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HARD Solids

Validating a Radiative Transfer Model for Optically Thin Deposits

PL14-V-HARD Solids-PD3UA

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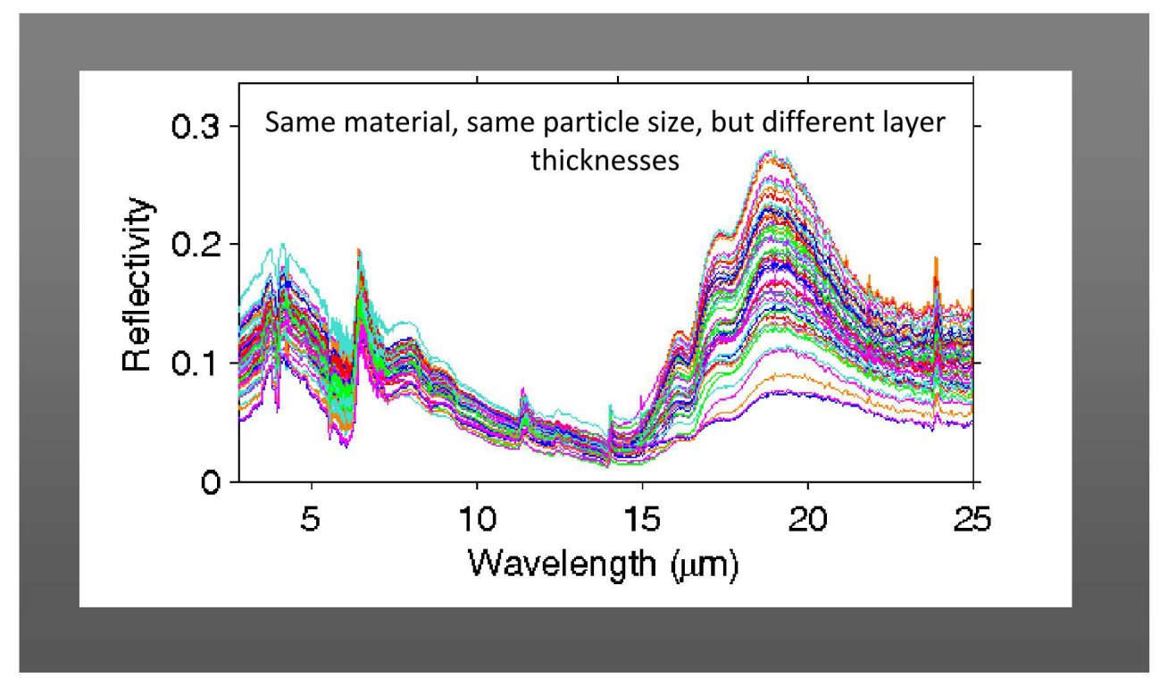
Goals and Objectives

- Develop physics-based models to compute spectra of complex solid materials
  - for use in algorithms leveraging these models and in spectral signature libraries
  - and supported by measurements that provide input data for models, validate models, and enable new models
- Model will incorporate fundamental physical properties (*n*,*k*) and account for morphological characteristics – particle size, shape, packing density, surface roughness, deposit thickness.

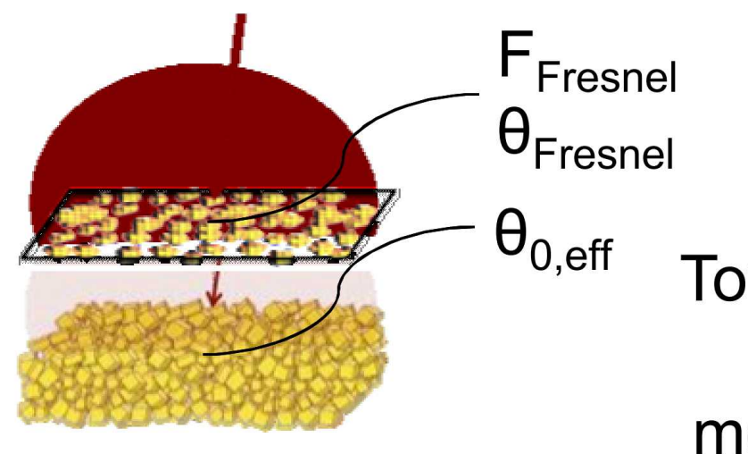
Introduction

Reflectance spectra of particulate media can exhibit strong dependence on morphology.

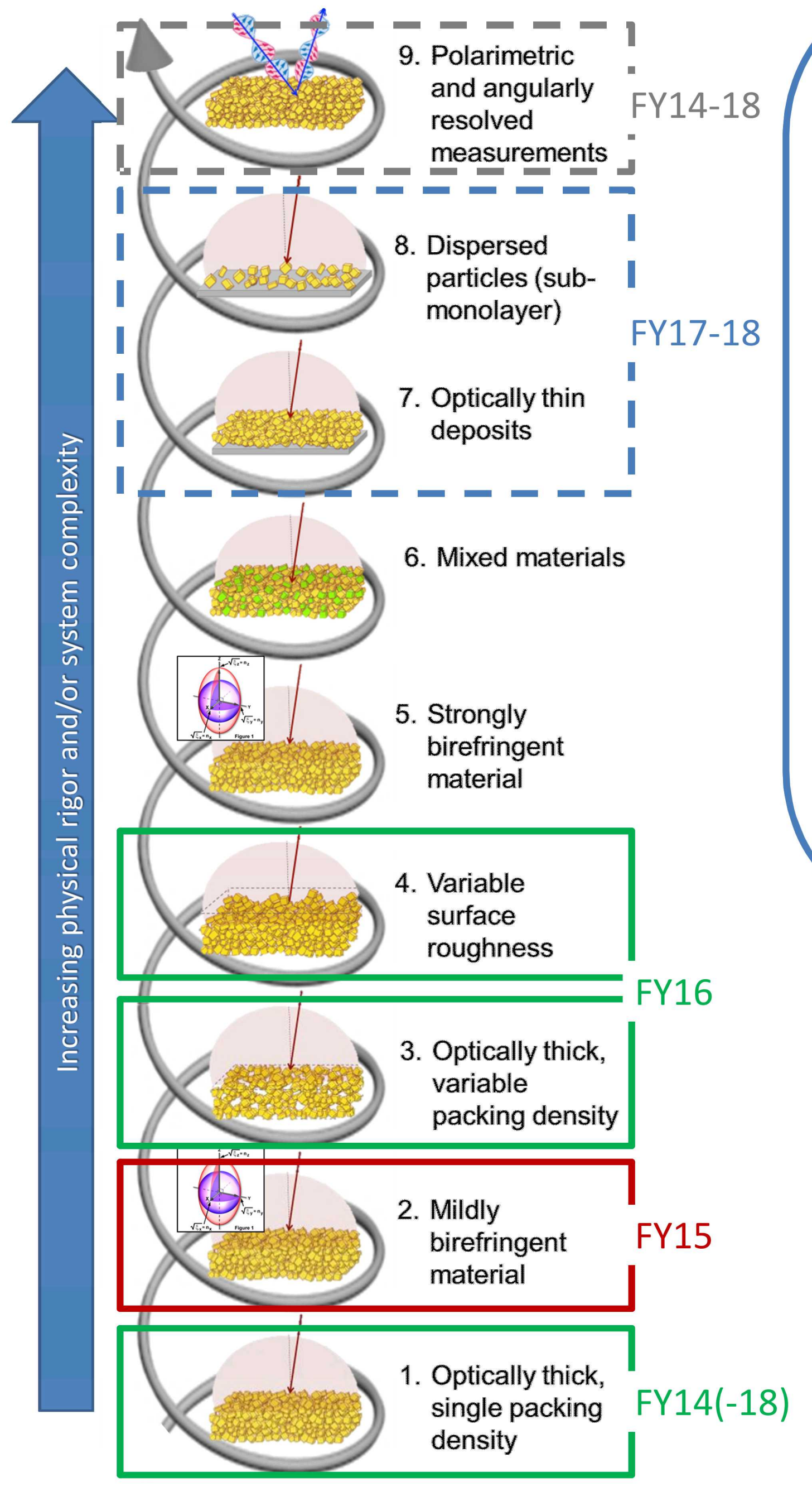


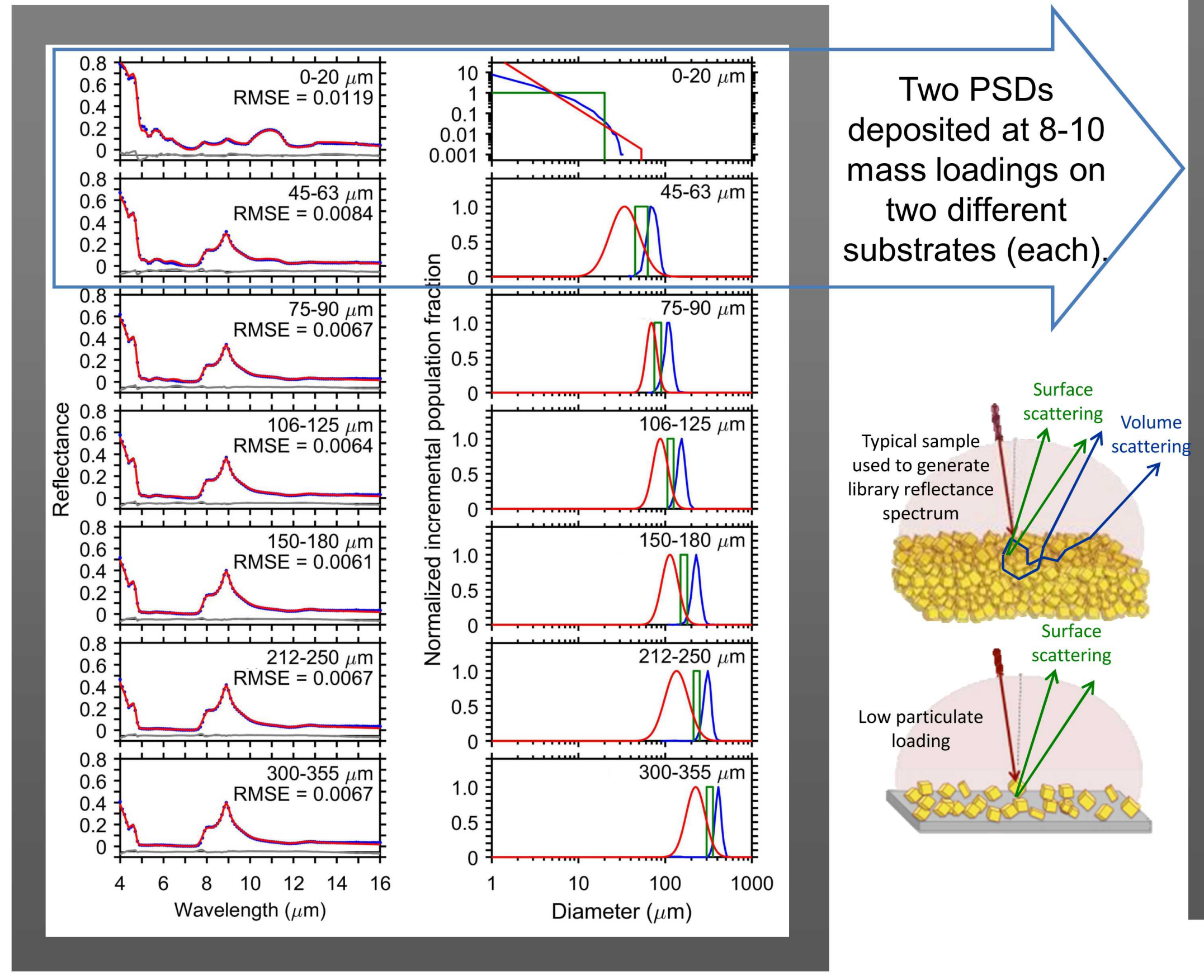
Varying the particle size, shape, packing density, surface roughness, and deposit thickness over entire parameter space is to be accomplished via modeling the interaction of incident radiation with the material deposit.

- Implement 1-D radiative transfer (RT) solutions
- Parameterize the particle size distribution (PSD) – e.g., lognormal
- Incorporate model "patches" to allow for application of RT to packed particulate media, specifically dealing with the 1st-surface reflection:



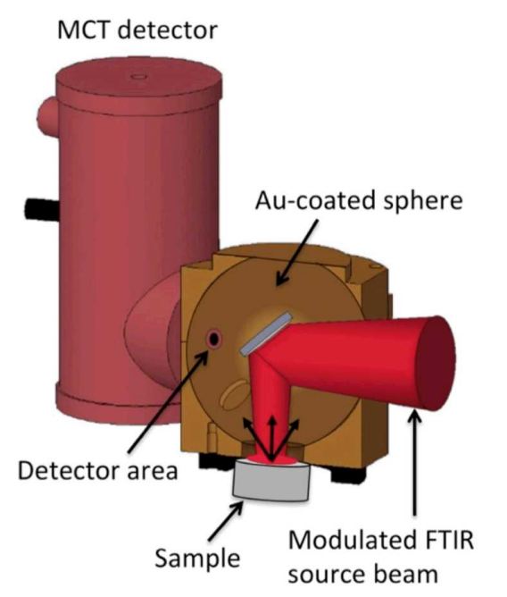
Project Progression





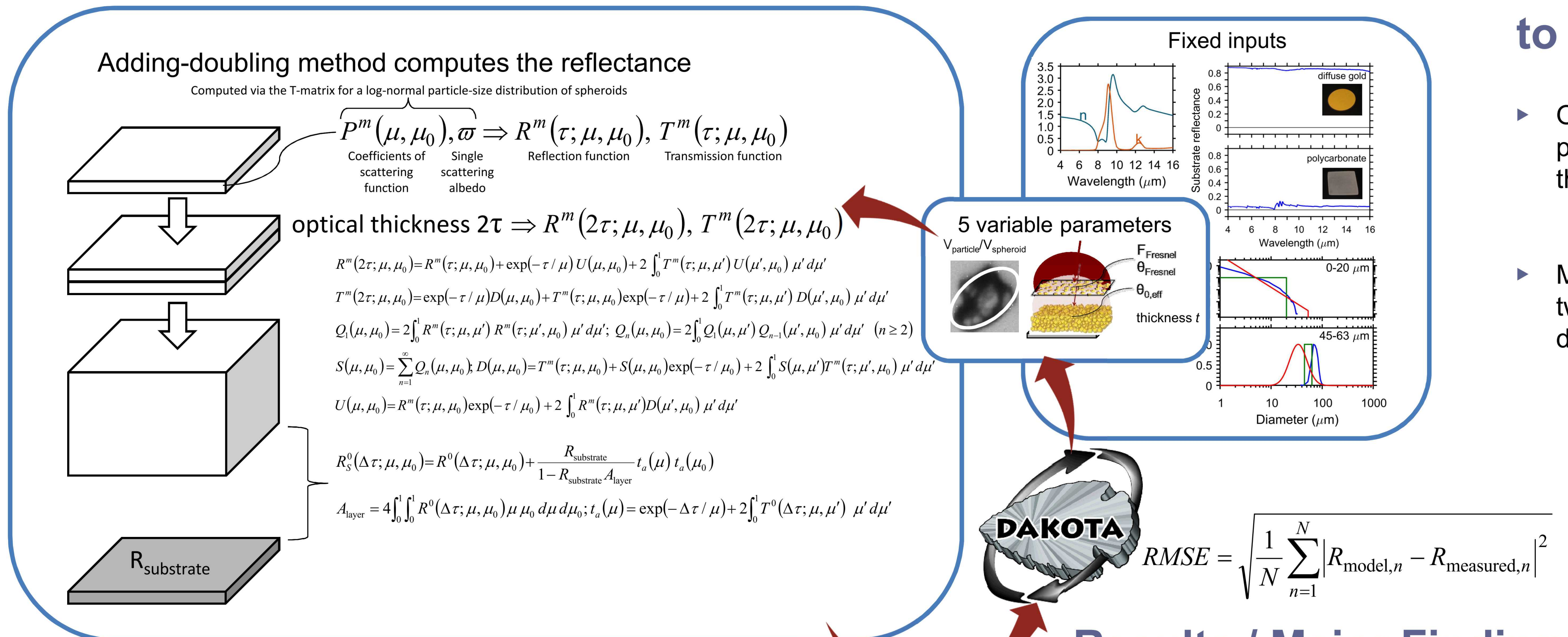
Two PSDs deposited at 8-10 mass loadings on two different substrates (each).

Total hemispherical reflectance measurements via FTIR with integrating sphere attachment



Particle sizing measurements via an automated optical microscope (Malvern Morphologi G3)

Methods



Adding-doubling method computes the reflectance

Computed via the T-matrix for a log-normal particle-size distribution of spheroids

$$\underbrace{P^m(\mu,\mu_0)}_{\text{Coefficients of scattering function}},\underbrace{\varpi}_{\text{Single scattering albedo}} \Rightarrow \underbrace{R^m(\tau;\mu,\mu_0)}_{\text{Reflection function}},\ \underbrace{T^m(\tau;\mu,\mu_0)}_{\text{Transmission function}}$$

optical thickness $2\tau \Rightarrow R^m(2\tau;\mu,\mu_0),\ T^m(2\tau;\mu,\mu_0)$

$$R^m(2\tau;\mu,\mu_0)=R^m(\tau;\mu,\mu_0)+\exp(-\tau/\mu)\,U(\mu,\mu_0)+2\int_0^1 T^m(\tau;\mu,\mu')\,U(\mu',\mu_0)\,\mu'\,d\mu'$$

$$T^m(2\tau;\mu,\mu_0)=\exp(-\tau/\mu)D(\mu,\mu_0)+T^m(\tau;\mu,\mu_0)\exp(-\tau/\mu)+2\int_0^1 T^m(\tau;\mu,\mu')\,D(\mu',\mu_0)\,\mu'\,d\mu'$$

$$Q_1(\mu,\mu_0)=2\int_0^1 R^m(\tau;\mu,\mu')\,R^m(\tau;\mu',\mu_0)\,\mu'\,d\mu';\ Q_n(\mu,\mu_0)=2\int_0^1 Q_1(\mu,\mu')\,Q_{n-1}(\mu',\mu_0)\,\mu'\,d\mu'\quad(n\geq 2)$$

$$S(\mu,\mu_0)=\sum_{n=1}^{\infty}Q_n(\mu,\mu_0);\ D(\mu,\mu_0)=T^m(\tau;\mu,\mu_0)+S(\mu,\mu_0)\exp(-\tau/\mu_0)+2\int_0^1 S(\mu,\mu')T^m(\tau;\mu',\mu_0)\,\mu'\,d\mu'$$

$$U(\mu,\mu_0)=R^m(\tau;\mu,\mu_0)\exp(-\tau/\mu_0)+2\int_0^1 R^m(\tau;\mu,\mu')D(\mu',\mu_0)\,\mu'\,d\mu'$$

$$R_S^0(\Delta\tau;\mu,\mu_0)=R^0(\Delta\tau;\mu,\mu_0)+\frac{R_{\text{substrate}}}{1-R_{\text{substrate}}A_{\text{layer}}}t_a(\mu)\,t_a(\mu_0)$$

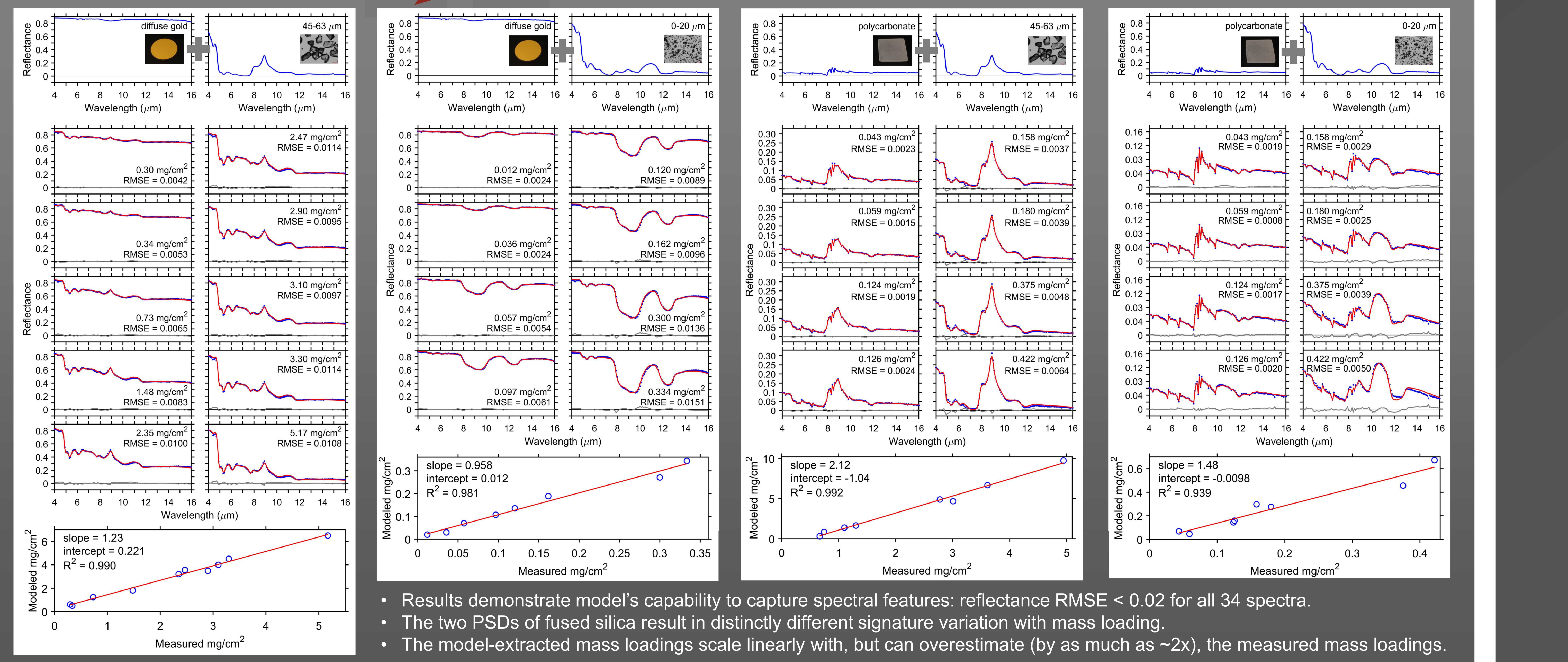
$$A_{\text{layer}}=4\int_0^1\int_0^1 R^0(\Delta\tau;\mu,\mu_0)\,\mu\,\mu_0\,d\mu\,d\mu_0;\ t_a(\mu)=\exp(-\Delta\tau/\mu)+2\int_0^1 T^0(\Delta\tau;\mu,\mu')\,\mu'\,d\mu'$$

$$RMSE=\sqrt{\frac{1}{N}\sum_{n=1}^{N}\left|R_{\text{model},n}-R_{\text{measured},n}\right|^2}$$

Conclusion and Relevance to Program Objectives

- Our baseline model for the reflectance of an optically thin deposit provides the means to account for particle-size and deposit thickness in the reflectance spectra of particulate media.
  - Based on fundamental material properties: complex refractive index (*n*,*k*) and material density
- Modeling results demonstrate excellent agreement with data acquired on two different size-selected fused silica powders, each deposited on two different substrates, representing two extremes:
  - Diffuse gold: High albedo, spectrally flat → Representative of metallic surfaces
  - Polycarbonate: Low albedo, spectrally featured → Representative of plastic surfaces

Results / Major Findings



- Results demonstrate model's capability to capture spectral features: reflectance RMSE < 0.02 for all 34 spectra.
- The two PSDs of fused silica result in distinctly different signature variation with mass loading.
- The model-extracted mass loadings scale linearly with, but can overestimate (by as much as ~2x), the measured mass loadings.

Discussion / Next Steps

- These results represent the first rigorous demonstration (to our knowledge) of extracting the mass loading of a particulate deposit from a reflectance spectrum using a physics-based model with only the pure material properties (complex refractive index and material density) as inputs
- Double-back to mid-points in the spiral: Mixed materials, birefringent materials

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