solid volume fraction and its spatial gradient. On the other hand, such distinction is not necessary for the fluid phase because we assume that the fluid material is a simple Newtonian fluid. As such, this material does not have any microstructure and it does exhibit scale segregation. Therefore, the thermodynamic state vectors for both fluid material and fluid phase are the same.

For illustrative purposes and for the sake of simplicity, in this dissertation we assume that: i) the fluid phase obeys the ideal gas equation of state and ii) the solid material obeys the stiffened gas equation of state which is the simplest equation of state that can be used for solids, (Saurel & Abgrall 1999). However, it is important to note that our analysis is not limited to the above expressions but can be directly applied with more general equations of state. Further, since the numerical methods that are presented in the next Chapters are concerned with constant density and constant temperature flows, the equations of state do not need to be taken into consideration.

As regards the fluid phase, the ideal-gas equation of state reads,

$$\hat{p}_f = (\gamma_f - 1)\hat{\rho}_f \hat{e}_f, \quad (2.2.10)$$

where $\gamma_f = \hat{c}_{p,f}/\hat{c}_{v,f}$ is the heat capacity ratio, with $\hat{c}_{p,f}$ and $\hat{c}_{v,f}$ being the specific heats of the fluid under constant pressure and constant volume, respectively. From the above equation, we readily obtain the thermal equation of state for an ideal gas,

$$\hat{p}_f = \hat{R}_f \hat{\rho}_f \hat{T}_f, \quad (2.2.11)$$

where $\hat{R}_f$ is the fluid constant, *i.e.* $\hat{R}_f = \hat{c}_{p,f} - \hat{c}_{v,f}$.

As regards the equation of state for the solid phase, we first observe that a given thermodynamic potential of this phase can be decomposed into two parts; one part that is independent of the additional variables ϕ_s and $\hat{\nabla}\phi_s$ and another part that is a function of them. Therefore, the first part relates to the thermodynamics of the solid material, *i.e.* the material that the grains consist of. It is a function of the solid density and temperature only and is referred to as the *pure part* of the thermodynamic potential. The remaining second part is a function of ϕ_s and $\hat{\nabla}\phi_s$ and possibly other thermodynamic variables, and is referred to as the *configuration part* of the thermodynamic potential.

Therefore, the following decompositions are introduced for the thermodynamic potentials of internal energy, entropy, and Helmholtz free energy,

$$\hat{e}_s = \hat{e}_s^p(\hat{\rho}_s, \hat{T}_s) + \hat{e}_s^c(\hat{\rho}_s, \hat{T}_s, \phi_s, \hat{\nabla}\phi_s), \quad (2.2.12)$$

$$\hat{\eta}_s = \hat{\eta}_s^p(\hat{\rho}_s, \hat{T}_s) + \hat{\eta}_s^c(\hat{\rho}_s, \hat{T}_s, \phi_s, \hat{\nabla}\phi_s), \quad (2.2.13)$$

$$\hat{\psi}_s = \hat{\psi}_s^p(\hat{\rho}_s, \hat{T}_s) + \hat{\psi}_s^c(\hat{\rho}_s, \hat{T}_s, \phi_s, \hat{\nabla}\phi_s). \quad (2.2.14)$$

The Helmholtz free energies $\hat{\psi}_s^p$ and $\hat{\psi}_s$ are defined as follows

$$\hat{\psi}_s^p = \hat{e}_s^p - \hat{T}_s \hat{\eta}_s^p, \quad (2.2.15)$$

$$\hat{\psi}_s = \hat{e}_s - \hat{T}_s \hat{\eta}_s. \quad (2.2.16)$$

From equations (2.2.15) and (2.2.16), and by virtue of the decompositions (2.2.12)–(2.2.14), we deduce that

$$\hat{\psi}_s^c = \hat{e}_s^c - \hat{T}_s \hat{\eta}_s^c. \quad (2.2.17)$$

Further, from the thermodynamics of the solid material, the following Gibbs relation holds

$$\hat{T}_s d\hat{\eta}_s^p = d\hat{e}_s^p - \frac{\hat{p}_s}{\hat{\rho}_s^2} d\hat{\rho}_s, \quad (2.2.18)$$

where, as mentioned earlier, it is assumed that elastic effects are negligible at length scales *smaller* than the grain diameter. Then, by subtracting (2.2.18) from (2.2.5) we obtain the Gibbs relation for the configuration part of the entropy of the granular material,

$$\hat{T}_s d\hat{\eta}_s^c = d\hat{e}_s^c + \frac{\hat{\beta}_s}{\hat{\rho}_s \phi_s} d\phi_s + \frac{1}{\hat{\rho}_s \phi_s} \hat{\mathbf{h}}_s \cdot d(\hat{\nabla} \phi_s). \quad (2.2.19)$$

Upon differentiation of (2.2.17) and introduction of the result in (2.2.19) we arrive at

$$d\hat{\psi}_s^c = -\hat{\eta}_s^c d\hat{T}_s - \frac{\hat{\beta}_s}{\hat{\rho}_s \phi_s} d\phi_s - \frac{1}{\hat{\rho}_s \phi_s} \hat{\mathbf{h}}_s \cdot d(\hat{\nabla} \phi_s), \quad (2.2.20)$$

from which we finally deduce that

$$\hat{\eta}_s^c = - \left(\frac{\partial \hat{\psi}_s^c}{\partial \hat{T}_s} \right)_{\hat{\rho}_s, \phi_s, \hat{\nabla} \phi_s}. \quad (2.2.21)$$

This relation implies that if $\hat{\psi}_s^c$ does not depend on the temperature $\hat{T}_s$, then the configuration entropy $\hat{\eta}_s^c$ is zero. Evidently, in the general case where the configuration free energy is a function of the temperature, then the configuration entropy is non-zero.

As mentioned above, the solid material is assumed to obey the stiffened-gas equation of state,

$$\hat{p}_s = -\gamma_s \hat{P}_\infty + (\gamma_s - 1) \hat{\rho}_s \hat{e}_s^p, \quad (2.2.22)$$

where $\hat{P}_\infty$ is a constant parameter, usually referred to as the “correction pressure”, and γ_s is the heat capacity ratio, $\gamma_s = \hat{c}_{p,s}/\hat{c}_{v,s}$, with $\hat{c}_{p,s}$ and $\hat{c}_{v,s}$ being the specific heats under constant pressure and constant volume, respectively, of the solid material, (Le Metayer *et al.* 2004).

From definition (2.2.22), one can readily obtain the thermal equation of state of a stiffened gas,

$$\hat{p}_s = -\hat{P}_\infty + \hat{R}_s \hat{\rho}_s \hat{T}_s, \quad (2.2.23)$$

where $\hat{R}_s$ is defined as the difference between the specific heats, $\hat{R}_s = \hat{c}_{p,s} - \hat{c}_{v,s}$. Usually, in the stiffened gas approximation the specific heats are considered constant. However, the above relations can be extended to the more general case where the specific heats are functions of the temperature.

After some simple algebraic manipulations involving definition (2.2.22) and standard thermodynamic relations, one can obtain the following canonical forms of the internal energy and entropy of a stiffened gas,

$$\hat{e}_s^p = \frac{\hat{P}_\infty}{\hat{\rho}_s} + \hat{c}_{v,s} T_s, \quad (2.2.24)$$

and

$$\hat{\eta}_s^p = \hat{c}_{v,s} \log \left(\left(\frac{\hat{T}_s}{T_0} \right) \left(\frac{\hat{\rho}_s}{\rho_0} \right)^{1-\gamma_s} \right) + \eta_0, \quad (2.2.25)$$

In the above equation T_0 , ρ_0 and η_0 are the temperature, density and entropy of the solid material in a reference state, respectively.

Finally, upon introduction of (2.2.24) and (2.2.25) in (2.2.15) we arrive at the canonical form of the Helmholtz free energy of a stiffened gas,

$$\hat{\psi}_s^p = \frac{\hat{P}_\infty}{\hat{\rho}_s} + \hat{c}_{v,s} \hat{T}_s \left(1 - \log \left(\left(\frac{\hat{T}_s}{T_0} \right) \left(\frac{\hat{\rho}_s}{\rho_0} \right)^{1-\gamma_s} \right) \right) - \hat{T}_s \eta_0. \quad (2.2.26)$$

As regards the configuration part of the Helmholtz free energy of the solid phase, the simplest choice is to consider a quadratic function of ϕ_s and $\hat{\nabla} \phi_s$, *i.e.*

$$\hat{\psi}_s^c = \frac{1}{2} \hat{k}_1 \phi_s^2 + \frac{1}{2} \hat{k}_2 |\hat{\nabla} \phi_s|^2, \quad (2.2.27)$$

where $\hat{k}_1$ and $\hat{k}_2$ are positive, material-dependent constants. It is interesting to note that the weighted (mass) integral of this function is a special case of the Ginzburg-Landau functional that is often used in statistical physics, (Landau & Lifshitz 1984).

According to (2.2.27), the configuration Helmholtz free energy is assumed to be independent of the temperature. As mentioned above, this implies that the configuration entropy is zero, $\hat{\eta}_s^c = 0$ and, therefore, $\hat{\psi}_s^c = \hat{e}_s^c$. Also, by employing relation (2.2.6) we arrive at the following expressions for the configuration pressure and configuration stress coefficient,

$$\hat{\beta}_s = \hat{k}_1 \hat{\rho}_s \phi_s^2, \quad \hat{\Gamma}_s = \hat{k}_2 \hat{\rho}_s \phi_s. \quad (2.2.28)$$

Finally, it is straightforward to verify that the expression for the Helmholtz free energy of the granular phase is a convex function and, therefore, the stability of thermodynamic equilibria is guaranteed, (Kondepundi & Prigogine 1998). Further, the second-order differential operator in the right-hand side of the compaction equation (2.2.8i) is elliptic.

Evidently, one can consider other, more elaborate and more accurate expressions for the pure and the configuration part of the Helmholtz free energy of the solid phase; see, for example, Passman *et al.* (1986), Powers (2004) and references therein. As regards the configuration stress vector $\hat{\beta}_s$, experimental studies on granular materials suggest that there is a critical value ϕ_c such that for $\phi_s > \phi_c$ shearing of the material causes expansion, while for $\phi_s < \phi_c$ it causes contraction, (Passman *et al.* 1986, Savage 1979). Intuitively, ϕ_c is the critical value of the solid volume fraction below which the grains are not expected to be in contact. This implies that the configuration pressure $\hat{\beta}_s$ should be zero, or generally

negligible, for $\phi_s < \phi_c$. The value of ϕ_c depends on the geometries and size distribution of the solid particles. For the simplest possible case, uniform spherical particles, a good estimate is $\phi_c \approx 0.52$. This number arises as the solution of the inverse sphere packing problem in an equidistant lattice. It follows that a more realistic constitutive relation for the configuration pressure $\hat{\beta}_s$ would be the following,

$$\hat{\beta}_s = \begin{cases} \hat{k}_1 \hat{\rho}_s (\phi_s - \phi_c)^2, & \phi_s \geq \phi_c, \\ 0, & \text{elsewhere.} \end{cases}$$

However, as regards the configuration stress coefficient $\hat{\Gamma}_s$, detailed experimental measurements in a variety of physical conditions currently do not exist in the literature. For this reason, in the past, researchers in the field of granular flows considered various *ad hoc* expressions for $\hat{\Gamma}_s$. Nonetheless, for the purpose of deriving low-Mach number asymptotics for two-phase granular mixtures, the expressions employed in this Chapter for the free energies of the solid phase are deemed to be adequate.

It is worth mentioning that by virtue of the continuity equation (2.2.1a) and the ideal-gas equation of state (2.2.11), the energy equation of the fluid phase (2.2.1c) can be written in terms of the fluid temperature as follows

$$\begin{aligned} \hat{\rho}_f \phi_f \hat{c}_{p,f} \frac{D_f \hat{T}_f}{D\hat{t}} - \frac{D_f \hat{p}_f \phi_f}{D\hat{t}} = & -\hat{p}_f^v \phi_f \hat{\nabla} \cdot \hat{\mathbf{u}}_f + \phi_f \hat{\mathbf{P}}_f^v : \hat{\mathbf{V}}_f^v - \hat{\nabla} \cdot (\phi_f \hat{\mathbf{q}}_f) \\ & + \hat{\mathbf{f}} \cdot (\hat{\mathbf{u}}_f - \hat{\mathbf{u}}_s) - \hat{E}. \end{aligned} \quad (2.2.29)$$

Similarly, the solid energy equation (2.2.1f) can be written in terms of the solid temperature as follows,

$$\begin{aligned} \hat{\rho}_s \phi_s \left(\hat{c}_{p,s} \frac{D_s \hat{T}_s}{D\hat{t}} + \frac{D_s \hat{\psi}_s^c}{D\hat{t}} \right) - \frac{D_s \hat{p}_s \phi_s}{D\hat{t}} = & -\hat{p}_s^v \phi_s \hat{\nabla} \cdot \hat{\mathbf{u}}_s + \phi_s \hat{\mathbf{P}}_s^v : \hat{\mathbf{V}}_s^v \\ & - \hat{\nabla} \cdot (\phi_s \hat{\mathbf{q}}_s) + \hat{E}. \end{aligned} \quad (2.2.30)$$

2.3 Derivation of the low-Mach number equations

Thus far, all equations have been given in dimensional form. In this section we first perform the non-dimensionalization of the balance equations, which is a necessary step before the derivation of their low-Mach number approximation. In what follows, the subscript “ r ” is used to denote the (dimensional) reference values with respect to which the non-dimensionalization is performed.

First, velocity vectors, length vectors, and time are non-dimensionalized with respect to the characteristic dimension of the flow domain $\hat{L}_r$, and the reference velocity of the

mixture $\hat{u}_r$, *e.g.* the average velocity over space and time, as follows

$$\mathbf{u}_i = \frac{\hat{\mathbf{u}}_i}{\hat{u}_r}, \quad \mathbf{x} = \frac{\hat{\mathbf{x}}}{\hat{L}_r}, \quad t = \hat{t} \frac{\hat{u}_r}{\hat{L}_r}. \quad (2.3.1)$$

Next, the non-dimensionalization of the thermodynamic variables, their derivatives, and the various transport and relaxation coefficients is performed with respect to a reference state of the material with the smallest speed of sound. We remark that, in most cases of interest, it is the fluid material that has the smallest speed of sound.

For illustration purposes, the speed of sound of some common solids and fluids is given in Table 2.1. We infer that, with the exception of cork and rubber, in all other cases the speed of sound of the solid material is larger than that of the fluid. Also, the ratio between the speeds of sound for the various solid-fluid pairs, varies from approximately 1.68, for concrete-glycerol, to 18.5, for aluminium-air.

Solids	Speed of sound (m/s)	Fluids	Speed of sound (m/s)
Aluminium	6420	Acetone	1174
Brick	4176	Air	346.3
Concrete	3200-3600	Alcohol, propyl	1144
Cork	366-518	Benzene	1298
Hardwood	3962	Castor oil	1474
Iron	5130	Chloroform	995
Rubber	40-150	Glycerol	1904
Silica	5760	Kerosene	1324
Steel	6100	Seawater	1560
Wood	3300-3600	Water	1497

Table 2.1: Speed of sound in some common solids and fluids at 25° C and atmospheric pressure.

Motivated by the above, and without loss of generality, we choose to perform the non-dimensionalization with respect to values that correspond to a *reference state of the fluid phase*. For example, if the flow domain is open, then the thermodynamic state of the fluid in the open boundary can be chosen as the reference state. By virtue of the ideal-gas equation of state for the fluid phase, (2.2.11), the following relation holds between the thermodynamic variables in the reference state

$$\hat{p}_r = \hat{R}_f \hat{\rho}_r \hat{T}_r, \quad (2.3.2)$$

Accordingly, the non-dimensionalization of the thermodynamic variables reads

$$p_i = \frac{\hat{p}_i}{\hat{p}_r}, \quad \rho_i = \frac{\hat{\rho}_i}{\hat{\rho}_r}, \quad T_i = \frac{\hat{T}_i}{\hat{T}_r}, \quad i = s, f, \quad (2.3.3)$$

and

$$c_{v,i} = \frac{\hat{c}_{v,i}}{\hat{c}_{v,r}}, \quad c_{p,i} = \frac{\hat{c}_{p,i}}{\hat{c}_{p,r}}, \quad i = s, f, \quad (2.3.4)$$

with $\hat{c}_{v,r} = \hat{c}_{v,f}(T_r)$ and $\hat{c}_{p,r} = \hat{c}_{p,f}(T_r)$.

Further, the non-dimensionalization of the transport coefficients is performed with respect to the values of the transport coefficients of the fluid at the reference thermodynamic state, *i.e.*

$$\mu_i = \frac{\hat{\mu}_i}{\hat{\mu}_r}, \quad \kappa_i = \frac{\hat{\kappa}_i}{\hat{\kappa}_r}, \quad \zeta_i = \frac{\hat{\zeta}_i}{\hat{\zeta}_r}, \quad i = s, f. \quad (2.3.5)$$

The Reynolds number Re , Prandtl number Pr and reference Mach number $M_{f,r}$ of the flow are defined as follows,

$$Re = \frac{\hat{\rho}_r \hat{u}_r \hat{L}_r}{\hat{\mu}_r}, \quad Pr = \frac{\hat{\mu}_r \hat{c}_{p,r}}{\hat{\kappa}_r}, \quad M_{f,r} = \frac{\hat{u}_r}{\hat{c}_{f,r}}. \quad (2.3.6)$$

In the above, $\hat{c}_{f,r}$ is the reference speed of sound of the fluid, defined by

$$\hat{c}_{f,r} = \sqrt{\gamma_{f,r} \hat{R}_f \hat{T}_r}, \quad (2.3.7)$$

with $\gamma_{f,r}$ being the value of the heat-capacity ratio of the fluid at the reference state, $\gamma_{f,r} = \hat{c}_{p,r}/\hat{c}_{v,r}$. Next, the interfacial drag coefficient $\hat{\delta}$, the interfacial heat transfer coefficient $\hat{h}$ and the dynamic compaction coefficient $\hat{\mu}_c$ are non-dimensionalized as follows,

$$\delta = \hat{\delta} \frac{\hat{L}_r}{\hat{\rho}_r \hat{u}_r}, \quad h = \hat{h} \frac{\hat{L}_r^2}{\hat{\mu}_r}, \quad \mu_c = \hat{\mu}_c \frac{\hat{T}_r}{\hat{\rho}_r \hat{u}_r \hat{L}_r}. \quad (2.3.8)$$

The expression for the interfacial force coefficient $\hat{\delta}$ for a monodisperse granular material consisting of spherical particles is provided in Section (5.4.1) of this dissertation.

As regards the non-dimensionalization of $\hat{\beta}_s$ and $\hat{\Gamma}_s$, we remark the following. Experience with incompressible flows of granular materials shows that the configuration pressure and configuration stresses are much smaller than the reference pressure of the carrier fluid $\hat{p}_r$; see Bagnold (1954), Passman *et al.* (1986) and Papalexandris (2004). In particular, it is expected that $\hat{\beta}_s$ and $\hat{\Gamma}_s$ scale with $\hat{\rho}_r \hat{u}_r^2$, which is also much smaller than $\hat{p}_r$ in the low-Mach number regime. On the other hand, it is convenient to perform the non-dimensionalization in a way that the non-dimensional variables are of order unity. For this reason, we chose to non-dimensionalize $\hat{\beta}_s$ and $\hat{\Gamma}_s$ with respect to $\hat{\rho}_r \hat{u}_r^2$ as follows,

$$\beta_s = \frac{\hat{\beta}_s}{\hat{\rho}_r \hat{u}_r^2}, \quad \Gamma_s = \frac{\hat{\Gamma}_s}{\hat{\rho}_r \hat{u}_r^2 \hat{L}_r^2}. \quad (2.3.9)$$

By performing the above non-dimensionalizations and by introducing the constitutive laws (2.2.8a)-(2.2.8h) to the balance equations (2.2.1a)-(2.2.1f), we arrive at the non-dimensional form of the two-phase flow model of reference. In particular, the balance equations of the fluid phase read,

$$\frac{D_f \rho_f \phi_f}{Dt} + \rho_f \phi_f \nabla \cdot \mathbf{u}_f = 0, \quad (2.3.10a)$$

$$\begin{aligned} \rho_f \phi_f \frac{D_f \mathbf{u}_f}{Dt} + \frac{1}{\epsilon} \nabla(p_f \phi_f) &= \frac{\xi}{Re} \nabla(\phi_f \zeta_f \nabla \cdot \mathbf{u}_f) + \frac{1}{Re} \nabla \cdot (2\phi_f \mu_f \mathbf{V}_f^v) \\ &\quad - \frac{1}{\epsilon} p_f \nabla \phi_s - \delta(\mathbf{u}_f - \mathbf{u}_s) + \rho_f \phi_f \mathbf{g}, \end{aligned} \quad (2.3.10b)$$

$$\begin{aligned} \rho_f \phi_f c_{p,f} \frac{D_f T_f}{Dt} - \frac{\gamma_{f,r} - 1}{\gamma_{f,r}} \frac{D_f p_f \phi_f}{Dt} &= \epsilon \frac{\xi}{Re} \zeta_f \phi_f (\nabla \cdot \mathbf{u}_f)^2 + \epsilon \frac{2}{Re} \phi_f \mu_f \mathbf{V}_f^v : \mathbf{V}_f^v \\ &\quad + \frac{\gamma_{f,r} - 1}{\gamma_{f,r}} p_f (\mathbf{u}_f - \mathbf{u}_s) \cdot \nabla \phi_s + \epsilon \delta(\mathbf{u}_f - \mathbf{u}_s)^2 \\ &\quad + \frac{1}{Pr Re} \nabla \cdot (\kappa_f \phi_f \nabla T_f) - \hbar \left(\frac{1}{T_s} - \frac{1}{T_f} \right). \end{aligned} \quad (2.3.10c)$$

The balance equations for the solid phase read,

$$\frac{D_f \rho_s \phi_s}{Dt} + \rho_s \phi_s \nabla \cdot \mathbf{u}_s = 0, \quad (2.3.10d)$$

$$\begin{aligned} \rho_s \phi_s \frac{D_s \mathbf{u}_s}{Dt} + \frac{1}{\epsilon} \nabla(p_s \phi_s) &= \frac{\xi}{Re} \nabla(\phi_s \zeta_s \nabla \cdot \mathbf{u}_s) + \frac{1}{Re} \nabla \cdot (2\phi_s \mu_s \mathbf{V}_s^v) \\ &\quad - \nabla \cdot (\Gamma_s \nabla \phi_s \otimes \nabla \phi_s) + \frac{1}{\epsilon} p_f \nabla \phi_s \\ &\quad + \delta(\mathbf{u}_f - \mathbf{u}_s) + \rho_s \phi_s \mathbf{g}, \end{aligned} \quad (2.3.10e)$$

$$\begin{aligned}
\rho_s \phi_s c_{p,s} \frac{D_s T_s}{Dt} - \frac{\gamma_{f,r} - 1}{\gamma_{f,r}} \frac{D_s p_s \phi_s}{Dt} + \epsilon \rho_s \phi_s \frac{D_s \psi_s^c}{Dt} = & -\epsilon \left(\frac{\Gamma_s}{3} |\nabla \phi_s|^2 - \frac{\xi}{Re} \phi_s \zeta_s \nabla \cdot \mathbf{u}_s \right) \nabla \cdot \mathbf{u}_s \\
& + \epsilon \left(\Gamma_s \Phi_s^v + \frac{2}{Re} \phi_s \mu_s \mathbf{V}_s^v \right) : \mathbf{V}_s^v \\
& + \frac{1}{Pr Re} \nabla \cdot (\kappa_s \phi_s \nabla T_s) \\
& + \hbar \left(\frac{1}{T_s} - \frac{1}{T_f} \right). \tag{2.3.10f}
\end{aligned}$$

Also, the compaction equation for the solid volume fraction (2.2.8i) in non-dimensional form is written as

$$\frac{D_s \phi_s}{Dt} = \frac{1}{\mu_c} \left(\frac{1}{\epsilon} \left(\frac{p_s}{T_s} - \frac{p_f}{T_f} \right) - \frac{\beta_s}{T_s} + \nabla \cdot \left(\frac{\Gamma_s}{T_s} \nabla \phi_s \right) \right). \tag{2.3.10g}$$

The parameter ϵ that appears in the above equations is defined as follows

$$\epsilon = \gamma_{f,r} M_{f,r}^2, \tag{2.3.11}$$

whereas, the parameter ξ is the ratio of the reference bulk viscosity to the reference shear viscosity, *i.e.* $\xi = \hat{\zeta}_r / \hat{\mu}_r$.

Finally, the non-dimensionalized state equation for the fluid phase (2.2.11) reads,

$$p_f = \rho_f T_f, \tag{2.3.12}$$

whereas the non-dimensionalized state equation for the solid material (2.2.23) reads,

$$p_s = -P_\infty + R_s \rho_s T_s, \tag{2.3.13}$$

with $P_\infty = \hat{P}_\infty / \hat{p}_r$ and $R_s = \hat{R}_s / \hat{R}_f$.

Each phase of the mixtures of interest has its own speed of sound and, therefore, its own Mach number. Evidently, a flow of the mixtures of interest is a low-Mach number flow if the reference velocity is much smaller than the speeds of sound of both phases. Consequently, it is the smaller of the phasial speeds of sound that determines whether the flow of interest is in the low-Mach number regime or not.

Next, we assume that the reference Mach number of the fluid phase is sufficiently small so as $\epsilon \ll 1$. Thus, the Mach numbers of both phases are much smaller than unity and, therefore, the flow of each phase is incompressible, in accordance with the incompressibility criterion that was mentioned in the introduction, (Gallavotti 2002). In turn, this implies that the governing system of equations (2.3.10a)-(2.3.13) is singularly

perturbed with respect to the parameter ϵ , *i.e.* with respect to the square of the reference Mach number $M_{f,r}^2$. As such, it is subject to singular perturbation analysis.

Next, each of the unknown variables of the system at hand is expanded into a perturbation series of ϵ , *i.e.* we assume expansions of the form,

$$\omega = \omega^0 + \epsilon \omega^1 + O(\epsilon^2), \quad (2.3.14)$$

whereas by the term “regular series” we mean series of non-negative powers. Moreover, similar expansions are considered for products, such as $p_s \phi_s$, and for functions, such as V_s^v .

Subsequently, we introduce the expansions of type (2.3.14) to equations (2.3.10a)-(2.3.13) and to the saturation relation (2.2.3). We also multiply equations (2.3.10b), (2.3.10c), (2.3.10e) and (2.3.10f) by the perturbation parameter ϵ , so that their leading-order terms are of order one, $O(1)$. Finally, we group terms of same order. The results are the following.

Saturation relation

At order $O(1)$, the saturation relation (2.2.3) reads,

$$\phi_s^0 + \phi_f^0 = 1. \quad (2.3.15)$$

Since ϕ_s and ϕ_f are positive, it follows that ϕ_s^0 and ϕ_f^0 are positive as well, for otherwise the overall perturbation series could be negative, which is a contradiction. Thus, the first-order terms of the perturbation expansion of the volume fractions ϕ_s^0 and ϕ_f^0 are both probability densities and convex coefficients, in analogy with the unperturbed variables ϕ_s and ϕ_f .

However, these properties do not hold for the higher-order terms. Indeed, at order $O(\epsilon)$ the saturation relation (2.2.3) takes the form,

$$\phi_s^1 + \phi_f^1 = 0, \quad (2.3.16)$$

which obviously implies that one of the second-order terms ϕ_s^1 and ϕ_f^1 must have negative sign.

Continuity equations

At order $O(1)$, the continuity equations for the solid phase (2.3.10d) and for the fluid phase (2.3.10a), respectively, read

$$\frac{D_s \rho_s^0 \phi_s^0}{Dt} + \rho_s^0 \phi_s^0 \nabla \cdot \mathbf{u}_s^0 = 0, \quad (2.3.17)$$

$$\frac{D_f \rho_f^0 \phi_f^0}{Dt} + \rho_f^0 \phi_f^0 \nabla \cdot \mathbf{u}_f^0 = 0. \quad (2.3.18)$$

In the above equations and throughout the remaining of this Chapter, we adopt the notation convention,

$$\frac{D_i}{Dt} = \frac{\partial}{\partial t} + \mathbf{u}_i^0 \cdot \hat{\nabla}, \quad i = s, f. \quad (2.3.19)$$

We observe that the structure of equations (2.3.17)–(2.3.18) is the same as the structure of the unperturbed continuity equations, just as in low-Mach number asymptotics for single phase flows. This is to be expected because all terms of the continuity equations are of the same order.

Momentum equations

At order $O(1)$, the momentum equation of the fluid phase (2.3.10b) reads,

$$\nabla(p_f^0 \phi_f^0) + p_f^0 \nabla \phi_s^0 = 0. \quad (2.3.20)$$

This equation yields, by virtue of (2.3.15),

$$\nabla p_f^0 = 0. \quad (2.3.21)$$

In other words, p_f^0 is a function of time only,

$$p_f^0 = p_f^0(t), \quad (2.3.22)$$

and is determined by the boundary conditions. In particular, if the domain is open, then p_f^0 is constant and equal to the open boundary pressure. If the domain is closed, then p_f^0 may vary in time.

At order $O(\epsilon)$, equation (2.3.10b) reads

$$\begin{aligned} \rho_f^0 \phi_f^0 \frac{D_f \mathbf{u}_f^0}{Dt} + \nabla(p_f^1 \phi_f^0 + p_f^0 \phi_f^1) &= \frac{\xi}{Re} \nabla(\phi_f^0 \zeta_f \nabla \cdot \mathbf{u}_f^0) + \frac{1}{Re} \nabla \cdot (2\phi_f^0 \mu_f \mathbf{V}_f^{v,0}) \\ &\quad - (p_f^1 \nabla \phi_s^0 + p_f^0 \nabla \phi_s^1) - \delta(\mathbf{u}_f^0 - \mathbf{u}_s^0) \\ &\quad + \rho_f^0 \phi_f^0 \mathbf{g}. \end{aligned} \quad (2.3.23)$$

Combining equation (2.3.23) with equations (2.3.15) and (2.3.21) we arrive at

$$\begin{aligned} \rho_f^0 \phi_f^0 \frac{D_f \mathbf{u}_f^0}{Dt} + \phi_f^0 \nabla p_f^1 &= \frac{\xi}{Re} \nabla(\phi_f^0 \zeta_f \nabla \cdot \mathbf{u}_f^0) + \frac{1}{Re} \nabla \cdot (2\phi_f^0 \mu_f \mathbf{V}_f^{v,0}) \\ &\quad - \delta(\mathbf{u}_f^0 - \mathbf{u}_s^0) + \rho_f^0 \phi_f^0 \mathbf{g}. \end{aligned} \quad (2.3.24)$$

At order $O(1)$, the momentum equation of the solid phase (2.3.10e) reads

$$\nabla(p_s^0\phi_s^0) + p_f^0\nabla\phi_f^0 = 0. \quad (2.3.25)$$

Combining this equation with (2.3.15) and (2.3.21) we obtain that

$$p_s^0 = p_f^0(t) \quad \text{or} \quad (2.3.26)$$

$$p_s^0 = p_f^0 + \frac{C(t)}{\phi_s^0}, \quad (2.3.27)$$

where $C(t)$ is function of time depending on the boundary conditions. Equation (2.3.27), however, becomes singular in the limit $\phi_s \rightarrow 0$. For this reason, equation (2.3.26) is chosen instead. In other words, the first-order pressures p_i^0 are equal and functions of time only, and are determined by the boundary conditions. This implies that in low-Mach number flows, the two phases are, to the first-order, in mechanical equilibrium with each other.

At order $O(\epsilon)$, the momentum equation of the solid phase (2.3.10e) reads

$$\begin{aligned} \rho_s^0\phi_s^0\frac{D_s\mathbf{u}_s^0}{Dt} + \nabla(p_s^1\phi_s^0 + p_s^0\phi_s^1) &= \frac{\xi}{Re}\nabla(\phi_s^0\zeta_s\nabla\cdot\mathbf{u}_s^0) + \frac{1}{Re}\nabla\cdot(2\phi_s^0\mu_s\mathbf{V}_s^{v,0}) \\ &\quad - \nabla\cdot(\Gamma_s^0\nabla\phi_s^0\otimes\nabla\phi_s^0) + (p_f^1\nabla\phi_s^0 + p_f^0\nabla\phi_s^1) \\ &\quad + \delta(\mathbf{u}_f^0 - \mathbf{u}_s^0) + \rho_s^0\phi_s^0\mathbf{g}. \end{aligned} \quad (2.3.28)$$

By virtue of (2.3.26), equation (2.3.28) takes the form

$$\begin{aligned} \rho_s^0\phi_s^0\frac{D_s\mathbf{u}_s^0}{Dt} + \nabla(p_s^1\phi_s^0) &= \frac{\xi}{Re}\nabla(\phi_s^0\zeta_s\nabla\cdot\mathbf{u}_s^0) + \frac{1}{Re}\nabla\cdot(2\phi_s^0\mu_s\mathbf{V}_s^{v,0}) \\ &\quad - \nabla\cdot(\Gamma_s^0\nabla\phi_s^0\otimes\nabla\phi_s^0) + p_f^1\nabla\phi_s^0 + \delta(\mathbf{u}_f^0 - \mathbf{u}_s^0) \\ &\quad + \rho_s^0\phi_s^0\mathbf{g}. \end{aligned} \quad (2.3.29)$$

The presence of p_f^1 in the last equation is due to the constitutive relation (2.2.8f) for the momentum exchange between the two phases, $\mathbf{f}$. According to this constitutive relation, one component of $\mathbf{f}$ is the non-conservative product of the fluid pressure and the gradient of the solid volume fraction, $\hat{p}_f\hat{\nabla}\phi_s$.

Equations of state

At order $O(1)$, the equation of state of the fluid phase (2.3.12) reads

$$p_f^0 = \rho_f^0 T_f^0. \quad (2.3.30)$$

Hence, since p_f^0 is constant in space, spatial variations in the first-order term of the fluid density ρ_f^0 result only from spatial variations of T_f^0 . We also observe that the structure of equation (2.3.30) is the same as the structure of the unperturbed equation of state (2.3.12).

Further, at order $O(\epsilon)$ the equation of state of the fluid phase (2.3.12) yields

$$p_f^1 = \rho_f^1 T_f^0 + \rho_f^0 T_f^1. \quad (2.3.31)$$

At order $O(1)$, the equation of state of the solid material (2.3.13) reads

$$p_s^0 = -P_\infty + R_s \rho_s^0 T_s^0. \quad (2.3.32)$$

Thus, by virtue of (2.3.26), we observe that spatial variations in the first-order term of the solid density ρ_s^0 are caused only by spatial variations of T_s^0 , in analogy with the fluid phase. Also, the structure of (2.3.32) is the same as the structure of the unperturbed solid equation of state (2.3.13).

Further, at order $O(\epsilon)$ the equation of state of the solid phase (2.3.13) yields

$$p_s^1 = R_s(\rho_s^1 T_s^0 + \rho_s^0 T_s^1). \quad (2.3.33)$$

According to typical terminology for single-phase flows, the first-order terms of the phasial pressures, p_i^0 , $i = f, s$, are referred to as “thermodynamic pressures” because they appear in the state equations of their corresponding phases, c.f. (2.3.30) and (2.3.32). Similarly, the second-order of the phasial pressures, p_i^1 , $i = f, s$, are referred to as “dynamic pressures” because their gradients act as forcing terms in the momentum equations, c.f. (2.3.24) and (2.3.29).

Compaction equation

At order $O(1)$, the compaction equation (2.3.10g) reads

$$\frac{p_s^0}{T_s^0} - \frac{p_f^0}{T_f^0} = 0, \quad (2.3.34)$$

which, by virtue of equation (2.3.26), yields

$$T_f^0 = T_s^0. \quad (2.3.35)$$

In other words, in low-Mach number flows and to the first-order approximation, the temperatures of the two phases are equal and, therefore, there is no heat exchange between the two phases. Nonetheless, the first-order temperature T_f^0 can exhibit strong spatial and temporal variations, similarly to single-phase low-Mach number flows.

At order $O(\epsilon)$, equation (2.3.10g) reads

$$\frac{D_s \phi_s^0}{Dt} = \frac{1}{\mu_c} \left(\frac{p_s^1 T_s^0 - p_s^0 T_s^1}{(T_s^0)^2} - \frac{p_f^1 T_f^0 - p_f^0 T_f^1}{(T_f^0)^2} - \frac{\beta_s^0}{T_s^0} + \nabla \cdot \left(\frac{\Gamma_s^0}{T_s^0} \nabla \phi_s^0 \right) \right). \quad (2.3.36)$$

Upon substitution of (2.3.26) and (2.3.35), this equation is written as follows

$$\frac{D_s \phi_s^0}{Dt} = \frac{1}{\mu_c} \left(\frac{p_s^1 - p_f^1}{T_s^0} - \frac{(T_s^1 - T_f^1) p_s^0}{(T_s^0)^2} - \frac{\beta_s^0}{T_s^0} + \nabla \cdot \left(\frac{\Gamma_s^0}{T_s^0} \nabla \phi_s^0 \right) \right). \quad (2.3.37)$$

We observe that second-order differences between the pressures and temperatures of the two phases act as forcing terms in the evolution of the solid volume fraction, even though *to the first order* the phasial pressures and temperatures are equal. In other words, second-order mechanical and thermal non-equilibrium between the two phases plays a critical role to the (irreversible) low-Mach number dynamics of the system, even though *to the first order* the two phases are in thermal and mechanical equilibrium with each other. This is analogous to the situation in the momentum equations, for both single and two-phase flows. In that case, the gradients of the second-order terms of the pressures act as forcing terms in the low-Mach number momentum equations, even though the first-order terms of the pressures are spatially uniform.

Energy equations

At order $O(1)$, and by virtue of (2.3.35), the energy equation of the fluid phase (2.3.10c) reads,

$$\begin{aligned} \rho_f^0 \phi_f^0 c_{p,f}^0 \frac{D_f T_f^0}{Dt} - \frac{\gamma_{f,r} - 1}{\gamma_{f,r}} \frac{D_f p_f^0 \phi_f^0}{Dt} &= \frac{\gamma_{f,r} - 1}{\gamma_{f,r}} p_f^0 (\mathbf{u}_f^0 - \mathbf{u}_s^0) \cdot \nabla \phi_s^0 \\ &+ \frac{1}{Pr Re} \nabla \cdot (\kappa_f^0 \phi_f^0 \nabla T_f^0). \end{aligned} \quad (2.3.38)$$

Similarly, the energy equation for the solid phase (2.3.10f) at order $O(1)$ reads

$$\rho_s^0 \phi_s^0 c_{p,s}^0 \frac{D_s T_s^0}{Dt} - \frac{\gamma_{f,r} - 1}{\gamma_{f,r}} \frac{D_s p_s^0 \phi_s^0}{Dt} = \frac{1}{Pr Re} \nabla \cdot (\kappa_s^0 \phi_s^0 \nabla T_s^0). \quad (2.3.39)$$

In analogy with single-phase flows, we define the two-phase low-Mach number equations as the set of equations that govern the evolution of the first-order terms of the

low-Mach number expansion. Under this definition, we arrive at the following system which corresponds to the low-Mach number equations for two-phase granular materials,

$$\phi_s^0 + \phi_f^0 = 1, \quad p_s^0 = p_f^0 = p_f^0(t), \quad T_f^0 = T_s^0, \quad (2.3.40a)$$

$$p_f^0 = \rho_f^0 T_f^0, \quad p_s^0 = -P_\infty + R_s \rho_s^0 T_s^0, \quad (2.3.40b)$$

$$\frac{D_f \rho_f^0 \phi_f^0}{Dt} + \rho_f^0 \phi_f^0 \nabla \cdot \mathbf{u}_f^0 = 0, \quad (2.3.40c)$$

$$\frac{D_s \rho_s^0 \phi_s^0}{Dt} + \rho_s^0 \phi_s^0 \nabla \cdot \mathbf{u}_s^0 = 0, \quad (2.3.40d)$$

$$\begin{aligned} \rho_f^0 \phi_f^0 \frac{D_f \mathbf{u}_f^0}{Dt} + \phi_f^0 \nabla p_f^1 &= \frac{\xi}{Re} \nabla (\phi_f^0 \zeta_f \nabla \cdot \mathbf{u}_f^0) + \frac{1}{Re} \nabla \cdot (2\phi_f^0 \mu_f \mathbf{V}_f^{v,0}) \\ &\quad - \delta(\mathbf{u}_f^0 - \mathbf{u}_s^0) + \rho_f^0 \phi_f^0 \mathbf{g}, \end{aligned} \quad (2.3.40e)$$

$$\begin{aligned} \rho_s^0 \phi_s^0 \frac{D_s \mathbf{u}_s^0}{Dt} + \nabla (p_s^1 \phi_s^0) &= \frac{\xi}{Re} \nabla (\phi_s^0 \zeta_s \nabla \cdot \mathbf{u}_s^0) + \frac{1}{Re} \nabla \cdot (2\phi_s^0 \mu_s \mathbf{V}_s^{v,0}) \\ &\quad - \nabla \cdot (\Gamma_s^0 \nabla \phi_s^0 \otimes \nabla \phi_s^0) + p_f^1 \nabla \phi_s^0 + \delta(\mathbf{u}_f^0 - \mathbf{u}_s^0) \\ &\quad + \rho_s^0 \phi_s^0 \mathbf{g}, \end{aligned} \quad (2.3.40f)$$

$$\begin{aligned} \rho_f^0 \phi_f^0 c_{p,f}^0 \frac{D_f T_f^0}{Dt} - \frac{\gamma_{f,r} - 1}{\gamma_{f,r}} \frac{D_f p_f^0 \phi_f^0}{Dt} &= \frac{\gamma_{f,r} - 1}{\gamma_{f,r}} p_f^0 (\mathbf{u}_f^0 - \mathbf{u}_s^0) \cdot \nabla \phi_s^0 \\ &\quad + \frac{1}{Pr Re} \nabla \cdot (\kappa_f^0 \phi_f^0 \nabla T_f^0), \end{aligned} \quad (2.3.40g)$$

$$\rho_s^0 \phi_s^0 c_{p,s}^0 \frac{D_s T_s^0}{Dt} - \frac{\gamma_{f,r} - 1}{\gamma_{f,r}} \frac{D_s p_s^0 \phi_s^0}{Dt} = \frac{1}{Pr Re} \nabla \cdot (\kappa_s^0 \phi_s^0 \nabla T_s^0), \quad (2.3.40h)$$

$$\frac{D_s \phi_s^0}{Dt} = \frac{1}{\mu_c} \left(\frac{p_s^1 - p_f^1}{T_s^0} - \frac{(T_s^1 - T_f^1) p_s^0}{(T_s^0)^2} - \frac{\beta_s^0}{T_s^0} + \nabla \cdot \left(\frac{\Gamma_s^0}{T_s^0} \nabla \phi_s^0 \right) \right). \quad (2.3.40i)$$

2.3.1 Properties of the low-Mach number equations

The low-Mach number equations (2.3.40c)-(2.3.40i) constitute a system of seven partial differential equations that is closed by the algebraic equations (2.3.40a) and (2.3.40b). The seven independent unknown variables are

$$\phi_s^0, \mathbf{u}_s^0, \mathbf{u}_f^0, p_s^1, p_f^1, T_s^0, \Delta T^1 = T_s^1 - T_f^1.$$

The above system has the following interesting properties.

1. The momentum equations (2.3.40e) and (2.3.40f) are decoupled from their corresponding energy equations (2.3.40g) and (2.3.40h), respectively. As mentioned in the introduction, this decoupling constitutes a major simplification over the unperturbed, compressible system (2.3.10a)-(2.3.13).
2. The first-order (thermodynamic) pressures p_f^0 and p_s^0 are equal and functions of time only. As such, their values are determined by the boundary conditions. In particular, in open domains, the thermodynamic pressures are constant.
3. The second-order difference between the phasial temperatures, ΔT^1 , appears as a forcing term in the compaction equation (2.3.40i). This implies that (2.3.40i) is not a convenient rate equation for the first-order term of the solid volume fraction. Instead, it is more convenient to consider it as an algebraic equation for ΔT^1 . However, in low-Mach number flows, we are typically interested in values only up to $O(1)$ and ΔT^1 does not appear in any other equation of the governing system. Therefore, we conclude that (2.3.40i), when viewed as an equation for ΔT^1 , essentially becomes redundant and does not need to be solved. In conclusion, for all practical purposes, the low-Mach number approximation consists of six equations with six unknowns. This can have important numerical implications because it means that the nonlinear and possibly stiff right-hand side of (2.3.40i) does not need to be integrated numerically.
4. Since the first-order phasial temperatures are equal, *i.e.* $T_f^0 = T_s^0$, one needs to solve only one of the energy equations (2.3.40g) and (2.3.40h) for T_s^0 . Then, the other energy equation can play the role of a rate equation for the ϕ_s^0 . In other words, one can integrate the other energy equation for the computation of ϕ_s^0 . In fact, from the numerical point of view, linear combinations of the two energy equations (addition, subtraction, etc) might be more advantageous for the computation of T_s^0 and ϕ_s^0 .
5. The viscous forces do enter the low-Mach number momentum equations (2.3.40e) and (2.3.40f). However, the work performed by these forces is of order $O(\epsilon)$ with respect to variations of the enthalpies of the two phases. Therefore, this work does not appear in the low-Mach number energy equations, just as in the low-Mach number approximation of single-phase flows.

6. The divergence of the tensor $(\Gamma_s^0 \nabla \phi_s^0 \otimes \nabla \phi_s^0)$, which models additional stresses associated with the micro-structure of the solid phase, appears in the low-Mach number solid momentum equation (2.3.40f). Moreover, this tensor does not vanish at equilibrium, which is expected because granular materials support shear stresses at equilibrium. However, the work of these stresses is also of $O(\epsilon)$ with respect to variations of the enthalpy of the solid phase. Therefore, this work does not appear in the low-Mach number solid energy equation (2.3.40g).
7. The configuration Helmholtz free energy of the solid phase $\psi^{c,0}$ is of order $O(\epsilon)$, with respect to the solid's pure-phase enthalpy, $c_{p,s}^0 T_s^0$. Therefore, its material derivative is neglected from the solid energy equation (2.3.40g).

As regards property 3, we observe that the dependence of the evolution of ϕ_s^0 on ΔT^1 , is a consequence of the following: i) the two phases are, in general, in non-equilibrium with each other, and ii) the evolution of the volume fraction is not a fully reversible process. As such, the forcing term of the compaction equation (2.2.8i) consists, in general, of a reversible and an irreversible part. As shown in Papalexandris (2004), consistency with the second thermodynamic law requires that the irreversible part be a function of difference between the temperatures of the two phases, *c.f.* (2.2.8i). This requirement is also reflected in the low-Mach number approximation (2.3.40i) of (2.2.8i), albeit in a subtle way, *i.e.* in the appearance of the second-order term of the difference of the phasial temperatures as a forcing term of (2.3.40i).

According to some models for two-phase granular mixtures, such as the one of Baer & Nunziato (1986) and its variations, the phasial temperatures do not appear in the right-hand side of the compaction equation. In other words, according to those models, the evolution of the volume fraction does not directly depend on the thermal non-equilibrium between the two phases. This implies that in those models, and in absence of configuration stress vector, the volume fraction evolution is a purely reversible process. This, however, is an additional constitutive *assumption* of questionable validity and not a constraint imposed by the second thermodynamic law or by any other thermodynamic argument. In any case, since the compaction equation in those models is independent of the phasial temperatures, it is expected that the low-Mach number approximation of those models would allow first-order differences between the phasial temperatures, *i.e.* $T_s^0 \neq T_f^0$, in general.

The situation is also different if ones makes a different constitutive assumption, namely that the two phases are in thermal equilibrium with each other, *i.e.* $T_s = T_f$, as is done in some other models; see, for example, Svendsen & Hutter (1995), Wang & Hutter (1999a) and Passman *et al.* (1986). Evidently, in this case, the forcing terms of the compaction equation are independent of the temperature and, furthermore, there is only one energy equation. Nonetheless, because of this additional assumption, the predictions of those models for the evolution of the mixture towards an equilibrium or stationary state are

different from the evolution predicted by the two-phase flow model of reference.

2.4 Special cases: constant density flows and the equilibrium limit

In this section we first examine the form of the low-Mach number equations in the special case of constant density flows, *i.e.* when the phasial densities ρ_s and ρ_f remain constant. The study of these equations has practical interest because such flows are encountered in various technological applications. It also has theoretical interest because these equations are the equivalent of the incompressible Navier-Stokes equations to two-phase granular mixtures.

In our study we focus in open domains and in closed domains under constant pressure, which are the cases that most often encountered in practice. In other words, we have that

$$p_f^0 = p_s^0 = \text{constant} . \quad (2.4.1)$$

Further, since the densities are constant, the first-order densities ρ_s^0 and ρ_f^0 are also constant. In turn, by virtue of the first-order approximation of the equations of state (2.3.40b), the last equation implies that

$$T_f^0 = T_s^0 = \text{constant} , \quad (2.4.2)$$

which means that, to the first order, the flow is isothermal. We note, however, that T_s^1 and T_f^1 are generally not constant and not equal to each other.

From the above equations it follows that the energy equation for the solid phase (2.3.40h) reduces to

$$\frac{D_s \phi_s^0}{Dt} = 0 . \quad (2.4.3)$$

This relation means that ϕ_s^0 is conserved along the streamlines of the solid phase. This, however, does not imply that in constant density flows the solid volume fraction becomes a passive scalar that is advected with the flow. Indeed, as is shown below, the configuration stress vector still appears in the momentum equation of the solid phase, *c.f.* (2.4.7). Therefore, ϕ_s^0 remains strongly coupled with both $\mathbf{u}_s^0$ and p_s^1 even in the case of constant density flows.

Substituting equation (2.4.3) to the solid continuity equation (2.3.40d), we deduce that the solid velocity is divergence free, *i.e.*

$$\nabla \cdot \mathbf{u}_s^0 = 0 . \quad (2.4.4)$$

This, in turn, implies that the solid continuity equation (2.3.40d) reduces to a kinematic constraint for the solid velocity, just as in the incompressible Navier-Stokes equations for single-phase flows.

Further, as regards the velocity of the fluid phase $\mathbf{u}_f^0$, by combining the energy equation (2.3.40g) and the continuity equation (2.3.40c), we arrive at

$$\nabla \cdot ((\mathbf{u}_s^0 - \mathbf{u}_f^0) \phi_f) = 0. \quad (2.4.5)$$

In other words, the velocity of the fluid phase is not divergence free but is subject to a different kinematic constraint. This “asymmetry” is due to the fact that, although the volume fraction is conserved along the streamlines of the granular phase, it is not conserved along the streamlines of the fluid phase but obeys a saturation relation instead.

Subsequently, by substituting (2.3.40a), (2.3.40b) and (2.4.3) in the compaction equation (2.3.40i), we arrive at

$$(T_s^1 - T_f^1) \frac{p_s^0}{T_s^0} = p_s^1 - p_f^1 - \beta_s^0 + \nabla \cdot (\Gamma_s^0 \nabla \phi_s^0). \quad (2.4.6)$$

We observe that the compaction equation has been reduced to an elliptic partial differential equation with respect to ϕ_s^0 . Further, the second-order terms of the phasial pressures and temperature differences still appear as forcing terms in the compaction equation (2.4.6) even though the phasial densities are constant and the flow is isothermal to the first order. We conclude that even in constant density flows, the distribution of the solid volume fraction depends on the second-order thermal non-equilibrium between the two phases. In any case, since we are interested only in first-order terms, then ϕ_s^0 can be computed via (2.4.3) and equation (2.4.6) becomes redundant.

Next, by introducing the divergence-free condition (2.4.4) in the solid momentum equation (2.3.40f) we obtain the following expression

$$\begin{aligned} \rho_s^0 \phi_s^0 \frac{D_s \mathbf{u}_s^0}{Dt} + \nabla(p_s^1 \phi_s^0) &= \frac{1}{Re} \nabla \cdot (2\phi_s^0 \mu_s \mathbf{V}_s^{v,0}) - \nabla \cdot (\Gamma_s^0 \nabla \phi_s^0 \otimes \nabla \phi_s^0) \\ &+ p_f^1 \nabla \phi_s^0 + \delta(\mathbf{u}_f^0 - \mathbf{u}_s^0) + \rho_s^0 \phi_s^0 \mathbf{g}. \end{aligned} \quad (2.4.7)$$

Finally, we note that the low-Mach number momentum equation for the fluid phase (2.3.40e) remains the same.

Summing up, the equations for constant density flows of two-phase granular mixtures are written as follows

$$\nabla \cdot ((\mathbf{u}_s^0 - \mathbf{u}_f^0) \phi_s^0) = 0, \quad (2.4.8a)$$

$$\nabla \cdot \mathbf{u}_s^0 = 0, \quad (2.4.8b)$$

$$\frac{D_s \phi_s^0}{Dt} = 0, \quad (2.4.8c)$$

$$\begin{aligned} \rho_f^0 \phi_f^0 \frac{D_f \mathbf{u}_f^0}{Dt} + \phi_f^0 \nabla p_f^1 &= \frac{\xi}{Re} \nabla (\phi_f^0 \zeta_f \nabla \cdot \mathbf{u}_f^0) + \frac{1}{Re} \nabla \cdot (2\phi_f^0 \mu_f \mathbf{V}_f^{v,0}) \\ &\quad - \delta(\mathbf{u}_f^0 - \mathbf{u}_s^0) + \rho_f^0 \phi_f^0 \mathbf{g}, \end{aligned} \quad (2.4.8d)$$

$$\begin{aligned} \rho_s^0 \phi_s^0 \frac{D_s \mathbf{u}_s^0}{Dt} + \nabla(p_s^1 \phi_s^0) &= \frac{1}{Re} \nabla \cdot (2\phi_s^0 \mu_s \mathbf{V}_s^{v,0}) - \nabla \cdot (\Gamma_s^0 \nabla \phi_s^0 \otimes \nabla \phi_s^0) \\ &\quad + p_f^1 \nabla \phi_s^0 + \delta(\mathbf{u}_f^0 - \mathbf{u}_s^0) + \rho_s^0 \phi_s^0 \mathbf{g}. \end{aligned} \quad (2.4.8e)$$

It is worth mentioning that by virtue of the divergence-free condition for the velocity of solid phase, the term containing the solid bulk viscous pressure has disappeared from the solid momentum equation (2.4.8e). However, this is not the case for the fluid momentum equation (2.4.8d).

As expected, the equations that govern constant density flows, (2.4.8a)–(2.4.8e), are much simpler than the general low-Mach number equations (2.3.40a)–(2.3.40i). For example, the continuity and momentum equations for the solid phase resemble the incompressible Navier-Stokes equations for simple fluids. This suggests that it could be possible to generalize the projection methods that are typically used for the Navier-Stokes equations and apply them for the numerical treatment of the balance equations for the solid phase (2.4.8a), (2.4.8c) and (2.4.8e). However, for the balance equations of the fluid phase (2.4.8b) and (2.4.8d), these methods are likely to require certain modifications, because of the different kinematic constraint that holds for the fluid phase, *cf.* (2.4.8a).

2.4.1 The equilibrium limit

At the equilibrium limit, all terms that describe dissipative effects vanish and the temperatures of the two phases become equal and constant. Also, the phasial velocities become zero everywhere. In this case, the low-Mach number equations (2.3.40a)–(2.3.40i) reduce to

$$p_s^0 = p_f^0 = \text{constant}, \quad \phi_s^0 + \phi_f^0 = 1, \quad (2.4.9a)$$

$$p_f^0 = \rho_f^0 T_f^0, \quad p_s^0 = -P_\infty + R_s \rho_s^0 T_s^0, \quad (2.4.9b)$$

$$\phi_f^0 \nabla p_f^1 = \rho_f^0 \phi_f^0 \mathbf{g}, \quad (2.4.9c)$$

$$\nabla(p_s^1 \phi_s^0) = p_f^1 \nabla \phi_s^0 - \nabla \cdot (\Gamma_s^0 \nabla \phi_s^0 \otimes \nabla \phi_s^0) + \rho_s^0 \phi_s^0 \mathbf{g}, \quad (2.4.9d)$$

$$p_s^1 - p_f^1 = \beta_s^0 - \nabla \cdot (\Gamma_s^0 \nabla \phi_s^0). \quad (2.4.9e)$$

Since the phasial temperatures are equal and constant, then their first-order approximations T_s^0 and T_f^0 are also equal and constant. Therefore, by virtue of (2.4.9a) and the state equations (2.4.9b), the first-order phasial densities ρ_s^0 and ρ_f^0 are also constant.

Further, we observe that equation (2.4.9c) can be integrated analytically for the computation of the fluid dynamic pressure p_f^1 . Consequently, the governing system reduces to equations (2.4.9d) and (2.4.9e) with respect to the two remaining unknown variables ϕ_s^0 and p_s^1 .

On the other hand, it is interesting to note that the same set of equations, (2.4.9a)–(2.4.9e), is recovered by a different procedure, see Chapter 3 for more details, which is summarized as follows.

- i. Consider the unperturbed, compressible two-phase flow model of reference and set all dissipative processes equal to zero, *i.e.* take its equilibrium limit.
- ii. Non-dimensionalize the resulting equations.
- iii. Employ standard hydrostatic-type arguments to show the smallness of the parameter

$$\epsilon' = \frac{|\mathbf{g}| L_r}{p_r / \rho_r}, \quad (2.4.10)$$

which appears in the non-dimensionalized equations.

- iv. Perturb singularly the non-dimensionalized equations with respect to ϵ' .

In other words, the operations of taking the equilibrium limit and perturbing singularly the two-phase flow model of reference commute. This should come at no surprise because, in the presence of a gravitational field, the term $u_r = \sqrt{|\mathbf{g}| L_r}$ plays the role of a reference velocity. Therefore, if one considers low-Mach number flows, this reference velocity is necessarily much smaller than $\sqrt{p_r / \rho_r}$ which is proportional to the reference speed of sound. We conclude that the smallness of ϵ' is included in the low-Mach number hypothesis. In particular, at equilibrium the parameter ϵ' controls the incompressibility of the mixture, which explains the observed commutation.

2.5 Remarks on the validation of the low-Mach number equations

As is the case for any new theory, both the two-phase flow model of reference and its low-Mach number approximation presented herein should be validated experimentally. In the past, constant density, isothermal granular flows have been studied experimentally

by various authors. On the other hand, and to the best of our knowledge, there have not been any experimental studies of granular flows in the presence of temperature gradients. Nonetheless, some of the isothermal experiments can be extended directly to conditions with temperature gradients. Below we briefly describe two of them, namely shear and gravity-driven flow experiments.

Shear flow experiments can be performed in viscometric shearing apparatus in planar or cylindrical configurations. In planar shear flow, a mixture of a granular medium and a fluid fills the space between parallel horizontal plates. Shear flow is caused by forcing the upper plate to move parallel to the lower one with a given velocity. On the other hand, cylindrical shear (Couette) flow consists of flow between two concentric and counter-rotating cylindrical drums; see Bagnold (1954), Savage & McKeown (1983) and references therein. Extension of these experimental configurations to flows with temperature gradients can be achieved by maintaining the two plates (or the drums) in different temperatures, thereby introducing a heat flux across the flow domain.

As regards gravity-driven flow experiments, there are two well-known variations that can be implemented directly. The first one is the free-surface flow of a granular material down an inclined plane; see Savage (1979), Savage & Lun (1988) and references therein. Extension of this experiment to non-isothermal conditions can be achieved by keeping the inclined plane at a temperature different than the ambient one. The second variation is the vertical channel flow, in which a granular material flows due to gravity between two parallel, vertical planes, Savage (1979). Extension of this set-up to flows with temperature gradients can be achieved by maintaining the two planes at different temperatures.

In the past, various authors have obtained numerical solutions for the above problems by employing different granular flow models; see, for example, Passman *et al.* (1986), Wang & Hutter (1999*a*), Wang & Hutter (2006) and references therein. All earlier numerical studies, however, were restricted to isothermal, steady-state, planar flows, for which the flow models reduce to a set of ordinary differential equations. Nonetheless, it is important to simulate numerically isothermal transient 3-D flows, so as to study the process of mechanical relaxation between the granular and fluid phases, in addition to low-Mach number flows with temperature gradients.

Despite the conceptual simplicity of the above experiments, the reader should be warned that validation of granular flow models is by no means an easy task. For example, one difficulty arises from the complexity of the mathematical models, which does not allow the derivation of analytical or even semi-analytical solutions. Thus, the mathematical models have to be discretized and solved numerically. However, the design of efficient and robust methods for these equations is challenging because they contain unconventional and highly non-linear differential and relaxation terms. Further, during numerical simulations, particular care has to be paid in the implementation of the boundary conditions. In fact, the issue of appropriate boundary conditions for granular materials is still open. For studies and discussion on this issue the reader is referred to Jenkins

& Richmann (1986), Richmann & Chou (1988), Wang & Hutter (2006) and references therein.

Further, another challenging issue is the large number of physical parameters appearing in two-phase flow models for granular materials. For some of these parameters, such as interfacial drag, there are empirical correlations which are considered to be sufficiently accurate. However, there are some transport coefficients of the granular phase for which generally accepted correlations are not available yet. Examples include the shear and bulk viscosity coefficients of the granular phase $\hat{\mu}_s$ and $\hat{\zeta}_s$, respectively, the dynamic compaction coefficient $\hat{\mu}_c$, and others.

Furthermore, currently there are no sufficiently accurate estimates for the coefficients appearing in the expression for the configuration part of the Helmholtz free energy, $\hat{k}_1$ and $\hat{k}_2$, *c.f.* (2.2.27). To this extend, it would be helpful if one could measure the normal and shear configuration stresses that are developed in a granular pile at equilibrium. Then, in principle one could use these measurements to deduce values for the coefficients $\hat{k}_1$ and $\hat{k}_2$. Alternatively, one could perform numerical simulations of the piles that are formed from discharging a granular material on a horizontal surface and determine the values of those coefficients so as the numerical predictions for the angle of repose of the piles match the experimentally measured angles.

Finally, another point that requires attention is to sufficiently approximate in experiments the numerous constitutive assumptions upon which the flow models are based. For example, the two-phase flow model of reference and its low-Mach number approximation treat the granular phase as a continuum. There are cases where this assumption is no longer valid, e.g. mixtures with very low concentrations of granular matter or with a small number of grains. Consequently, experiments designed for the validation of the models in hand should include large numbers of particles. Further, the grains used in the experiments should be cohesionless, of approximately the same size, without humidity and free of electrostatic forces.

2.6 Conclusions

In this Chapter we have presented a generalization of low-Mach number asymptotics to multi-phase flows and applied it to derive the low-Mach number approximation of the two-phase flow model of reference. Our methodology amounts to non-dimensionalizing the governing system with respect to a reference thermodynamic state of the phase with the smallest speed of sound and expanding all variables in power series of the Mach number in this reference state. As in the case of single-phase flows, the multi-phase low-Mach number equations are considerably simpler than the unperturbed, compressible models. In particular, the momentum equations of the two phases are essentially decoupled from their corresponding energy equations.

The low-Mach number approximation, when applied to the above mathematical model

for two-phase granular mixtures, requires that the phasial temperatures be equal to the first order. Nonetheless, the second-order term of the temperature difference appears as a forcing term in the rate equation for the volume fraction (compaction equation). Thus, this equation becomes essentially redundant and the solid volume fraction is computed from one of the two energy equations.

In the special but important cases of constant density flows and of equilibrium limit the governing equations are further simplified. In particular, in constant density flows, the velocity of the solid phase is divergence free, and the solid continuity and momentum equations resemble the classical incompressible Navier-Stokes equations. Also, the volume fraction is constant along the streamlines of the solid phase. On the other hand, the velocity of the fluid phase is not divergence free but subject to a different kinematic constraint.

It is expected that the low-Mach number equations that have been derived herein are easier to study than the unperturbed compressible model, both from the numerical and the theoretical point of view.

Chapter 3

Numerical analysis of hydrostatics of two-phase granular mixtures

3.1 Introduction

A necessary condition for the validity of any model that aims to describe two-phase flows of granular materials is the accurate prediction of the equilibrium distributions. However, a numerical framework for the computation of the multi-dimensional structure of two-phase granular mixtures at equilibrium is currently not available. Consequently, multi-dimensional numerical results for equilibria of such mixtures are available only for very special cases.

In this Chapter we present and analyze an algorithm for the numerical approximation of the equilibrium limit of two-phase flow model of reference. At the limit of thermodynamic equilibrium, this model reduces to a system of equations that describe the hydrostatics of two-phase granular mixtures. This is an overdetermined system of nonlinear elliptic equations for the volume fraction and the pressure of the granular material. Since granular materials support shear at equilibrium, the equilibrium equations admit spatially structured solutions for both the pressure and the volume fraction and, therefore, their study is far from trivial.

Based on standard hydrostatic-type scaling arguments we first perform a perturbation analysis for the system in hand. The perturbed system is then supplemented by an appropriate compatibility condition which arises from the cohomologies of the gradient operator. Subsequently, we design a projection-type, Successive-Over-Relaxation algorithm for the perturbed system based on the combination of the Helmholtz decomposition and Ladyzhenskaya's theorem for the construction of the orthogonal complement

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of the Lebesgue square-integrable solenoidal vector fields.

This Chapter is organized as follows. In Section 3.2 we present the equilibrium equations and we develop the theoretical framework for the numerical method. In Section 3.3 the numerical algorithm is presented in detail. Section 3.4 is devoted to the stability and consistency analysis. In Section 3.5 we discuss possible approaches for cases not covered by the perturbation analysis. Finally, in Section 3.6, we present some representative results from the numerical experiments that we conducted in the course of our study.

3.2 The equilibrium equations

Let us consider a saturated mixture of an isotropic granular material and a simple fluid occupying a Lipschitz domain Ω . Throughout this Chapter, we assume that the volume fractions of the two phases ϕ_s, ϕ_f are uniformly bounded away from zero. This assumption is made because the passage to the single phase equations is highly singular and beyond the scope of the present study. Further, all functions are assumed to be sufficiently smooth in their arguments.

At equilibrium, the temperatures of the two phases $\hat{T}_s, \hat{T}_f$ are equal and uniform, the velocities of the two phases are zero everywhere, and all the terms that describe dissipative processes are zero. Therefore, the two-phase flow model of reference (2.2.1a)–(2.2.1f), (2.2.8a)–(2.2.8i) reduces to the following overdetermined system of partial differential equations,

$$\hat{\nabla}((\hat{p}_s - \hat{p}_f)\phi_s) = -\hat{\nabla} \cdot (\hat{\Gamma}_s \hat{\nabla} \phi_s \otimes \hat{\nabla} \phi_s) + \phi_s(\hat{\rho}_s - \hat{\rho}_f)\hat{\mathbf{g}}, \quad (3.2.1)$$

$$\hat{\nabla} \hat{p}_f = \hat{\rho}_f \hat{\mathbf{g}}, \quad (3.2.2)$$

$$\hat{p}_s - \hat{p}_f = \hat{\beta}_s - \hat{\nabla} \cdot (\hat{\Gamma}_s \hat{\nabla} \phi_s), \quad (3.2.3)$$

Equations (3.2.1) and (3.2.2) result from the momentum equations for the solid and fluid phase, respectively, and express the balance of forces acting on each phase at equilibrium. Further, equation (3.2.3) is the equilibrium limit of the compaction equation.

As regards equations of state, following Chapter 2 we assume that the fluid phase obeys the ideal gas equation of state,

$$\hat{p}_f = R_f \hat{\rho}_f \hat{T}_f, \quad (3.2.4)$$

whereas the solid material follows the stiffened gas equation of state,

$$\hat{p}_s + \hat{P}_\infty = R_s \hat{\rho}_s \hat{T}_s, \quad (3.2.5)$$

As it will be shown later, the detailed expression for the equation of states does not play a role either in the derivation of the numerical method or in the acquisition of numerical results. Further, as regards $\hat{\beta}_s$ and $\hat{\Gamma}_s$, we adopt the expressions given in Chapter 2,

$$\hat{\beta}_s = \hat{k}_1 \hat{\rho}_s \phi_s^2, \quad \hat{\Gamma}_s = \hat{k}_2 \hat{\rho}_s \phi_s. \quad (3.2.6)$$

where $\hat{k}_1, \hat{k}_2 > 0$ are constants related to the granular medium under study.

We remark that under this choice i) $\hat{\Gamma}_s$ and $\hat{\beta}$ are bounded, and ii) $\hat{\Gamma}_s$ is strictly positive in Ω . Further, the symmetric configuration stress tensor $\hat{\sigma}$ has the analytical representation,

$$\hat{\sigma} = \begin{pmatrix} \hat{\sigma}_{11} & \hat{\sigma}_{12} & \hat{\sigma}_{13} \\ \hat{\sigma}_{12} & \hat{\sigma}_{22} & \hat{\sigma}_{23} \\ \hat{\sigma}_{31} & \hat{\sigma}_{32} & \hat{\sigma}_{33} \end{pmatrix} = \hat{k}_2 \hat{\rho}_s \phi_s \begin{pmatrix} \frac{\partial \phi_s}{\partial \hat{x}} \frac{\partial \phi_s}{\partial \hat{x}} & \frac{\partial \phi_s}{\partial \hat{x}} \frac{\partial \phi_s}{\partial \hat{y}} & \frac{\partial \phi_s}{\partial \hat{x}} \frac{\partial \phi_s}{\partial \hat{z}} \\ \frac{\partial \phi_s}{\partial \hat{x}} \frac{\partial \phi_s}{\partial \hat{y}} & \frac{\partial \phi_s}{\partial \hat{y}} \frac{\partial \phi_s}{\partial \hat{y}} & \frac{\partial \phi_s}{\partial \hat{y}} \frac{\partial \phi_s}{\partial \hat{z}} \\ \frac{\partial \phi_s}{\partial \hat{x}} \frac{\partial \phi_s}{\partial \hat{z}} & \frac{\partial \phi_s}{\partial \hat{y}} \frac{\partial \phi_s}{\partial \hat{z}} & \frac{\partial \phi_s}{\partial \hat{z}} \frac{\partial \phi_s}{\partial \hat{z}} \end{pmatrix}.$$

Moreover, since $\hat{\beta}_s$ appears only as a lower-order forcing term in (3.2.3), its precise functional form has no impact in our analysis and algorithm development, for as long as $\hat{\beta}_s$ remains bounded.

As regards the system of equations in hand, we observe that the solid phase density is a function of the solid pressure only, $\hat{\rho}_s = F(\hat{p}_s)$, because at equilibrium the temperature is constant and uniform. This implies that the only unknowns in the equilibrium equations are the solid volume fraction ϕ_s and the phasial pressures $\hat{p}_f, \hat{p}_s$. However, the distribution of the fluid pressure $\hat{p}_f$ can be written in analytic form after straightforward integration of equation (3.2.2),

$$\hat{p}_f = \hat{p}_0 e^{\frac{-|\mathbf{g}|}{R_f T} \hat{z}}, \quad (3.2.7)$$

where $\hat{p}_0$ is the fluid pressure at the ground level $\hat{z} = 0$, and $|\mathbf{g}|$ is the amplitude of the gravity vector $\mathbf{g}$.

Next, we introduce the difference of the phasial pressures $\hat{p}$,

$$\hat{p} = \hat{p}_s - \hat{p}_f = \hat{p}_s - \hat{p}_0 e^{-\frac{|\mathbf{g}|}{R_f T} \hat{z}}. \quad (3.2.8)$$

and rewrite the equilibrium equations as

$$\hat{\nabla}(\hat{p}\phi_s) = -\hat{\nabla} \cdot (\hat{k}_2 \hat{\rho}_s \phi_s \hat{\nabla} \phi_s \otimes \hat{\nabla} \phi_s) + \phi_s (\hat{\rho}_s - \hat{\rho}_f) \hat{\mathbf{g}}, \quad (3.2.9)$$

$$\hat{p} = \hat{k}_1 \hat{\rho}_s \phi_s^2 - \hat{\nabla} \cdot (\hat{k}_2 \hat{\rho}_s \phi_s \hat{\nabla} \phi_s). \quad (3.2.10)$$

This system has to be solved for ϕ_s and $\hat{p}$. Once $\hat{p}$ is known, the solid pressure $\hat{p}_s$ is calculated via (3.2.7) and (3.2.8). It is useful to remark that since $\hat{p}$ is merely the difference of the phasial pressures, it is not subject to any positivity constraint.

3.2.1 Ellipticity of the governing equations

Henceforth, we limit ourselves to $n = 2$, *i.e.* we are going to study the two-dimensional problem in the XZ -plane, while taking into account the presence of gravitational forces. Nonetheless, the analysis can be applied to the three-dimensional case too, after certain minor modifications.

Next, assuming that $\hat{p}$ is given as a source term, we identify in (3.2.10) the classical quasilinear modified Helmholtz equation in terms of the volume fraction ϕ_s . Since $\hat{\Gamma}_s$ is by definition non-negative and uniformly bounded, it follows that equation (3.2.10) is elliptic with respect to ϕ_s .

Next, we show that each component of the vector equation (3.2.9) is elliptic with respect to ϕ_s . For this, we first introduce the decomposition

$$\hat{\nabla} \cdot (\hat{k}_2 \hat{\rho}_s \phi_s \hat{\nabla} \phi_s \otimes \hat{\nabla} \phi_s) = \hat{\nabla} \cdot (\hat{k}_2 \hat{\rho}_s \phi_s \hat{\nabla} \phi_s) \cdot \hat{\nabla} \phi_s + \hat{k}_2 \hat{\rho}_s \phi_s H(\phi_s) \hat{\nabla} \phi_s,$$

where $H(\phi_s)$ stands for the Hessian matrix of ϕ_s . Applying this decomposition to (3.2.9) and further assuming that $\partial \phi_s / \partial \hat{x} \neq 0$ and $\partial \phi_s / \partial \hat{z} \neq 0$, we arrive in the following system of equations,

$$\begin{aligned} \hat{p} + \phi_s \frac{\partial \hat{p} / \partial \hat{x}}{\partial \phi_s / \partial \hat{x}} + \hat{\nabla} \cdot (\hat{k}_2 \hat{\rho}_s \phi_s \hat{\nabla} \phi_s) + \hat{k}_2 \hat{\rho}_s \phi_s \left(\frac{\partial^2 \phi_s}{\partial \hat{x}^2} + \frac{\partial^2 \phi_s}{\partial \hat{x} \partial \hat{z}} \right) &= 0, \\ \hat{p} + \phi_s \frac{\partial \hat{p} / \partial \hat{z}}{\partial \phi_s / \partial \hat{z}} + \hat{\nabla} \cdot (\hat{k}_2 \hat{\rho}_s \phi_s \hat{\nabla} \phi_s) + \hat{k}_2 \hat{\rho}_s \phi_s \left(\frac{\partial^2 \phi_s}{\partial \hat{z}^2} + \frac{\partial^2 \phi_s}{\partial \hat{x} \partial \hat{z}} \right) &= \frac{\phi_s (\hat{\rho}_s - \hat{\rho}_f) \hat{g}}{\partial \phi_s / \partial \hat{z}}. \end{aligned}$$

Under the same reasoning as above for equation (3.2.10), each equation of the above system is elliptic in terms of ϕ_s .

At this point, it is important to note that herein we have employed the definition of ellipticity for second order, scalar equations; see, for example, Gilbarg & Trudinger (1983). Evidently, one can study the ellipticity properties of the overdetermined system as a whole, however, such an analysis is beyond the scopes of the present study.

Further, we observe the presence of $\hat{\rho}_s$ in the coefficients inside the differential operators of the system (3.2.9)-(3.2.10). But since $\hat{\rho}_s$ and $\hat{p}$ are functionally dependent via the equation of state for the solid phase (3.2.5), then $\hat{p}$ enters explicitly the expression of the coefficients of the differential operators of the system. Thus, the system (3.2.9)-(3.2.10) is strongly coupled. Furthermore, this strong coupling is present even with the simplest possible equation of state for the solid material, that of a stiffened gas. It is therefore,

expected that more complicated equations of state will increase the complexity of the coupling.

In order to overcome the coupling that arises from the presence of the pressure $\hat{p}$ in the coefficients of the differential operators, we perform a perturbation analysis of the system (3.2.9)-(3.2.10), guided by standard scaling arguments of hydrostatics. Besides its usefulness for numerical purposes, this analysis provides physical insight on the relative contribution of each force to the equilibrium configuration of the mixtures of interest.

3.2.2 Perturbation analysis

First, we write the system of equations (3.2.9)-(3.2.10) in non-dimensional form. To this extent, we use the fluid pressure $\hat{p}_0$, and the fluid density $\hat{\rho}_0$, at ground level as reference values. Thus,

$$\hat{p}_s = \hat{p}_0 p_s, \quad \hat{p}_f = \hat{p}_0 p_f, \quad \hat{P}_\infty = \hat{p}_0 P_\infty, \quad (3.2.11)$$

$$\hat{\rho}_s = \hat{\rho}_0 \rho_s, \quad \hat{\rho}_f = \hat{\rho}_0 \rho_f. \quad (3.2.12)$$

Further, the temperature $\hat{T}$ is non-dimensionalized via the state equation of the fluid, (3.2.4),

$$\hat{T} = \frac{\hat{p}_0}{R_f \hat{\rho}_0} T. \quad (3.2.13)$$

Since the temperature is constant at equilibrium, we have $T = 1$ everywhere.

Moreover, the spatial variables $\hat{x}, \hat{z}$ are non-dimensionalized by the characteristic length of the domain Ω , $\hat{L}_{ref}$.

$$\hat{x} = \hat{L}_{ref} x, \quad \hat{z} = \hat{L}_{ref} z. \quad (3.2.14)$$

It is important to note that $\hat{L}_{ref}$ is assumed to be at least two orders of magnitude larger than the characteristic length-scale of the grains, a necessary condition for the continuum hypothesis to be valid. Also, the constants $\hat{k}_1, \hat{k}_2$ are non-dimensionalized as follows,

$$\hat{k}_1 = |\mathbf{g}| \hat{L}_{ref} k_1, \quad \hat{k}_2 = |\mathbf{g}| \hat{L}_{ref}^3 k_2. \quad (3.2.15)$$

Finally, we define the parameter $\epsilon > 0$,

$$\epsilon = \frac{|\mathbf{g}| \hat{L}_{ref}}{\hat{p}_0 / \hat{\rho}_0}. \quad (3.2.16)$$

With the above non-dimensionalization, the equilibrium equations are written in the following, non-dimensional, form

$$\nabla(p\phi_s) = \epsilon(-\nabla \cdot (k_2\rho_s\phi_s\nabla\phi_s \otimes \nabla\phi_s) + \phi_s(\rho_s - \rho_f)\mathbf{z}), \quad (3.2.17)$$

$$p = \epsilon(k_1\rho_s\phi_s^2 - \nabla \cdot (k_2\rho_s\phi_s\nabla\phi_s)). \quad (3.2.18)$$

The system (3.2.17)-(3.2.18) is closed with the state equations in non-dimensional form. As mentioned above, for the non-dimensional temperature at equilibrium we have $T = 1$ everywhere. Thus, the non-dimensionalized equations of state at equilibrium read

$$p_f = \rho_f, \quad (3.2.19)$$

and

$$p_s = -P_\infty + \frac{R_s}{R_f}\rho_s. \quad (3.2.20)$$

It is important to stress once again that these particular non-dimensional forms of the state equations are valid only for isothermal conditions, such as the equilibrium distributions considered herein. Finally, from equation (3.2.7) we obtain directly the analytical expression of the dimensionless fluid pressure p_f ,

$$p_f = e^{-\epsilon z}. \quad (3.2.21)$$

Next, we observe that the denominator in (3.2.16), $\hat{p}_0/\hat{\rho}_0$, is at the order of magnitude of the square of the sound speed of the fluid phase. In turn, this implies that in most industrial applications and natural phenomena involving granular materials, the parameter ϵ is very small, *i.e.* $\epsilon \ll 1$. In fact, since the denominator in (3.2.16) is typically at least as large as the acceleration of gravity, the parameter ϵ may be at the order of unity only if $\hat{L}_{ref}$ is very large. Such conditions, however, are highly unlikely to occur in equilibrium distributions of two-phase mixtures. One possible exception is a mixture whose fluid constituent is a rarefied gas (small $\hat{p}_0/\hat{\rho}_0$).

Such extreme cases, however, are beyond the scope of the present study. Thus, from now on we assume that ϵ is at least an order of magnitude smaller than unity. This, in turn, suggests that we can perform a perturbation expansion of the governing equations in powers of ϵ . Therefore, we assume the following, generally divergent, regular perturbation expansion,

$$p_s = p_s^0 + \epsilon p_s^1 + O(\epsilon^2), \quad (3.2.22)$$

$$p_f = p_f^0 + \epsilon p_f^1 + O(\epsilon^2), \quad (3.2.23)$$

$$\rho_s = \rho_s^0 + \epsilon \rho_s^1 + O(\epsilon^2), \quad (3.2.24)$$

$$\phi_s = \phi_s^0 + \epsilon \phi_s^1 + O(\epsilon^2). \quad (3.2.25)$$

By the uniqueness of the perturbation expansion we can easily obtain the perturbation expansions for the rest of the variables which appear as products and differences. For p we have

$$p = p^0 + \epsilon p^1 + O(\epsilon^2), \quad (3.2.26)$$

where $p^0 = p_s^0 - p_f^0$ and $p^1 = p_s^1 - p_f^1$ respectively. Similarly for $p\phi_s$ and $\rho_s\phi_s$ we have

$$p\phi_s = (p\phi_s)^0 + \epsilon (p\phi_s)^1 + O(\epsilon^2), \quad (3.2.27)$$

$$\rho_s\phi_s = (\rho_s\phi_s)^0 + \epsilon (\rho_s\phi_s)^1 + O(\epsilon^2), \quad (3.2.28)$$

where

$$(p\phi_s)^0 = p^0\phi_s^0,$$

$$(p\phi_s)^1 = p^0\phi_s^1 + p^1\phi_s^0,$$

$$(\rho_s\phi_s)^0 = \rho_s^0\phi_s^0,$$

$$(\rho_s\phi_s)^1 = \rho_s^0\phi_s^1 + \rho_s^1\phi_s^0.$$

Using exactly the same approach we can also obtain the expansions for triple products and higher order products.

Inserting the expansions (3.2.22)-(3.2.28) to equations (3.2.17)-(3.2.18), grouping terms of the same order and applying the fundamental theorem of perturbation theory (Kato 1966), we obtain the following expressions for the zero-order terms,

$$p_f^0 = 1, \quad p_s^0 = 1, \quad (3.2.29)$$

$$\rho_f^0 = 1, \quad \rho_s^0 = (1 + P_\infty) \frac{R_f}{R_s}, \quad (3.2.30)$$

and the following closed system of equations for the first order terms,

$$p_f^1 = -z, \quad (3.2.31)$$

$$p^1 = k_1\rho_s^0(\phi_s^0)^2 - \nabla \cdot (k_2\rho_s^0\phi_s^0\nabla\phi_s^0), \quad (3.2.32)$$

$$\nabla(p^1\phi_s^0) = -\nabla \cdot (k_2\rho_s^0\phi_s^0\nabla\phi_s^0 \otimes \nabla\phi_s^0) + \phi_s^0(\rho_s^0 - \rho_f^0)\mathbf{z}. \quad (3.2.33)$$

We observe that the coefficients of the differential operators in the perturbed system (3.2.32)-(3.2.33) do not depend on the pressure term p^1 . Instead, only the (constant) zero-order solid density, ρ_s^0 , enters the expressions for these coefficients. Therefore, the perturbation analysis has allowed us to overcome the problematic coupling caused by the

presence of p in the coefficients of the differential operators and in β_s , in equations (3.2.9)-(3.2.10). In other words, the perturbed system (3.2.32)-(3.2.33) is a fully decoupled set of PDEs.

Indeed, multiplying (3.2.32) by ϕ_s , taking the gradient and combining with (3.2.33) results in the third-order vector equation for ϕ_s^0 ,

$$\begin{aligned} k_2 \rho_s^0 H(\phi_s^0) + \phi_s^0 (\rho_s^0 - \rho_f^0) \mathbf{z} = & -k_2 \rho_s^0 \phi_s^0 \nabla(\nabla \cdot (\nabla(\phi_s^0)^2)) \\ & + 3 k_1 \rho_s^0 (\phi_s^0)^2 \nabla \phi_s^0, \end{aligned} \quad (3.2.34)$$

where $H(\cdot)$ is the Hessian operator. This equation is obviously independent of p^1 . The study of existence and regularity of (3.2.34) is by itself an important step towards a better understanding of the equilibrium behavior of granular mixtures and it will be addressed in a future work.

Further, it is interesting to note that ϕ_s^0 inherits the properties of ϕ_s and, particularly, it is also a probability density. On the other hand, the higher-order terms of the perturbation expansion of ϕ_s are not probability densities. Since in our study we will be dealing with the perturbed problem, we will refer to ϕ_s^0 as the "solid volume fraction".

Finally, we observe that the decoupling resulted from the perturbation analysis depends only on the denominator of (3.2.16), $\hat{p}_0/\hat{\rho}_0$, being large, under the isothermal conditions of thermodynamic equilibrium. Therefore, the analysis presented above is independent of the choice of the solid phase equation of state. Indeed, a different choice of state equation would result to the same perturbed problem, since the pressure $\hat{p}_s$ would still be a function of $\hat{\rho}_s$ only.

3.2.3 Integrability Analysis

The governing system (3.2.9)-(3.2.10) is overdetermined in spatial dimensions higher than one. Moreover, the overdeterminacy carries over to the perturbed system (3.2.32)-(3.2.33) as well. Overdetermined systems of PDEs need to be supplemented with compatibility conditions and, more specifically, with differential conditions that are necessary for the solvability of the system. Also, it is useful to remark that an overdetermined system of PDEs and its compatibility conditions can be represented as a "portion" of a complex of differential operators. Then, if the corresponding cohomology space is zero, the necessary compatibility conditions become sufficient as well; see, for example, Dudnikov & Samborski (1996) for the case of linear systems.

At first sight, the overdeterminacy might seem strange and give the impression that the system (3.2.9)-(3.2.10) and its perturbed version (3.2.32)-(3.2.33) are ill-posed. However, this is not the case.

In fact, in our case the overdeterminacy stems from the momentum equation (3.2.9) and is explained as follows. The momentum equation is a vector equation that expresses

the balance of forces in each spatial dimension. On the other hand, at equilibrium it degenerates to an equation for the solid pressure, which is a scalar. However, since the momentum equation (3.2.9) has a clear physical meaning (balance of forces), the compatibility condition for the system (3.2.32)-(3.2.33) arises naturally and is remarkably simple.

Since the system (3.2.32), (3.2.33) is decoupled, ϕ_s^0 can be obtained by solving equation (3.2.34). This equation is also overdetermined, but it is integrable by construction. Indeed, the symmetry of the higher-order mixed derivatives is satisfied identically, as one can verify by simple cross-differentiation. Once ϕ_s^0 is known, the unknown variable p^1 can be obtained via equation (3.2.33). We observe that this is an equation of the form

$$\nabla f = g. \quad (3.2.35)$$

It is well known, that such an equation is integrable if and only if its right-hand side is curl-free, *i.e.* $\nabla \times (g) = 0$. To put it simply, this criterion says that the equality of the mixed second-order derivatives of f must carry over to the right-hand side of (3.2.35). Applying this to (3.2.33) we conclude that it is integrable if and only if,

$$-\nabla \cdot (k_2 \rho_s^0 \phi_s^0 \nabla \phi_s^0 \otimes \nabla \phi_s^0) + \phi_s^0 (\rho_s^0 - \rho_f^0) \mathbf{z} \in \text{Ker}(\text{curl}). \quad (3.2.36)$$

We also remark that since the right-hand side of (3.2.33) stands for the source term g of equation (3.2.35), its precise functional form does not affect the integrability condition (3.2.36).

As an additional point of mathematical interest, it is worth noting that the system (3.2.35) and equation $\nabla \times (g) = 0$ can be represented as the initial portion of the De Rham complex, which is exact if Ω is contractible. Consequently, the compatibility condition $\nabla \times (g) = 0$ is both sufficient and necessary; see, for example, Dudnikov & Samborski (1996) and also Flanders (1989) for an implicit discussion.

Next, let us assume that

$$-\nabla \cdot (k_2 \rho_s^0 \phi_s^0 \nabla \phi_s^0 \otimes \nabla \phi_s^0) + \phi_s^0 (\rho_s^0 - \rho_f^0) \mathbf{z} \in L^{2,2}(\Omega), \quad (3.2.37)$$

and recall the well known Helmholtz decomposition,

$$L^{2,2}(\Omega) = L_{\text{div}}^{2,2}(\Omega) \oplus L_{\text{curl}}^{2,2}(\Omega), \quad (3.2.38)$$

where $L_{\text{div}}^{2,2}(\Omega)$ is the space of the *solenoidal* vector fields, *i.e.* divergence-free vector fields obeying a no-slip condition in the boundary. Also, in (3.2.38), $L_{\text{curl}}^{2,2}(\Omega)$ is the orthogonal complement of $L_{\text{div}}^{2,2}(\Omega)$, *i.e.* the space of curl-free vector fields that can be expressed in the form of a potential. By virtue of the Helmholtz decomposition and of assumption (3.2.37), the integrability condition (3.2.36) can be reformulated as

$$-\nabla \cdot (k_2 \rho_s^0 \phi_s^0 \nabla \phi_s^0 \otimes \nabla \phi_s^0) + \phi_s^0 (\rho_s^0 - \rho_f^0) \mathbf{z} \in L_{\text{curl}}^{2,2}(\Omega). \quad (3.2.39)$$

Therefore, we have, in a sense, the reciprocal of the Leray projector used in the incompressible Navier-Stokes equations; see Gallavotti (2002). The curl-free part of an $L^{2,2}$ -vector field can be uniquely determined, up to an additive constant, via the use of Ladyzhenskaya's theorem (Ladyzhenskaya 1969), which states that:

Theorem 3.2.1. (*Ladyzhenskaya's theorem*). *Given an $L^{2,2}$ -vector field F in Ω , its curl-free part is the solution of the Neumann problem,*

Find $u \in H^1(\Omega)$ such that

$$\begin{aligned} \nabla \cdot (\nabla u) &= \nabla \cdot (F), \quad \text{in } \Omega, \\ \frac{\partial u}{\partial n} &= \frac{\partial F}{\partial n}, \quad \text{in } \partial\Omega. \end{aligned}$$

With the use of Ladyzhenskaya's theorem, we apply the divergence operator in all terms of (3.2.33) which transforms it to the following equivalent Poisson equation with Neumann data,

$$\nabla \cdot (\nabla(p^1\phi_s^0)) = \nabla \cdot (-\nabla \cdot (k_2\rho_s^0\phi_s^0\nabla\phi_s^0 \otimes \nabla\phi_s^0) + \phi_s^0(\rho_s^0 - \rho_f^0)\mathbf{z}), \text{ in } \Omega, \quad (3.2.40)$$

$$\nabla(p^1\phi_s^0) \cdot \mathbf{n} = (-\nabla \cdot (k_2\rho_s^0\phi_s^0\nabla\phi_s^0 \otimes \nabla\phi_s^0) + \phi_s^0(\rho_s^0 - \rho_f^0)\mathbf{z}) \cdot \mathbf{n}, \text{ in } \partial\Omega. \quad (3.2.41)$$

The main advantage of Ladyzhenskaya's theorem is that it allows us to overcome the overdeterminacy of the momentum equation (3.2.33) by projecting the right-hand side of (3.2.33) to the correct space. Moreover, the new equation is equivalent to the original one, thus, no information is lost from this projection. Further, it provides compatibility conditions on the boundary for both the volume fraction ϕ_s and the pressure difference p . Finally, it can be extremely useful for numerical purposes because it transforms the momentum equation to a Poisson equation, which can be easily treated numerically.

At this point it is important to mention that the system in hand admits *multiple* solutions even after imposing compatibility conditions. This non-uniqueness implies that the two-phase mixtures of interest can support multiple equilibrium distributions. This, in turn, implies that the equations of the full model that describe the evolution of the mixture towards equilibrium, *c.f.* Chapter 2, constitute a non-ergodic dynamical system since ergodicity is equivalent with the existence and uniqueness of an equilibrium distribution, (Sinai 1993). In fact, since an equilibrium distribution is the large-time solution of the initial-boundary value problem associated with the full model, it depends strongly on the initial conditions.

Further, by Ladyzhenskaya's theorem and by the existence and uniqueness results for the Neumann problem of the Poisson equation (Gilbarg & Trudinger 1983), it follows that for every smooth solution of (3.2.34) ϕ_s^0 , we obtain only one, up to a constant, equilibrium pressure distribution. This implies that the perturbed problem admits an one-parameter family of solutions. Thus, we arrive to the important conclusion that non-physical solutions, such as two different pressure distributions corresponding to the same volume fraction distribution, are not admitted by the system of equations in hand.

3.3 The numerical method

As mentioned earlier, Ladyzhenskaya's theorem can be used in the design of a projection method for the computation of p^1 from the momentum equation (3.2.33). This implies that ϕ_s^0 must be computed first. One method to perform the computation of ϕ_s^0 is to solve numerically equation (3.2.34). Nonetheless, this is a third-order vector equation and, therefore, its numerical approximation is cumbersome.

A more efficient and robust method is to compute ϕ_s^0 from the compaction equation (3.2.32), which is the method adopted herein. This suggests the use of a Successive-Over-Relaxation (SOR) method for the compaction equation (3.2.32) via the introduction of a pseudo-temporal derivative and, thus, by the transformation of the original boundary problem to a Cauchy problem. The desired solution is then the steady-state solution of the initial value problem. The temporally relaxed compaction equation has the form

$$\frac{\partial \phi_s^0}{\partial t} = p^1 - k_1 \rho_s^0 (\phi_s^0)^2 + \nabla \cdot (k_2 \rho_s^0 \phi_s^0 \nabla \phi_s^0). \quad (3.3.1)$$

The temporally relaxed compaction equation (3.3.1) is a diffusion equation with a forcing term, *i.e.* an equation of the form

$$\frac{\partial u}{\partial t} = \Delta u^m - u^p.$$

Such equations are often encountered, among other applications, in models of flows through porous media, (Kalashnikov 1987, Galaktionov & Vazquez 2002).

In our case, the variable u is the solid volume fraction, which is positive and bounded, $\phi_s^0 \in [0, 1]$. This fact and the convexity of β_s^0 with respect to ϕ_s^0 imply that blow-up of the classical-strong solutions is not to be expected. The temporal relaxation of ϕ_s^0 further implies the temporal relaxation of p^1 due to the coupling between (3.2.32) and (3.2.33).

Due to its simplicity and straightforward implementation we employ the second approach for the numerical solution of the system. Summing up, the proposed numerical method consists of the following major steps,

- i. Predictor-corrector SOR algorithm for the compaction equation (3.2.32).
- ii. Predictor-corrector projection method, based on Ladyzhenskaya's theorem for the momentum equation (3.2.33).

The use of a predictor-corrector algorithm is motivated by the fact that such methods are well known for their stability and robustness in nonlinear parabolic equations, (Douglas & Jones 1963). Also, such methods have been successfully applied to systems containing stiff reaction-diffusion equations, (Lessani & Papalexandris 2006).

3.3.1 Spatio-temporal discretization and flow-chart of the algorithm

In order to simplify the algebra, and without loss of generality, we assume that Ω is discretized via an equidistant mesh $T_{\Delta x, \Delta y}$ with mesh size $\Delta x = \Delta y$, *i.e.* $T_{\Delta x, \Delta y} = T_{\Delta x}$. Also, following standard practices, we assume that $T_{\Delta x}$ is equipped with a lexicographic ordering relation. Further, $T_{\Delta x}$ is assumed to consist of $N \times M$ grid points, N generally being non-equal to M . Finally, we adopt the following notation convention:

- The superscripts $n, n + 1$ denotes the *corrected* values in times $t_n = n \Delta t$ and $t_{n+1} = (n + 1) \Delta t$ respectively.
- The superscript $*$ refers to the predicted value in the time step t_n .
- Spatial coordinates are represented as ordered sub-indices $\{ij\}$
- All differential operators appearing in the flow chart of the algorithm are assumed to be *finite difference operators*.
- Due to the presence of multiple superscripts, we drop the exponents 0 and 1 from ϕ_s^0 and p^1 , respectively, without risk of confusion.

In the proposed algorithm, spatial differential operators are discretized via 2nd-order accurate, central finite differences. Further, temporal differential operators are discretized via forward finite differences, with time step $\Delta t \leq F(\Delta x)$. As usual, the function F will be calculated during the stability analysis. The use of forward finite differences reflects the fact that equation (3.2.32) is parabolic, hence central or backward differences offers no advantage. Finally, we define the function $\text{Res}(p^i, \phi^i)$ as follows,

$$\text{Res}(p^i, \phi_s^i) = p^i - k_1 \rho_s^0 (\phi_s^i)^2 + \nabla \cdot (k_2 \rho_s^0 \phi_s^i \nabla \phi_s^i), \quad i = n, n + 1, *. \quad (3.3.2)$$

The flow-chart of the algorithm is the following.

Prediction step

1. The predicted value ϕ_s^* of the volume fraction in the $(n + 1)$ -th step is computed from the compaction equation as follows:

$$\frac{\phi_s^* - \phi_s^n}{\Delta t} = \text{Res}(p^n, \phi_s^n). \quad (3.3.3)$$

2. The predicted value p^* is computed by taking the divergence of (3.2.33), solving the resulting Neumann problem of the Poisson equation for the product $(p\phi_s)$,

$$\nabla \cdot (\nabla(p\phi_s)^*) = \nabla \cdot (-\nabla \cdot (k_2\rho_s^0\phi_s^*\nabla\phi_s^* \otimes \nabla\phi_s^*) + \phi_s^*(\rho_s^0 - \rho_f^0)\mathbf{g})), \quad (3.3.4)$$

$$\nabla(p\phi_s)^* \cdot \mathbf{n} = (-\nabla \cdot (k_2\rho_s^0\phi_s^*\nabla\phi_s^* \otimes \nabla\phi_s^*) + \phi_s^*(\rho_s^0 - \rho_f^0)\mathbf{z}) \cdot \mathbf{n}. \quad (3.3.5)$$

and then dividing by ϕ_s^* .

Correction step

1. The corrected value ϕ_s^{n+1} of the volume fraction in the $(n+1)$ -th step is computed from the compaction equation as follows:

$$\frac{\phi_s^{n+1} - \phi_s^n}{\Delta t} = \text{Res}(p^*, \phi_s^*). \quad (3.3.6)$$

2. The corrected value p^{n+1} is computed by taking the divergence of (3.2.33), solving the resulting Neumann problem of the Poisson equation,

$$\begin{aligned} \nabla \cdot (\nabla(p\phi_s)^{n+1}) &= \nabla \cdot (-\nabla \cdot (k_2\rho_s^0\phi_s^{n+1}\nabla\phi_s^{n+1} \otimes \nabla\phi_s^{n+1}) \\ &\quad + \phi_s^{n+1}(\rho_s^0 - \rho_f^0)\mathbf{z}), \end{aligned} \quad (3.3.7)$$

$$\begin{aligned} \nabla(p\phi_s)^{n+1} \cdot \mathbf{n} &= -\nabla \cdot (k_2\rho_s^0\phi_s^{n+1}\nabla\phi_s^{n+1} \otimes \nabla\phi_s^{n+1}) \cdot \mathbf{n} \\ &\quad + \phi_s^{n+1}(\rho_s^0 - \rho_f^0)\mathbf{z} \cdot \mathbf{n}, \end{aligned} \quad (3.3.8)$$

and then dividing by ϕ_s^{n+1} .

3.4 Stability, consistency and convergence

In this Section we present the stability and consistency analysis of the proposed numerical method. The numerical solutions that the method produces in the various time-steps are interpreted as vectors, according to the lexicographic relation that $T_{\Delta x}$ is equipped with. Moreover, for reasons concerning the invertibility of operators, we will assume that $N = M$.

Solutions throughout this Section are understood as strong solutions with “sufficient smoothness” in space and time. Further, we recall that ϕ_s^0 is a positive and bounded function. As usual, and for the sake of simplicity, the analysis focuses on the pure Cauchy problem with periodic boundary conditions. The following notation convention for the discrete version of the spatial differential operators is adopted.

- $M(\phi_s)$ denotes the finite difference operator that approximates

$$\nabla \cdot (k_2 \rho_s^0 \phi_s \nabla \phi_s) .$$

- $A(\phi_s)$ denotes the finite difference operator that approximates

$$\nabla \cdot (-\nabla \cdot (k_2 \rho_s^0 \phi_s \nabla \phi_s \otimes \nabla \phi_s)) .$$

- $B(\phi)$ denotes the finite difference operator that approximates

$$\nabla \cdot (\phi_s (\rho_s^0 - \rho_f^0) \mathbf{z}) .$$

Finally, due to the use of the multiples sub-indices in the representation of ϕ_s as a vector, we drop the subscript s , *i.e.* $\phi_s = \phi$, without the risk of confusion.

3.4.1 Stability

We begin the stability analysis of the numerical method by proving the following Lemmas.

Lemma 3.4.1. *Let*

$$\begin{aligned} F : [0, 1]^{N^2} \times \mathbb{R}^{N^2} &\longrightarrow \mathbb{R}^{N^2} \\ (\phi^n, p^n) &\longmapsto \phi^* , \end{aligned}$$

denote the non-linear function of the iteration equation

$$\phi^* = F(\phi^n, p^n) ,$$

defined through the spatio-temporal discretization of the temporally relaxed compaction equation (3.3.1). Then, F is globally Lipschitz, with Lipschitz constant $K = K(\Delta x, \Delta t)$.

Proof. The function F is, by definition, affine and polynomial in the variables that take values in $\mathbb{R}^{N^2}$ and in $[0, 1]^{N^2}$, respectively. Therefore, it is globally Lipschitz. In view of (3.3.1), the Lipschitz constant $K = K(\Delta x, \Delta t)$ which completes the proof. $\square$

Lemma 3.4.2. *Assume that $\phi^n \in [0, 1]^{N^2}$. Then, there exists a constant $C = C(\Delta(x))$ such as*

$$\|p_{ij}^n\|_{\max} \leq C \|\phi_{ij}^n\|_{\max} .$$

Proof. The right-hand side of the Poisson equation (3.2.40) is approximated by the operators $A(\phi^n)$ and $B(\phi^n)$. In fact, $A(\phi^n)$ is a matrix and each of its elements is a polynomial function of ϕ^n in the domain $[0, 1]^{N^2}$. By standard continuity arguments there exists a constant $C_1 = C_1(\Delta x)$ such that

$$A_{k,l}(\phi^n) \leq C_1 \|\phi^n\|_{\max}, \quad \forall \{k, l\}. \quad (3.4.1)$$

Moreover, $A(\phi^n)$ is of the form $A(\phi^n) = \frac{1}{\Delta x^4} \tilde{A}(\phi^n)$, where $\tilde{A}(\phi^n)$ is an operator which does not depend on Δx . Thus, $C_2 = \frac{1}{\Delta x^4} C_1$ and (3.4.1) becomes

$$A_{k,l}(\phi^n) \leq \frac{C_2}{\Delta x^4} \|\phi^n\|_{\max}, \quad \forall \{k, l\}. \quad (3.4.2)$$

Analogously, for $B(\phi^n)$ we have that there exists a constant C_3 such as

$$B_{k,l}(\phi^n) \leq \frac{C_3}{\Delta x} \|\phi^n\|_{\max}, \quad \forall \{k, l\}. \quad (3.4.3)$$

Now, let $L/\Delta x^2$ denote the finite difference operator that discretizes the Laplacian in the left-hand side of (3.2.40). L is a tri-diagonal matrix whose element do not depend on Δx . From (3.4.2) and (3.4.3) we have

$$\|(p\phi)^n\|_{\max} \leq \|L^{-1}\|_{\infty} \frac{C_2}{\Delta x^2} \|\phi^n\|_{\max}.$$

Since ϕ^n , is bounded there exists a constant C_4 such as

$$C_4 \|p^n\|_{\max} \leq \|(p\phi)^n\|_{\max} \leq \|L^{-1}\|_{\infty} \left(\frac{C_2}{\Delta x^2} + C_3 \Delta x^3 \right) \|\phi^n\|_{\max},$$

therefore,

$$\|p^n\|_{\max} \leq C(\Delta x) \|\phi^n\|_{\max},$$

where

$$C(\Delta x) = \|L^{-1}\|_{\infty} \left(\frac{C_2}{\Delta x^2} + C_3 \Delta x^3 \right), \quad (3.4.4)$$

and thus the proof is completed. $\square$

We can now prove the stability Theorem.

Theorem 3.4.3. *Let ϕ^n, ϕ^*, p^n, p^* stand for the predicted and corrected solution vectors that are obtained in the n -th step. Assume that $\phi^0 \in [0, 1]^{N^2}$, where ϕ^0 is the initial condition of the volume fraction. Then if the following condition holds,*

$$K(\Delta(x), \Delta(t))(1 + C(\Delta x)) \leq 1, \quad (3.4.5)$$

the numerical method is stable.

Proof. First we show the stability of (3.3.3). From Lemmas (3.4.1) and (3.4.2) we have

$$\|\phi^*\|_{\max} \leq K(\Delta(x), \Delta(t))(1 + C(\Delta x)) \|\phi^n\|_{\max}.$$

Now, fix $n = 0$. By the Theorem's assumption on the initial conditions we have that

$$\|\phi^*\|_{\max} \leq K(\Delta(x), \Delta(t))(1 + C(\Delta x)),$$

therefore, if

$$K(\Delta(x), \Delta(t))(1 + C(\Delta x)) \leq 1, \quad (3.4.6)$$

we have that $\|\phi^*\|_{\max} \leq 1$. Since the prediction and correction steps have the same structure, we also have $\|\phi^1\|_{\max} \leq 1$. Induction completes the proof for arbitrary n .

The stability of the Poisson equation (3.2.40) follows from the stability of the finite difference approximation, (Mitchell & Griffiths 1980). $\square$

Apart from the stability properties of the proposed algorithm it is important to show that the nonlinear function F is positivity preserving, *i.e.* it maps probability densities to probability densities. To this extent, we first observe that condition (3.4.6) is of the form $\Delta t \leq G_1(\Delta x)$. In fact, positivity of ϕ^* and, thus of ϕ^{n+1} , follows directly by writing the coordinate-wise analytical expression for F and by using i) the fact that ϕ^n is bounded and ii) Lemma (3.4.2). Upon doing so, one arrives at a similar condition of the form $\Delta t \leq G_2(\Delta x)$. In other words, the following proposition is true.

Proposition 3.4.4. *Assume that Δx are chosen so as $G_1(\Delta x)$ and $G_2(\Delta x)$ are strictly smaller than one. Further, let $G(\Delta x) = \min\{G_1(\Delta x), G_2(\Delta x)\}$. Then, if*

$$\Delta t \leq G(\Delta x), \quad (3.4.7)$$

the function $F : [0, 1]^{N^2} \times \mathbb{R}^{N^2} \rightarrow \mathbb{R}^{N^2}$ is positivity preserving.

Equation (3.4.7) states the condition that must be satisfied by Δt and Δx so as for the numerical method to be stable and positivity preserving. A rough computation shows that, asymptotically, equation (3.4.7) has the analytical form $\Delta t \leq \Delta x^2 \min\{k_1, k_2\}$.

The exact formulation for arbitrary Δx and Δt , throughout this approach is very challenging for two reasons. First, (3.4.7) is rational in its arguments and, therefore, one needs to perform a series of complicated algebraic manipulations in order to transform it into a more manageable form. Second, calculation of the optimal constants is not straightforward. To see this, we recall that each row of the matrices A and $B_{i,j}$ gives rise to non-linear polynomial functions of the ϕ_{ij} arguments. Therefore, the optimal constants for the bounds obtained in Theorem (3.4.3) and Proposition (3.4.4) are the solutions to the corresponding non-linear optimization problems over the unit N^2 -dimensional cube. However, solving such problems is far from trivial and, in any case, time-consuming.

In our case it is sufficient to use the asymptotical formulation $\Delta t \leq \Delta x^2 \min\{k_1, k_2\}$, which corresponds to a *feasible* solution of the non-linear optimization problem. This feasible solution can be obtained easily due to the special structure of the domain.

3.4.2 Consistency

The consistency of the numerical method is demonstrated in the following theorem.

Theorem 3.4.5. *Let us assume the conditions of Theorem (3.4.3), Proposition (3.4.4) and that the condition (3.4.7) is satisfied. Further, we assume that the unique solution pair $\phi(x, t), p(x, t)$ of the Cauchy problem with initial data $\phi^0 = \phi(x, 0)$ and $p^0 = p(x, 0)$ in the range $(0, T)$ has the following properties,*

1. $\phi(x, t) \in C^3((0, T) : C^3(\Omega))$,
2. $p(x, t) \in C^3((0, T) : L^2(\Omega))$,
3. $p\phi \in C^3((0, T) : H^2(\Omega))$.

Then, the numerical method proposed is consistent both in space and in time.

Proof. As usual, we will treat spatial and temporal consistency separately. First we show temporal consistency by assuming that the method is exact in the spatial level. Assuming that the method is exact in the time step n , the local truncation error reads in the time-step $n + 1$

$$\begin{aligned} \|\phi^{n+1} - \phi(t_{n+1})\|_{\max} &= \|\phi^{n+1} + \phi^* - \phi^* - \phi(t_{n+1})\|_{\max} \\ &\leq \|\phi^* - \phi(t_{n+1})\|_{\max} + \|\phi^{n+1} - \phi^*\|_{\max}. \end{aligned} \quad (3.4.8)$$

We will treat the two components of (3.4.8) separately.

For the first component of (3.4.8), $\|\phi^* - \phi(t_{n+1})\|_{\max}$, exact Taylor expansion of $\phi(t_{n+1})$ around t_n combined with the definition of ϕ^* in (3.3.3) gives

$$\begin{aligned} \|\phi^* - \phi(t_{n+1})\|_{\max} &= \\ \|\phi^n + \Delta t \text{Res}(\phi^n, p^n) - (\phi(t_n) + \Delta t \frac{\partial \phi}{\partial t}(t_n) + \Delta t^2 \frac{\partial^2 \phi}{\partial t^2}(\xi))\|_{\max}, \end{aligned}$$

where $\xi \in (t_n, t_{n+1})$. The assumption that the method is exact in the spatial level, and in the n -th time-step, implies that

$$\begin{aligned} \|\phi^n + \Delta t \text{Res}(\phi^n, p^n) - (\phi(t_n) + \Delta t \frac{\partial \phi}{\partial t}(t_n) + \Delta t^2 \frac{\partial^2 \phi}{\partial t^2}(\xi))\|_{\max} \\ \leq \|\Delta t^2 \frac{\partial^2 \phi}{\partial t^2}(\xi)\|_{\max}. \end{aligned} \quad (3.4.9)$$

Since $\phi \in C^3((0, T) : C^3(\Omega))$ it follows that (3.4.9) can be bounded by

$$\|\Delta t^2 \frac{\partial^2 \phi}{\partial t^2}(\xi)\|_{\max} \leq \Delta t^2 \|\frac{\partial^2 \phi}{\partial t^2}\|_{C^3((0, T) : C^3(\Omega))} = O(\Delta t^2). \quad (3.4.10)$$

For the second component of (3.4.8) $\|\phi^{n+1} - \phi^*\|_{\max}$ we have

$$\begin{aligned} \|\phi^{n+1} - \phi^*\|_{\max} &= \Delta t \|\text{Res}(\phi^*, p^*) - \text{Res}(\phi^n, p^n)\|_{\max} \\ &= \Delta t \|k_1(\rho_s^0(\phi^*)^2 - \rho_s^0(\phi^n)^2) + (p^* - p^n) \\ &\quad + M(\phi^*) - M(\phi^n)\|_{\max} \\ &\leq \Delta t (\|k_1(\rho_s^0(\phi^*)^2 - \rho_s^0(\phi^n)^2)\|_{\max} + \|(p^* - p^n)\|_{\max}) \\ &\quad + \Delta t \|M(\phi^*) - M(\phi^n)\|_{\max}. \end{aligned} \quad (3.4.11)$$

We study the three components of (3.4.11) separately. For the component $\|(p^* - p^n)\|_{\max}$ we have,

$$\begin{aligned} \|((p\phi)^* - (p\phi)^n)\|_{\max} &= \|A(\phi^n) - A(\phi^*) + B(\phi^n) - B(\phi^*)\|_{\max} \\ &\leq \|A(\phi^n) - A(\phi^*)\|_{\max} + \|B(\phi^n) - B(\phi^*)\|_{\max}. \end{aligned}$$

The continuity of the functions $A(.,.), B(.,.)$ and (3.4.10) imply that as $\Delta t \rightarrow 0$ the following holds.

$$\|((p\phi)^* - (p\phi)^n)\|_{\max} \rightarrow 0.$$

This, in turn implies that

$$\|(p^* - p^n)\|_{\max} \rightarrow 0.$$

The rate of consistency follows from the rate of $\|\phi^* - \phi^n\|_{\max}$, *i.e.*

$$\|(p^* - p^n)\|_{\max} = O(\Delta t^2). \quad (3.4.12)$$

Finally, (3.4.10) implies that

$$\|M(\phi^*) - M(\phi^n)\|_{\max} = O(\Delta t^2), \quad (3.4.13)$$

$$\|k_1(\rho_s^0(\phi^*)^2 - \rho_s^0(\phi^n)^2)\|_{\max} = O(\Delta t^2), \quad (3.4.14)$$

Summing up (3.4.12)-(3.4.14) we obtain

$$\|\phi^{n+1} - \phi^*\|_{\max} = O(\Delta t^2), \quad (3.4.15)$$

and therefore, combining (3.4.10) and (3.4.15) we have

$$\|\phi^{n+1} - \phi(t_{n+1})\|_{\max} = O(\Delta t^2),$$

Hence, the method is second order consistent in time. Spatial consistency for $\phi, p\phi$ follows from the standard estimates for Poisson equations, (Mitchell & Griffiths 1980). $\square$

We conclude this Section with the convergence corollary.

Corollary 3.4.6. *Under the assumptions of Theorems (3.4.3), (3.4.5) and Proposition (3.4.4) the discrete solution pair (ϕ^n, p^n) produced by the numerical method, converges to the unique solution pair of the Cauchy problem $(\phi(x, t), p(x, t))$ in the max-norm as $\Delta t, \Delta x \rightarrow 0$.*

Proof. The proof follows by the Lax-Richtmyer generalized equivalence principle for non-linear systems. This, well known, principle states that stability and consistency imply convergence (Rosinger 1980, Stetter 1980). $\square$

3.5 Remarks on the unperturbed problem

The numerical method that we propose is formally valid for the perturbed system (3.2.32)-(3.2.33), *i.e.* when $\epsilon \ll 1$. Nonetheless, we have also applied the proposed algorithm to the unperturbed problem, in order to study the validity of the perturbation expansion derived in Section 3.2.2. The only modification that the algorithm requires is to update the density of the solid phase ρ_s , which is not constant. This is performed by solving the solid equation of state for ρ_s (3.2.5), immediately after the computation of the pressure difference p .

Our numerical experiments showed virtually no difference between the solutions of the original system (3.2.9) and (3.2.10) and its perturbed version (3.2.32) and (3.2.33). The agreement of these numerical results provides evidence for the validity of the perturbation expansion of Section 3.2.2.

Further, the numerical experiments showed that when $\epsilon \ll 1$, the solid density variations predicted by the unperturbed problem are negligible. This allows the direct application of the proposed method to the unperturbed problem. However, when ϵ grows larger, the solid density variations are no longer negligible. Also the unperturbed system (3.2.9) and (3.2.10) is endowed with a different set of compatibility conditions, which are given below. Therefore, the direct application of our numerical method to the unperturbed (3.2.9) and (3.2.10) without modification will might lead to incorrect results.

As mentioned earlier, the parameter ϵ is very small in all industrial applications and natural phenomena involving granular materials that we are aware of. However, the case where ϵ is not small is still interesting from the theoretical point of view (and possibly from the practical point of view as well, since this type of equations might arise in other areas of physical sciences). For this reason it is worth discussing possible ways to treat the governing system (3.2.9) and (3.2.10) numerically when ϵ is not small.

It is clear that in this case the perturbation expansion is no longer valid, unless the convergence of the expansion is formally proven. However, if ϵ is neither in the limit range of zero nor at the order of unity (for example, if $\epsilon = 0.15$) it is possible to extend the perturbation analysis via Padé approximation. This amounts to reconstruct the perturbation expansion as a series of Padé approximates. Such series are known to successfully approximate the corresponding functions for values of ϵ in the range $0.1 - 0.2$; see, for example, Baker & Graves-Morris (1996). Despite the obvious disadvantage of having to compute higher order terms of the original perturbation expansion, the proposed numerical method can in principle be applied to the new perturbed problem, thanks to the constructive definition of the Padé coefficients.

Further, if $\epsilon = O(1)$, then the full, unperturbed, problem has to be considered. In this case, as we mentioned before, the presence of $\hat{p}$ in the coefficients of the differential operators results in a strongly coupled system of equations. As a consequence, the momentum equation (3.2.9) no longer takes the simple form $\nabla f = g$ and, therefore, the Helmholtz decomposition (3.2.38) is not helpful anymore. Instead, equation (3.2.9), in two dimensions, has the following form,

$$\left(\frac{\partial}{\partial x} + A_1(x, z)\right)f = \omega_1, \quad (3.5.1)$$

$$\left(\frac{\partial}{\partial z} + A_2(x, z)\right)f = \omega_2. \quad (3.5.2)$$

Such equations have been used as examples of the classical Frobenius integrability theorem. Their compatibility condition reads

$$\left(\frac{\partial}{\partial x} + A_1(x, z)\right)\omega_2 = \left(\frac{\partial}{\partial z} + A_2(x, z)\right)\omega_1, \quad (3.5.3)$$

which is the classical commutation relation accounted in Lie theory (Krein & Shikhvatov 1970). This new compatibility condition acts as a constraint on (3.5.1), (3.5.2), thus taking care of the overdeterminacy problem.

However, the design of an algorithm for the numerical treatment of the new constrained system is much more challenging. This is because the new compatibility condition, (3.5.3), when combined with the Helmholtz decomposition (3.2.38), does not produce a simple condition for the right-hand sides of (3.5.1) and (3.5.2), contrary to the outcome of the perturbed case, see equation (3.2.39). Therefore, the momentum equation

can no longer be transformed into an equivalent Poisson equation by simply applying the divergence operator. In this case, taking the divergence of the momentum equation will give rise to incompatibilities on the boundary.

A possible approach for the numerical treatment of the unperturbed problem is to simultaneously solve all equations, including the compatibility condition, via a Newton-Raphson method. However, the implementation of this approach is very challenging. The main difficulty of this approach comes from the discretization of the momentum equation. If one chooses one-sided finite differences for the approximation of the gradient operator, then the corresponding linear system is well-posed; however one order of accuracy is lost. This can be detrimental when the problem involves non-linear, high-order terms, like the tensor product of the gradients that appears in the expression for the configuration stresses. On the other hand, if one chooses 2nd or higher-order central differences, as is often the case, then the corresponding linear system becomes ill-posed because the diagonal of the matrix has zeros everywhere. A possible straightforward way to overcome the ill-posedness of the linear-system is the use of Tikhonov regularization, (Tikhonov & Arsenin 1977). This method, roughly speaking, transforms the linear system in a regularized least-square minimization problem. Further, with this approach certain classical technical difficulties of the Newton-Raphson method must be resolved, such as the analytic derivation of the corresponding Jacobian matrix and a judiciously chosen initial guess.

3.6 Numerical results

The efficiency of the proposed numerical method has been investigated in a series of numerical experiments, part of which will be presented in this Section. In these numerical experiments we have used a mixture of water and sand as the mixture of reference.

3.6.1 Set up of the numerical experiments

The first issue that arises in the numerical treatment of equations for granular mixtures is the values of the constants $\hat{k}_1$ and $\hat{k}_2$ in the expressions for $\hat{\beta}_s$ and $\hat{\Gamma}_s$; *cf.* equation (3.2.6). Ideally, for a given granular material, these values should be obtained experimentally. However, as mentioned in Chapter 2, accurate experimental data for these parameters are not yet available. For this reason, we resorted in considering values from earlier numerical studies.

In particular, we have used the same physical parameters as the ones given by the authors in (Passman *et al.* 1986), who studied numerically shearing motions of a saturated sand-water mixture. These values are $\hat{k}_1 = 0.02 \text{ m}^2/\text{s}^2$ and $\hat{k}_2 = 4 \times 10^{-8} \text{ m}^4/\text{s}^2$. It should be mentioned that Passman *et al.* (1986) did not elaborate on how these values were prescribed. However, they noted that the acquisition of values for these parameters

is problematic. The same values were later adopted in Wang & Hutter (1999a) who studied the same problem as in Passman *et al.* (1986), but with a different constitutive model.

It should also be noted that the above value of $\hat{k}_2$ is very small. Indeed, a heuristic order-of-magnitude analysis of the momentum equation (3.2.33) shows that, with this choice of $\hat{k}_2$, the amplitude of the configuration stresses $\hat{\boldsymbol{\sigma}}$ is three to five orders smaller than that of the gravitational forces $\phi_s(\hat{\rho}_s - \hat{\rho}_f)\hat{\mathbf{g}}$. For such small values of $\hat{k}_2$, the effect of the configuration stresses on $\hat{p}^1\phi_s^0$ is expected to be non-negligible only inside boundary or transition layers. Since the limit $\hat{k}_2 \rightarrow 0$ is singular, solutions of the governing equations (3.2.32) and (3.2.33), for such small values of $\hat{k}_2$, can also be studied via singular perturbation techniques. For the sake of completeness, we also note that the extreme case where $\hat{k}_2 = 0$ admits solutions in closed form. This limit case, however, refers to granular materials that do not support shear at equilibrium and, therefore, has no physical interest.

In our simulations, the uniform temperature of the mixture $\hat{T}$ is set equal to 300 K. The computational domain is a square with sides equal to $\hat{L} = 0.1$ m. As mentioned in Subsection 3.2.2, the water pressure and density at ground level, $\hat{z} = 0$ m, are used as reference values. Thus, $\hat{p}_0 = 1$ atm and $\hat{\rho}_0 = 1000$ kg/m³. Also, we use the length of the side of the computational domain as characteristic length; $\hat{L}_{ref} = 0.1$ m. With this choice of reference values, the perturbation parameter is $\epsilon = 0.0098$, which is a small value, as required for the validity of the perturbation expansion. Finally, an equidistant mesh of 200×200 cells has been used for our simulations and the time-step Δt has been chosen so that $\Delta t = \Delta x^2$.

For the initial condition of ϕ_s^0 we proceed as follows. First, we note that there exists a maximum value of particle packing. This corresponds to the maximum value of the volume fraction in absence of plastic deformations of the grains, which we denote by ϕ_m . As $\phi_s^0 \rightarrow \phi_m$, the solid particles are in such strong contact that the solid phase behaves like a rigid body. For spherical grains, ϕ_m corresponds to the solution of the so-called “minimum packing problem” and is approximately equal to 0.74. Second, the volume fraction has the trend to decrease with $\hat{z}$ due to gravitational forces (sand is more dense than water). This trend should be reflected in the initial profile. Further, the initial condition of ϕ_s^0 must be positive everywhere.

Motivated by these criteria, we have used profiles of the form

$$\phi_s^0(\hat{x}, \hat{z}, 0) = 0.74 - F(\hat{z}) G(\hat{x}), \quad (3.6.1)$$

and perturbations thereof, where $F(\hat{z})$ is a decreasing function in $\hat{z}$. Simple choices for $F(\hat{z})$ and $G(\hat{x})$ are appropriately scaled trigonometric functions or second-order polynomials. In our numerical experiments we have made extensive use of the following profile,

$$\phi_s^0(\hat{x}, \hat{z}, 0) = \left(0.74 - W \hat{x} (L - \hat{x}) \sin \left(\frac{\pi \hat{z}}{2L} \right) \right) \left(1 + 0.1 \sin \left(\frac{\hat{x} \pi}{L} \right) \right), \quad (3.6.2)$$

where W is a constant of order one.

As regards the assignment of boundary conditions, we must caution the reader that imposing physically meaningful boundary values for ϕ_s^0 can be problematic. This has been acknowledged by many authors; see, for example, the recent discussion of Massoudi (2007). More specifically, we are aware of no evidence, experimental or otherwise, that can guide the choice of boundary conditions for the volume fraction. In fact, this is the case with all additional thermodynamic variables, since such variables are generally not controllable on the boundary, (Lebon *et al.* 2008).

For the particular problem in hand, and following previous works on steady-state granular flows, we have chosen to assign Dirichlet boundary conditions to the volume fraction. In particular, the boundary conditions for ϕ_s^0 are obtained by evaluating the corresponding initial conditions to the boundary points. On the other hand, Neumann boundary conditions are assigned to the pressure difference $\hat{p}^1$, as dictated by Ladyzhenskaya's theorem.

3.6.2 Representative results and numerical convergence

We now present the results from numerical simulations that correspond to a mixture of sand and water whose parameter values, initial and boundary conditions follow the set-up formulated above.

Figure 3.1 shows the equilibrium distribution of the solid volume fraction, ϕ_s^0 ; when the initial condition is given by (3.6.2). We observe that the concentration of the granular material decreases with $\hat{z}$, due to the density differences between the two phases. In particular, at the top of the domain, ϕ_s^0 has been reduced to approximately 60% of its value at ground level. Moreover, the concentration of the granular material is higher at the boundaries as reflected by the convexity of the volume fraction's profile.

Figure 3.2 shows the difference between the solid and fluid pressures, $\hat{p} = \hat{p}_s - \hat{p}_f$, measured in N/m^2 . We observe the presence of boundary layers in the top and bottom boundaries of the domain. As mentioned above, the role of the configuration stresses is non-negligible inside these layers. However, outside these layers the pressure difference $\hat{p}$ is dominated by the gravitational forces and decreases monotonically with $\hat{z}$. Further, $\hat{p}$ varies little with $\hat{x}$, due to the small value of $\hat{k}_2$. We also observe that the maximum value of $\hat{p}$ is equal to, approximately, $100 N/m^2$, whereas its minimum value is negative and equal to, approximately, $-40 N/m^2$. In other words, the overall variation of $\hat{p}$ is at the order of 0.1% of the reference pressure $\hat{p}_0 = 1 atm$. This fact is in accordance with our assumption that the correction terms in the perturbation expansion of Subsection 3.2.2 are small, of order ϵ , with respect to the leading order terms.

Figures 3.3(a)-3.3(c) show the components of the configuration stress tensor $\hat{\sigma}$. We observe that the magnitudes of both the normal and the configuration stresses components are very small; $\|\hat{\sigma}_{11}\| = O(10^{-3})$, $\|\hat{\sigma}_{22}\| = O(10^{-3})$, and $\|\hat{\sigma}_{12}\| = O(10^{-4})$. In other

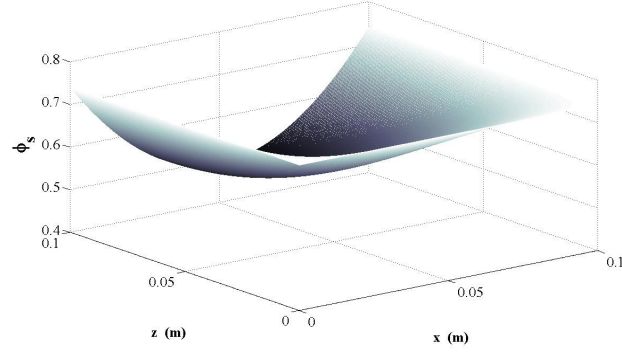


Figure 3.1: Solid volume fraction ϕ_s^0 . The concentration of the granular material is higher in the lower boundary of the domain and decreases with $\hat{z}$ due to the density differences between the two phases. In fact, at the top of the domain, the concentration of the granular material has been reduced to 60% of its value at ground level.

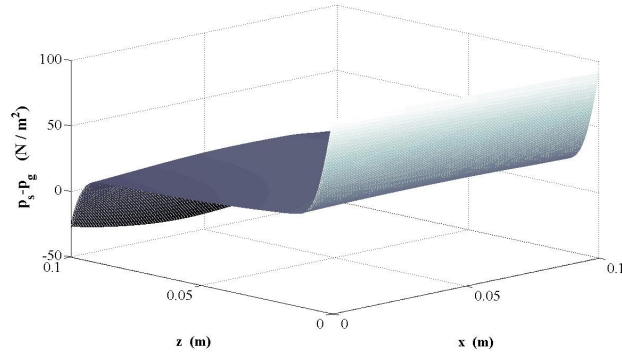
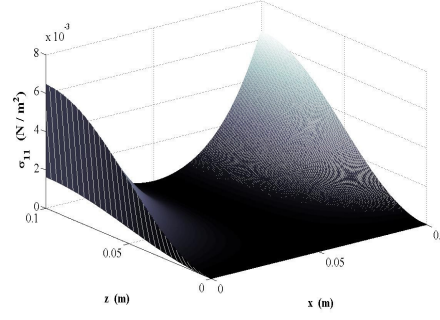
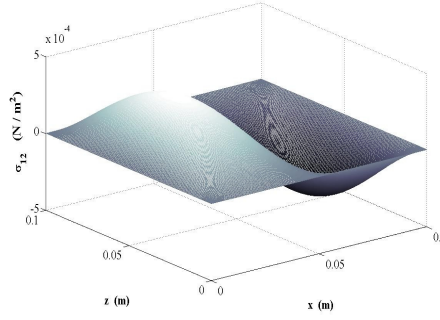


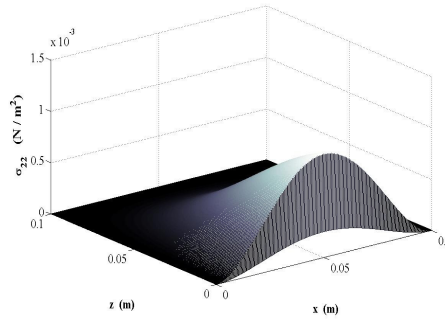
Figure 3.2: Pressure difference $\hat{p}$. We observe the formation of thin transition layers in the top and bottom boundaries of the domain which reflect the contribution of the configuration stresses to the pressure difference. Outside these layers, the pressure difference is dominated by the gravitational forces. We also note that the overall variation of the difference between the phasial pressures remains the order of 0.1% of the reference pressure $\hat{p}_0 = 1 \text{ atm}$.



(a)



(b)



(c)

Figure 3.3: Configuration stresses (a) $\hat{\sigma}_{11}$, (b) $\hat{\sigma}_{22}$, (c) $\hat{\sigma}_{12}$. The configuration stresses remain three to five orders of magnitude smaller than the gravitational forces, which can be attributed to the smallness of $\hat{k}_2$. Both the normal and the shear configuration stresses assume their maximum values near the boundaries of the domain where the granular material has the highest particle concentration.

words, the configuration stresses remain three to five orders of magnitude smaller than the gravitational forces; this is in agreement with our estimates above, regarding the consequences of the smallness of $\hat{k}_2$. Additionally, the contribution of all configuration stresses maximizes at the boundary of the domain, where the concentration of the granular material is higher.

For the case presented here, we have also performed a grid-convergence study. The numerical convergence was tested via the use of the mesh-dependent l^1 norm of the error of the volume fraction ϕ_s^0 and the pressure difference $\hat{p}$, respectively. The mesh-dependent l^1 norm of the numerical error is defined as

$$Er(F) = \frac{1}{N} \sum_{i=1}^N |f_i - F_i|, \quad (3.6.3)$$

where N is the number of computational cells, F stands for the exact solution, and f stands for the numerical solution. In absence of an analytical solution we used as "exact solution" the numerical result obtained with a very fine grid with 1600×1600 points. The four numerical solutions that have been used for the convergence study correspond to grids of 100×100 , 200×200 , 400×400 and 800×800 points respectively.

Figures 3.4 and 3.5 show the results of the grid-convergence study for the variables ϕ_s^0 and $\hat{p}$, respectively. It can be directly observed that numerical convergence is achieved with grid-refinement, thus confirming the theoretical results of Section 3.4.

3.6.3 Parametric studies

In the course of our numerical experiments we have performed parametric studies with respect to $\hat{k}_1$ and $\hat{k}_2$. These studies are a straightforward way of testing the robustness of the proposed numerical method but they also provide insight on the dependence and sensitivity of the solutions to the values that these parameter take. The results of these parametric studies are summarized below.

First, we fix $\hat{k}_2 = 4 \times 10^{-8} \text{ m}^4/\text{s}^2$ and let $\hat{k}_1$ vary between $0.002 - 20 \text{ m}^2/\text{s}^2$. Changes in $\hat{k}_1$ translate directly into changes of the stiffness of the compaction equation (3.2.32) but leave (3.2.33) unaffected. Our numerical experiments showed that the changes in the solid volume fraction distribution ϕ_s^0 are very small, at the order of $O(10^{-4})$. Moreover, the variation of $\hat{k}_1$ has virtually no effect on the magnitude and shape of the profile of the configuration stresses $\hat{\sigma}_{ij}$.

However, as Figures 3.6(a)-3.6(d) show, the profile of the pressure difference $\hat{p}$ is much more sensitive to change of $\hat{k}_1$. First we observe that the magnitude of $\hat{p}$ increases with $\hat{k}_1$. Further, as $\hat{k}_1$ increases, the gradients of $\hat{p}$ in the top and bottom boundaries are smoothed out, *i.e.* the boundary layers become thicker. This implies that the configuration stresses play a non-negligible role everywhere in the domain. Moreover, as $\hat{k}_1$ increases, the variations of $\hat{p}$ in the $\hat{x}$ direction become larger. This trend can be explained by the fact

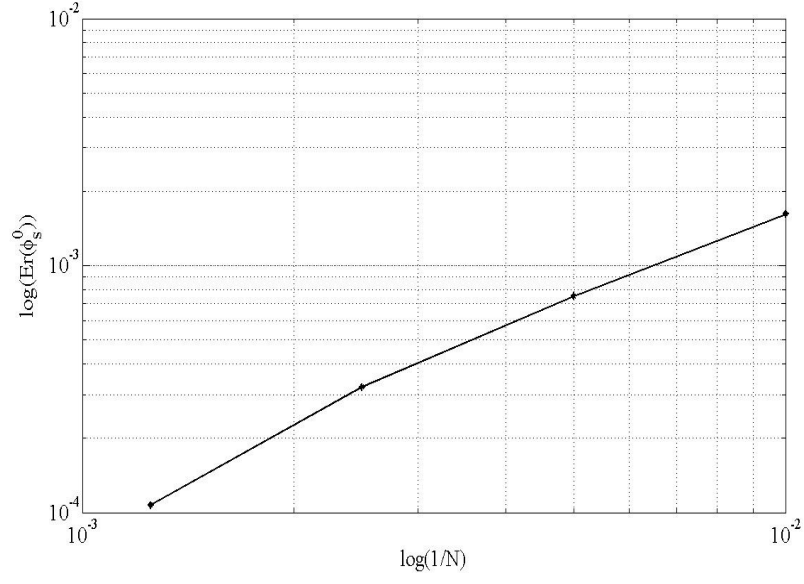


Figure 3.4: Grid-convergence study for the solid volume fraction ϕ_s^0 .

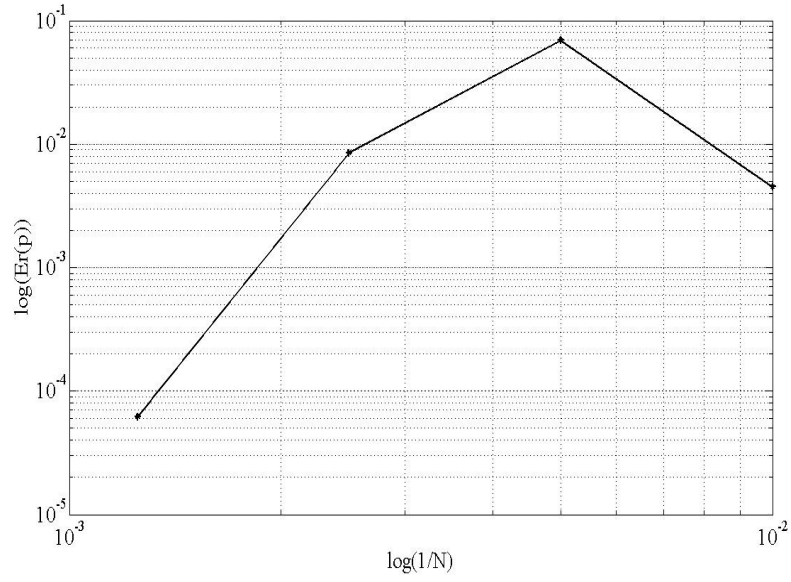


Figure 3.5: Grid-convergence study for the pressure difference $\hat{p}$.

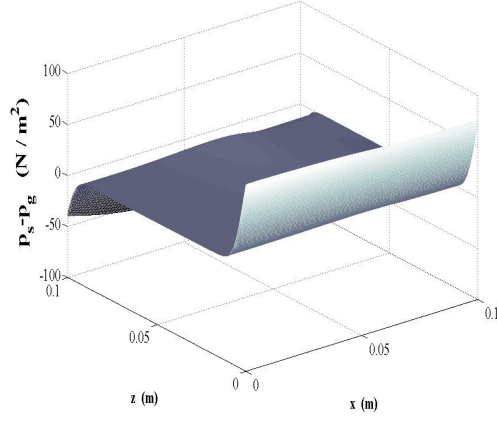
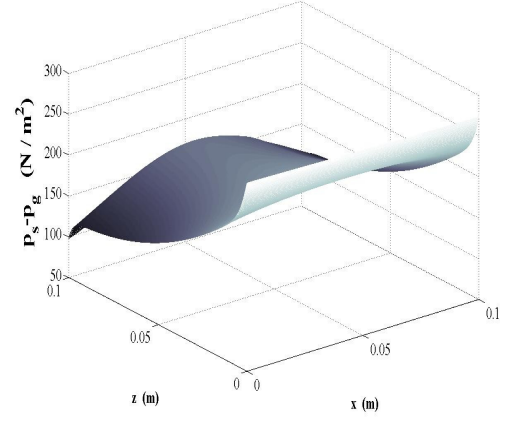
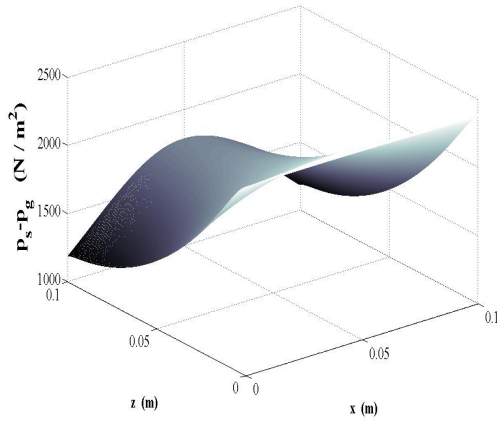
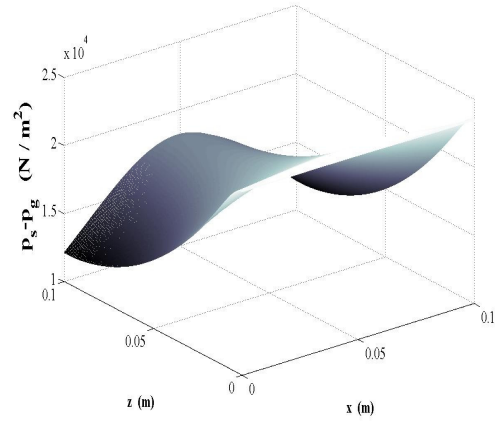
(a) $\hat{k}_1 = 0.002 \text{ m}^2/\text{s}^2$.(b) $\hat{k}_1 = 0.2 \text{ m}^2/\text{s}^2$.(c) $\hat{k}_1 = 2 \text{ m}^2/\text{s}^2$.(d) $\hat{k}_1 = 20 \text{ m}^2/\text{s}^2$.

Figure 3.6: Pressure difference $\hat{p}$, $\hat{k}_2 = 4 \times 10^{-8} \text{ m}^4/\text{s}^2$. As $\hat{k}_1$ increases, so does the magnitude of the configuration pressure $\hat{\beta}_s$. This, in turn, results in an increase of the solid phase pressure and, therefore, in the magnitude of the pressure difference $\hat{p}$.

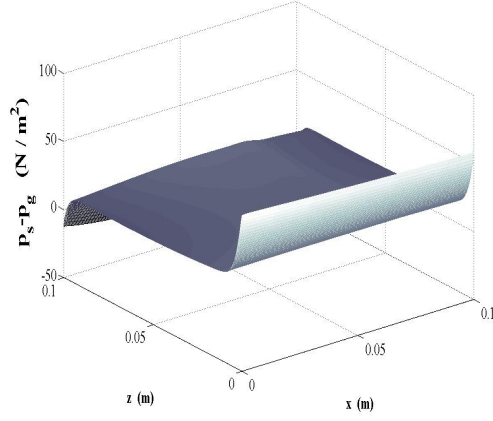
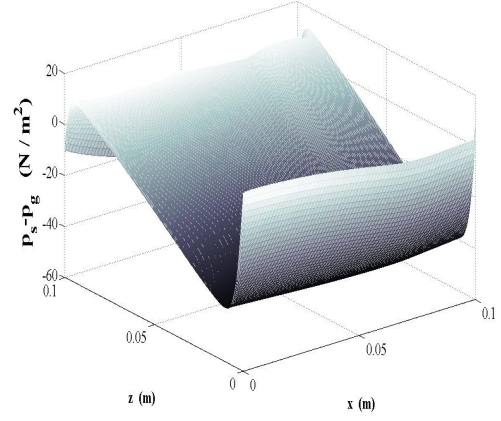
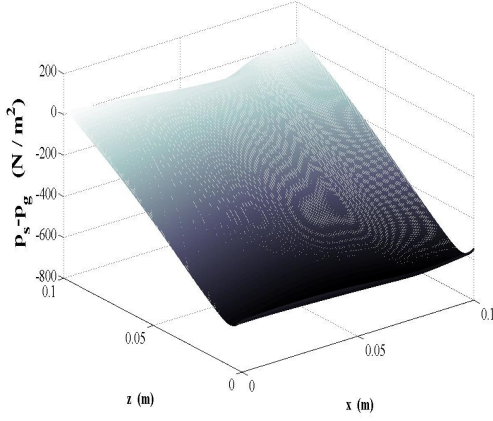
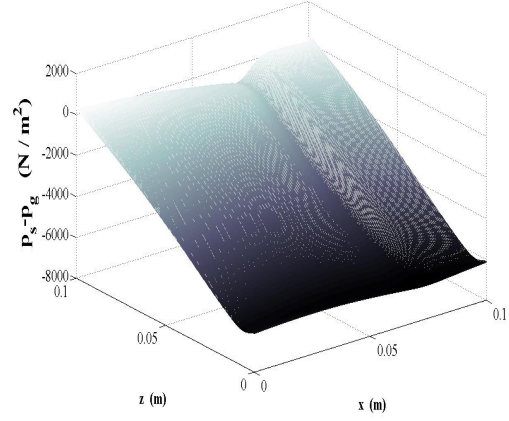
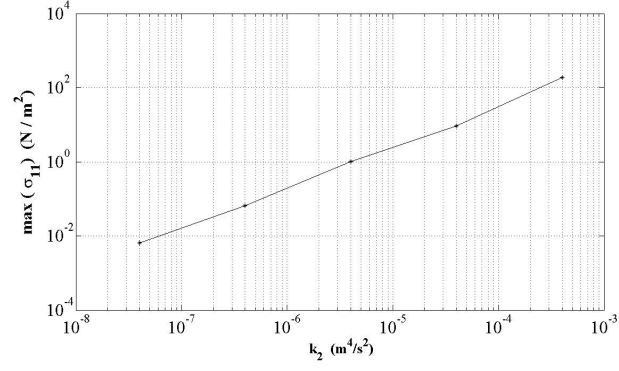
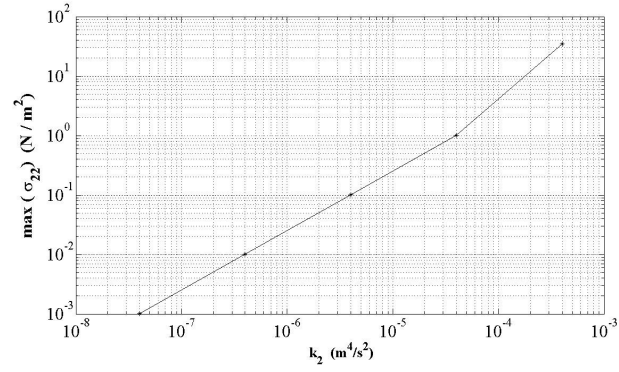
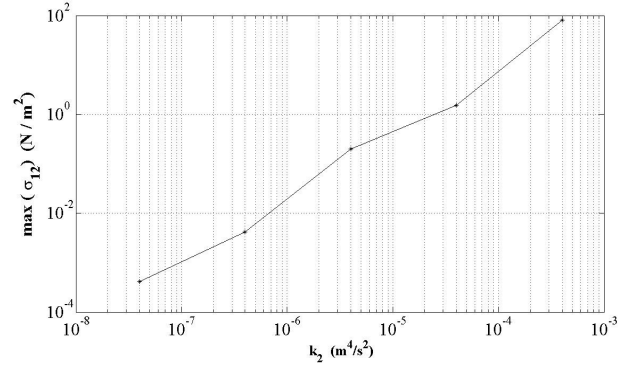
(a) $\hat{k}_2 = 4 \times 10^{-7} \text{ m}^4/\text{s}^2$.(b) $\hat{k}_2 = 4 \times 10^{-6} \text{ m}^4/\text{s}^2$.(c) $\hat{k}_2 = 4 \times 10^{-5} \text{ m}^4/\text{s}^2$.(d) $\hat{k}_2 = 4 \times 10^{-4} \text{ m}^4/\text{s}^2$.

Figure 3.7: Pressure difference $\hat{p}$, $\hat{k}_1 = 0.02 \text{ m}^2/\text{s}^2$. The magnitude of the configuration stresses increases with $\hat{k}_2$ and so does the thickness of the boundary layers in the pressure difference profile. For $\hat{k}_2$ larger than $10^{-6} \text{ m}^4/\text{s}^2$, the boundary layers disappear and the configuration stresses become more dominant than gravitational forces.



(a)



(c)

Figure 3.8: Max-plot of configuration stress (a) $\hat{\sigma}_{11}$, (b) $\hat{\sigma}_{22}$, (c) $\hat{\sigma}_{12}$. The amplitude of both normal and shear configuration stresses increases considerably with $\hat{k}_2$. However, the configuration stresses remain always at least two orders of magnitude smaller than the pressure difference $\hat{p}$.

that as $\hat{k}_1$ increases, the configuration pressure $\hat{\beta}_s$ in the compaction equation eventually becomes dominant over the diffusion term. It is also interesting to note that the monotonic decrease of $\hat{p}$ in the $\hat{z}$ direction is essentially unaffected by variations of $\hat{k}_1$. However, the presence of gradients in the $\hat{x}$ direction results in the appearance of points where the gradient becomes zero in the interior of the domain.

We also considered values of $\hat{k}_1$ smaller than $0.002 \text{ m}^2/\text{s}^2$. Our numerical predictions showed that after a certain threshold, around $\hat{k}_1 = 0.001 \text{ m}^2/\text{s}^2$, there is very little change on the solution profiles. This can be explained by the fact that as the value of $\hat{k}_1$ gets smaller, so does the configuration pressure $\hat{\beta}_s$ which eventually becomes negligible with respect to the other terms of the compaction equation.

As regards the parametric study for $\hat{k}_2$, we fix $\hat{k}_1 = 0.02 \text{ m}^2/\text{s}^2$ and let $\hat{k}_2$ take values in the range $10^{-8} - 10^{-4} \text{ m}^4/\text{s}^2$. Similarly to the parametric study for $\hat{k}_1$, we observe very small changes in the profile of the solid volume fraction. In particular, our numerical experiments predict that the changes in ϕ_s^0 with $\hat{k}_2$ are at the order of 10^{-4} .

On the other hand, as Figures 3.7(a)-3.7(d) and 3.8(a)-3.8(c) show, the pressure difference $\hat{p}$ and the configuration stresses $\hat{\sigma}_{ij}$ are considerably more sensitive to variations of $\hat{k}_2$. In particular, in Figures 3.7(a)-3.7(d) we observe that for values of $\hat{k}_2$ larger than approximately $10^{-6} \text{ m}^4/\text{s}^2$, the order of magnitude of the pressure difference $\hat{p}$ increases with $\hat{k}_2$. For values of $\hat{k}_2$ smaller than $10^{-6} \text{ m}^4/\text{s}^2$, the total variation of $\hat{p}$ remains at the order of 100 N/m^2 .

Further, we observe that the above value, $\hat{k}_2 \sim 10^{-6} \text{ m}^4/\text{s}^2$, also acts as a threshold for the behavior of the variation of $\hat{p}$ with $\hat{z}$. Indeed, for values of $\hat{k}_2$ below this threshold, $\hat{p}$ decreases monotonically with $\hat{z}$ because the gravitational forces are larger than the configuration stresses $\hat{\sigma}_{ij}$ everywhere in the domain. In contrast, for values of $\hat{k}_2$ above this threshold, the configuration stresses can balance out the effect of the gravitational forces, thereby changing the monotonicity of $\hat{p}$ along the $\hat{z}$ direction. Also, as $\hat{k}_2$ increases, so does the thickness of the boundary layers. For $\hat{k}_2$ larger than the above threshold, the boundary layers disappear in the sense that the configuration stresses $\hat{\sigma}_{ij}$ have non-negligible effect everywhere in the domain.

Also, our parametric study indicates that the shapes of the configuration stresses $\hat{\sigma}_{ij}$ are largely unaffected by changes of $\hat{k}_2$. (A similar observation was drawn in the parametric study of $\hat{k}_1$). Nonetheless, the amplitude of all three configuration stresses increase considerably with $\hat{k}_2$, as can be observed in Figures 3.8(a)-3.8(c). These figures show the variation of the maxima of $\hat{\sigma}_{ij}$ with $\hat{k}_2$. Nonetheless, these configuration stresses remain always at least two order of magnitude smaller than the pressure difference $\hat{p}$.

3.7 Conclusions

In this Chapter we have presented a numerical analysis for the equilibrium limit of the two-phase flow model of reference. At this limit, the model reduces to a coupled, overdetermined system of nonlinear elliptic PDEs that describes the hydrostatics of granular materials. However, at equilibrium, the variations of the phasial densities are expected to be small, which allows a perturbation analysis and, subsequently, decoupling of the system in hand. The perturbed system is supplemented by a compatibility condition which arises naturally and is based on the cohomologies of the gradient operator. Further, we have developed a projection-type, SOR predictor-corrector algorithm for the numerical treatment of the equations based on Ladyzhenskaya's decomposition theorem. As shown herein, the proposed algorithm is both stable and consistent hence, under some standard assumptions, convergent.

We have also conducted a series of numerical experiments by using a water- sand mixture as reference. Our numerical studies showed that the configuration stresses, which result from non-local effects related to the micro-structure of the mixture, lead to the formation of thin transition or boundary layers. Overall, our numerical experiments indicated that the equilibrium limit of the two-phase flow model of reference admits solutions that are, intuitively, physically correct. This numerical evidence however, can only serve as a preliminary test of the validity of the model in hand. The crucial validity test is to compare numerical predictions with experimental data.

Finally, we recall that throughout this Chapter we have assumed that the volume fraction is uniformly bounded away from zero. In fact, at this limit, the equations locally degenerate and the performance of the proposed numerical method deteriorates considerably. Our numerical experiments indicate that, for the particular boundary value problem that we have considered herein, if the initial volume fraction distribution is bounded away from zero then its evolution remains bounded away from zero as well. However, in general, one cannot *a priori* exclude the existence of solutions where the volume fraction becomes zero locally.

Chapter 4

Existence theory for hydrostatics of two-phase granular mixtures

4.1 Introduction

For a comprehensive study of the properties of the equilibrium limit of the two-phase flow model of reference, the numerical analysis presented in Chapter 3 should be supplemented with a well-posedness analysis. To this end, since the equilibrium limit consists of an overdetermined system of nonlinear partial differential equations (PDEs), the existence of solutions is by no means an obvious fact.

In this Chapter we present an existence and regularity theory for the equilibrium limit of the two-phase flow model of reference. The overdeterminacy of the system in hand imposes that, prior to the development of an existence theory, an integrability analysis needs to be performed. As it will be shown later, the integrability analysis in this case is straightforward. This analysis, in turn, allows us to transform the overdetermined system to a singular elliptic PDE with natural growth. Next, by applying weak convergence methods and by using suitably chosen nonlinear test-functions, we show that the transformed elliptic PDE admits weak solutions, in the sense of distributions. Subsequently, we proceed to establish an existence theory for the original overdetermined system.

It is worth noting that the well-posedness of continuum models for hydrostatics of granular mixtures has been an open problem. Therefore, the existence theory presented herein gives a positive answer to this problem.

The results of this Chapter can also be found in the article Varsakelis, C. & Papalexandris, M. V. 2012 Existence of solutions to a continuum model for hydrostatics of fluid-saturated granular materials, which has been submitted for publication and is currently under review.

4.2 Mathematical formulation

Let us consider a saturated mixture of an isotropic granular material and a simple Newtonian fluid occupying a bounded domain $\mathbb{R}^{n-1} \times \mathbb{R}^+$, $n = 2, 3$. We are interested in proving the existence of solutions to equations (3.2.31)–(3.2.33), *i.e.* the perturbed version of the equilibrium limit. Dropping the superscripts, in order to simplify notation, allows us to write equations (3.2.31)–(3.2.33) as follows,

$$p_f = -z, \quad (4.2.1)$$

$$\nabla((p_s - p_f)\phi_s) = -\nabla \cdot (\Gamma_s \nabla \phi_s \otimes \nabla \phi_s) + \phi_s(\rho_s - \rho_f) \mathbf{g}, \quad (4.2.2)$$

$$p_s - p_f = \beta_s - \nabla \cdot (\Gamma_s \nabla \phi_s). \quad (4.2.3)$$

Since p_f is explicitly given, the unknowns in the above equations are p_s and ϕ_s . We recall that p_s, p_f are the “dynamic” pressures of the solid and fluid phase, respectively; they are equivalent to the pressure that appears in the incompressible Navier-Stokes equations. Also, ρ_s and ρ_f are the phasial densities related to the phasial temperatures and the “thermodynamic” pressures via the equations of state. At equilibrium, the phasial temperatures are constant and equal to each other, and so are the thermodynamic pressures; for more details see Chapter 2. Therefore, ρ_s and ρ_f are constant and known in Ω .

Further, the configuration pressure β_s and the configuration stress coefficient Γ_s are given by the familiar expressions,

$$\beta_s = k_1 \rho_s \phi_s^2 \quad \Gamma_s = k_2 \rho_s \phi_s, \quad (4.2.4)$$

As mentioned above, p_f is a known quantity and, thus, equation (4.2.1) is redundant. Henceforth, the analysis will be focused on the reduced system (4.2.2) and (4.2.3). Next, by adopting the notation convention $\phi = \phi_s$, $p = p_s - p_f$, $\rho = \rho_s - \rho_f$, $\kappa_1 = k_1 \rho_s$ and $\kappa_2 = k_2 \rho_s$ the system (4.2.2) and (4.2.3) is rewritten as follows,

$$\nabla(p\phi) = -\nabla \cdot (\kappa_2 \phi \nabla \phi \otimes \nabla \phi) + \phi \rho \mathbf{g}, \quad (4.2.5)$$

$$p = \kappa_1 \phi^2 - \nabla \cdot (\kappa_2 \phi \nabla \phi) \quad (4.2.6)$$

with p and ϕ as unknown variables.

The above system needs to be supplemented with suitable boundary conditions. As regards the volume fraction, in this Chapter, and in order to simplify the presentation, zero Dirichlet conditions are assigned to ϕ , namely

$$\phi = 0, \quad \mathbf{x} \in \partial\Omega. \quad (4.2.7)$$

However, our analysis can be extended to more general Dirichlet conditions as well. Further, as shown in Chapter 3, appropriate Neumann boundary conditions for the pressure term p are obtained by virtue of Ladyzhenskaya's decomposition theorem. This approach is completely equivalent to the assignment of Neumann data for the pressure in the incompressible Navier-Stokes equations, (Ladyzhenskaya 1969).

We proceed with the definition of solutions for the system (4.2.5)–(4.2.6). In this respect, the pair $(\phi, p) \in H_0^1(\Omega) \times W_{\text{loc}}^{1,1}(\Omega)$ is said to be a weak solution of (4.2.5)–(4.2.6) if

$$\phi > 0, \quad \text{a.e.} \quad (4.2.8)$$

$$\int_{\Omega} \nabla(p\phi) \cdot \mathbf{h} \, d\mathbf{x} = \int_{\Omega} \kappa_2 \phi \nabla \phi \otimes \nabla \phi : \nabla \mathbf{h} \, d\mathbf{x} + \int_{\Omega} \phi \rho \mathbf{g} \cdot \mathbf{h} \, d\mathbf{x}, \quad (4.2.9)$$

$$\int_{\Omega} p \zeta \, d\mathbf{x} = \int_{\Omega} \kappa_1 \phi^2 \zeta \, d\mathbf{x} + \int_{\Omega} \kappa_2 \phi \nabla \phi \cdot \nabla \zeta \, d\mathbf{x}, \quad (4.2.10)$$

for all test-functions $\mathbf{h} \in (H_0^1(\Omega))^n$ and $\zeta \in H_0^1(\Omega)$, where $(H_0^1(\Omega))^n$ stands for the n -copies of $H_0^1(\Omega)$.

4.2.1 Integrability analysis

In spatial dimensions $n > 1$, the system (4.2.5)–(4.2.6) becomes overdetermined. Therefore, prior to the development of an existence theory, an integrability analysis needs to be performed. In other words, we have to investigate whether the equations in hand are compatible with each other and whether the system in hand needs to be supplemented with additional constraints (compatibility conditions) to ensure its solvability.

First, it is interesting to recall that an integrability analysis has been presented in Chapter 3, which is based on the Helmholtz decomposition and Ladyzhenskaya's decomposition theorem. This approach, although it has significant advantages from the numerical point of view, it is not expedient from the theoretical point of view. Nonetheless, and perhaps surprisingly, it turns out that an alternative integrability analysis of (4.2.5)–(4.2.6) can be carried in a relatively straightforward manner. More precisely, we prove the following integrability theorem.

Theorem 4.2.1. *The system (4.2.5)–(4.2.6) is Frobenius integrable.*

Proof. First, we observe that $\nabla \cdot (\kappa_2 \phi \nabla \phi \otimes \nabla \phi)$ can be decomposed as follows

$$\nabla \cdot (\kappa_2 \phi \nabla \phi \otimes \nabla \phi) = \nabla \cdot (\kappa_2 \phi \nabla \phi) \nabla \phi + \kappa_2 \phi \nabla(\nabla \phi) \nabla \phi. \quad (4.2.11)$$

Next, upon introduction of equations (4.2.11) and (4.2.6) to (4.2.5), we arrive at

$$\nabla(p\phi) = (p - \kappa_1 \phi^2) \nabla \phi - \kappa_2 \phi \nabla(\nabla \phi) \nabla \phi + \phi \rho \mathbf{g}.$$

This equation is further simplified to

$$\nabla p = -\kappa_1 \phi \nabla \phi - \kappa_2 \nabla(\nabla \phi) \nabla \phi + \rho \mathbf{g}. \quad (4.2.12)$$

Equation (4.2.12) can be cast in the form of a gradient as follows

$$\nabla \left(p + \frac{\kappa_1}{2} \phi^2 + \frac{\kappa_2}{2} |\nabla \phi|^2 - \rho \mathbf{g} z \right) = 0. \quad (4.2.13)$$

Evidently, equation (4.2.13) is integrable which, in turn, implies that the system (4.2.5)–(4.2.6) is integrable as well. $\square$

It can be shown that the above equation holds for general expressions for β_s and Γ_s and not only those given by (4.2.4). It is also worth mentioning that in the absence of gravity, in which case the gaseous pressure is constant, the above relation reduces to $\nabla(p_s + \frac{\kappa_1}{2} \phi^2 + \frac{\kappa_2}{2} |\nabla \phi|^2) = 0$. The quantity in the left-hand side of this relation is identified as the gradient of the Gibbs free energy of the granular material multiplied by the material's density, under constant temperature; see Chapter 2. In other words, the integrability of the system in hand has the physical meaning of the minimization of the Gibbs free energy of the granular material under constant temperature.

Further, it should be also remarked that by carrying the above integrability analysis we implicitly assume more regularity for the unknown variables. Consequently, the possibility of throwing away solutions of lower regularity cannot be excluded.

4.3 Existence results

First, let us fix the notation $f = \rho z + C_{\text{in}}$, where C_{in} is a constant that comes from the integration of equation (4.2.13). By integrating equation (4.2.13) and combining it with equation (4.2.6), we readily arrive at the following PDE for the volume fraction

$$-\nabla \cdot (\kappa_2 \phi \nabla \phi) = -\frac{3\kappa_1}{2} \phi^2 - \frac{\kappa_2}{2} (\nabla \phi)^2 + f. \quad (4.3.1)$$

The above equation belongs to the class of nonlinear second-order equations with natural growth. However, it is not generally coercive and, therefore, the operator $-\nabla \cdot (\kappa_2 \phi \nabla \phi)$ does not fulfill the Leray-Lions conditions, (Leray & Lions 1965). This is a significant drawback because it implies that the standard weak convergence methods cannot be applied directly; see, for example, Boccardo *et al.* (1982) and Boccardo *et al.* (1992).

In principle, this difficulty can be by-passed with two approaches. The first approach is to consider a sequence of coercive approximations for (4.3.1) and, subsequently, derive uniform *a priori* estimates. This procedure has been employed, for example, in Droniou (2002) and in Zou & Li (2010) for linear and nonlinear elliptic problems, respectively.

However, this approach requires ϕ to be uniformly bounded away from zero, which is difficult to establish beforehand in our case.

The second approach is based on transforming equation (4.3.1) to a singular non-linear, elliptic equation with natural growth. This is easily performed by applying the transformation $\omega = \sqrt{\phi}$ and by normalizing the higher-order term. In turn, this leads to the following form of our boundary-value problem,

$$-\nabla \cdot (\nabla \omega) = -a\omega - \frac{(\nabla \omega)^2}{2\omega} + \tilde{f}, \quad \mathbf{x} \in \partial\Omega, \quad (4.3.2)$$

$$\omega = 0, \quad \mathbf{x} \in \partial\Omega. \quad (4.3.3)$$

In the above equation, $a = \frac{3\kappa_1}{\kappa_2} > 0$, whereas

$$\tilde{f} = \frac{2}{\kappa_2} f = \frac{2}{\kappa_2} (C_{\text{in}} - \rho z). \quad (4.3.4)$$

Evidently, the difficulty has moved to the quadratic gradient term $\frac{(\nabla \omega)^2}{2\omega}$ which is no longer a Caratheodory function in its arguments because of the possible singularity in the denominator; see Korkut *et al.* (1999) for general nonlinear elliptic equations.

Equations of the type of (4.3.2), albeit without the linear term in the right-hand side, have been studied in the past by Arcoya *et al.* (2009) and Boccardo (2008) who proved existence of solutions in $H_{0,\text{loc}}^1(\Omega)$ and $H_0^1(\Omega)$, respectively. The authors of these papers replace the singular term by a well-controlled approximation of Caratheodory functions and, via the use of suitably chosen test-functions, prove that the approximate solutions converge to the solution of the original equation. In this Chapter we adopt the same strategy. However, the arguments that we employ are different because of the presence of the linear term in the right-hand side of (4.3.2).

Finally, we mention that, in what follows, C will denote a generic constant, whose exact value does not affect the derivation of the required estimates. This is to distinguish the various constants that will appear from the integration constant C_{in} .

We now proceed to the definition of weak solutions for the transformed problem (4.3.2)–(4.3.3).

Definition 4.3.1. A function $\omega \in H_0^1(\Omega) \cap L^\infty(\Omega)$ is a weak solution, in the sense of distributions, of (4.3.2)–(4.3.3) if

1. $\omega > 0$, in Ω ,
2. $\frac{(\nabla \omega)^2}{2\omega} \in L^1(\Omega)$,
3. The following integral identity is satisfied

$$\int_{\Omega} \nabla \omega \nabla h \, d\mathbf{x} = - \int_{\Omega} a\omega h \, d\mathbf{x} - \int_{\Omega} \frac{(\nabla \omega)^2}{2\omega} h \, d\mathbf{x} + \int_{\Omega} \tilde{f} h \, d\mathbf{x}, \quad (4.3.5)$$

$$\forall h \in H_0^1(\Omega) \cap L^\infty(\Omega).$$

We note that requirement (2) of the above definition, namely, $\frac{(\nabla\omega)^2}{2\omega} \in L^1(\Omega)$, allows for ω to be chosen as a test-function in (4.3.5).

Next, since we are interested in non-negative solutions everywhere in Ω , we assume that the source term $\tilde{f}$ is non-negative. Since $z \in \mathbb{R}^+$, the non-negativity of $\tilde{f}$ is equivalent to setting the integration constant C_{in} such as $C_{\text{in}} \geq \|\rho z\|_{L^\infty(\Omega)}$.

We now proceed to formulate the main theorem of this section.

Theorem 4.3.1. *The boundary value problem (4.3.2)–(4.3.3) has at least one weak solution in the sense of Definition 4.3.1.*

In order to simplify the presentation, the proof is divided into a number of Lemmas. More specifically, the proof consists of the following steps.

1. Construction of a sequence of approximate problems. The limit of this sequence is the problem in hand, (4.3.2)–(4.3.3).
2. The approximate problems are chosen so that the singular term of (4.3.2) is replaced by a regularized one which is easier to control. Further, the approximate problems should be such that a unique solvability theory exists for them. In other words, each approximate problem should admit a unique solution.
3. Derivation of *a priori* regularity estimates for the sequence of solutions of the approximate problems.
4. Passage to the limit of the sequence of approximate problems and deduction of existence of a weak solution for the problem in hand (4.3.2)–(4.3.3).

First, we construct a sequence of approximate problems for (4.3.2). They are obtained via a regularization of the singular term of (4.3.2), which can be found, among others, in Leray & Lions (1965).

First, for all $n \in \mathbb{N}$ we define the positive truncation of a function τ at level n as follows

$$g_n(\tau) = \begin{cases} \tau & \text{if } 0 < \tau < n, \\ n & \text{if } \tau \geq n, \\ 0 & \text{else.} \end{cases}$$

Further, for all $n \in \mathbb{N}$, and under the above notation, we consider the following sequence of regularized problems

$$-\nabla \cdot (\nabla \omega_n) + a\omega_n + g_n\left(\frac{1}{\omega_n}\right) F_n = \tilde{f}, \quad \text{in } \Omega, \quad (4.3.6)$$

$$\omega_n = 0, \quad \mathbf{x} \in \partial\Omega, \quad (4.3.7)$$

where F_n is defined as follows

$$F_n = \frac{\nabla \omega_n \cdot \nabla \omega_n}{2 + \frac{2}{n}(\nabla \omega_n)^2} \geq 0. \quad (4.3.8)$$

We remark that it is not necessary to extend the above regularization to $\tilde{f}$ because in our case $\tilde{f}$ is smooth and bounded by definition. However, we remark that if $\tilde{f}$ was an L^p -function, with $p < \infty$ or more generally a measure, the regularization scheme would need to be extended to $\tilde{f}$ as well.

Next, we observe that since the right-hand side of (4.3.6) is by construction bounded, the classical Leray-Lions result Leray & Lions (1965) guarantees the unique solvability of (4.3.6) for all $n \in \mathbb{N}$, in the weak sense. Also, for the sequence of solutions $\{\omega_n\}$, the same result yields that $\omega_n \in H_0^1(\Omega) \cap L^\infty(\Omega)$. In particular, we establish the following.

Lemma 4.3.2. *The sequence of solutions $\{\omega_n\}$ is uniformly bounded in $H_0^1(\Omega)$ and $L^\infty(\Omega)$.*

Proof. For the H_0^1 boundedness, we choose ω_n as a test-function in (4.3.6). This results in

$$\int_{\Omega} (\nabla \omega_n)^2 d\mathbf{x} = - \int_{\Omega} a \omega_n^2 d\mathbf{x} - \int_{\Omega} g_n \left(\frac{1}{\omega_n} \right) F_n \omega_n d\mathbf{x} + \int_{\Omega} \tilde{f} \omega_n d\mathbf{x}.$$

We observe that the first two integrals of the right-hand side of the above equation are always non-negative, by construction. This fact and the Cauchy-Schwarz inequality give

$$\int_{\Omega} (\nabla \omega_n)^2 d\mathbf{x} \leq \|\tilde{f}\|_{L^2(\Omega)} \|\omega_n\|_{L^2(\Omega)}.$$

The proof is completed by applying the Poincaré inequality to $\|\omega_n\|_{L^2(\Omega)}$.

For the L^∞ boundedness, we choose $(\omega_n - \Lambda)_+$, as a test-function, where Λ is the scaled $L^\infty(\Omega)$ norm of $\tilde{f}$: $\Lambda = \|\tilde{f}\|_{L^\infty(\Omega)}/a$. (This choice is motivated by the presence of the coefficient a as a multiplier of ω_n). Then, we have

$$\begin{aligned} \int_{\Omega} \nabla \omega_n \nabla (\omega_n - \Lambda)_+ d\mathbf{x} &= - \int_{\Omega} a \omega_n (\omega_n - \Lambda)_+ d\mathbf{x} \\ &\quad - \int_{\Omega} g_n \left(\frac{1}{\omega_n} \right) F_n (\omega_n - \Lambda)_+ d\mathbf{x} \\ &\quad + \int_{\Omega} \tilde{f} (\omega_n - \Lambda)_+ d\mathbf{x}. \end{aligned}$$

The left-hand side of the above equation is always non-negative, whereas the second term in the right-hand side is always non-positive. This yields the following inequality,

$$\int_{\Omega} a\omega_n(\omega_n - \Lambda)_+ d\mathbf{x} \leq \int_{\Omega} \tilde{f}(\omega_n - \Lambda)_+ d\mathbf{x}.$$

By adding the term $-a\Lambda(\omega_n - \Lambda)_+$ in both sides of the above inequality, we arrive at

$$\int_{\Omega} a(\omega_n - \Lambda)_+(\omega_n - \Lambda) d\mathbf{x} \leq \int_{\Omega} (\tilde{f} - a\Lambda)(\omega_n - \Lambda)_+ d\mathbf{x}.$$

The right-hand side of the above relation is always non-positive by virtue of the definition of Λ . Therefore, we deduce that

$$\omega_n \leq \Lambda.$$

In turn, this implies that $|\{\omega_n \geq \Lambda\}| = 0$, with $||$ being the Lebesgue measure of the set, which completes the proof. $\square$

Subsequently, we prove that the sequence of solutions $\{\omega_n\}$ consists of positive terms.

Lemma 4.3.3. *For all $n \in \mathbb{N}$, $\omega_n > 0$.*

Proof. First, we show that ω_n is non-negative. To this end, we take the negative part of ω_n , $\omega_n^- = \min\{\omega_n, 0\}$, as a test-function in (4.3.6). This gives

$$\int_{\Omega} (\nabla \omega_n^-)^2 d\mathbf{x} = - \int_{\Omega} a(\omega_n^-)^2 d\mathbf{x} - \int_{\Omega} g_n \left(\frac{1}{\omega_n} \right) F_n \omega_n^- d\mathbf{x} + \int_{\Omega} \tilde{f} \omega_n^- d\mathbf{x}.$$

By construction, the second term of the right-hand side of the above equation is zero, which yields

$$\int_{\Omega} (\nabla \omega_n^-)^2 d\mathbf{x} + \int_{\Omega} a(\omega_n^-)^2 d\mathbf{x} \leq \int_{\Omega} \tilde{f} \omega_n^- d\mathbf{x} \leq 0,$$

because $\tilde{f} \geq 0$ and $a > 0$. Therefore, $\omega_n^- \equiv 0$, i.e. $\omega_n \geq 0$. To show the strict positivity of ω_n we employ the following standard argument. There exists a $C = C(n)$ such as

$$a\omega_n + g_n \left(\frac{1}{\omega_n} \right) F_n \leq \omega_n n C(n).$$

Then, it follows from (4.3.6) that ω_n satisfies, in the sense of distributions, the inequality

$$-\nabla \cdot (\nabla \omega_n) + C(n) n \omega_n \geq \tilde{f}.$$

Further, since $\tilde{f} > 0$, application of the strong maximum principle yields that $\omega_n > 0$ which completes the proof. $\square$

Summing up our results thus far, the sequence of solutions $\{\omega_n\}$ consists of positive terms and is bounded in $H_0^1(\Omega) \cap L^\infty(\Omega)$. Passing if necessary to a subsequence, still denoted by $\{\omega_n\}$, we conclude that there exists a function $\omega \geq 0$ such as

$$\omega_n \rightharpoonup \omega, \quad \text{in } H_0^1(\Omega), \quad (4.3.9)$$

$$\omega_n \xrightarrow{*} \omega, \quad \text{in } L^\infty(\Omega), \quad (4.3.10)$$

and by Rellich's theorem we additionally get that

$$\omega_n \rightarrow \omega, \quad \text{in } L^2(\Omega), \quad (4.3.11)$$

$$\omega_n \rightarrow \omega, \quad \text{a.e. in } \Omega. \quad (4.3.12)$$

In view of Lemma 4.3.3 and (4.3.12), we can prove that ω is actually positive in Ω , *i.e.* that $\{\omega_n\}$ is uniformly bounded away from zero. This is established in the next Lemma.

Lemma 4.3.4. *The limit-function ω is strictly positive in Ω .*

Proof. Let $\eta \in C_c^\infty(\Omega)$ be a non-negative function and fix $1/2 \leq \theta < 1$. We choose η/ω_n^θ as a test-function in (4.3.6). Indeed, this is an admissible test-function by virtue of Lemma 4.3.3 which guarantees that η/ω_n^θ is bounded for every n . Equation (4.3.6) yields, upon rearrangement,

$$\begin{aligned} \int_{\Omega} \frac{\nabla \omega_n \nabla \eta}{\omega_n^\theta} d\mathbf{x} + \int_{\Omega} a \eta \omega_n^{1-\theta} d\mathbf{x} - \int_{\Omega} \frac{\tilde{f} \eta}{\omega_n^\theta} d\mathbf{x} \\ = \theta \int_{\Omega} \frac{(\nabla \omega_n)^2 \eta}{\omega_n^{\theta+1}} d\mathbf{x} - \int_{\Omega} g_n \left(\frac{1}{\omega_n} \right) F_n \frac{\eta}{\omega_n^\theta} d\mathbf{x}. \end{aligned} \quad (4.3.13)$$

We observe that, by construction, the right-hand side of (4.3.13) is non-negative. Next, we fix $k > 0$ such as $|\{\omega_n = k\}| = 0$. We note that this assumption holds for almost all $k \in \mathbb{R}^+$, since $\omega_n \in L^2$ and, therefore, in L^1 also by virtue of the L^p -embedding theorem. For such a k , and upon factorization, we arrive at

$$\int_{\Omega} \frac{1}{(1-\theta)} \nabla \omega_n^{1-\theta} \nabla \eta d\mathbf{x} + \int_{\Omega} a \eta \omega_n^{1-\theta} d\mathbf{x} \geq \int_{\Omega} \chi(\omega_n \leq k) \frac{\tilde{f} \eta}{k^\theta} d\mathbf{x}, \quad (4.3.14)$$

where $\chi()$ is the characteristic function of a set. The comparison principle for (4.3.14) yields that $\omega_n^{1-\theta} \geq \varphi_n$, where $\varphi_n \in H_0^1(\Omega)$ is the distributional solution of

$$\int_{\Omega} \frac{1}{(1-\theta)} \nabla \varphi_n \nabla \eta d\mathbf{x} + \int_{\Omega} a \eta \varphi_n d\mathbf{x} = \int_{\Omega} \chi(\omega_n \leq k) \frac{\tilde{f} \eta}{k^\theta} d\mathbf{x}.$$

Because of (4.3.12) we deduce that $\chi(\omega_n \leq k) \rightarrow \chi(\omega \leq k)$ a.e. in Ω . This, in turn, implies that $\varphi_n \rightarrow \varphi$ in $H_0^1(\Omega)$, where φ is the solution of

$$\int_{\Omega} \frac{1}{(1-\theta)} \nabla \varphi \nabla \eta d\mathbf{x} + \int_{\Omega} a\eta \varphi d\mathbf{x} = \int_{\Omega} \chi(\omega \leq k) \frac{\tilde{f}\eta}{L^{\theta}} d\mathbf{x}.$$

Finally, by virtue of the strong maximum principle we infer that $\varphi > 0$. Therefore, we have that

$$0 < \varphi_n \leq \omega_n^{1-\theta}, \quad (4.3.15)$$

and by sending $n \rightarrow \infty$ we conclude that $\omega > 0$, since $\omega_n \rightarrow \omega$ a.e. in Ω . $\square$

We add that, as a consequence of Lemma 4.3.4, there exists a strictly positive constant c_l such as $c_l \leq \omega_n$ uniformly in n and $c_l \leq \omega$. Next, we observe that, in order to take limits in (4.3.6), we have to show that the sequence $\{g_n(\frac{1}{\omega_n})F_n\}$ and the nonlinear term $\frac{(\nabla\omega)^2}{2\omega}$ are bounded in $L^1(\Omega)$ and that

$$\lim_{n \rightarrow \infty} \int_{\Omega} g_n \left(\frac{1}{\omega_n} \right) F_n d\mathbf{x} = \int_{\Omega} \frac{(\nabla\omega)^2}{2\omega} d\mathbf{x}. \quad (4.3.16)$$

In the next Lemma, we show the required L^1 boundedness.

Lemma 4.3.5. *Both the sequence of the nonlinear approximations $g_n \left(\frac{1}{\omega_n} \right) F_n$ and the function $\frac{(\nabla\omega)^2}{2\omega}$ are bounded in $L^1(\Omega)$. Also, the following inequalities are true:*

$$\int_{\Omega} g_n \left(\frac{1}{\omega_n} \right) F_n d\mathbf{x} \leq \int_{\Omega} \tilde{f} d\mathbf{x}, \quad (4.3.17)$$

$$\int_{\Omega} \frac{(\nabla\omega)^2}{2\omega} d\mathbf{x} \leq \int_{\Omega} \tilde{f} d\mathbf{x}. \quad (4.3.18)$$

Proof. Since $\tilde{f}$ is smooth, we can use exactly the same arguments as in the proof of Theorem 1.1 of Arcoya *et al.* (2009). This amounts to:

- i) take $\frac{1}{\epsilon} g_{\epsilon} \left(\frac{1}{\omega_n} \right)$ as test-function in (4.3.6),
- ii) take the limit $\epsilon \rightarrow 0$, and
- iii) apply Fatou's Lemma.

The proof follows. $\square$

Next, in order to demonstrate the equi-integrability of the sequence $\{g_n(\frac{1}{\omega_n})F_n\}$, we first show the strong convergence of $\{\omega_n\}$ in $H_0^1(\Omega)$.

Lemma 4.3.6. *The sequence of approximate solutions $\{\omega_n\}$ converges strongly to ω in $H_0^1(\Omega)$.*

Proof. First, we consider a constant $B > 0$ whose precise value is to be fixed later. We observe that for all $n \in \mathbb{N}$ the following identity is true.

$$\begin{aligned} & \int_{\Omega} B \cosh(B(\omega_n - \omega)) |\nabla(\omega_n - \omega)|^2 \, d\mathbf{x} \\ &= - \int_{\Omega} B \cosh(B(\omega_n - \omega)) \nabla \omega \nabla(\omega_n - \omega) \, d\mathbf{x} \\ & \quad + \int_{\Omega} B \cosh(B(\omega_n - \omega)) \nabla \omega_n \nabla(\omega_n - \omega) \, d\mathbf{x}. \end{aligned} \quad (4.3.19)$$

We will treat each term of the right-hand side of (4.3.19) separately. The first term goes to zero as $n \rightarrow \infty$ by virtue of (4.3.9)–(4.3.12). For the second term, we take $\sinh(B(\omega_n - \omega))$ as a test-function in (4.3.6) which gives

$$\begin{aligned} & \int_{\Omega} B \nabla \omega_n \cosh(B(\omega_n - \omega)) \nabla(\omega_n - \omega) \, d\mathbf{x} \\ &= - \int_{\Omega} a \omega_n \sinh(B(\omega_n - \omega)) \, d\mathbf{x} \\ & \quad - \int_{\Omega} g_n \left(\frac{1}{\omega_n} \right) F_n \sinh(B(\omega_n - \omega)) \, d\mathbf{x} \\ & \quad + \int_{\Omega} \tilde{f} \sinh(B(\omega_n - \omega)) \, d\mathbf{x}. \end{aligned} \quad (4.3.20)$$

By introducing (4.3.20) to (4.3.19) we get

$$\begin{aligned} & \int_{\Omega} B \cosh(B(\omega_n - \omega)) |\nabla(\omega_n - \omega)|^2 \, d\mathbf{x} \\ &= o(1) - \int_{\Omega} a \omega_n \sinh(B(\omega_n - \omega)) \, d\mathbf{x} \\ & \quad - \int_{\Omega} g_n \left(\frac{1}{\omega_n} \right) F_n \sinh(B(\omega_n - \omega)) \, d\mathbf{x} \\ & \quad + \int_{\Omega} \tilde{f} \sinh(\omega_n - \omega) \, d\mathbf{x}. \end{aligned} \quad (4.3.21)$$

Next, we observe that

$$\begin{aligned} - \int_{\Omega} g_n \left(\frac{1}{\omega_n} \right) F_n \sinh(\omega_n - \omega) d\mathbf{x} &\leq \int_{\Omega} \frac{1}{\omega_n} \frac{(\nabla \omega_n)^2}{2} |\sinh(\omega_n - \omega)| d\mathbf{x} \\ &\leq \int_{\Omega} \frac{(\nabla \omega_n)^2}{2c_l} |\sinh(\omega_n - \omega)| d\mathbf{x}. \end{aligned} \quad (4.3.22)$$

Combining (4.3.22) and (4.3.21) we get

$$\begin{aligned} \int_{\Omega} B \cosh(B(\omega_n - \omega)) |\nabla(\omega_n - \omega)|^2 d\mathbf{x} \\ = o(1) - \int_{\Omega} a \omega_n \sinh(\omega_n - \omega) d\mathbf{x} \\ + \int_{\Omega} \frac{(\nabla \omega_n)^2}{2c_l} |\sinh(B(\omega_n - \omega))| d\mathbf{x} \\ + \int_{\Omega} \tilde{f} \sinh(B(\omega_n - \omega)) d\mathbf{x}. \end{aligned} \quad (4.3.23)$$

We observe that, in view of (4.3.11) and (4.3.12), the second and fourth terms of the right-hand side of (4.3.23) go to zero as n goes to infinity. Next, by expanding the third term and by using the inequalities $|\sinh x| \leq \cosh x$ and $1 \geq \cosh x$, we arrive at

$$\left(B - \frac{2}{c_l} \right) \int_{\Omega} |\nabla(\omega_n - \omega)|^2 d\mathbf{x} = o(1). \quad (4.3.24)$$

The proof is concluded by setting $B > 2/c_l$. □

We now proceed to prove the equi-integrability of the sequence $\{g_n \left(\frac{1}{\omega_n} \right) F_n\}$.

Lemma 4.3.7. *The sequence $\{g_n \left(\frac{1}{\omega_n} \right) F_n\}$ is equi-integrable.*

Proof. Let $E \subset \Omega$. Then, for any $k > 0$,

$$\begin{aligned} \int_E \left| g_n \left(\frac{1}{\omega_n} \right) F_n \right| d\mathbf{x} &\leq \int_{E \cap \omega_n \geq k} \left| g_n \left(\frac{1}{\omega_n} \right) F_n \right| d\mathbf{x} \\ &\quad + \int_{E \cap \omega_n \leq k} \left| g_n \left(\frac{1}{\omega_n} \right) F_n \right| d\mathbf{x}. \end{aligned} \quad (4.3.25)$$

We will treat each term of the right-hand side of (4.3.25) separately. For the first term,

we take $(e^{k-\omega_n} - 1)_-$ as a test-function in (4.3.6), which yields

$$\begin{aligned} \int_{\Omega} \nabla \omega_n \nabla (e^{k-\omega_n} - 1)_- d\mathbf{x} &= -a \int_{\Omega} \omega_n (e^{k-\omega_n} - 1)_- d\mathbf{x} \\ &\quad - \int_{\Omega} g_n \left(\frac{1}{\omega_n} \right) F_n (e^{k-\omega_n} - 1)_- d\mathbf{x} \\ &\quad + \int_{\Omega} \tilde{f} (e^{k-\omega_n} - 1)_- d\mathbf{x}, \end{aligned}$$

and upon rearranging and simplifying terms we arrive at

$$\begin{aligned} \int_{\omega \geq k} g_n \left(\frac{1}{\omega_n} \right) F_n d\mathbf{x} &\leq \int_{\omega \geq k} (\nabla \omega_n)^2 d\mathbf{x} + a \int_{\omega \geq k} \omega_n e^{k-\omega_n} d\mathbf{x} \\ &\quad + \int_{\omega \geq k} g_n \left(\frac{1}{\omega_n} \right) F_n e^{k-\omega_n} d\mathbf{x} + \int_{\omega \geq k} \tilde{f} d\mathbf{x}. \end{aligned}$$

Next, by employing Lemma 4.3.5 and the fact that $\{\omega_n\}$ is bounded by Λ , we obtain

$$\begin{aligned} \int_{\omega \geq k} g_n \left(\frac{1}{\omega_n} \right) F_n d\mathbf{x} &\leq \int_{\omega \geq k} (\nabla \omega_n)^2 d\mathbf{x} + a \int_{\omega \geq k} \omega_n e^{k+\Lambda} d\mathbf{x} \\ &\quad + \int_{\omega \geq k} \tilde{f} (e^{k+\Lambda} + 1) d\mathbf{x} \end{aligned} \quad (4.3.26)$$

Next, by taking $(\omega_n - k)_+$ as a test-function in (4.3.6) and by dropping the negative terms, we deduce that

$$\int_{\omega \geq k} (\nabla \omega_n)^2 d\mathbf{x} \leq \int_{\omega \geq k} \tilde{f} \omega_n d\mathbf{x}. \quad (4.3.27)$$

Upon introduction of (4.3.27) to (4.3.26), we arrive at

$$\int_{\omega \geq k} g_n \left(\frac{1}{\omega_n} \right) F_n d\mathbf{x} \leq a \int_{\omega \geq k} \omega_n e^{k+\Lambda} d\mathbf{x} + \int_{\omega \geq k} \tilde{f} (e^{k+\Lambda} + 1 + \omega_n) d\mathbf{x}. \quad (4.3.28)$$

Since $\{\omega_n\}$ is bounded in L^∞ we can let $k \rightarrow \infty$ and conclude that the left-hand side of (4.3.26) goes to zero uniformly with respect to n .

For the second term of the right-hand side of (4.3.25), we proceed as follows. Let $\epsilon > 0$ and choose k sufficiently large so that

$$\int_{\omega \geq k} g_n \left(\frac{1}{\omega_n} \right) F_n d\mathbf{x} \leq \frac{\epsilon}{2}.$$

It follows that

$$\begin{aligned} \int_{E \cap \omega_n \leq k} \left| g_n \left(\frac{1}{\omega_n} \right) F_n \right| d\mathbf{x} &\leq \int_{E \cap \omega_n \leq k} \left| g_n \left(\frac{1}{\omega_n} \right) \frac{(\nabla \omega_n)^2}{2} \right| d\mathbf{x} \\ &\leq \frac{1}{c_l} \int_{E \cap \omega_n \leq k} \left| \frac{(\nabla \omega_n)^2}{2} \right| d\mathbf{x}, \end{aligned} \quad (4.3.29)$$

where we have used the fact that $0 < c_l \leq \omega_n$ uniformly with respect to n . Next, by applying Lemma 4.3.6, we can choose E to be sufficiently small so that

$$\frac{1}{c_l} \int_{E \cap \omega_n \geq k} \left| \frac{1}{2} (\nabla \omega_n)^2 \right| d\mathbf{x} \leq \epsilon,$$

for all $n \in \mathbb{N}$ and, therefore, the proof is concluded. $\square$

It remains to show that we can pass to the limit in the nonlinear terms. This is established in the following Lemma.

Lemma 4.3.8.

$$\lim_{n \rightarrow \infty} \int_{\Omega} g_n \left(\frac{1}{\omega_n} \right) F_n \zeta d\mathbf{x} = \int_{\Omega} \left(\frac{(\nabla \omega)^2}{2\omega} \right) \zeta d\mathbf{x},$$

for all test-functions $\zeta \in H_0^1(\Omega) \cap L^\infty(\Omega)$.

Proof. By Lemma 4.3.7, the sequence $\{g_n \left(\frac{1}{\omega_n} \right) F_n\}$ is equi-integrable. Further, since $\omega_n \rightarrow \omega$ in $H_0^1(\Omega)$, then $\nabla \omega_n \rightarrow \nabla \omega$ almost everywhere. This fact, combined with relation (4.3.12), implies that $\{g_n \left(\frac{1}{\omega_n} \right) F_n\}$ converges almost everywhere to $\frac{1}{\omega} \frac{(\nabla \omega)^2}{2}$. Moreover, by virtue of Lemma 4.3.5, both the sequence $\{g_n \left(\frac{1}{\omega_n} \right) F_n\}$ and the function $\frac{1}{\omega} \frac{(\nabla \omega)^2}{2}$ are bounded in $L^1(\Omega)$. Thus, by employing Vitali's convergence theorem the proof is concluded. $\square$

We now have all the ingredients to prove Theorem 4.3.1.

Proof. (of Theorem 4.3.1)

By virtue of (4.3.9)–(4.3.12) and by employing Lemmas 4.3.8 and 4.3.5, we take limits in (4.3.6) and deduce that the limit-function $\omega \in H_0^1(\Omega) \cap L^\infty(\Omega)$ is a weak solution in the sense of Definition (4.3.1). Therefore, the proof is completed. $\square$

4.4 Existence results for the original system (4.2.9)–(4.2.10)

We now return to the study of the original system (4.2.9)–(4.2.10). In this respect, we first observe that since ω is a weak solution of equation (4.3.2), the function $\sqrt{\omega}$ is a weak solution of the original equation (4.3.1). It remains to establish the existence of a function $p \in W_{\text{loc}}^{1,1}(\Omega)$ that satisfies (4.2.9)–(4.2.10). This is demonstrated in the next two Lemmas.

Lemma 4.4.1. *Let p be the function satisfying (4.2.10). Then, $p \in L^1_{\text{loc}}(\Omega)$.*

Proof. Let $U \subset\subset \Omega$ and assume that U is open. Also, let W such as $U \subset\subset W \subset\subset \Omega$. We define a cut-off function η such that

$$\eta = \begin{cases} 1, & \forall \mathbf{x} \in U, \\ 0, & \forall \mathbf{x} \in \Omega \setminus W, \\ 0 \leq \eta \leq 1, & \forall \mathbf{x} \in \Omega, \end{cases}$$

Further, we assume that $\|\nabla \eta\|_{L^\infty(\Omega)} < \infty$. Next, we take η as a test-function in (4.2.10). By virtue of the smoothness of η , the application of the Cauchy-Schwarz inequality to the right-hand side of (4.2.10) yields,

$$\int_{\Omega} p \eta \, d\mathbf{x} \leq \|\kappa_1 \phi^2\|_{L^2(\Omega)} \|\eta\|_{L^2(\Omega)} + \|\nabla \eta\|_{L^\infty(\Omega)} \int_{\Omega} |\kappa_2 \phi \nabla \phi| \, d\mathbf{x}. \quad (4.4.1)$$

Also, application of the Cauchy-Schwarz inequality to the second integral of the right-hand side of (4.4.1) gives

$$\begin{aligned} & \|\kappa_1 \phi^2\|_{L^2(\Omega)} \|\eta\|_{L^2(\Omega)} + \|\nabla \eta\|_{L^\infty(\Omega)} \int_{\Omega} |\kappa_2 \phi \nabla \phi| \, d\mathbf{x} \\ & \leq \|\kappa_1 \phi^2\|_{L^2(\Omega)} \|\eta\|_{L^2(\Omega)} \\ & \quad + \|\nabla \eta\|_{L^\infty(\Omega)} \|\kappa_2 \phi\|_{L^2(\Omega)} \|\nabla \phi\|_{L^2(\Omega)}. \end{aligned} \quad (4.4.2)$$

Combining (4.4.2) and (4.4.1), and since $\phi \in H_0^1(\Omega)$, we deduce that

$$\int_{\Omega} p \eta \, d\mathbf{x} \leq C. \quad (4.4.3)$$

For the L^2 -inner product of the left-hand side of (4.4.3), the polarization identity yields

$$\int_{\Omega} p \eta \, d\mathbf{x} = \frac{1}{4} \left(\|p + \eta\|_{L^2(\Omega)}^2 - \|p - \eta\|_{L^2(\Omega)}^2 \right). \quad (4.4.4)$$

Further, the following relation holds, by virtue of the triangle inequality,

$$\begin{aligned}
\|p + \eta\|_{L^2(\Omega)}^2 - \|p - \eta\|_{L^2(\omega)}^2 &\geq \|p + \eta\|_{L^2(\Omega)}^2 - \|p\|_{L^2(\Omega)}^2 - \|\eta\|_{L^2(\Omega)}^2 \\
&= 2 \int_{\Omega} \eta |p| \, d\mathbf{x} - \|\eta\|_{L^2(\Omega)}^2 \\
&\geq 2 \int_U |p| \, d\mathbf{x} - \|\eta\|_{L^2(\Omega)}^2.
\end{aligned} \tag{4.4.5}$$

By combining (4.4.4) and (4.4.5) and by using the fact that η is smooth, we finally arrive at

$$\int_U |p| \, d\mathbf{x} \leq C, \tag{4.4.6}$$

and, therefore, the Lemma has been proved. $\square$

Having proven Lemma 4.4.1, it remains to establish the integrability of ∇p . This is performed in the following Lemma.

Lemma 4.4.2. *For the function p of the previous Lemma, the following is true: $p \in W_{loc}^{1,1}(\Omega)$.*

Proof. We begin by recalling equation (4.2.9),

$$\int_{\Omega} \nabla(p\phi) \cdot \mathbf{h} \, d\mathbf{x} = \int_{\Omega} \kappa_2 \phi \nabla \phi \otimes \nabla \phi : \nabla \mathbf{h} \, d\mathbf{x} + \int_{\Omega} \phi \rho \mathbf{g} \cdot \mathbf{h} \, d\mathbf{x},$$

for all test-functions $\mathbf{h} \in (H_0^1(\Omega))^n$. Next, let U , W and $\boldsymbol{\eta}$ defined as in the proof of Lemma (4.4.1). Setting the test-function $\mathbf{h}$ equal to $\boldsymbol{\eta}$ we get

$$\int_{\Omega} \nabla(p\phi) \cdot \boldsymbol{\eta} \, d\mathbf{x} = \int_{\Omega} \kappa_2 \phi \nabla \phi \otimes \nabla \phi : \nabla \boldsymbol{\eta} \, d\mathbf{x} + \int_{\Omega} \phi \rho \mathbf{g} \cdot \boldsymbol{\eta} \, d\mathbf{x}. \tag{4.4.7}$$

We will treat each term of the right-hand side of (4.4.7) separately. For the first term, the presumed bound $\|\nabla \boldsymbol{\eta}\|_{L^\infty(D)} < \infty$ implies that

$$\int_{\Omega} \kappa_2 \phi \nabla \phi \otimes \nabla \phi : \nabla \boldsymbol{\eta} \, d\mathbf{x} \leq C \int_{\Omega} \kappa_2 \phi (\nabla \phi \cdot \mathbf{1})^2 \, d\mathbf{x}, \tag{4.4.8}$$

Next, since $\phi \in L^\infty$ and by using the inequality $|a + b|^2 \leq C(|a|^2 + |b|^2)$, we arrive at

$$\int_{\Omega} \kappa_2 \phi \nabla \phi \otimes \nabla \phi : \nabla \boldsymbol{\eta} \, d\mathbf{x} \leq C \int_{\Omega} |\nabla \phi|^2 \, d\mathbf{x} \leq C. \tag{4.4.9}$$

As regards the second term of the right-hand side of (4.4.7), the Cauchy-Schwarz inequality yields

$$\int_{\Omega} \phi \rho \mathbf{g} \cdot \boldsymbol{\eta} \, d\mathbf{x} \leq C \|\phi\|_{L^2(\Omega)} \|\boldsymbol{\eta}\|_{L^2(\Omega)}, \quad (4.4.10)$$

and since $\phi \in H_0^1(\Omega)$ and $\boldsymbol{\eta}$ is smooth, we conclude that

$$\int_{\Omega} \phi \rho \mathbf{g} \cdot \boldsymbol{\eta} \, d\mathbf{x} \leq C. \quad (4.4.11)$$

Finally, by combining (4.4.9) and (4.4.11), we arrive at

$$\int_{\Omega} \nabla(p\phi) \cdot \boldsymbol{\eta} \, d\mathbf{x} \leq C. \quad (4.4.12)$$

Next, we identify the integral $\int_{\Omega} \nabla(p\phi) \cdot \boldsymbol{\eta} \, d\mathbf{x}$ as the L^2 -inner product of $\nabla(p\phi)$ with $\boldsymbol{\eta}$. Therefore, for the left-hand side of (4.4.12), the polarization identity gives,

$$\int_{\Omega} \nabla(p\phi) \cdot \boldsymbol{\eta} \, d\mathbf{x} = \frac{1}{4} \|\nabla(p\phi) + \boldsymbol{\eta}\|_{L^2(\Omega)}^2 - \frac{1}{4} \|\nabla(p\phi) - \boldsymbol{\eta}\|_{L^2(\Omega)}^2.$$

Applying the triangle inequality and expanding the sum of the squares in the above identity yields,

$$\begin{aligned} \int_{\Omega} \nabla(p\phi) \cdot \boldsymbol{\eta} \, d\mathbf{x} + \|\boldsymbol{\eta}\|_{L^2(\Omega)}^2 &\geq \int_{\Omega} |\boldsymbol{\eta} \nabla(p\phi)| \, d\mathbf{x} \geq \int_W |\boldsymbol{\eta} \nabla(p\phi)| \, d\mathbf{x} \\ &\geq \int_U |\nabla(p\phi)| \, d\mathbf{x}. \end{aligned} \quad (4.4.13)$$

By combining (4.4.12) and (4.4.13) we readily arrive at

$$\int_U |\nabla(p\phi)| \, d\mathbf{x} \leq C + \|\boldsymbol{\eta}\|_{L^2(D)}^2, \quad (4.4.14)$$

and since $\boldsymbol{\eta}$ is smooth and ϕ is bounded away from zero, we finally obtain that

$$\int_U |\nabla p| \, d\mathbf{x} \leq C, \quad (4.4.15)$$

which completes the proof. $\square$

4.5 Conclusions

In this Chapter we have presented an existence and regularity theory for hydrostatics of granular materials, as predicted by the equilibrium limit of the two-phase flow model of reference. First, we conduct an integrability analysis which allows to transform the original system to a singular nonlinear elliptic PDE with natural growth. By applying the so-called weak convergence methods and by employing suitable nonlinear test-functions, we have proved that this elliptic PDE admits at least on weak solution, in the sense of distributions. Based on this result, we have established an existence theory for the original overdetermined system.

The analysis that has been presented herein is confined to dimensions two and three. However, as a point of mathematical interest, we mention that our results are valid for any dimension $n > 1$. Further, in our studies, we have chosen to investigate the case of zero Dirichlet conditions for the volume fraction. From the mathematical point of view, this is the simplest case and, therefore, represents a natural starting point. From the physical point of view, zero Dirichlet conditions are not likely to be encountered in presence of gravitational forces but they could be justified in their absence; in which case the analysis presented herein applies as well. Additionally, it is worth adding that our theory can be applicable to more general Dirichlet conditions provided that suitable, possibly different, test functions are chosen.

For the zero Dirichlet problem, the solution obtained herein has a volume fraction that is uniformly bounded away from zero. However, since the uniqueness of solutions has not been established, one cannot *a priori* exclude the existence of other solutions, where the volume fraction can become zero locally. For such cases, our analysis is no longer valid and one has to resort to different strategies. One possible methodology can be found in Arcoya *et al.* (2009), in which the authors introduce assumptions on the growth of the singular term and employ a different definition for weak solutions. By doing so, they succeed in proving the existence of finite energy (H_0^1) solutions.

Finally, since Chapter 3 and Chapter 4 are complementary to each other, an important question is whether the solution obtained in this Chapter can be recovered numerically by the algorithm presented in Chapter 3. To this extend, since the uniqueness of the solutions has not been proved, there is no guarantee that the results of the theoretical and the numerical analysis will coincide.

Chapter 5

A numerical method for incompressible flows of two-phase granular mixtures

5.1 Introduction

Along with the development of elaborate and sophisticated mathematical models for two-phase granular flows, there have been efforts towards the numerical simulation of these flows as well. To date, considerable emphasis has been given to dilute mixtures, as reflected by the extensive reference list for both compressible and incompressible flows; see, for example, Lun (2000), Huilin *et al.* (2003a), Huanpenga *et al.* (2004), Benavides & van Wachem (2008), Levy & Sayed (2008), Bisi *et al.* (2012) and the references therein.

In addition, various authors have developed numerical methods for dense compressible granular flows, (Saurel & Abgrall 1999, Gonthier & Powers 2000, Gavriluk & Saurel 2002b, Schwendeman *et al.* 2006, Cochran & Powers 2008, Tokareva & Toro 2010, Thanh *et al.* 2012). However, the validity of the numerical results obtained by these algorithms is questionable. This is because of the presence of non-conservative products in the governing equations, *i.e.* first-order differential terms that are not fluxes but they arise from the modeling of the interactions between the two phases. The presence of non-conservative products implies that weak solutions in the standard sense of distributions can no longer be defined. Also, the Riemann problem of the hyperbolic, diffusion-free equations is ill-posed; there are initial conditions for which the problem admits zero solutions, as well as initial conditions for which the problem admits multiple entropy-satisfying solutions, (Deledicque & Papalexandris 2007).

The results of this Chapter can also be found in the article Varsakelis, C. & Papalexandris, M. V. 2012 A numerical method for unsteady flows of fluid-saturated granular materials, which has been submitted for publication and is currently under review.

As regards dense incompressible granular flows, there is a notable dearth of numerical methods. Consequently, numerical results for such flows are available only for very special cases. For example, there exist results for simple shear flows (Passman *et al.* 1986, Wang & Hutter 1999*a*, Massoudi & Phuoc 2005), Poiseuille flows (Fang *et al.* 2006) and gravity-driven flows (Savage 1979, Gudhe *et al.* 1994, Wang & Hutter 1999*b*, Fang *et al.* 2006, Fang 2008). However, all these studies focus on one-dimensional, steady-state flows in a simple planar geometry. Under these assumptions, the governing equations reduce to a system of ordinary differential equations that can be easily solved. By contrast, numerical results for multi-dimensional, incompressible, unsteady flows are currently not available in the literature. Therefore, the predictive value of continuum models for incompressible flows of two-phase granular mixtures remains unclear.

In this Chapter we present an algorithm for the numerical treatment of the low-Mach number equations for two-phase granular flows that have been derived in Chapter 1, in the case where both constituents have constant density. The proposed algorithm belongs to the class of generalized projection methods and employs a fractional-step, predictor-corrector scheme for the integration in time. A Poisson equation and a second-order elliptic equation with variable coefficient are solved at both the predictor and corrector steps for the computation of the pressures of the solid and fluid phase, respectively.

It is important to note that any algorithm that aims to treat numerically continuum models for incompressible two-phase granular flows should be able to deal with strong material interfaces. In fact, an important characteristic of such flows is the formation of zones of high-particle concentrations. These structures change in size and shape as they are convected by the flow. Further, and depending on the flow conditions, they can merge or break up. Thus, the boundaries of these high-particle concentration zones are propagating and deforming interfaces whose geometry changes significantly over time. In turn, these changes are reflected in the spatial gradient of the solid phase volume fraction which becomes very large across such interfaces, thereby, producing spurious oscillations. For this reason, the proposed algorithm is coupled with an interface detection and treatment methodology, based on a local regularization methodology.

This Chapter is organized as follows. In Section 5.2 we present the governing equations and discuss their properties and the critical issues concerning their numerical treatment. In Section 5.3 we describe the numerical algorithm in detail. In Section 5.4 we present representative results of numerical simulations of unsteady, two-dimensional shear flows that illustrate the stability and robustness of the algorithm. Also, we present the results of a comparison study between the results predicted by our simulations and those of Passman *et al.* (1986), Wang & Hutter (1999*a*), Massoudi & Phuoc (2005) for steady-state, one-dimensional shear flows.

5.2 Governing equations

Let us consider a saturated mixture of an isotropic granular material and a simple fluid occupying a Lipschitz domain $\Omega \subset \mathbb{R}^N$, $N \geq 1$. We assume that both phases have constant density. Then, according to Chapter 2, and upon dropping the superscripts in order to simplify the presentation, the non-dimensional governing equations of the mixture are the following.

Mass and momentum balance equations for the solid (granular) phase,

$$\nabla \cdot \mathbf{u}_s = 0, \quad (5.2.1)$$

$$\begin{aligned} \rho_s \frac{\partial \phi_s \mathbf{u}_s}{\partial t} + \rho_s \nabla \cdot (\phi_s \mathbf{u}_s \otimes \mathbf{u}_s) + \nabla(p_s \phi_s) &= \frac{1}{Re} \nabla \cdot (2\mu_s \phi_s \mathbf{V}_s^v) \\ &\quad - \nabla \cdot (\Gamma_s \nabla \phi_s \otimes \nabla \phi_s) \\ &\quad + p_f \nabla \phi_s + \delta(\mathbf{u}_f - \mathbf{u}_s) \\ &\quad + \rho_s \phi_s \mathbf{g}. \end{aligned} \quad (5.2.2)$$

Mass and momentum balance equations for the fluid phase,

$$\nabla \cdot ((\mathbf{u}_s - \mathbf{u}_f) \phi_f) = 0, \quad (5.2.3)$$

$$\begin{aligned} \rho_f \frac{\partial \phi_f \mathbf{u}_f}{\partial t} + \rho_f \nabla \cdot (\phi_f \mathbf{u}_f \otimes \mathbf{u}_f) + \nabla(\phi_f p_f) &= \frac{1}{Re} \nabla \cdot (2\mu_f \phi_f \mathbf{V}_f^v) - p_f \nabla \phi_s \\ &\quad - \delta(\mathbf{u}_f - \mathbf{u}_s) + \rho_f \phi_f \mathbf{g}. \end{aligned} \quad (5.2.4)$$

Compaction equation,

$$\frac{\partial \phi_s}{\partial t} + \mathbf{u}_s \cdot \nabla \phi_s = 0. \quad (5.2.5)$$

The above balance laws are supplemented with the saturation condition,

$$\phi_s(\mathbf{x}) + \phi_f(\mathbf{x}) = 1, \quad \mathbf{x} \in \Omega. \quad (5.2.6)$$

The unknowns in the above equations are the volume fraction ϕ_s , the dynamic pressures p_s and p_f and the phasial velocities $\mathbf{u}_s$ and $\mathbf{u}_f$. Also, we recall that Re is the Reynolds number defined with respect to the fluid's density and viscosity coefficient; *cf.* Chapter 2.

We observe that, due to (5.2.1), the compaction equation (5.2.5) is actually a conservation law for the volume fraction. Further, we note that, although the velocity of the solid phase $\mathbf{u}_s$ is divergence-free, the velocity of the fluid phase $\mathbf{u}_f$ obeys a different kinematic constraint, (5.2.3). As discussed in Chapter 1, this is because of the introduction of the volume fraction ϕ_s as an additional variable and the saturation condition. In fact, by combining (5.2.1), (5.2.3) and (5.2.6), we deduce that $\mathbf{u}_f$ is divergence-free only when it is equal to $\mathbf{u}_s$.

Finally, we adopt the notation convention $\boldsymbol{\sigma}$ for the configuration stress tensor $\nabla \cdot (\Gamma_s \nabla \phi_s \otimes \nabla \phi_s)$ that appears in the right-hand side of equation 5.2.2.

5.2.1 Development of a projection method: critical issues

The presence of two momentum equations in the system of equations (5.2.1)-(5.2.5) suggests the use of a double projection; one for each velocity vector. However, this idea, despite its conceptual simplicity, cannot be applied directly because of the following challenging issues.

- (i) the velocity vector of the fluid phase $\mathbf{u}_f$ is not divergence-free. Instead, it satisfies a different kinematic constraint that has to be accommodated. Further, neither (5.2.1) nor (5.2.3) can be directly employed in a projection method. In fact, taking the divergence of equations (5.2.2) and (5.2.4) does not yield terms that can be simplified by (5.2.1) and (5.2.3), respectively, as is the case with projection methods.

As a first option, one can cast equations (5.2.2) and (5.2.4) in a form that they are solvable with respect to $\mathbf{u}_s$ and $(\mathbf{u}_s - \mathbf{u}_f)\phi_f$, correspondingly. In turn, this reformulation allows for the direct accommodation of the kinematic constraints (5.2.1) and (5.2.3); this is the main idea of the Bell and Marcus algorithm for Boussinesq flows Bell & Marcus (1992), see also the more recent study of Nicoud (2000). However, it can be shown, after some algebra, that this procedure amounts to dividing the right-hand side of (5.2.1) by ϕ_s and that of (5.2.3) by ϕ_f . Consequently, this approach requires ϕ_s and ϕ_f to be uniformly bounded away from zero and, therefore, cannot be applied to the governing equations in hand.

An alternative strategy, that is adopted herein, is to derive kinematic constraints for $\phi_s \mathbf{u}_s$ and $\phi_f \mathbf{u}_f$ by combining equations (5.2.1) and (5.2.3) with the compaction equation (5.2.5). Upon doing so, we readily obtain,

$$\nabla \cdot (\phi_s \mathbf{u}_s) = -\frac{\partial \phi_s}{\partial t}, \quad (5.2.7)$$

$$\nabla \cdot (\phi_f \mathbf{u}_f) = \frac{\partial \phi_s}{\partial t}. \quad (5.2.8)$$

The above equations show that the projection operation can still be employed for computational purposes if it is supplemented with an approximation for the time

derivative of ϕ_s . A similar situation appears in the study of single-phase low-Mach number flows; see, for example, Knikker (2011) and the references therein.

Mathematically, equations (5.2.7) and (5.2.8) imply that $\phi_s \mathbf{u}_s$ and $\phi_f \mathbf{u}_f$ are not projected to the space of divergence-free vector fields but to vector fields whose non-solenoidal part is known and can be computed. Therefore, from the algorithmic point of view, the kinematic constraints (5.2.7) and (5.2.8) can be as efficient as the divergence-free constraint, depending on the accuracy that the right-hand sides of (5.2.7) and (5.2.8) are computed.

- (ii) An additional challenging point is the presence of moving and deforming material interfaces. In fact, an important characteristic of such flows is the formation of zones of high-particle concentration. These structures change in size and shape as they are convected by the flow. Further, and depending on the flow conditions, they can merge or break up. In other words, the boundaries of these structures are propagating and deforming interfaces whose geometry changes significantly over time. In the vicinity of such interfaces the gradient of the volume fraction $\nabla \phi_s$ becomes very steep and renders equations (5.2.2) and (5.2.4) stiff. This can result in spurious oscillations across material interfaces which deteriorate the performance of the numerical method. Consequently the numerical method for the governing system should be supplemented with an interface-treatment strategy.

Further, we remark that the treatment of a material interface becomes more difficult as the ratio of the phasial densities increases. For example, the treatment of an air-sand interface, $\rho_s/\rho_f = O(1000)$ is much harder than that of a water-sand interface, $\rho_s/\rho_f = O(1)$. Therefore, the treatment of the interfaces has to be robust enough to handle large ratios of the phasial densities.

In this Chapter, the numerical treatment of material interfaces is performed via a local and selective regularization scheme. In particular, the employed scheme is variation of the regularization schemes that are presented and analyzed in Tornberg & Engquist (2004).

- (iii) The discretization of the divergence of the configuration stress tensor $\boldsymbol{\sigma}$ represents an additional critical issue. This is a highly nonlinear differential operator that, additionally, becomes singular in the vicinity of material interfaces. For the discretization of this term, we propose herein a generalization of the flux-interpolation technique of Lessani & Papalexandris (2006) to differential operators as well.
- (iv) Another challenging issue is the large viscosity ratios of the two phases. For example, in a mixture of air with natural angular sand, the viscosity ratio μ_s/μ_f is at the order of $O(10^8)$. This makes the viscous flux of the granular phase and the interphasial drag coefficient δ very stiff. To avoid such stiffness problems, time integration in the prediction stage is performed with a Cranck-Nicolson scheme for the

above viscous flux combined with an Adams-Bashforth method for the source terms. On the other hand, in the correction stage the time integration of all terms is performed via a modified Adams-Bashforth method. However, it should be underlined that, because of the strong coupling between the two phases and the complicated structure of the equations in hand, the use of implicit schemes should be kept at a minimum.

- (v) Finally, it should not go unnoticed the fact that the governing system (5.2.1)-(5.2.5) consists of a large number $(2N + 3)$ of highly nonlinear PDEs. This increases the computational complexity of the algorithm. Therefore, the implementation of the algorithm should be carried out in an efficient and well-orchestrated manner.

5.3 The numerical method

The proposed numerical method is based on a predictor-corrector time-integration scheme which employs a projection method for the computation of the phasial pressures p_s and p_f . This section is devoted to the detailed description of the numerical method, with time and space discretization discussed separately.

Before presenting the components of the algorithm, it is convenient to write the momentum equations (5.2.2) and (5.2.4) in a form in which the phasial pressures p_s, p_f appear only in gradients. To this end, combining the product differentiation identity for $p_f \nabla \phi_s$ and the saturation relation (5.2.6) with equations (5.2.2) and (5.2.4), readily yields,

$$\begin{aligned} \rho_s \frac{\partial \phi_s \mathbf{u}_s}{\partial t} + \rho_s \nabla \cdot (\phi_s \mathbf{u}_s \otimes \mathbf{u}_s) + \nabla p &= \frac{1}{Re} \nabla \cdot (2\mu_s \phi_s \mathbf{V}_s^v) \\ &\quad - \nabla \cdot (\Gamma_s \nabla \phi_s \otimes \nabla \phi_s) \\ &\quad - \phi_s \nabla p_f + \delta(\mathbf{u}_f - \mathbf{u}_s) \\ &\quad + \rho_s \phi_s \mathbf{g}, \end{aligned} \tag{5.3.1}$$

$$\begin{aligned} \rho_f \frac{\partial \phi_f \mathbf{u}_f}{\partial t} + \rho_f \nabla \cdot (\phi_f \mathbf{u}_f \otimes \mathbf{u}_f) + \phi_f \nabla p_f &= \frac{1}{Re} \nabla \cdot (2\mu_f \phi_f \mathbf{V}_f^v) - \delta(\mathbf{u}_f - \mathbf{u}_s) \\ &\quad + \rho_f \phi_f \mathbf{g}, \end{aligned} \tag{5.3.2}$$

where we have used the notation $p = (p_s - p_f)\phi_s$.

5.3.1 Time discretization

In what follows, we will make use of the following notation convention. The time step is assumed to be Δt . Further, the superscripts $n, *$ and $n + 1$ will denote the computed

values at time $n \Delta t$, the predicted values and the corrected values at time $(n + 1) \Delta t$, respectively.

Predictor stage

- i) The predicted value of the volume fraction ϕ_s^* is computed from the compaction equation (5.2.5) with the use of a forward Euler method,

$$\frac{\phi_s^* - \phi_s^n}{\Delta t} = -\mathbf{u}_s^n \cdot \nabla \phi_s^n. \quad (5.3.3)$$

- ii) In this step, the predicted values of the solid phase velocity $\mathbf{u}_s^*$ and pressure p_s^* are computed. First, an intermediate variable $\tilde{\mathbf{u}}_s$ is introduced that has the dimensions of velocity. The value of $\tilde{\mathbf{u}}_s$ is computed by solving the convective and diffusive parts of the momentum equation of the solid phase (5.3.1). A Cranck-Nicolson scheme is employed for the viscous fluxes whereas an Adams-Bashforth method is used for the remaining terms,

$$\begin{aligned} \frac{\rho_s \phi_s^* \tilde{\mathbf{u}}_s - \rho_s \phi_s^n \mathbf{u}_s^n}{\Delta t} &= \frac{1}{Re} \nabla \cdot \left(\frac{2\mu_s^* \phi_s^* \tilde{\mathbf{V}}_s^v + 2\mu_s^n \phi_s^n (\mathbf{V}_s^v)^n}{2} \right) \\ &+ \frac{3\text{Res}_s^n - \text{Res}_s^{n-1}}{2}, \end{aligned} \quad (5.3.4)$$

where Res_s is defined as

$$\begin{aligned} \text{Res}_s &= -\nabla \cdot (\rho_s \phi_s \mathbf{u}_s \otimes \mathbf{u}_s) - \nabla \cdot (\Gamma_s \nabla \phi_s \otimes \nabla \phi_s) - \phi_s \nabla p_f \\ &+ \delta(\mathbf{u}_f - \mathbf{u}_s) + \rho_s \phi_s \mathbf{g}. \end{aligned} \quad (5.3.5)$$

The time-discretization scheme for the momentum equation of the solid phase (5.3.1) in the predictor stage is completed by setting,

$$\rho_s \phi_s^* \mathbf{u}_s^* - \rho_s \phi_s^* \tilde{\mathbf{u}}_s = -\Delta t \nabla p^*. \quad (5.3.6)$$

Next, we proceed to the projection step. Taking the divergence of (5.3.6) gives, upon rearrangement,

$$\nabla \cdot (\Delta t \nabla p^*) = -\nabla \cdot (\rho_s \phi_s^* \mathbf{u}_s^*) + \nabla \cdot (\rho_s \phi_s^* \tilde{\mathbf{u}}_s). \quad (5.3.7)$$

The term $-\nabla \cdot (\rho_s \phi_s^* \mathbf{u}_s^*)$ is equal to $\rho_s \frac{\partial \phi_s^*}{\partial t}$ because of the kinematic constraint (5.2.7), derived in subsection 5.2.1. For the temporal derivative of ϕ_s^* the following second-order backward approximation is employed,

$$\frac{\partial \phi_s^*}{\partial t} = \frac{3\phi_s^* - 4\phi_s^n + \phi_s^{n-1}}{2\Delta t}. \quad (5.3.8)$$

Combining (5.3.7), (5.2.7) and (5.3.8) yields the following Poisson equation for p^* ,

$$\nabla \cdot (\nabla p^*) = \rho_s \frac{3\phi_s^* - 4\phi_s^n + \phi_s^{n-1}}{2\Delta t^2} + \frac{\nabla \cdot (\rho_s \phi_s^* \tilde{\mathbf{u}}_s)}{\Delta t}. \quad (5.3.9)$$

The predicted value p^* is computed by numerically solving equation (5.3.9). Then, the predicted value $\mathbf{u}_s^*$ is calculated from (5.3.6).

- iii) The predicted values of the velocity and pressure of the fluid phase, $\mathbf{u}_f^*$ and p_f^* , respectively, are computed from the momentum equation of the fluid phase (5.3.2). Similarly to step (ii), an intermediate velocity $\tilde{\mathbf{u}}_f$ is introduced and calculated by integrating the convection-diffusion part of equation (5.3.2). For this integration, an Adams-Bashforth method is used,

$$\frac{\rho_f \phi_f^* \tilde{\mathbf{u}}_f - \rho_f \phi_f^n \tilde{\mathbf{u}}_f^n}{\Delta t} = \frac{3\text{Res}_f^n - \text{Res}_f^{n-1}}{2}, \quad (5.3.10)$$

where Res_f is defined as,

$$\begin{aligned} \text{Res}_f = & -\nabla \cdot (\rho_f \phi_f \mathbf{u}_f \otimes \mathbf{u}_f) + \frac{1}{Re} \nabla \cdot (2\mu_f \phi_f^n \mathbf{V}_f^v) \\ & - \delta(\mathbf{u}_f - \mathbf{u}_s) + \rho_f \phi_f \mathbf{g}. \end{aligned} \quad (5.3.11)$$

The time discretization scheme for the momentum equation of the fluid phase (5.3.2) in the predictor stage is completed by setting,

$$\rho_f \phi_f^* \mathbf{u}_f^* - \rho_f \phi_f^* \tilde{\mathbf{u}}_f = -\Delta t \phi_f^* \nabla p_f^*, \quad (5.3.12)$$

In the projection step, we take the divergence of (5.3.12) which, upon rearrangement, yields,

$$\Delta t \nabla \cdot (\phi_f^* \nabla p_f^*) = -\nabla \cdot (\rho_f \phi_f^* \mathbf{u}_f^*) + \nabla \cdot (\rho_f \phi_f^* \tilde{\mathbf{u}}_f). \quad (5.3.13)$$

From the kinematic constraint (5.2.8), the divergence of $\rho_f \phi_f^* \mathbf{u}_f^*$ equals $\rho_f \frac{\partial \phi_s^*}{\partial t}$. As in step (ii), $\frac{\partial \phi_s^*}{\partial t}$ is approximated by the second-order scheme of (5.3.8). Therefore, the following second-order elliptic PDE for p_f^* is obtained,

$$\nabla \cdot (\phi_f^* \nabla p_f^*) = -\rho_f \frac{3\phi_s^* - 4\phi_s^n + \phi_s^{n-1}}{2\Delta t^2} + \frac{\nabla \cdot (\rho_f \phi_f^* \tilde{\mathbf{u}}_f)}{\Delta t}. \quad (5.3.14)$$

The predicted value p_f^* is computed by numerically solving the above equation (5.3.14). Then, the predicted value of $\mathbf{u}_f^*$ is calculated from equation (5.3.12).

Corrector stage

- i) The corrected value of the volume fraction ϕ_s^{n+1} is computed from the compaction equation (5.2.5) with the use of the trapezoidal method,

$$\frac{\phi_s^{n+1} - \phi^n}{\Delta t} = -\frac{\mathbf{u}_s^* \nabla \phi_s^* + \mathbf{u}_s^n \nabla \phi_s^n}{2}. \quad (5.3.15)$$

- ii) For the corrected value of the solid phase velocity $\mathbf{u}_s^{n+1}$ and pressure p_s^{n+1} , an updated intermediate variable $\check{\mathbf{u}}_s$ that has the dimensions of velocity is introduced. The value of $\check{\mathbf{u}}_s$ is computed by the convection-diffusion part of the solid phase momentum equation (5.3.1). In this step, a trapezoidal rule is used for the viscous flux whereas an Adams-Bashforth method is employed for the remaining terms. More precisely,

$$\begin{aligned} \frac{\rho_s \phi_s^{n+1} \check{\mathbf{u}}_s - \rho_s \phi_s^n \mathbf{u}_s^n}{\Delta t} &= \frac{1}{Re} \nabla \cdot \left(\frac{2\mu_s^* \phi_s^* \tilde{\mathbf{V}}_s^v + 2\mu_s^n \phi_s^n (\mathbf{V}_s^v)^n}{2} \right) \\ &\quad + \frac{3\text{Res}_s^n - \text{Res}_s^{n-1}}{2}. \end{aligned} \quad (5.3.16)$$

The time discretization scheme for the momentum equation of the solid phase (5.3.1) in the corrector stage is completed by setting,

$$\rho_s \phi_s^{n+1} \mathbf{u}_s^{n+1} - \rho_s \phi_s^{n+1} \check{\mathbf{u}}_s = -\Delta t \nabla p^{n+1}. \quad (5.3.17)$$

Next, by taking the divergence of (5.3.17) and by rearranging, we arrive at

$$\nabla \cdot (\nabla p^{n+1}) = -\frac{\nabla \cdot (\rho_s \phi_s^{n+1} \mathbf{u}_s^{n+1})}{\Delta t} + \frac{\nabla \cdot (\rho_s \phi_s^{n+1} \check{\mathbf{u}}_s)}{\Delta t}. \quad (5.3.18)$$

From the kinematic constraint (5.2.7), the first term of the right-hand side of (5.3.18) equals $\rho_s \frac{\partial \phi_s^{n+1}}{\partial t}$. As in step (ii) of the predictor stage, this temporal derivative is approximated with the second-order scheme of (5.3.8). Combining (5.3.18), (5.2.7) and (5.3.8) yields the following Poisson equation for p^{n+1} ,

$$\nabla \cdot (\nabla p^{n+1}) = \rho_s \frac{3\phi_s^{n+1} - 4\phi_s^n + \phi_s^{n-1}}{2\Delta t^2} + \frac{\nabla \cdot (\rho_s \phi_s^{n+1} \check{\mathbf{u}}_s)}{\Delta t}. \quad (5.3.19)$$

Similarly to the predictor stage, the corrected value p^{n+1} is computed by solving numerically equation (5.3.19). Subsequently, the corrected value $\mathbf{u}_s^{n+1}$ is calculated from equation (5.3.17).

- iii) For the corrected values of the velocity and pressure of the fluid phase, $\mathbf{u}_f^{n+1}$ and p_f^{n+1} , respectively, we first introduce an updated intermediate variable $\tilde{\mathbf{u}}_f$ that has the dimensions of velocity. The value of $\tilde{\mathbf{u}}_f$ is computed by solving the convection-diffusion part of the fluid phase momentum equation (5.3.2) with an Adams-Bashforth method,

$$\frac{\rho_f \phi_f^{n+1} \tilde{\mathbf{u}}_f - \rho_f \phi_f^n \mathbf{u}_f^n}{\Delta t} = \frac{3\text{Res}_f^n - \text{Res}_f^{n-1}}{2}. \quad (5.3.20)$$

The time discretization scheme for the momentum equation of the fluid phase (5.3.2) in the corrector stage is completed by setting,

$$\phi_f^{n+1} \mathbf{u}_f^{n+1} - \phi_f^{n+1} \tilde{\mathbf{u}}_f = \Delta t \phi_f^{n+1} \nabla p_f^{n+1}, \quad (5.3.21)$$

Taking the divergence of (5.3.21) yields, upon rearrangement,

$$\nabla \cdot (\phi_f^{n+1} \nabla p_f^{n+1}) = -\frac{\nabla \cdot (\rho_f \phi_f^{n+1} \mathbf{u}_f^{n+1})}{\Delta t} + \frac{\nabla \cdot (\rho_f \phi_f^{n+1} \tilde{\mathbf{u}}_f)}{\Delta t}. \quad (5.3.22)$$

From the kinematic constraint (5.2.8), the term $\nabla \cdot (\rho_f \phi_f^{n+1} \mathbf{u}_f^{n+1})$ equals $\rho_f \frac{\partial \phi_s^{n+1}}{\partial t}$. As in step (iii) of the predictor stage, the time derivative of ϕ_s^{n+1} is approximated by the second-order scheme of (5.3.8). Therefore, we arrive at the following second-order elliptic PDE for p_f^{n+1} ,

$$\nabla \cdot (\phi_f^{n+1} \nabla p_f^{n+1}) = -\rho_f \frac{3\phi_s^{n+1} - 4\phi_s^n + \phi_s^{n-1}}{2\Delta t^2} + \frac{\nabla \cdot (\rho_f \phi_f^{n+1} \tilde{\mathbf{u}}_f)}{\Delta t}. \quad (5.3.23)$$

Similarly to the predictor stage, the corrected value p_f^{n+1} is computed by solving numerically equation (5.3.23). Then, the corrected value $\mathbf{u}_f^{n+1}$ is obtained from equation (5.3.21).

According to the proposed algorithm, $p = (p_s - p_f)\phi_s$ is treated as an independent variable and, thus, the precise value of p_s is not required for the advancing of the algorithm in time. However, the exact value of p_s can be readily obtained at any time level once $(p_s - p_f)\phi_s$ is computed.

We remark that for the computation of the phasial pressures p_s and p_f two Poisson equations and two second-order elliptic PDEs, respectively, have to be solved at each time step. The presence of the second-order elliptic PDEs results from the reformulation of the momentum equations (5.3.1) and (5.3.2). In other words, solving two second-order elliptic PDEs, instead of two (constant coefficient) Poisson equations, is the price for casting the momentum equations in a form that contains only the gradients of the pressures. For the sake of completeness, we note that the linear systems that result from

the discretization of the Poisson and the second-order elliptic PDEs are solved via the bi-conjugate, stabilized gradient algorithm.

A worth-noting feature of the proposed algorithm is the treatment of the viscous flux of the solid phase. In the predictor stage this viscous flux is treated in an implicit manner while in the corrector stage, it is treated explicitly. As discussed in subsection 5.2.1, the viscous flux of the solid phase is rendered stiff for high viscosity ratios. In the predictor stage this is remedied via the use of the Cranck-Nicolson scheme. Preliminary numerical experiments showed that the use of the Cranck-Nicolson scheme is not necessary to be extended to the corrector stage as well, as no stability problems have been observed. Consequently, in the step (ii) of the corrector stage, the Cranck-Nicolson scheme is replaced by an explicit trapezoidal rule, which is computationally cheaper.

We also remark that the approximation for the temporal derivative $\frac{\partial \phi_s}{\partial t}$ is a critical issue for the overall efficiency of the projection method. In the proposed algorithm, we employ the second-order backward scheme of (5.3.8). Numerical experiments showed that this choice works well in practice. Further, it has been successfully used in the past in projection methods for variable-density flows; see, for example, Lessani & Papalexandris (2006), Sewall & Tafti (2008). Evidently, other higher-order schemes can be chosen; see, for example, Cook & Riley (1996) for a comparison between even-order and odd-order schemes.

Finally, the intermediate variables $\tilde{\mathbf{u}}_s, \tilde{\mathbf{u}}_f, \tilde{\mathbf{u}}_s$ and $\tilde{\mathbf{u}}_f$ have to be assigned boundary conditions. These variables have the dimensions of velocity and are sometimes referred to as *provisional* velocities, (Knikker 2011). For this reason, it is customary to set $\tilde{\mathbf{u}}_i = \tilde{\mathbf{u}}_i = \mathbf{u}_i$, $i = s, f$ on the boundary. However, other options also exist; see, for example, the discussion in Knikker (2011) and references therein.

5.3.2 Spatial discretization

For the sake of simplicity, we assume that the mesh $\mathcal{M}$ consists of a finite number of N -dimensional rectangles K_i such that $\Omega = \cup_i \{K_i\}$. Further, we suppose that the mesh is $(\Delta x_1, \dots, \Delta x_N)$ -regular where $\Delta x_i, i = 1, \dots, N$ is the mesh-width in the x_i direction.

The proposed algorithm employs a collocated grid system for the spatial discretization of the equations in hand. The main advantages of collocated grid systems over staggered ones are ease of implementation and direct extension to curvilinear coordinate systems. However, collocated grid systems suffer from the odd-even decoupling problem which results in spurious oscillations for the phasial pressure. This phenomenon has its origins in the numerical treatment of convective terms and can be remedied by the use of flux interpolation methods, (Rhie & Chow 1983). Herein, we propose a generalized version of this approach for systems containing high-order differential operators, such as the divergence of the stress configuration tensor in our system.

For the spatial discretization of the compaction equation (5.2.5), we employ the

Corner-Transport-Upwind (CTU) scheme of Colella (1990). This is a second-order generalization of the standard upwind scheme for the multi-dimensional advection equation; for a detailed description the reader is referred to Colella (1990), LeVeque (2002). Additionally, this is a positivity-preserving algorithm, a property which is important in our case since the volume fraction ϕ_s must remain non-negative.

Next, we give the definition of two discrete operators that will be used below. The finite-difference operator acting on a function $f(x_1, \dots, x_N)$ in the x_1 -direction is given by,

$$\frac{\delta_n f(x_1, \dots, x_N)}{\delta_n x_1} = \frac{f(x_1 + n \frac{\Delta x_1}{2}, \dots, x_N) - f(x_1 - n \frac{\Delta x_1}{2}, \dots, x_N)}{n \Delta x_1}, \quad (5.3.24)$$

and the interpolation operator along the x_1 -direction is given by,

$$\bar{f}^{n x_1}(x_1, \dots, x_N) = \frac{f(x_1 + n \frac{\Delta x_1}{2}, \dots, x_N) + f(x_1 - n \frac{\Delta x_1}{2}, \dots, x_N)}{2}. \quad (5.3.25)$$

Completely analogous definitions stand for the above operators acting on the other directions.

The second-order differential operators that describe the viscous fluxes are discretized via second-order centered finite differences. For the discretization of the convective terms, the following auxiliary fluxes are introduced,

$$F_{s_i} = \rho_s \phi_s u_{s_i}, \quad i = 1, \dots, N, \quad (5.3.26)$$

$$F_{f_i} = \rho_f \phi_f u_{f_i}, \quad i = 1, \dots, N, \quad (5.3.27)$$

where $\mathbf{u}_j = (u_{j_1}, \dots, u_{j_N})$, $j = s, f$. The fluxes F_{j_i} are staggered with respect to the other variables in space, *i.e.* they are computed at the center of the cell's interface normal to the i -th direction. In other words, the auxiliary fluxes F_{j_i} live in a dual grid and, numerically, they are calculated via interpolation. Finally, it is assumed that their index is the same as the associated computational cell.

The auxiliary fluxes F_{j_i} are computed at both the predictor and the corrector stage of the algorithm. In the predictor stage, the F_{j_i} are computed from equations (5.3.6) and (5.3.12) for the solid and fluid phase, respectively, as follows,

$$F_{s_i}^* = \overline{\rho_s \phi_s^* \tilde{u}_{s_i}}^{1 x_i} - \Delta t \frac{\delta_1 p^*}{\delta_1 x_i}, \quad i = 1, \dots, N, \quad (5.3.28)$$

$$F_{f_i}^* = \overline{\rho_f \phi_f^* \tilde{u}_{f_i}}^{1 x_i} - \Delta t \frac{\delta_1 p^*}{\delta_1 x_i}, \quad i = 1, \dots, N. \quad (5.3.29)$$

Further, by applying the δ_1 finite difference operator to equations (5.2.7) and (5.2.8) and

by using the definition of F_{j_i} , we arrive at,

$$\rho_s \frac{3\phi_s^* - 4\phi_s^n + \phi_s^{n-1}}{2\Delta t^2} + \frac{\delta_1 F_{s_i}^*}{\delta_1 x_i} = 0, \quad i = 1, \dots, N, \quad (5.3.30)$$

$$-\rho_f \frac{3\phi_s^* - 4\phi_s^n + \phi_s^{n-1}}{2\Delta t^2} + \frac{\delta_1 F_{f_i}^*}{\delta_1 x_i} = 0, \quad i = 1, \dots, N. \quad (5.3.31)$$

Combining equations (5.3.28), (5.3.29) with (5.3.30) and (5.3.31), yields the following discretization scheme for the Poisson equation (5.3.9) and the second-order elliptic PDEs (5.3.14) of the prediction stage,

$$\begin{aligned} \frac{\delta_1}{\delta_1 x_i} \left(\frac{\delta_1 p^*}{\delta_1 x_i} \right) &= \rho_s \frac{3\phi_s^* - 4\phi_s^n + \phi_s^{n-1}}{2\Delta t^2} + \frac{\delta_1 \overline{\rho_s \phi_s^* \tilde{u}_{i,s}}^{1x_i}}{\Delta t \delta_1 x_i}, \\ \frac{\delta_1}{\delta_1 x_i} \left(\frac{\overline{\phi_f^{*1x_i}} \delta_1 p_f^*}{\delta_1 x_i} \right) &= -\rho_f \frac{3\phi_s^* - 4\phi_s^n + \phi_s^{n-1}}{2\Delta t^2} + \frac{\delta_1 \overline{\rho_f \phi_f^* \tilde{u}_{i,f}}^{1x_i}}{\Delta t \delta_1 x_i}. \end{aligned}$$

A completely analogous procedure yields the discretization scheme for the Poisson equation (5.3.19) and the second-order elliptic PDE (5.3.23) of the correction stage. The final relations read,

$$\frac{\delta_1}{\delta_1 x_i} \left(\frac{\delta_1 p^{n+1}}{\delta_1 x_i} \right) = \rho_s \frac{3\phi_s^{n+1} - 4\phi_s^n + \phi_s^{n-1}}{2\Delta t^2} + \frac{\delta_1 \overline{\rho_s \phi_s^{n+1} \tilde{u}_{i,s}}^{1x_i}}{\Delta t \delta_1 x_i}, \quad (5.3.32)$$

$$\frac{\delta_1}{\delta_1 x_i} \left(\frac{\overline{\phi_f^{n+1} 1x_i} \delta_1 p_f^{n+1}}{\delta_1 x_i} \right) = -\rho_f \frac{3\phi_s^{n+1} - 4\phi_s^n + \phi_s^{n-1}}{2\Delta t^2} + \frac{\delta_1 \overline{\rho_f \phi_f^{n+1} \tilde{u}_{i,f}}^{1x_i}}{\Delta t \delta_1 x_i}. \quad (5.3.33)$$

Finally, the auxiliary fluxes F_{j_i} are employed for an efficient discretization of the convective terms of the momentum equations,

$$\frac{\partial \rho_s \phi_s u_{s_i} u_{s_k}}{\partial x_k} \approx \frac{\delta_1 F_{s_k} \overline{u}_{s_i}^{1x_k}}{\delta_1 x_k}, \quad (5.3.34)$$

$$\frac{\partial \rho_f \phi_f u_{f_i} u_{k,f}}{\partial x_k} \approx \frac{\delta_1 F_{f_k} \overline{u}_{f_i}^{1x_k}}{\delta_1 x_k}. \quad (5.3.35)$$

Discretization of the divergence of the configuration stress tensor

For the discretization of the divergence of the configuration stress tensor $\boldsymbol{\sigma}$, appearing in the right-hand side of equation (5.2.2), the divergence theorem gives,

$$\int_K \nabla \cdot (\Gamma_s \nabla \phi_s \otimes \nabla \phi_s) d\mathbf{x} = \int_{\partial K} \Gamma_s \nabla \phi_s \otimes \nabla \phi_s \cdot \mathbf{n} dS, \quad \forall K \in \mathcal{M}, \quad (5.3.36)$$

where the divergence and the inner product with the normal vector $\mathbf{n}$ are applied on the rows of the tensor $\Gamma_s \nabla \phi_s \otimes \nabla \phi_s$. Since each $K \in \mathcal{M}$ is an N -dimensional rectangle (with 2^N faces), equation (5.3.36) can be rewritten as,

$$\int_{\partial K} \Gamma_s \nabla \phi_s \otimes \nabla \phi_s \cdot \mathbf{n} \, dS = \sum_{k=1}^{2^N} \int_{\partial^k K} \Gamma_s \nabla \phi_s \otimes \nabla \phi_s \cdot \mathbf{n} \, dS, \quad (5.3.37)$$

where $\partial^k K$ represents the k -face of the rectangle K . By virtue of the second mean-value theorem of integral calculus, the following holds,

$$\sum_{k=1}^{2^N} \int_{\partial^k K} \frac{\partial \phi_s}{\partial x_i} \Gamma_s \nabla \phi_s \cdot \mathbf{n} \, dS = \sum_{k=1}^{2^N} \Phi_i^k \int_{\partial^k K} \Gamma_s \nabla \phi_s \cdot \mathbf{n} \, dS, \quad i = 1, \dots, N, \quad (5.3.38)$$

where Φ_i^k is the mean value of $\frac{\partial \phi_s}{\partial x_i}$ on the k -face of K . The mean value Φ_i^k is approximated by interpolation,

$$\Phi_i^k = \frac{\overline{\partial \phi_s}^{-1x_j}}{\partial x_i}, \quad (5.3.39)$$

where j is the direction normal to the k -face of K . Next, by applying the difference operator δ_1 , we obtain the following discretization scheme,

$$\sum_{k=1}^{2^N} \Phi_i^k \int_{\partial^k K} \nabla \phi_s \cdot \mathbf{n} \, dS \approx \frac{\delta_1}{\delta_1 x_j} \left(\bar{\Gamma}^{1x_j} \frac{\delta_1 \phi_s}{\delta_1 x_j} \frac{\overline{\partial \phi_s}^{-1x_j}}{\partial x_i} \right). \quad (5.3.40)$$

The above relation represents a generalization of the flux-interpolation technique of Lessani & Papalexandris (2006). In this generalized version, auxiliary fluxes are employed for functions involving differential operators as well. Also, by employing the divergence theorem and repeating the arguments of this subsection, one can obtain an alternative derivation of the original flux-interpolation method of Rhie & Chow (1983) for the convective fluxes.

5.3.3 Numerical treatment of material interfaces

As mentioned above, in the vicinity of material interfaces equations (5.2.2) and (5.2.4) are rendered stiff because of the presence of large volume fraction gradients. In order to remedy such stiffness problems, the proposed algorithm is combined with a regularization scheme. According to it, the step i of the prediction stage is modified as follows.

- 1) Compute the predicted value of the volume fraction ϕ_s^* from the compaction equation,

$$\frac{\phi_s^* - \phi_s^n}{\Delta t} = -\frac{1}{2} \mathbf{u}_s^n \cdot \nabla \phi_s^n. \quad (5.3.41)$$

- 2) For every computational cell A , compute the differences between the value of ϕ_s^* in A with the values of ϕ_s^* in the adjusted cells, *i.e.* compute $|\phi_s^*(A) - \phi_s^*(B)|$, for all $B \in \mathcal{M}$ that they have a common face with A . Then, an interface exists in the direction normal to the common face of A and B if,

$$|\phi_s^*(A) - \phi_s^*(B)| > M,$$

where M is a control-parameter to be determined. Since $\phi_s \in [0, 1]$, a reasonable choice is $M = 0.1$. Numerical experiments have showed that this choice works well in practice.

- 3) Compute the regularized values ϕ_s^r as follows,

$$\frac{\phi_s^r - \phi_s^*}{\Delta t} = -\frac{1}{2} \mathbf{u}_s^n \cdot \nabla \phi_s^n + \epsilon \nabla \cdot (\mathbf{C} \nabla \phi_s), \quad (5.3.42)$$

where ϵ is a regularization parameter and $\mathbf{C}$ is a symmetric 3×3 matrix that for each cell is defined as follows,

- a. For the diagonal components, set $\mathbf{C}_{ii} = 1$ if there is an interface along the i -th direction of the cell's boundaries. Otherwise, set $\mathbf{C}_{ii} = 0$.
- b. For the off-diagonal component, set $\mathbf{C}_{ij} = \mathbf{C}_{ji} = 1/2$, $i \neq j$, if there is an interface along both the i -th and the j -th direction of the cell's boundaries. Otherwise, set $\mathbf{C}_{ij} = \mathbf{C}_{ji} = 0$.

- 4) Proceed to Step ii of the predictor stage.

The parameter ϵ in equation (5.3.42) determines the width of the regularization and, as such, has to be as narrow as possible in order to avoid excessive numerical diffusion. Further, in order to ensure the consistency of the modified equation (5.3.42) with the original compaction equation (5.2.5), ϵ should depend on the grid resolution so that $\epsilon \rightarrow 0$ as $(\Delta x_1, \dots, \Delta x_N) \rightarrow (0, \dots, 0)$. For our purposes we have used $\epsilon = \min\{(\Delta x_1)^3, \dots, (\Delta x_N)^3\}$ which meets these requirements.

The above regularization scheme belongs to the class of splitting methods and employs a viscous modification selectively, at the interface points only. The splitting part does not introduce additional discretization errors, due to the linearity of the compaction equation (5.2.5). Therefore, only the viscous modification can introduce any additional errors. Even so, these errors remain well-controlled by the size of ϵ .

As regards the discretization of the compaction equation (5.2.5) and its modification (5.3.42), the CTU scheme can still be employed for the discretization of the convective terms, without the need for more elaborate schemes. As regards the newly introduced diffusion terms, they are discretized via centered, second-order differences.

Finally, it is important to remark that the regularization of ϕ_s^* that is employed herein is a variation of one of the techniques presented in Tornberg & Engquist (2004). Evidently, other more elaborate schemes could be employed instead. For example, one could directly replace the values of ϕ_s , in the vicinity of interfaces, by those of a smoother, compactly supported function. As shown in Tornberg & Engquist (2004), this procedure yields a formally convergent regularization scheme. In addition, it is possible to represent the discontinuity in an integral form via the use of Dirac functions. Then, a regularization scheme based on the convolution with a mollifier could also be employed.

5.4 Numerical results

The efficiency of the proposed numerical method has been investigated in a series of numerical tests some of which are presented and discussed below. These tests concern the evolution of a granular bulb, immersed in an interstitial fluid, under shear. As mentioned above, simulations of unsteady or multi-dimensional flows of dense granular mixtures have yet to appear in the literature. For this reason, our tests are concentrated on numerical-convergence studies and comparisons with previously published results of steady-state, 1-D flows (to the extent that such comparisons can be made since the previous results have been obtained with different flow models).

All quantities in this Section are given in dimensional form; however we have maintained exactly the same notation as in the previous sections which concerned only non-dimensional variables. In particular, we have dropped the hat symbol to denote dimensional variables.

5.4.1 Mixture parameters

In our study, the various parameters are estimated so as to correspond to a mixture of water with sand. In particular the sand is assumed to be monodisperse with grain diameter $d_p \approx 0.4 \text{ mm}$. The densities of water ρ_f and sand ρ_s are taken equal to 1000 kg/m^3 and 2200 kg/m^3 , respectively. Below we provide expressions for the configuration stress coefficient Γ_s and all transport and relaxation coefficients that appear in the governing equations.

For the configuration stress coefficient Γ_s , we choose the expression that has been employed throughout this dissertation,

$$\Gamma_s = k_2 \rho_s \phi_s, \quad (5.4.1)$$

where k_2 is a material-dependent, strictly positive constant. As mentioned in Chapter 2, the value of k_2 is a common issue that arises in the numerical treatment of equations for granular mixtures. In this study, we again employ the value given in Passman *et al.*

(1986), namely, $k_2 = 4 \times 10^{-8} m^4/s^2$. The effects of varying the value of k_2 are also investigated herein via a parametric study.

For the viscosity coefficient of the granular phase μ_s , we adopt the expression proposed in Savage (1979),

$$\mu_s = \frac{\bar{\mu}_s \phi_s}{(\phi_{\max} - \phi_s)^2}. \quad (5.4.2)$$

In this relation, following Passman *et al.* (1986), the value of $\bar{\mu}_s$ is set at $\bar{\mu}_s = 723 \text{ kg/ms}$. Also $\phi_{\max}$ is the value of the volume fraction that corresponds to the maximum packing of grains. The above expression has a singularity at $\phi_s = \phi_{\max}$, which is supposed to represent the “jamming” effect (rigid-body motion) that grains experience upon attaining their maximum packing. However, the suitability of the functional form of (5.4.2) is yet to be confirmed. More important, the effects of its singularity have not been explored either mathematically or numerically. For this reason, in this study, we assume that $\phi_{\max} = 1$.

On the other hand, since the interstitial medium (water) is a simple Newtonian fluid kept at constant temperature, the fluid viscosity is assumed to be constant and equal to $\mu_f = 1 \times 10^{-3} \text{ kg/(m s)}$.

Further, we assume that the force density $\mathbf{f}$ exerted by the fluid on the particles is given by the following expression,

$$\mathbf{f} = -\phi_s 18 \frac{\mu_f}{d_p^2} (\mathbf{u}_s - \mathbf{u}_f) g(Re_p). \quad (5.4.3)$$

For the function $g(Re_p)$, the empirical relationship of Rowe (1961) is used,

$$g(Re_p) = \begin{cases} 1 + 0.15 Re_p^{0.687}, & Re_p < 1000, \\ 0.01833 Re_p, & Re_p \geq 1000, \end{cases} \quad (5.4.4)$$

where Re_p is the Reynolds number of the grains,

$$Re_p = \frac{\rho_f d_p}{\mu_f} |\mathbf{u}_s - \mathbf{u}_f|. \quad (5.4.5)$$

The function $g(Re_p)$ provides a correction to Stokes law; in fact, it is related to the interfacial drag coefficient C_D as follows,

$$C_D = \frac{24}{Re_p} g(Re_p), \quad (5.4.6)$$

where $\frac{24}{Re_p}$ is the interfacial drag coefficient obtained from the Stokes law at low Reynolds numbers ($Re_p \ll 1$).

Next, since $\mathbf{f} = \delta(\mathbf{u}_f - \mathbf{u}_s)$, the following expression for δ is finally obtained,

$$\delta = \phi_s 18 \frac{\mu_f}{d_p^2} \mathcal{G}(Re_p). \quad (5.4.7)$$

Finally, it is noted that strictly speaking the relation (5.4.7) is applicable to dilute mixtures. As the concentration of the granular materials increases, one expects that the drag coefficient C_D should depend on the volume fraction as well. However, for the purpose of testing the efficiency of the proposed algorithm, the relation (5.4.7) is deemed adequate.

5.4.2 Numerical setup

We consider the flow between two parallel plates in the xz -Cartesian plane, kept at a distance $h = 0.1 \text{ m}$. The flow is driven by the horizontal motion of the upper plate with constant velocity $U_w = 1 \text{ m/s}$. The flow is assumed to be periodic in the streamwise (x) direction with period $l = 0.5 \text{ m}$. The gravity vector points to the negative z direction. Finally, an equidistant mesh of 1000×200 computational cells is used and we employ a CFL number of 5×10^{-3} based on the upper plate's velocity.

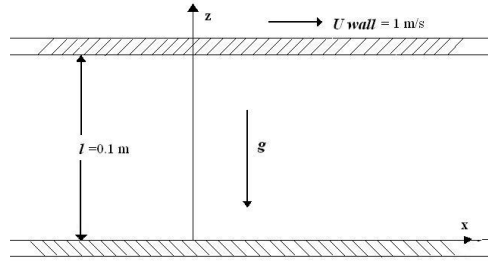


Figure 5.1: Geometry of simple shear flow.

As regards boundary conditions on the two plates, no-slip conditions are prescribed for the phasial velocities $\mathbf{u}_s = (u_s, v_s)$ and $\mathbf{u}_f = (u_f, v_f)$. More specifically, $\mathbf{u}_i \cdot \boldsymbol{\tau} = U_w$ and $\mathbf{u}_i \cdot \boldsymbol{\tau} = 0, i = s, f$ on the upper and lower plates, respectively, where $\boldsymbol{\tau}$ is the tangent vector. Still, experiments with granular materials indicate that no-slip conditions on walls have to be employed with caution. In fact, they are not always appropriate because a non-negligible slip can develop. In these cases, one possibility is to replace the no-slip conditions by a Navier slip-type condition (Artoni *et al.* 2009). Such cases, however, are beyond the scope of the present work. Further, for the phasial pressures, reflecting (zero-Neumann) conditions are prescribed on both plates, in analogy with the incompressible Navier-Stokes equations. Zero-Neumann conditions have also been prescribed for the volume fraction ϕ_s on both plates. Such a boundary condition allows for rearrangements

in the distribution of the granular material in the vicinity of the plates, a property which is important for unsteady flows.

In our simulations, the initial distribution of the volume fraction is given by the following relation,

$$\phi_s^0(x, z) = \begin{cases} 0.2 + 0.6 \sin\left(\frac{\pi(x-a)}{2(b-a)}\right) \sin\left(\frac{\pi(z-c)}{(d-c)}\right), & a \leq x \leq b, c \leq z \leq d, \\ 0.2, & \text{otherwise,} \end{cases}$$

with $0 \leq a, b \leq l$, $0 \leq c, d \leq h$ and is showed in Figure 5.2. This expression represents

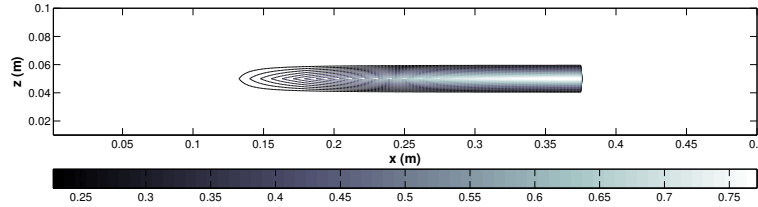


Figure 5.2: Initial distribution for the granular material. A granular bulb of high-particle concentration is placed between the plates and the rest of the domain is filled with a dilute water-sand mixture.

a granular bulb of high-particle concentration embedded in a rectangle of dimensions $[a, b] \times [c, d]$. According to this profile, in the downstream direction there is a sharp interface between this bulb and the surrounding mixture. Across this interface, the volume fraction has a jump equal to $(\phi_s^0)_{\max} - (\phi_s^0)_{\min} = 0.6$. In the other directions, this bulb has a diffuse interface; in other words, there is a smooth transition from the low-particle concentration of the surrounding mixture to the high-particle concentration of the bulb.

In the simulations presented below we have chosen $a = 0.125 m$, $b = 0.375 m$, $c = 0.04 m$ and $d = 0.06 m$. The rectangle that initially encloses the granular bulb accounts for 10% of the computational domain Ω . Initially, the entire mixture is at rest and the flow is induced by the impulsive motion of the upper plate.

5.4.3 Results for unsteady shear flow and numerical convergence

We now present results of our simulations with the parameters and numerical set-up given above. Contour plots of the flow variables at $t = 0.5 s$ are presented in Figures 5.3-5.7(c).

In particular, Figure 5.3 shows the distribution of the volume fraction ϕ_s . We observe that the shearing of the granular material results in a decrease in the volume fraction's values inside the granular bulb. More specifically, the maximum value of ϕ_s has dropped from the initial 0.8 to 0.721, which represents a decrease of the order of 10%. In other words, the granular bulb expands as it is sheared; this phenomenon is known as *Reynold's dilatancy*, (Massoudi & Mehrabadi 2001). Also, due to the onset of the Rayleigh-Taylor instability at the interface between the bulb and the surrounding mixture, the bulb has deformed into a wavy finger-type shape. At the same time, the right upper front of the granular bulb is pulled towards the upper plate due to shear and the bulb's main body descends towards the bottom plate due to gravity.

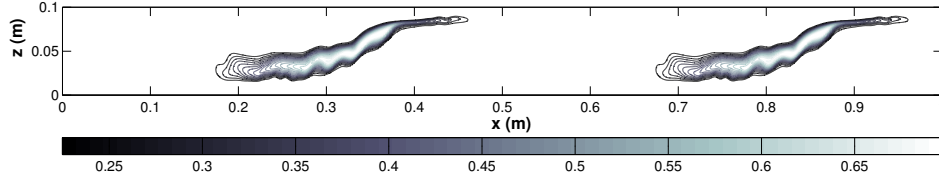
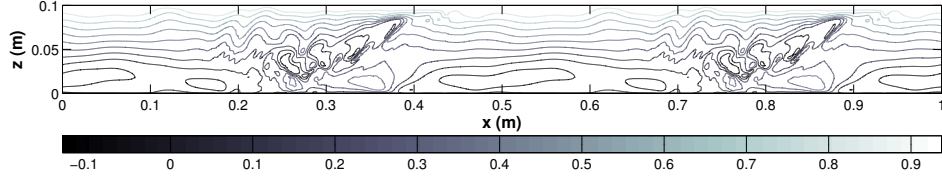


Figure 5.3: Contour plot of ϕ_s at $t = 0.5$ s. Two periods in the x -direction are plotted. The particle concentration inside the granular bulb has decreased due to Reynold's dilatancy. Also, due to the onset of the Rayleigh-Taylor instability, the bulb has deformed into a wavy filamentary shape. Further, due to the applied shear, the right-upper front of the granular bulb is pulled towards the upper plate whereas the bulb's main body descends due to gravity.

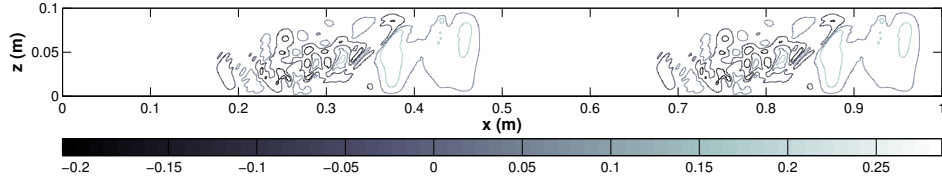
Figures 5.4(a)-5.4(d) display contour plots of the phasial velocities. As expected, the two phases respond in a different manner under shear due to the density and viscosity differences. This results in substantial differences in the distributions of $\mathbf{u}_s$ and $\mathbf{u}_f$ at the early stages of the flow. Further, in the vicinity of the bulb's main body, away from the upper-right front, the motion of the surrounding mixture resembles flow past a bluff body. Indeed, the figure plots show that the surrounding, and less dense, mixture circumvents the bulb and is displaced upwards. Also, these figures confirm that both the fluid and the granular phase exhibit high shear rate close to the upper plate.

The magnitude of the vorticity field of the fluid phase is shown in Figure 5.5. We observe the formation of vortex sheets emanating from the edge of the granular bulb. Further, upon comparison with Figure 5.3, we infer that regions of high vorticity are constrained within areas of low-particle concentration. This is because of the inertial bias between the denser solid particles and the lighter interstitial fluid.

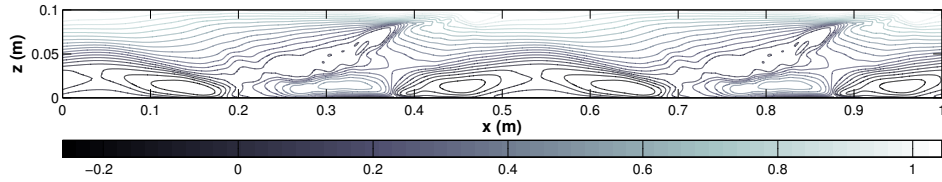
The phasial pressures p_s and p_f are displayed in Figures 5.6(a)-5.6(b), respectively. We observe that the magnitude of p_s is substantially larger than the magnitude of p_f



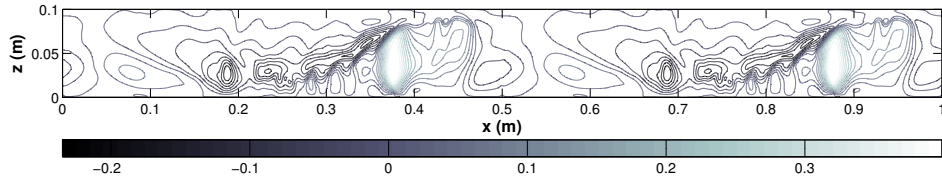
(a)



(b)



(c)



(d)

Figure 5.4: Contour plots of velocities (m/s) at $t = 0.5 s$. Two periods in the x -direction are plotted. (a) u_s , (b) v_s , (c) u_f , (d) v_f . The two phases respond differently under shear, because of the density and viscosity differences. In the vicinity of the bulb's main body, the surrounding, lighter, mixture circumvents the bulb and is displaced upwards, resembling flow past a bluff body. Also, both the fluid and the granular phase exhibit high shear rate close to the upper plate.

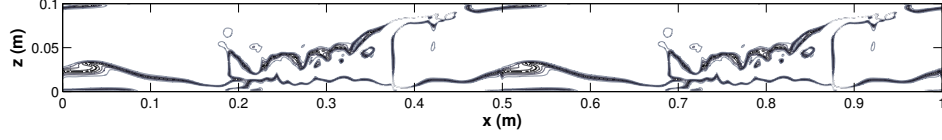
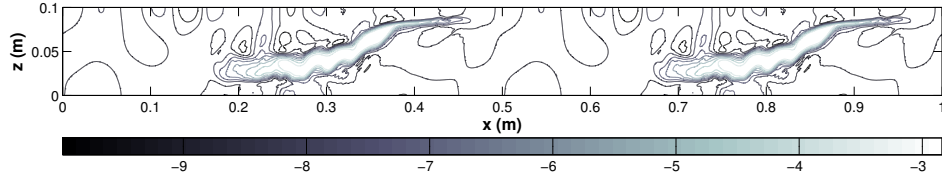
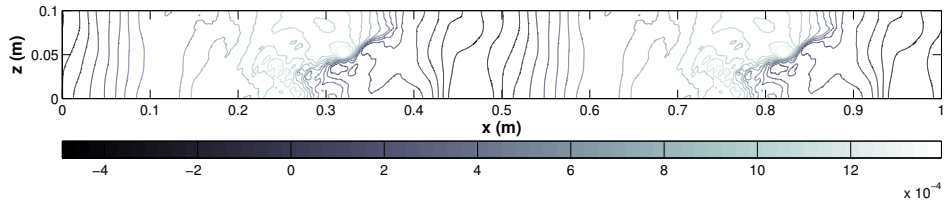


Figure 5.5: Contour plot of the magnitude of the fluid phase vorticity at $t = 0.5$ s. Two periods in the x -direction are plotted. One can observe the formation of vortex sheets emanating from the edge of the granular bulb. Further, due to the inertial bias between the denser solid particles and the lighter interstitial fluid, the zones of high vorticity are constrained within regions of low-particle concentration.

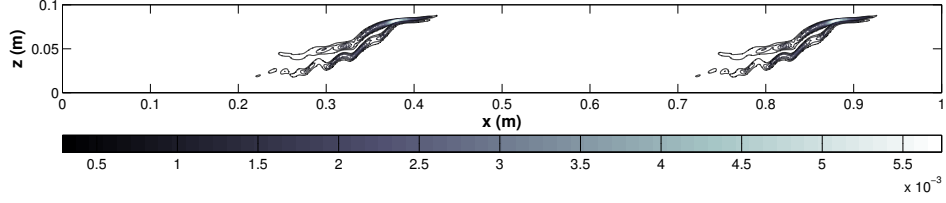


(a)

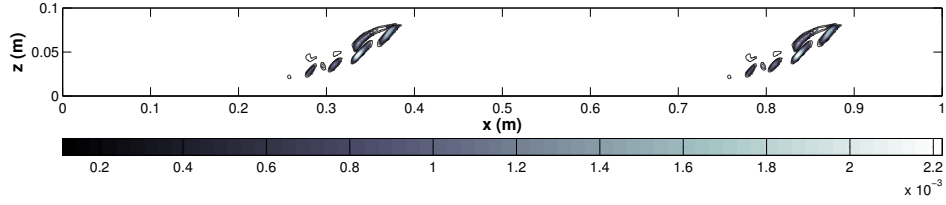


(b)

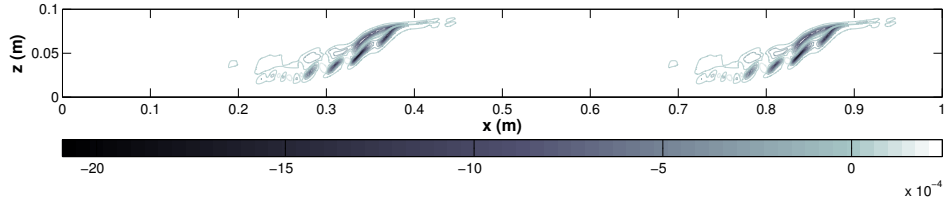
Figure 5.6: Contour plots of phasial pressures p_s and p_f (kPa) at $t = 0.5$ s. Two periods in the x -direction are plotted. (a) p_s , (b) p_f . The phasial pressures are maintained at different levels with a difference at the order of 10 kPa. The magnitude of p_s is larger than that of p_f throughout the domain. Inside the granular bulb, the pressure of the granular phase increases with the particle concentration.



(a)



(b)



(c)

Figure 5.7: Contour plots of configuration stresses (kPa) at $t = 0.5$ s. Two periods in the x -direction are plotted. (a) σ_{11} , (b) σ_{22} , (c) σ_{12} . The contribution of both the normal and the shear configuration stresses is confined in the vicinity of the edge of the granular bulb, where the volume fraction gradients are high. Away from the edge, the configuration stresses decay rapidly to zero.

throughout the domain. In fact, their difference is at the order of 10 kPa . Additionally, it is worth noting that, inside the granular bulb, p_s increases with the particle concentration and its peak value occurs near the points of maximum particle concentration.

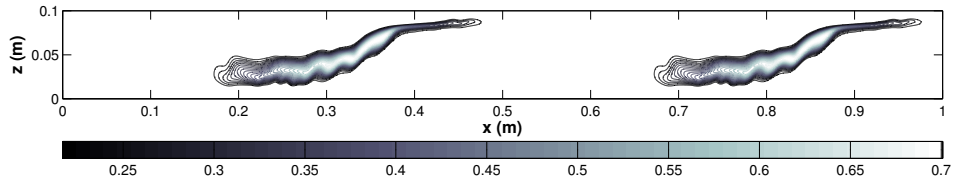
Contour plots of the configuration stress tensor's components are presented in figures 5.7(a)–5.7(c). As expected, the contribution of the configuration stresses maximizes on the edge of the granular bulb, where the gradients of ϕ_s are larger. Interestingly, the maximum values of both normal and shear configuration stresses are of the same order of magnitude, 1 Pa ; this is still three orders of magnitude smaller than the pressure of the granular phase p_s . The smallness of the configuration stresses can be attributed to the small value of k_2 that is employed in the simulations, namely $k_2 = 4 \times 10^{-8} \text{ m}^4/\text{s}^2$. Consequently, away from material interfaces, *i.e.* regions of steep volume fraction gradients, the configuration stresses approach rapidly zero.

In order to obtain further insight on the interplay between gravity, shear and interfacial drag, we have prolonged the simulation until $t = 3.5 \text{ s}$. Some of our numerical predictions at these times are presented below. Figures 5.8(a)–5.8(f) show contours of the volume fraction's distribution in six different time levels, namely, $t = 1, 1.5, 2, 2.5, 3, 3.5 \text{ s}$. It can be verified that the peak value of particle concentration decreases with time, due to dilatancy and particle dispersion. Thus, at $t = 3.5 \text{ s}$, the peak value is $\phi_s = 0.53$ which represents a 34% decrease from the initial peak value of 0.8. The granular bulb continues its descent until it reaches the lower plate where it forms a granular pile. At the same time, the upper-right front of the bulb continues to be pulled by the upper plate due to shear. However, it does not detach from the bulb's main body, leading to the formation of a very long granular finger. The particle concentration inside this granular finger is lower, compared to the bulb's main body one, and reduces continuously with time.

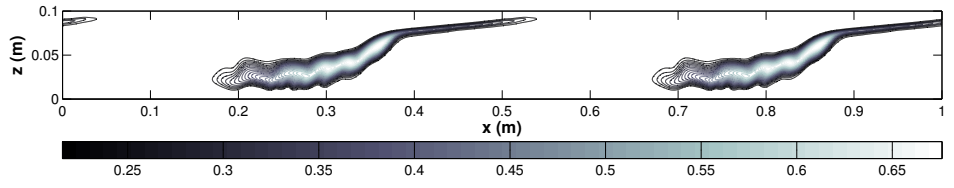
The main characteristics of the phasial velocities do not change much as time evolves, until the formation of the granular pile on the lower plate. In order to study the effect of the relaxation term $\delta(\mathbf{u}_s - \mathbf{u}_f)$, we have computed the evolution of the L^1 -norm of $(\mathbf{u}_s - \mathbf{u}_f)$ which is shown in Figure 5.9. It can be inferred that the difference of the phasial velocities is always non-zero. Instead, it decreases slowly with time. However, when the granular bulb reaches the lower plate, there is an increase in $(\mathbf{u}_s - \mathbf{u}_f)$, due to the deceleration of the bulb and the ensuing pile formation.

At this point, it is worth remarking that this flow is maintained by an external forcing acting on the mixture and, therefore, the mixture remains out of thermodynamic equilibrium. This, in turn, implies that there is no *a priori* guarantee that the two velocities will eventually become equal. In fact, according to earlier studies of *stationary, one-dimensional* shear flows of granular mixtures, the phasial velocities can be maintained at different levels, (Passman *et al.* 1986, Wang & Hutter 1999a).

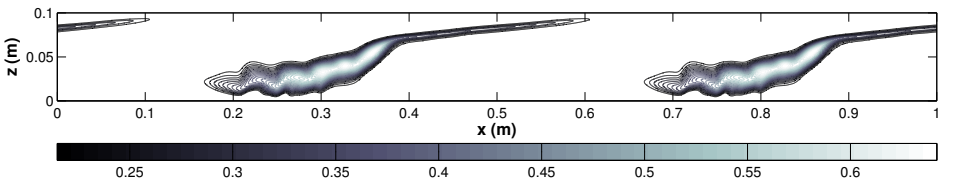
The magnitude of the vorticity field of the fluid phase is shown in Figure 5.10. We can readily infer that the vortex sheets, observed at $t = 0.5 \text{ s}$, have been suppressed because of the dispersion of the solid particles in the interstitial fluid. Still, areas of high vorticity



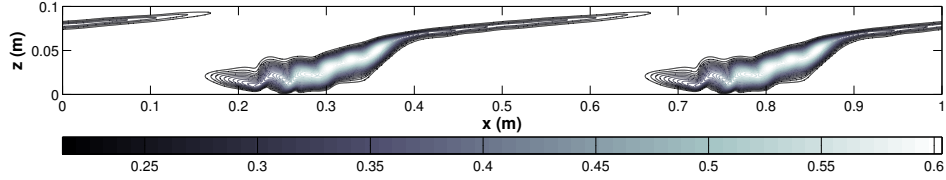
(a)



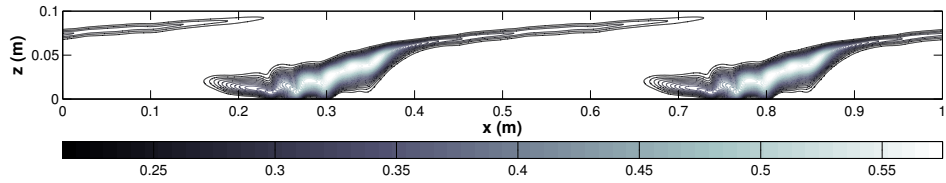
(b)



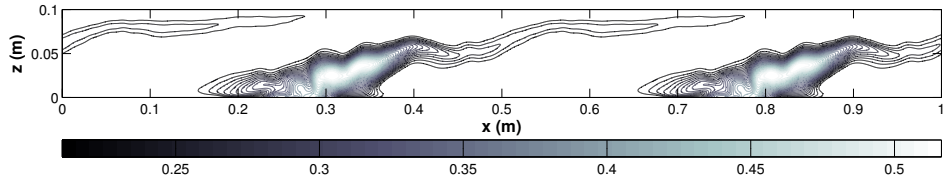
(c)



(d)



(e)



(f)

Figure 5.8: Contour plots of ϕ_s . Two periods in the x -direction are plotted. (a) $t = 1$ s, (b) $t = 1.5$ s, (c) $t = 2$ s, (d) $t = 2.5$ s, (e) $t = 3$ s, (f) $t = 3.5$ s. The particle concentration inside the bulb reduces with time due to dilatancy and particle dispersion. The bulb continues to descend and when it reaches the lower plate a granular pile is formed. Also, the right-upper front continues to be pulled by the upper plate due to shear. However, it remains attached to the main body of the bulb and thus a long granular filament is formed.

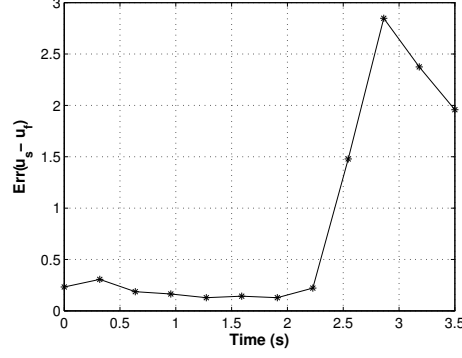


Figure 5.9: Evolution of L^1 -norm of $\mathbf{u}_s - \mathbf{u}_f$. The two phases continue to respond differently under shear. The difference between the phasial velocities decreases slowly but increases, temporarily, due to the deceleration of the granular bulb and the formation of the granular pile.

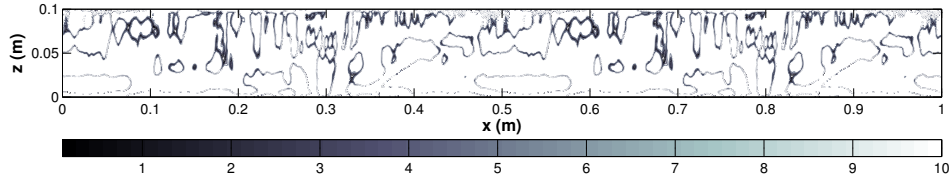


Figure 5.10: Contour plot of the magnitude of the fluid phase vorticity at $t = 3.5$ s. Two periods in the x -direction are plotted. The vortical structures observed at $t = 0.5$ s, have been suppressed due to the dispersion of the solid particles in the interstitial fluid. As in earlier times, the zones of high vorticity are constrained in zones of low-particle concentration.

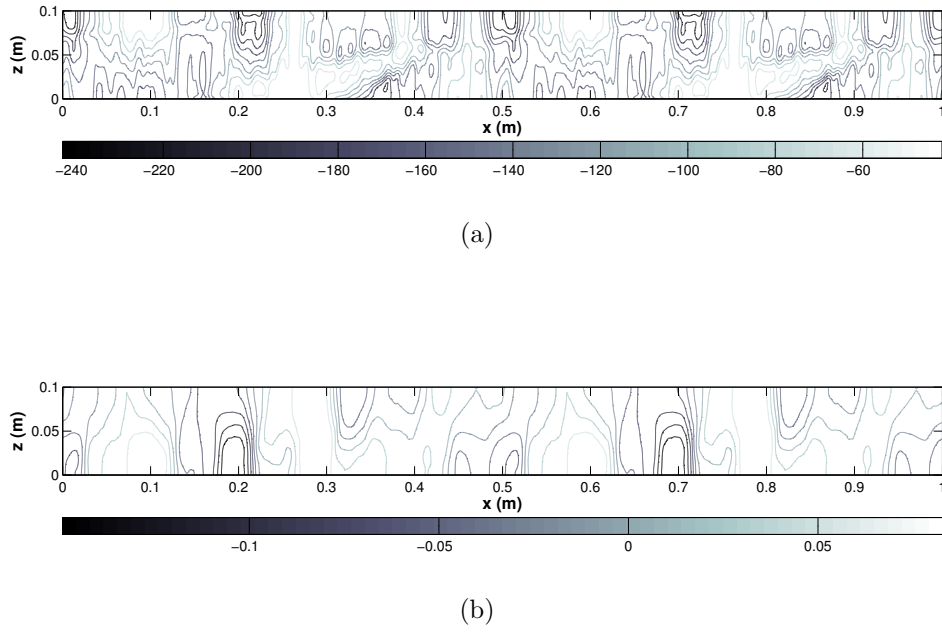
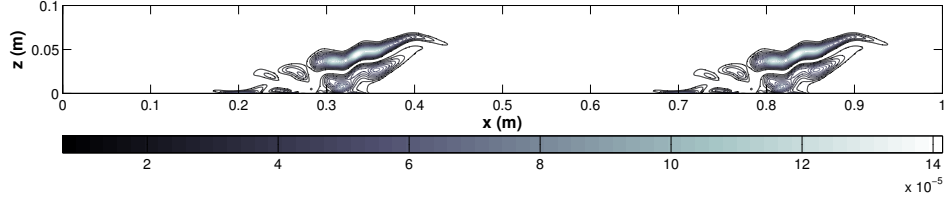
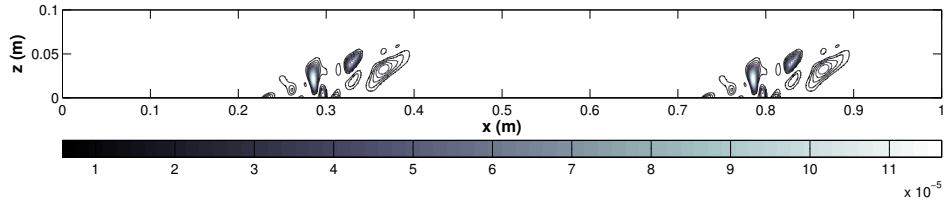


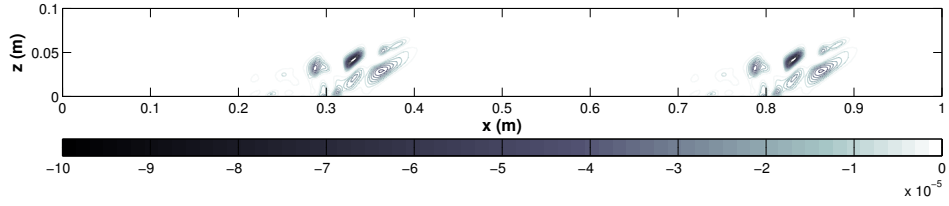
Figure 5.11: Contour plots of the phasial pressures p_s and p_f (kPa) at $t = 3.5$ s. Two periods in the x -direction are plotted. (a) p_s , (b) p_f . The phasial pressures increase until the granular pile is formed, by which time their values are stabilized. The pressure of the granular phase continues to be larger than the pressure of the fluid phase throughout the domain and their difference is at the order of 100 kPa .



(a)



(b)



(c)

Figure 5.12: Contour plots of the configuration stresses (kPa) at $t = 3.5$ s. Two periods in the x -direction are plotted. (a) σ_{11} , (b) σ_{22} , (c) σ_{12} . In analogy with the earlier stages of the flow, the contribution of the configuration stresses is confined in the vicinity of the edge of the granular bulb. However, their magnitude has decreased. This is due to the diffusion of the granular bulb in the carrier fluid which results in lower volume fraction gradients.

are concentrated away from clusters of high-particle concentration.

Figures 5.11(a)-5.11(b) display the phasial pressures at $t = 3.5$ s. According our numerical predictions, both p_s and p_f increase until the formation of the granular pile, at which time their values are stabilized. The pressure of the granular phase continues to be larger than the pressure of the fluid phase and at $t = 3.5$ s, the difference between their peak values has been increased by an order of magnitude and has become equal to, approximately, 100 kPa.

Finally, the components of the configuration stress tensor at $t = 3.5$ s, are shown in Figures 5.12(a)-5.12(c). We observe that the magnitude of both the normal and the shear configuration stresses has decreased to the order of 0.1 Pa. This decrease is due to the diffusion of the grains to the interstitial fluid which, in turn, results in smaller volume fraction gradients. Further, the peak values of both normal and shear configuration stresses always occur on the interface between the granular bulb and the surrounding mixture, *i.e.* in the area where the volume fraction gradients are steeper.

For the case presented here, a grid-convergence study has also been performed. The numerical convergence of the proposed algorithm is examined via the use of the mesh-dependent L^1 -norm of the error for the phasial pressures p_s , p_f , the phasial velocities $\mathbf{u}_s$, $\mathbf{u}_f$ and the (non-constant) mixture density $\rho_{\text{mix}} = \rho_s \phi_s + \rho_f \phi_f$. The mesh-dependent L^1 norm of the numerical error is defined as,

$$Err(F) = \frac{1}{N} \sum_{i=1}^N |f_i - F_i|, \quad (5.4.8)$$

where N is the total number of computational cells, F stands for the exact solution and f is the numerical solution. In absence of an exact solution for the problem in hand, we have replaced F by the numerical prediction obtained with a very fine grid with 2000×400 points.

The following grid sizes were considered in this convergence study: 250×50 , 500×100 and 1000×200 . Figures 5.13(a)-5.14(c) show the results of the grid-convergence study for the variables p_s , p_f , $\mathbf{u}_s$, $\mathbf{u}_f$ and ρ_{mix} , respectively. It can be directly observed that numerical convergence is achieved with refinement of the grid.

5.4.4 Parametric study

In the course of our numerical experiments we have performed a parametric study with respect to k_2 . This is not only a robustness test for the proposed algorithm but it also provides useful insight on the effect that the configuration stresses can have. Herein, we have considered values between $k_2 = 4 \times 10^{-8}$ and $k_2 = 10^{-1} \text{ m}^4/\text{s}^2$ and we compare the numerical predictions at $t = 0.5$ s. The results of our study are summarized below.

As shown in Figures 5.15(a)-5.15(c), the increase of k_2 inhibits the diffusion of the granular bulb in the surrounding mixture. In fact, as k_2 increases so do the configuration

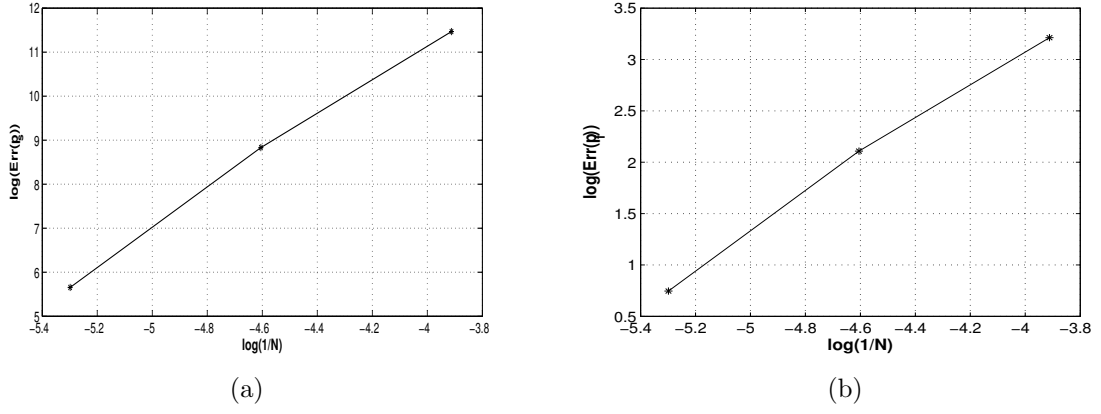


Figure 5.13: Grid-convergence study at $t = 0.5$ s. (a) p_s , (b) p_f .

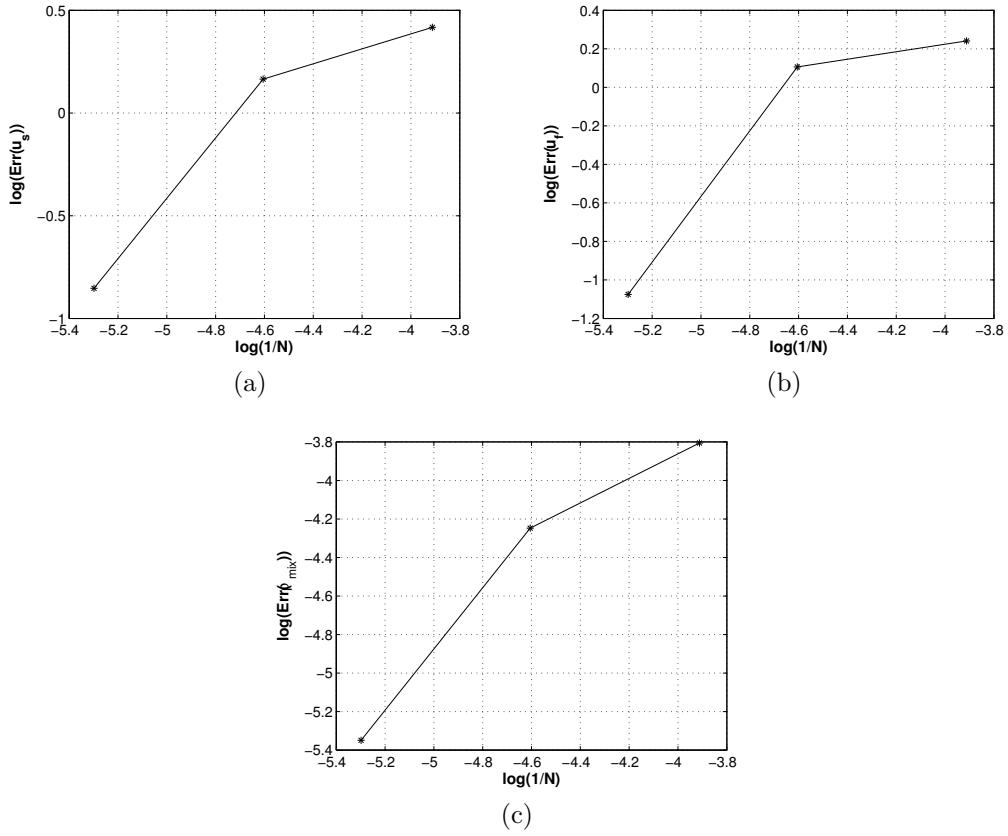


Figure 5.14: Grid-convergence study at $t = 0.5$ s. (a) u_s , (b) u_f , (c) ρ_{mix} .

stresses, *cf.* Figures 5.18(a)-5.18(c), and eventually they dominate in the interplay with the developed shear and the interphasial drag. Consequently, relative grain motions become increasingly more difficult. In other words, as k_2 increases, the granular bulb resembles a rigid body.

Figures 5.16(a)-5.17(c) display p_s and p_f for different values of k_2 . We observe that both p_s and p_f increase with k_2 , however, p_s continues to be larger than p_f for all that values of k_2 that have been employed. In addition, our numerical predictions show that the value $k_2 = 10^{-3} \text{ m}^4/\text{s}^2$ acts as a threshold. For values below this threshold changes in k_2 have a small effect in the peak values of the phasial pressures. By contrast, for values above this threshold, the peak values of both p_s and p_f change considerably with k_2 . Finally, it is worth noting that pressure of the granular phase continue to increase with ϕ_s and attains its peak value on the edge of the granular bulb.

According to our numerical simulations, the variation of k_2 has small effects in the shapes of the configuration stresses. However, the amplitude of both the normal and the shear stresses increases considerably with k_2 , as can be observed in Figures 5.18(a)-5.18(c). These figures show the variation of the configuration stresses maximum values with respect to k_2 .

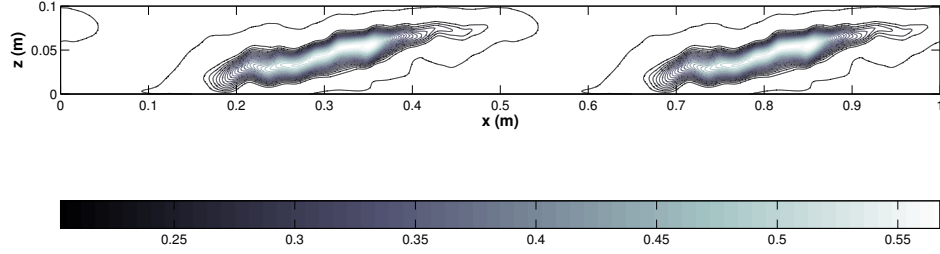
Finally, and for the sake of completeness, vector plots of the normalized velocities $\mathbf{u}_s$ and $\mathbf{u}_f$ for different values of k_2 are shown in in Figures 5.19(a)-5.20(c). It is interesting to observe that, as the contribution of the configuration stresses increases, it becomes more difficult for the surrounding fluid to penetrate the granular bulb. This, in turn, results in the formation of vortices whose diameter increases with k_2 as well.

At this point, it is worth noting that, in our parametric study, we have assessed the effects of increasing the value of k_2 from the initial $k_2 = 4 \times 10^{-8} \text{ m}^4/\text{s}^2$. Evidently, it is possible to conduct a parametric study for smaller values as well. Nonetheless, our numerical predictions have shown that, for $k_2 = 4 \times 10^{-8} \text{ m}^4/\text{s}^2$, the contribution of the configuration stresses is small. Consequently, much smaller values of k_2 are expected to require very fine resolutions, so that the effects of the configuration stresses are properly resolved. However, values of k_2 for which the configuration stresses have a practically negligible contribution are not deemed physically relevant.

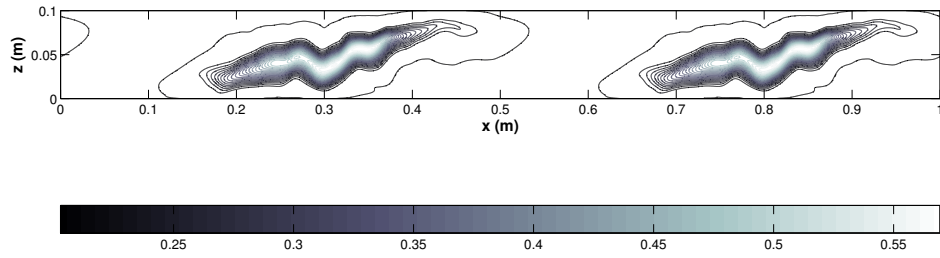
5.4.5 Numerical results for steady-state, 1-D shear flow

Numerical results for steady-state, 1-D shear flows of sand - water mixtures were previously presented in Passman *et al.* (1986), Wang & Hutter (1999a), Massoudi & Phuoc (2005). These results were obtained with three different mathematical models. In this section we present numerical predictions for the same flow, for by using the model (5.2.1)-(5.2.5)

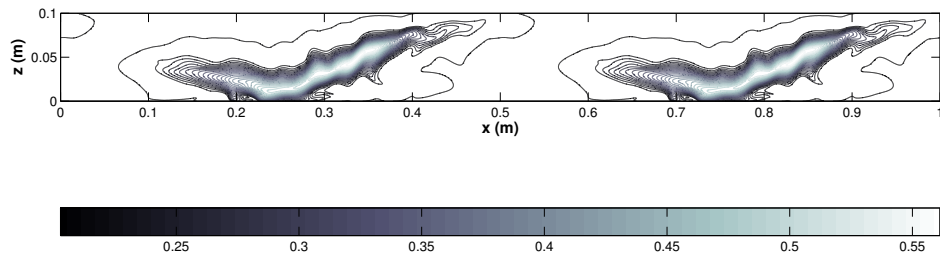
As an additional verification test, we present numerical results for steady-state 1-D shear flows, as predicted by equations and make a qualitative comparison with those of



(a)

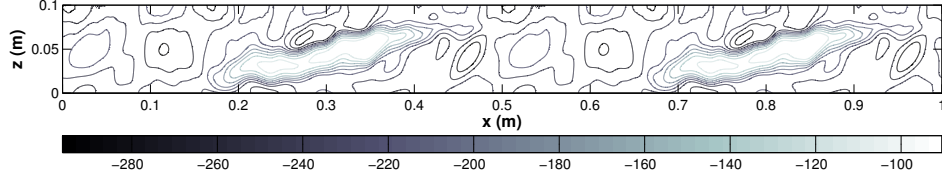


(b)

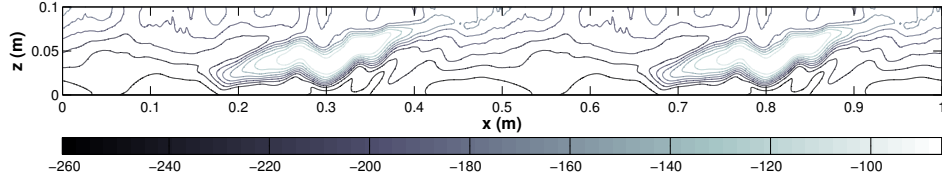


(c)

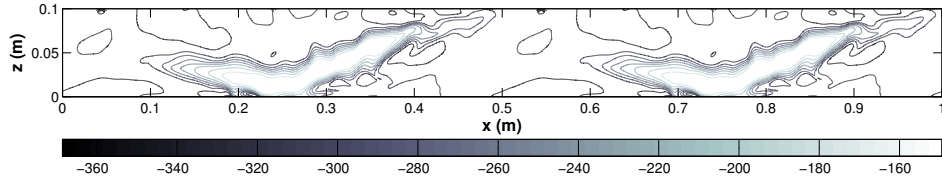
Figure 5.15: Contour plots of ϕ_s for different values of k_2 at $t = 0.5$ s. Two periods in the x -direction are plotted. (a) $k_2 = 10^{-5} \text{ m}^4/\text{s}^2$, (b) $k_2 = 10^{-3} \text{ m}^4/\text{s}^2$, (c) $k_2 = 10^{-1} \text{ m}^4/\text{s}^2$. We observe that the increase of k_2 inhibits the diffusion of the granular bulb in the surrounding mixture. As k_2 increases, so do the configuration stresses which, in turn, makes relative grain motions more difficult; for sufficiently large values of k_2 the behavior of the bulb resembles that of a rigid body.



(a)

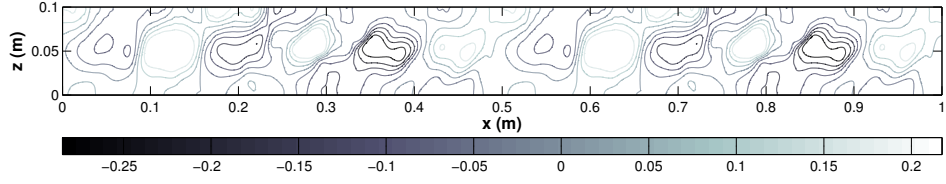


(b)

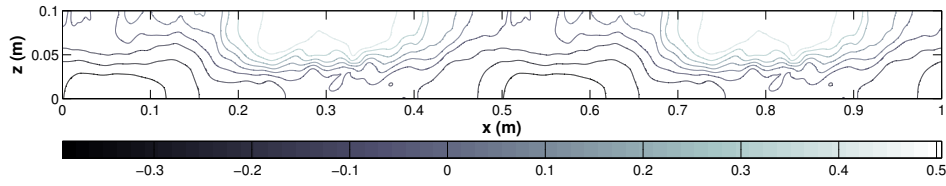


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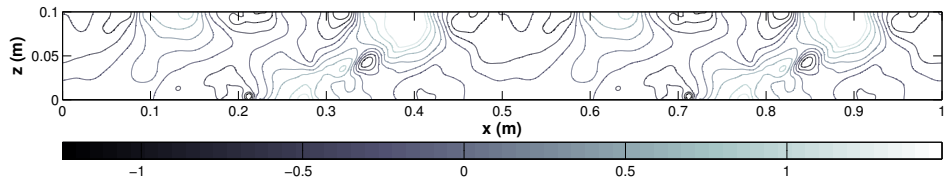
Figure 5.16: Contour plots of p_s (kPa) for different values of k_2 at $t = 0.5$ s. Two periods in the x -direction are plotted. (a) $k_2 = 10^{-5} \text{ m}^4/\text{s}^2$, (b) $k_2 = 10^{-3} \text{ m}^4/\text{s}^2$, (c) $k_2 = 10^{-1} \text{ m}^4/\text{s}^2$. The pressure of the granular phase increases with k_2 . According to our numerical experiments the value $k_2 = 10^{-3} \text{ m}^4/\text{s}^2$ acts as threshold. The peak values of p_s increases with k_2 for values above this threshold. However, it remains rather insensitive for values of k_2 below this threshold.



(a)



(b)



(c)

Figure 5.17: Contour plots of p_f (kPa) for different values of k_2 at $t = 0.5 \text{ s}$. Two periods in the x -direction are plotted. (a) $k_2 = 10^{-5} \text{ m}^4/\text{s}^2$, (b) $k_2 = 10^{-3} \text{ m}^4/\text{s}^2$, (c) $k_2 = 10^{-1} \text{ m}^4/\text{s}^2$. Similarly to the pressure of the granular phase, the value $k_2 = 10^{-3} \text{ m}^4/\text{s}^2$ acts as a threshold for the fluid pressure as well.

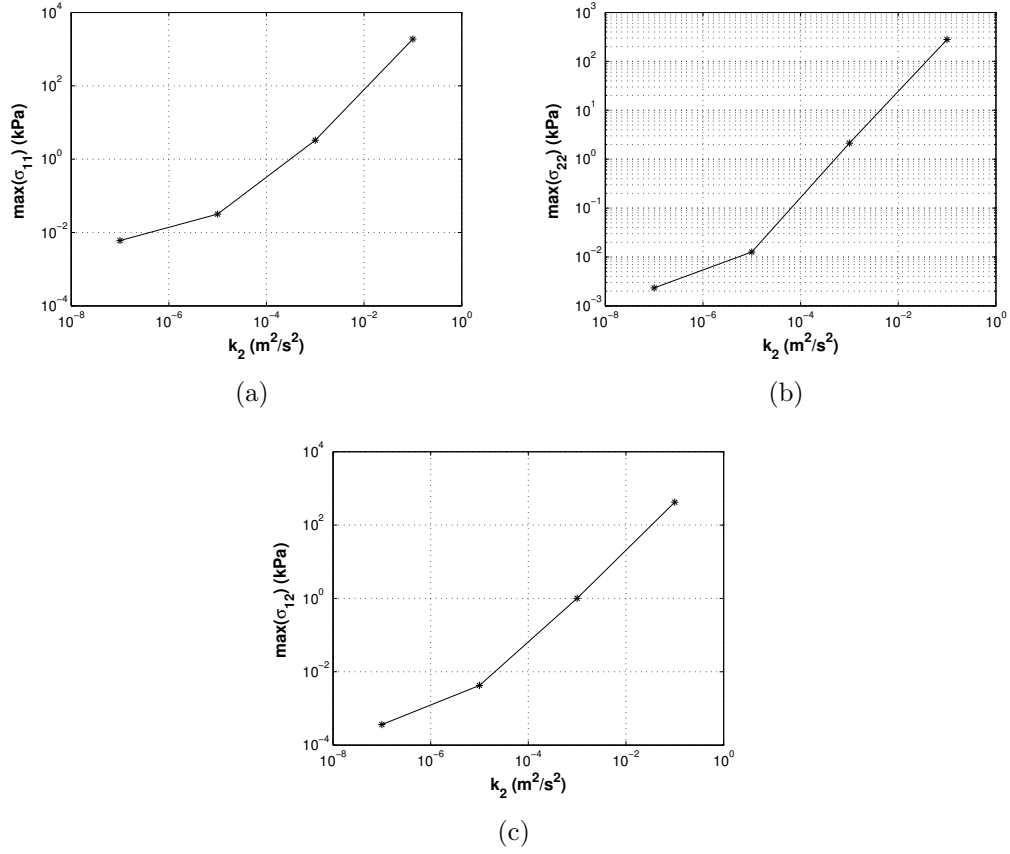
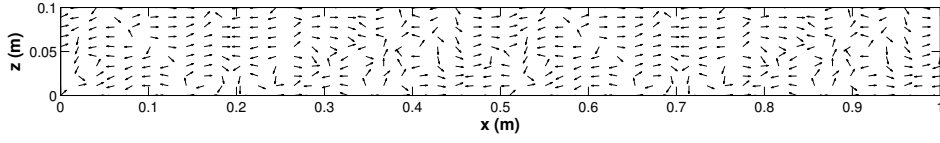
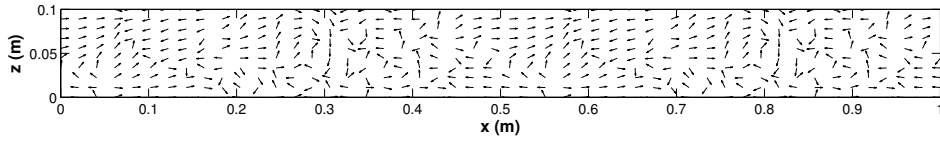


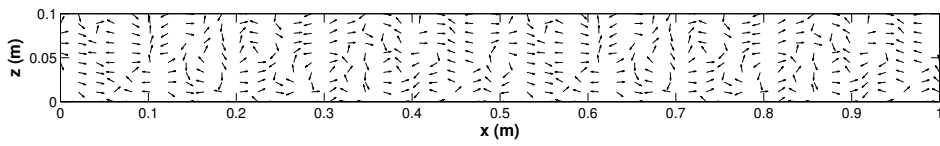
Figure 5.18: Variation of the maximum values of the configuration stresses with respect to k_2 at $t = 0.5$ s. (a) σ_{11} , (b) σ_{22} , (c) σ_{12} . The magnitude of all configuration stresses is quite sensitive to changes in k_2 . In fact, for $k_2 = 10^{-1} \text{ m}^4/\text{s}^2$ the configuration stresses have the same order of magnitude with the pressure of the granular phase.



(a)

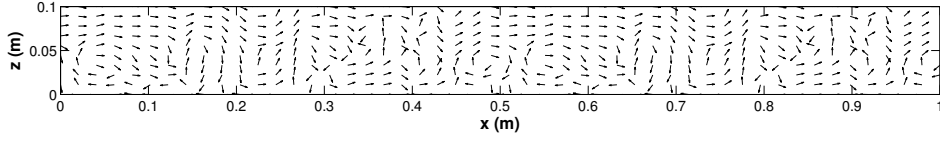


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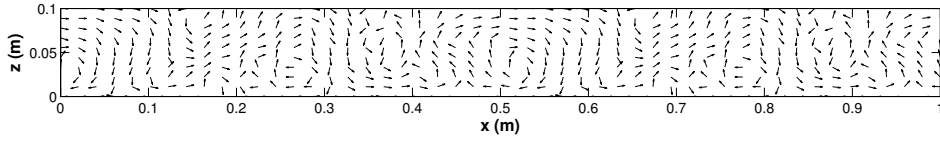


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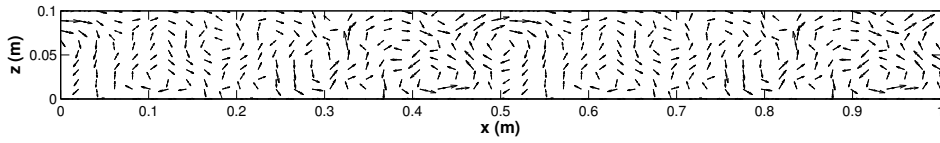
Figure 5.19: Vector plots of normalized $\mathbf{u}_s$ for different values of k_2 at $t = 0.5$ s. Two periods in the x -direction are plotted. (a) $k_2 = 10^{-5} \text{ m}^4/\text{s}^2$, (b) $k_2 = 10^{-3} \text{ m}^4/\text{s}^2$, (c) $k_2 = 10^{-1} \text{ m}^4/\text{s}^2$. As k_2 increases, the regions of high shear rate, close to the upper plate, become thinner. This is due to the higher values of the configuration stresses.



(a)



(b)



(c)

Figure 5.20: Vector plots of normalized $\mathbf{u}_f$ for different values of k_2 at $t = 0.5$ s. Two periods in the x -direction are plotted. (a) $k_2 = 10^{-5} \text{ m}^4/\text{s}^2$, (b) $k_2 = 10^{-3} \text{ m}^4/\text{s}^2$, (c) $k_2 = 10^{-1} \text{ m}^4/\text{s}^2$. We observe that, due to the increase of the configuration stresses with k_2 , it becomes more difficult for the interstitial fluid to penetrate the bulb which enhances the vortex formation.

Passman *et al.* (1986), Wang & Hutter (1999a), Massoudi & Phuoc (2005).

In the previous works the authors have assumed solutions of the form $\phi_s = \phi_s(z)$, $\mathbf{u}_i = (u_i(z), 0, 0)$, $p_i = p_i(z)$, $i = s, f$. Nonetheless, this represents an *ad hoc* assumption. In fact, our numerical simulations have shown that the flow is two-dimensional for the problem in hand. However, in order to enable comparison, in this section we also use these assumptions.

Following Passman *et al.* (1986) and Wang & Hutter (1999a), Dirichlet boundary conditions are assigned to the volume fraction; $\phi_s(0) = 0.7$ and $\phi_s(l) = 0.3$; slightly different values are employed in Massoudi & Phuoc (2005). Further, a linear profile is chosen as an initial condition for the volume fraction. Also, the coefficient δ is set constant and equal to $\delta = 0.1 \text{ kg/m}^3$ whereas for the viscosity of the fluid phase (water) we employ the linear expression that is given in Passman *et al.* (1986), *i.e.* $\mu_f = 1 \times 10^{-3} \phi_f \text{ kg/m}$. Boundary conditions for the other flow variables and material parameters are kept the same as in the two-dimensional simulations. For this study, Ω is assumed to be a square with dimensions $l = h = 0.1 \text{ cm}$. The velocity of the upper plate is set to $U_w = 1 \text{ m/s}$. Finally, a computational grid of 200×200 cells is used. The results presented below correspond to the steady state that is reached shortly after the initiation of the computation.

Figures 5.21-5.23 show the volume fraction, the phasial velocities and the normal stresses of the two phases, where by normal stresses we refer to the quantities, $\tau_{sN} = -\phi_s p_s - \Gamma_s (\frac{\partial \phi_s}{\partial z})^2$ and $\tau_{fN} = -\phi_f p_f$.

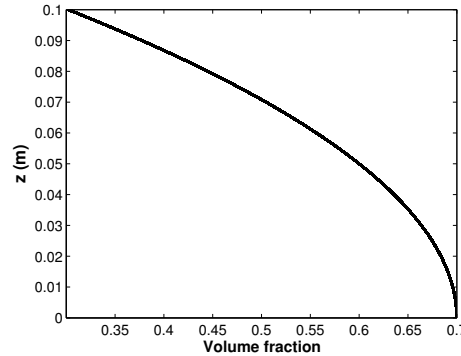


Figure 5.21: Volume fraction profile for steady-state, 1-D shear flow. The volume fraction decreases monotonically from the upper to the lower plate due to the density differences between the two phases.

The volume fraction decreases monotonically from its value at $\phi_s(0) = 0.7$. Further, ϕ_s scales with the square root of x and, in particular, with $\sqrt{(0.7 - x)}$. We note that the value of 0.7 inside the square root is the maximum value of ϕ_s . The phasial velocities are very similar to each other with the fluid phase velocity being slightly larger. Both

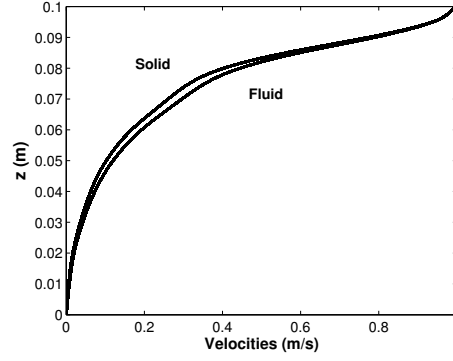


Figure 5.22: Phasial velocities for steady-state, 1-D shear flow (m/s). The phasial velocities are have very similar profiles, however, the velocity of the fluid phase is slightly larger. Close to the upper plate, both phases are subject to high shear rates.

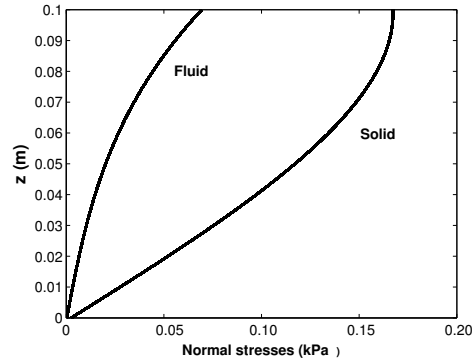


Figure 5.23: Normal stresses for steady-state, 1-D shear flow (kPa). The normal stresses of the two phases increase monotonically with z . The normal stress of the granular phase remains larger than the normal stress of the fluid phase throughout the domain. A similar trend has been predicted in the unsteady flow simulations.

velocity profiles show the existence of a thin bottom layer, with thickness approximately 25 grain diameters, where rigid motion is exhibited. Similarly to the two-dimensional case, this motion transforms smoothly into a high shear rate as we move towards the upper plate. Finally, the normal stress of the granular phase is larger than that of the fluid phase, for all values of z . Their difference maximizes in the upper plate, where $\tau_{s_N} - \tau_{f_N} = 0.978 \text{ kPa}$, and minimizes in the lower plate, where $\tau_{s_N} - \tau_{f_N} = 0.2 \text{ Pa}$. Further, both normal stresses increase monotonically with z .

As regards the volume fraction, the profiles presented in Passman *et al.* (1986), Wang & Hutter (1999a), Massoudi & Phuoc (2005) are in good agreement with the one given in Figure 5.21. We remark, however, that the profiles of Passman *et al.* (1986), Wang & Hutter (1999a) exhibit a sharper decrease than the profile of Massoudi & Phuoc (2005) and the one predicted herein. The velocity profiles of Passman *et al.* (1986), Wang & Hutter (1999a), Massoudi & Phuoc (2005) are qualitatively very similar to the ones predicted by equations (5.2.1)-(5.2.5). Finally, as regards the normal stresses, there are discrepancies between the predictions of all four mathematical models.

The overall qualitative agreement between the predictions of the model in hand with those of Passman *et al.* (1986), Wang & Hutter (1999a), Massoudi & Phuoc (2005) is good. However, since the four models employ different constitutive expressions for the dissipative and relaxation mechanisms of the flow, detailed quantitative comparisons are not possible.

5.5 Conclusions

In this paper we have presented a numerical method for the calculation of constant density flows of fluid-saturated granular materials. The proposed algorithm belongs to the class of generalized projection methods and employs a predictor-corrector scheme for the integration in time. A Poisson equation and a second-order elliptic equation are solved at both the predictor and corrector steps for the computation of the pressures of the granular and fluid phase, respectively. Further, due to the presence of material interfaces in the flows of interest, the algorithm is combined with a local regularization scheme for their numerical treatment.

The efficiency and robustness of the proposed algorithm has been assessed through numerical simulations of a two-dimensional shear flow for a mixture of sand with water. A granular bulb of high-particle concentration has initially been placed between two parallel plates and the rest of the domain has been filled with the interstitial fluid (water). Our numerical results have shown that because of the developing shear stresses and the onset of the Rayleigh-Taylor instability, the granular bulb deforms to a wavy finger-like shape whose length increases with time. At the same time, the bulb descends due to gravity and once it reaches the lower plate it forms a granular pile. Such results had not been published in the literature before.

Finally, results from one-dimensional, steady-state shear flows have also been presented. Our results show that the velocities and the volume fraction are qualitatively very similar to those reported in Passman *et al.* (1986), Wang & Hutter (1999*a*), Mas-soudi & Phuoc (2005). However, the predictions of the normal stresses are different in all four models. This can be attributed to the different constitutive expressions that the four mathematical models employ for the modeling of the dissipative processes that occur in the mixture.

Concluding remarks and perspectives

The objective of this dissertation has been the theoretical and numerical analysis of two-phase flows of granular materials. In the first part, we have generalized the concept of the low-Mach number approximation to multi-phase flows. In our approach we non-dimensionalize the governing equations with respect to a reference thermodynamic state of the phase with the smallest speed of sound and expand all variables in regular perturbation series of the Mach number in this reference state. Further, we have applied it to the two-phase flow model of reference to derive the low-Mach number equations for two-phase flows of granular materials. Similarly to the single-phase case, the low-Mach number equations are simpler than the full, compressible model and, in particular, the momentum equations of the two phases decouple from the corresponding energy equations. Interestingly, for the two-phase flow model of reference, the low-Mach number approximation requires for the phasial temperatures to be equal at the first order. This is because of the appearance of the temperature difference in the compaction equation, whose presence is dictated by thermodynamic considerations. The special cases of constant density flows and of equilibrium limit have also been discussed. As expected, in both cases the low-Mach number equations are further simplified.

In the second part, we have developed a numerical framework for the equilibrium limit of the two-phase flow of reference. At this limit, the model reduces to an overdetermined, albeit integrable, system of nonlinear PDEs that describes the hydrostatics of granular materials. The numerical algorithm that we have proposed is a projection type, successive-over-relaxation predictor-corrector method based on Ladyzhenskaya's decomposition theorem. We have proved that this algorithm is stable and consistent and, therefore, convergent. This algorithm has been employed in a series of numerical experiments in which a mixture of sand with water has been used as a reference. The numerical results have indicated that at the equilibrium limit the two-phase flow model of reference admits solutions which are, intuitively, physically correct. However, comparison with experimental data remains the real verification test.

The third part has also been concerned with the hydrostatics of granular materials. In particular, we have developed an existence and regularity theory for the equilibrium

limit of the two-phase flow model of reference. More precisely, based on weak-convergence methods, we have shown that the equilibrium limit admits at least one weak solution in the sense of distributions. A key role in the existence theory is played by the integrability analysis that we have conducted which has two important corollaries. First, the fortuitous result that the overdetermined system of PDEs is equivalent to a nonlinear PDE with natural growth. Second, the integrability of the system in hand has the physical meaning of the minimization of the Gibbs free energy of the granular material under constant temperature.

The second and third parts of the dissertation are complimentary to each other. When combined, they provide a positive answer to the open question concerning the well-posedness of continuum models for granular materials at equilibrium.

In the fourth part of the dissertation we have proposed a numerical method for the calculation of constant density flows of two-phase granular mixtures. This algorithm employs a predictor-corrector scheme for the integration in time and a projection method for the computation of the phasial pressures. Further, it is combined with an interface detection and treatment scheme based on a local regularization method. The proposed algorithm has been used to investigate numerically a two-dimensional, unsteady shear flow for mixture of sand with water. For these simulations, a granular bulb of high particle concentration has initially been placed between two parallel plates and the rest of the domain has been filled with the interstitial fluid (water). Our numerical results have shown that because of the developing shear stresses and the onset of the Rayleigh-Taylor instability, the granular bulb deforms to a wavy finger-like shape whose length increases with time. At the same time, the granular bulb descends due to gravity and once it reaches the lower plate it forms a granular pile. Results of multi-dimensional, unsteady granular flows had not appeared in the literature before.

In what follows, we describe some research tasks that represent future directions. For the sake of simplicity, theoretical, numerical and experimental tasks are discussed separately.

Theoretical tasks

The volume fraction is axiomatically defined as a normalized Radon-Nikodym density whose integral over a measurable set gives the probability of finding the granular phase inside the set. In the compressible regime, the compaction equation which governs its evolution is a nonlinear reaction-diffusion equation along the streamlines of the granular phase. It is, therefore, interesting to study the compaction equation from the dynamical system point of view. This will help to identify the ergodic properties of the system, which are important for the irreversible evolution of the two-phase mixtures towards equilibrium.

Further, for various types of single phase flows, the low-Mach number expansion has been proved to be convergent, *cf.* Chapter 2. Therefore, it is deemed useful to examine the

conditions under which the low-Mach number expansion for two-phase granular materials is convergent as well.

Finally, it is important to extend the mathematical analysis of the two-phase flow model of reference to flowing conditions, besides hydrostatics, as well. Two such flows that represent a natural next step are steady-state flows and time-dependent Stokes flows, *i.e.* viscosity dominated flows at low Reynolds numbers with negligible convective effects. In both cases the velocities enter the picture, however, the absence of temporal derivatives in steady-state flows and of the nonlinear convective term in Stokes flows are expected to simplify the analysis.

Numerical tasks

The numerical method proposed in Chapter 5 can be employed for the direct numerical simulation of flows over inclined, Poiseuille flows and chute flows. These simulations can provide valuable insight in the behavior of two-phase granular materials and shed light to a number of phenomena that are not currently understood, *e.g.* formation of arches, grain segregation and others. Further, these flows are important for practical applications. For example, simulations of flows over inclined planes can be used for the derivation of criteria of avalanche formation and they can also be used to study the characteristics of avalanche propagation.

In addition, it is important to extend the algorithm for constant density flows to account for the full low-Mach number equations as well. The extended algorithm can be used for the study of transient flows with temperature gradients. For example, one can study numerically anisothermal shearing motions induced by sliding parallel plates, when the two plates are maintained in different temperatures. Such simulation can advance our understanding of some important issues such as: the response of fluid-saturated granular materials to thermal loads, the effects of the thermal non-equilibrium to the flow properties and, in particular, to the evolution of material interfaces, the required time for thermal equilibrium between the phases, *etc.*

Experimental tasks

As mentioned in Chapter 2, there are currently no sufficiently accurate estimates for the configuration part of the Helmholtz free energy. To this end, it is deemed useful to measure experimentally the normal and shear configuration stresses that are developed in a pile at equilibrium. From such measurements empirical correlations for the configuration part of the Helmholtz free energy can be derived.

Further, notwithstanding that isothermal shear and gravity driven flows have been studied experimentally in the past, there is a dearth of such studies for flows with temperature gradients. Since a proposed future direction concerns the numerical study of granular flows with temperature gradients, it would be useful to conduct experimental

studies on such flows as well. Evidently, the comparison between the numerical and experimental results would provide an important means for the validation of the two-phase flow model of reference and its low-Mach number approximation.

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