

The Gray-Thornton Model of Granular Segregation

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Abstract. In this paper, we explore properties of the Gray-Thornton model for particle size segregation in granular avalanches. The model equation is a single conservation law expressing conservation of mass under shear for the concentration of the smaller of two types of particle in a bidisperse mixture. Sharp interfaces across which the concentration jumps are shock wave solutions of the partial differential equation. We show that they can form internally from smooth data, as well as propagate in from boundaries of the domain. We prove a general stability result that expresses the physically reasonable notion that an interface should be stable only if the concentration of small particles is larger below the interface than above. Once shocks form, they are sheared by the flow, leading to loss of stability when an interface becomes vertical. The subsequent evolution of a mixing zone, a two-dimensional rarefaction solution of the equation that replaces the unstable part of the shock can be tracked explicitly for a short time. We conducted experiments to test the continuum model against real flow in a Couette geometry, in which a bidisperse mixture is confined in the annular region between concentric vertical cylinders. Initially, the material is placed in the annulus with a layer of large particles below a layer of small particles. The sample is then sheared by rotating the bottom confining plate, while a heavy top plate is allowed to move vertically to accommodate Reynolds dilatancy. Comparison to predictions of the model show reasonable agreement with the rate at which the sample mixes, and with the rate of the subsequent re-segregation. However, the model naturally fails to capture short-time dilatancy, finite size effects, or three-dimensional effects.

Keywords: Segregation, granular materials, shock waves, hyperbolic conservation laws

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INTRODUCTION

The mechanisms of kinetic sieving and squeeze-exclusion, that induce granular materials of different size but same density to segregate, were incorporated into a mathematical model by Savage and Lun in their classic paper [10] on steady chute flow. More recently, Gray and Thornton [4] gave a different derivation of a time-dependent continuum model using mixture theory. In this paper, we consider the Gray-Thornton model in two space variables (x, z) , and time t . The model is a scalar conservation law describing the evolution of the volume fraction $\varphi(x, z, t)$ of small particles as the material is sheared by a given depth-dependent velocity $u(z)$ in the x -direction (for example down a chute). The velocity $u(z)$, assumed to be time-independent, transports particles down the slope, and induces shear through the shear rate $u'(z)$. The Gray-Thornton equation takes the form

$$\varphi_t + u(z)\varphi_x + (S\varphi(\varphi - 1))_z = 0, \quad -\infty < x < \infty, \quad -1 < z < 1, \quad t > 0, \quad (1)$$

In this equation, segregation is driven by the normal velocity of small particles, taken to be proportional to the volume fraction $1 - \varphi$ of large particles. The constant of proportionality S sets the time scale, the segregation rate. In avalanche flow, the parallel velocity $u(z)$ is roughly linear, and a constant segregation rate is a reasonable assumption. However, for shear induced through a boundary, such as provided by a moving confining plate, the velocity is known to be more closely exponential than linear [9]. In this circumstance, segregation occurs significantly faster in regions of high shear than in those with low shear rate, so that S is properly taken to be a function of z .

Properties of equation (1), and related models, have been explored in a series of papers [3, 8, 12]. The equation is interesting partly because, being a scalar first order equation, it is a simple macroscopic model for segregation, a complicated dynamic process at the grain diameter scale. Moreover, it is a continuum model that seeks to approximate fluid-like flow of a granular material in a context in which flow typically occurs only within a depth of a small number of grains. Nonetheless, the model captures the phenomenon of segregation under shear in a reasonably convincing way.

The equation is also interesting mathematically. Although scalar equations are well understood in many ways, equation (1) has some unusual features that create novel solution structures. The structure of the equation is that it transports particles linearly parallel to the x -axis, but with a speed that is depth dependent, giving a non-constant

coefficient in the transport term. As a consequence, characteristics are curved. A more subtle effect of the non-constant coefficient is seen on shock waves. These are interfaces in space-time across which the solution has a jump discontinuity. We show in this paper that shocks are stable if there is a greater concentration of large particles above the shock than below. The novel feature that appears in solutions is that, because of the shearing, stable shock waves can become vertical, and then lose stability. The emerging solution structure is still not fully understood, but in this paper we report on some progress in understanding what happens immediately after the shock loses stability.

In [6, 7], we considered equation (1) with exponential function $u(z)$ and $S(z) = s|u'(z)|$. However, we restricted attention to solutions independent of x , mimicking conditions in a Couette cell, in which layers of large and small particles are sheared by rotating a lower confining plate.

In §, we consider a general equation

$$\varphi_t + u(z)\varphi_x + (S(z)f(\varphi))_z = 0, \quad -\infty < x < \infty, \quad -1 < z < 1, \quad t > 0, \quad (2)$$

Here, $f(\varphi)$ models segregation normal to the x -axis. We assume it is a smooth convex function on the interval $0 \leq \varphi \leq 1$, with $f(0) = f(1) = 0$, consistent with the idea that the normal flux of small particles should be zero if there are either no large particles or no small particles at that location.

CHARACTERISTICS AND SHOCKS

In this section, we present the basic building blocks of solutions of equation (2), and prove a very general stability result.

We write equation (2) as

$$\varphi_t + u(z)\varphi_x + S(z)f'(\varphi)\varphi_z = -S'(z)f(\varphi) \quad (3)$$

If the solution $\varphi(x, z, t) = \varphi_0$ is known at the point $x = x_0, z = z_0$, and time $t = t_0$, then the PDE shows how to continue the solution to $t > t_0$, by tracing the solution along *characteristics*, given by the ODE system

$$\begin{aligned} \frac{dx}{dt} &= u(z); & \frac{dz}{dt} &= S(z)f'(\varphi); & \frac{d\varphi}{dt} &= -S'(z)f(\varphi); \\ x(t_0) &= x_0; & z(t_0) &= z_0; & \varphi(x_0, z_0, t_0) &= \varphi_0. \end{aligned} \quad (4)$$

Since the final two ODE are independent of x , they form a vector field in the (z, φ) -plane, with a first integral:

$$S(z)f(\varphi) = \text{const.} \quad (5)$$

In particular, when $\varphi = \varphi(z, t)$ is independent of x , this equation is a useful representation of characteristics.

Shock waves are smooth surfaces $z = \hat{z}(x, t)$ across which $\varphi(x, z, t)$ has a jump discontinuity. Let $\varphi_{\pm}(x, t) = \varphi(x, \hat{z}(x, t) \pm, t)$. Since equation (2) is in divergence (i.e., conservative) form in space-time, the normal component of the divergence-free function $(\varphi, u(z)\varphi, S(z)f(\varphi))$ is continuous across the shock:

$$\hat{z}_t[\varphi] + \hat{z}_x u(\hat{z})[\varphi] - S(\hat{z})[f(\varphi)] = 0. \quad (6)$$

Here, we have used the normal $(\hat{z}_t, \hat{z}_x, -1)$ at the shock; the notation $[g(\varphi)] = g(\varphi_+) - g(\varphi_-)$ signifies the jump of a function $g(\varphi)$ across the shock. Consequently, the evolution of the shock, coupled to that of the weak solution $\varphi(x, z, t)$ on either side of it, is given by the PDE

$$\hat{z}_t + u(\hat{z})\hat{z}_x = S(\hat{z})G(\varphi_+, \varphi_-), \quad (7)$$

where

$$G(\varphi_+, \varphi_-) = \begin{cases} \frac{f(\varphi_+) - f(\varphi_-)}{\varphi_+ - \varphi_-}, & \varphi_+ \neq \varphi_- \\ f'(\varphi_-), & \varphi_+ = \varphi_- \end{cases} \quad (8)$$

This equation can be solved by the method of characteristics, once $\varphi_{\pm}(x, t)$ are known. More generally, these functions are found in conjunction with the evolution of the shock wave, as in [1]. To assess stability of the shock, in the sense of hyperbolic conservation laws, we use the Lax entropy condition, which ensures that, for a given initial condition with

a shock, the solution can be continued at least for a short time with the same structure, i.e., the solution φ evolves, and the shock evolves with it. The Lax entropy condition simply guarantees that the characteristic surfaces that would emanate from points on the shock would immediately cross. As a consequence, the solution would be double-valued in the overlapping region, but in fact well-posedness is recovered by constructing a shock lying within the region, and satisfying (7). This construction is standard in the hyperbolic equations literature [11] when the solution is constant along characteristics; it corresponds to *structural* stability (i.e., short-time persistence) of the solution rather than the *asymptotic* (i.e., long-time) stability, commonly referred to in dynamical systems.

Stability of shocks

Since φ is not constant along characteristics, the treatment of stability is not completely standard. Nonetheless, for a stable shock, the two characteristic surfaces in space-time overlap, and the single-valuedness of the solutions has to be recovered by continuing the shock into this region.

We suppose there is a shock wave $z = \hat{z}(x, t)$, with well-defined values of φ on either side at time $t = t_0$. Let $\varphi_{\pm}^0(x) = \varphi_{\pm}(x, t_0)$.

Theorem 1 *The interface $z = \hat{z}(x, t)$ is dynamically stable if $\varphi_+^0 < \varphi_-^0$; it is unstable if $\varphi_+^0 > \varphi_-^0$.*

Proof: The idea of stability is that the characteristic surfaces generated by characteristics originating on the shock at time $t = t_0$, with initial conditions $\varphi = \varphi_{\pm}^0$, should overlap for small $t > t_0$, so that a shock can be fit in between, satisfying the Rankine-Hugoniot condition. To verify this condition, we calculate the speeds of the two characteristic surfaces, and of the shock, normal to the shock at time $t = t_0$. The normal \hat{N} to the shock $z = \hat{z}(x, t)$ is given by

$$\hat{N} = (1, -\hat{z}_x)/(1 + \hat{z}_x^2)^{1/2}. \quad (9)$$

The characteristic speeds λ_{\pm} normal to the shock are given by

$$\lambda_{\pm} = (x', z') \cdot \hat{N}, \quad (10)$$

where $x'(t), z'(t)$ are given by the characteristic equations (4). Thus,

$$\lambda_{\pm} = \frac{1}{(1 + \hat{z}_x^2)^{1/2}} (-u(\hat{z})\hat{z}_x + S(\hat{z})f'(\varphi_{\pm})). \quad (11)$$

The velocity of the shock at fixed $x = x_0$ is given by $(\dot{x}, \dot{z}) = (0, \hat{z}_t)$. Thus, the normal speed σ is given by

$$\sigma = \hat{N} \cdot (\dot{x}, \dot{z}) = \hat{z}_t/(1 + \hat{z}_x^2)^{1/2}. \quad (12)$$

Now, $\hat{z}(x, t)$ satisfies the PDE (7), so that

$$\hat{z}_t = -u(\hat{z})\hat{z}_x + S(\hat{z})G(\varphi_+, \varphi_-).$$

Substituting into (12), we find

$$\sigma = \frac{1}{(1 + \hat{z}_x^2)^{1/2}} (-u(\hat{z})\hat{z}_x + S(\hat{z})G(\varphi_+, \varphi_-)). \quad (13)$$

Comparing (11) and (13), we see that, from convexity of $f(\varphi)$, $\lambda_- > \sigma > \lambda_+$ is equivalent to $\varphi_+ < \varphi_-$, as claimed. ■

Shock formation

In this section, we examine the tendency of shocks to form in the interior of the flow. Shock formation is associated with finite-time blow-up of the gradient of the solution, so that the slope of the graph becomes infinite as a shock forms.

Thus, it makes sense to examine the evolution of the gradient $\nabla\varphi(x, z, t) = (\varphi_x, \varphi_z)$ in a smooth solution $\varphi(x, z, t)$. We do this by differentiating the PDE (2) with respect to x and z :

$$\frac{dv}{dt} = -S(z)f''(\varphi)v - S'(z)f'(\varphi)v \quad (14a)$$

$$\frac{dw}{dt} = -u'(z)v - S(z)f''(\varphi)w^2 - 2S'(z)f'(\varphi)w - S''(z)f(\varphi). \quad (14b)$$

The derivatives on the left hand side are along characteristics, but note that both z and φ evolve along the characteristics, so that in general, the system of ODE has to include the characteristic equations. In general, this is a complicated system to analyze, and complete results are not available. However, we can treat special cases. For the original Gray-Thornton model, in which $u(z)$ is linear, and $S(z) > 0$ is constant, a complete characterization of shock formation is given in [1]. Here, we consider the case of exponential $S(z)$, which is consistent with the experimental configuration described below. Specifically, we assume

$$u'(z) > 0; \quad S(z) = se^{\beta(z+1)}, \quad -1 \leq z \leq 1, \quad (15)$$

with $s > 0$ constant. We prove the following result.

Theorem 2 *Suppose the conditions (15) hold. If either (a) $\phi_x^0(x_0, z_0) \geq 0$, and $\phi_z^0(x_0, z_0) < 0$, then either a shock forms in finite time, or the characteristic emanating from (x_0, z_0) reaches a boundary $z = \pm 1$ before $\nabla\varphi$ becomes singular.*

Proof: First, observe that the w -axis $v = 0$ is invariant for equation (14a). In case (a), it follows from the assumption $v(0) = \phi_x^0(x_0, z_0) > 0$, that $v(t) > 0$ for all $t > 0$ for which the solution of (14) remains bounded. This is the only information we need concerning v in case (a) in order to analyze finite time blow-up of w in equation (14b).

Differentiating equation (5), we obtain

$$S'(z)f'(\varphi)w = -\frac{S'(z)^2}{S}f(\varphi) \quad (16)$$

Substituting into equation (14b), we get,

$$\frac{dw}{dt} = -S(z)f''(\varphi)w^2 + \left(\frac{S'(z)^2}{S(z)} - S''(z)\right)f(\varphi) - u'(z)v < -S(z)f''(\varphi)w^2, \quad (17)$$

since $v > 0$, $\frac{S'(z)^2}{S(z)} - S''(z) = s\beta^2 e^{\beta(z+1)} > 0$ and $f(\varphi) \leq 0$. Now z and φ are evolving on the characteristic emanating from (x_0, z_0) , but both $S(z) > 0$ and $f''(\varphi) > 0$ are bounded from below by positive constants, in the physical domain $-1 < z < 1, 0 \leq \varphi \leq 1$. Thus, there is $k > 0$ such that

$$\frac{dw}{dt} < -kw^2, \quad (18)$$

at least until the characteristic reaches the boundary.

Since $w(0) = \phi_z^0(x_0, z_0) < 0$, then (18) implies that $w(t) \rightarrow -\infty$ in finite time, since

$$w(t) \leq \frac{w(0)}{1 + kw(0)t}.$$

■

Remarks: 1. If $w(0) > 0$, then the dynamics are somewhat more complicated, with the characteristics rolling over as $w(t) = \varphi_z$ changes sign. Once this happens, the conditions of the theorem are satisfied, and a shock forms. However, to prove this rigorously, we would need to establish that $w(t^*) < 0$ for some finite time $t = t^*$, in order to show that $w(t) \rightarrow -\infty$. The evolution of $w(t)$ is controlled by $v(t)$:

$$\frac{dw}{dt} < -u'(z)v. \quad (19)$$

Now, $u'(z) \geq k_0 = \min_{-1 \leq z \leq 1} u'(z) > 0$. Provided $v(t) > 0$ is bounded away from $v = 0$, then $w(t)$ crosses the v -axis in finite time.

2. In the simpler case of the original Gray-Thornton model, in which $u(z)$ is linear, $S(z)$ is constant, and $f(\varphi) = \varphi(\varphi - 1)$, system (14) simplifies considerably. Solutions φ are constant on characteristics, and the various terms that are now constants rather than variable can be eliminated from the equations by scaling, leaving the system

$$\frac{dv}{dt} = -2vw \tag{20a}$$

$$\frac{dw}{dt} = -v - 2w^2. \tag{20b}$$

Somewhat surprisingly, this system can be solved explicitly:

$$v(t) = \frac{v_0}{q(t)}, \quad w(t) = \frac{w_0 - v_0 t}{q(t)}, \quad q(t) = 1 + 2w_0 t - v_0 t^2, \tag{21}$$

where $v(0) = v_0, w(0) = w_0$. Consequently, conditions for shock formation can be specified precisely, and the time at which the shock forms can be expressed exactly in terms of the initial conditions [1]: shocks form if and only if $q(t)$ has a positive zero.

Shock breaking

Once a shock wave forms, it evolves according to the PDE (7), as discussed above. In this subsection, we show that certain shocks lose stability, due to being sheared by the flow. To avoid the complicated problem of how the solution evolves on either side of the shock, let's simplify the issue. In fact, let's take $\varphi_+ = 0, \varphi_- = 1$, so that the shock is stable. Then $G(\varphi_+, \varphi_-) = 0$ in equation (7). Furthermore, if we take $u(z) = z$, the original form of the Gray-Thornton model, then (7) becomes the inviscid Burgers equation [13] for the shock location $z = \hat{z}(x, t)$:

$$\hat{z}_t + \hat{z}\hat{z}_x = 0. \tag{22}$$

Now solutions of Burgers equation are known to break in finite time, unless they are monotonically increasing. Consequently, any shock wave solution satisfying (22) will become vertical in finite time if $\hat{z}_x < 0$ anywhere, at any time. This makes sense, because the interface is being sheared by the depth-dependent velocity. In the classical theory of Burgers equation, the solution can be continued as a shock wave, but here, the solution itself is a shock, and as it breaks, it loses stability because a middle section is now unstable: it has $\varphi_+ < \varphi_-$, but because the section has turned over, $\varphi = \varphi_+ = 0$ below the shock, and $\varphi = \varphi_- = 1$ above the shock. (See Theorem 1.)

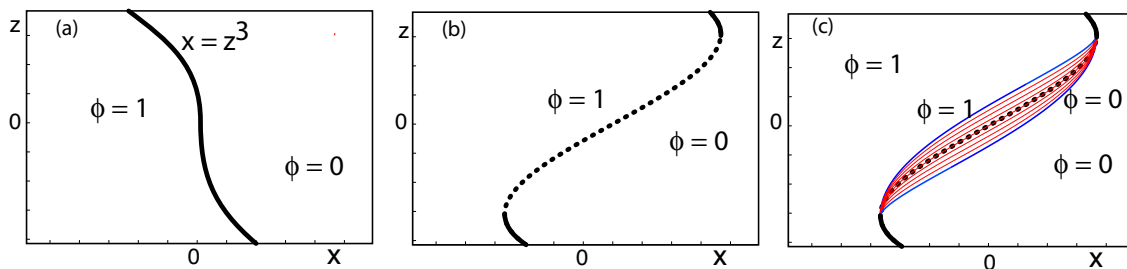


FIGURE 1. Solutions of (1), with $u(z) = z$ and initial condition (23). (a) Initial condition. (b) Evolved shock showing unstable section. (c) Solution with rarefaction wave, $t < 1/12$.

The solution is in fact continued using the method of characteristics to introduce a rarefaction wave, corresponding to a mixing zone. Consider an initial condition

$$\varphi(x, z, 0) = \begin{cases} 1, & x < -z^3, \\ 0, & x > -z^3. \end{cases} \tag{23}$$

in which the interface $x = -z^3$ is already vertical at $z = 0$ in the initial condition. Then to see the shock breaking, it is convenient to consider the parameterization of the shock by z rather than x : $x = \hat{x}(z, t) = -z^3 + zt$ satisfies the evolution equation for \hat{x} :

$$\hat{x}_t + z\hat{x}_z = 0. \quad (24)$$

Then for $t > 0$, $\hat{x}(z, t)$ is non-monotonic; it is increasing between $z = \pm\sqrt{\frac{t}{3}}$, the unstable section of the evolved shock wave, and decreasing outside this interval. The solution with a rarefaction wave is valid for $t < \frac{1}{12}$, and is shown in Fig. 1. Beyond $t = \frac{1}{12}$, the solution becomes more complicated, but can be calculated with a simple numerical algorithm, as described in a forthcoming paper [1].

EXPERIMENTS WITH A COUETTE CELL

Experiments were conducted in an annular Couette cell, in which a mixture of small and large particles is sheared between concentric vertical cylinders. Here, we summarize results that will appear in a pair of papers [6, 7]. The experimental setup and protocol are described in detail in [2]. A bottom confining plate is rotated at constant frequency $f = 49 \pm 0.5$ mHz, approximately 3 rpm, and a top plate exerts a controlled pressure on the particles (0.36 ± 0.008) *mg*, where *mg* is the total weight of the particles and the variation in force is due to the stretching of springs partially supporting the plate. The top plate is free to move vertically, thereby accommodating dilation and consolidation. Experiments reported here were carried out with spherical glass beads, of diameters 3 mm and 6 mm. Different size ratios, and variations in other experimental conditions are described in [2].

The purpose of the experiment is to compare predictions of the Gray-Thornton model quantitatively with experimental data. We find that the model captures the gross behavior of mixing and segregation as the material is sheared, even though it cannot reproduce significant features of the flow. To reflect conditions in the experiments, we make several assumptions concerning the model. First, we assume that, although mixing and segregation involve three-dimensional motion of particles, we consider solutions that depend only on the vertical variable z . This assumption is reflected in the initial configurations chosen for the experiments, in which a layer of small particles is placed above a layer of large particles. Second, we assume that the segregation rate is proportional to the shear rate, reflecting the notion that there should be more segregation when the sample is sheared faster. As the beads mix, they occupy significantly less volume, so that the top plate falls slightly. Later, as the mixture resegregates, they begin to occupy more volume, and the top plate rises. We assume that the degree of segregation is quantitatively measured by the height of the top plate, with the connection between model solutions and the height of the top plate being provided by a packing fraction density.

In the experiment, we take two types of measurements. From high speed images we extract particle trajectories, which lead to an average velocity profile $u(z)$ that is roughly independent of time and ϕ . The second measurement is to record the height $H(t)$ of the top plate as a function of time t .

Figure 2(a) summarizes averaged velocity data, and a fit by an exponential function $u(z)$. The horizontal bars indicate the spread of the data, using the width of a parabolic fit at half height. In Fig. 2(b), we show the corresponding shear rate plot and a fit by an exponential function. The solid line in Fig. 2(a) is derived from the same exponential function. Near the top (resp. bottom) of the cell, a layer of large (resp. small) particles forms quickly, creating an effective boundary. Consequently, the velocity profile and shear rate are determined from data in the middle section shown in the figure, normalized to $0 \leq z \leq 1$.

In Figure 3 we show the time series of the height $H(t)$, together with the result of solving the mathematical initial value problem with shear rate given by the experimental data. The mathematical problem yields a function $\phi(z, t)$, the volume fraction of small particles on a fixed domain $0 < z < 1$. To extract a physical height from this function, we employ a volume packing fraction $\rho(\phi)$, based on results from MD simulations of static packings [5]. The packing fraction allows us to translate the local particle fraction into a real volume. Since the cross-sectional area of the apparatus is constant, and the initial volume of particles is known, we then simply have to integrate the effective volume over the fixed domain $0 \leq z \leq 1$ in order to compute a height function $h(t)$, which we refer to as the proxy height. In Fig. 3, we observe that the mixing rate (where $H(t)$ is decreasing) is well captured by the model. Moreover, although the resegregation in the model is delayed, compared to the experimental observation, nonetheless the model and experiment agree remarkably well in the rate of resegregation. In particular, both model and experiment suggest different rates for mixing and resegregation.

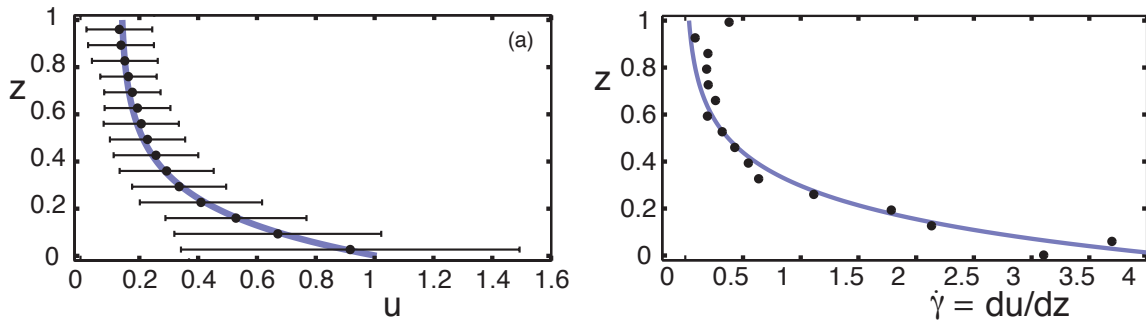


FIGURE 2. (a) Measured velocity profile $u(z)$ (\bullet) in the region $0 \leq z \leq 1$, showing the exponential fit to the shear rate data in (b). Velocities are scaled so that $u(0) = 1$. (b) Shear rate $\dot{\gamma} = |du/dz|$ within the region $0 \leq z \leq 1$. The solid line is the fit to an exponential function.

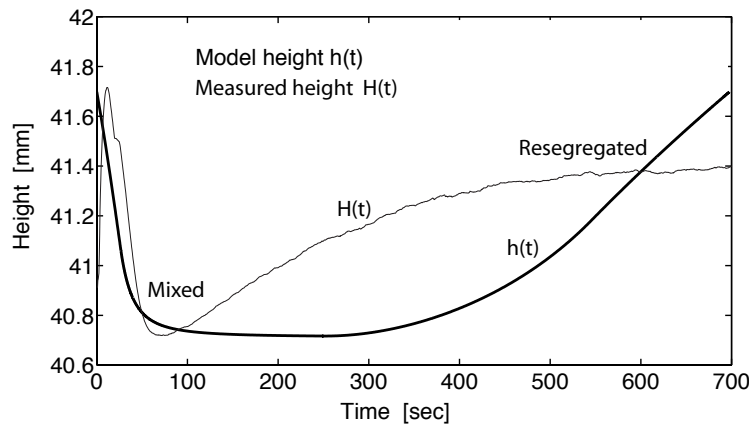


FIGURE 3. The experimentally-measured height $H(t)$ and the calculated height $h(t)$.

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