**Check One: X Project ☐Review ☐Collaboration**

 **☐Workshop ☐Other**

| **Descriptive Title** | Numerical Modeling Approach to Heterogeneous Particle Wetting and Fish-Eye Avoidance. |
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| **Working Title[[1]](#footnote-0)** | Numerical Modeling- Reconstitution of Wetting |
| **Technical Area[[2]](#footnote-1)** | Wet |
| **Date** | 6/17/25 |
| **Short Description** | Building on the strong support for experimental approaches to powder/particle wetting voiced at the 2024 reconstitution workshop, we propose a critical numerical modeling project. This project will directly complement the upcoming experimental work by Luccio Isa and Pat Spicer, focusing on the wetting of heterogeneous particles and, secondarily, preventing specific reconstitution failures like 'fish eyes.' Our numerical modeling effort will deliver powerful tools to quantify, validate, and iteratively advance models for predicting and optimizing reconstitution system behavior. This synergistic coupling of modeling and experimental systems will not only provide unprecedented insights into complex wetting phenomena but also rapidly accelerate our fundamental understanding of powder wetting and dispersion, enabling targeted solutions to pressing industry challenges. |
| **Objectives** | 1. Develop numerical models to predict and validate heterogeneous particle wetting and fish-eye mechanisms, working with experimentalist approaches in model systems.
2. Simulate “single” particle wetting and more complex, multiple particle wetting systems, specifically targeting fish-eye formation and avoidance.
3. Determine the controlling variables of a powder that determines the rate of movement across a liquid/gas interface. This may include but is not limited to:
	1. porosity, density, of the released powder
	2. interfacial tension of the liquid interface
	3. density ratio
	4. particle mobility in the agglomerate
	5. rate of escape of trapped gas
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| **Scope** | Numerical modeling and simulations of: * Tunable heterogeneous particles and their transport across gas/liquid interface
* Fish eye formation & avoidance.
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| **Recommended Contractors (2 or 3)** |
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1. Title used in meeting agendas and file archives [↑](#footnote-ref-0)
2. One or more from the following list: W = wet systems; D = dry systems; F = particle formation; SR = size reduction; M = modeling; SE = systems engineering [↑](#footnote-ref-1)