The Effect of Shear Thinning on Splatting Behavior of Molten Polymer Droplets under Thermal Spray Conditions

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Introduction

This abstract presents theoretical analysis of the effect of shear thinning on impact and deformation of non-Newtonian droplets. Previously published results [1] indicated that shear thinning plays an important role in the splatting behavior of High Velocity Oxy-Fuel sprayed polymer particles. This is primarily due to the high impact velocity (> 100 m/s) of micron-sized particles, which generates high shear rates (> 10^6 s^{-1}) during particle impact.

Reynolds number is the most commonly used dimensionless quantity governing the spreading of droplets during inertially induced flows when surface tension and capillary effect can be neglected as described elsewhere [2]. The Reynolds number scales the relative importance of inertia to viscous forces ($Re = \rho\ V_o\ D_o/\mu_o$) during droplet spreading and can be defined by the droplet density (ρ), original diameter (D_o), impact velocity (V_o) and dynamic viscosity (μ). It is not obvious what would be appropriate value for the viscosity (μ) in this equation so that the Reynolds number (Re) can effectively describe the spreading dynamics of a shear thinning droplet. The zero shear rate viscosity (μ_o) would be an obvious choice, however; impact viscosity of a shear thinning droplet is often much lower than the zero shear rate viscosity so that a high shear rate viscosity is also a reasonable selection.

In the following section the zero shear rate Reynolds number ($Re_o = \rho\ V_o\ D_o/\mu_o$) and high shear rate Reynolds number ($Re^* = \rho\ V_o\ D_o/\mu^*$) are derived by scaling the momentum equation for the fluid flow. A molten polymer droplet was modeled as a generalized Newtonian fluid with shear rate dependent viscosity. The extent of droplet spreading (D_{splat}/D_o) was predicted through a parametric study as a function of both Reynolds numbers (Re_o and Re^*). The maximum spreading diameter of a droplet (D_{splat}) was based on the diameter of a fully spread static splat and D_o was the original diameter of the droplet. Droplet spreading and the extent of droplet spreading was predicted using a volume-of-fluid computational fluid mechanics package, Flow-3D® version 9.0 as reported earlier [1, 2].

Theoretical Approach

The shear thinning effect on droplet spreading is analyzed using the momentum Equation 1 for generalized Newtonian flow where the dynamic viscosity (μ) is a function of the rate of the deformation tensor ($\mathbf{\Gamma} = 0.5(\nabla v + \nabla v^T)$).

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\,\mathbf{v}\right) = \rho\,\mathbf{g} - \nabla\,p + \nabla\cdot\left[\mu\left(\mathbf{\Gamma}\right)\left(\nabla\mathbf{v} + \nabla\mathbf{v}^T\right)\right] \tag{1}$$

A scalar measure of the rate of strain in shearing, or shear rate, is $\dot{\gamma} = 2\Gamma \equiv (\mathbf{\Gamma}:\mathbf{\Gamma})^{1/2}$ so that the viscosity is often described in a simplified form as a function of shear rate ($\mu = f(\dot{\gamma})$).

The logical scales for length, velocity and time are droplet diameter (D_o), impact velocity (V_o) and their ratio ($t^* = D_o/V_o$) so that scaled variables are of the form:

$$\tilde{\nabla} = D_o \nabla\,; \qquad \tilde{\mathbf{v}} = \frac{\mathbf{v}}{V_o}\,; \qquad \tilde{t} = \frac{t}{t^*} = t\frac{V_o}{D_o}\,; \tag{2}$$

The scaled pressure and dynamic viscosity are of the form:

$$\tilde{P} = \frac{P}{P_i^*} = \frac{P}{\rho V_o^{\,2}}\,, \qquad \tilde{\mu} = \frac{\mu(\dot{\gamma})}{\mu^*} = \tilde{\mu}(\tilde{\dot{\gamma}}) \tag{3}$$

Substitution of the dimensional variables ($\mathbf{v}$, t, P, μ and ∇) with scaled variables ($\tilde{\mathbf{v}}, \tilde{t}, \tilde{P}, \tilde{\mu}$ and $\tilde{\nabla}$) into Equation 1, rearranging and dividing it by $\rho V_o^2/D_o$, yields the following scaled equation:

$$\left[\frac{\partial \tilde{\mathbf{v}}}{\partial \tilde{t}} + \tilde{\mathbf{v}} \bullet \tilde{\nabla}\tilde{\mathbf{v}}\right] = -\tilde{\nabla}\tilde{P} + \tilde{\nabla} \bullet \left[\overbrace{\frac{\mu^*}{\rho V_o D_o}}^{\frac{1}{Re^*}} \tilde{\mu}\left(\tilde{\nabla}\tilde{\mathbf{v}} + \tilde{\nabla}\tilde{\mathbf{v}}^{T}\right)\right], \tag{4}$$

The resulting Reynolds number (Re*), that emerges as an inverse coefficient in Equation 4, includes viscosity scale μ^*. As mentioned earlier it is not obvious what values would be appropriate for this scale so that the characteristic Reynolds number (Re*) can effectively describe the spreading dynamics of a deforming droplet. A simplified version of the four parameter isothermal Carreau model [3] was used to derive the scale for characteristic viscosity at droplet impact (Equation 5).

$$\frac{\mu}{\mu_o} = \left[1 + (\lambda\dot{\gamma})^2\right]^{\frac{n-1}{2}} \tag{5}$$

where n is shear thinning ("power law") exponent and λ relaxation time constant. The characteristic viscosity μ^* at the characteristic impact shear rate ($\dot{\gamma}^* = V_o/D_o$) can be defined using this model (Equation 5) as follows:

$$\frac{\mu^*}{\mu_o} = \left[1 + (\lambda\dot{\gamma}^*)^2\right]^{\frac{n-1}{2}} = \left[1 + \left(\lambda\frac{V_o}{D_o}\right)^2\right]^{\frac{n-1}{2}} \tag{6}$$

Substituting the characteristic viscosity μ* (Equation 6) into the Reynolds number obtained from equation 4, yields the following relationship:

$$Re^* = \frac{\rho\, V_o\, D_o}{\mu_o}\left[1+\left(\lambda\frac{V_o}{D_o}\right)^2\right]^{\frac{1-n}{2}} = Re_o\left[1+\left(\lambda\frac{V_o}{D_o}\right)^2\right]^{\frac{1-n}{2}} \qquad (7)$$

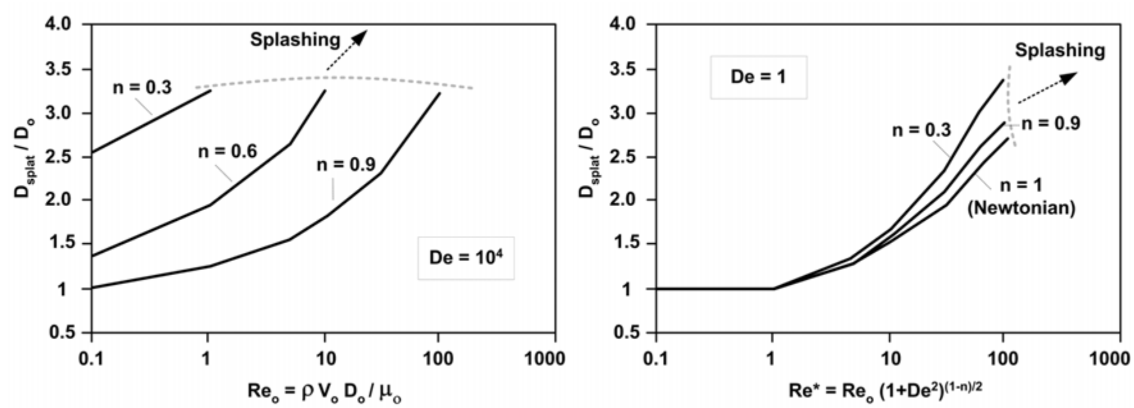
Equation 7 defines a high shear rate Reynolds number (Re*) which takes into account the shear thinning effect based on the Carreau model. An additional correlation can be created by introducing the Deborah number ($De = \lambda V_o/D_o$) [3] into Equation 7 as follows:

$$Re^* = Re_o\left[1+De^2\right]^{\frac{1-n}{2}} \qquad (8)$$

According to Equation 8, the three key parameters that define the flow dynamics of a shear thinning droplet are: (i) the Deborah number — De, (ii) the shear thinning exponent – n, and (iii) the Reynolds number that can be either high shear rate Reynolds number ($Re^* = Re_o\,[1 + De^2]^{1-n/2}$) or the zero shear rate Reynolds number ($Re_o = \rho\ V_o\, D_o/\mu_o$). In the following section the extent of droplet spreading (D_{splat}/D_o) was predicted through a parametric study where two of the parameters were varied while the third was kept constant.

Numerical Predictions

The maximum spreading ratio of a droplet predicted as a function of the shear thinning exponent (n), Deborah number (De) and both Reynolds numbers (Re* and Re_o) are shown in Figures 1.



(a) (b)

Figure 1 Predicted splatting ratio of a shear thinning droplet as a function of n, a constant Deborah number (a) Re_o and (b) Re*.

The splatting predictions based on a zero shear rate Reynolds number (Re_o) (Figure 1a) confirmed that at higher Deborah numbers (i.e. higher shear rates) the spreading predictions were very sensitive to the shear thinning exponent (n). In other words, even for a rough estimate of droplet spreading ratio, precise rheological properties of the given material, particularly the shear thinning exponent and relaxation time, are necessary which is often not practically feasible. The spreading predictions based on Re* indicated that they were largely insensitive to variations in the shear thinning exponent (Figure 1b). This result was fundamentally different from the predictions based on Re_o (Figure 1a) indicating that Re* can better capture the flow dynamics during impact of a shear thinning droplet.

In all cases, splashing of the shear thinning droplets started when the spreading ratio of the droplet reached a value in the range 3.0 to 3.5. These predictions do not account for any surface tension effects, as justified earlier [1, 2]. Increases in surface tension will typically reduce the degree of droplet spreading and stimulate flow instabilities and splashing.

Conclusions

It was found that a Reynolds number based on zero shear rate viscosity ($Re_o = \rho V_o D_o / \mu_o$) which is often readily available, does not properly capture the flow dynamics during impact of a shear thinning droplet. This was primarily because the viscosity of a shear thinning droplet at impact is often much lower than the zero shear rate viscosity, particularly at high shear rates, and changes constantly until the droplet is fully deformed into a static splat.

A theoretical relationship (Equation 8), combining the Reynolds number with a shear thinning Carreau model and Deborah number, was proposed in order to better capture the dynamics of shear thinning droplet. The predicted spreading ratios based on Re* were relatively insensitive to the values of the Deborah number and shear thinning exponent. The key conclusion of this analysis is that high shear rate Reynolds number (Re*), proposed by equation 8, can better describe the flow dynamics during the splatting of a shear thinning droplet than zero shear rate Reynolds number (Re_o).

References

[1] Ivosevic, M., Cairncross, R. A., and Knight, R., 3D Predictions of Thermally Sprayed Polymer Splats: Modeling Particle Acceleration, Heating and Deformation on Impact with a Flat Substrate, *Int. Journal of Heat and Mass Transfer*, In Press 2006.

[2] Ivosevic, M., Splat Formation during Thermal Spraying of Polymer Particles: Mathematical Modeling and Experimental Analysis, *PhD Thesis*, Drexel University, Philadelphia, PA 19104, 2006.

[3] Bird, R. B., Armstrong R. C. and Hassager, O., *Dynamics of Polymeric Liquids*, Volume 1: Fluid Mechanics, 2nd Ed., John Wiley & Sons, Inc., 1987.

Acknowledgment of support: This research has been supported by the National Science Foundation (NSF) under collaborative grant number DMI 0209319. The views expressed in this paper do not necessarily reflect those of NSF.