Title

Bayesian non-linear mixed effects model for safer powder storage

Authors & Bio:

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Abstract

Powders are ubiquitous in the chemical industry, from pharmaceutical powders for tablet production to food powders like sugar. In these applications, powders are often stored in silos where the powder builds up stress under its own weight. The Janssen model describes this build up, but this model has unknown parameters that must be estimated from experimental data. This parameter estimation involves several challenges, such as structural unidentifiability and correlated measurements. To overcome these challenges, a Bayesian non-linear mixed effects model, that incorporates data from two different measurement set-ups, is implemented in Turing.jl.

Summary

Powders are ubiquitous in the chemical industry, from pharmaceutical powders for tablet production, to food powders like sugar. Powder flowability is a crucial aspect for smooth processing in all these applications. When powder is stored in silos, it builds up stress under its own weight. This stress can affect its flowability, leading to problems like arching or ratholing.

Janssen's approach is the most used stress model for silos [1]. This model contains unknown parameters that must be estimated from experimental data at lab scale. One of these parameters is the relation between horizontal and vertical stress in the system. This parameter enables the correct prediction of the stress propagation throughout the system. To estimate this parameter, measurements of both stresses need to be linked. However, no commercial set-ups are readily available to measure the relation between the horizontal and vertical stress directly. Data from a new experimental protocol was published in [2], extracting the stress relationship from wall friction measurements and an analytical set-up measuring the vertical stress propagation in a vertical pipe. This data will be used in the analyses in this presentation.

In this presentation, we will perform a Bayesian non-linear mixed effects analysis on these data. The non-linear model is derived from a force balance. Random effects are introduced because high variability between repetitions of experiments under the same set of conditions is observed, compared to the measurement noise within a set of conditions.

The choice for the Bayesian paradigm is twofold. First, because we have physical bounds available for most parameters of interest, which can serve as prior information in the Bayesian estimation. Second, because data from two different measurement setups must be combined to be able to identify all the parameters of interest. The joint likelihood over both measurement setups is readily calculated, as are posterior densities. In contrast, incorporating data from both setups would be less straightforward in the frequentist framework. The presence of prior information and an easily calculated likelihood thus makes the Bayesian framework a natural choice.

The Bayesian inference is implemented in Turing.jl. The choice of Turing and the Julia programming language was motivated by the close resemblance of the code to the mathematical description of the Janssen equation.

References

[1] Schulze, Dietmar (2008). "Stresses in vertical channels (Janssen's approach)". In: Powders And Bulk Solids. Springer, pp. 259–262.
[2] Coppens, Margot et al. (2023). "Combination and analysis of the lateral stress ratio and wall friction measurements". In: Powder Technology 418, p. 118286.