AI-Assisted Powder Characterization for Predicting Bulk Flow and Packing Behavior

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1. Vision

This research applies state-of-the-art Vision AI methodologies to establish and interpret correlations between particle-level properties and bulk powder behavior in flow and packing applications. The approach utilizes hybrid tabular and imagery data from a wide range of powder characterization instruments, some of which are unique to the University of Leeds. The work will later be extended to include processes of interest to the IFPRI members, such as compaction and triboelectrification.

2. Industrial Challenge and Background

Powder characterization remains a critical bottleneck across pharmaceutical, food, chemical and advanced manufacturing industries. Conventional methods require 50-100+ grams of material and time-intensive protocols including rheometry, shear testing and compressibility measurements that assess fundamental properties governing handling and processing performance [1]. This presents severe challenges for early-stage development where material quantities are limited to sub-gram levels [2] and for specialty materials where cost constraints limit extensive testing. Characterization campaigns cost tens of thousands of dollars per formulation and extend development timelines by several months.

The University of Leeds possesses a comprehensive suite of powder characterization instruments with access to the state-of-the-art Bragg Centre for material and surface characterization. Available instruments include Morphologi G3 automated imaging, Freeman FT4 powder rheometer, Schulze ring shear tester, Malvern Mastersizer, Sympatec QicPic, Retsch Camsizer, Geldart angle of repose apparatus, scanning electron microscopy with energy dispersive X-ray spectroscopy, and Raman spectroscopy. Unique methodologies developed at Leeds include the Ball Indentation Method for assessing cohesive powder flowability at low stress levels, the Drop Test Method for measuring particle adhesion force through impact detachment, and aerodynamic dispersion for triboelectrification. This infrastructure provides unique multi-scale assessment from individual particle interactions to bulk assembly behavior.

We have accumulated comprehensive characterization data from over 50 diverse powders spanning pharmaceutical, food, chemical and manufacturing sectors through ongoing research activities. Our preliminary investigations demonstrate prediction errors as low as 20% for key flowability metrics using machine learning models integrating features from dispersion images with small-scale test data (Figure 1), with up to 99% reduction in required material. In consultation with IFPRI members, we will characterize additional powders of specific interest to ensure the framework encompasses the full breadth of industrial powder systems.

3. Research Objectives

The primary objective is to identify the most influential powder attributes that are critical in manufacturing and processing of particulate-based products. Through systematic application of machine learning to comprehensive powder characterization data, we will establish quantitative structure-property relationships governing bulk powder behavior. Specific objectives include:

1. Develop multi-modal AI frameworks integrating microscopic imaging with material properties to predict bulk powder behavior including flow and packing characteristics.
2. Identify critical powder attributes through feature importance analysis that determine which particle and material characteristics most strongly influence processing performance.
3. Establish probabilistic predictions with quantified uncertainty supporting risk-based industrial decision making.
4. Create validated, generalizable prediction tools applicable across pharmaceutical, food, chemical and manufacturing sectors.
5. Deliver demonstration software that IFPRI members can apply to their own powder systems with minimal material requirements.

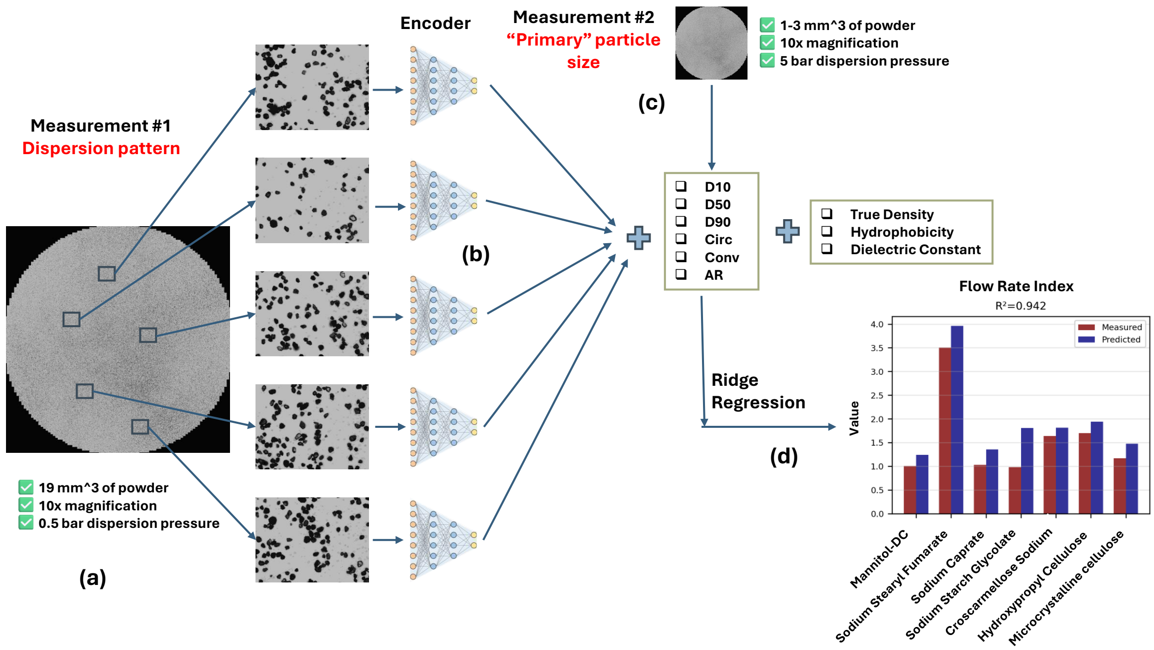

Figure 1: Prototype AI framework showing dual measurement strategy with weakly and well-dispersed powder images, feature extraction from dispersion patterns, integration with particle descriptors, and prediction of Flow Rate Index (R^2=0.942).

4. Innovation

Three key innovations distinguish this research. First, the Bayesian data fusion framework handles missing data through probabilistic inference (Figure 2). When partial characterization information is available, the framework draws on learned correlations between features while widening confidence intervals. As additional measurements are provided (electron microscopy, adhesion tests, surface energy), predictions update and uncertainty decreases systematically. This flexibility is critical for industrial deployment where data availability varies across development stages.

Second, the multi-modal approach extracts features from three complementary imaging modalities: Morphologi G3 dispersion patterns capturing agglomeration behavior, electron microscopy revealing surface characteristics, and drop test adhesion quantification. These visual features combine with explicit particle properties (size distributions, shape descriptors, density, surface characteristics including hydrophobic, hydrophilic and hygroscopic nature) in the predictive framework.

Third, explainable AI establishes trust through visualization of learned structure-property relationships (Figure 3). Sensitivity analysis reveals how image features correlate with bulk properties, converting opaque models into interpretable frameworks essential for industrial adoption. This explainability enables particle technologists to validate that learned relationships align with fundamental powder mechanics principles, converting black-box neural networks into interpretable frameworks [3].

5. Alignment with IFPRI Member Needs

This research directly addresses critical challenges facing multiple IFPRI member sectors. For pharmaceutical industry, material scarcity in early-stage development necessitates sample-efficient characterization while probabilistic predictions support risk-based formulation decisions. Additionally, the approach can help in selecting surrogate materials based on the similarity of their predicted bulk powder behaviour. For food processing, rapid assessment informs process design for mixing, conveying and packaging while supporting reformulation efforts. For specialty chemicals and advanced materials, applications span additive manufacturing powder qualification, battery materials assessment and catalyst handling predictions where material costs make sample-efficient characterization economically compelling.

Models trained on one powder class can predict properties of different powder classes when adjusted through

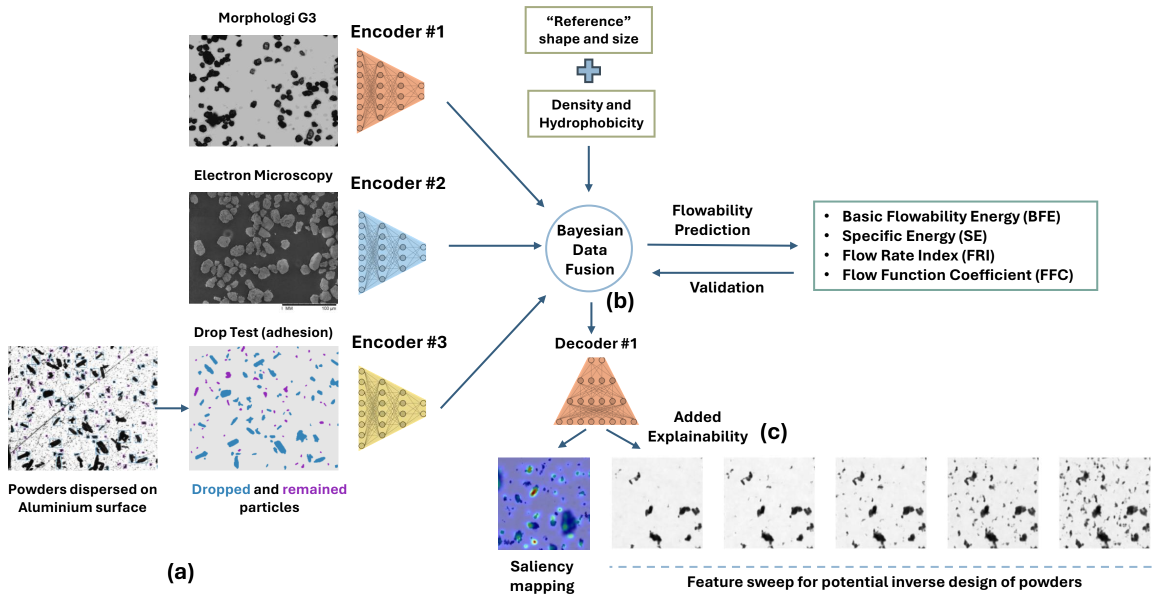

Figure 2: Multi-modal Bayesian data fusion framework showing three imaging modalities (Morphologi G3, electron microscopy, drop tests), feature extraction combining with particle properties, and predictions with quantified uncertainty for multiple powder behavior metrics.

domain adaptation techniques. This demonstrates that fundamental structure-property relationships apply across industry boundaries, enabling IFPRI members to benefit from characterization data contributed by members from different industrial sectors.

6. Approach

6.1. Overall Research Strategy

The research follows systematic progression through three work packages: multi-modal architecture development (WP1), Bayesian framework optimization (WP2) and industrial validation (WP3). The approach integrates multi-scale experimental characterization with machine learning methodologies.

Powders will be characterized using the comprehensive suite of instruments at Leeds. Small-scale characterization (less than 5 mg) employs Morphologi G3 automated imaging at multiple air pressures yielding particle size distributions and shape descriptors [4]. Scanning electron microscopy provides surface morphology characterization and detailed shape features not visible in optical images [5, 6]. Drop tests quantify adhesion following established protocols [7]. Surface characterization employs X-ray photoelectron spectroscopy and inverse gas chromatography to determine surface energy and hydrophobic, hydrophilic and hygroscopic characteristics.

Bulk behavior characterization (50-100 g) employs Freeman FT4 rheometer quantifying Basic Flowability Energy, Specific Energy, Flow Rate Index, Compressibility and permeability. Schulze ring shear tester determines Flow Function Coefficient, cohesion, internal friction angle and wall friction. Geldart apparatus measures angle of repose, while tap density will measure the packing behaviour. Characterization of additional powders to expand the dataset will form part of Work Package 1, while validation experiments using IFPRI member powders will form part of Work Package 3.

The machine learning framework integrates features extracted from microscopic images with explicit particle properties. The Bayesian interface handles missing input data by marginalizing over possible values, yielding wider confidence intervals reflecting increased uncertainty. As additional data modalities become available, predictions update and uncertainty decreases. Explainable AI methods identify which features drive predictions and visualize learned structure-property relationships [8].

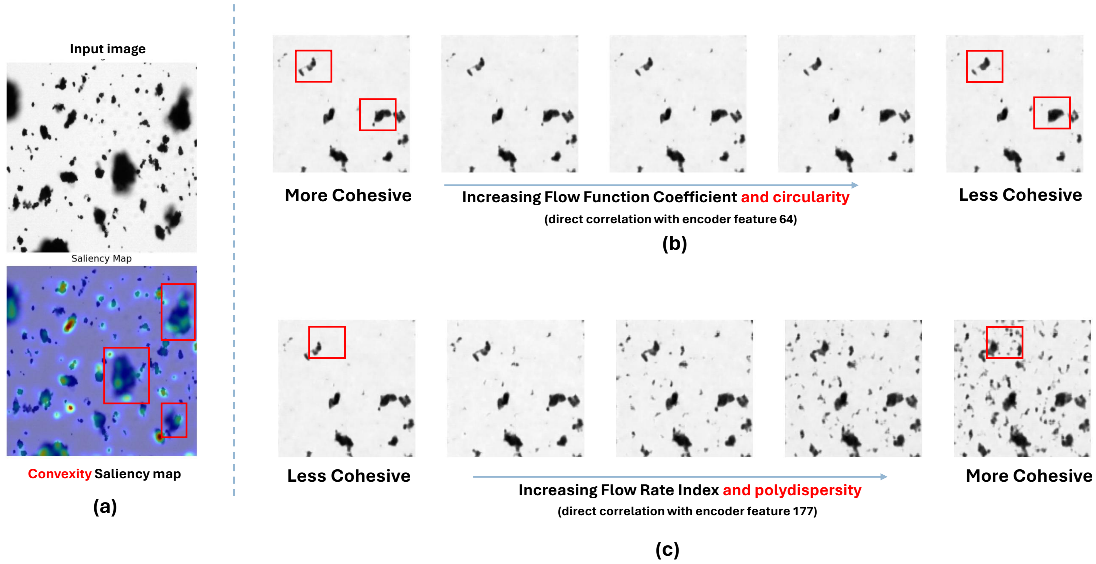

Figure 3: Explainability analysis revealing learned structure-property relationships through saliency mapping and systematic feature manipulation demonstrating correlation between image features and powder behavior metrics.

6.2. Validation Criteria

Validation employs stratified k-fold cross-validation with rigorous separation between training and test sets across powder chemistry classes. The ultimate assessment will be the external validation, conducted using powder samples provided by IFPRI members. Acceptance criteria are normalized root mean square error less than 15% for primary flow properties and less than 20% for secondary properties.

6.3. Work Packages

WP1: Multi-Modal Feature Engineering (Months 1-12). Develop comprehensive feature extraction methodologies capturing powder characteristics from microscopic imaging. Systematic optimization will determine optimal architecture parameters through cross-validation. Correlation analysis will identify relationships between microscopic features and bulk properties. Additional powders selected in consultation with IFPRI members will be characterized to expand the dataset. *Deliverables:* Validated feature extraction architectures, technical report and presentation at IFPRI Annual General Meeting.

WP2: Bayesian Predictive Model Development (Months 13-24). Develop and optimize predictive models with Bayesian uncertainty quantification for flow and packing behavior. Model comparison uses cross-validation and predictive performance on held-out test sets. *Deliverables:* Complete predictive framework, demonstration interface with explainability visualizations, peer-reviewed publication, presentation at IFPRI Annual General Meeting.

WP3: Industrial Validation and Deployment (Months 25-36). Conduct comprehensive validation across diverse industrial powder classes provided by IFPRI member companies. Active learning strategies identify which powders provide maximum information gain. Software development focuses on user-friendly interfaces that accept microscopic images and characterization data, generate predictions with confidence intervals and provide explainability visualizations. *Deliverables:* Comprehensive validation report, demonstration software tools with documentation, final report, peer-reviewed publication and presentation at IFPRI Annual General Meeting with live software demonstration (Figure 4).

7. Research Team and Infrastructure

Dr. Arash Rabbani is Assistant Professor in Artificial Intelligence at the School of Computer Science, University of Leeds. Trained as a chemical engineer with a PhD from the University of Manchester, he has interdisciplinary expertise in image-driven characterization of granular materials with 50+ peer-reviewed publications. He currently leads a £330K EPSRC project on AI-assisted powder characterization, which has generated the preliminary results and comprehensive dataset underpinning this proposal.

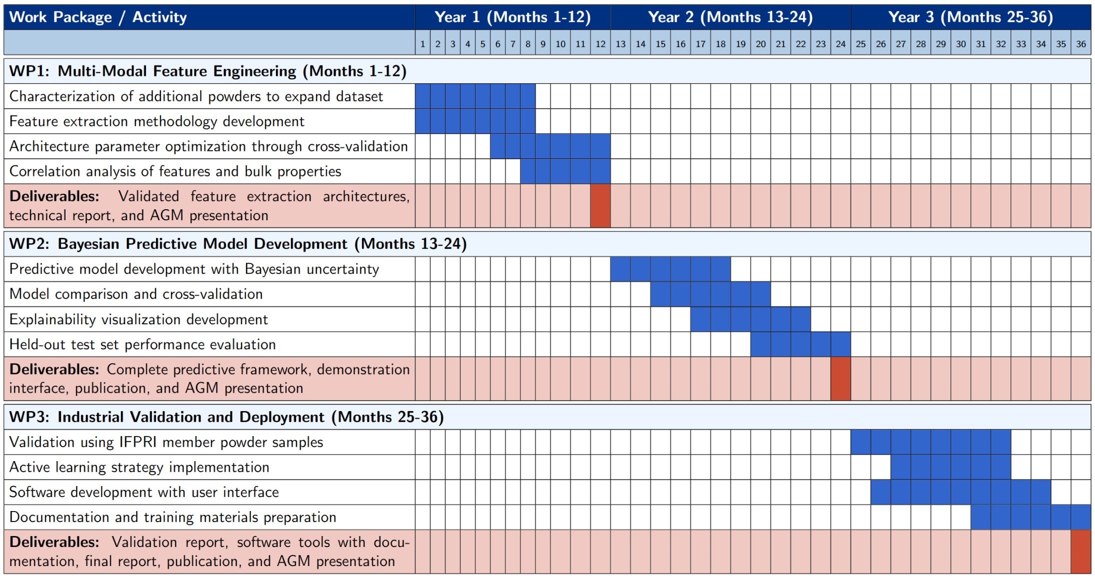

Figure 4: Project timeline showing three work packages spanning 36 months with deliverables including presentations at all IFPRI Annual General Meetings.

Collaborators Prof. Mojtaba Ghadiri and Dr. Ali Hassanpour at the School of Chemical Engineering, University of Leeds, provide essential expertise on the particle technology. Prof. Ghadiri brings over 30 years of research experience in powder flowability, triboelectrification and structure-property relationships. Dr. Hassanpour has extensive expertise in powder adhesion and additive manufacturing applications. Additional collaborations span surface characterization through the Bragg Centre for Materials Research at Leeds (Dr. Sven Schroeder for X-ray photoelectron spectroscopy, Dr. Anuradha Pallipurath for Raman spectroscopy), collaboration with Prof. Jerry Heng at Imperial College London for complementary surface energy measurements, and collaboration with Plansee Austria for metal powder characterization in additive manufacturing.

The School of Computer Science has agreed to waive PhD tuition fees for a student recruited to this project (Home students prioritized), enabling IFPRI funding to support student stipend with remaining resources allocated to enhance the project through complementary characterizations, dissemination and impact activities. This project is part of a broader research program on AI-assisted powder characterization. We currently have a PhD studentship investigating machine learning for triboelectrification prediction, a studentship with Plansee Austria examining compaction behavior of metal powders, and a studentship with Johnson & Johnson on powder mixing. These parallel activities create a collaborative environment that maximizes knowledge exchange, ensuring IFPRI members gain access to a broader range of powder behavior predictions.

8. Dissemination and Impact

Research findings will be disseminated through 2-3 peer-reviewed publications targeting *Powder Technology*, *Chemical Engineering Science* or *AIChE Journal*. Demonstration software tools will be made available to IFPRI members for testing their own powder systems and collaboration on external validation.

Principal Investigator Rabbani will attend all three Annual General Meetings to present progress, demonstrate tools and engage with members regarding application challenges. We will actively solicit member involvement in validation studies through powder sample contributions. Selected findings will be presented at conferences including World Congress on Particle Technology. Training workshops for IFPRI members on using the demonstration software will be organized during the final year.

9. Future Directions

Success in achieving prediction accuracy targets will position the project for extension along several paths. Extended property predictions could broaden the framework to encompass triboelectric charge generation (building on concurrent studentship research), spreadability in additive manufacturing, wettability and dissolution behavior. Chemistry-aware modeling could integrate molecular-level chemical descriptors enabling inverse design capabilities for optimal formulation compositions. Multi-component system extension could address binary and ternary powder blends predicting segregation propensity and mixture flowability [9]. The specific extension direction will be determined based on initial results and IFPRI member priorities.

10. Budget Justification

The requested annual funding of $42,000 will be allocated to support a PhD student stipend at UK rates (£19,000 annually, approximately $24,000) with the School of Computer Science waiving tuition fees. The remaining budget ($18,000 annually) supports characterization consumables and equipment time for IFPRI member powder samples ($8,000), travel to IFPRI Annual General Meetings and member site visits ($4,000), computing resources and software licenses ($2,000), open-access publication fees ($3,000) and contingency ($1,000).

11. Conclusion

This proposal addresses critical industrial challenges in powder characterization through an innovative AI-driven approach that dramatically reduces material requirements while providing probabilistic predictions with quantified uncertainty. Our preliminary results (prediction errors less than 20% using only milligrams of material) demonstrate technical feasibility.

The research combines state-of-the-art machine learning methodologies with comprehensive powder characterization capabilities, some unique to Leeds, advancing both practical applications and scientific understanding by identifying the most influential powder attributes critical for manufacturing and processing.

We are committed to IFPRI's collaborative, pre-competitive research model. The project will actively engage IFPRI members through powder sample contributions, validation studies and feedback on demonstration software. Deliverables include publications, presentations and demonstration software tools that IFPRI members can use to characterize and predict behavior of their own powder systems with minimal material requirements.

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