Peristaltic transport of a particulate suspension in the small intestine

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Food transport through different sections of the gastrointestinal tract for the purposes of digestion and waste removal is an essential physiological function for life. Mechanical and chemical breakdown of food takes place throughout the gastrointestinal tract. Periodic muscular contraction and relaxation of the intestinal walls agitate, mix and propel the multiphase digesta along the intestines. Experimental measurement of flow inside the intestines is difficult therefore understanding of food transport through the majority of the gut is limited. Computational models for predicting the transient behaviour of intestinal content subject to peristaltic activity offer the possibility for assessing the digestive performance of different foods. We present a numerical model for peristalsis in the duodenum using a suspension of rigid particulates in a viscous Newtonian fluid to represent simple digesta. This consists of a thin viscoelastic membrane representing the gut wall coupled to the particle-based methods Smoothed Particle Hydrodynamics (SPH) and Discrete Element Method (DEM) which are used to predict the motion of liquid and solids content respectively. Peristaltic waves travel along the gut wall resulting in active muscular contractions and relaxations of the gut. The bulk motion of the content shows both phases move together due to the laminar nature of the flow with only very short-term inter-phase differences found in the relaxation region and in the wake of the contraction. Propulsive events were found to cause significant non-homogeneity of the solids distribution along the length of the duodenum. The inclusion of solids mildly modifies the overall propulsive flow behaviour and the retrograde jet in the wake of the contraction. In the absence of solids and connective tissue constraints, a transverse wobbling instability in the fluid filled viscoelastic tube is observed.

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1. Introduction

There is great interest in the formulation of new food structures [1,2] to improve digestive health by providing targeted digestive functionality, improved food tolerance response, enhanced nutritional uptake, and reduced salt, sugar and fat levels while maintaining a desirable sensory experience. The design and development of such structures requires comprehensive knowledge about the effects of manufacturing methods on the matrix of a given food and how this food is digested via physical and biochemical processes at each stage along the gastrointestinal (GI) tract. For example, baking has been found

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to affect the digestibility of gluten proteins [3] and the availability of glucose for intestinal absorption can be increased with an appropriate formulation [4].

Digesta composition, physiological structure and function, and the type of motor patterns present all differ along the length of the GI tract. Our understanding of transport and mixing mechanisms in less accessible regions of the gut (such as the small bowel and proximal colon) is relatively poor. In the past decade, there have been many important technical advances related to *in vivo* monitoring of gut motility [5]. Of these, the measurement techniques that appear most relevant to intestinal flow are high-resolution manometry [6], impedance measurements of bolus transit [7], ingested wireless capsules [8], and mapping of GI electrical activity [9]. This research is generally motivated by two principle aims: clinical studies which seek to identify abnormal motor patterns responsible for functional gastrointestinal disorders [10,11]; and to understand the digestive properties of different food structures for improved nutritional outcomes [12,2,13]. *In vitro* studies of isolated segments of animal gut suspended in an organ bath allow for more detailed direct measurement of bolus transport, pressures and wall shape [14,15]. As pioneers of this methodology, Costa et al. [16] have recently demonstrated that active and passive contractions and relaxations can be sufficiently differentiated based purely on manometric pressure measurements and spatiotemporal imaging of wall distension. *In vitro* studies of content mixing in the small bowel indicate that mixing does not occur optimally in small sections of the gut but rather is a slow process distributed over the full length of intestine [17]. This facilitates the slow timescales of diffusion of enzymes into the digesta for nutrient digestion.

A complementary approach to *in vivo* measurement and *in vitro* lab studies is the development of mathematical models that can describe the relationships between changing wall geometry, content pressures and flow. Models of digestive processes [18,19] based on Computational Fluid Dynamics (CFD) methods provide a means for studying healthy and abnormal digestion. Models of esophageal flow tend to be more mature due to the availability of direct measurement of bolus transport. Consequently, such models can now provide valuable insights into the function of circular and longitudinal muscle contractions during swallowing [20] as well as the role of the mucosal layer [21]. The remainder of the GI tract is less well studied by direct measurement and in silico models may be used together with CFD models to study digestive function. Models of content mixing and gastric emptying from the stomach have been undertaken by Ferrua et al. [12] and Harrison et al. [22]. Multiscale models linking cellular function to muscle activation and flow of digesta have been developed for the stomach [23] and the intestine [24]. Lim et al. [25] used a Lattice Boltzmann model to study mixing around small intestine villi and their effect on nutrient absorption. Under muscular tension the gut wall changes both at a macroscopic and a microscopic scale by the formulation of microfolds [26]. These generate a cyclic approximation and separation of villi with strong flow consequences. Hari et al. [27] studied peristaltic transport in the duodenum coupled to porous transport of glucose across the gut wall. Love et al. [28] compared mixing patterns for segmentation and propulsive motor patterns for different rheologies. Trusov et al. [29] have proposed a meso-level model framework for multiphase flow through the stomach and duodenum which incorporates peristaltic mass transport, chemical absorption and secretion of digestive juices. None of these preceding models attempt to solve for the two-way fluid-structure interaction (FSI) between digesta and the deformable tissues of the gut wall but rather use prescribed wall kinematics so that the wall shape and motion are inputs to the model. The gut wall is compliant and its shape changes in response to content pressures and the changes in muscular tension during active contractions and relaxations. The deformation of the gut wall in turn modifies the flow of content until the wall tension and content pressures equilibrate. Particle-based methods provide a natural framework for solving such FSI problems. Sinnott et al. [30] used this type of method to identify the role of descending inhibitory reflex in generating a toroidal vortex within the large intestine and showed that this is an important mechanism for intestinal transport and mixing. The mixing of different viscosity Newtonian content for this peristalsis model was investigated in [18]. The study presented here uses a similar model to investigate flow through the duodenum.

Partially digested food in the form of a slurry of solids and liquid exits the stomach though the pyloric sphincter [22] and discharges into the duodenum, which is the first section of the small intestine. Gastric digestion typically reduces solid food down to 1-2 mm size fragments [31] which become the input material for the next stages of mechanical and chemical digestion in the small intestine. The majority of enzymatic breakdown of food and significant nutrient absorption occurs in the short (roughly 25 cm) duodenal section. Following this, digesta are transported downstream into the jejunum. Bile and pancreatic juices are secreted in the duodenum and aid chemical digestion. Receptors in the duodenal wall regulate the rate at which the stomach empties [32] for different food compositions. Fluid content can pass from the stomach into the duodenum without muscular restriction [33]. In particular, large amplitude tonic contractions of the duodenum due to the presence of acids or lipids result in delayed gastric emptying [34]. In general, individual sections of the gastrointestinal (GI) tract have unique motor control and can synchronize their motor activity with neighbouring sections. This occurs throughout the GI tract except in the transition from stomach to small intestine. There is a lack of continuity in the coordination of peristaltic activity from the antrum of the stomach into the duodenum due to a lack of pacemaker cells in the pylorus [35].

Motor patterns in the first part of the small intestine are peristaltic (propulsive in nature), segmentative (non-propulsive and short duration), and may also include pendular activity (non-propagating longitudinal contractions) [36]. Segmentation patterns are near-stationary sequences of alternating muscular contractions and relaxations of the gut wall. These motor patterns are believed to be responsible for mixing digesta which is essential for maintaining uniform food/enzyme composition along the length of the duodenum. Although no significant evidence of their mixing ability has been demonstrated based on CFD models [37] they may play a role in mechanical agitation and breakdown of digesta. Conversely, propulsive patterns in the small intestine are generally believed to be more important for axial transport than mixing.
To develop greater understanding in order to control the flow of non-Newtonian multiphase slurries is also important for a wide range of process industries. CFD simulations using similar mixture models to the one proposed here have been used to study the behaviour of suspensions in stirred vessels using DEM coupled with an Eulerian representation of the fluid phase [38,39]. This type of model has also been used to develop a particle suspension rheology model for Herschel–Bulkley slurries [40]. Robinson et al. [41] developed a fully resolved DEM-SPH two-phase suspension model (rather than the interphase, drag mediated, two fluid, unresolved model used here) and validated their model for sedimentation and Rayleigh–Taylor instability test cases. Prakash et al. [42] studied mixing of a suspension of discrete particulates in a stirred tank using a fully resolved DEM-SPH model.

The aim of this study is to develop a 3D model framework for a two-phase suspension of rigid particulates to represent simple digesta in the small intestine subject to propulsive motor patterns in the gut wall which can be easily extended to represent more complex foods in future studies. We vary the solids concentration which modifies the apparent viscosity of the content and investigate how this affects the flow behaviour of the solid and liquid phases and its interaction with the gut wall. The motivation for this is that digesta composition with complex and spatially varying solids distribution may have significant effect on flow and mixing. For example, reduced vortical flow due to increased content viscosity has been found to reduce radial advection of digesta [30] to the wall for nutrient absorption, and reduce mixing rates and axial transport. The flow of the solids and fluid phases and the gut wall are solved using computational particle-based methods. This provides a natural framework for calculation of fluid-structure interactions between digesta and the wall, as well as the coupling forces between solids and fluid phases. The wall is represented here as a thin viscoelastic membrane which dynamically deforms in response to forces exerted by the digesta and the applied peristaltic waves. The particulate solids are represented as a simple monodisperse suspension of neutrally buoyant spheres. For this study, we consider three different compositions of digesta: a fluid only content, a thin suspension of 2% solids by volume, and a moderately concentrated suspension of 20% solids. We report on differences in the fluid flow field, the resulting solids distribution and the mass transport rates for each case.

2. Computational model

2.1. Smoothed particle hydrodynamics (fluid phase)

The fluid phase of the intestinal content is modelled with the Smoothed Particle Hydrodynamics (SPH) method using the CSIRO SPH solver [43]. The SPH method is a Lagrangian continuum method which uses a meshless spatial discretisation to convert systems of PDEs into coupled systems of ODEs that can then be solved using suitable time integration methods. See [44] for a detailed review of this method. SPH particles represent discrete regions of fluid whose motions are governed by local fluid stresses produced by interactions with other particles. The basis of this method is that any continuous function $A$ can be expressed in an SPH form so that the interpolated value of this function at any position $r$ becomes

$$A(r) = \sum_b m_b \frac{A_b}{\rho_b} W(r - r_b, h),$$  \hspace{1cm} (1)

where $m_b$ is the mass, $\rho_b$ is the density and $r_b$ is the position of particle $b$. $W$ is a cubic-spline interpolation kernel with smoothing length $h$ that approximates a Gaussian function. This smoothing kernel allows physical properties of the fluid to be converted from discrete particle data to smooth continuous interpolation fields. The gradient of the SPH function is simply given by differentiating Eq. (1):

$$\nabla A(r) = \sum_b m_b \frac{A_b}{\rho_b} \nabla W(r - r_b, h)$$ \hspace{1cm} (2)

For fluids, the continuity equation may therefore be formulated as

$$\frac{d\rho_a}{dt} = \sum_b m_b v_{ab} \cdot \nabla_{a} W_{ab},$$ \hspace{1cm} (3)

where $\rho_a$ is the density of particle $a$ with velocity $\mathbf{v}_a$. We denote the position vector from particle $b$ to particle $a$ by $r_{ab} = r_a - r_b$ and the velocity difference by $v_{ab} = \mathbf{v}_a - \mathbf{v}_b$. This form of the continuity equation is not affected by density discontinuities such as at free surfaces and has excellent numerical conservation properties.

The SPH method used here for fluids is a quasi-compressible formulation with an equation of state specifying the relationship between particle density and fluid pressure. A form suitable for weakly compressible fluids is

$$P = \frac{c^2 \rho_0}{\gamma} \left( \left( \frac{\rho}{\rho_0} \right)^{\gamma} - 1 \right),$$ \hspace{1cm} (4)

where $P_0$ is the magnitude of the pressure given by

$$\frac{\gamma P_0}{\rho_0} = 100 V^2 = c^2$$ \hspace{1cm} (5)
and $V$ is the characteristic or maximum fluid velocity and $c$ is the speed of sound [45]. This means that the sound speed is ten times the characteristic speed and ensures that the density variation is less than 1% and that the flow is close to incompressible. $\rho_0$ is the reference density and $\gamma = 7$.

The SPH form of the momentum equation becomes the acceleration for each particle $a$

$$
\frac{d\mathbf{v}_a}{dt} = -\sum_b m_b \left[ \frac{P_a}{P_b} \left( \frac{P_b}{P_a} + \frac{P_a}{P_b} \right) - \frac{\xi}{\rho_a \rho_b} \frac{4 \mu_a \mu_b}{\rho_a + \rho_b} \frac{\mathbf{v}_a \cdot \mathbf{r}_{ab}}{r_{ab}^2 + \eta^2} \right] + \mathbf{g},
$$

where $P_a$ is the fluid pressure for particle $a$ derived from the equation of state (Eq. (4)) and $\mu_a$ is the particle viscosity. $\xi$ is a factor associated with the viscous term, and $\eta$ is a small parameter used to smooth out the singularity at $\mathbf{r}_{ab} = 0$. With respect to the standard form of the Navier–Stokes equation, the first two terms here represent the pressure gradient term and the third term represents the Newtonian viscous stress term. The SPH viscous stress formulation used here allows for accurate momentum transfer when there are very large spatial variations or discontinuities of viscosity within the domain [46].

The method uses an explicit integration scheme and the simulation timestep $\Delta t$ is governed by the Courant condition

$$
\Delta t = \min_a \left( \frac{0.5h}{c + 2\xi \mu_a / \rho_0} \right).
$$

2.2. Discrete element method (solids phase)

The particulate solids are represented here using the Discrete Element Method (DEM) and are modelled using the CSIRO DEM solver [47,48]. DEM is a Lagrangian method used for simulating the flow of granular materials at the particle scale. This involves following the motion of every particle or object in the flow and modelling each collision between the particles and between the particles and their environment. The methodology is well established and detailed reviews are given in [49,50]. The general algorithm is straightforward and has three main stages:  

1. A search grid is used to periodically build a near-neighbour interaction list that contains all the particle pairs and object-particle pairs that are likely to experience collisions in the short term.
2. The forces on each pair of colliding particles and/or boundary objects are evaluated in their local reference frame using a suitable contact force model (which is described in more detail below) and then transformed into the simulation.
3. All the forces and torques on each particle and object are summed and the resulting equations of motion are integrated to give the resulting motion of these bodies. The motion of the DEM particles is thus defined by

$$
\dot{\mathbf{x}}_i = \mathbf{u}_i, \\
\dot{\mathbf{u}}_i = \sum_j \frac{\mathbf{F}_{ij}}{m_i} + \mathbf{g}, \\
\dot{\mathbf{w}}_i = \sum_j \frac{\mathbf{M}_{ij}}{I_i},
$$

where $\mathbf{x}_i$, $\mathbf{u}_i$, and $\mathbf{F}_{ij}$ are the position, velocity and collisional vector forces for each particle $i$ with mass $m_i$ and principle moments of inertia $I_i$. This gives a particle spin vector $\mathbf{w}_i$ when acted on by torques $\mathbf{M}_{ij}$. Note that Eq. (10) is solved in the canonical frame of the particles.

The entities are allowed to overlap and the amount of overlap $\Delta x$, and normal $v_n$ and tangential $v_t$ relative velocities determine the collisional forces via a contact force law. A linear spring-dashpot model is used where the normal and tangential forces are given by

$$
F_n = -k_n \Delta x + C_n v_n, \\
F_t = \min \left\{ \mu F_n, k_t \sum v_t \Delta t + C_t v_t \right\}.
$$

The normal force consists of a linear spring to provide the repulsive force and a dashpot to dissipate a proportion of the relative kinetic energy. The maximum overlap between particles is determined by the stiffness $k_n$ of the spring in the normal direction. Typically, average overlaps of $< 0.5\%$ of the particle diameter are desirable. The normal damping coefficient $C_n$ is chosen to give the required coefficient of restitution $\varepsilon$. The vector force $F_t$ and velocity $v_t$ are defined in the plane tangent to the surface at the contact point. The tangential summation term represents an incremental spring that stores energy from the relative tangential motion and models the elastic tangential deformation of the contacting surfaces, while the dashpot dissipates energy and models tangential plastic deformations. The total tangential force $F_t$ is limited by the Coulomb frictional limit $\mu F_n$, at which point the surface contact shears and the particles begin to slide over each other. A comparison between this and other contact models for inelastic collisions can be found in [51]. For this study we treat the particulates as spheres but a strength of the method is that the model is easily extensible to include broad size and shape distributions.
2.3. Coupling of phases

For full details of the two-way coupling of the DEM and SPH methods for particulate solids and fluid phases, see Cleary [52]. Briefly, for the purpose of coupling the solids and fluid phases, the particulate DEM solids in the digesta is represented as a continuous field in the SPH multiphase calculation. The drag force on each solid particulate from the liquid phase is given by the empirical relationship of [53]. The coupling force applied to the fluid phase from the averaged continuum representation of the solids is given by Darcy’s law:

\[ F_{\text{darcy}} = \varepsilon_{\text{DEM}}^2 \mu_a \frac{(V_a - V_{\text{DEM}})}{\rho_a K_{\text{DEM}}}, \]

where \( \varepsilon_{\text{DEM}} \) is the porosity (void fraction) of the solids phase, \( \mu_a \) is the viscosity, \( V_a \) is the velocity, and \( \rho_a \) is the density for SPH fluid particle \( a \), and \( V_{\text{DEM}} \) is the DEM solids velocity at that point.

The permeability \( K \) of the solids phase can be calculated from the porosity using the Koseny–Carman relationship

\[ K = \frac{\varepsilon^3}{CT(1-\varepsilon)^2S^2}, \]

where \( (1-\varepsilon) \) is the solid fraction of the particulates, \( C \) is their shape factor (typically 2–3), \( T \) is the tortuosity of the fluid pathways through the solids phase and \( S \) is the ratio of surface area to particle volume (for the solids phase). This force is then added to the SPH momentum equation (Eq. (6)). The pressure solution of the SPH method has been shown to be robust across transitions from free-flowing fluid to drag-controlled flow in particulate dominated flows [52].

2.4. Viscoelastic wall model and peristaltic waves

The duodenum wall is passively compliant and can accommodate peristaltic waves of active contraction and relaxation of circular muscle. The model uses a viscoelastic membrane representation and peristaltic wave control which are fully described in [30]. The duodenum model geometry is a cylindrical tube with closed rigid walls at each end in order to maintain a constant volume of digesta. In vivo, the real physiology consists of a pyloric sphincter at the proximal end which opens only during gastric emptying but otherwise which is closed and the distal end is open. Due to the long length of the tube the pressure distribution and flow field local to the contraction is unaffected provided the peristaltic wave terminates sufficiently before reaching the end. Therefore the approximation of closing the distal end of the model geometry is not an unreasonable one. The curved boundary wall is viscoelastic and therefore generates tensile forces if stretched beyond its natural length in any direction. The setup of this closed tube geometry follows the same process used in [54]. The tube is filled with just enough content to ensure that there are no void spaces which means that there are no tensile forces in the wall when it is at rest.

The surface of the duodenum is discretised into SPH boundary particles. A viscoelastic bond is constructed between each pair of adjacent boundary particles. This consists of a linear spring (for elastic deformation) in parallel with a dashpot (for viscous damping) for the normal direction. This is very similar to the DEM contact model (Eq. (11)). There is no non-normal contribution to the force. Gao et al. [55] measured the elasticity of healthy passive duodenum tissue and found it to be linearly dependent on stretch ratio over the range 1–2 giving wall tensions ranging from 5–10 N/m. Accordingly we set the stiffness of the wall springs to be 10 N/m. The damping coefficient was set to 1.9 to give a coefficient of restitution of 0.5. These values have been used in previous gut motility studies [30, 54].

The extension of the springs and their motion is the result of the balance of hydrodynamic forces applied to it by the digesta within the intestine and the viscoelastic wall force. The resulting cylindrical network of these boundary particles with wall bonds provides a compliant boundary which is able to flex in response to variations in internal content pressures. Muscular forces within the intestine wall which cause it to contract or relax are modelled by changing the natural lengths of the bonds which models the contraction of the intestine wall muscle fibres [30]. The instantaneous shape of the wall is therefore a direct prediction from the fluid-structure interaction between content pressures and tensile wall forces. This contrasts with most modelling in the GI tract where the shapes are assumed.

A sequence of moving sinusoidal peristaltic waves is generated in the intestinal wall at various locations and travel axially from the pylorus (oral end) towards the jejunum (anal end). Each wave consists of a contraction region with a leading relaxation region that is in advance of the contraction. The contraction/relaxation pattern is cylindrically symmetric and varies axially. These influence the instantaneous local wall tensions in each part of the duodenum wall. The operation of the model emulates the real behaviour of propulsive motor patterns in the intestines.

2.5. Rheology of digesta in the small intestine

Digesta that flows into the duodenum is referred to as “chyme” and consists of a thick particulate suspension containing <2 mm size food fragments combined with gastric juices from the stomach. The physical properties of chyme depend on the composition of food matter being digested and can vary considerably. The liquid phase generally has low viscosity and is often considered to be Newtonian [56] but the presence of substantial particulate matter raises the apparent viscosity of whole chyme resulting in strongly non-Newtonian behaviour. When treated as a single phase, chyme is pseudoplastic in
nature [56] and at sufficient solids density may behave as a weak viscoelastic gel [57] but will thin when subject to high shear rates. The size, shape and orientation of the particulates will also influence any non-Newtonian behaviour. Elongated particles in a suspension produce higher apparent viscosities than the same volume fraction of spheres [58]. For example dietary fibre is known to increase content viscosity [59] and non-Newtonian behaviour. Solid food fragments can be viscoelastic and deform macroscopically which will further modify the overall digesta rheology. Their surface chemistry can also cause fragments to be adhesive leading to agglomeration and significant changes to the particulate microstructure. For further details on the influence of different food structures on gastric digestion and chyme composition see [31,2].

Phenomenological non-Newtonian rheology models are often desirable for researchers to study the flow of digesta when using a single continuum phase. These are reasonable provided the composition of the material remains relatively homogeneous. Different rates of mixing and digestion in the stomach for different food types ingested result in differences in residence time. The gastric emptying rate for liquids is rapid so that half of a purely liquid meal can empty in 10–60 min [31]. However gastric digestion of solids is biphasic with a significant lag before solids are sufficiently reduced in size to allow them to pass through the pyloric opening. This means that full gastric emptying of solids can take up to 3–4 h. Differences in emptying rate even for a single meal of multiple food components will necessarily lead to time-variation in the composition of the content presented to the small intestine [60]. Consequently digesta can be highly non-homogeneous with large variations in both solids concentration and composition. This can produce significant spatial variations in digesta rheological behaviour. A particle-based solid/liquid model framework for digesta allows for discrete particulates to be modelled directly and collisional interactions between particulates and hydrodynamic interactions between solids and liquid phases to be directly predicted. With this type of methodology, non-Newtonian behaviour is a model prediction based on the mechanics of the system rather than imposed by a phenomenological rheology model. It enables the study of complex materials with large spatial variations in viscosity which progressively transition from dilute suspensions to semi-solid paste-like materials. The rheological behaviour of the interstitial fluid is significantly simpler than that of the overall digesta and is often Newtonian in behaviour. Separating the representations of the solid phase (which is the cause of a significant amount of observed non-Newtonian behaviour) from that of the interstitial fluid (which has a simpler and often Newtonian rheology) is a key advantage of the proposed model.

In this study we use a simple suspension of identical rigid spheres in a viscous Newtonian fluid. This is a first step in developing a coupled particle model framework for chyme that is suitable for high liquid content in the duodenum. This is not intended to specifically represent the composition or rheology of any particular digested food structure but rather to be a model that is suitable for investigating the response of a suspension of solid food fragments subject to peristaltic dynamics. This model can be easily extended to represent more realistic and more specific digesta by modifying particle attributes (size, density, shape and surface properties) and including additional physics such as adhesive forces (electrostatic) and cohesive forces.

From [61] a system comprising of identical hard spheres will have an apparent viscosity of

$$\mu(\phi) = \mu_0 [1 + 2.5\phi + k\phi^2],$$  

where \(\mu_0\) is the viscosity of the suspending fluid, \(\phi\) is the volume fraction of the particulate solids, and \(k\) is a constant which depends on the flow field and thus on the hydrodynamic forces exerted on the particles. For pure straining motion \(k = 7.6\); and for an incompressible solid suspension \(k = 5.2\). A suspension with \(\phi = 0.2\) will therefore have an apparent viscosity of \(\sim 1.7–1.8\ \mu_0\).

2.6. Biomechanical model of the duodenum and content

The 3D duodenum geometry used in this study represents a human adult and is (at rest) a closed cylindrical tube with diameter 2.5 cm and an axial length of 25 cm as shown in Fig. 1. In vivo, the oral end of the real duodenum is closed due to constriction of the pylorus but the downstream end leading into the jejunum is open. As discussed earlier this is not an unreasonable assumption provided the motor patterns terminate well before the closed distal end. Alternatively, the model in this paper could also be considered to represent an in vitro lab preparation of a section of intestine with tied ends similar to a previous study [54]. This geometry is filled with a stationary Newtonian fluid having a density of water (1000 kg/m\(^3\)) and viscosity of 0.01 Pa.s. We choose values here to reflect representative properties of a typical liquid phase found in the duodenum.

![Duodenum geometry](image)

Fig. 1. Duodenum geometry (grey) with closed ends. Particulate solids occupy 20% of the volume of the first half of the tube and are coloured as axial bands according to their initial position. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
The 3D SPH model uses a fluid resolution of 1.25 mm giving 110,000 SPH particles in the domain. A boundary particle spacing of 0.625 mm is used and is finer than for the fluid so that the maximum separation between boundary particles at peak extension remains smaller than the SPH fluid resolution. This spacing gives 53,000 boundary particles. The dispersed particulate solids phase consists of 1 mm diameter neutrally buoyant DEM spheres (representative of typical particle sizes following gastric digestion). Three cases are investigated in this study for different content:

1) a fluid only case;
2) a thin suspension case which is a suspension with 2% solids loading by volume in the 1st half at the entry side of the duodenum and fluid only in the latter half. Based on Eq. (15) regions of the flow where the solids fraction is 2% will have an apparent viscosity of 1.05 x that of the fluid only case; and
3) a thick suspension case which is a suspension with 20% solid loading by volume in the 1st half at the entry side of the duodenum (as shown in Fig. 1) with fluid only in the latter half. Based on Eq. (15), this material will have an apparent viscosity that is \(1.7 - 1.8\) base fluid viscosity.

DEM particles are coloured into axial bands based on their starting position along the duodenum. This provides a visual way of tracking the mixing and transport of the solids content. Computation timesteps of \(4.7 \times 10^{-5}\) s and \(4.3 \times 10^{-5}\) s are used for the fluid only and multiphase simulations respectively.

Observed peristaltic wave speeds for the proximal intestine range from 0.5-2 cm/s [62]. In our model, waves are set up in the duodenal wall with a duration of 5 s and wave speed of 2 cm/s. They commence at the same location (5 cm from the start of the tube) for each cycle and repeat every 6 s allowing a 1 s of relaxation period in between successive waves giving a sequence of 10 waves during the computational period. The relaxation period was chosen so that the wave dissipates well before approaching the closed end of the tube and the downstream pressures near the closed end do not become excessively high, as was observed in [63]. An 80% shortening of elastic wall elements define the maximum active contraction (which will be almost lumen occluding) while a matching 80% lengthening of the elements define the maximum active relaxation of the wall. The axial length of the full wave (including both contractile and relaxation parts of equal length) is 8 cm following the model in [21]. This is consistent with the 4 cm contraction only wave used in [29].

### 2.7. The need for validation

Each of the DEM and SPH methods has been independently validated by many authors over the last two decades. It is equally important to validate the specific code implementations used in such a study. For the CSIRO solvers used here:

- DEM validation has been considered in the context of predicting particle motions in mills [64] who compared the charge structure predicted with experimental photographs for a laboratory scale mill and found very good agreement. Gowendar et al. [65] found extremely good agreement for the charge solid fraction and velocity distributions in a laboratory scale ball mill using PEPT. Owen et al. [66] showed good agreement in predicting the time dependent run-out of a collapsing slope. Owen et al. [67] showed very good agreement for the mass transfer rates in a screw conveyor at angles varying from horizontal to vertical by comparison to experimentally measured values.
- SPH validation has been considered in free surface flows induced by collapse of water in a tank [68] and in die casting [69–71]. Prakash et al. [42] showed excellent agreement between a fully resolved DEM-SPH model and experiment for mixing of buoyant non-round pellets in a 1 m diameter mixing tank with an off-center vertical impeller.
- The fully coupled DEM-SPH model has only recently been proposed so the coupling of this combined method remains as a future challenge. In vitro validation of this coupled model in the context of GI transport remains a specific need.

### 3. Fluid only flow and mixing in the small intestine

Fig. 2 shows the flow field for the fluid only content at different times during the passage of the 1st peristaltic wave along the length of the duodenum. This shows the deformation of the wall and the fluid content both coloured by axial speed. The wave travels from left (oral end) to right (anal end).

At 1.5 s (Fig. 2a), the contraction and relaxation components are substantially developed. High axial speeds (red) up to 50% greater than the wave speed occur at the centre of the relaxation region. Here the walls dilate due to the high pressures generated in front of the advancing contraction (see [54] for the relationship between pressure field and axial velocities). Near the wall, speeds are lower (green) at roughly half of the wave speed. This radial dependence on axial speed results in a toroidal vortex shown in Fig. 3. The development of this vortical flow was discussed in detail in [30] in the context of transport of viscous liquid in the large intestine. The vortex (located inside the relaxation region) is important for radial transport of nutrients to the wall for absorption as well as radial and axial mixing of content.

At 3 s (Fig. 2b) the relaxation region is now less elongated in the axial direction and more spherical in shape and the flow field inside is more symmetrical. A strongly developed retrograde jet is present inside the contraction region. This reverse jet is important for redistributing content back along the length of the duodenum and for the re-pressurization of the duodenum walls near the oral end.

At 4.5 s (Fig. 2c) the wave has nearly finished dissipating and the previous flow pattern is rapidly decaying so that flow is now entirely in the reverse direction. Downstream pressures near the closed anal end of the tube relax and content axially
redistributes back towards the oral end. Due to the closed ends there is no net axial flow inside this model as a consequence. This restricts the degree of axial transport for the particulate solids in the next section but results in enhanced mixing of the solids in the first half of the tube.

4. Flow and mixing of thin (2% solids) and thick (20% solids) suspensions

For the case of a thin suspension (2%) of fine particulate solids the flow field appears very similar to the previous fluid only case. Fig. 4 shows the passage of the same peristaltic wave shown in Fig. 2 and at the same times for easy comparison. In addition, the distribution of particulate solids along the axial length of the tube is shown at each time. The Reynolds number ($Re$) for the fluid flow is 80, based on a maximum flow speed of 0.03 m/s, viscosity of 0.01 Pa s, characteristic diameter of 0.025 m and fluid density of 1000 kg/m$^3$. The particle Reynolds number $Re_p = 3.0$ based on a particle diameter of 1 mm, a maximum particle speed of 0.03 m/s, and the fluid density and viscosity as stated above. Since $Re_p$ is small, there is limited opportunity for the fluid and solids phases to move differentially during the passage of a peristaltic wave. The particle $Re$ is defined for a single object in a fluid. The flow of the fluid and solids phases will remain very tightly coupled for very dilute suspensions where the rate of collisions between particulates is low. At higher concentrations, collisions between particles may lead to differences between the two phases.

At 1.5 s (Fig. 4a) and 4.5 s (Fig. 4c), the flow field for the thin suspension is almost identical to the fluid only case. At 3.0 s (Fig. 4b) there are some very small differences apparent in the size and shape of the high speed fluid region which is slightly more rounded and smaller than for the fluid only case. The high speed fluid transports fine particulates downstream
Fig. 3. Vortical flow of fluid content inside the region of active muscular relaxation of the gut wall at $t = 3.0$ s. Fluid is coloured by axial speed. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 4. The passage of a single peristaltic wave along the length of the duodenum for content with 2% solids loading at three different times. The left column shows fluid phase coloured by axial speed. The right column shows the solids coloured by their initial position. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
along the length of duodenum until the wave dissipates. The distribution of solids along the duodenum after a single wave passage is not at all uniform. The particulates are pushed downstream, ahead of the contraction, and accumulate inside the relaxation region resulting in a greater concentration of solids towards the front of the wave. A small amount of particulates are carried upstream by the retrograde jet resulting in a significantly reduced solid fraction in the wake of the wave. This suggests that peristaltic motor patterns do not necessarily guarantee homogeneity of multiphase digesta along the length of the intestine. Complexities in real motor patterns such as variations in frequency, amplitude and starting locations of successive waves will tend to further modify the solids distribution.

Increasing the concentration of fine particulates to a thick suspension of 20% solids produces some additional small scale but interesting changes to the propulsive transport. Fig. 5 shows the passage of the same peristaltic wave shown in Figs. 2 and 4. Again, the distribution of particulate solids along the axial length of the tube is shown at each time. The concentration of particulates is greater than for the previous case and therefore the rate of collisions between particulates is higher. Particles “bunch up” inside the relaxation region and the local solid fraction increases to around 0.25 at the front of the wave. The non-uniformity of the solids distribution results in spatial variation of local drag forces on the fluid phase. This in turn causes modification of the pressure distribution of the digesta resulting in a combined solids/liquid flow field with some differences to the fluid only case as outlined below.

At 1.5 s (Fig. 5a), the peak fluid speed inside the relaxation region is reduced relative to the fluid only case and the size of the high speed flow region shrinks. Fluid content in the wake of the contraction occupies a central region whereas the solids tend to spread sideways towards the wall. The nature of the mixing is much easier to determine for the higher concentration of particulates than it was for the thin suspension. Mixing of the solids occurs by stretching of content in the axial direction due to the passage of the peristaltic wave. Transverse layering of the solids then occurs within the toroidal vortex in the relaxation region. In this region the green/blue solids migrate to the wall and are then entrained behind the
wave by low axial flow at the wall. This results in a radial stratification of the coloured bands of particles after the passage of each wave.

At 3 s (Fig. 5b), the fluid flow field inside the relaxation region is very similar to the fluid only case but the shape of the dilated wall is somewhat different (with the trailing edge near the contraction is slightly steeper in gradient) indicating that the pressure distribution along the duodenal wall has been modified by the presence of the solids. The reverse jet from the rear of the contraction region is not as strong as for the fluid only case and is narrower and more centralised. Inside the relaxation region, the solids are more centrally located and are only sparsely distributed near the dilated wall. The mixing state of the solids has developed further with radial migration of the pink particles to the walls as well as extending back to the contraction region.

By 4.5 s (Fig. 5c) the radial stratification of the solids extends along almost the full axial length of the duodenum. The wall upstream of the contraction takes longer to relax back to its original diameter than the fluid only case. This indicates that fluid pressures take longer to equilibrate upstream as a consequence of the reduced strength in the reverse flow caused by the presence of the solids.

Fig. 6 shows the flow field for the fluid phase of each case represented as 1-D axial flow velocity profiles. Each profile contains the radial variation of axial velocity plotted at different axial locations throughout the contraction and relaxation regions of a fully developed wave. The addition of 20% solids modifies the fluid flow field in three specific locations:

1) the retrograde jet starting on the downstream side of the contraction is initially stronger but becomes similar in strength to that of the fluid only content further upstream inside the contraction region;
2) the downstream flow from the end of the contraction into the start of the relaxation region is weaker. This results in the modified wall shape in Fig. 5b; and
3) the flow downstream near the end of the relaxation region becomes stronger and more plug-like.

The presence of solids in the digesta acts to thicken the fluid and mildly increase the effective viscosity. For content containing up to at least 20% solids, the changes to the vortical flow appear to be mild. The toroidal vortex in the recirculation region is therefore largely similar in size and strength for all three cases. So one might reasonably anticipate that the mixing and rate of radial transport of nutrients to the gut wall for absorption will not be strongly dependent on solids fraction at low concentration but may become more significant with increased solids loading. Vortex strength and radial transport are greatly reduced for high viscosity content [30]. Therefore for digesta with very high solids loading one might expect that nutrient absorption will be adversely affected. In fact, intestinal permeability and glucose absorption have been found to be reduced for high viscosity digesta [72].

Fig. 7 compares the mass flow rates for the three cases. These are measured at a vertical cross-sectional data collection plane located halfway along the length of the model duodenum. The masses and velocities of DEM solid and SPH fluid particles are recorded as they cross this plane. For the fluid only case, the peak antegrade and retrograde flow rates are both 0.021 kg/s giving no net mass flow after each wave. This is due to the closed ends of the model duodenum. For the thick suspension, the peak mass flow rate of the total solid/liquid content is about 35% lower than the peak rate for the fluid only case. The solids phase contributes roughly 20% to the overall peak mass flow rate which is consistent with the 20% solids loading by mass for the neutrally buoyant material. The thin suspension has a very low solids mass flow rate which
is consistent with the low 2% solids loading. The fluid mass flow rate is similar to that for the thick suspension (0.012–0.014 kg/s). So the addition of solids to the digesta appears to reduce the peak mass flow rate.

Fig. 8 shows the axial flow velocities spatially averaged over the data collection plane used for Fig. 7 for the multiphase and fluid only cases. For both the thin and thick suspension cases, the average velocities for the solid and fluid phase are almost identical for the majority of the period of each wave indicating that the two phases are strongly coupled together for most of the time. However, for the thick suspension case, inside the relaxation region the solids have higher forwards velocities of 30 mm/s compared to speeds of 10-20 mm/s for the fluid phase. This is mostly a consequence of the radial distribution of the solids inside the relaxation region since they are more sparsely distributed near the wall. Therefore more of the solids are located in the high velocity central flow region (see Fig. 4b). The low particle Reynolds number could lead
Fig. 8. The time variation of the average axial velocities crossing a plane located halfway along the length of the duodenum. The velocities are shown for waves 2 and 3 for: (a) fluid only content; (b) 2% solids; and c) 20% solids.

to the interpretation that the solids completely move with the fluid. However, there are non-trivial short-term differences between phases which may impact on the digestion of the solids and diffusion of resulting species to the wall for absorption. The peak retrograde velocities for the fluid only case are about 90% higher in the absence of solids. This results in transverse motion of the duodenum wall and is the focus of the next section.

5. Low pressure induced “wobbling” instability

For the fluid only content case, the duodenum was found to experience significant transverse mobility in the reduced pressure region in the wake of each of the peristaltic waves (see Fig. 9). There is a residual low pressure region that is
generated in the wake of the compression zone of the contracting wall. This persists for a reasonable time as it takes time for the viscous fluid to flow back towards the oral end in response to the weak axial pressure gradient and to equilibrate the pressures in the system. This can be characterised as a relaxation process for the system. During this time while the viscoelastic wall behind the contraction is not fully pressurised it becomes subject to this transverse “wobbling” instability. The instability develops after 5–6 waves have traversed the duodenum.

**Fig. 9**. Development of a transverse wobbling instability observed in the fluid only case, (a) 37 s, (b) 43 s, (c) 46 s, and (d) 52 s. It begins to develop only after the passage of several peristaltic waves which creates a strong axial variation in content and pressure.

Fig. 9a & b show the first second of waves 7 and 8 while Fig. 9c & d show one second before the end of waves 8 and 9. They show the degree of vertical movement in the walls which oscillate transversely with a period that is longer than the period of the peristaltic waves (which reflects the long relaxation time of the system). This wobbling instability arises because there is not sufficient overpressure in this part of the tube to increase pressures in the wake of the contraction. If one wanted, this instability could be inhibited by increasing the fluid pressures in the tube, but since the duodenum does not necessarily have to be pressurised this instability can manifest.

Interestingly, the presence of solids seems to inhibit the development of this instability with no transverse movement identified up to 10 full wave passages. The damping out of this instability is due to a reduction in the strength of the retrograde when a solids phase is added to the digesta as shown in Fig. 8. The movement of the intestines in *vivo* is restricted with attachments within the abdomen via thin connective tissue called the mesentery which will moderate such movements. Connective tissue restraints will therefore need to be incorporated into future models of the intestines.

### 6. Conclusions

This paper introduces a particle-based CFD model using a two-way coupling of fluid and solids in a particulate suspension to study peristaltic flow dynamics in the duodenum. Propulsive peristaltic waves containing muscular contraction and relaxation components were applied to the compliant wall of a closed section of intestine. Model predictions were made of the flow of digestive content in response to these motor patterns as well as predictions of the gut wall shape in response to changes in content pressures. Differences in transport and mixing of content due to different solids concentration were investigated.

For purely liquid content, high fluid pressures in front of the moving contraction cause significant dilation of the walls immediately downstream inside the relaxation region. A radial velocity gradient in this region results in a vortical flow structure that is important for advective transport of nutrients to the gut wall, and for radial and axial mixing of content. A retrograde jet inside the contraction region redistributes content axially back towards the oral end. This results in re-pressurization of the oral end of the tube back to its original diameter once the wave has dissipated.

At sufficiently high solids loading (20%) inter-particle collisions in the digesta lead to variations in local concentration along the length of the duodenum and spatial variations in drag forces (and effective local viscosity) of the fluid phase. In
turn this modifies the fluid pressures inside the relaxation region mildly changing the dilated wall shape and fluid flow field. The bulk motion of the content shows both phases generally move together due to the laminar nature of the flow but with some differences found in the relaxation region and in the wake of the contraction. In particular the strength of the retrograde jet through the contraction is reduced. The presence of a solids phase in the digesta leads to a mild reduction in overall axial mass transport due to a reduction in peak axial velocities (both in the downstream and upstream directions) compared to the fluid only content.

The propulsive wave results in strong axial mixing of the solids content but also leads to significant non-uniformity of solids content along much of the length of the duodenal section. This suggests that peristaltic motor patterns do not guarantee homogeneity of multiphase digesta throughout the intestines. Over a moderate range of solids loading (< 20%), the vortical flow appears to be only mildly sensitive to solids concentration. For digesta with much higher solids loading than we have considered here, we expect the much higher drag forces to result in higher effective viscosity content which will tend to reduce the strength of the recirculation vortex and radial transport rates, as well as the degree of nutrient absorption by the gut wall consistent with other empirical studies. This suggests potential nutritional benefits in maintaining more fluid-like content in the small intestine.

A transverse wobbling instability can develop inside the residual low pressure region of purely fluid content in the wake of each contraction. The walls of the duodenum oscillate at a period greater than the period of the peristaltic waves due to the long relaxation time of the system. The addition of mesenteric connective tissue attachments in the model would prevent the instability from arising. The presence of a solids phase in the content was found to inhibit this instability by reducing the strength of the retrograde jet.

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