Implementation of a self-consistent slab model of a membrane bilayer structure in the SasView suite

Objective:

- Complex bilayer systems such as multicomponent lipid bilayers, lipid extracts, or living cells have a lamellar structure which can be modeled using a slab model.
- Existing implementations of these models often provide unreliable results due to covariance of scattering length density and bilayer thickness. We address this by introducing additional constraints.

Approach:

- We have implemented a model for lamellar structures in the commonly used small angle scattering suite, SasView.
- This model introduces constraints to the lamellar structure based on the molecular volume and scattering length of the molecules in the bilayer, as shown in Figure 1.

Results:

- We implement the model and demonstrate its use to fit scattering data from common lipid bilayers across a series of temperatures and contrast conditions.
- The python code implemented in SasView code is published in the Supporting Information and submitted for inclusion in next release of SasView.

Significance:

- Provides the scattering community a useful implementation of the slab model which provides physically meaningful (and self-consistent) descriptions of lamellar structure. This should improve small angle scattering curve fitting.
- Establishes a basis for the subsequent development of structural models to incorporate the complexity of lipid bilayers in the presence of co-solvents.

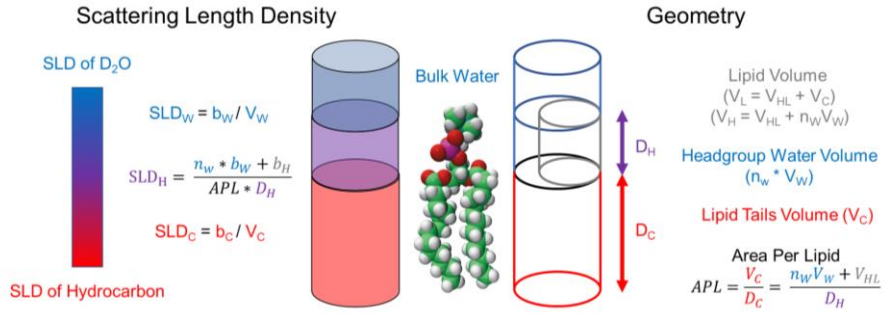

Figure 1. A self-consistent lamellar slab model has been developed which improves existing models of small angle scattering data by including constraints of the molecular volumes and scattering lengths of the constituent molecules.

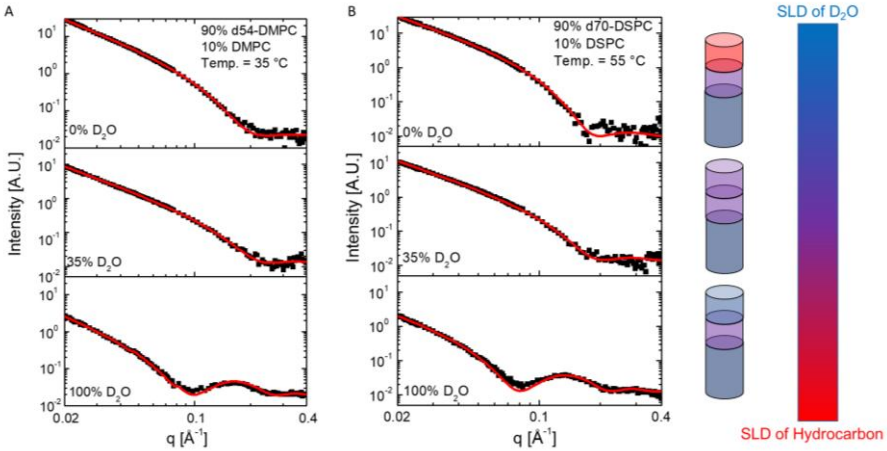

Figure 2. The self-consistent lamellar slab model is validated against data from multiple lipids (A) DMPC at 35C and (B) DSPC at 55C. Here we show the implementation of the model to solve the structure by simultaneously fitting different solvent contrast conditions for the same lipid bilayers with structural results in good agreement to prior work.

L. Tan et al. “Implementation of a self-consistent slab model of bilayer structure in the SasView suite.” 2020, in press. *J Appl Crystal,* https://doi.org/10.1107/S1600576720015526 *Supported by the ORNL Biofuels SFA.*