



IFPRI Project Abstract

Adhesion of powders to metal surfaces during compaction

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Project Objective (from project brief):

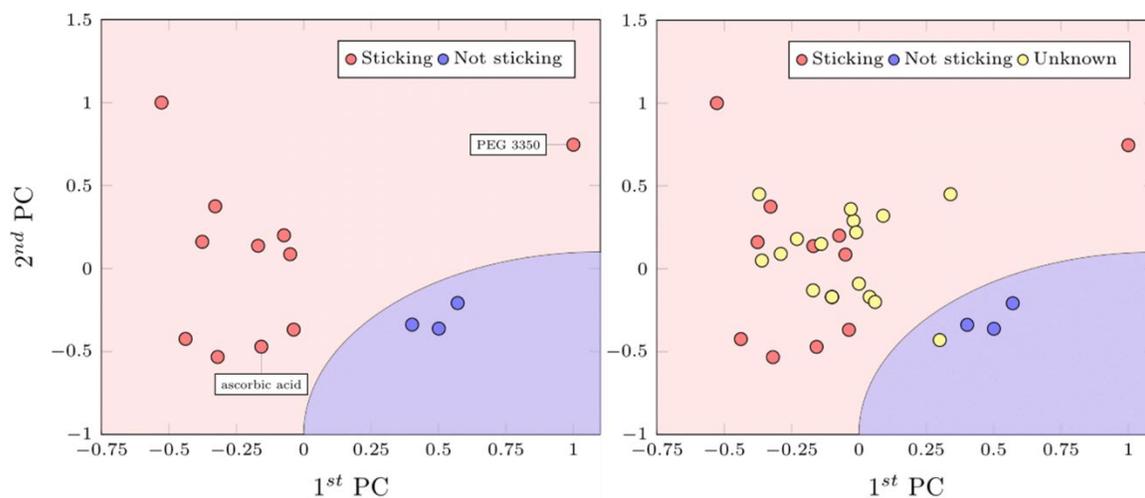
- Establishment of a test method to quantify material adhesion on compaction tooling over an industrially relevant range of process and environmental conditions
 - Identification of key factors affecting the amount and/or rate of powder adhesion on compaction tooling
 - Establish predictive criteria for the propensity of adhesion given a set of molecular/crystal properties and process/environmental conditions
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Approach:

- Construct a database of sticking behavior under different levels of compaction stress (20, 50, 75, 100, 150, 250 MPa), loading rate (10 mm/min and drop test frame), temperature (room and 50 °C) and relative humidity (33% RH and 75% RH). The database also includes powder properties (chemical formula, physical characteristics, mechanical properties of particles, interaction properties between particles, thermal properties).
 - Formulate sticking hypotheses and identify key factors responsible for sticking
 - Identify a suitable correlation method to relate a chemical formula to sticking behavior.
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Recent Results:

- The database was completed following comprehensive characterisation of 7 materials.
- The sticking hypotheses/mechanisms were rationalised: compaction pressure, rate, temperature, humidity effects, supported by additional characterization methods including: AFM for topology, AFM Kelvin probe, SEM/EDX, particle size measurement, and contact angle measurement
- To link chemical formula to sticking behaviour, Mordred descriptors were identified as suitable to describe a chemical formula.
- Principal Component Analysis (PCA) was performed to predict sticking of a new molecule. A parameter space was determined for sticking (please see Figure below). Initial validation tests were performed using the diagnostic test developed.



Next Steps:

Work remaining (to be completed before the final report):

- Identify key Mordred categories (20 => 5): e.g. polarity, acid/base, autocorrelation
- Identify key Mordred descriptors (1800 => 100): e.g. molecular weight, no. of H donors/acceptor, no of cyclic structures
- Refine sticking prediction maps. Consider particle and bulk properties (e.g. physical, mechanical and thermal properties).

Deliverable: Python package:

- Input: SMILES representation (new molecule)
 - Output: yes/no sticking prediction and representation on sticking map
 - Graphical user interface
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