From Microscales to Macroscales: Fundamental Modeling and Simulations of Granular Media

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Computations performed on the Jet Propulsion Laboratory supercomputers

Outline

- Definition of granular media

- Governing equations
  - Carrier medium
    - Definition of a phase indicator
    - Definition of the ensemble average of the phase indicator
  - Particles
    - Collision dynamics
    - Particle dynamics
    - The moment equations
    - Modeling of unclosed terms in the particle equations
    - Particle friction

- Results for application to a fluidized bed
  - Comparisons with experiments
  - Predictions for reactive-particle simulations

- Future needs in modeling and simulations

Definition of a granular medium

- Particle containing volume having a large particle volumetric fraction, i.e. $V_p /(V_f+V_p)=O(1)$

- Consequences of the definition
  - A distribution function of the particles can be defined
  - The particles will have close range interactions
    - Collisions
    - Friction
    - Chemical reactions
  - Particle morphology may be changed by breakup and erosion
  - The chemical composition of the surface may change

Carrier medium

- Assumptions must be made about the medium
  - Rarefied gas?
  - Satisfies the continuum gas assumption?
  - Liquid?
  - Supercritical fluid?
- The mathematical framework depends upon the medium
- Current mathematical framework is for an atmospheric-pressure gas satisfying the continuum assumption
  - Neglect pressure work
  - Neglect viscous dissipation

Generic equation describing the evolution of a flow

$$\underbrace{\frac{\partial(\rho\psi)}{\partial t}}_{\text{transient}} + \underbrace{\nabla\cdot(\rho\psi u)}_{\text{convective}} = \underbrace{\nabla\cdot Q}_{\text{diffusive}} + \underbrace{\mathbf{S}}_{\text{sources}}$$

- Ψ is a scalar (e.g. mass fraction, energy) → Q is a vector
- Ψ is a vector (e.g. velocity) → Q is a tensor

Gas-phase governing equations, 1 of 3

Define a field quantity $\Psi(\mathbf{x},t)$.

The general ensemble average of $\Psi(\mathbf{x},t)$ is

$$< \Psi(\mathbf{x},t) >= \int \Psi(\mathbf{x},t) P(\Pi) d\Pi$$

where $P(\Pi)$ is the probability that a specific realization Π is encountered

Denote (Drew 1983)

- ρ_g as the density
- χ_g as the phase indicator (1 for gas, 0 elsewhere)
- $\alpha_g = < \chi_g >$ as the ensemble average of the phase indicator function

One may define

$$\overline{\Psi} \equiv < \chi_g \Psi(\mathbf{x},t) > / \alpha_g$$

$$\widetilde{\Psi} \equiv < \chi_g \rho_g \Psi(\mathbf{x},t) > / \alpha_g \overline{\rho}_g$$

Multiply NS+energy+species+EOS by α_g and ensemble average →

Gas-phase governing equations, 2 of 3

$$\frac{\partial(\alpha\overline{\rho})_g}{\partial t} + \nabla\cdot(\alpha\overline{\rho}\tilde{\mathbf{u}})_g = \Gamma_g$$

$$\frac{\partial(\alpha\overline{\rho}\tilde{\mathbf{u}})_g}{\partial t} + \nabla\cdot(\alpha\overline{\rho}\tilde{\mathbf{u}}\tilde{\mathbf{u}})_g = -\alpha_g\nabla\overline{p}_g + \nabla\cdot\alpha_g[\overline{\boldsymbol{\tau}} + \boldsymbol{\Sigma}^{\mathrm{Re}}]_g + \alpha_g\overline{\rho}_g\mathbf{f}_g + \mathbf{M}_g + \Gamma_g\mathbf{u}_g^i$$

$$\frac{\partial(\alpha\rho\tilde{h})_g}{\partial t} + \nabla\cdot(\alpha\overline{\rho}\tilde{\mathbf{u}}\tilde{h})_g = -\nabla\cdot\alpha_g[\overline{\mathbf{q}} + \mathbf{q}^{\mathrm{Re}}]_g + F_g + \Gamma_g h_g^i$$

$$\frac{\partial(\alpha\overline{\rho}\tilde{Y}_\xi)_g}{\partial t} + \nabla\cdot(\alpha\overline{\rho}\tilde{\mathbf{u}}\tilde{Y}_\xi)_g = -\nabla\cdot\alpha_g[\overline{\mathbf{j}}_\xi + \mathbf{j}_\xi^{\mathrm{Re}}]_g + \alpha_g\overline{\rho}_g\tilde{R}_{g\xi} + H_{g\xi} + \Gamma_g Y_{g\xi}^i.$$

$$\overline{p}_g = R_u\overline{\rho}_g\sum_\xi(\tilde{Y}_\xi/W_\xi)\tilde{T}_g$$

$\mathbf{f}_g$ Gravitational acceleration

$R_{g\xi}$ Reaction rate

$\mathbf{M}_g$, F_g, and $H_{g\xi}$ Diffusive interfacial transfer $H_{g\xi} \equiv < \mathbf{j}_{g\xi}\cdot\nabla\chi_g >$

Γ_g, $\Gamma_g\mathbf{u}_g^i$, $\Gamma_g Y_{g\xi}^i$, and $\Gamma_g h_g^i$ Convective interfacial transfer

$$\Gamma_g \equiv < \rho_g(\mathbf{u}_g - \mathbf{u}_g^i)\cdot\nabla\chi_g >$$

$\boldsymbol{\Sigma}_g^{\mathrm{Re}}$, $\mathbf{j}_{g\xi}^{\mathrm{Re}}$, $\mathbf{q}_g^{\mathrm{Re}}$ Turbulent flux of conserved quantities

$$\alpha_g\boldsymbol{\Sigma}_g^{\mathrm{Re}} \equiv -< \chi_g\rho_g\mathbf{u}_g'\mathbf{u}_g' >$$

Gas phase governing equations, 3 of 3

Molecular fluxes

$$\overline{\boldsymbol{\tau}}_g = 2\mu_g \mathbf{S}_g \qquad \mathbf{S}_g = (\nabla\tilde{\mathbf{u}}_g + \nabla\tilde{\mathbf{u}}_g^T)/2 - (\nabla \bullet \tilde{\mathbf{u}}_g)/3$$

$$\overline{\mathbf{j}}_\xi = -\overline{\rho}_g \mathcal{D}_\xi \nabla\widetilde{Y}_\xi$$

$$\overline{\mathbf{q}}_g = -\lambda_g \nabla\widetilde{T}_g - \sum_\xi h_\xi \overline{\mathbf{j}}_\xi$$

To solve the equations, we need:

- values of the molecular transport coefficients
- models for the turbulent fluxes

Particle-phase governing equations, 1 of 4

- Methodology similar to dense gases using kinetic theory concepts
  - no assumption of equipartition of granular energy according to particle mass ratio because the collisions may be inelastic
  - must derive separate equations for each class *i*
  - no assumption that Δu (relative velocity between particle classes) $\ll \Theta_c$ (rms velocity; related to temperature in molecular context)
- Define the single-particle distribution function for class *i*

$$f_i(\mathbf{x}, \mathbf{c}, Y_\xi, T, m, t)$$

- Compute the number of particles of class *i*

$$n_i(\mathbf{x}, t) = \int f_i d\mathbf{c} dY_\xi dT dm$$

- Define a particle-ensemble average for variable Ψ

$$\overline{\Psi}_i(\mathbf{x}, t) = \frac{1}{n_i} \int \Psi_i f_i d\mathbf{c} dY_\xi dT dm$$

Particle-phase governing equations, 2 of 4

- Definition of mass-weighted particle-ensemble average

α_i denotes the local phase fraction of class i (where pores are excluded) and $\overline{\rho}_i$ its corresponding average particle density

$\widehat{\alpha}_i$ and $\widehat{\rho}_i$ where the pores of the particles are counted as volume belonging to the particle

$$\alpha_i \overline{\rho}_i = \widehat{\alpha}_i \widehat{\rho}_i$$

$$\alpha_i \overline{\rho}_i = n_i \overline{m}_i = \int m_i f_i d\mathbf{c} dY_\xi dT dm$$

$$\widetilde{\Psi}_i(\mathbf{x},t) = \frac{1}{\alpha_i \overline{\rho}_i} \int m_i \Psi_i f_i d\mathbf{c} dY_\xi dT dm \qquad < \Psi >_i \equiv \widetilde{\Psi}_i$$

- Define particle-ensemble quantities
  - Average velocity $\mathbf{u}_i = < \mathbf{c}_i >$
  - Fluctuating velocity component $\mathbf{C}_i = \mathbf{c}_i - \mathbf{u}_i$
  - Granular temperature $\Theta_i = \frac{1}{3} < C^2 >$
  - Solidity ($\eta = 1 - \epsilon$) $\eta_i = m_i / V_i \sum \frac{Y_\xi}{\rho_\xi}$ V_i includes pores
- We assume that the volume of the particle is constant (no break-up or erosion)

Particle-phase governing equations, 3 of 4

Use analogy to the Boltzmann equations: multiply an analog equation by mΨ and integrate over space

$$\frac{\partial \alpha_i \overline{\rho}_i \widetilde{\Psi}_i}{\partial t} + \nabla \cdot (\alpha_i \overline{\rho}_i < \mathbf{c}_i \Psi_i >) = \sum_{k=A,B} C_{ik}(m_i \Psi_i) +$$

$$\alpha_i \overline{\rho}_i < \frac{\mathbf{F}_i}{m_i} \frac{\partial \Psi_i}{\partial \mathbf{c}_i} > + \alpha_i \overline{\rho}_i < \frac{dT_i}{dt} \frac{\partial \Psi_i}{\partial T_i} > +$$

$$\alpha_i \overline{\rho}_i \sum_{\xi} < \frac{dY_{i\xi}}{dt} \frac{\partial \Psi_i}{\partial Y_{i\xi}} > + \alpha_i \overline{\rho}_i < \frac{dm_i}{dt} [\frac{\partial \Psi_i}{\partial m_i} + \frac{\Psi_i}{m_i}] >$$

Mean collisional rate of change of Ψ

$$C_{ik}(m_i \Psi_i) = \chi_{ik}(m_i \Psi_i) - \nabla \cdot \theta_{ik}(m_i \Psi_i)$$

Integral over all binary collisions   Source-like   Flux term; transport by collisions

➡ Difference for soils from Boltzmann equations:

-multiple particle collisions

-no Maxwellian distribution

-collisions yield elastic and plastic stresses

Particle-phase governing equations, 4 of 4

To solve the equations we need to know:

- the result of collision dynamics (assumed binary collision; but this is not necessarily the case)
    - are particles smooth?
    - what is the particle shape?
- the result of particle dynamics: rate of change for each particle of various particle properties (mass, composition, temperature, velocity) as the particle moves on its trajectory
- values for the transport properties of the particle phase

Particle-collision dynamics

Particles of masses m_1 and m_2, and radii σ_1 and σ_2

Define $\mathbf{g} \equiv \mathbf{c}_1 - \mathbf{c}_2$

$$(\mathbf{g}' \cdot \mathbf{k}) = -e_{ik}(\mathbf{g} \cdot \mathbf{k})$$

restitution coefficient

Momentum

$$\mathbf{c}_1' - \mathbf{c}_1 = -M_k(1 + e_{ik})(\mathbf{g} \cdot \mathbf{k})\mathbf{k} \qquad M_i = m_i/m_{ik} \qquad m_{ik} = m_i + m_k$$

Energy

$$\Delta E = \frac{5.36(m/G)^{3/5}(\sigma g)^{7/10}(T_1 - T_2)}{(\rho C_p \lambda)_1^{-1/2} + (\rho C_p \lambda)_2^{-1/2}}$$

Sun & Chen (1988)

elastic deformation of spheres during contact and heat conduction

g is the magnitude of **g**

$$\sigma = \frac{\sigma_1 \sigma_2}{\sigma_1 + \sigma_2}; \quad m = \frac{m_1 m_2}{m_1 + m_2}; \quad G = \frac{4/3}{\frac{1-\nu_1^2}{G_1} + \frac{1-\nu_2^2}{G_2}}$$

G: Young modulus

ν: Poisson ratio

Particle dynamics: Lagrangian frame

Particle mass

$$\frac{dm_i}{dt} = \sum_\xi \frac{dm_{i,\xi}}{dt} = m_i \sum_\xi R_{i,\xi}$$

Species mass fractions

$$\frac{dm_{i,\xi}}{dt} = \frac{dm_i Y_{i,\xi}}{dt} = m_i R_{i,\xi}$$

Single particle momentum

$$m_i \frac{d\mathbf{c}_i}{dt} = \mathbf{F}_i = m_i \mathbf{f}_g - V_i \nabla \overleftrightarrow{p}_g + \frac{m_i}{\tau_{i,12}}(\overleftrightarrow{\mathbf{u}}_g - \mathbf{c}_i)$$

Relaxation time of particle (correlation: single particle drag + multiparticle correction)

Velocity of undisturbed flow at particle location

Energy (pressure inside and outside particle are equal)

$$(mC_p)_i \frac{dT_i}{dt} = Q_{cd,i} + Q_{r,i} + \sum \frac{dm_{i,\xi}}{dt}(h_v - h_\xi)$$

Conductive heat transfer (Nusselt)

radiative

reaction

Particle moment equations, 1 of 2

- $\Psi = 1$: mass eq.

$$\frac{\partial(\alpha_i \overline{\rho}_i)}{\partial t} + \nabla \cdot (\alpha_i \overline{\rho}_i \mathbf{u}_i) = \Gamma_i$$

$$\Gamma_i = \alpha_i \overline{\rho_i} < \frac{1}{m_i}\frac{dm_i}{dt} >= \alpha_i \overline{\rho_i} \sum_{\xi} < R_{i,\xi} >$$

- $\Psi = c$: momentum eq.

$$\frac{\partial(\alpha_i \overline{\rho}_i \mathbf{u}_i)}{\partial t} + \nabla \cdot (\alpha_i \overline{\rho}_i \mathbf{u}_i \mathbf{u}_i) = \alpha_i \overline{\rho}_i < \frac{\mathbf{F}_i}{m_i} > + \alpha_i \overline{\rho}_i < \frac{dm_i}{dt}\frac{\mathbf{c}_i}{m_i} > - \nabla \cdot \mathbf{\Sigma}_i + \boldsymbol{\phi}_i$$

effective stress tensor — collisional source

$$\mathbf{\Sigma}_i = \alpha_i \overline{\rho}_i < \mathbf{C}_i \mathbf{C}_i > + \sum_{k=A,B} \theta_{ik}(m_i \mathbf{C}_i) \qquad \phi_i = \sum_{k=A,B} \chi_{ik}(m_i \mathbf{C}_i)$$

- $\Psi = Y_\xi$: species mass fractions eqs.

$$\frac{\partial(\alpha_i \overline{\rho}_i \widetilde{Y}_{i\xi})}{\partial t} + \nabla \cdot (\alpha_i \overline{\rho}_i \mathbf{u}_i \widetilde{Y}_{i\xi}) = -\nabla \cdot (\alpha_i \overline{\rho}_i < \mathbf{C}_i Y'_{i\xi} >) + \Gamma_{i\xi}$$

$$\Gamma_{i\xi} = \alpha_i \overline{\rho}_i < R_{i,\xi} >$$

(no collisional terms as the mass fractions are assumed invariant in a collision)

Particle moment equations, 2 of 2

- $\Psi = (1/2)C^2$: granular temperature eq.

$$\frac{3}{2}\left[\frac{\partial(\alpha_i\overline{\rho}_i\Theta_i)}{\partial t} + \nabla\cdot(\alpha_i\overline{\rho}_i\mathbf{u}_i\Theta_i)\right] = -\mathbf{\Sigma}_i : \nabla\mathbf{u}_i - \nabla\cdot\mathbf{q}_i + \gamma_i + \alpha_i\overline{\rho}_i < \frac{dm_i}{dt}\frac{1/2C_i^2}{m_i} > + \alpha_i\overline{\rho}_i < \frac{\mathbf{F}_i}{m_i}\cdot\mathbf{C}_i >$$

granular temperature

$$\Theta_i = 1/3 < C_i^2 >$$

average heat flux

$$\mathbf{q}_i = \alpha_i\overline{\rho}_i < 1/2C_i^2\mathbf{C} > + \sum_{k=A,B}\theta_{ik}(1/2m_iC_i^2)$$

velocity fluctuations

collisions

source term

$$\gamma_i = \sum_k \chi_{ik}(\tfrac{1}{2}m_iC_i^2)$$

energy redistribution among classes and dissipation due to inelastic collisions

- $\Psi = h$: energy eq.

$$\frac{\partial(\alpha_i\overline{\rho}_i\tilde{h}_i)}{\partial t} + \nabla\cdot(\alpha_i\overline{\rho}_i\mathbf{u}_i\tilde{h}_i) = \alpha_i\overline{\rho}_i < \frac{Q_{cd,i}+Q_{r,i}}{m_i} > + \alpha_i\overline{\rho}_i < \frac{1}{\rho_i}\frac{dp_g}{dt} > + \alpha_i\overline{\rho}_i < \frac{dm_i}{dt}\frac{h_v}{m_i} >$$

$$-\nabla\cdot\alpha_i\overline{\rho}_i < \mathbf{C}_i h_i' >$$

'turbulent' flux
(collisions: negligible)

Closure of particle-phase equations

Correlations which must be closed:

- collisional contributions to both transport and source terms
- exchange terms between gas and solids
- in-phase transport terms and transport properties

Assume that the hydrodynamic problem can be uncoupled from chemistry

$$f_i(\mathbf{x}, \mathbf{c}_i, Y_{\xi,i}, m_i, T_i, t) = f_i(\mathbf{x}, \mathbf{c}_i, t)\delta(m_i - \overline{m}_i)\delta(T_i - \widetilde{T}_i)\sum_\xi \delta(Y_{\xi,i} - \widetilde{Y}_{\xi,i})$$

↑ velocity distribution function

Collisional and kinetic contributions

Assumptions

- Maxwellian distribution
- drift between particles is small, i.e.

$$\Delta \mathbf{u}_{ik} = \mathbf{u}_i - \mathbf{u}_k \ll (\Theta_i + \Theta_k)^{1/2}$$

- neglect products of spatial gradients
- neglect products of spatial gradients and $(1 - e_{ik})$
- neglect products of spatial gradients and $\Delta \mathbf{u}_{ik}$

Invoke the radial distribution function (describes how the particle density varies as a function of the distance from one particle)

$$h_{ik} = \frac{1}{1 - \hat{\alpha}/\alpha_{max}} + 6 \frac{\sigma_i \sigma_k}{\sigma_i + \sigma_k} \frac{\xi}{(1 - \hat{\alpha}/\alpha_{max})^2} + 8 \left(\frac{\sigma_i \sigma_k}{\sigma_i + \sigma_k} \right)^2 \frac{\xi}{(1 - \hat{\alpha}/\alpha_{max})^2}$$

$$\xi = 2\pi/3 \sum n_i \sigma_i^2$$

Constitutive particle-phase equations

Collisional momentum source

$$\boldsymbol{\phi}_i = \sum_k F_{ik} \left\{ \tfrac{4}{3}\sqrt{2\pi}\,(\Theta_i + \Theta_k)^{1/2}(\mathbf{u}_k - \mathbf{u}_i) + \tfrac{\pi}{3}\sigma_{ik}(\Theta_i + \Theta_k)\nabla \ln \tfrac{n_i}{n_k} \right\}$$

solid/solid drag diffusion

Stresses due to collisions

$$\boldsymbol{\Sigma}_i = n_i m_i \Theta_i \mathbf{I} + \sum_k \left\{ p_{ik}\mathbf{I} - \mu_i^{ik}[2\mathbf{S}_i + \tfrac{5}{3}\nabla \cdot \mathbf{u}_i] - \mu_i^{kk}[2\mathbf{S}_k + \tfrac{5}{3}\nabla \cdot \mathbf{u}_k] \right\}$$

shear rate due to collisions (not streaming): Gaussian conseq.

Heat flux due to collisions

$$\mathbf{q}_i = \sum_k \left\{ \kappa_i^{ik}\nabla\Theta_i + \kappa_i^{kk}\nabla\Theta_k \right\}$$

conductivity due to collisions

Granular temperature source term due to collisions

$$\gamma_i = \sum_k -2\sqrt{2\pi}\,F_{ik}(\Theta_i + \Theta_k)^{1/2}\{2(M_i\Theta_i - M_k\Theta_k) + M_k(1 - e_{ik})(\Theta_i + \Theta_k)\}$$

$$F_{ik} = n_i n_k m_i M_k (1 + e_{ik}) h_{ik} \sigma_{ik}^2$$

Granular pressure and transport coefficients

collisions with class k

pertinent velocity gradient

class i

$$p_{ik} = \frac{1}{3}\pi n_i n_k m_i M_k (1 + e_{ik}) h_{ik} \sigma_{ik}^3 (\Theta_i + \Theta_k)$$

$$\mu_i^{ik} = \frac{1}{15}\sqrt{2\pi}\, n_i n_k m_i M_k^2 (1 + e_{ik}) h_{ik} \sigma_{ik}^4 (\Theta_i + \Theta_k)^{3/2} / \Theta_i$$

$$\mu_i^{kk} = \frac{1}{15}\sqrt{2\pi}\, n_i n_k m_k M_i^2 (1 + e_{ik}) h_{ik} \sigma_{ik}^4 (\Theta_i + \Theta_k)^{3/2} / \Theta_k$$

$$\kappa_i^{ik} = \frac{1}{3}\sqrt{2\pi}\, n_i n_k m_i M_k (1 + e_{ik}) h_{ik} \sigma_{ik}^4 (\Theta_i + \Theta_k)^{1/2} (M_k \Theta_k / \Theta_i)$$

$$\kappa_i^{kk} = \frac{1}{3}\sqrt{2\pi}\, n_i n_k m_i M_k (1 + e_{ik}) h_{ik} \sigma_{ik}^4 (\Theta_i + \Theta_k)^{1/2} (M_i \Theta_i / \Theta_k)$$

Gas-particles exchange terms: examples, 1 of 2

- Mass and species

$$\Gamma_g = -\sum_i \Gamma_i$$

$$\Gamma_i = \alpha_i \overline{\rho}_i \sum_\xi \widetilde{R}_{i,\xi}^{s \to g} = \alpha_i \overline{\rho}_i \sum_\xi R_{i,\xi}(\{\widetilde{Y}\}, \widetilde{T}_i)$$

neglects correlations between T and Y_i's

- Momentum

Mass transfer

$$\Gamma_g \mathbf{u}_g^i = \sum_i < \frac{dm_i}{dt} \frac{\mathbf{c}_i}{m_i} >= \sum_i \Gamma_i \tilde{\mathbf{u}}_i.$$

Force interaction

$$\alpha_i \overline{\rho}_i < \frac{\mathbf{F}_i}{m_i} >= \alpha_i \overline{\rho}_i [\mathbf{f}_g -< \frac{V_p}{m_i} \nabla \overleftrightarrow{p}_g > - < \frac{1}{\tau_{i,12}} (\mathbf{c}_i - \overleftrightarrow{\mathbf{u}}_g) >].$$

$$-\alpha_i \overline{\rho}_i < \frac{V_p}{m_i} \nabla \overleftrightarrow{p}_g > \approx -\widehat{\alpha}_i \nabla \overline{p}_g$$

$$-\alpha_i \overline{\rho}_i < \frac{1}{\tau_{i,12}} (\mathbf{c}_i - \overleftrightarrow{\mathbf{u}}_g) > \approx -\frac{\alpha_i \overline{\rho}_i}{\tau_{i,12}} (\mathbf{u}_i -< \overleftrightarrow{\mathbf{u}}_g >_i)$$

Gas-particles exchange terms: examples, 2 of 2

- Granular energy

mass transfer related correlation (negligible Θ fluctuations assumed)

$$\alpha_i \overline{\rho}_i < \frac{dm_i}{dt} \frac{1/2 C_i^2}{m_i} >= \frac{3}{2} \Gamma_i \Theta_i$$

interaction with the gas phase (p_g fluctuations neglected; $\overleftrightarrow{\mathbf{u}}_g = < \overleftrightarrow{\mathbf{u}}_g >_i + \mathbf{u}_g''$)

$$\alpha_i \overline{\rho}_i < \frac{\mathbf{F}_i}{m_i} \cdot \mathbf{C}_i' >= \frac{\alpha_i \overline{\rho}_i}{\tau_{i,12}} (< \mathbf{C}_i' \cdot \mathbf{u}_g'' >_i - < \mathbf{C}_i' \cdot \mathbf{C}_i' >_i)$$

(term negligible if the particle/flow interaction time is much larger than the collisional time)

In-phase transport fluxes

- solid-phase closure
- correlations between the velocity of the respective class and a variable, not explicitly considered in the distribution function
- transport fluxes arise from the self-diffusive transport of the respective property, carried by the particles

$$-\nabla \cdot (\alpha_i \overline{\rho}_i < \mathbf{C}_i Y'_{i\xi} >) = \nabla \cdot (\alpha_i \overline{\rho}_i \mathcal{D}_{ii} \nabla \widetilde{Y}_{i\xi})$$

$$-\nabla \cdot (\alpha_i \overline{\rho}_i < \mathbf{C}_i h'_i >) = \nabla \cdot (\alpha_i \overline{\rho}_i C_{p,i} \mathcal{D}_{ii} \nabla \widetilde{T}_i)$$

Transport of mean particle mass and computation of solidity

• transport theorem, used for the particle mass, gives a transport equation for $\widetilde{m}_i$ not $\overline{m}_i$

• however, it is $\overline{m}_i$ that is required by the model for calculation of the average solidity and the collision terms

$$\frac{\partial(\alpha\rho\overline{m})_i}{\partial t} + \nabla \cdot (\alpha\rho\mathbf{u}\overline{m})_i = \nabla \cdot \alpha_i \overline{\rho}_i \mathcal{D}_{ii} \nabla \overline{m}_i - 2\Gamma_i \overline{m}_i$$

$$\overline{\eta}_i = \overline{m}_i / V_i \sum_\xi \widetilde{Y}_\xi / \rho_\xi$$

Frictional transfer

- So far, stress model based on collisional transfer
- As the volumetric fraction approaches α_{max}, stresses are transmitted at points of sliding or rolling contact
- Where shear rates are very small, Θ_i is too small to support the solids
- Must propose an additional stress based on friction for $\alpha > \alpha_{min}$

Johnson and Jackson (1987) $\boldsymbol{\Sigma}^{tot} = \boldsymbol{\Sigma}^{f} + \boldsymbol{\Sigma}^{c}$ ← collisional and kinetic

$$\boldsymbol{\Sigma}_i^f = -p_i^f \mathbf{I} + 2\mu_i^f \mathbf{S}_i$$

Anderson and Jackson (1992) $$p_i^f = \frac{\alpha_i \rho_i}{\sum \alpha_i \rho_i} Fr \frac{(\hat{\alpha} - \alpha_{min})^p}{(\alpha_{max} - \hat{\alpha})^n}$$ (p=2, n=5)

$$\mu_i^f = p_i^f \sin(\phi)/2\sqrt{I_2}$$

angle of internal friction (25°) → ϕ

second invariant of the strain rate tensor → I_2

Fr ≡ material constant =0.005; $\alpha_{min} \simeq 0.55\text{-}0.6$, $\alpha_{max} = 0.64$

Results on dynamics, 1 of 4

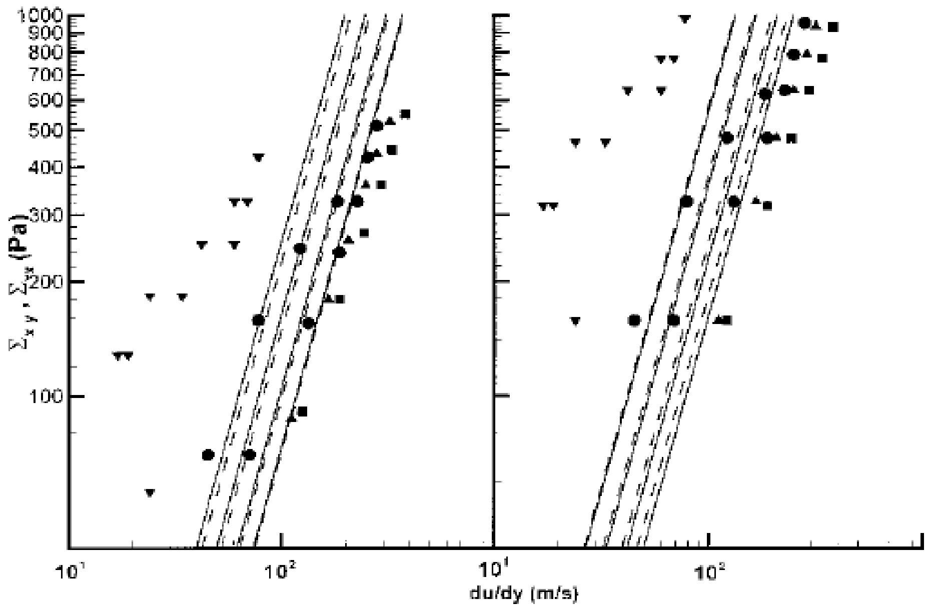


FIG. 1. Predictions of the total shear (left) and normal stresses (right) generated in a simple shear flow of a binary mixture as function of shear rate for various bulk solids fractions, compared with the experimental data from Ref. [20]. Predictions: ——, binary model; - - - -, monodisperse model. Experimental data: ■, α_{tot} = 0.498; ▲, α_{tot} = 0.512; ●, α_{tot} = 0.528; ▼, α_{tot} = 0.542.

20. Savage, S. B., and Sayed, M., *J. Fluid Mech.* 142:391–430 (1984).

- No frictional transfer; problem at high α_{tot}
- Difference from data at lower α_{tot} is attributed to the Gaussian distributions and the form of the radial distribution function

Results on dynamics, 2 of 4

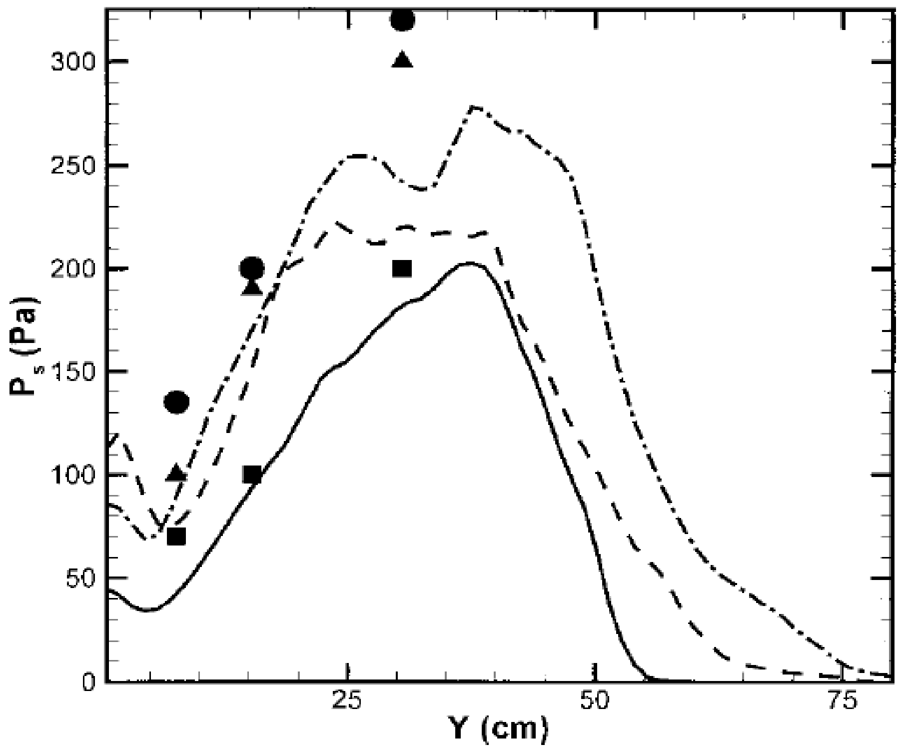


FIG. 2. Predictions of the total time-averaged solids pressure along the wall compared to experimental data of Ref. [21] at different superficial gas velocities. Predictions: $V_g = 0.4$, ——; $V_g = 0.6$, - - -; $V_g = 0.8$, –·–. Experimental data: $V_g = 0.4$, ■; $V_g = 0.6$, ▲; $V_g = 0.8$, ●.

21. Campbell, C. S., and Wang, D. G., *J. Fluid Mech.* 227:495–508 (1991).

All results from now on include friction

- Bubbling bed homogeneously fluidized with air
- Increase in solids p with height; null when there are no particles
- Increase in p_s with superficial gas velocity

Discrepancies with data attributed to
- 2D simulation vs 3D experiment
- insufficient period of averaging (9 s), causing scatter

Results on dynamics, 3 of 4

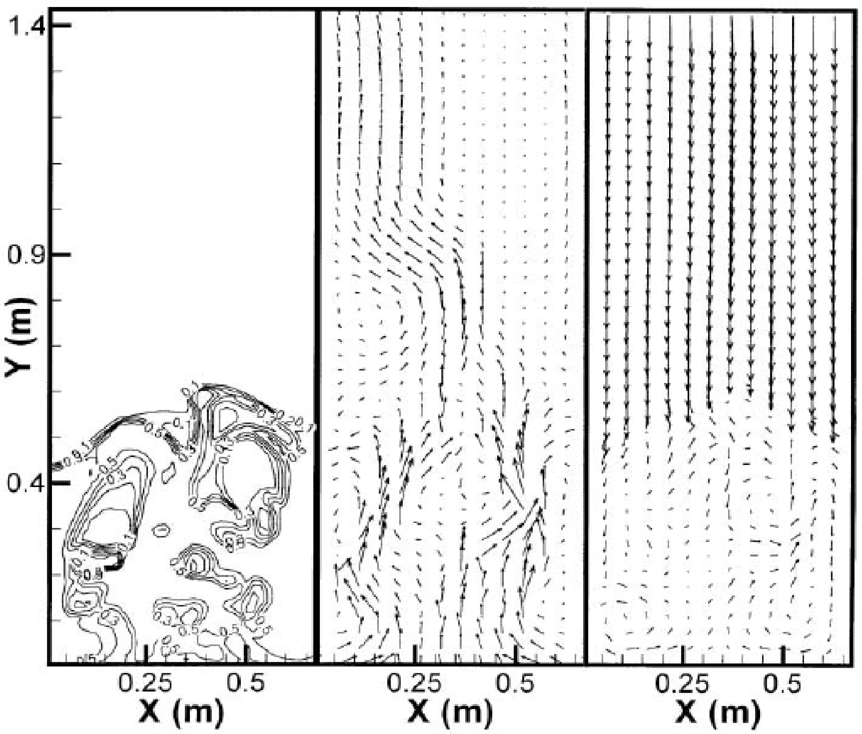


FIG. 3. Instantaneous fields of the solid phase fraction (left), gas velocity (middle), and solids velocity (right) at $t = 3$ s. Only one out of every nine velocity vectors is shown.

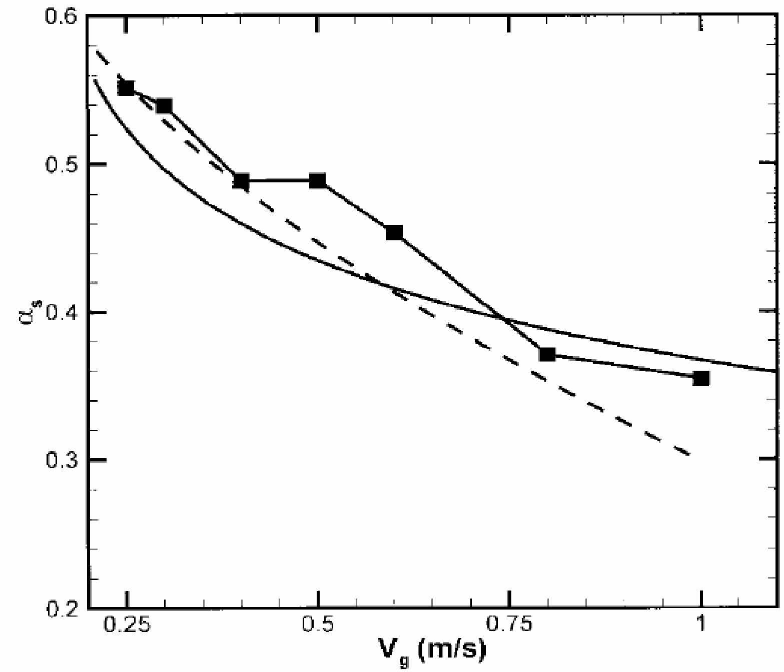


FIG. 4. Solid-phase volume fraction in the lower bed as function of the superficial gas velocity: ■, present model; ——, experimental correlation of Ref. [22]; - - -, equilibrium solution of two-fluid equations.

22. Johnsson, F., Anderson, S., and Leckner, B., *Powder Technol.* 68:117–123, (1991).

volumetrically 2/3 sand, 1/3 biomass

Results on dynamics, 3 of 4

$$S = (0.2\alpha_s - 0.4\alpha_b)/(0.2\alpha_s + 0.4\alpha_b)$$

S = 0, no segregation; S = ±1, complete segregation

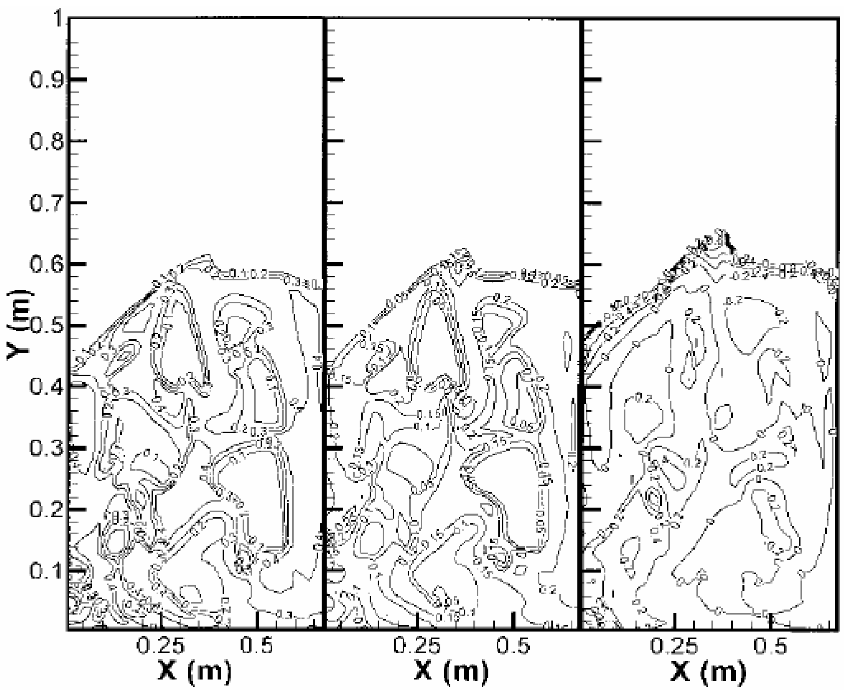


FIG. 5. Instantaneous distributions of sand (left) and biomass (middle) concentrations, and of the segregation parameter (right) at $t = 6$ s.

$S \in [-0.2, 0.2]$

(S<0 inside the bubbles)

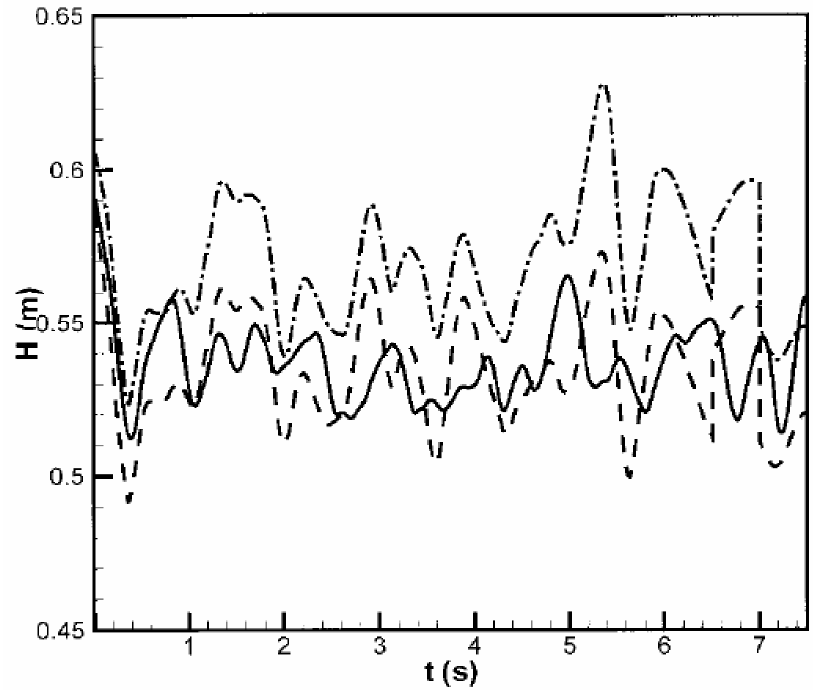


FIG. 6. Time evolution of the y coordinate of center of mass of sand and biomass compared to that of a monodispersed simulation: monodisperse, ——; sand, - - -; biomass, —·—.

Segregation increases with decreasing biomass particle size

Results on dynamics and reaction, 1 of 3

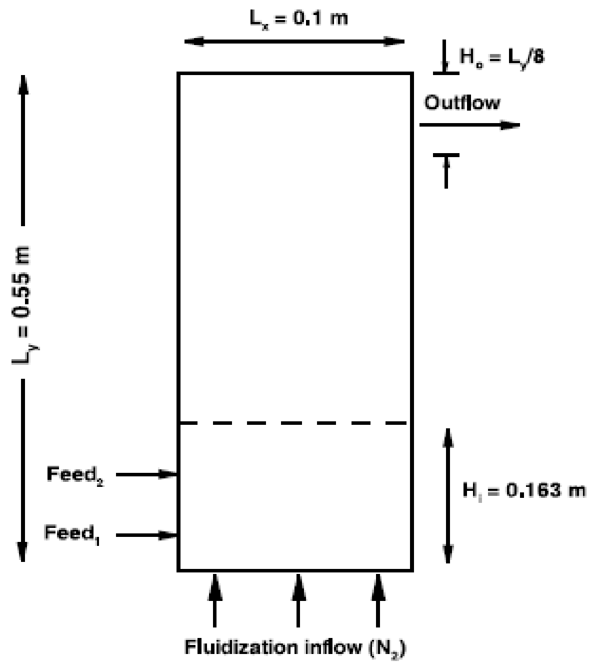
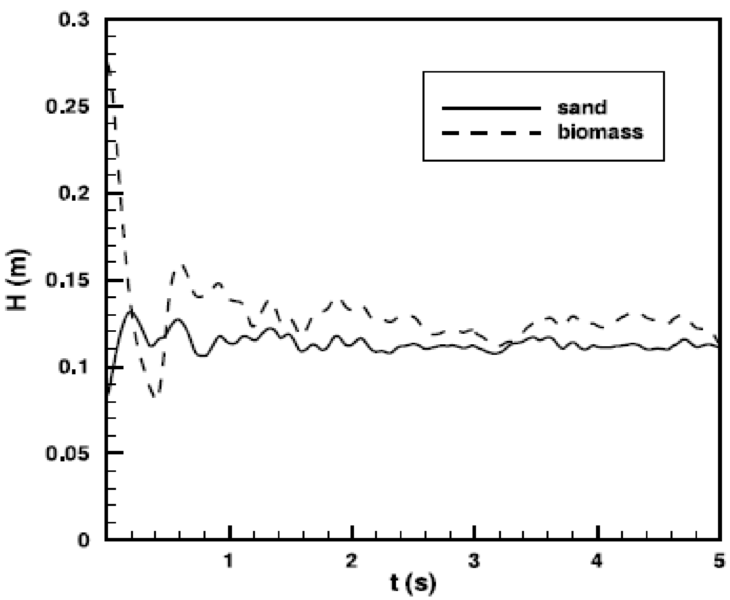


Fig. 1. Schematic of the fluidized bed.



Average vertical coordinate of center of mass; Run 3

Table 3
Summary of operating parameters in the simulations performed

Run no.	T_g (K)	T_b (K)	Feedpoint	Feedstock	Feed rate	V_g (m/s)	d_p (mm)
1	600	400	1	Bagasse	1	0.5	0.5
2	700	400	1	Bagasse	1	0.5	0.5
3[a]	750	400	1	Bagasse	1	0.5	0.5

Results on dynamics and reaction, 2 of 3

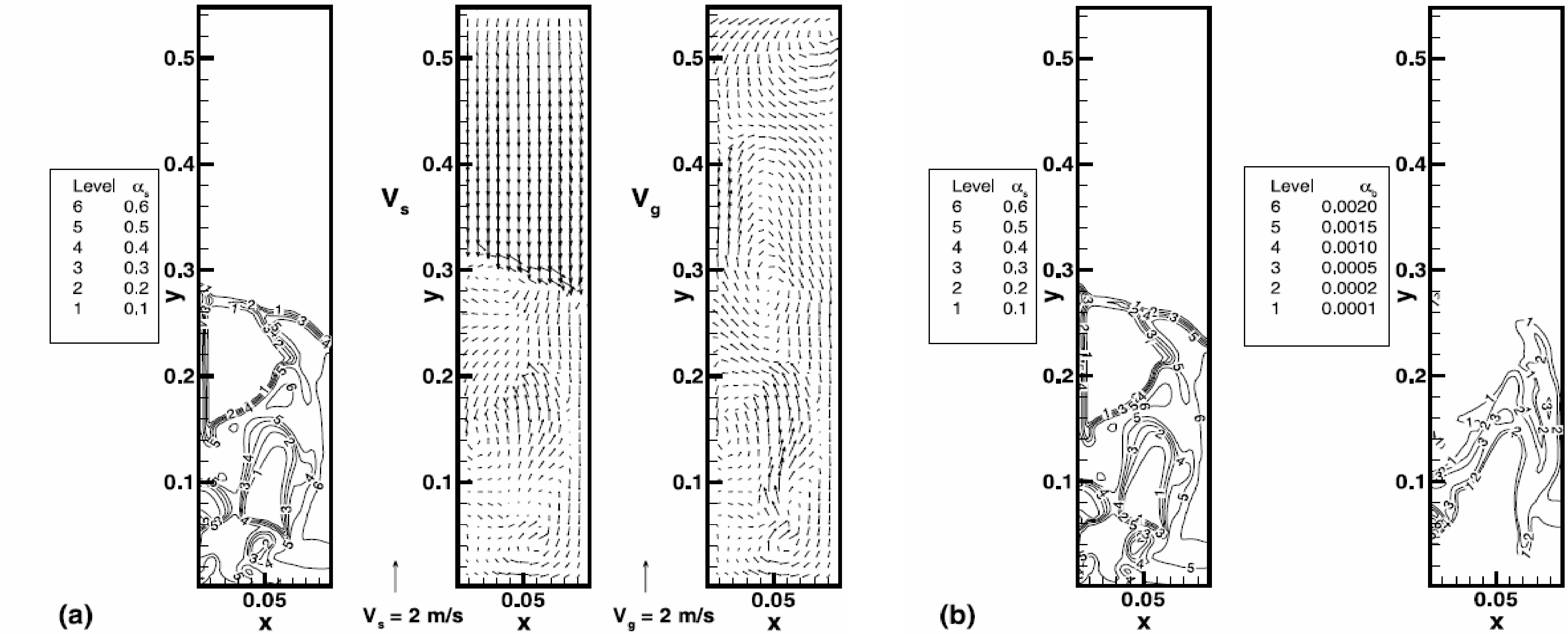
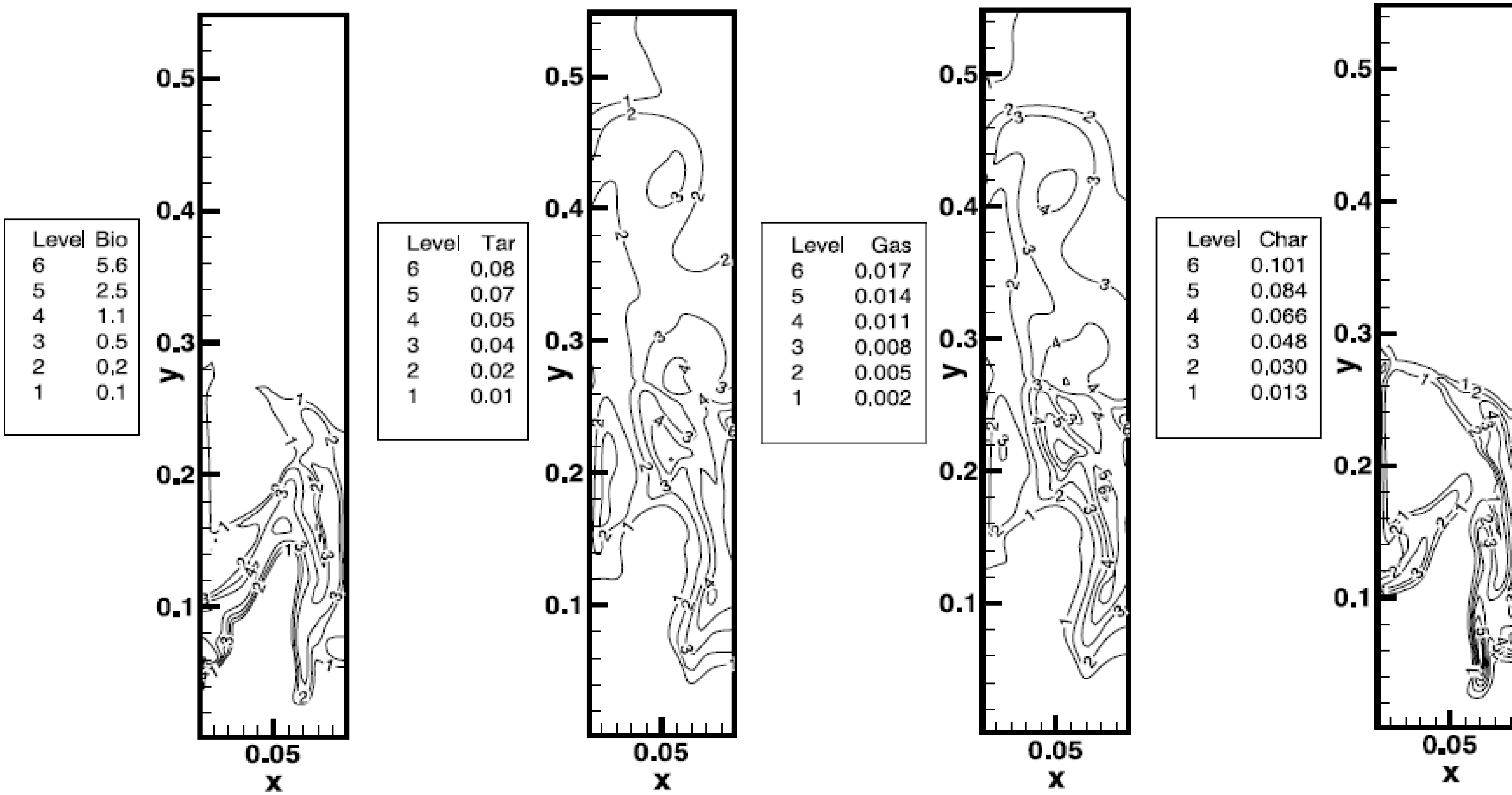


Fig. 2. (a) Volume fraction distribution of solids, carrier gas velocity and solids velocity at $t = 1.5$ s, for Run 3, and (b) volume fraction distribution of sand and biomass at $t = 1.5$ s, for Run 3. The conditions for Run 3 are listed in Table 3.

Results on dynamics and reaction, 3 of 3



Partial macroscopic densities: $\alpha\rho Y$

Summary

What is available:

- granular flow theory; no equipartition of granular energy assumed
- incorporates assumptions which must be modified for soils:
    - Maxwellian (i.e. Gaussian) distribution of particles
    - stresses result from either collisions or friction, or both
    - binary particle collisions
- transfer of mass, momentum, energy and granular temperature during collisions or friction allows computation of the granular pressure, granular viscosity and granular thermal conductivity

What is needed:

- information about particle shape and morphology
- radial distribution function
- experimental data to compare to predictions
- couple a trustworthy model with uncertainty quantification