Functional Data Analysis and DOE Applied to Food Milling Processes

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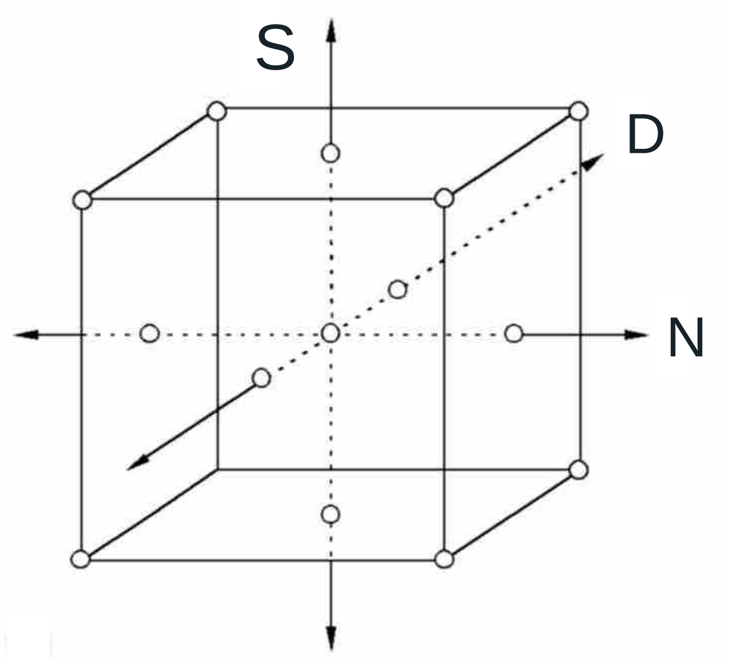
Introduction & Objectives

- Nearly all pharmaceutical production, fermentation and other cell-cultivation processes and the processes of the food industry are carried out in batch.
- The Design Space (DS) of batch processes is dynamic since the process is nonstationary.
- Experimental designs with time dependent responses are typically run to study such systems.
- In this work, functional data analysis (FDA) and design of experiments (DOE) are used together to develop the design space of a typical batch milling process, the refining of a spreadable cocoa and hazelnut product.

Methods

- Ingredients used to prepare 100 g of the hazelnut-and-cocoa-based anhydrous paste: seed oil (27 g), hazelnut paste (8 g), cacao powder (11 g), milk powder and derivatives (7.5 g), lecithin (0.6 g), sugar (31 g), ice sugar (14 g), other (0.9 g).
- Grinding equipment: a pilot stirred ball mill model wafa20 (Mazzetti Renato, Italy).
- Experiments:
  - ✓ Experimental design: face-centered central composite design.
  - ✓ Factors: shaft rotation speed (N), ball diameter (D), overall mass of balls (S).
  - ✓ Responses: fineness (size of the largest solid particles) and milling energy vs. time.
  - ✓ Response constraints: to avoid the gritty sensation in the mouth, fineness < 30 µm; to avoid over-milling, fineness > 20 µm.
- Software: JMP Pro 14.3.0 (SAS Institute, NC, USA).

Face-centered central composite design

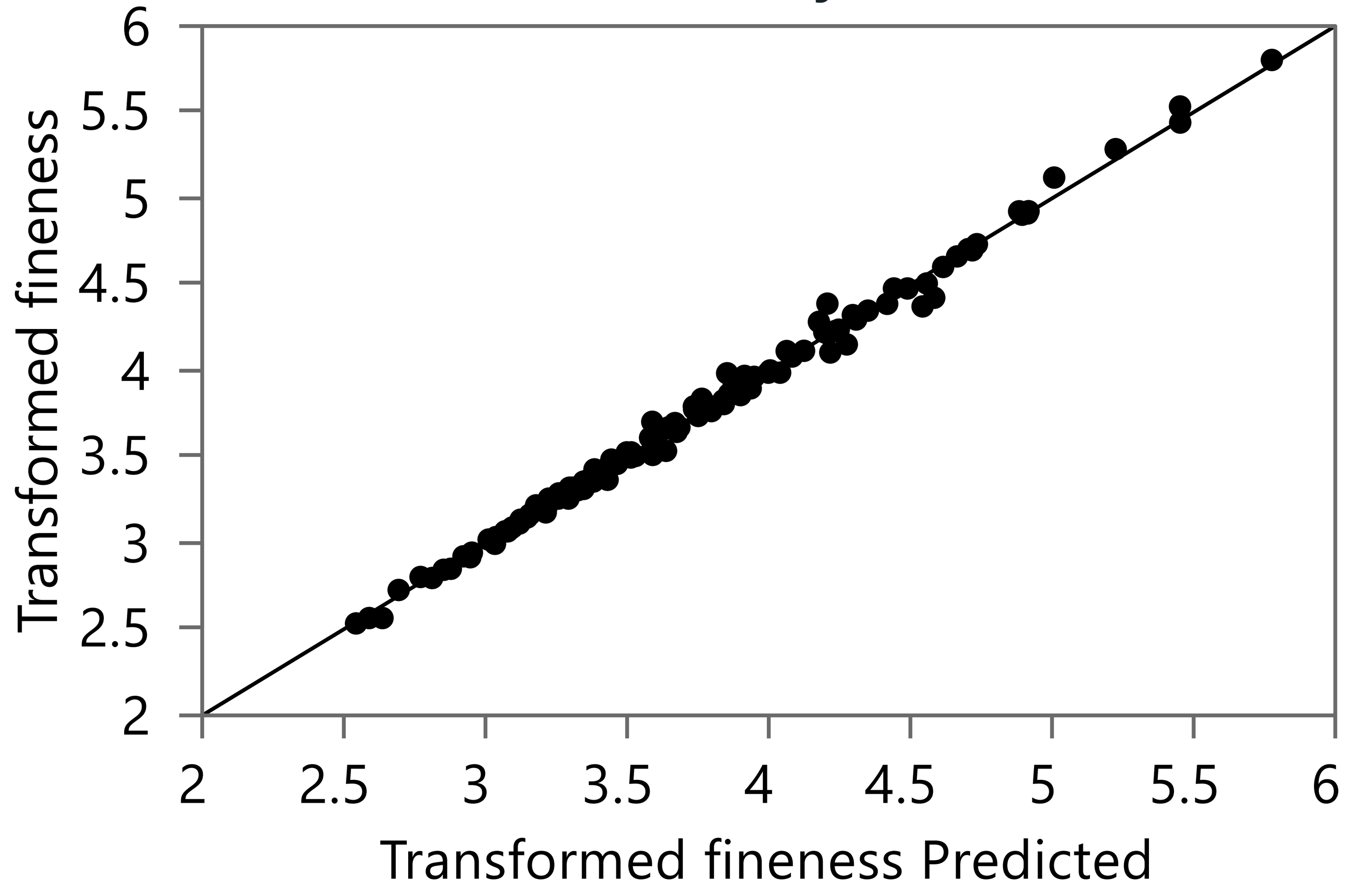


Detail of a stirred ball mill

Results

Click graphs to enlarge

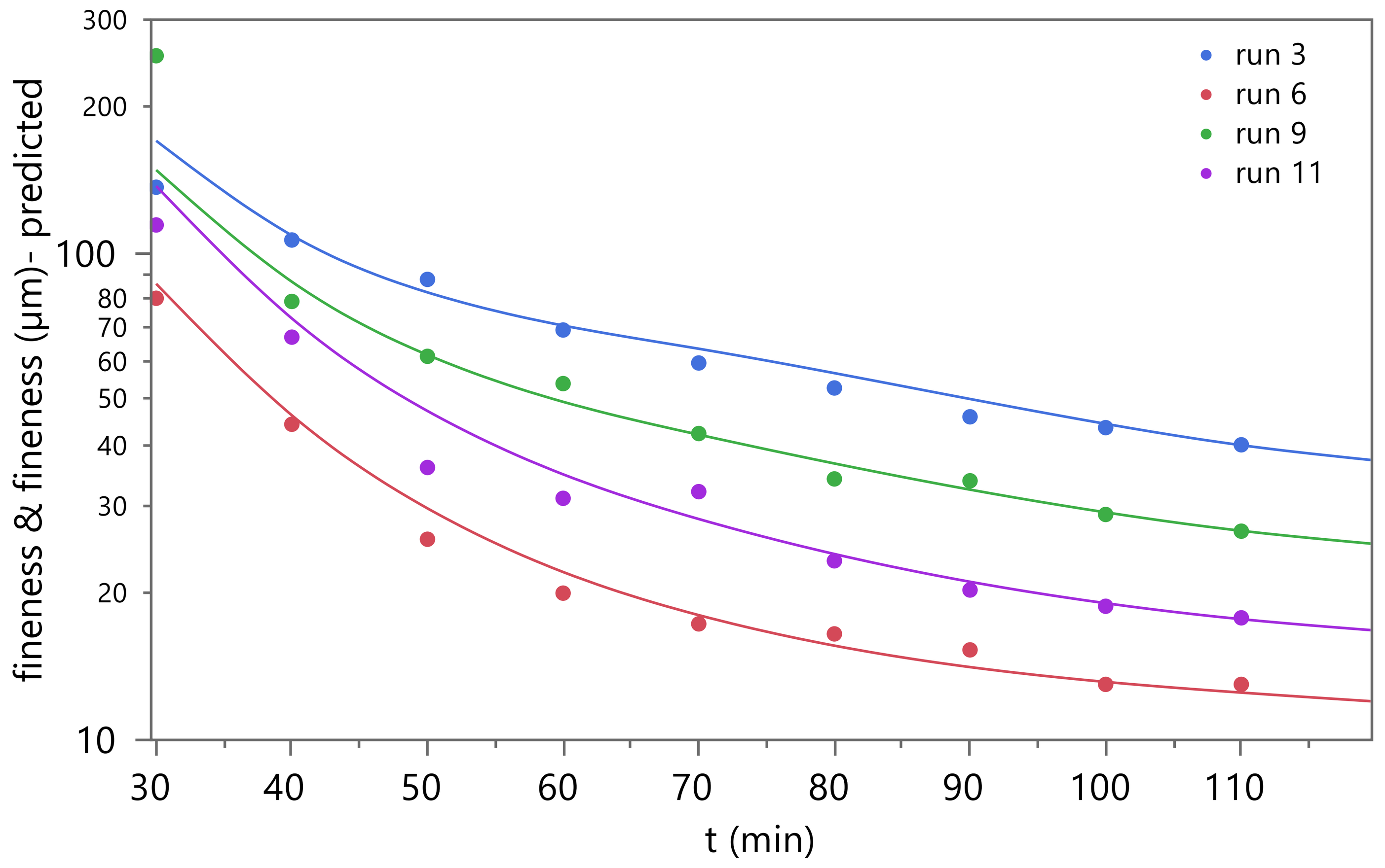
Functional data analysis



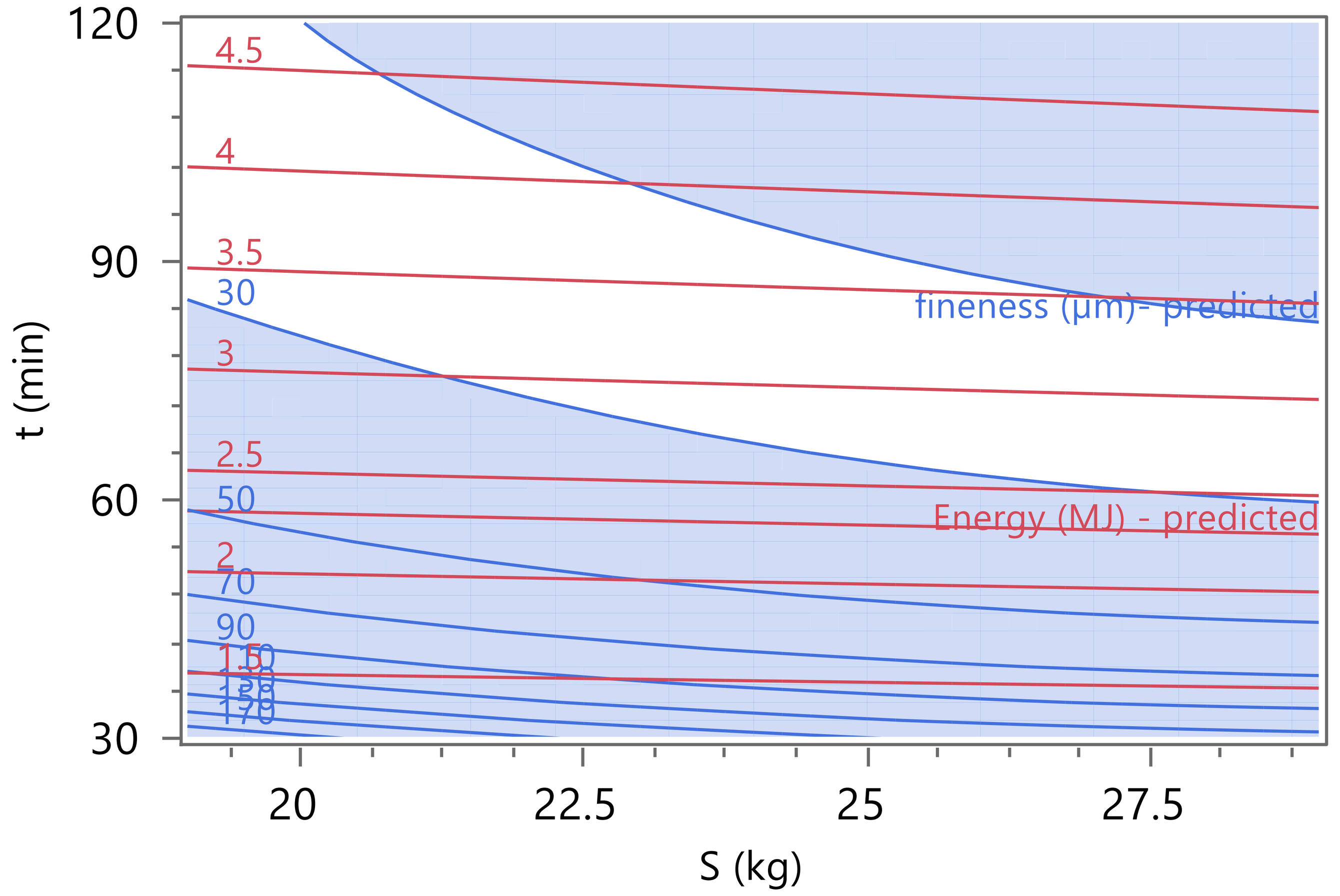
Functional principal component analysis

FPC	Eigenvalue	20 40 60 80	Percent
1	5.7896		78.1%
2	1.3455		18.1%
3	0.2613		3.52%

Model development



Design space identification



Conclusions

- Functional data analysis applied to functional designed experiments appears to be a straightforward, robust and easy to use approach to build the dynamical design space of a batch process.

References & Acknowledgements

- Fidaleo, M. (2020) Functional data analysis and design of experiments as efficient tools to determine the dynamical design space of food and biotechnological batch processes. Food and Bioprocess Technology, 13, 1035–1047.
- Fidaleo, M., Mainardi, S., Nardi, R. (2017) Modeling the refining process of an anhydrous hazelnut and cocoa paste in stirred ball mills. Food and Bioproducts Processing 105, 147-156.

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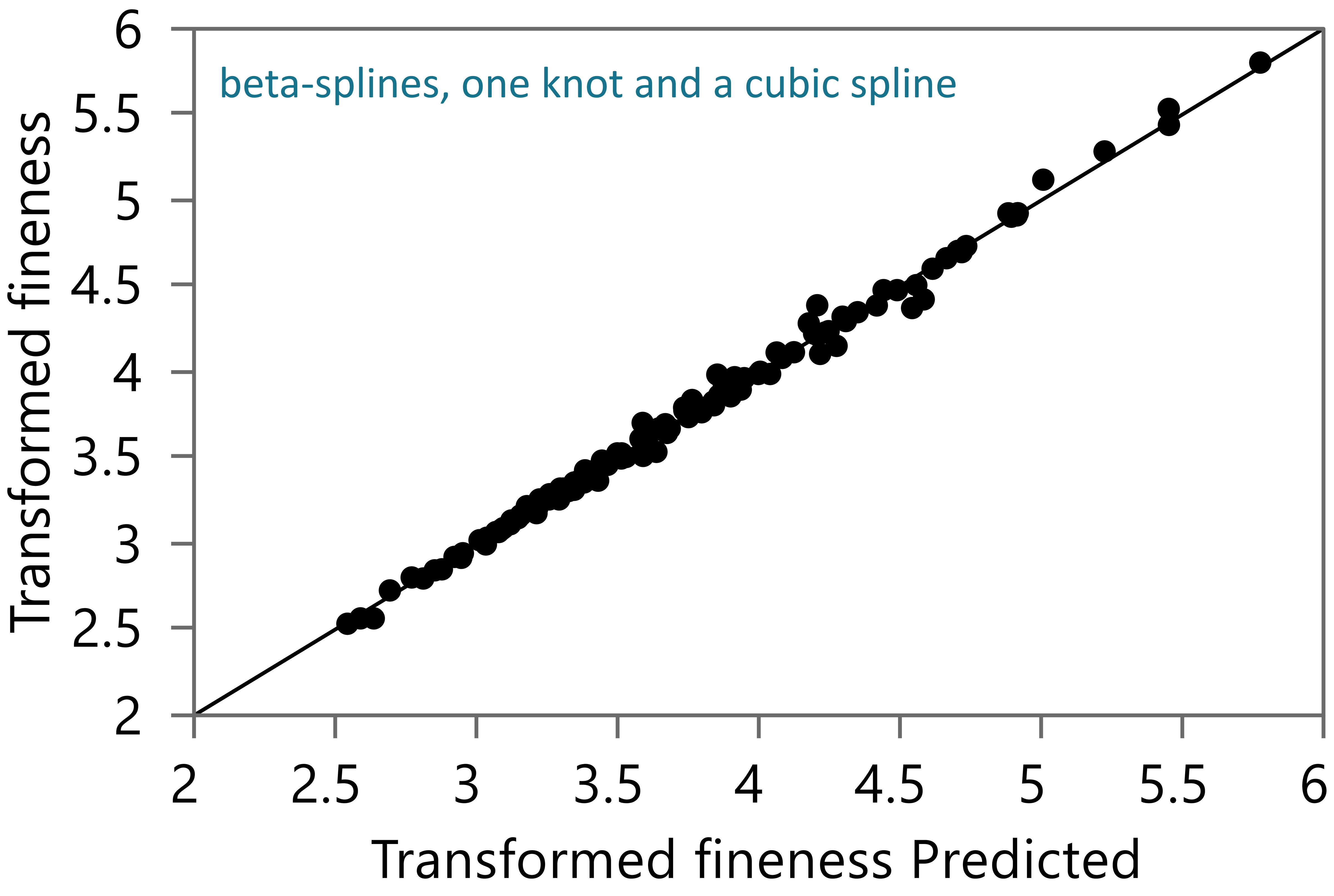
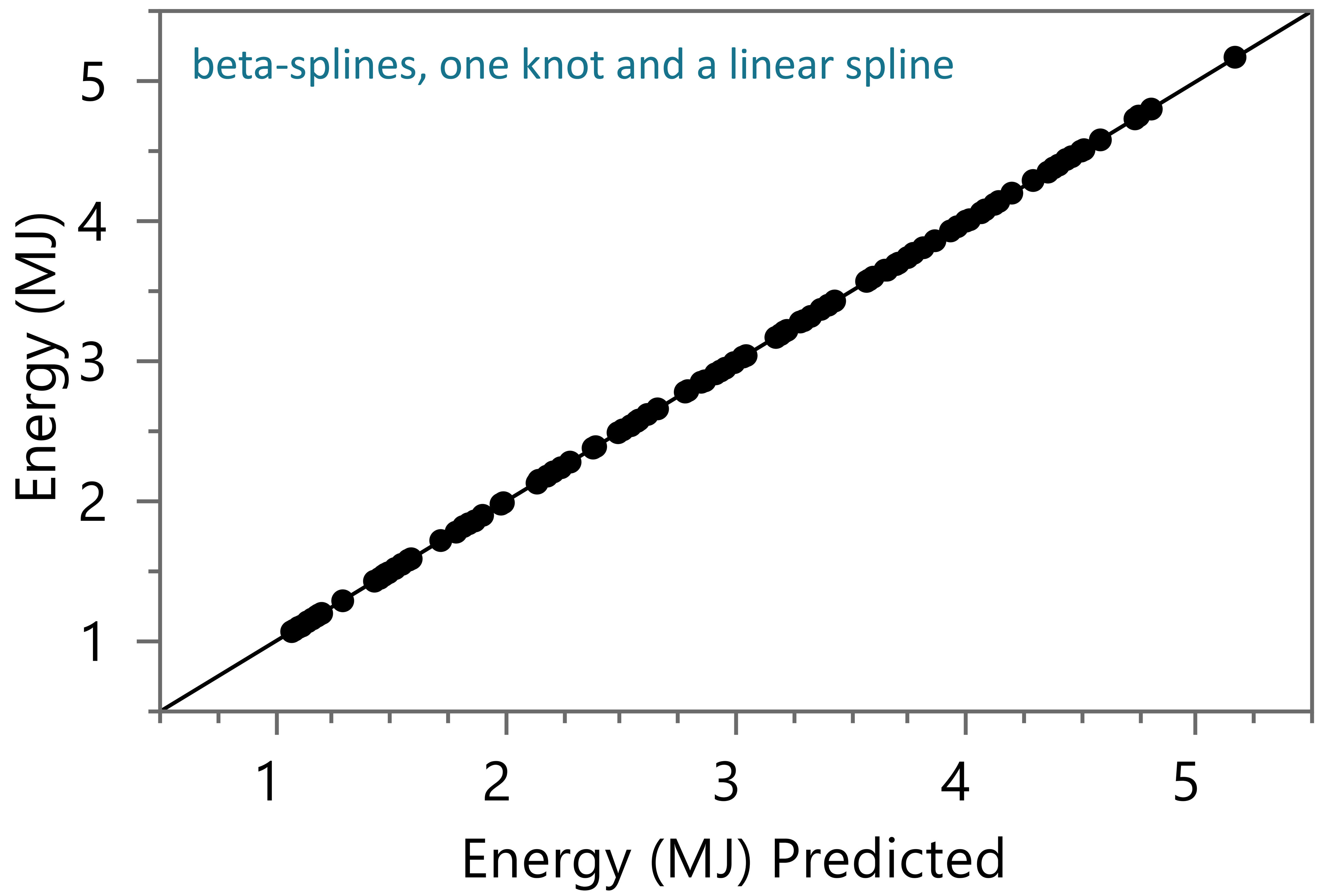
Functional data analysis (FDA)

1. DATA SMOOTHING THROUGH FDA

$$y_i(t) = \sum_{k=1}^{K} \alpha_{k,i}\, \gamma_k(t)$$

- i refers to the experimental batch run
- $\alpha_{k,i}$ are the linear combination coefficients that change from one batch to the other
- $\gamma_k(t)$ are the basis functions.





Functional principal component analysis (FPCA)

2. PARTITION INTO SCORES AND EIGENFUNCTIONS THROUGH FPCA

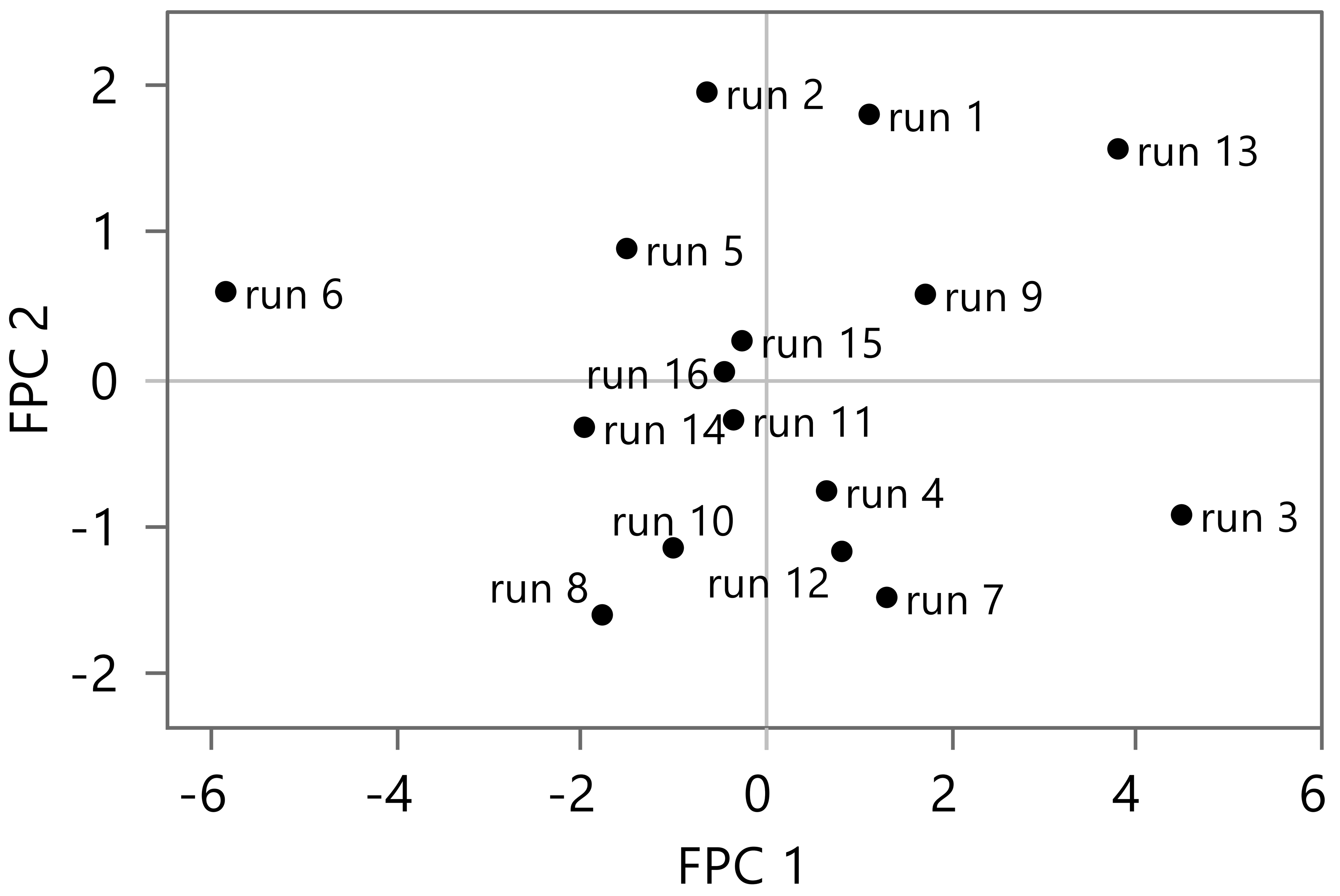
$$y_i(t) = \mu(t) + \sum_m FPC_{m,i}\, f_m(t)$$

- i refers to the experimental batch run
- μ(t) is the overall mean of the functional responses
- m is the component number
- $FPC_{m,i}$ and $f_m(t)$ are the m-th FPC score and the m-th eigenfunction

Fineness data

FPC	Eigenvalue	20 40 60 80	Percent	Cumulative
1	5.7896		78.1%	78.1%
2	1.3455		18.1%	96.2%
3	0.2613		3.52%	99.8%

Fineness data



3. MODELING SCORES AS A FUNCTION OF FACTORS

$$FPC = \beta_0 + \sum_{j=1}^{p} \beta_j x_j + \sum_{j=1}^{p} \beta_{jj} x_j^2 + \sum_{j=1}^{p} \sum_{k=1}^{p} \beta_{jk} x_j x_k$$

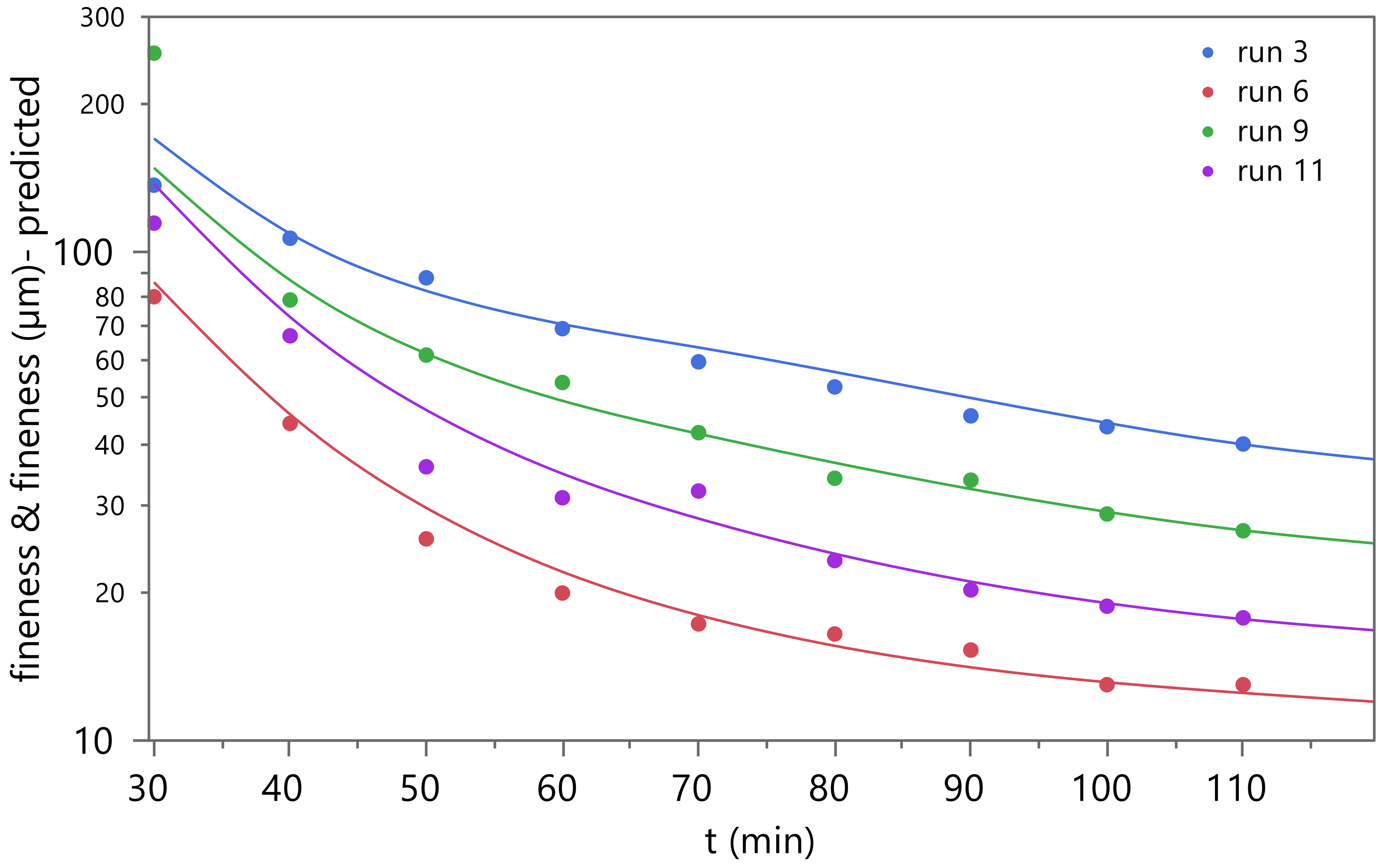
- j refers to the experimental factor
- x_j are the experimental factors
- β_{jk} are the response surface polynomial coefficients
- $\gamma_k(t)$ are the basis functions.

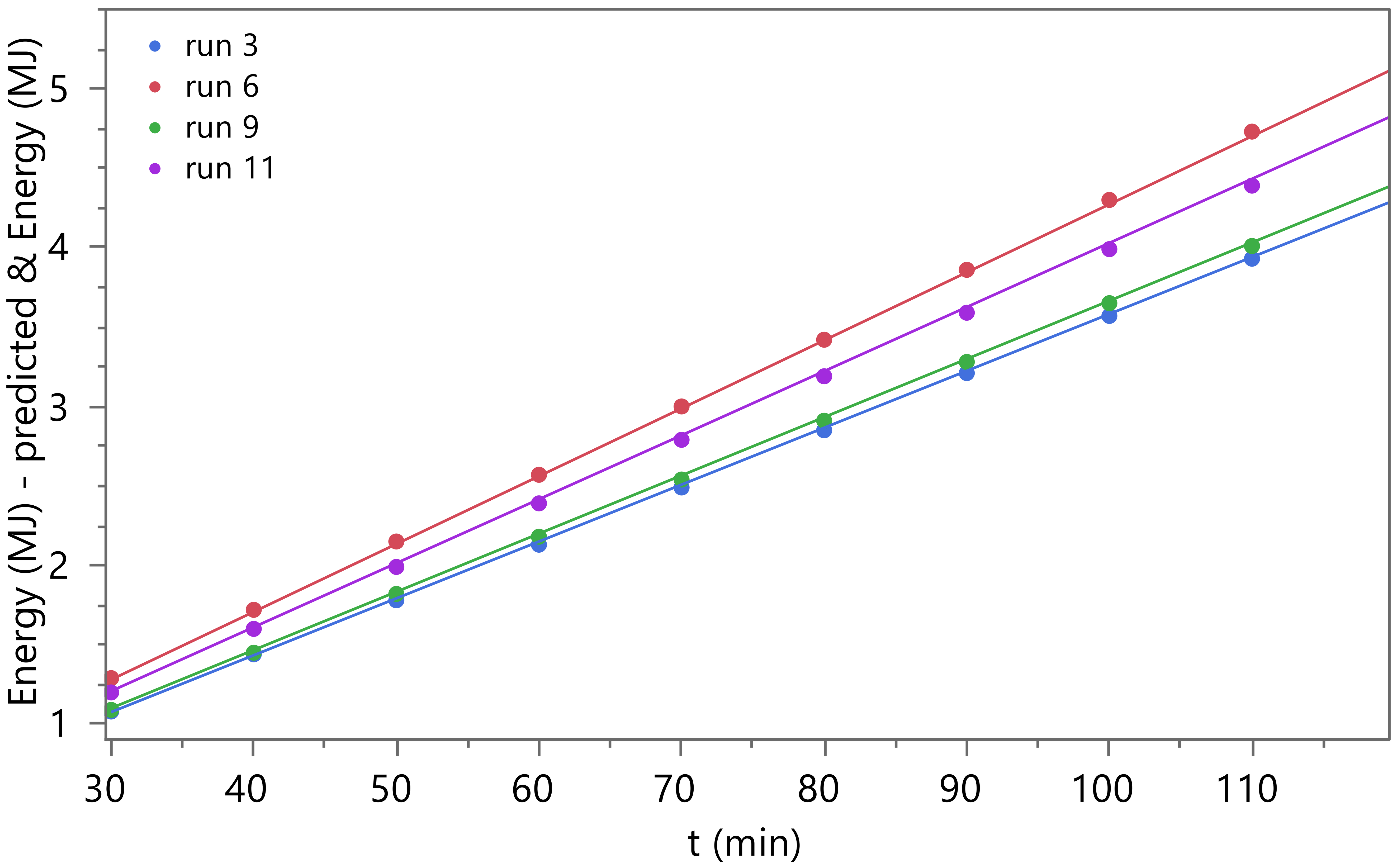
Model development

4. BUILDING FINAL MODEL

$$y_i(t) = \mu(t) + \sum_m FPC_{m,i}\, f_m(t)$$

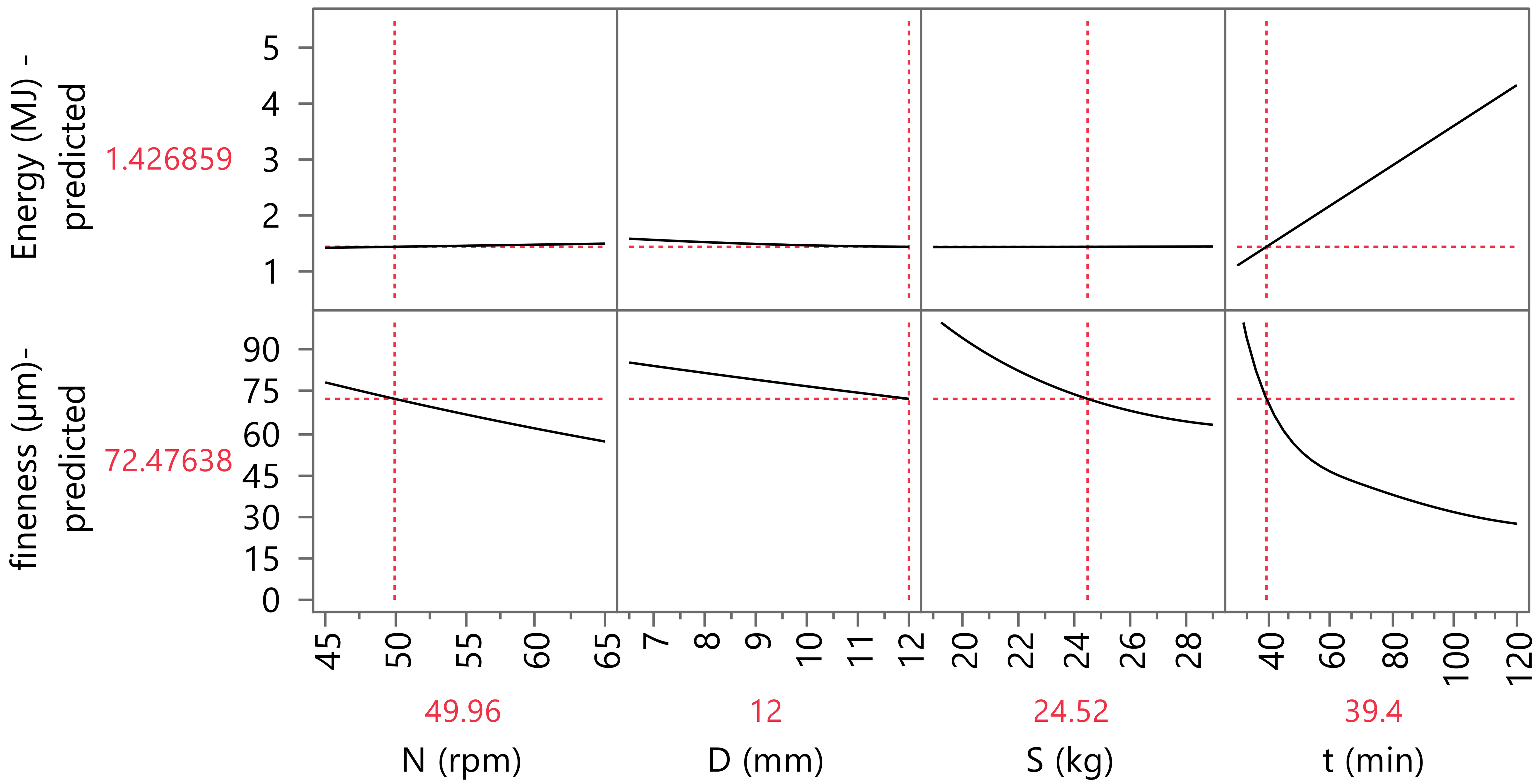
- i refers to the batch run
- μ(t) is the overall mean of the functional responses
- m is the component number
- $FPC_{m,i}$ and $f_m(t)$ are the m-th FPC score and the m-th eigenfunction

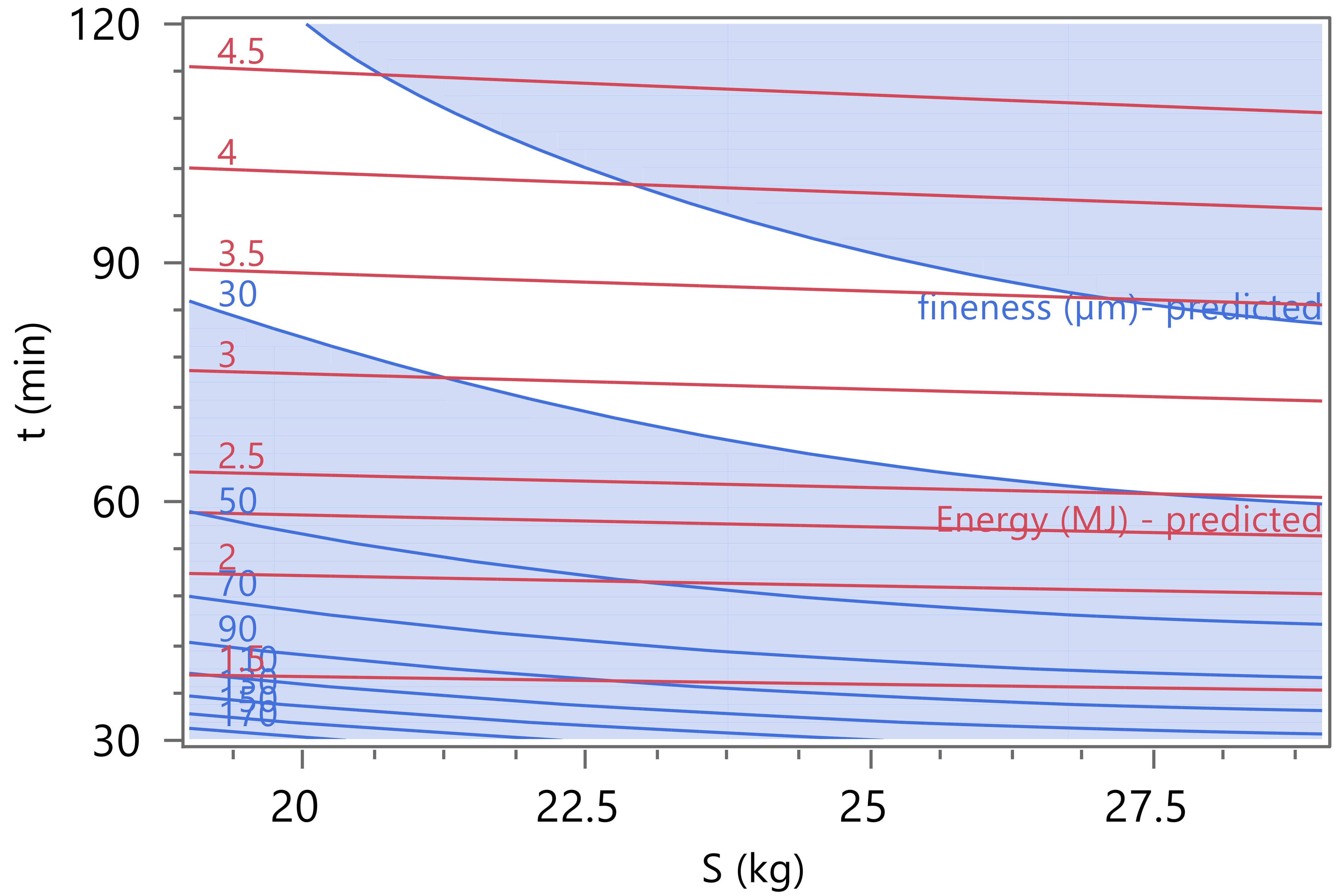




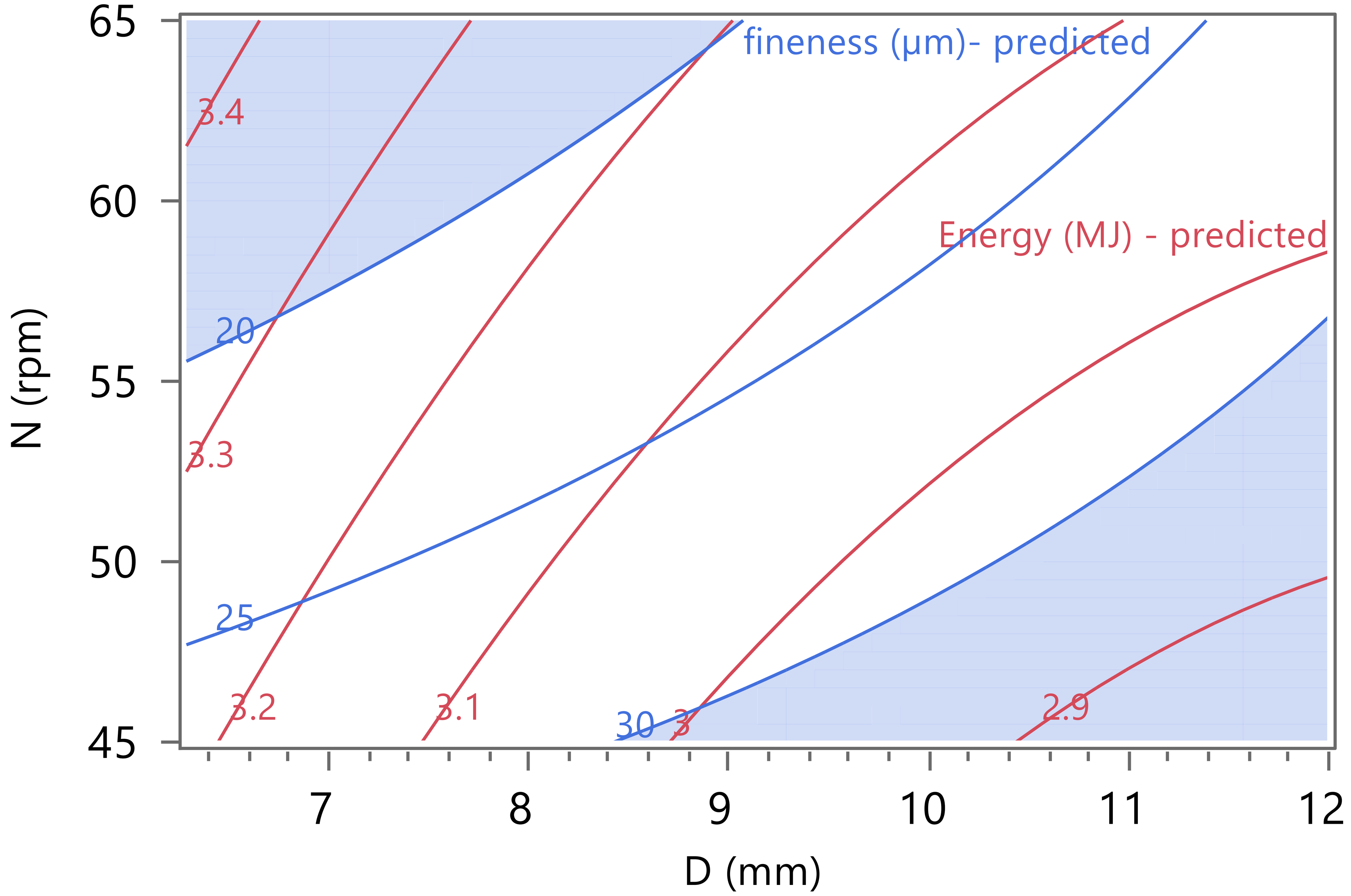
Design space identification

5. USE FINAL MODEL TO DEVELOP DESIGN SPACE





N = 55 rpm
D = 6.5 mm



S = 29 kg
t = 80 min