Automated parameter estimation approach for predicting the flow behavior of time-evolving materials

In different industries and in our daily lives, a wide range of soft materials and products present intriguing behaviors under applied stresses, and these behaviors can be described by rheological models that consider a set of parameters [1]. For example, ketchups are usually difficult to get out of the bottles, hair gels can have quite large bubbles indefinitely trapped inside, and toothpastes are easily extruded from the tubes, but usually do not drain out of the brush even if the brush is turned around. Other classical examples of products and soft materials presenting intriguing and complex behaviors are: shampoos, body creams, mayonnaise, yoghurt, bread dough, chocolate, printing inks, paints, plastics, adhesives, cements, muds, greases, waxy crude oils, biological tissues, and blood (see Fig.1).

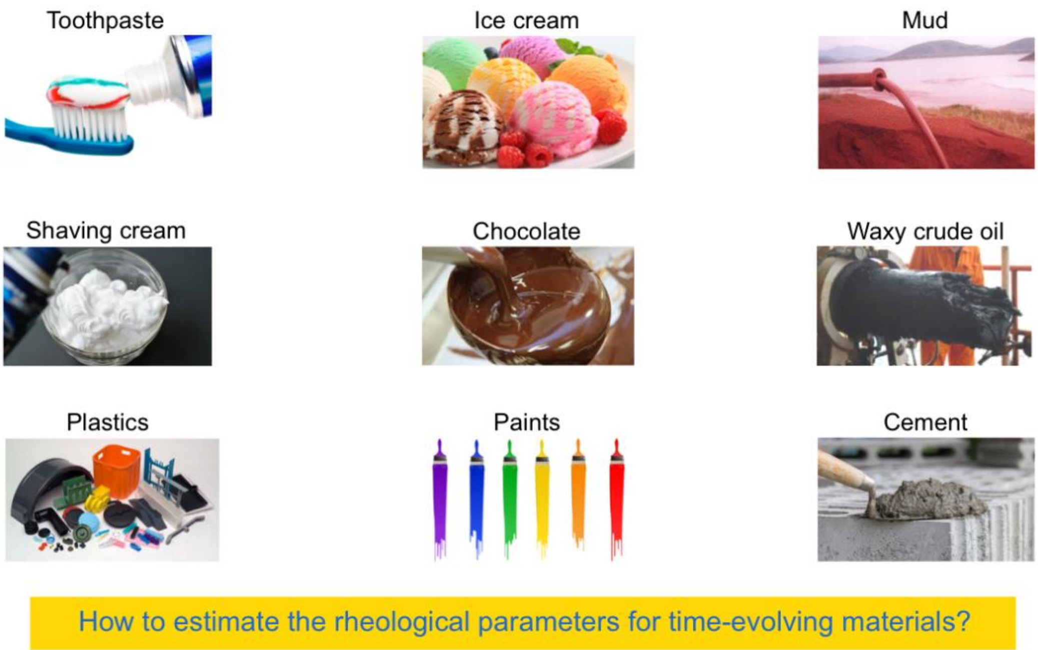

Fig. 1 – Examples of products and materials presenting complex rheological behavior.

All these materials and products experience different transport processes either in nature or during production and end use. In these processes, many of these materials undergo chemical reactions and/or irreversible physical changes, which modify the behavior of the material as time evolves. To better understand, predict, design, and control these transport processes it is crucial to (i) select a proper rheological model to describe the behavior of the material of interest and (ii) estimate the parameters of these models in an accurate way by fitting the model to rheological data. In particular, rheological parameters estimation is a challenging task that needs to be automated and improved. Examples of parameters to be estimated include yield stress, consistency index, structural shear modulus, thixotropic equilibration time, and reaction rate coefficients [2], [3].

In this thesis, we employ advanced parameter estimation techniques to fit a state-of-the-art rheological model to experimental data available for time-evolving materials.

The student will have access to a database of experimental results and will focus on parameter estimation strategies and fundamental understanding of the observed behaviors. The rheological model considers a structural kinetic equation to describe the evolution of the material's behavior, which is based on the structure variable λ [4]. An example of equation to be considered following a simple chemical reaction is provided below.

$$A + B \rightarrow C$$

$$\frac{d\lambda}{dt} = \frac{1}{t_{eq}}\left\{(1-\lambda) - (1-\lambda_{eq})\left(\frac{\lambda}{\lambda_{eq}}\right)\right\} + \xi\ k\ [C_C]^m$$

References:

[1] J. Mewis and N. J. Wagner, *Adv. Colloid Interface Sci.* 147-148, 2009.

[2] P. R. de Souza Mendes, *Soft Matter* 7, 2011.

[3] F. H. Marchesini et al., *J. Rheol.* 63(2), 2019.

[4] K. Dullaert and J. Mewis, *J. Non-Newton. Fluid Mech.* 139, 2006.

Key words:

Parameter estimation, rheological behavior, time-evolving materials, structural kinetics, flows, transport phenomena

Goal:

-Automating and improving rheological parameters estimation for time-evolving materials to allow for proper description, understanding and design of transport processes and products.