Multiphysics Simulations Of Shear Thickening & Clogging In Prefilled Syringes

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Abstract

Clogging can occur when particulates suspended in a viscous carrier fluid flow through confined geometries. Examples include the blockage of inkjet printer nozzles in additive manufacturing processes, the clogging in medical injection devices by highly concentrated injectables, and the occlusion of pores by organic contaminants in water filtration membranes. Computer simulations provide a useful tool to understand clogging mechanisms and elucidate design strategies to minimize or avoid clogging. Here, we present COMSOL Multiphysics® simulations of the injection of a highly concentrated particulate suspension through a syringe needle to determine the conditions that lead to clogging.

We coupled the Creeping Flow and Phase Transport interfaces in COMSOL Multiphysics® to simulate the flow of a particulate suspension through a needle syringe under a steady applied plunger force. Clogging is said to occur above a threshold plunger force of 20 N. The fluid velocity, fluid pressure, and particle phase volume fraction were tracked during the simulation. The suspension viscosity varied with local particle volume fraction and local shear stress, imparting non-Newtonian fluid mechanics. Rheological data for a surrogate fluid [1], cornstarch in a glycerol-water mixture, were used to calibrate a non-Newtonian constitutive model [2] for use in the simulation (Figure 1). The model exhibits discontinuous shear thickening - a sudden jump in the suspension viscosity above a critical onset stress.

Fluid mechanics simulations with the calibrated constitutive model show a rise in the plunger force for large particles at high volume fraction. The microscopic mechanism of this rise in plunger force is depicted in Figure 2. As the suspension flows from the barrel hub into the needle, initially well-lubricated particles are brought into frictional contact. When a sufficient number of particles are in frictional contact, the suspension clogs. Simulations of needle flow at various particle diameters and volume fractions enable prediction of the 20 N threshold for clogging (Figure 3). Larger, more densely packed particles increase the risk of clogging. Smaller particle diameters (< 1 μm) clog above a volume fraction of 47%, whereas larger particles (> 1 μm) clog above around 40%.

In summary, we employed multiphysics simulations to predict clogging of a particulate suspension through a syringe needle. Needle clogging in prefilled syringes can impede drug product injection and negatively impact drug product quality. Our simulations furnished an operating diagram based on a maximum allowable plunger force, which predicts clogging for large, densely packed particles. The onset of clogging was correlated to the transition from lubricated to frictional particle contacts in the suspension. Simulations such as these can help predict and remediate clogging in prefilled syringes, which ultimately lead to savings in development time and reduced risk.

Reference

[1] E. Brown & H. M. Jaeger, "The role of dilation and confining stresses in shear thickening of dense suspensions," Journal of Rheology 56.4, 875-923 (2012).
[2] M. Wyart & M. E. Cates, "Discontinuous shear thickening without inertia in dense non-Brownian suspensions," Physical Review Letters 112.9, 098302 (2014).

Figures used in the abstract

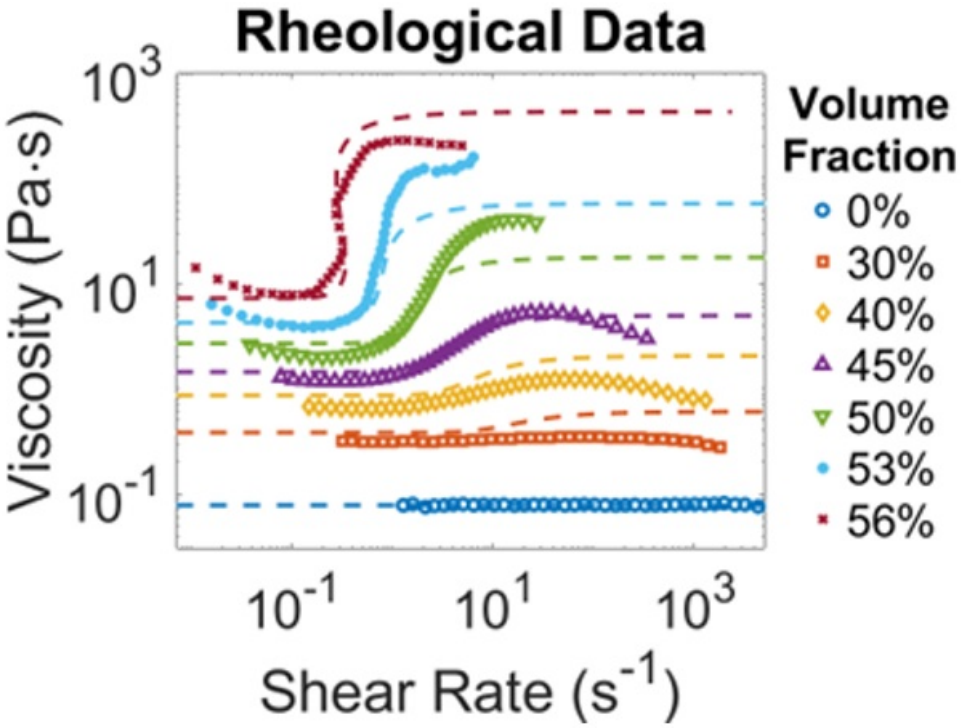

Figure 1 : Shear rheology of cornstarch suspension at various volume fractions [1]. Dashed lines show model fits [2].

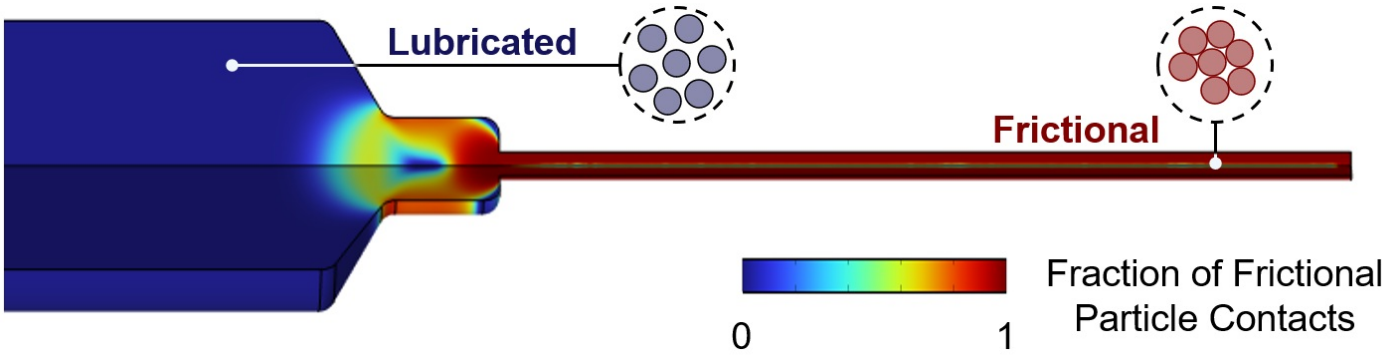

Figure 2 : CFD simulation of a particulate suspension through a syringe needle (particle volume fraction of 50%, particle diameter of 10 μm). Contours show transition from lubricated to frictional particle contacts, which leads to shear thickening and clogging.

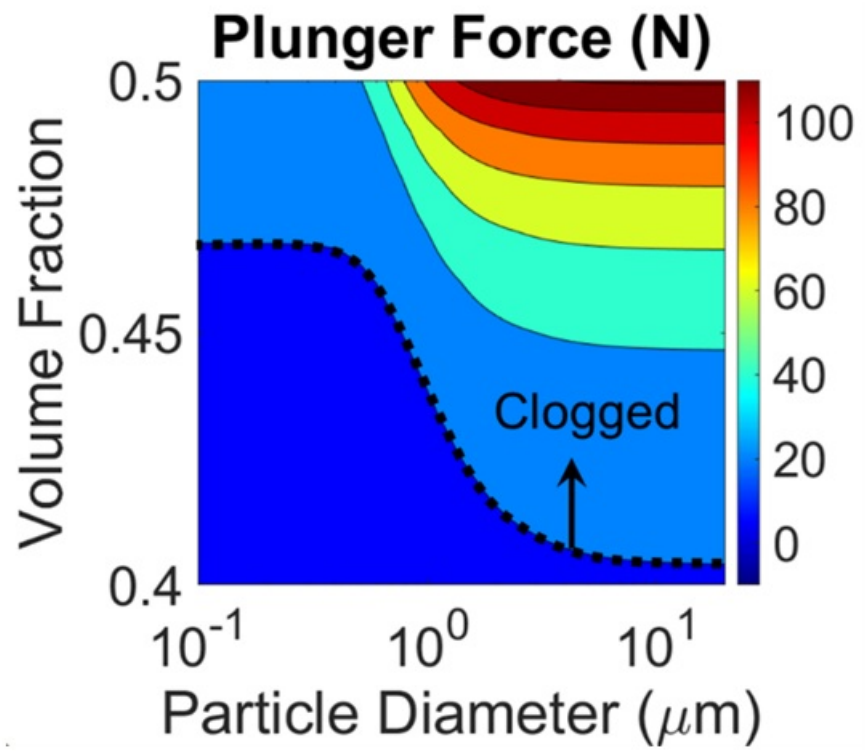

Figure 3 : Contours of plunger force as a function of suspension properties predict the 20 N threshold for clogging.