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Formulation and validation of an efficient computational model for a dilute, settling suspension undergoing rotational mixing

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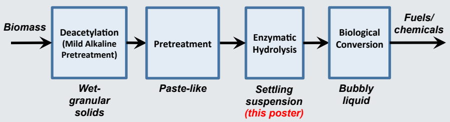
Executive Summary

- Designing processing equipment for the mixing of settling suspensions is a challenging problem.
- We developed a mixture model to describe the hydrodynamics of a settling cellulose suspension.
- The solids are represented by a scalar volume-fraction field that undergoes transport due to particle diffusion, settling, fluid advection, and shear stress.
- Simulation results were in quantitative agreement with experimentally obtained torque and mixing-rate data, including a characteristic torque bifurcation.
- The CFD model will be coupled with reaction-kinetics models and will be useful for designing economical biochemical conversion reactors.

Background

Biochemical conversion of cellulosic biomass

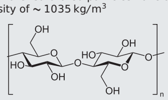
- The conversion of cellulosic biomass into fuels and chemicals has the potential to provide renewable alternatives to those derived from fossil carbon sources (oil, natural gas, and coal).
- The deconstruction, fractionation, and biochemical conversion of cellulosic biomass involves process streams with widely varying material properties (see diagram below).
- Proper mixing during biomass conversing is vital to achieving maximum process yields and economic success.

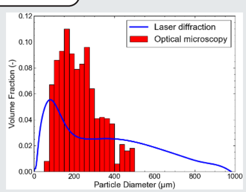


Experimental

Material

- 5 wt% α-cellulose (Sigma-Aldrich) in DI water
- The porous fibers and particles have a broad size range and form aggregates
- The water-saturated particles have a density of $\sim 1035\,\mathrm{kg/m^3}$





Rheometry

- TA Instruments (New Castle, DE) AR-G2 stress controlled rheometer
- Stainless-steel vane with 4 blades that are 38 mm in height and 1.25 mm thick, with an overall diameter of 15 mm

Vane-and-Cup Setup

- 15 mm diameter vane inside TA Instruments' standard stainless steel cup (30 mm inner diameter)

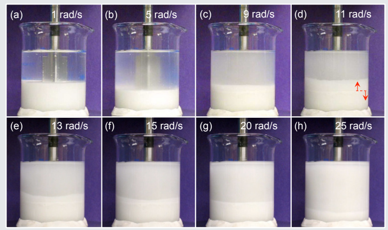
Vane-and-Beaker Setup

- 15 mm vane inside a 100 mL glass beaker (70 mm height and 47 mm diameter) fastened to the rheometer Peltier plate with adhesive putty

Procedure

- The angular velocity of the vane was increased and then decreased in steps for the range of 1 to 45 rad/s
- Each velocity was held constant for a maximum of 10 min and data was gathered every 3 s
- The system was considered to have achieved "steady-state" once the instrument recorded 5 consecutive torque measurements all within 5% of one another
- Rheometer data was averaged over a 15 s data collection window

Results

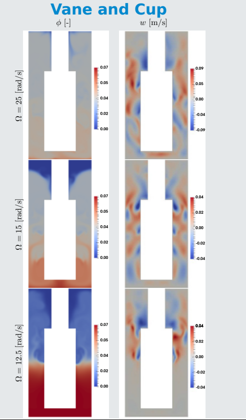


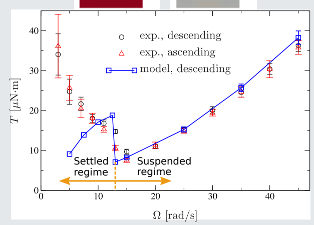
(above) Photographs of the suspension undergoing mixing at incremental mixing speeds across the settled-suspended transition. As the speed of the vane is increased, particles are convected into suspension. At intermediate speeds, some particles resettle near the beaker wall, as indicated in panel (d).

(top right) CFD simulation snapshot slices of the particle volume fraction (ϕ) and vertical velocity component (w) at the rotational speeds (Ω) indicated. Qualitative agreement of the solids distribution is observed between the simulations and experiments.

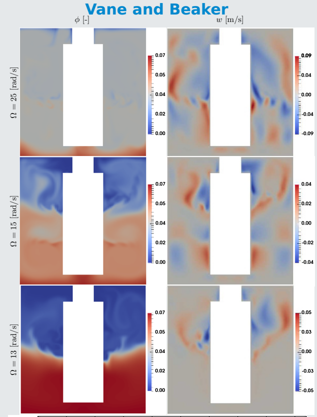
(bottom right) Steady torque vs. rotational speed of the CFD predictions and experimentally measured values. The CFD model predictions are in close agreement for the suspended regime ($15 \le \Omega \le 35$ rad/s). The simulations predict a bifurcated torque response at rotation rates that are quite close to the experimental observations. However, the simulation torque profiles do not match experimental profiles in the suspended flow regime. This is not surprising given the absence of yield-stress behavior in our model, and hence the predicted torque goes to zero as $\Omega \to 0$.

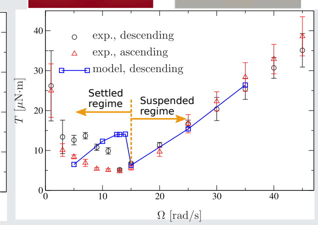
Vane and Cup





Vane and Beaker





Computational Methods

- CFD employing a *mixture model*
- Single velocity field $\mathbf{u}(\mathbf{x},t) = (u,v,w)$ in an Eulerian framework ($\mathbf{x} \in R^3$)
- Solids volume fraction $\phi(\mathbf{x},t)$ is a scalar field that undergoes transport due to *particle diffusion, settling, fluid advection,* and *shear-stress*
- *Boussinesq approximation* is used because particle density is a small perturbation from water density
- Given the axisymmetric vessels, a reference frame rotating about the z axis with angular rotation rate Ω was used
- Simulations performed with open-source *Nek5000* software that is based on the high-order spectral-finite-element method

$$\frac{\partial \mathbf{u}}{\partial t} = -\mathbf{u}\cdot\nabla\mathbf{u} - \frac{1}{\rho_w}\nabla p - 2\Omega\mathbf{z}\times\mathbf{u} + \frac{1}{\rho_w}\nabla\cdot(\mu_{ef}\nabla\mathbf{u}) - \phi\left(\frac{\rho_s}{\rho_w}-1\right)\left[g\mathbf{z} + \Omega^2\mathbf{z}\times(\mathbf{z}\times\mathbf{x})\right] \quad (1)$$

$$\nabla\cdot\mathbf{u} = 0 \quad (2)$$

$$\frac{\partial\phi}{\partial t} = -\nabla\cdot(\mathbf{F}_{adv} + \mathbf{F}_{diff} + \mathbf{F}_{shear} + \mathbf{F}_{settle}) \quad (3)$$

$$(\mathbf{F}_{adv} + \mathbf{F}_{diff} + \mathbf{F}_{shear} + \mathbf{F}_{settle})\cdot\mathbf{n} = 0, \quad \mathbf{x}\in\Gamma$$

$$\mathbf{F}_{adv} = \mathbf{u}\phi \quad (4)$$

$$\mathbf{F}_{diff} = -D\nabla\phi \quad (5)$$

$$\mathbf{F}_{settle} = \mathbf{z}\phi w_{settle} \quad (6)$$

$$\mathbf{F}_{shear} = -C_\phi a^2\phi\nabla(\dot\gamma\phi) - C_\mu a^2\phi^2\dot\gamma\nabla\left[\log(\mu_{ef})\right] \quad (7)$$

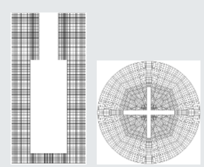
$$w_{settle} = C_1\frac{\exp(-\phi C_2) - \exp(-\phi_{max}C_2)}{1-\exp(-\phi_{max}C_2)}H(\phi_{max}-\phi) \quad (8)$$

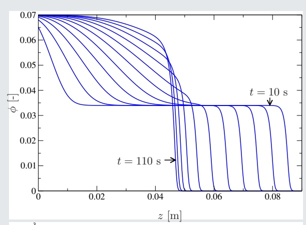
$$\mu_{ef} = \mu_w\left(1-\frac{\phi}{\phi_\infty}\right)^{-n} \quad (9)$$

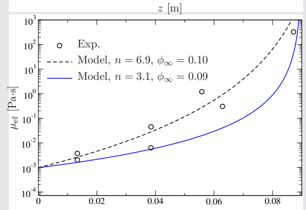
(top right) Solids-volume-fraction (ϕ) profiles for a simulation with no mixing ($\Omega = 0$) to test settling model.

(bottom right) Viscosity model. The best fit (dashed line) to independently measured viscosity (via rough parallel-plate measurements) resulted in predicted torque values that were too high. "Tuning" the viscosity model (blue line) resulted in excellent quantitative agreement as shown in the results.

(below) Mesh for the vane and cup with ~ 8000 hexahedral elements.







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