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Predicting biomass comminution: Physical experiment, population balance model, and deep learning

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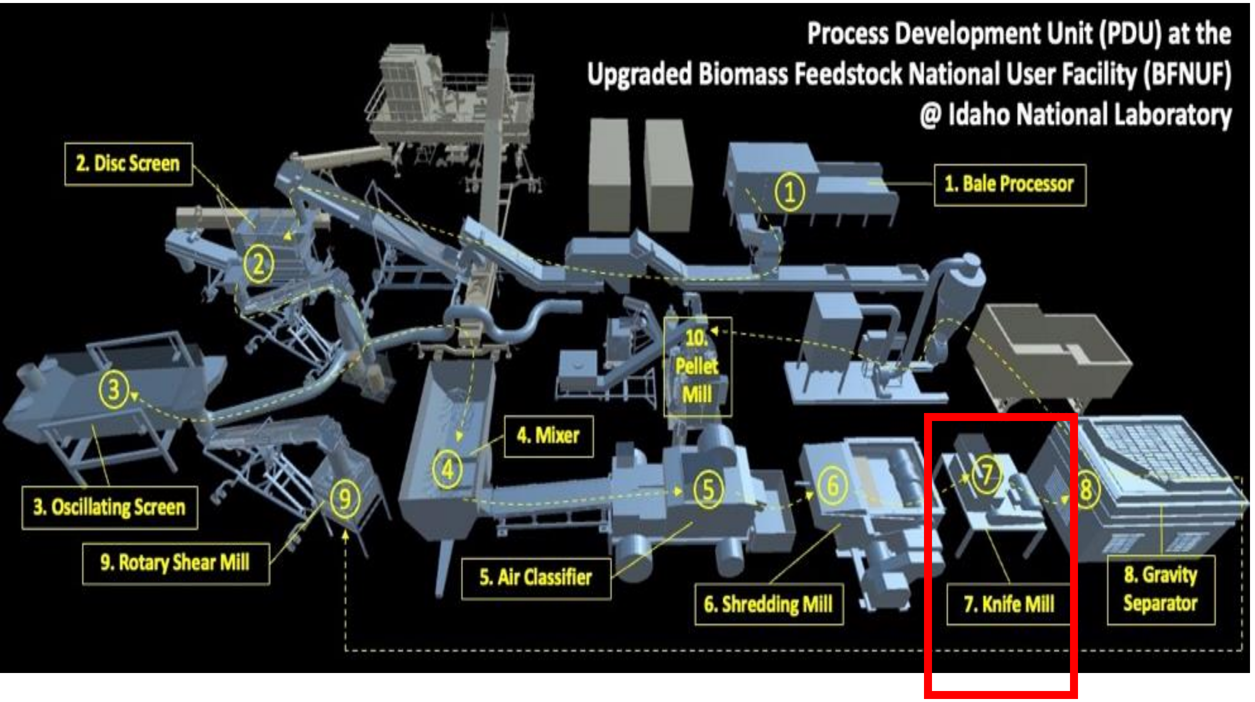
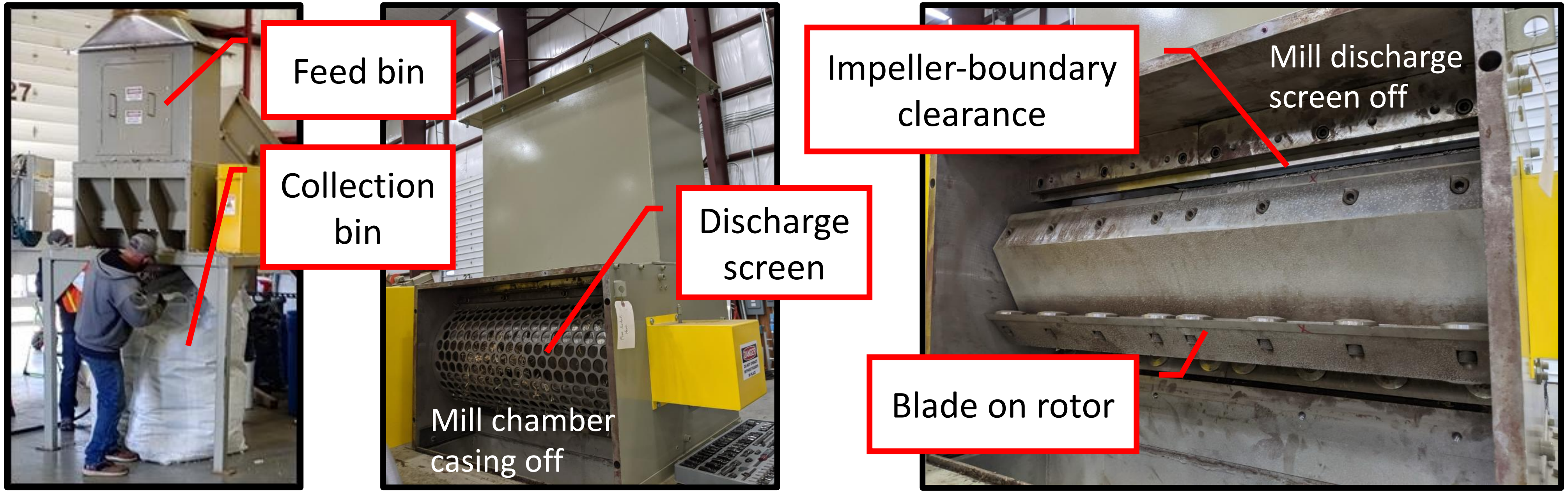
Ground transportation to processing facilities, e.g., INL's BFNUF

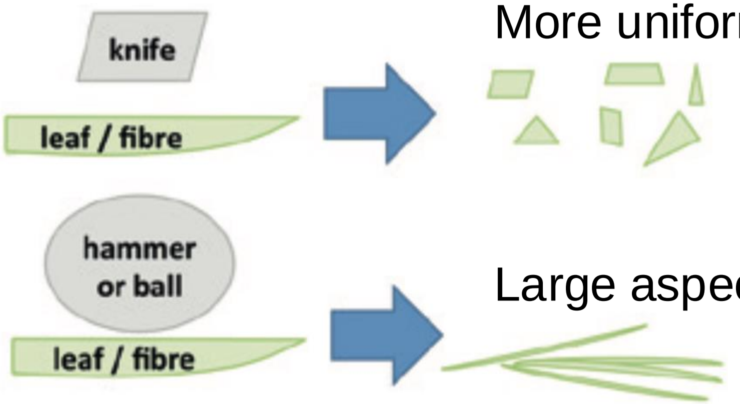


<u>Processes:</u>
conditioning,
screening,
size reduction,
separation, etc.

<u>Outcome:</u>
conversion-ready
biomass feedstocks

Large-scale knife mill at Idaho National Laboratory's Biomass Feedstock National User Facility (BFNUF)



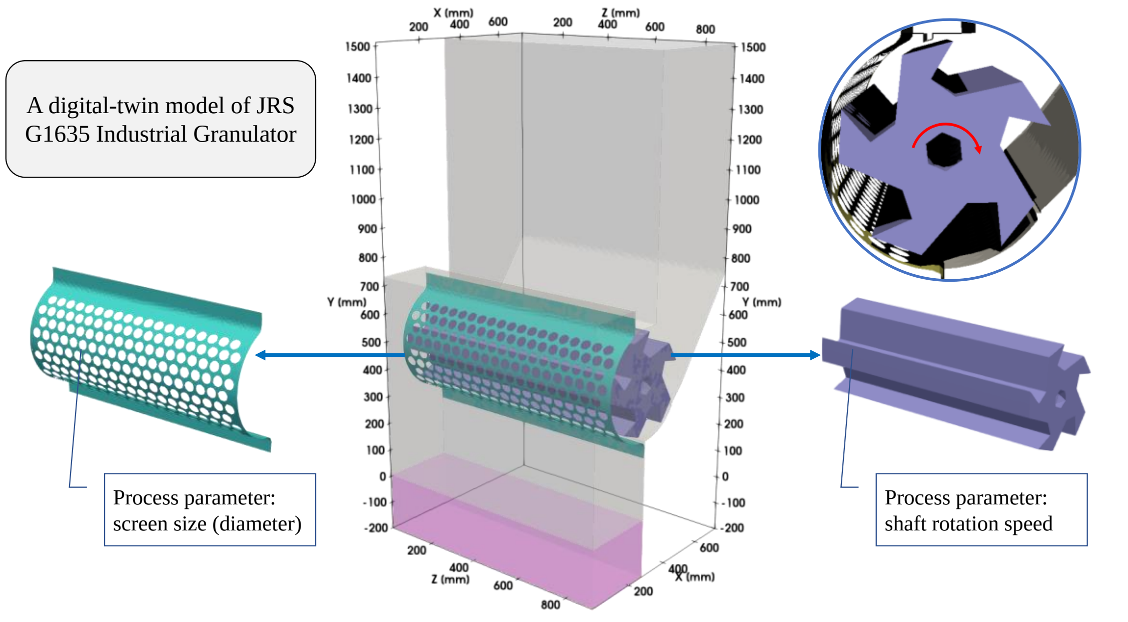


More uniform particle shapes (good flowability)

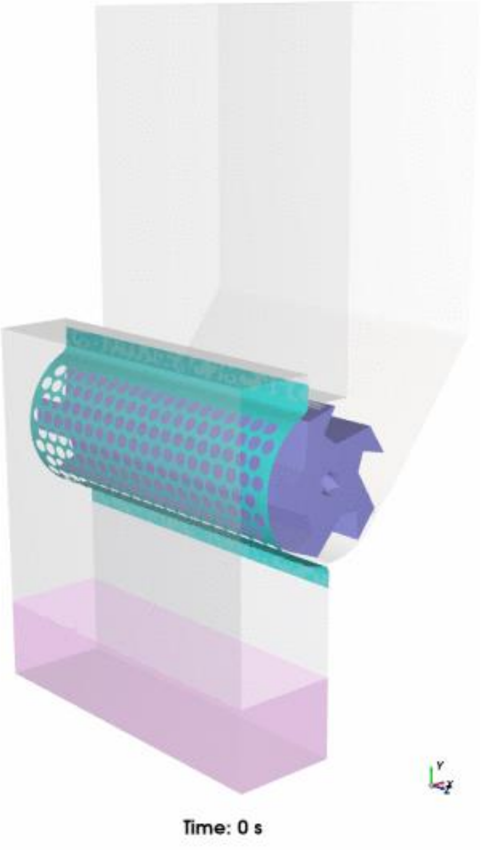
Choice for comminution of corn stover

Large aspect ratio particle shapes (poor flowability)

Previous work: computational physics-based digital-twin model for the knife milling unit operation



A digital-twin model of the JRS knife mill and Discrete Element Method (DEM) simulations.



Pros

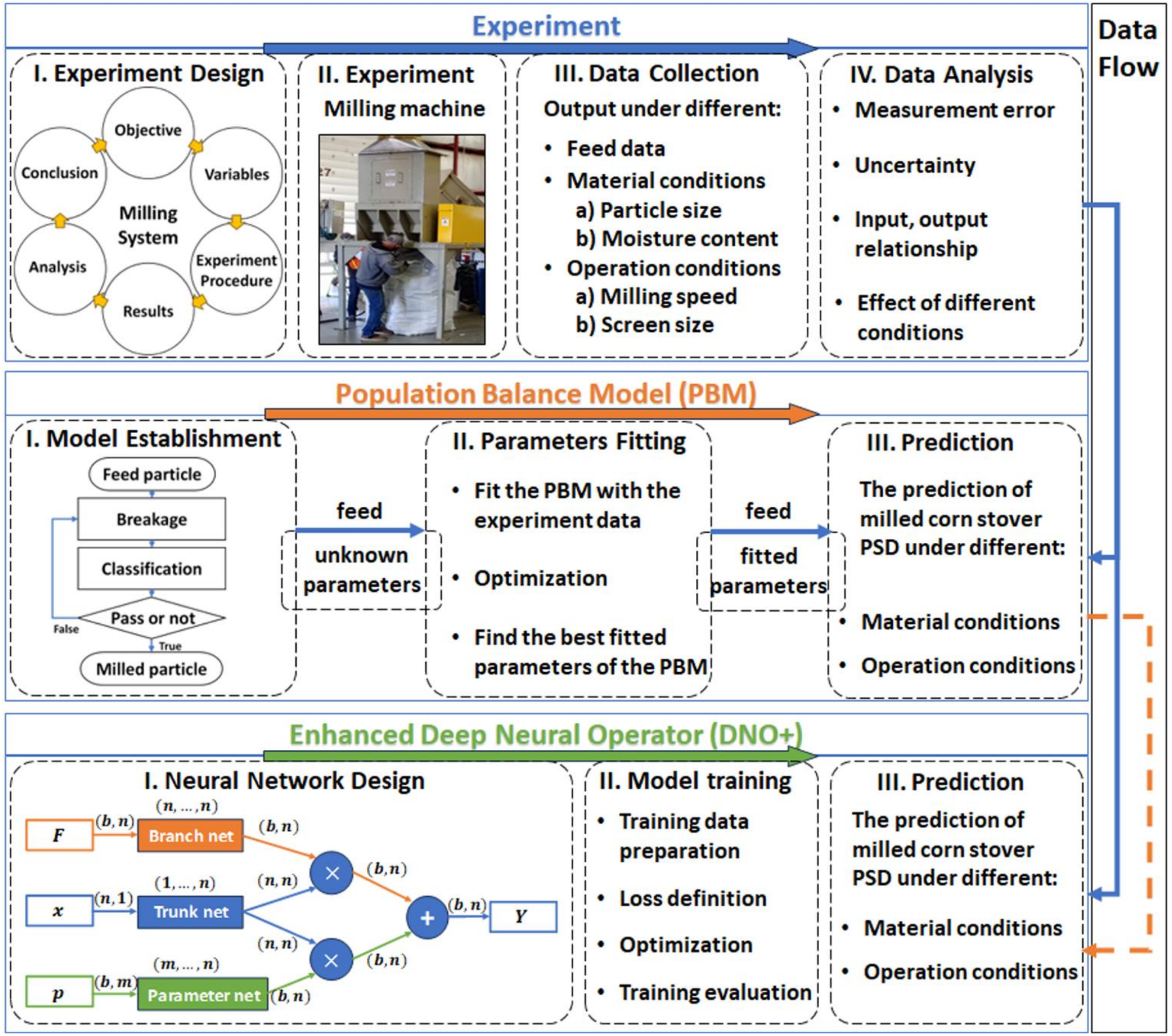
- Track the motion, deformation, and breakage of feed materials.
- Diagnose operation problems and explore parameter limits.
- Determine criticality of material properties and operation parameters.

Cons

- Expensive in computing cost even with top-tier GPUs (e.g., Nvidia RTX 4090).
- Long learning curves for entry-level process engineers.

Y. Xia et. al. (2023). An experiment-informed discrete element modelling study of knife milling for flexural biomass feedstocks. *Biosystems Engineering*, 236, 39-53. https://doi.org/10.1016/j.biosystemseng.2023.10.008

Analytical and machine learning-based prediction models



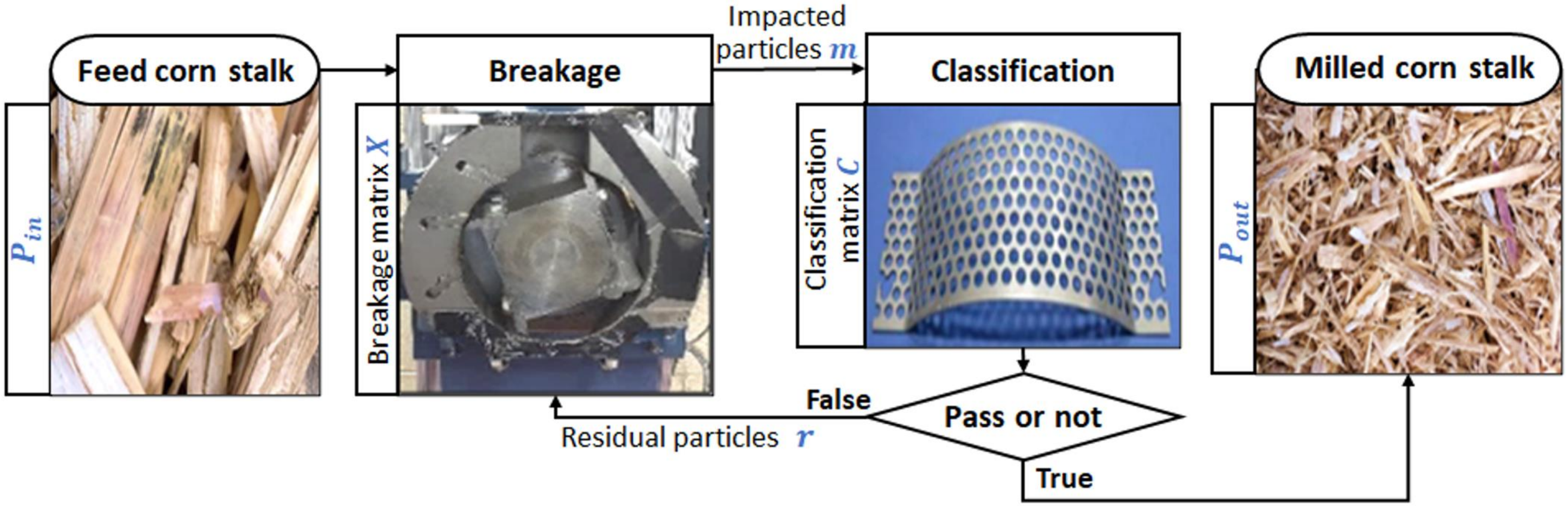
New models developed in this work:

- Analytical: extended population balance model (PBM)
- ML model: enhanced deep neural operator (DNO+)

Keynotes:

- Cannot replace the benefits of computational physics-based models like DEM.
- Provide fast estimate of particle size distribution of milled materials and guide physical operations.
- Model accuracy eventually depends on source physical test data. The more source data the more reliable.
- Large-scale physical test data is expensive to produce – a common challenge for scale-up engineering!

Brief intro to the extended* population balance model (PBM)



Extended PBM

Original PBM

- Discharge screen size
- Mill blade speed
- Mass distribution regarding sieve size

Individually fitted

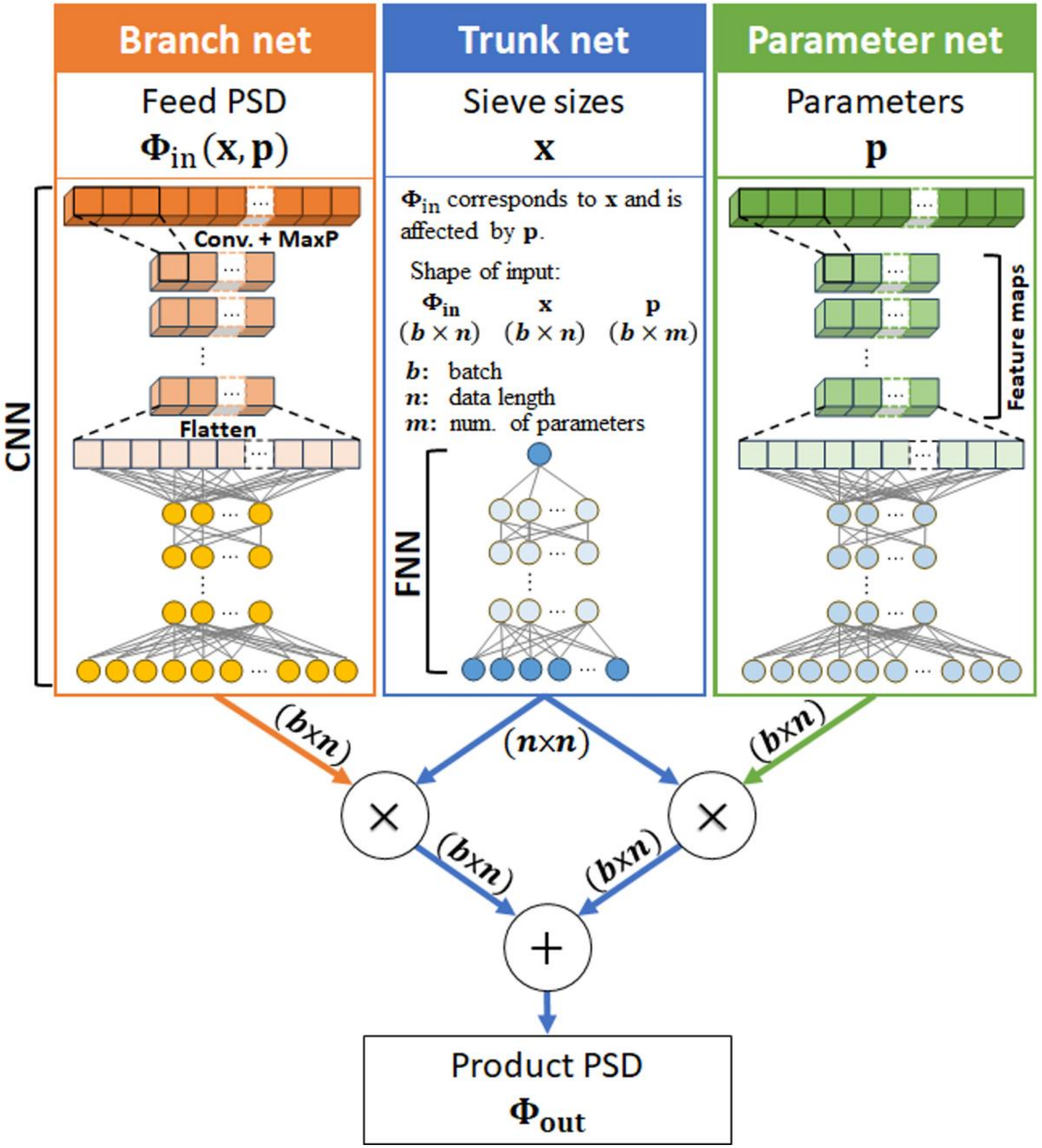
PBM model fitting parameters: f_{res}, $\mathbf{x} \cdot \mathbf{w}_{\min}/n$, γ, α, c/d

Extra material properties
- Moisture content

Random forest regression (RFR) to estimate fitting parameters on-the-fly

Outcome
- Discharged mass distribution regarding sieve size

Brief intro to enhanced* deep neural operator (DNO+)



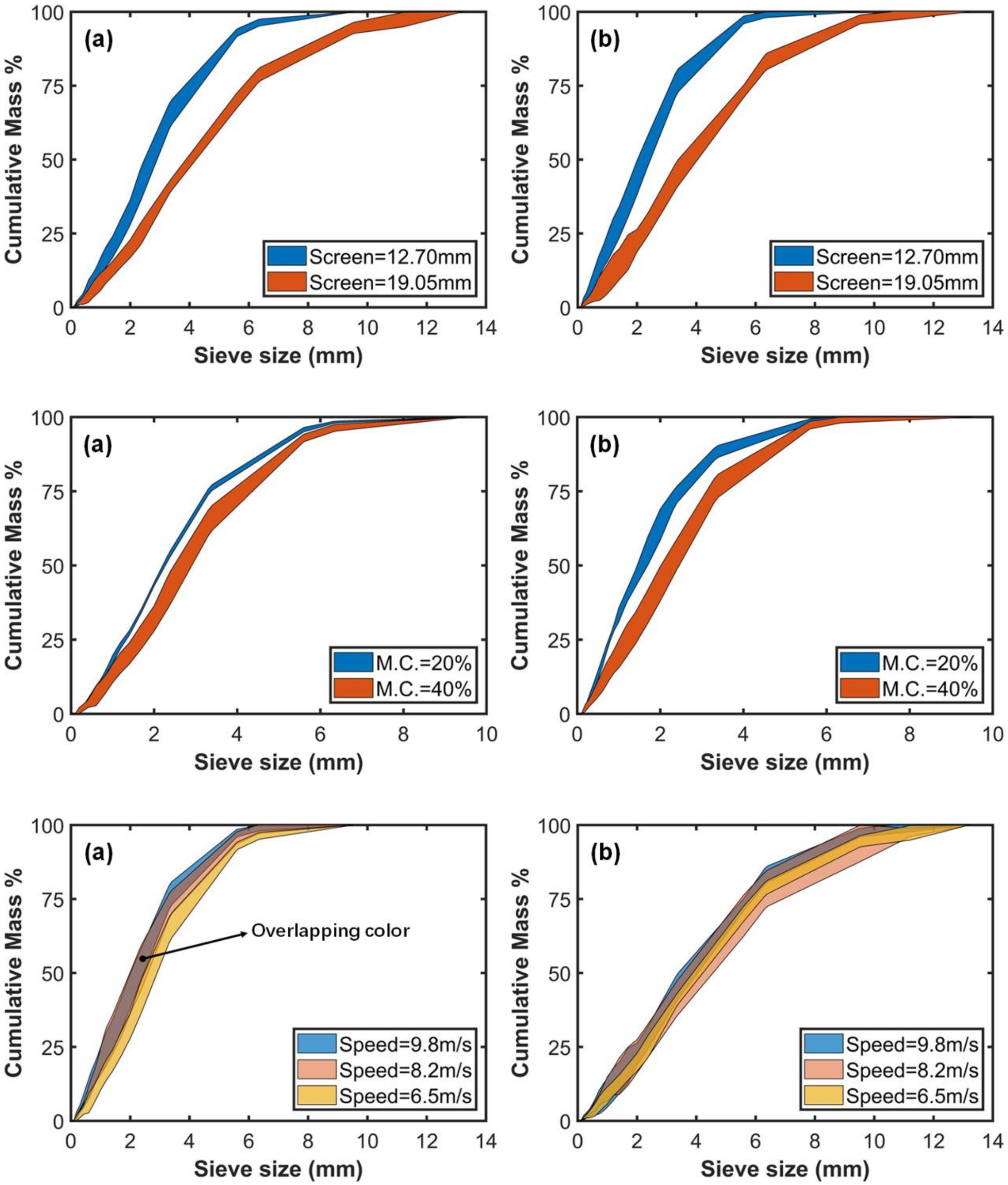
The original deep neural operator (DNO) model identifies an operator between the single type of input and output sequences of a system (e.g., feed PSD vs. outcome PSD) and cannot involve other different types of input.

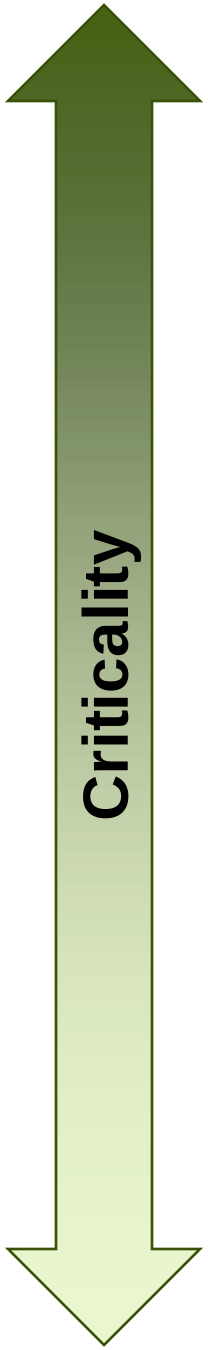
DNO+ model structure that contains three different DNNs

- Trunk net handles sieve size that runs through system.
- Branch net processes cumulative mass vs. sieve size.
- Parameter network processes the influence of material properties and operating conditions on system.

DNO+ can include additional types of input such as feed moisture content and discharge screen size that exert influence on the system behavior.

Physical parametric tests of corn stalk knife milling



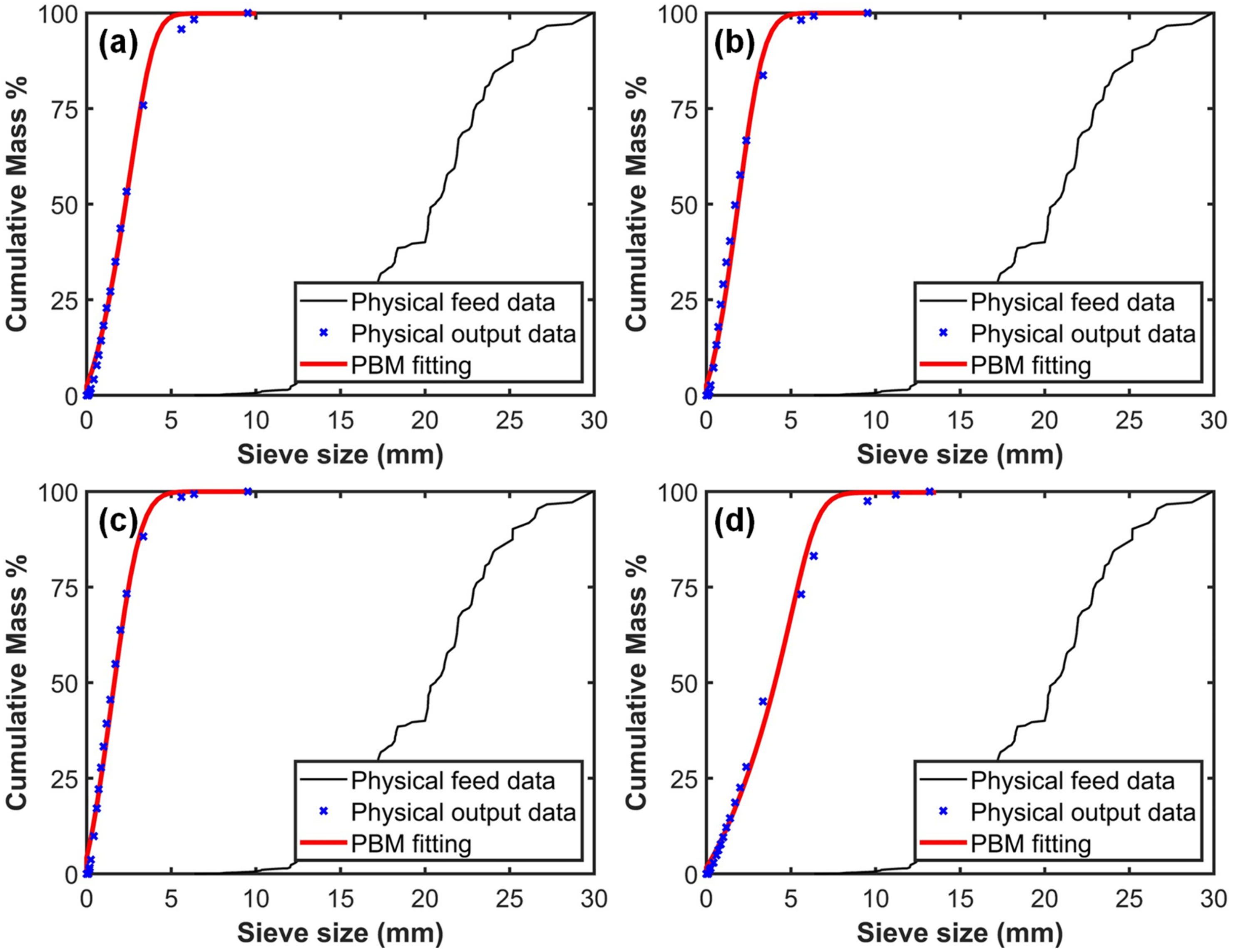


Discharge screen size
- This is as expected

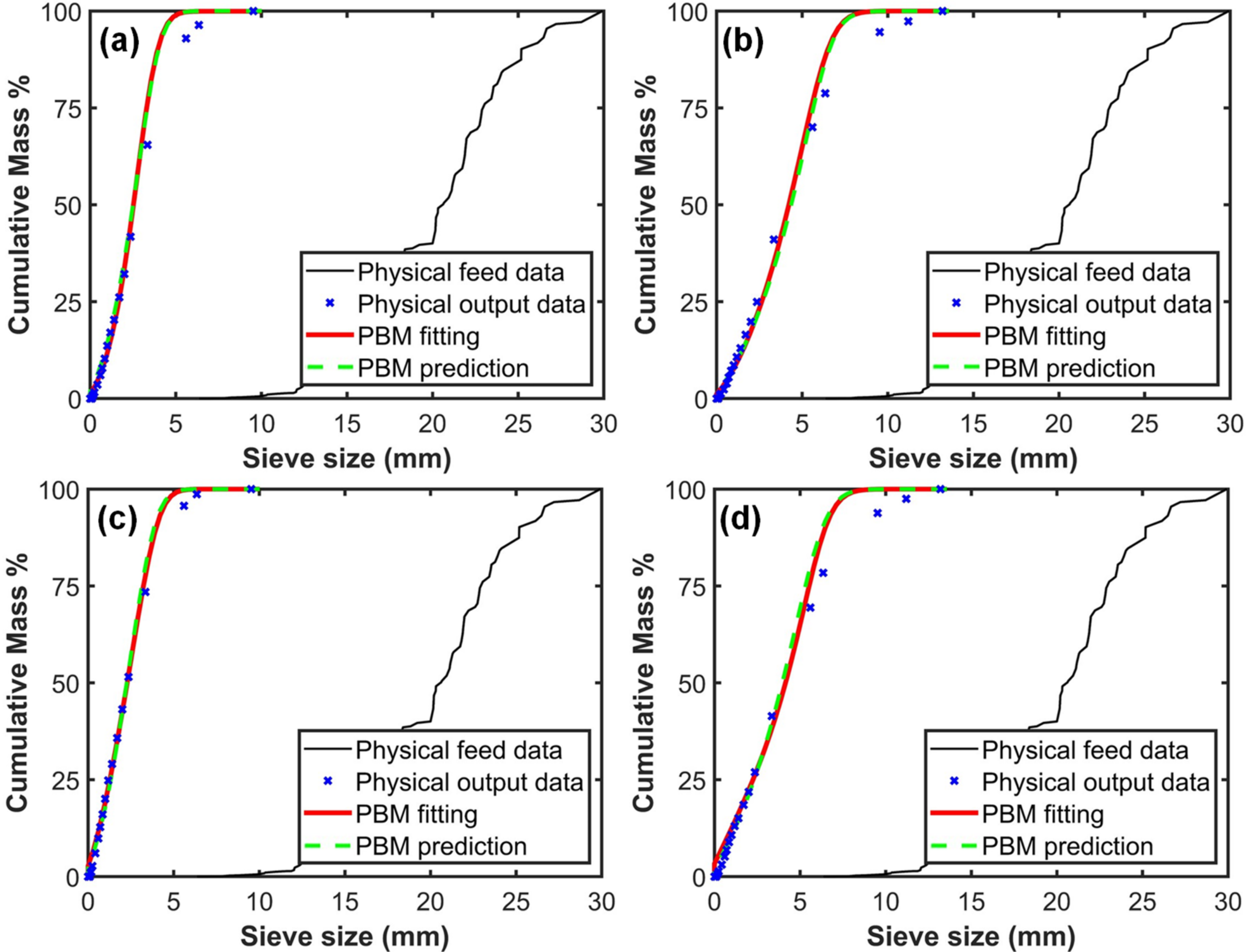
Feed moisture content
- Special to biomass materials

Blade tip speed
- Energy cost can be reduced by using lower power rate

Examples of the PBM fitting accuracy in four test conditions

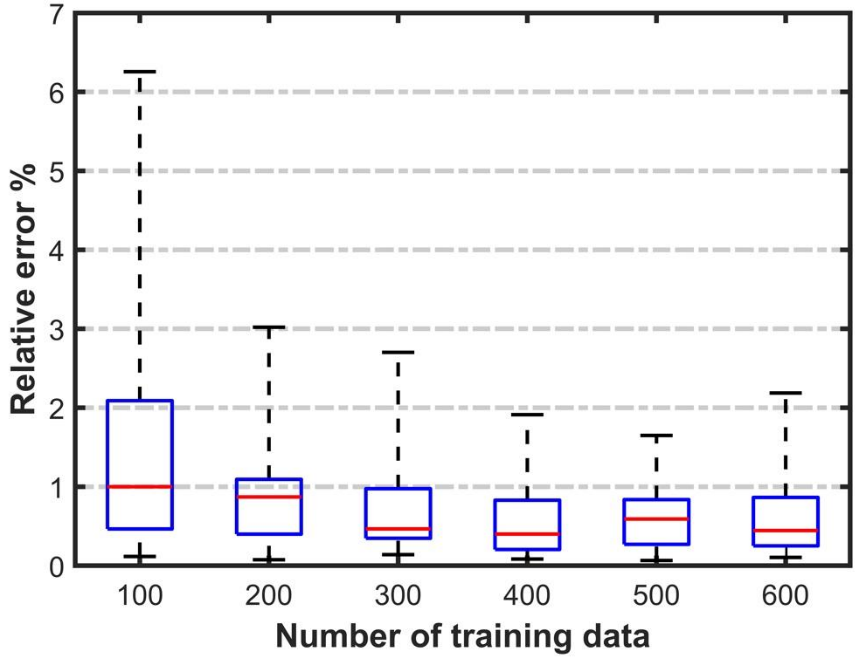


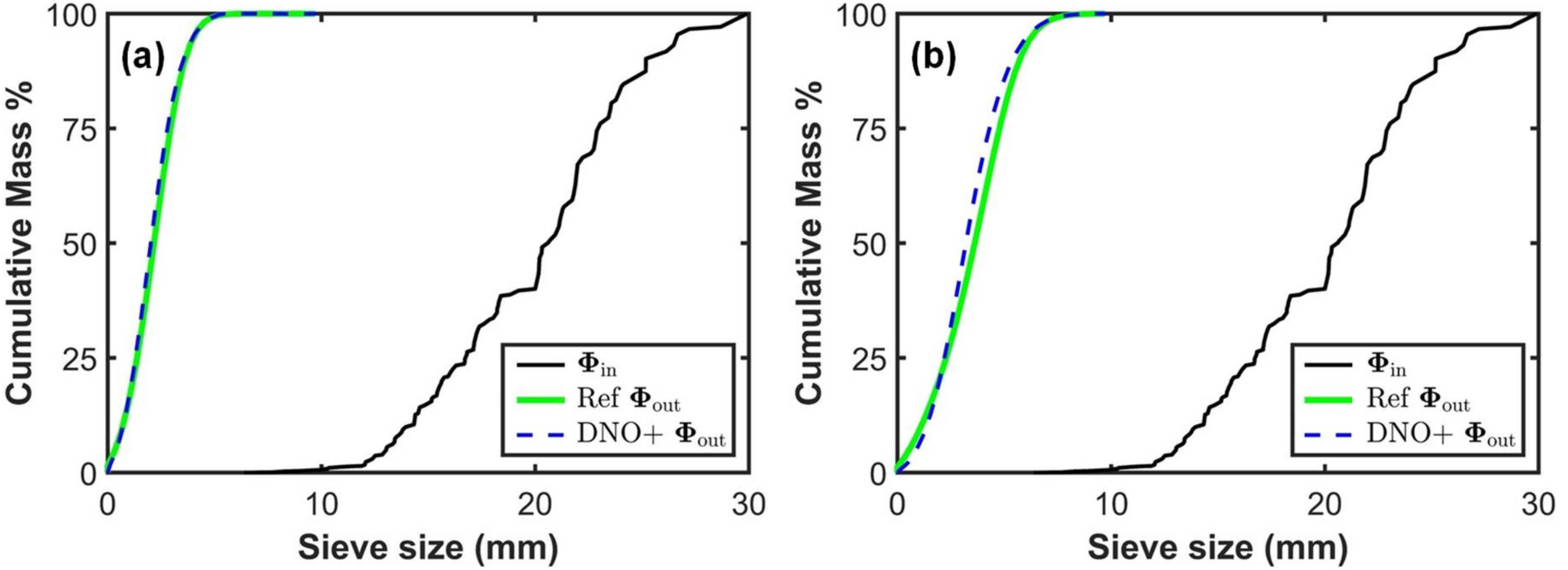
Comparison between PBM using individually determined fitting parameters and PBM using trained mapping operator



Observation: “Parameter free” (fitting parameters calculated on the fly) is possible in the extended PBM to deliver satisfying accuracy

Training and accuracy of DNO+

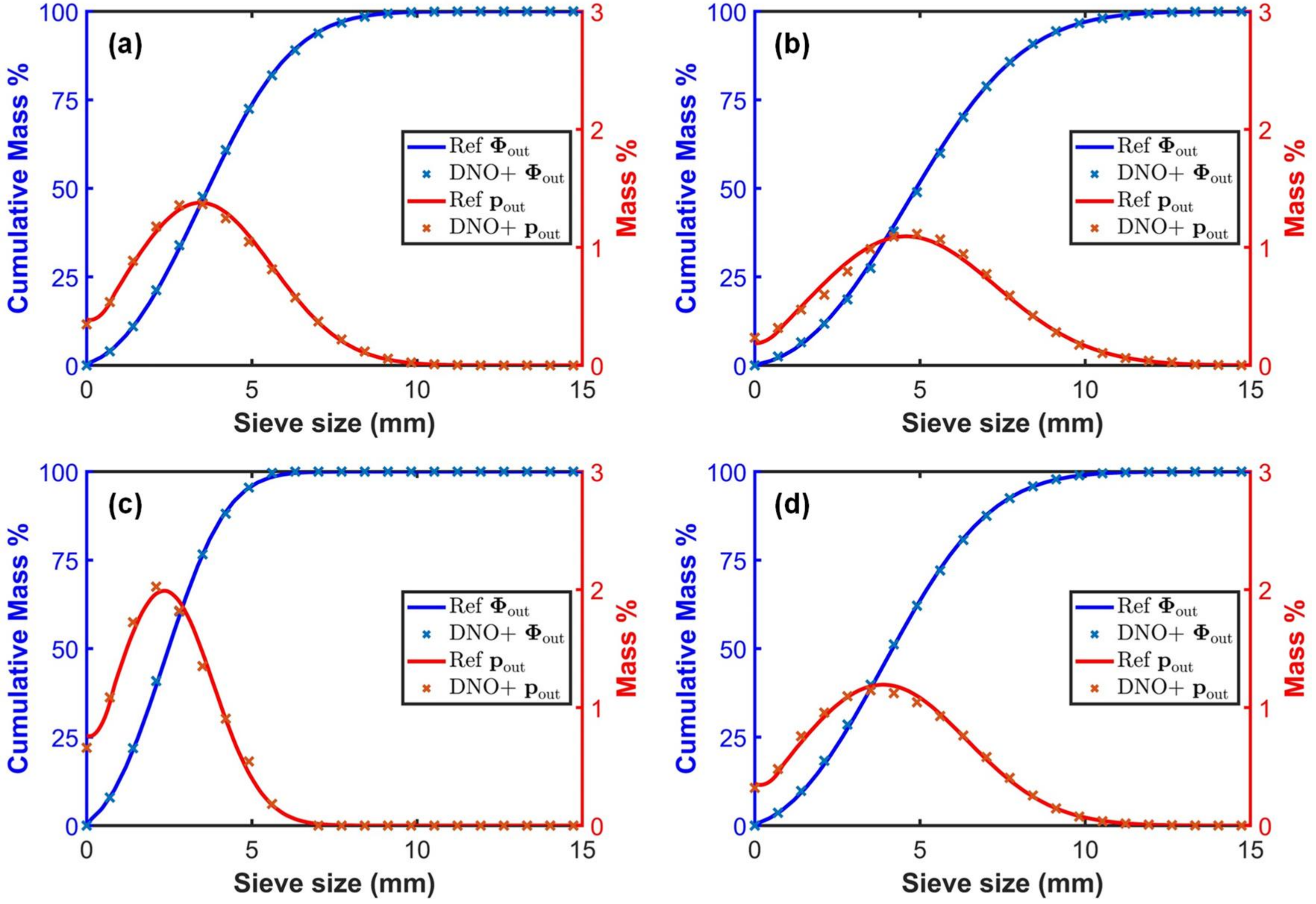




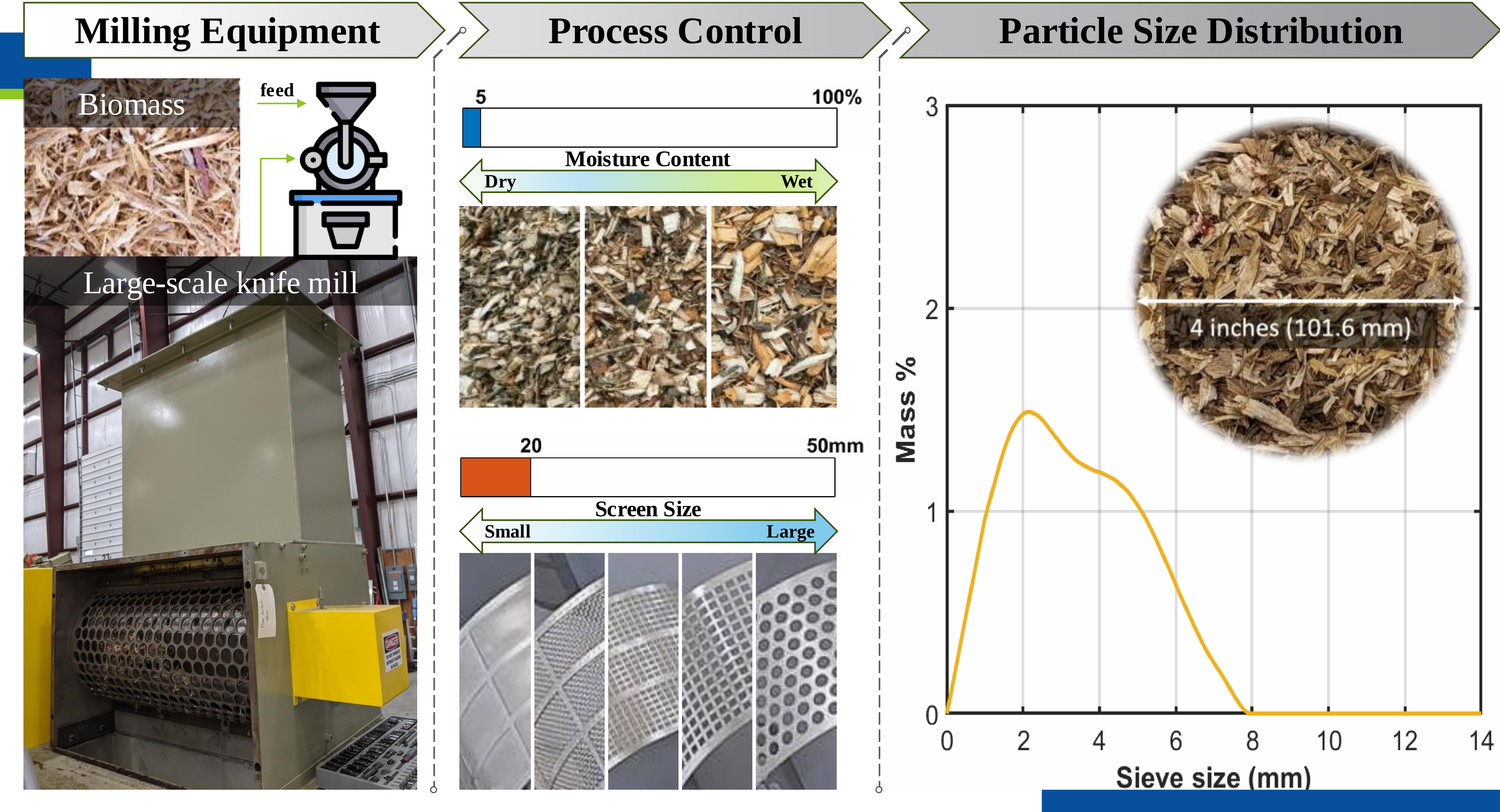
- Limited number of physical tests (12) indicates the need to use PBM predictions to generate source data for training DNO+.
- Error sensitivity study indicates 300 data sets are enough

Predictive accuracy: examples of DNO+ predictions for two test cases from the physical experiments

Examples of DNO+ predictions for four test cases in the expanded and refined parameter space



Additional thoughts: Though both the extended PBM model and the DNO+ model achieved accurate predictions for large-scale knife milling of corn stover, the extension and application of DNO+ do not require strong subject matter expertise. Thus, it would be easier to adapt the DNO+ model for other preprocessing operations with different physical mechanisms.



Milling Equipment
Process Control
Particle Size Distribution
Biomass
feed
Large-scale knife mill
5
100%
Moisture Content
Dry
Wet
20
50mm
Screen Size
Small
Large
3
2
1
0
Mass %
0
2
4
6
8
10
12
14
Sieve size (mm)
4 inches (101.6 mm)

Conclusions

Lu, M., Xia, Y., Bhattacharjee, T., Klinger, J., & Li, Z. (2024). Predicting biomass comminution: Physical experiment, population balance model, and deep learning. *Powder Technology*, *441*, 119830.

- An extended population balance model (PBM) is developed for biomass comminution.
- Biomass feed moisture is added in the PBM as a new input parameter.
- An enhanced deep neutral operator (DNO+) model is developed for biomass comminution.
- DNO+ allows for influencing factors such as moisture and screen size as extra inputs.
- Both models are remarkably accurate in the calibration or training parameter space.

Acknowledgements

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