Machine Learning and Hybrid Modelling of Particle Breakage in a Jet Mill

Carl Jackson

Johnson Matthey

About Us

Carl Jackson
Senior Digital Chemical Engineer
Core Capabilities
Group Technology
Johnson Matthey

Mingzhe Yu PhD
Senior Solids Engineer
Core Capabilities
Group Technology
Johnson Matthey

Johnson Matthey

A global leader in advanced materials and sustainable technologies, established in 1817 and listed on the London Stock Exchange as a constituent of the FTSE 250 Index.

Addressing three markets...

We deliver through our four businesses...

Energy
Designing technologies of sustainable energy sources, including hydrogen, sustainable aviation fuel, methanol and ammonia.

Chemicals
Process and catalysts technologies that enable the production of chemicals helping customers lower their carbon and environmental footprint.

Automotive
Emission control systems that reduce NO_x and other particulates that harm people and the environment.

Clean Air
Leading in autocatalyst markets

Catalyst Technologies*
#1 in syngas-based chemicals and fuels technology

*sale agreed to Honeywell

Hydrogen Technologies
Market leader in performance components for fuel cells and electrolysers

Platinum Group Metal Services
#1 Global PGM refiner

c. 80%
PGMs used in our products are internally refined

Driving down automotive emissions

- Global leader in autocatalysts for diesel and gasoline vehicles

Market leader in high-performance components for hydrogen fuel cells

Advances

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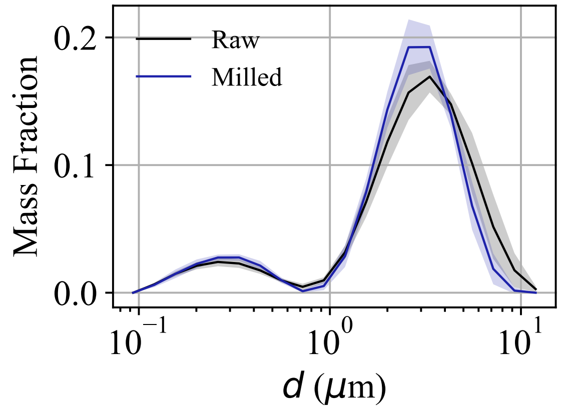
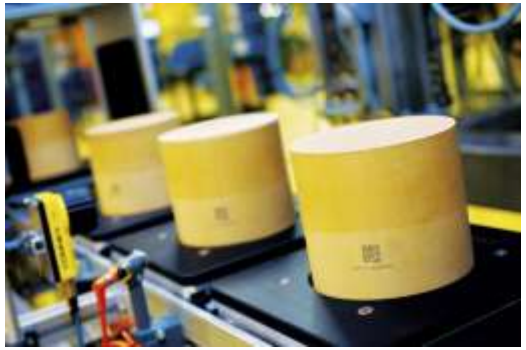
Agenda

- Background
- Population Balance Models and Hybrid Modelling
- Method
- Model Performances and Predictions
- Key Learnings
- Questions

Importance of Particle Size Distributions





Both product performance and manufacturing capability are sensitive to PSD

Motivations for modelling

1. Reduce trial and error of mill settings
   - At scale->material wastage and time
2. Model to inform toll manufacturers
3. Troubleshooting

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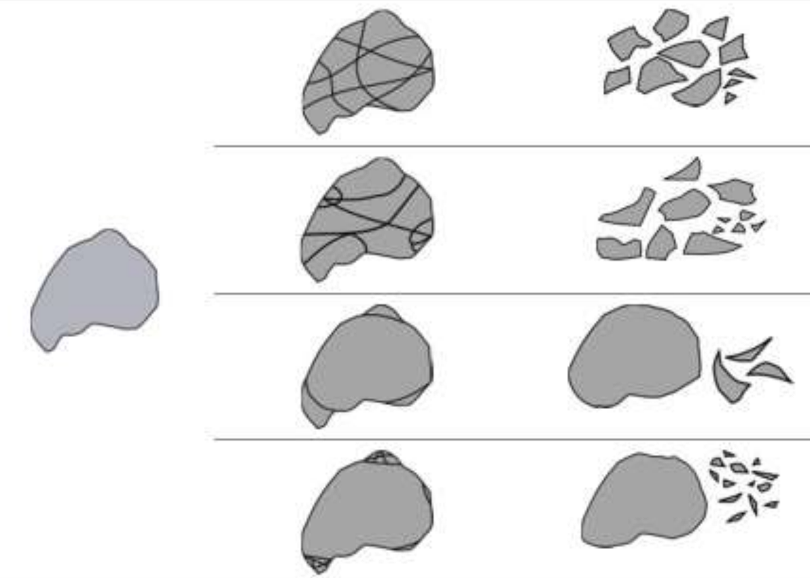
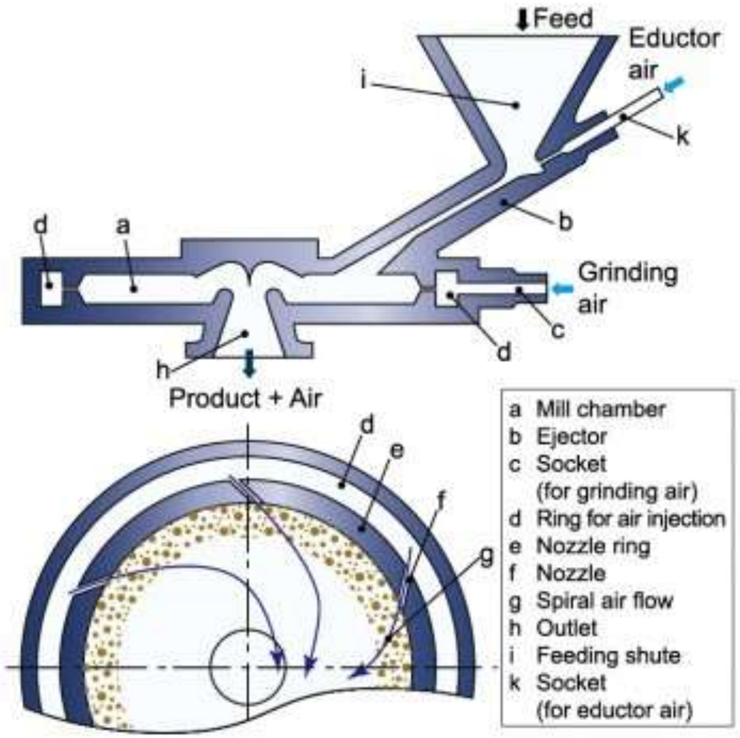
Jet Mills

Feed particle	Breakage pattern	Product particles	Breakage mechanism
			Shattering
			Cleavage
			Chipping
			Abrasion



Wet Mill

Dry Mill



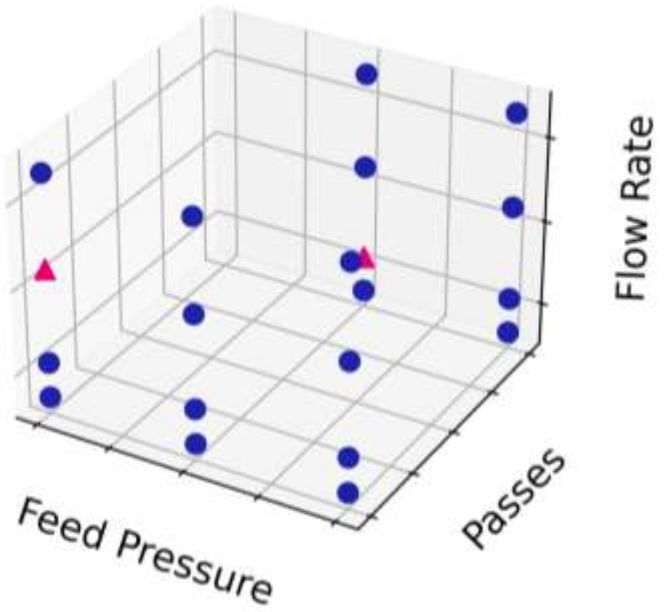
Hosokawa jet mill [1]

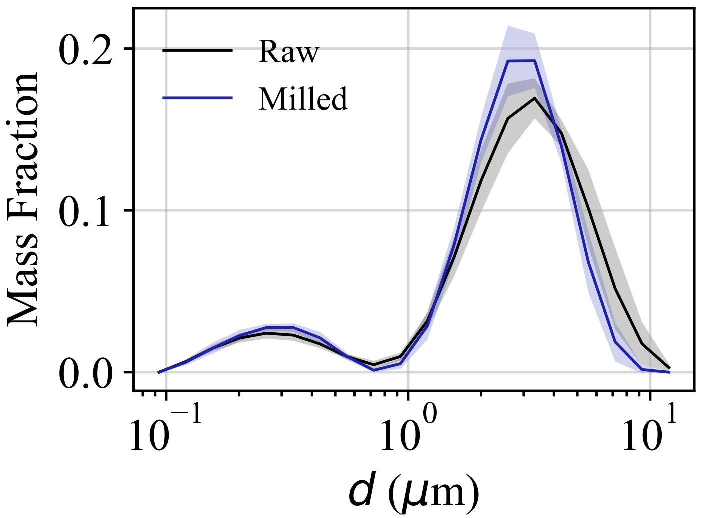
[1] Spiral Jet Mill AS Technical Documentation. Hosokawa Micron Corporation

Dataset

Features	
Initial PSD	Average of 3 measurements 30 bins
Feed pressure	Pressure going into the mill. Grind pressure is always 80% of feed pressure
Feed rate	Mass feed rate into the mill
Run duration	Duration of the batch
Number of passes	Passes through the mill previously. 1-3

Targets	
Product PSD	Average of 3 measurements 30 bins
Yield	Mass of product relative to feed. Typically 75-90%





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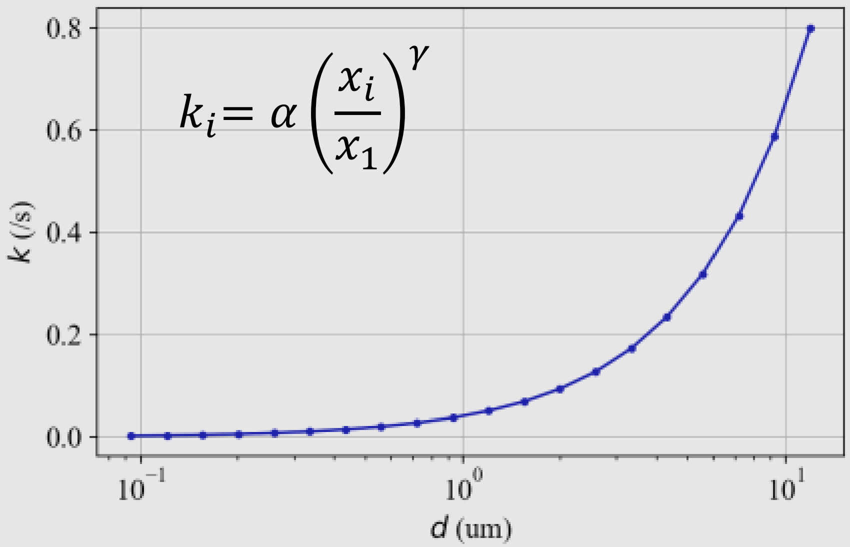
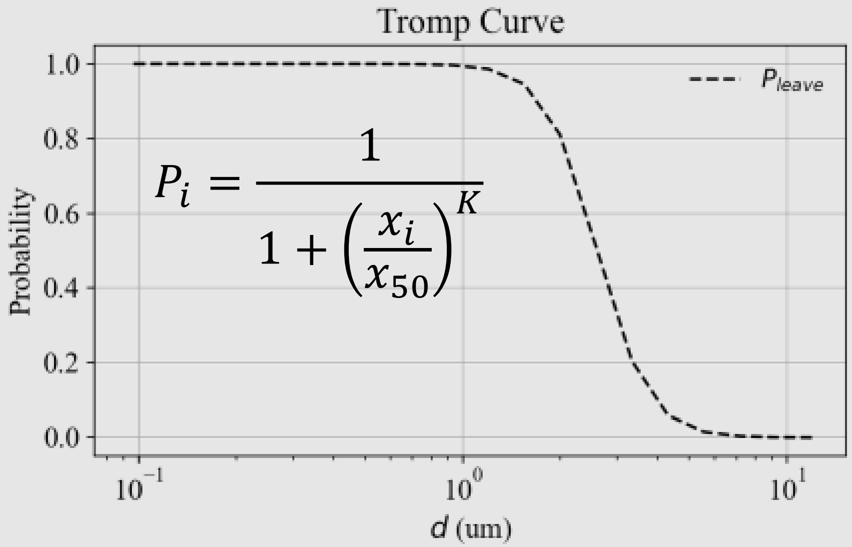
Population Balance Model (PBM)

$$\underbrace{\frac{dm_i}{dt}}_{\text{Chamber}} = \underbrace{f_{in,i}\dot{m}}_{\text{In}} - \underbrace{\frac{P_i m_i}{\tau}}_{\text{Out}} \underbrace{- k_i m_i}_{\text{Death}} + \underbrace{\sum_{j=1}^{i} b_{ij} k_j m_j}_{\text{Birth}}$$

Breakage rate



Classification function



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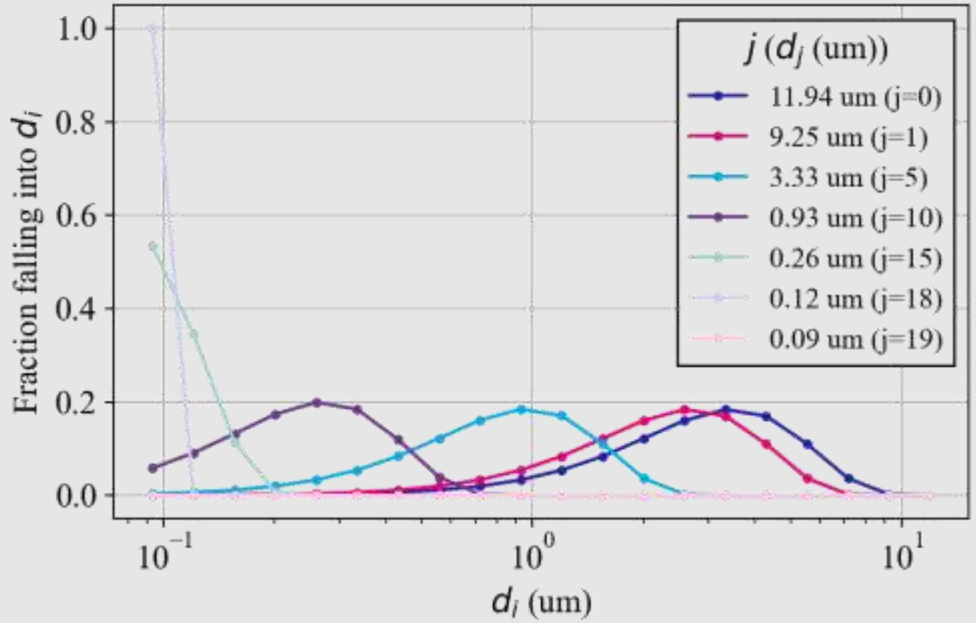
Breakage distribution function

$$b_{ij} = \left(\frac{x_i}{x_j}\right)^{\beta} \left(1 - \frac{x_i}{x_j}\right)^{q}$$

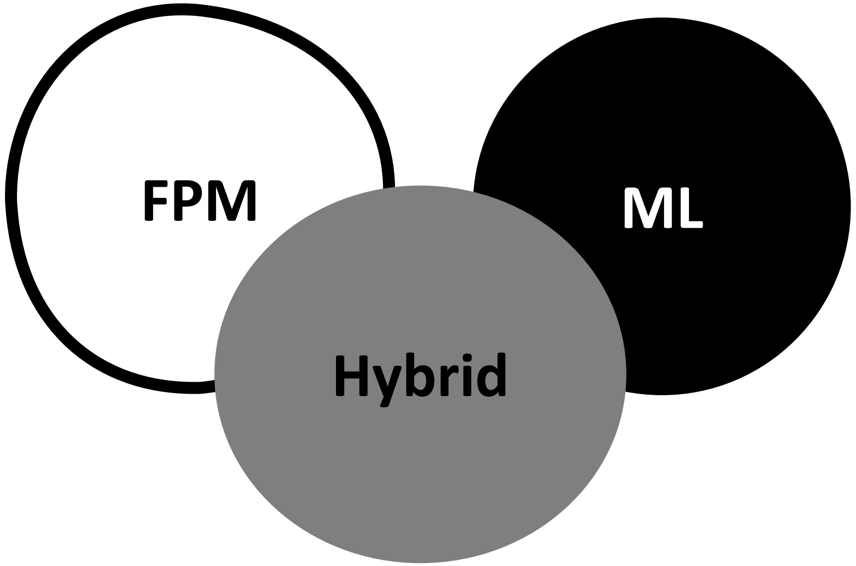
	i=1	i=2	i=3	...	i=n
j=1	0	0	0	...	0
j=2	$b_{1,2}$	0	0	...	0
j=3	$b_{1,3}$	$b_{2,3}$	0	...	0
...	...	...	...	...	0
j=n	$b_{1,n}$	$b_{2,n}$	$b_{3,n}$	...	0



Hybrid models

Consists of 2 parts…

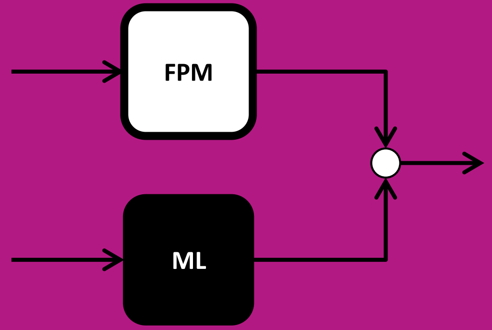
1. First principles model (mechanistic, white-box model)
2. ML model (data-driven, black-box model)



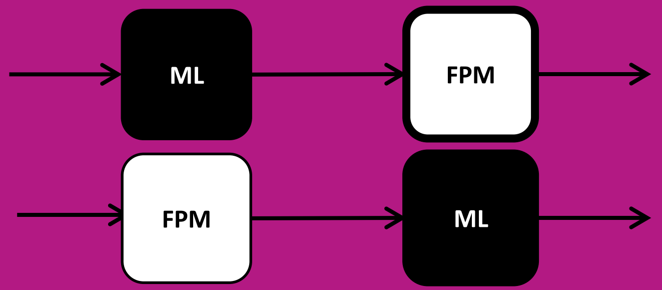
- Data
- Extrapolation
- General performance
- Time/expertise to develop

Different structures

Parallel arrangement

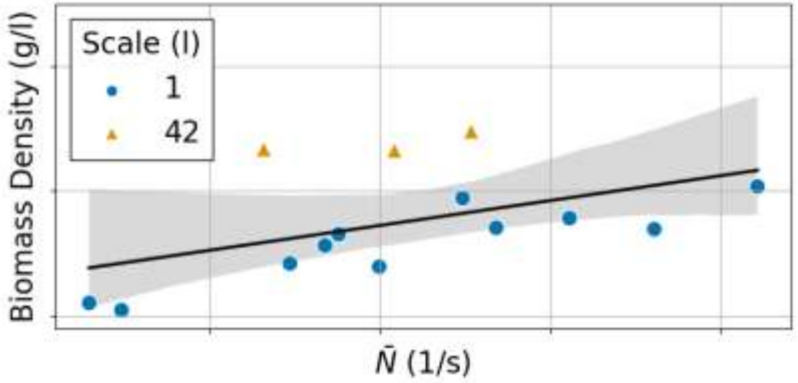


Series arrangement



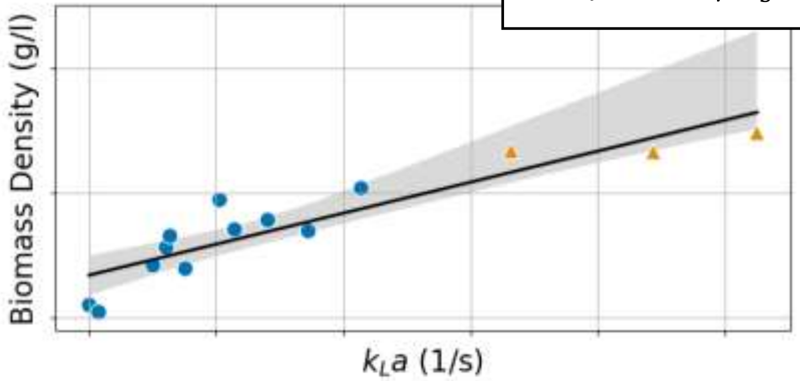
M. von Stosch et al. Chem. Eng. Sci. 60, 86-101 (2016)

Hybrid models



$$P_V = \frac{N_p \rho (N)^3 D^5}{V_w}$$

$$k_l a = A P_V^{\alpha} u_s^{\beta}$$



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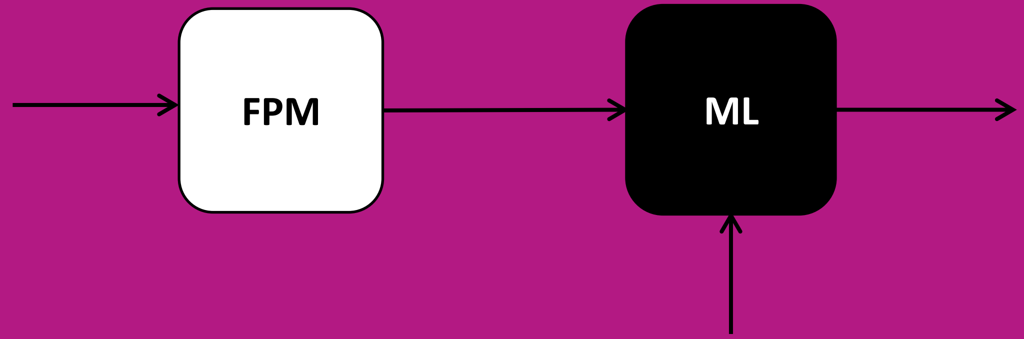
Small fermentation dataset across different scales

"Which phenomena are important for biomass density (yield)?"

Oxygen mass transfer

- More bugs → More oxygen uptake → More agitation to maintain DO_2

Derive a soft-sensor for final fermentation batch yield across multiple scales



van't Reit K. Ind. Eng. Chem. Process Des. Dev. 18(3) 1979: 357–364

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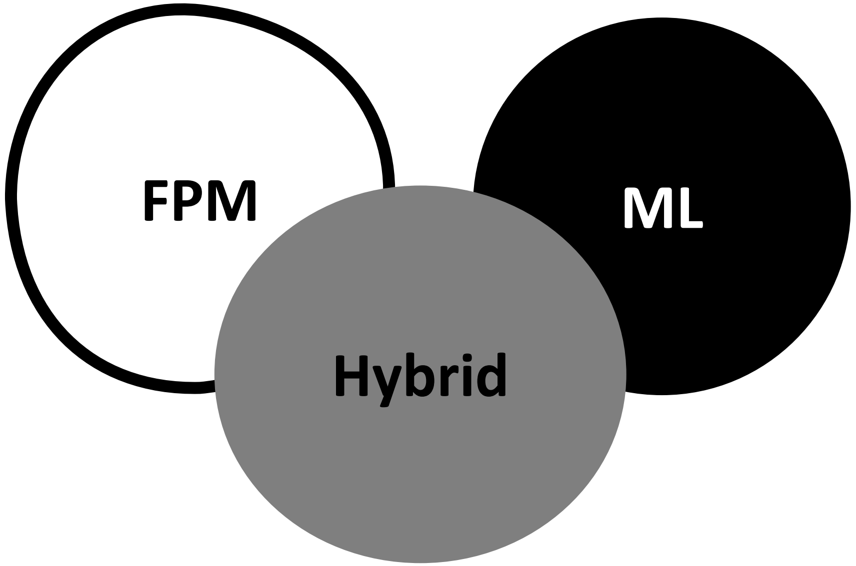

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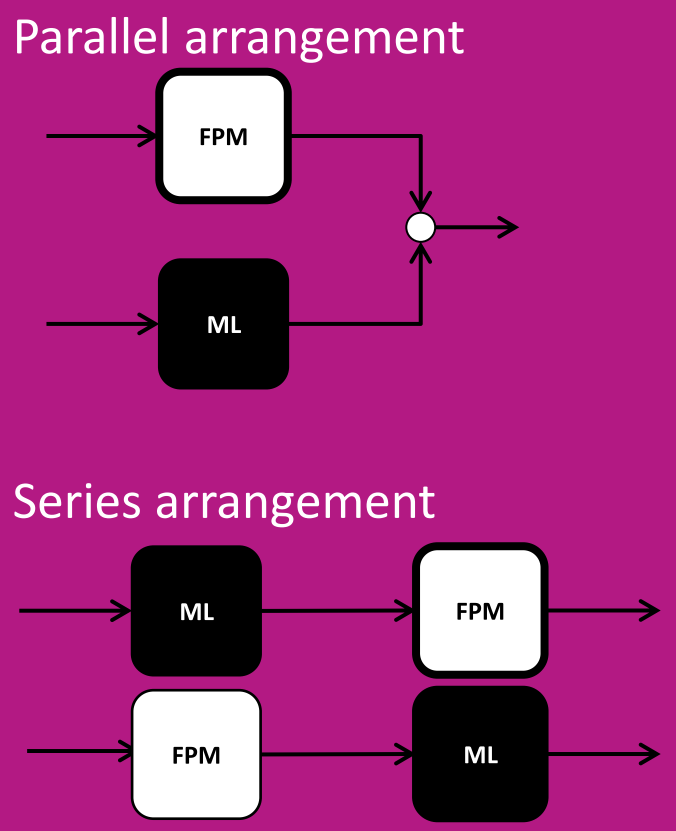
Different structures



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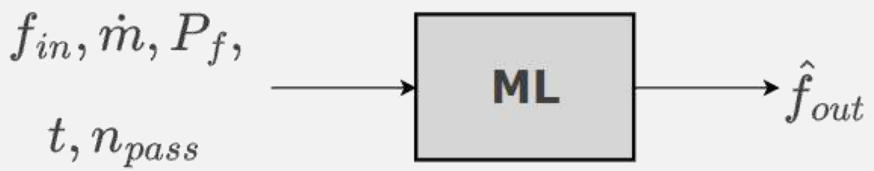
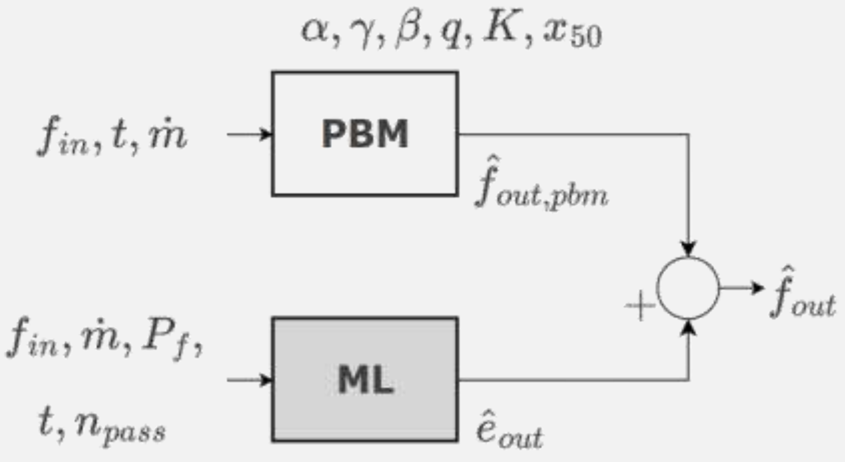
Model Architectures

Data-driven model



Corrective hybrid model

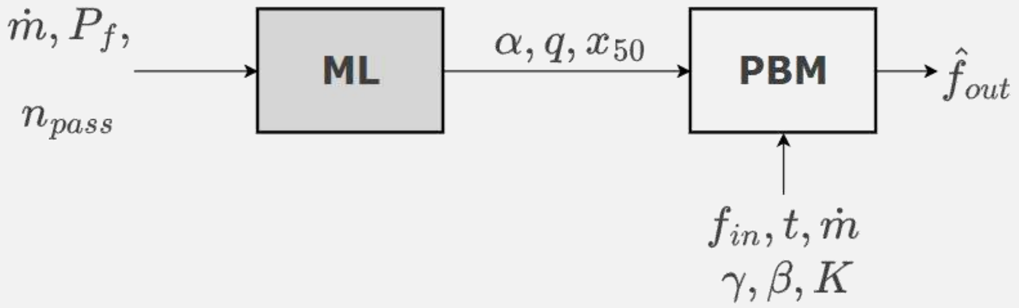
ML model predicts error of PBM



Series hybrid model

ML model predicts parameters of the PBM

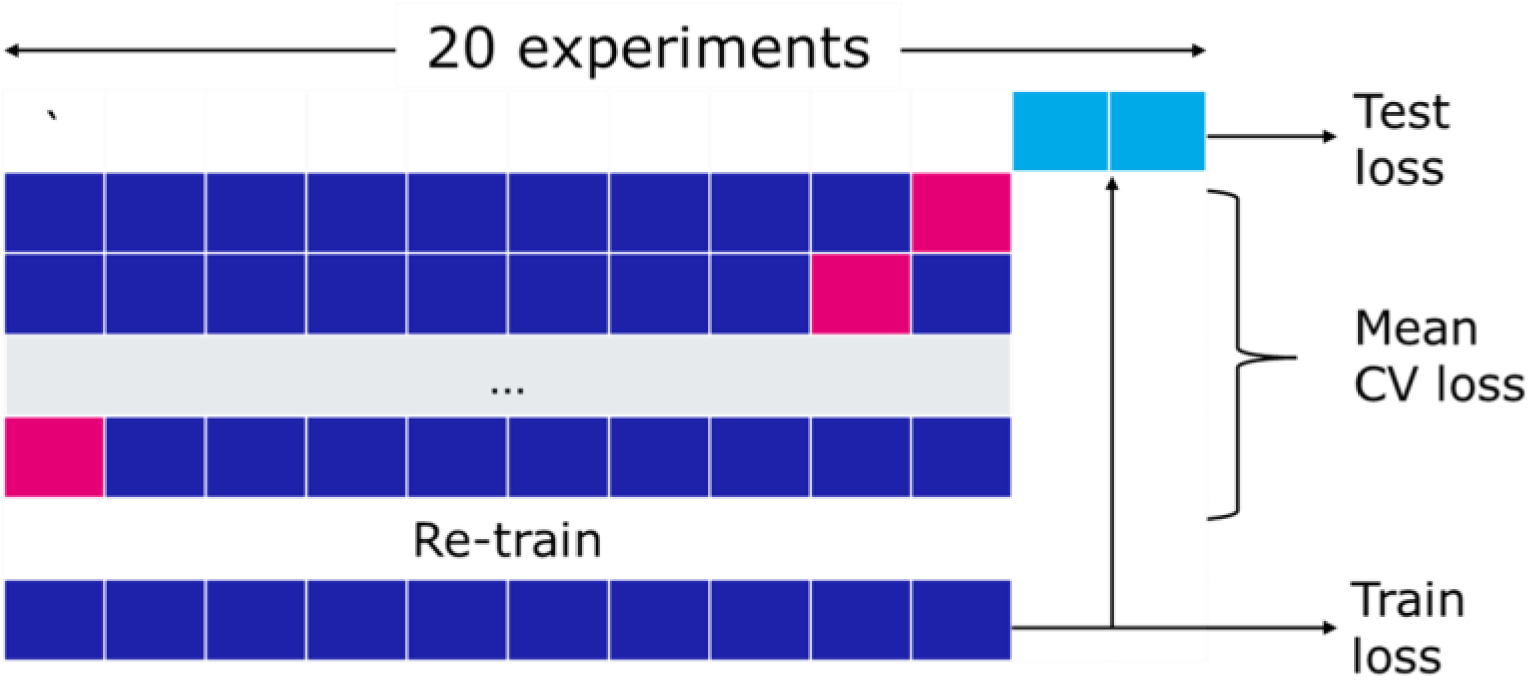
- α (overall breakage intensity / selection severity)
- x_{50} (classification cut size)
- q (fine tail)



Model Evaluation and Optimisation

Hyperparameters of each model optimised using Optuna™ [2]

Loss metric is mean absolute error (MAE) between true and predicted PSD



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[2] Akiba et al. 2019. Optuna: A Next-generation Hyperparameter Optimization Framework. In KDD.

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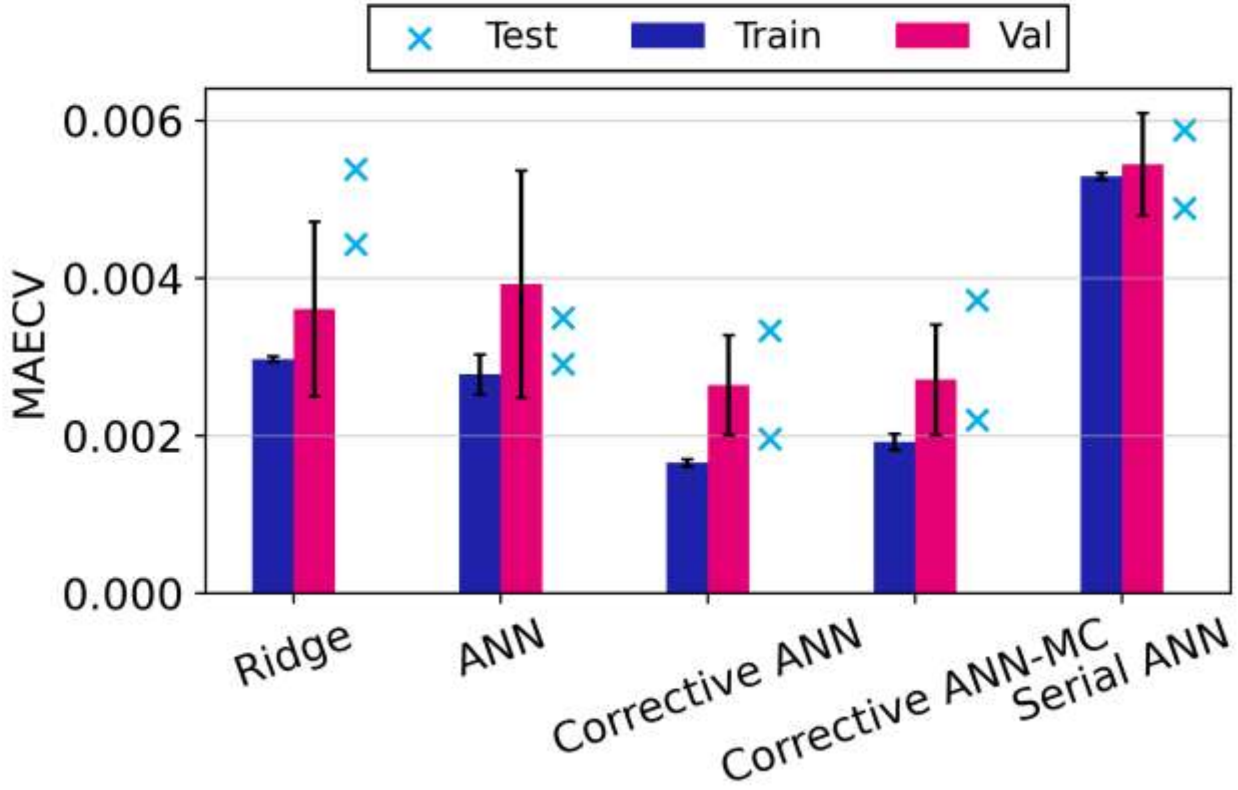
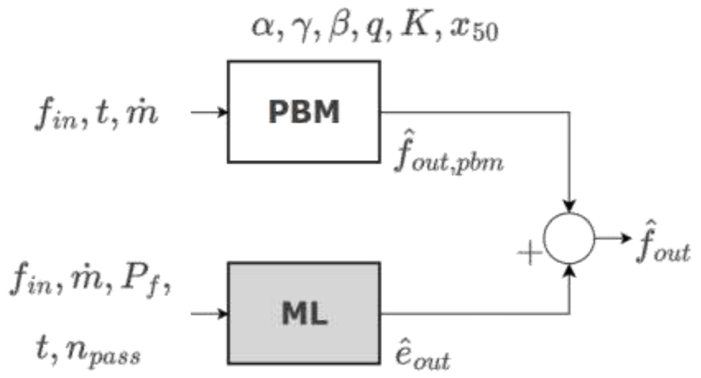
Results

$$\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \lambda \sum_{j=1}^{P} w^2$$

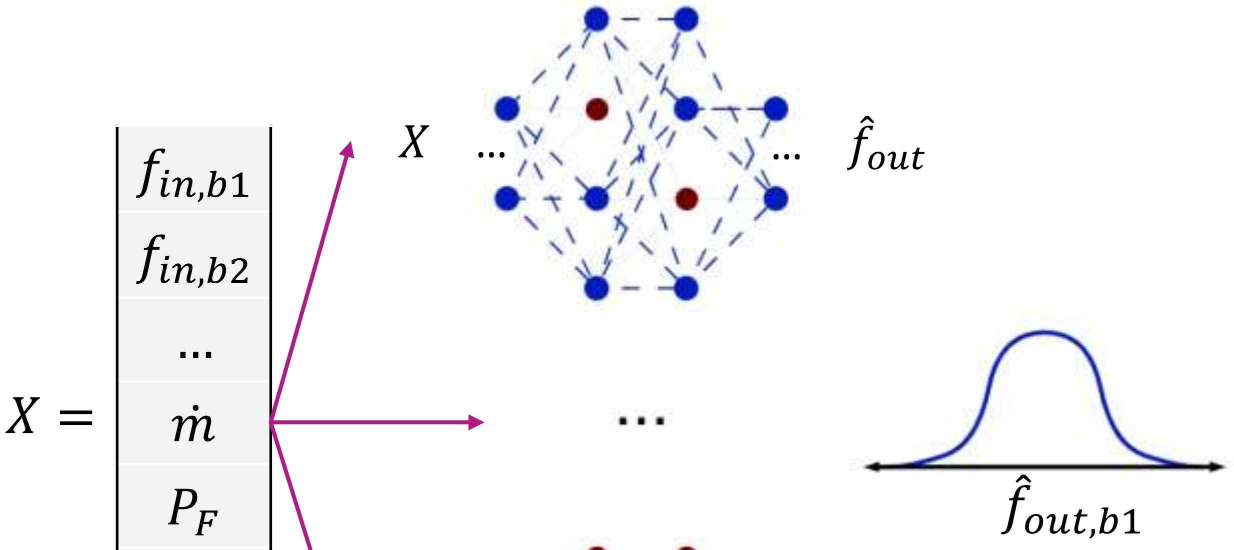




Neural networks built and trained in PyTorch. Torch ODE solved with torchdiffeq

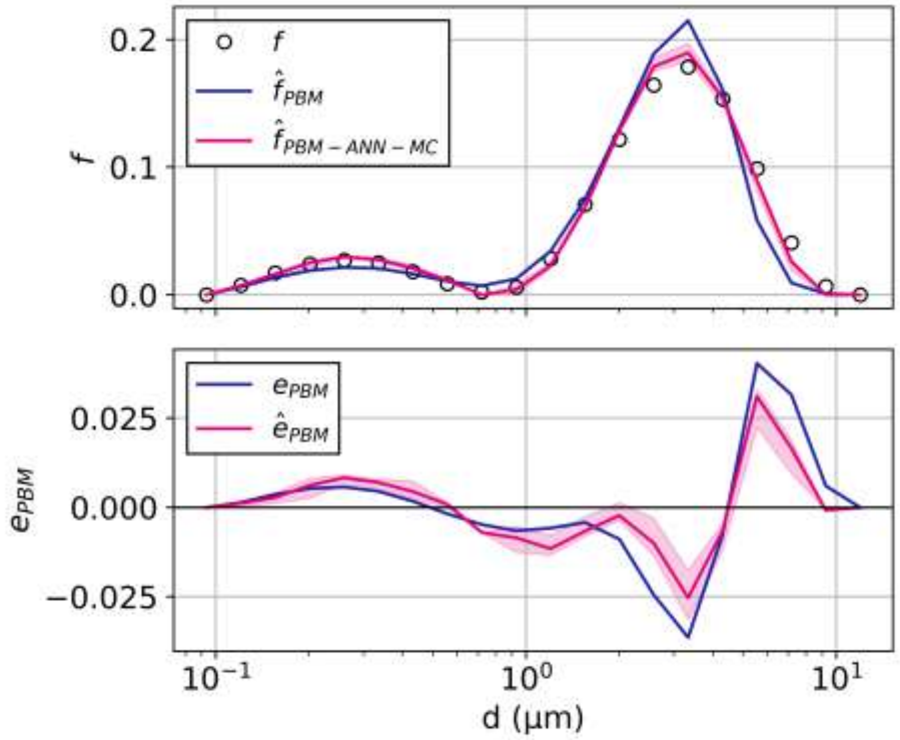
Results

- Monte Carlo Dropout Neural Network



Approximation of posterior distribution of each PSD bin

Corrective ANN-MC performance on test experiment



Gal, Y., & Ghahramani, Z. 2016. Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning.

Results

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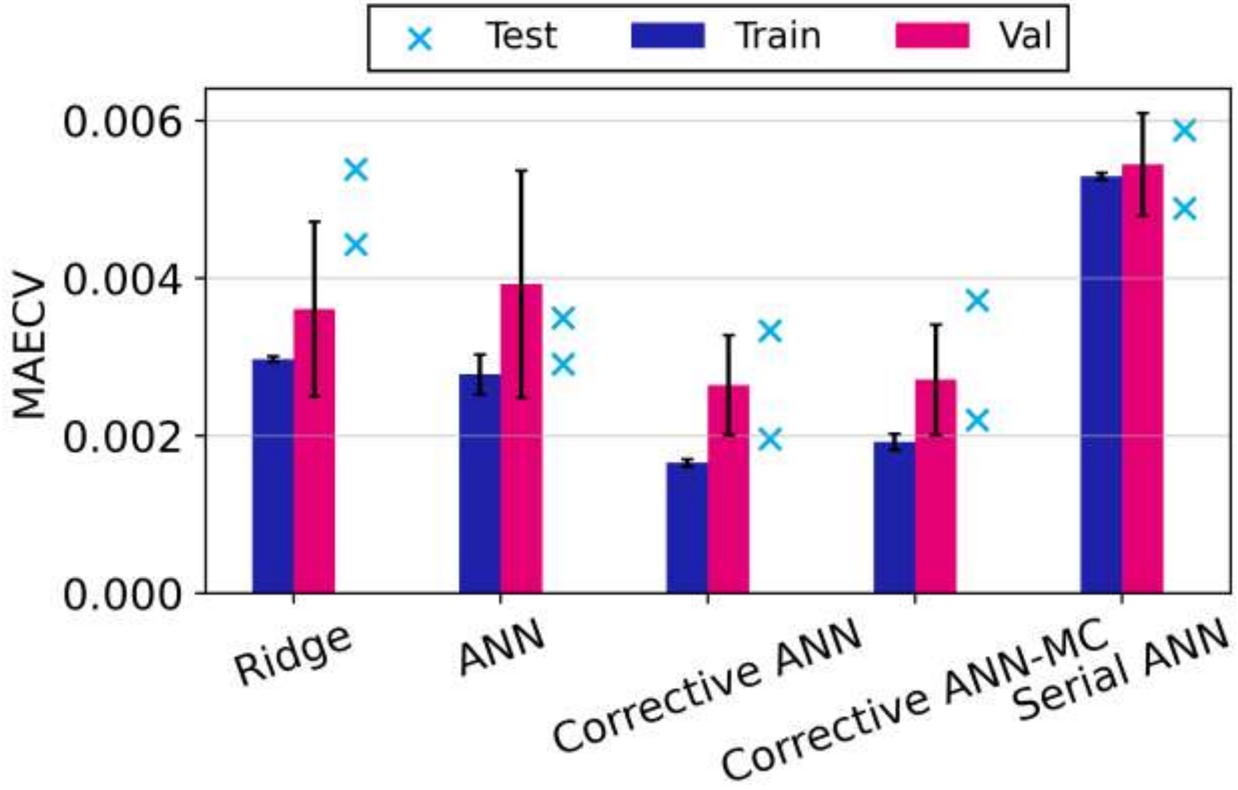

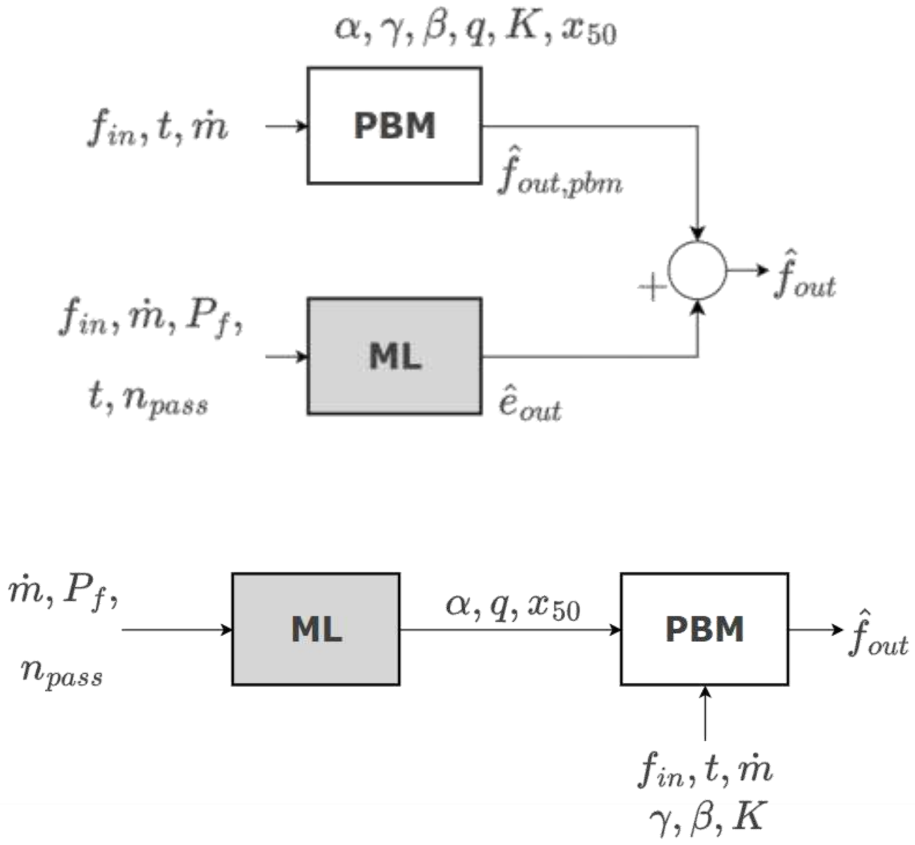

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Key Learnings

- A bad analogy of inductive bias in hybrid modelling

Imagine you're cooking from a recipe…

Which will produce the best dish:

a. **Strictly** follow a recipe
b. **Minor deviations** from the recipe
c. **Major deviations** from the recipe

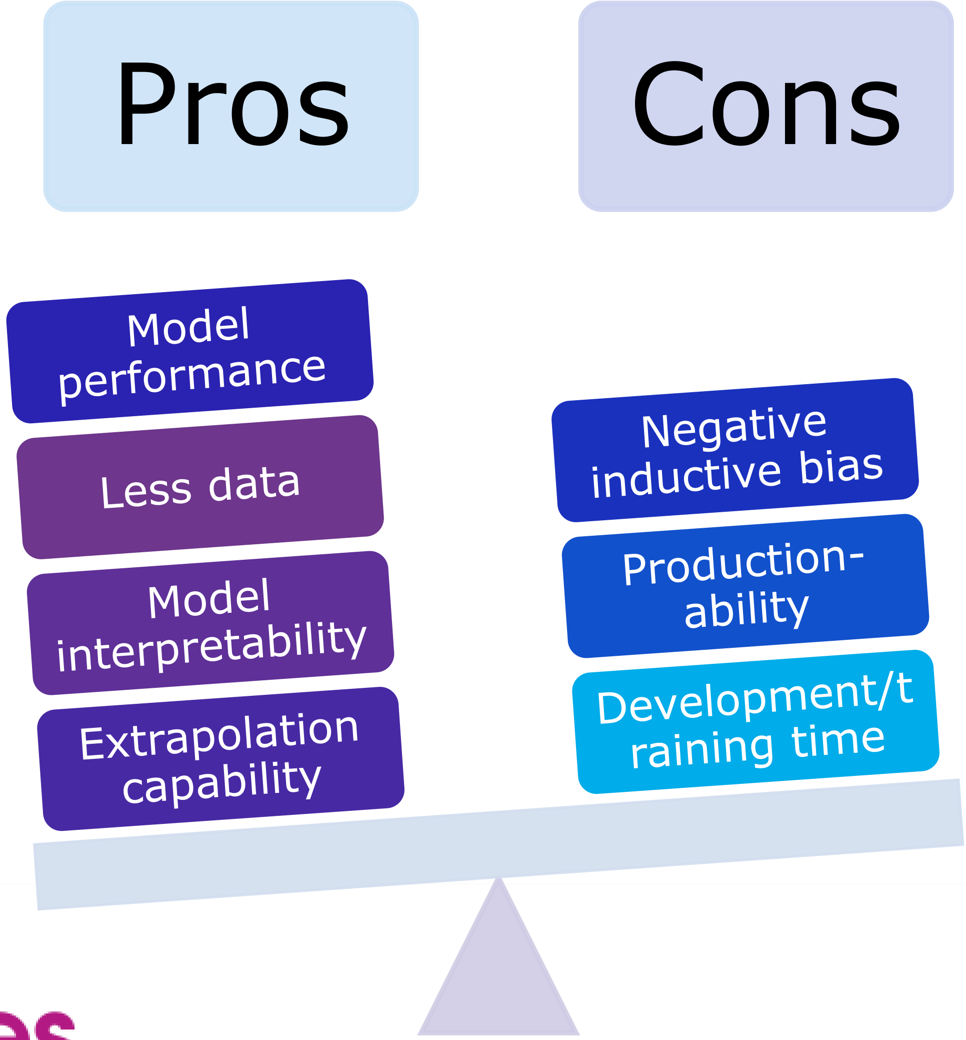
Depends on:

- Quality of the **recipe**
    - Quality of the **first-principles model**
- Your **past experiences and skill** as a chef
    - Quantity and quality of the **data**

Advances

Terrifying image generated with Microsoft Copilot

Key Learnings



Advances

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Conclusions

Corrective hybrid modelling has been beneficial in predicting milled product PSD
Series hybrid modelling…not so much

- Negative inductive bias owing to the challenges of PBMs

Corrective hybrid models with Monte Carlo neural nets show equal performance and provide CI

- But longer inference times make it impractical for series hybrid modelling

Considerations for future hybrid modelling work

- Revisit PBM
- Hybrid model structure
    - How confident are you in the first-principles model?
    - Are all of the likely phenomena captured?
    - Optimise the hybrid architecture
- What are the requirements for implementing into production

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carl.jackson@matthey.com

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