Value Chain Optimization for Metal Recycling Processes Through Causal Modeling

Software Competence Center Hagenberg

Valeria Fonseca Diaz - Recy & DepoTech 2024

Industrial state of the art when optimizing recycling processes

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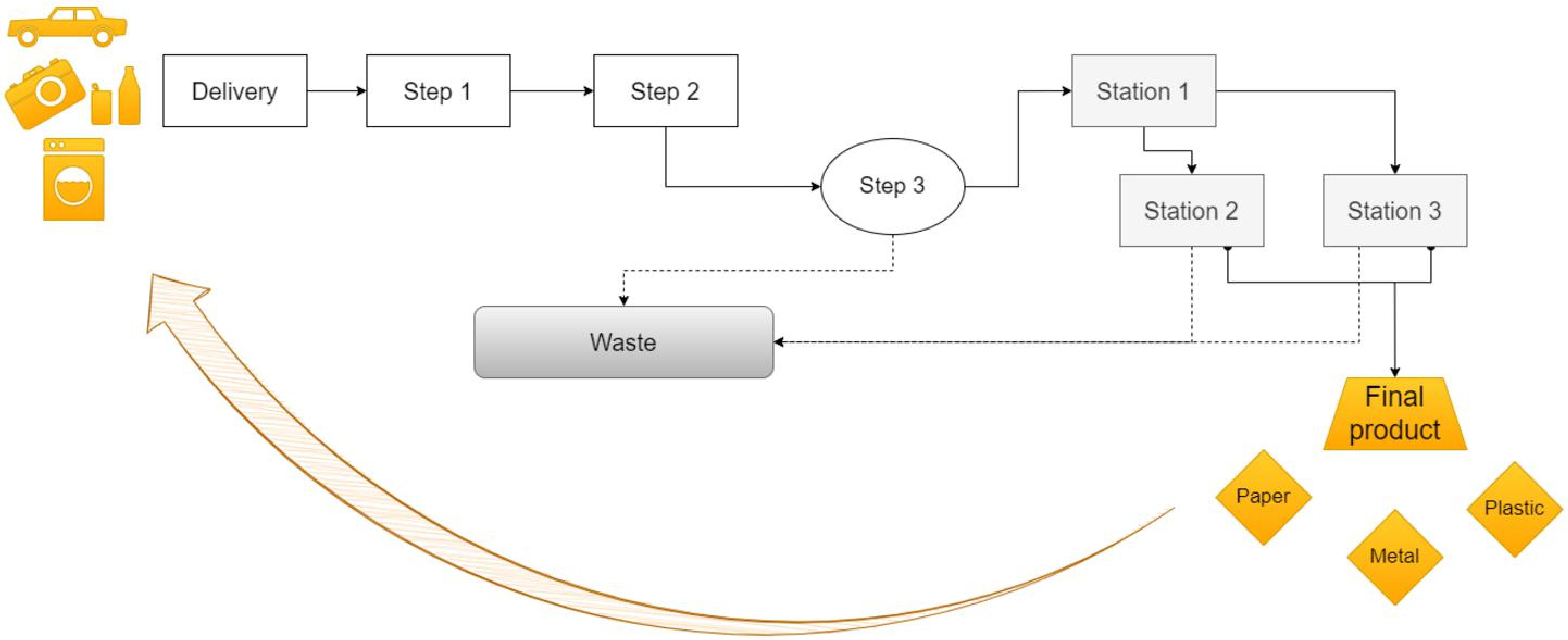
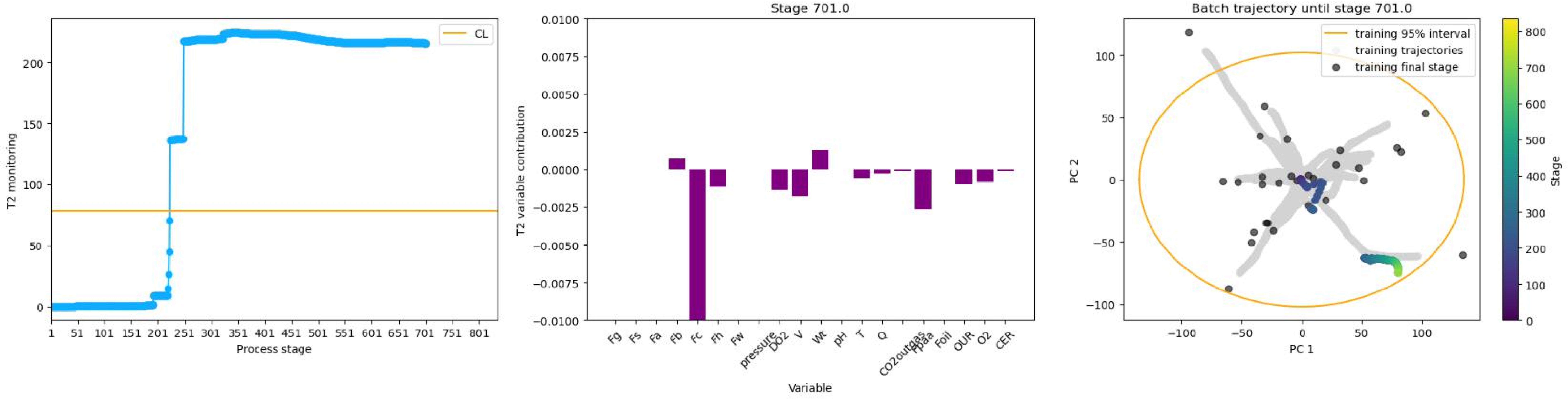
From input material to final products



How to model these processes?

- State of the art: Multivariate analysis, MSPC
- A monitoring dashboard: Progress of one specific batch



J.M. Prats-Montalbán, A. de Juan, A. Ferrer, Multivariate image analysis: A review with applications, Chemometr Intell Lab Syst, 2011,https://doi.org/10.1016/j.chemolab.2011.03.002

Stepping forward

For industrial processes that are still not digitalized:

- Account for the conditional dependencies through the entire process
- Quantify the standard error of predictions
- Equip industrial solutions with explainability/interpretability for root cause analysis

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Our work

We are redefining the framework of process modeling for *the digital era*, so that:

- On a theoretical level:
  - The modeling framework is easily adjustable for complex and deep model architectures
  - We quantify also the uncertainty of a prediction
  - All the conditional dependencies through the real process are adequately considered in the model
  - We set a new basis for explainable artificial intelligence (XAI)
- On a practical level:
  - Obtain accurate predictions of the process performance
  - Find accurate and precise root causes when monitoring and analyzing the process behavior

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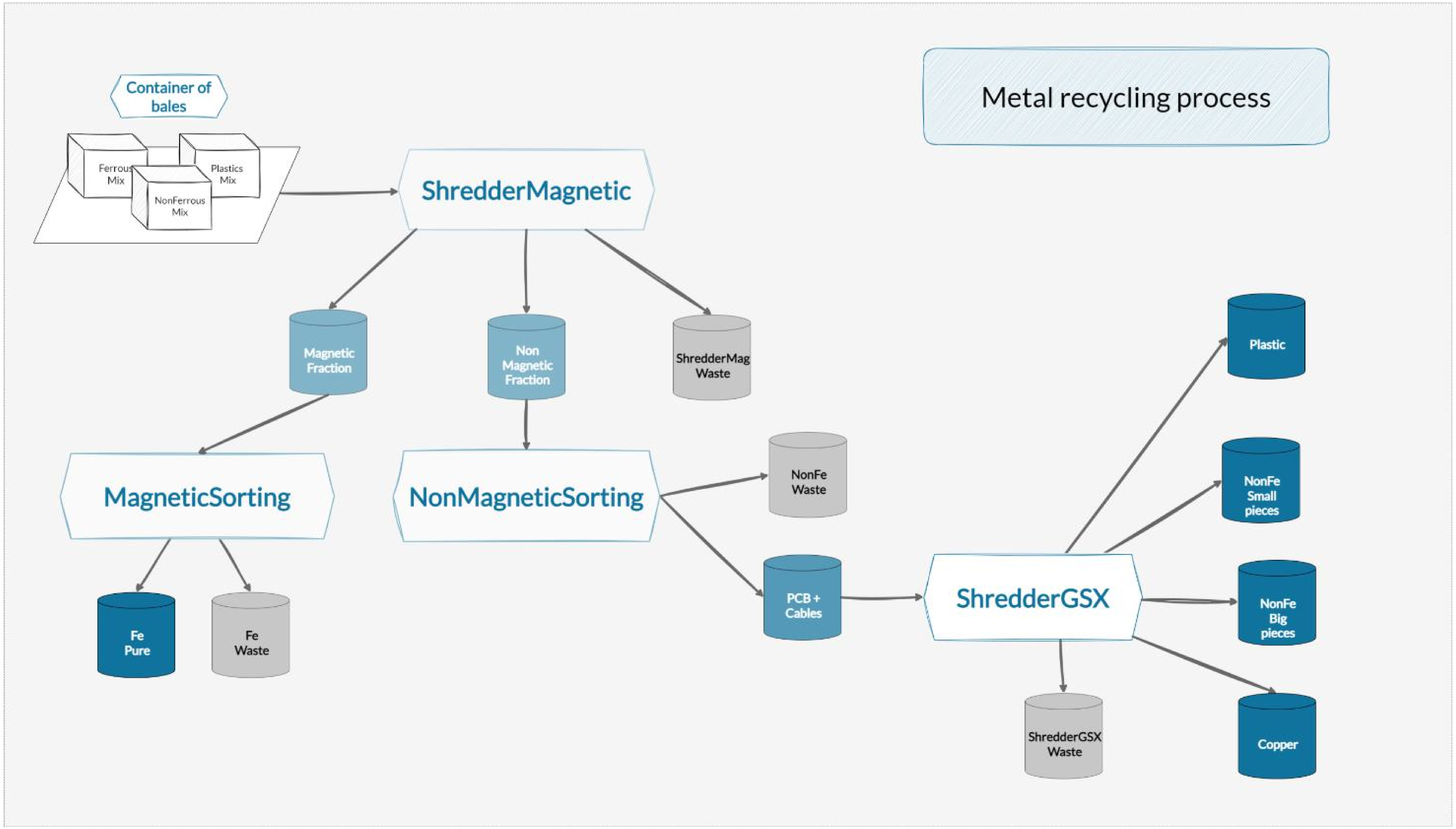
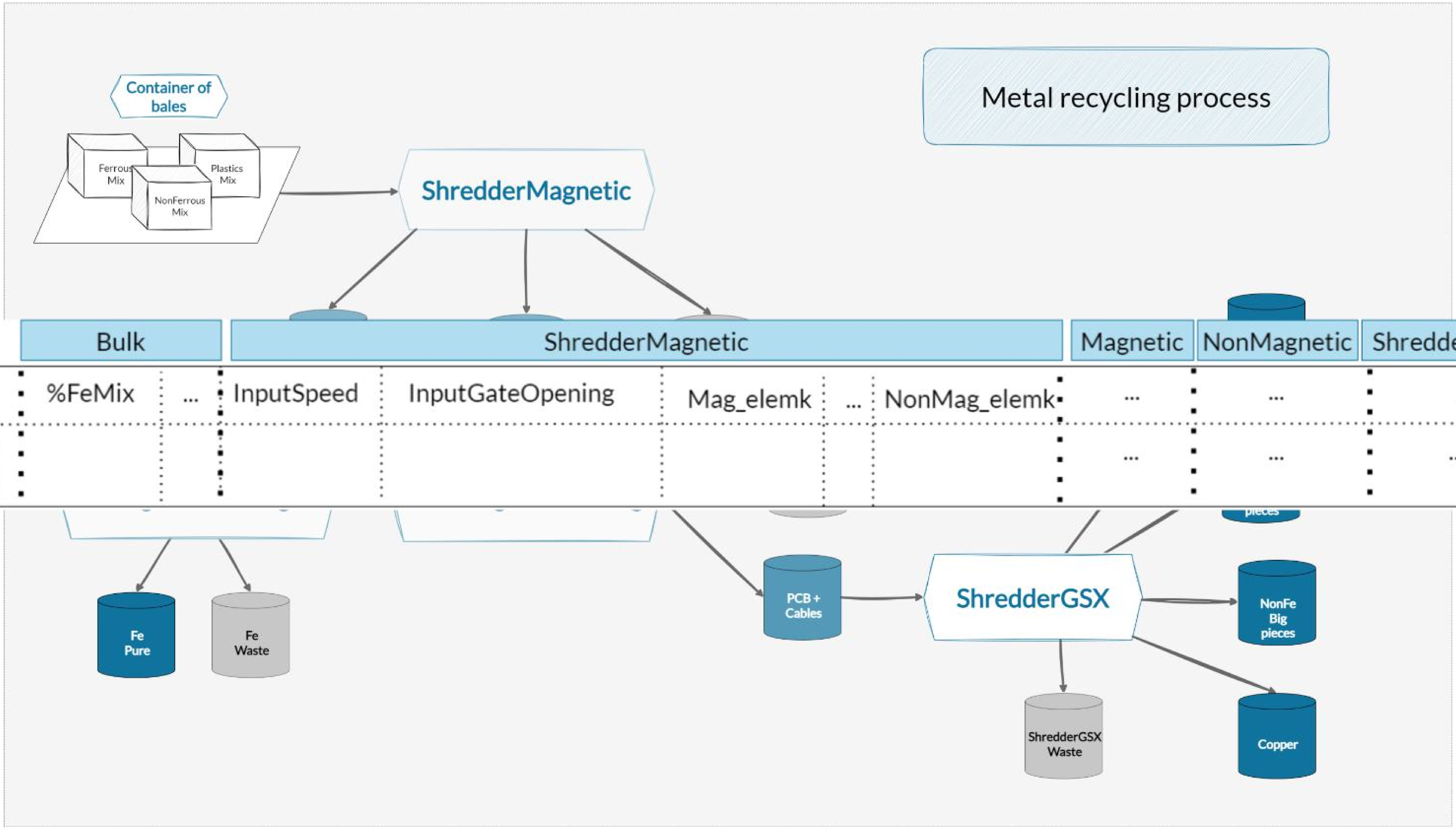
Model process between input and final output in one step

Our case study

Our case study



Our case study



Bulk			ShredderMagnetic					Magnetic	NonMagnetic	ShredderGSX
Bulk ID	%FeMix	...	InputSpeed	InputGateOpening	Mag_elemk	...	NonMag_elemk	...	...	...
0001								...	...	...
0002										

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Process conceptualization in one stage

Marco Johannes Maier, Dirichlet Regression Models: Theory, Implementation and Applications, Doctoral thesis, Alpen-Adria-Universität Klagenfurt Fakultät für Kulturwissenschaften, June 2020.

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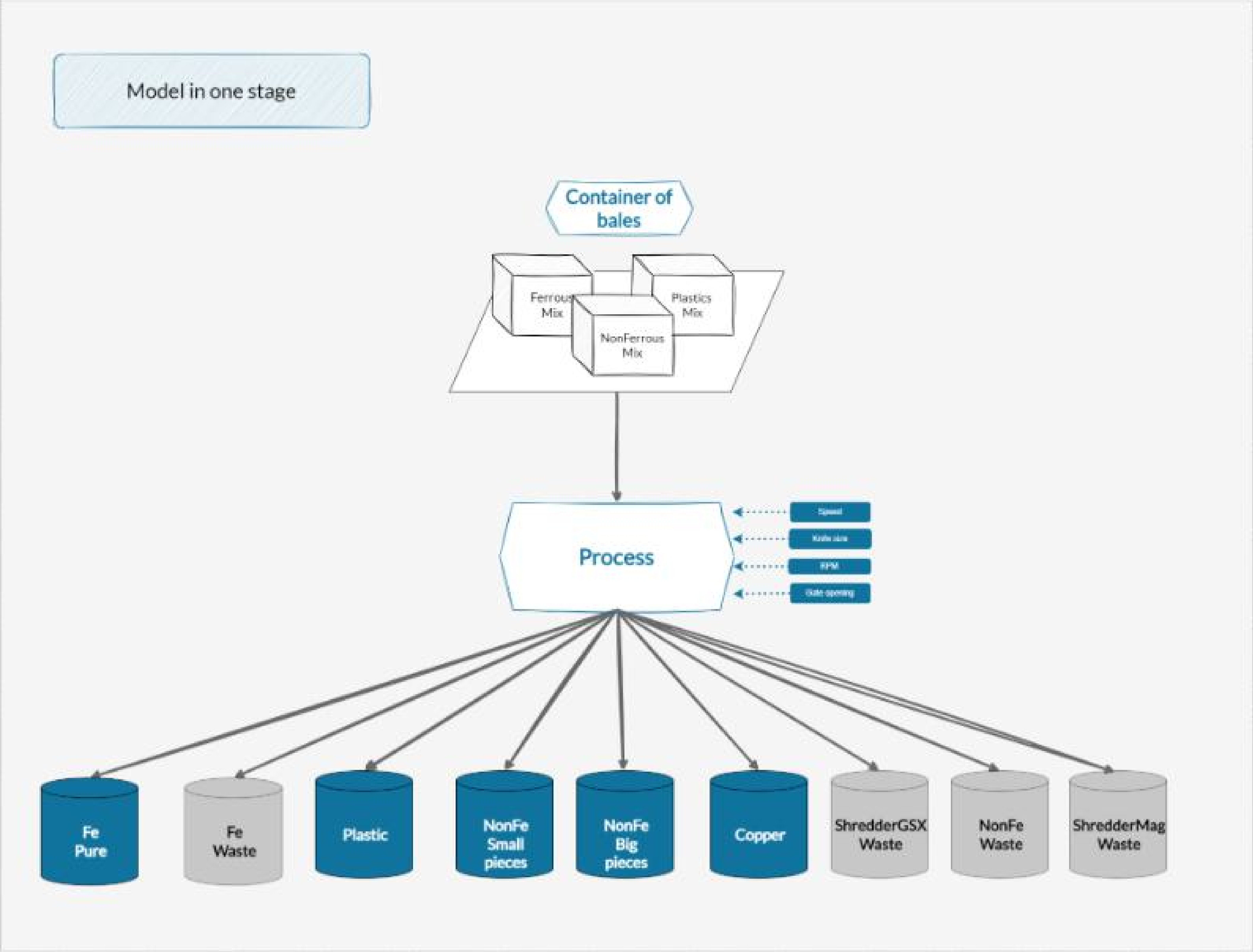
Process conceptualization in one stage



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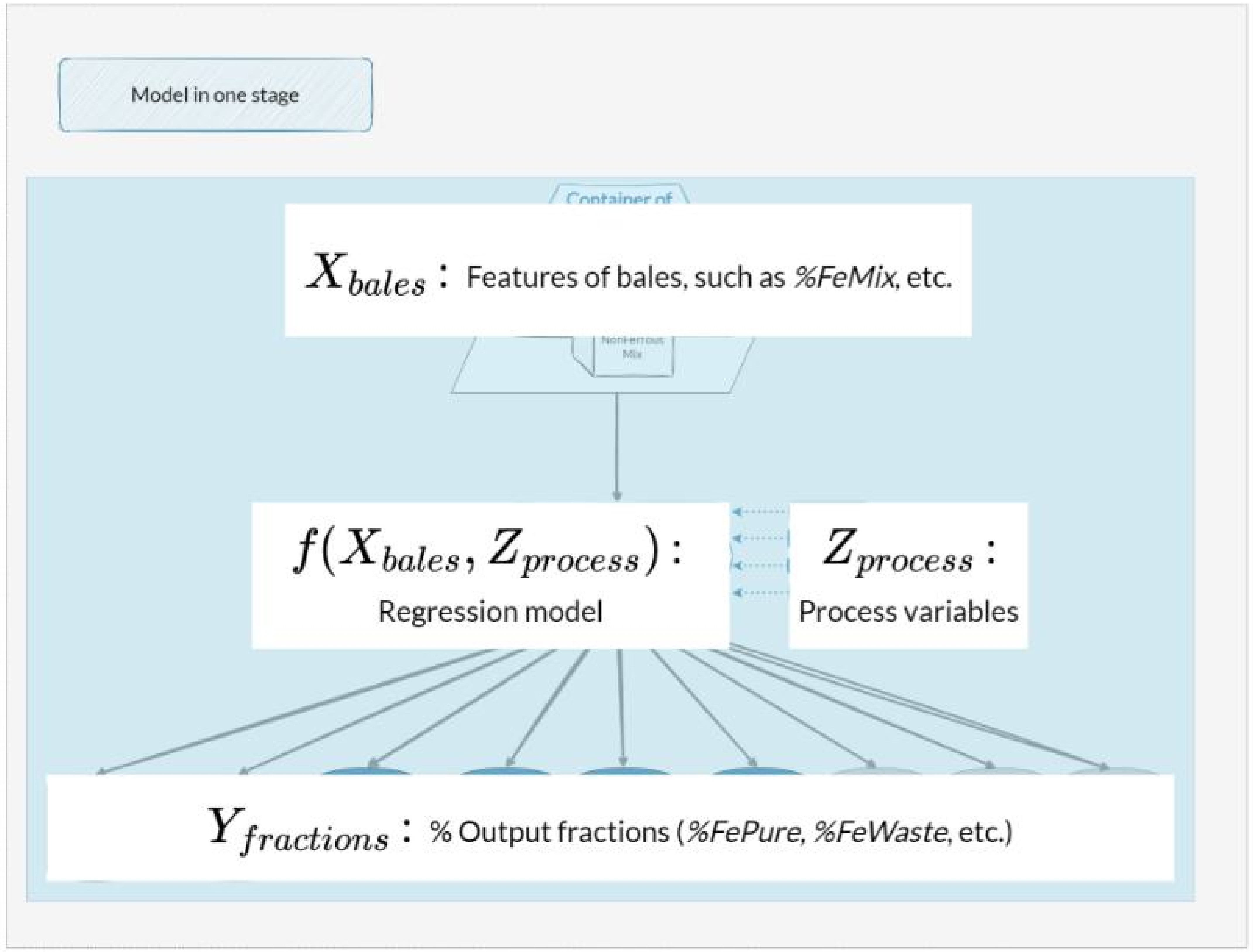

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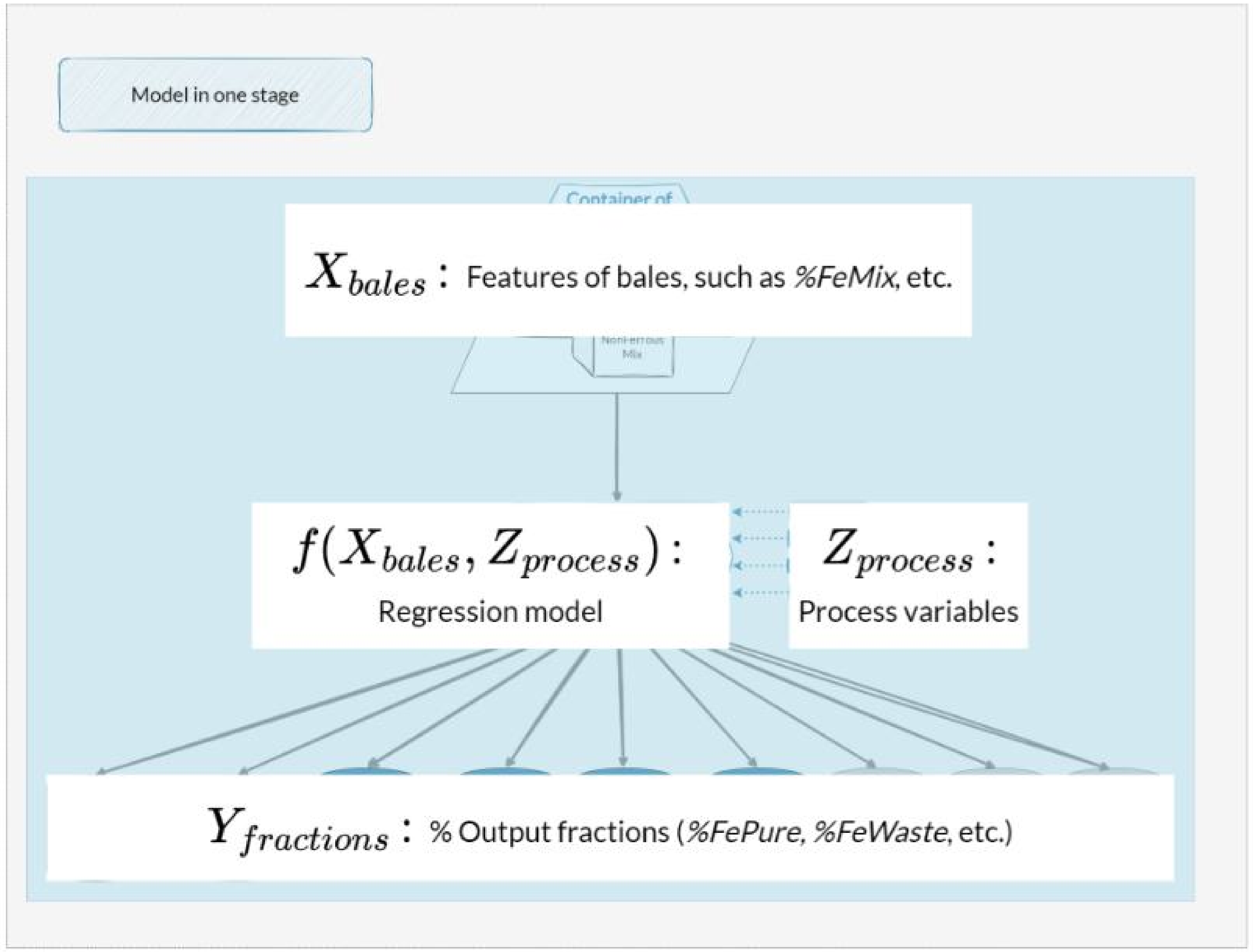

Let's define a Bayesian model

- Priors: $\beta_X, \beta_Z \sim Normal(0, \Sigma)$
- Regression model:
  $Y \sim Dirichlet(X\beta_X + Z\beta_Z)$

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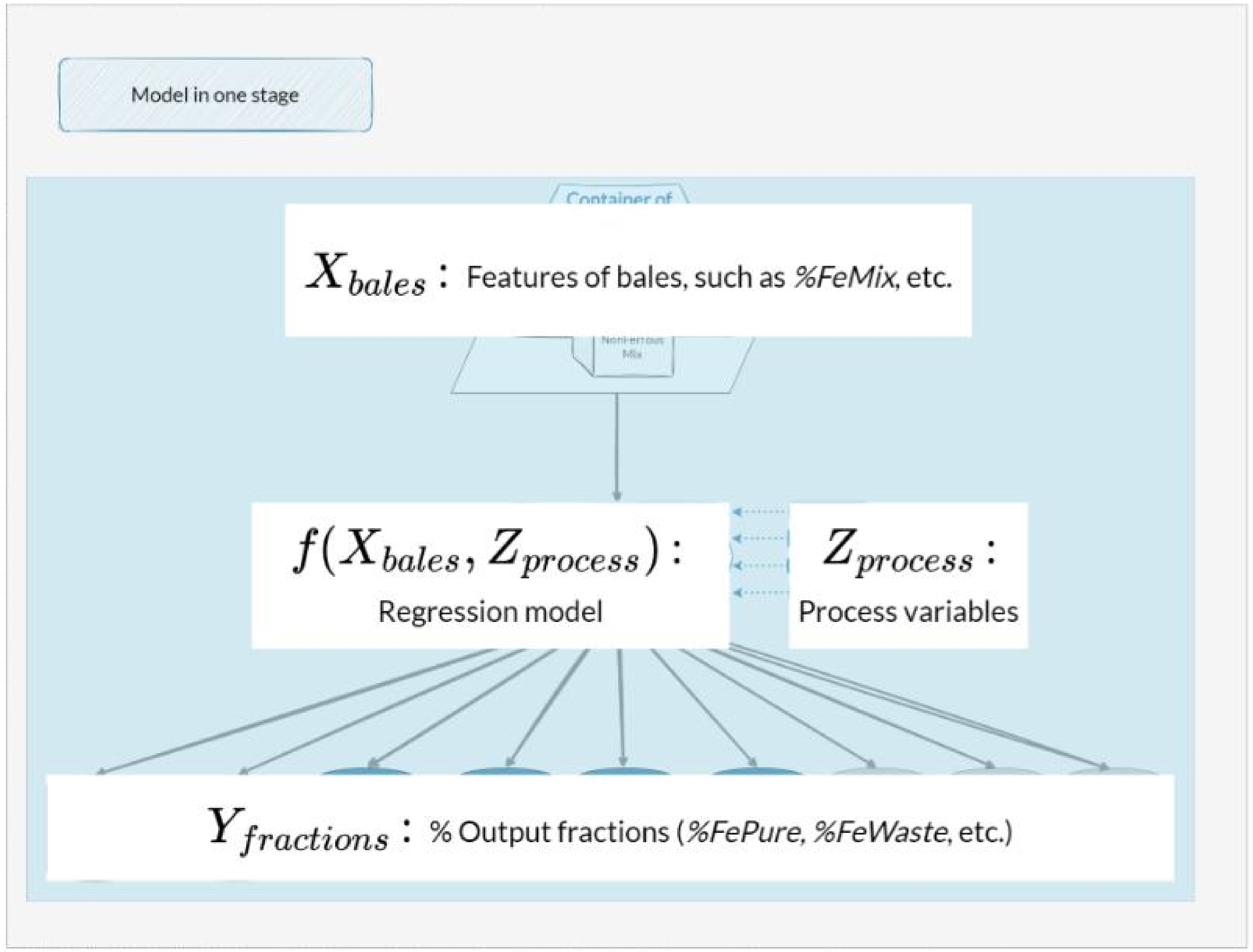

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With a probabilistic programming approach, we obtain posterior and posterior predictive distributions

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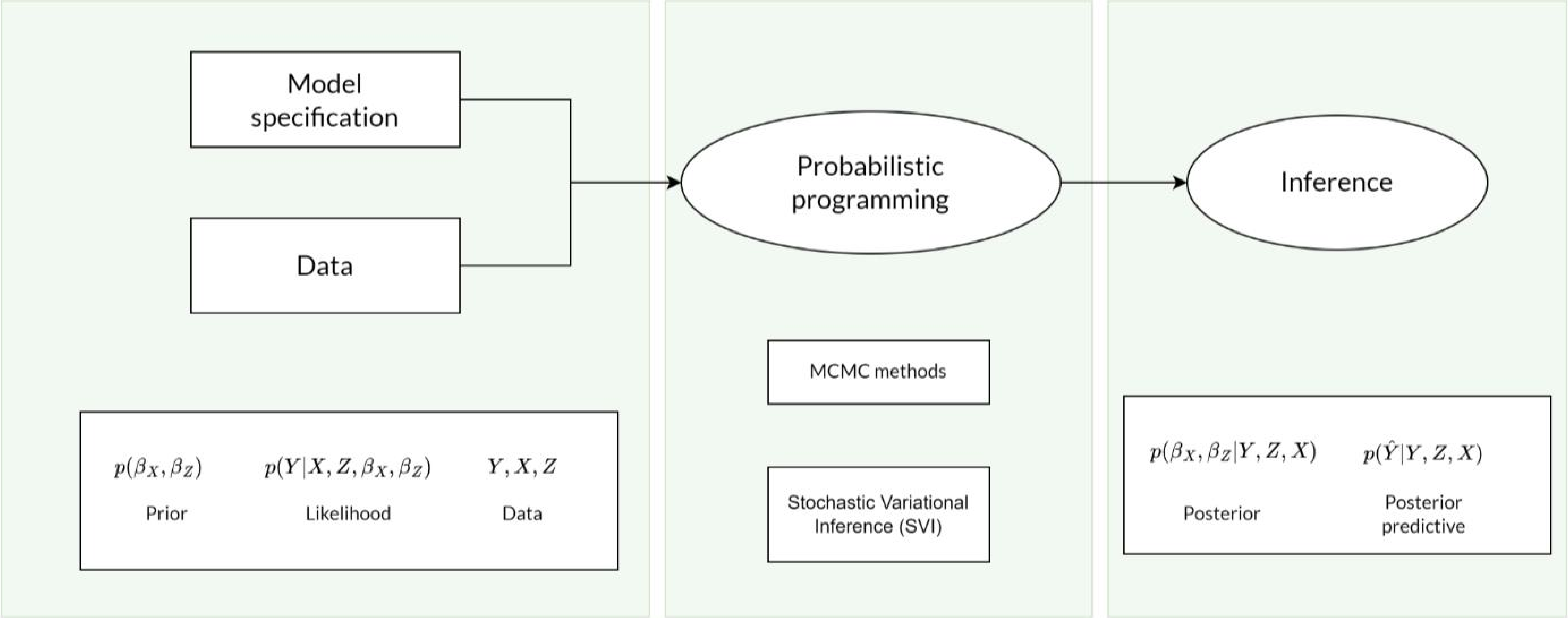
Probabilistic programming approach



M. Hoffman, D. M. Blei, C. Wang, J. Paisley, Stochastic Variational Inference, arXiv, 2013, https://arxiv.org/abs/1206.7051

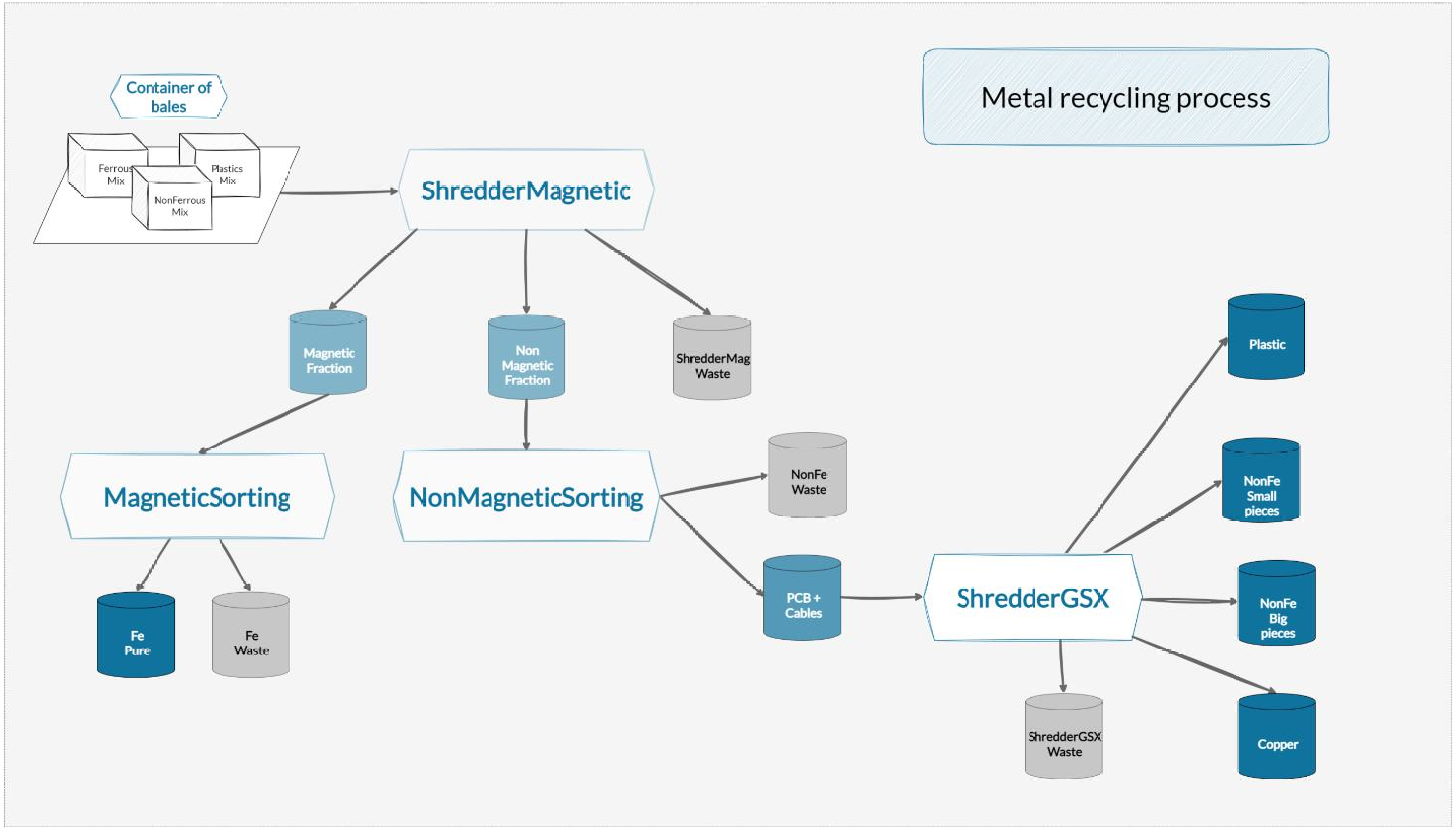
D. Wingate, T. Weber, Automated Variational Inference in Probabilistic Programming, arXiv, 2013, https://arxiv.org/abs/1301.1299

Pyro Programming Language https://docs.pyro.ai/en/stable/

Exploiting the model of the entire process

Process conceptualization

Process conceptualization



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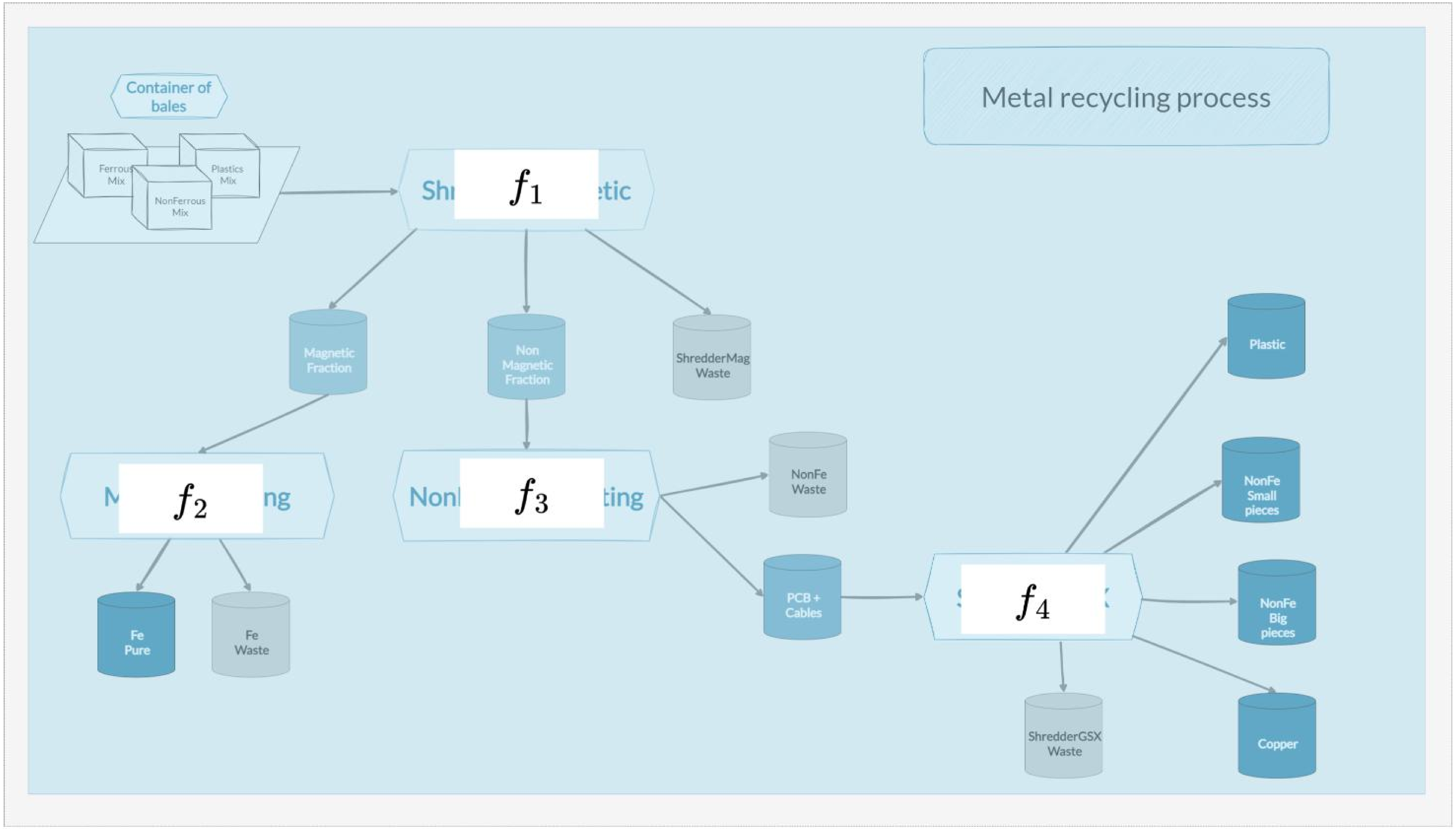

(Deeper) Bayesian structural model

Ranganath, R. and Gerrish, S. and Blei, D., Black Box Variational Inference, Proceedings of the Seventeenth International Conference on Artificial Intelligence and Statistics, 2014, http://proceedings.mlr.press/v33/ranganath14.pdf

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(Deeper) Bayesian structural model

- Priors for all parameters: $\beta_{\mathbf{g_1}}, \beta_{\mathbf{g_2}}, \beta_{\mathbf{g_3}}, \beta_{\mathbf{g_4}}$

- $f_1 : [Y_{sh-m}, Y_{sh-nm}, Y_{sh-w}] \sim Dir(\mathbf{g_1}(X, Z_{sh}))$

- $f_2 : [Y_{m-fe}, Y_{m-w}] \sim Dir(\mathbf{g_2}(Y_{sh-m}))$

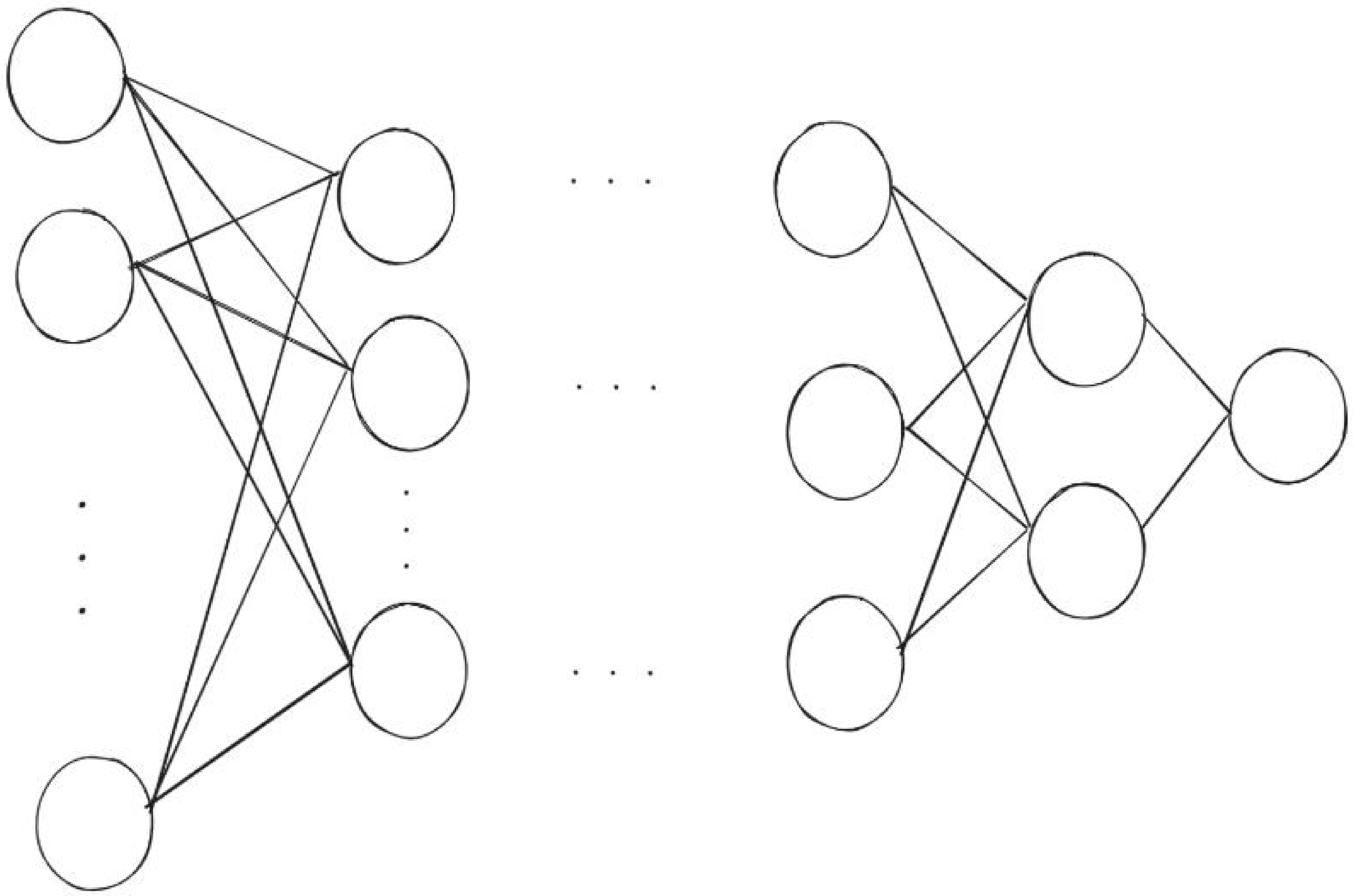
- $f_3 : [Y_{nm-pcbcab}, Y_{nm-w}] \sim Dir(\mathbf{g_3}(Y_{sh-nm}))$

- $f_4 : [Y_{gsx}, Y_{gsx-w}] \sim Dir(\mathbf{g_4}(Y_{nm-pcbcab}, Z_{gsx}))$

Ranganath, R. and Gerrish, S. and Blei, D., Black Box Variational Inference, Proceedings of the Seventeenth International Conference on Artificial Intelligence and Statistics, 2014, http://proceedings.mlr.press/v33/ranganath14.pdf

(Deeper) Bayesian structural model

$$\mathbf{g_j} : g_k(\mathbf{W}_k \cdot \mathbf{Z}_{k-1} + \mathbf{b}_k)$$
$$\mathbf{Z}_{k-1} = g_{k-1}(\mathbf{W}_{k-1} \cdot \mathbf{Z}_{k-2} + \mathbf{b}_{k-1})$$
$$\ldots$$
$$\mathbf{Z}_2 = g_1(\mathbf{W}_1 \cdot \mathbf{Z}_1 + \mathbf{b}_1)$$



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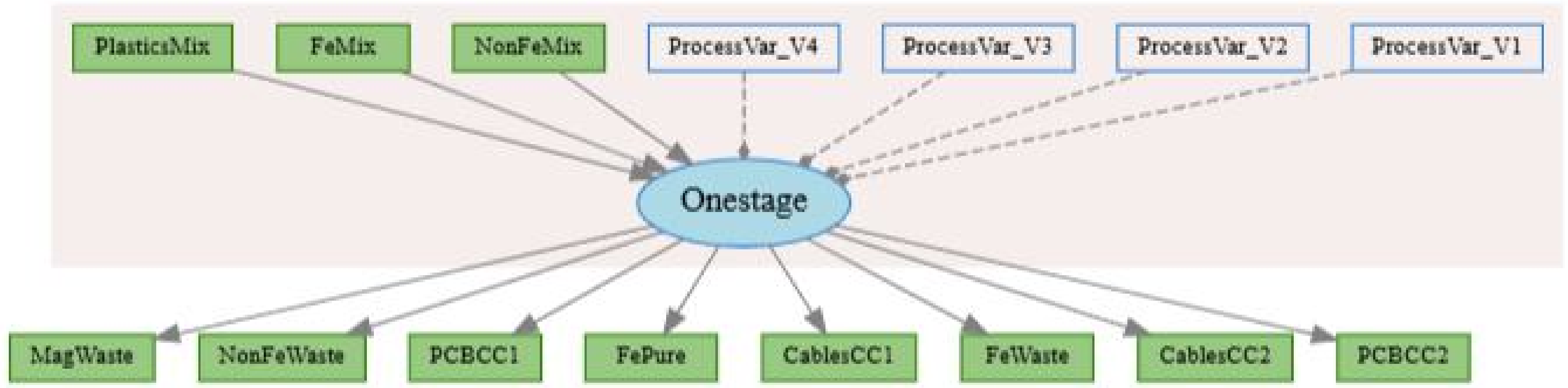
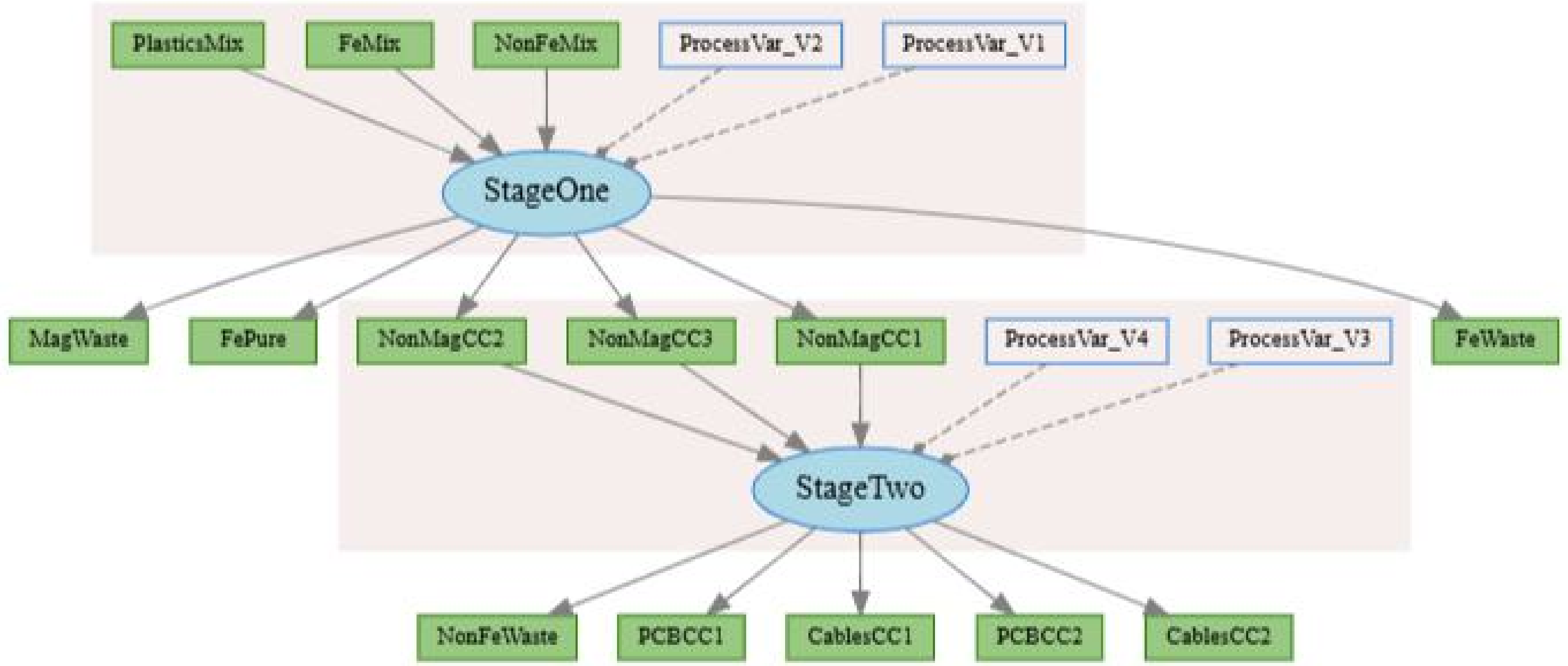
Experimental

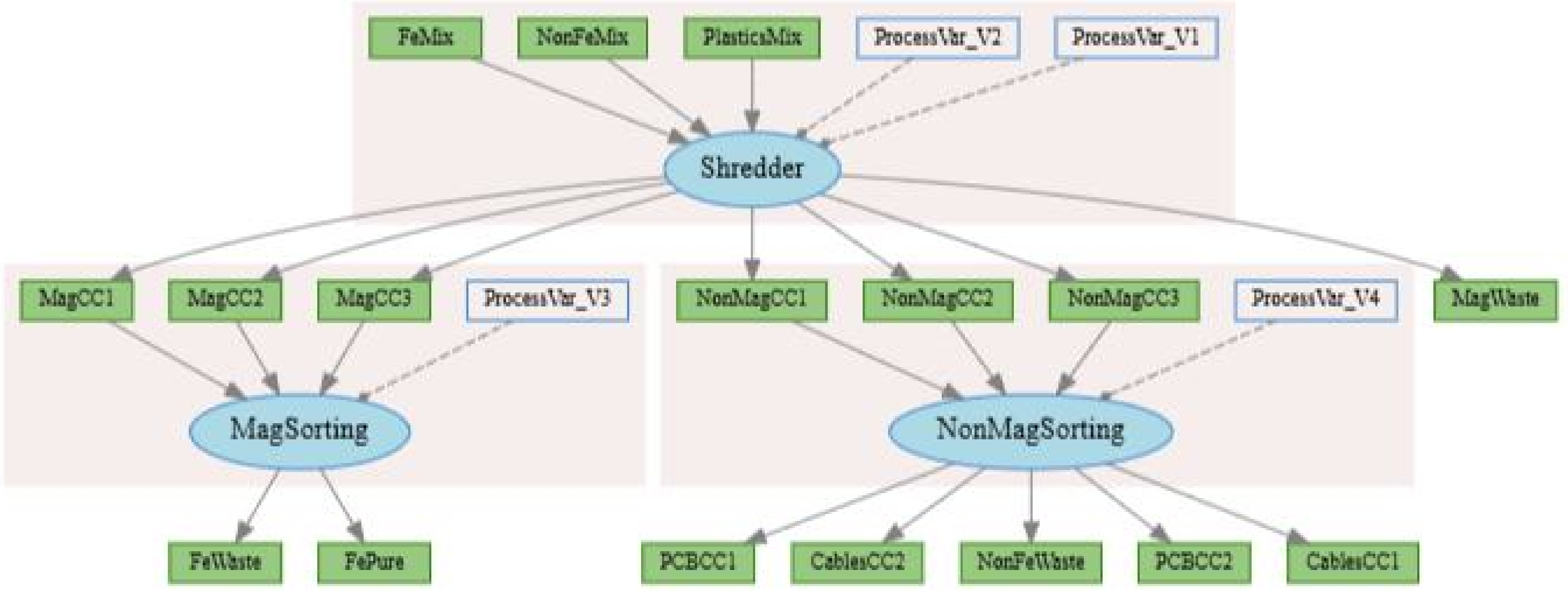
Three models



Model 1

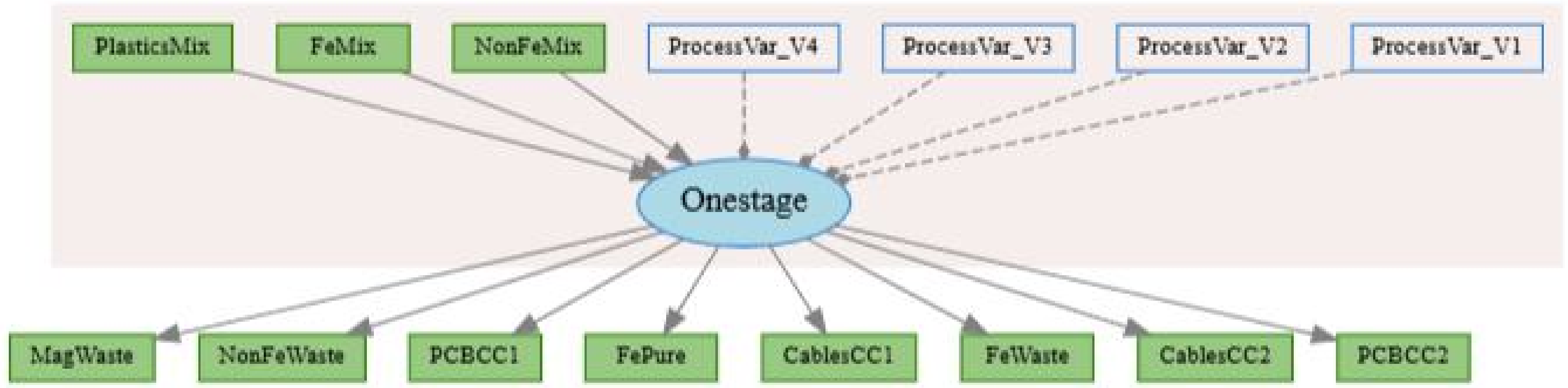


Model 2



Model 3

Three models



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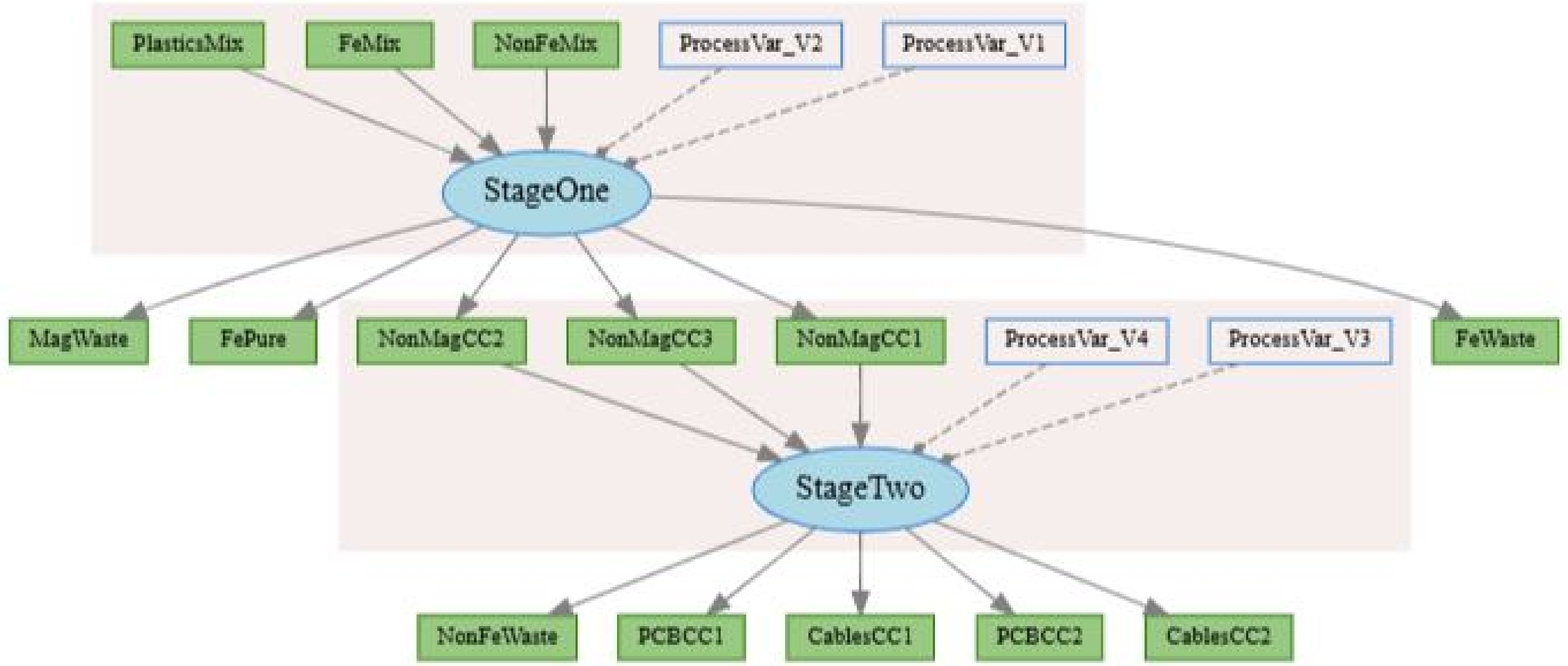
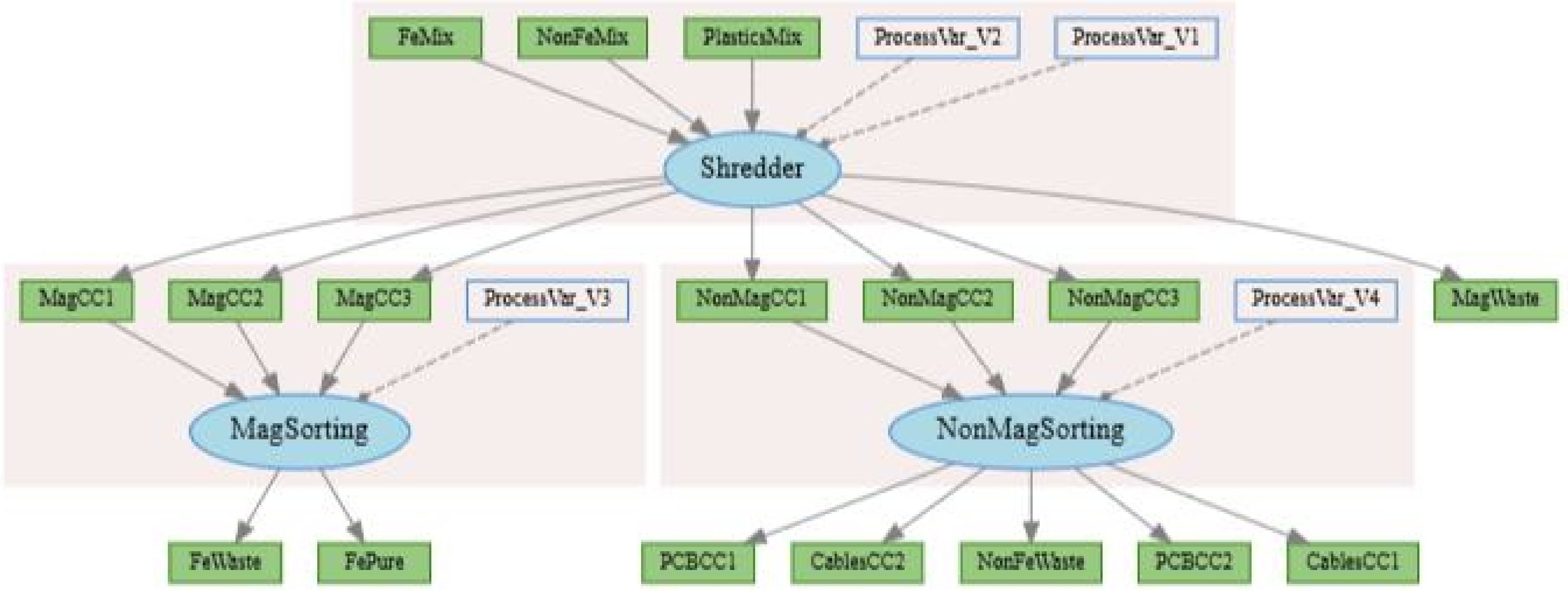


Model 2

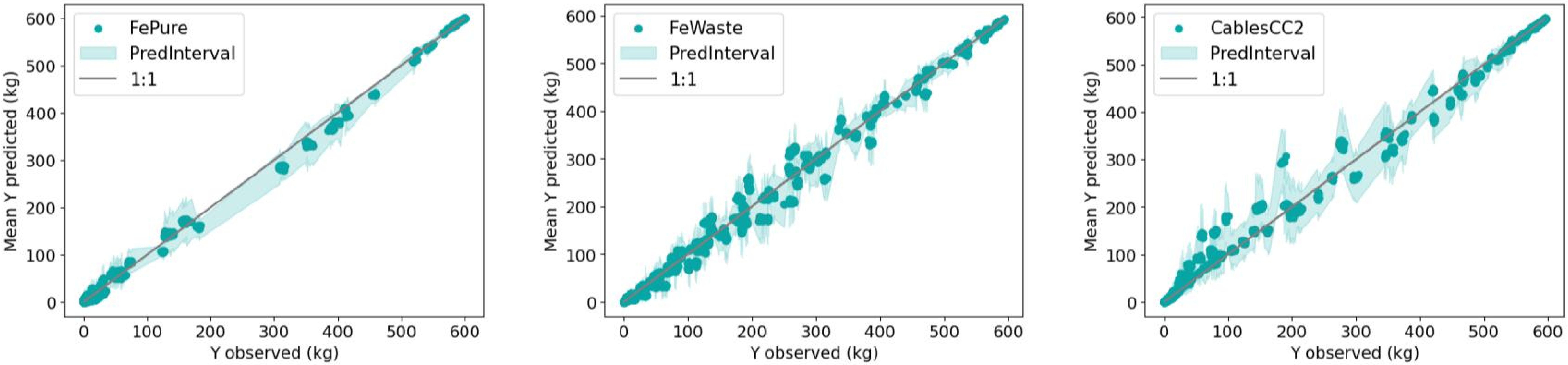


Model 3

For simplicity, we will focus on the performance of *FePure*, *FeWaste*, and *CablesCC2* which have the largest variance.

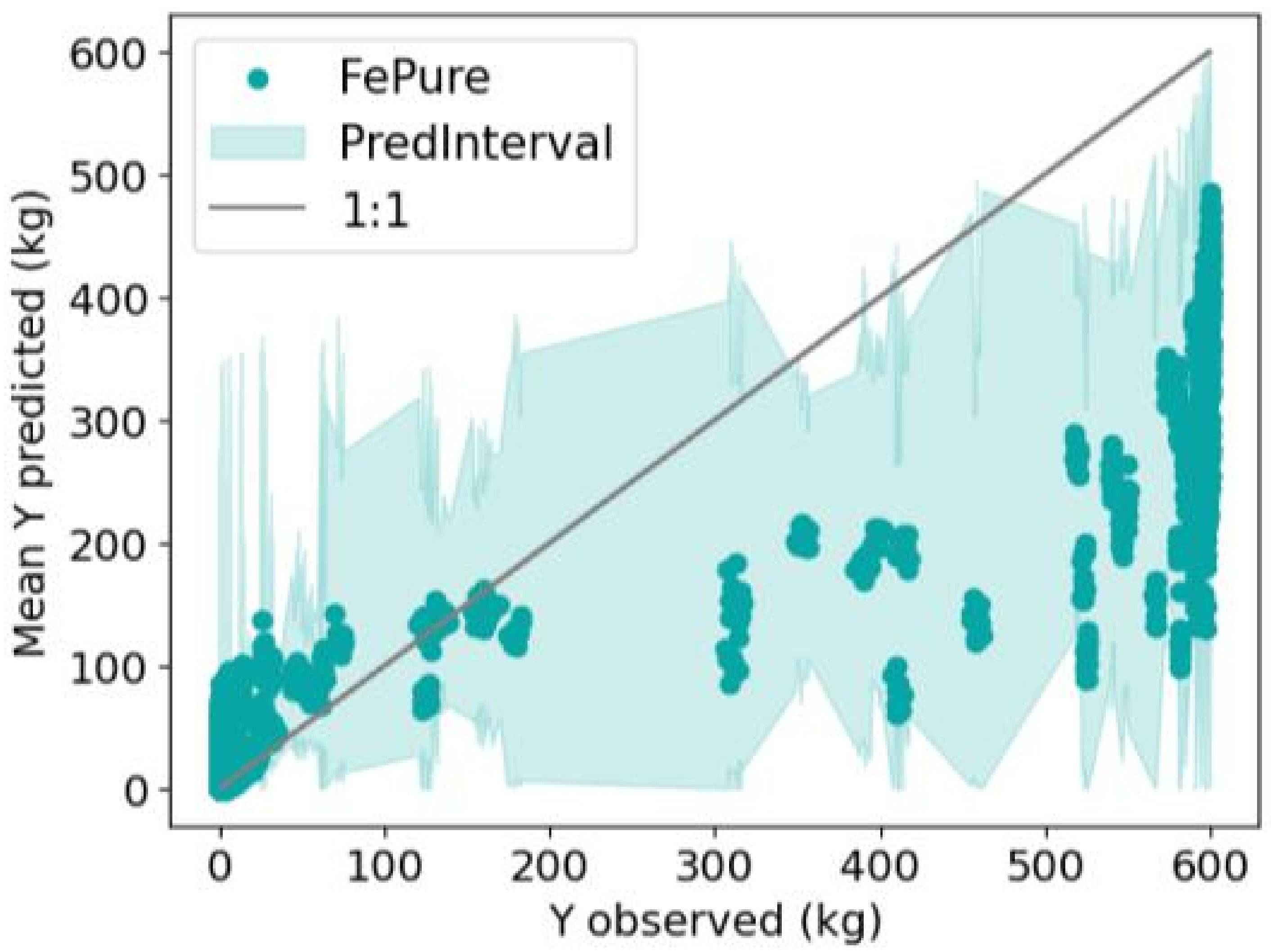
Overview of prediction performance

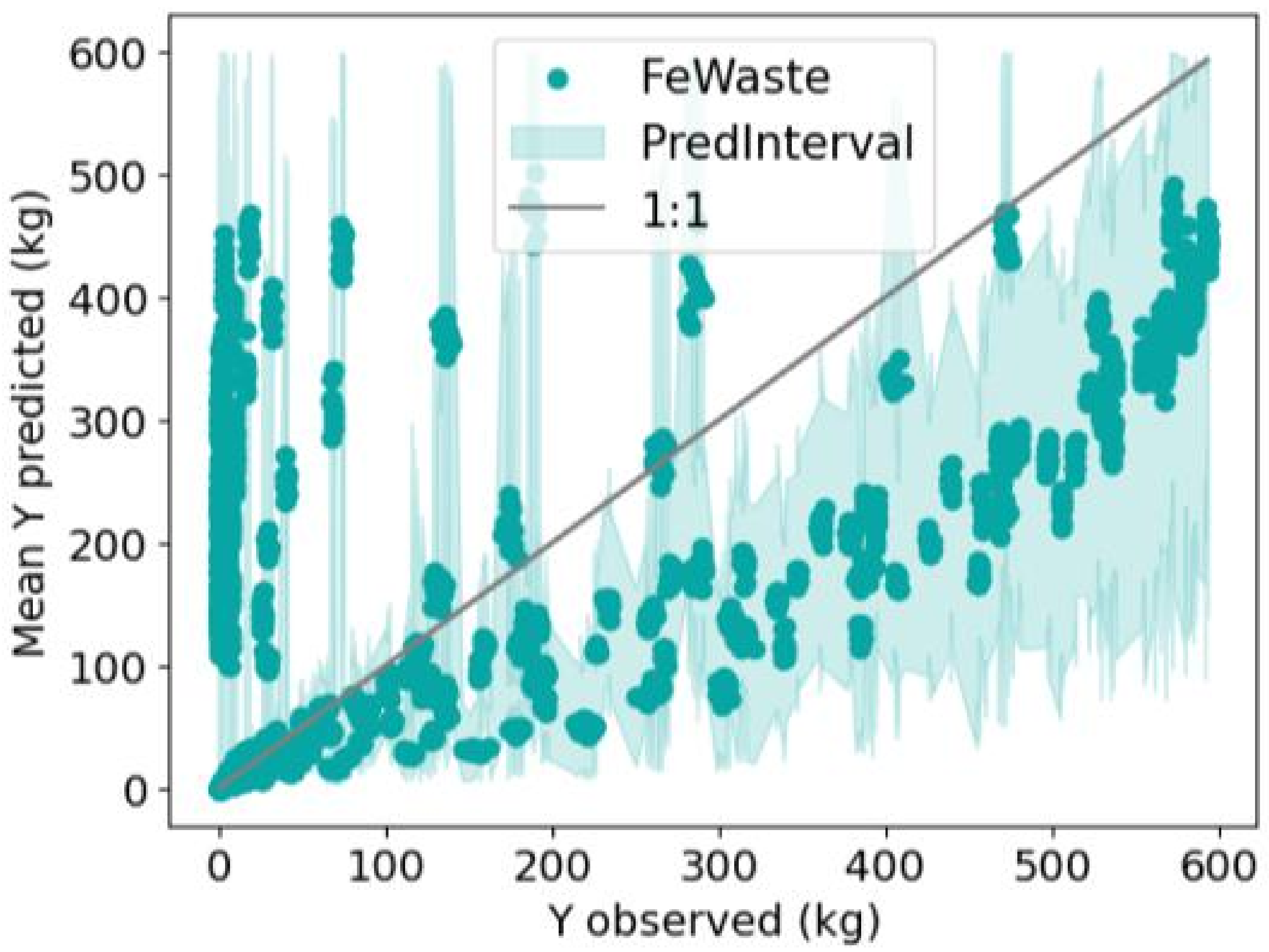
> Model 1: Neural network 2 hidden layers with 5 neurons each and sigmoid activation functions

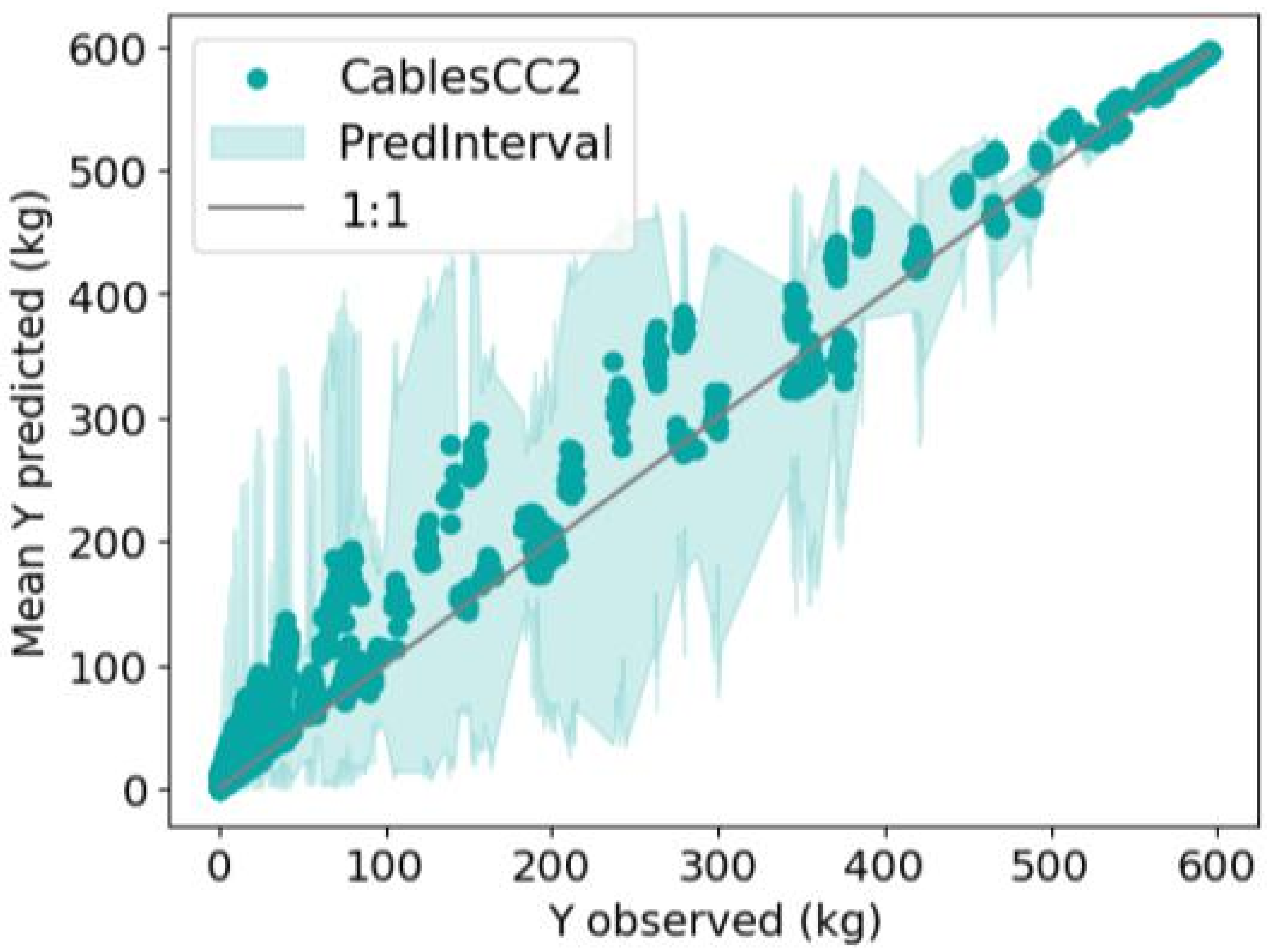


Overview of prediction performance

Model 2: Linear functions and 1 conditional model

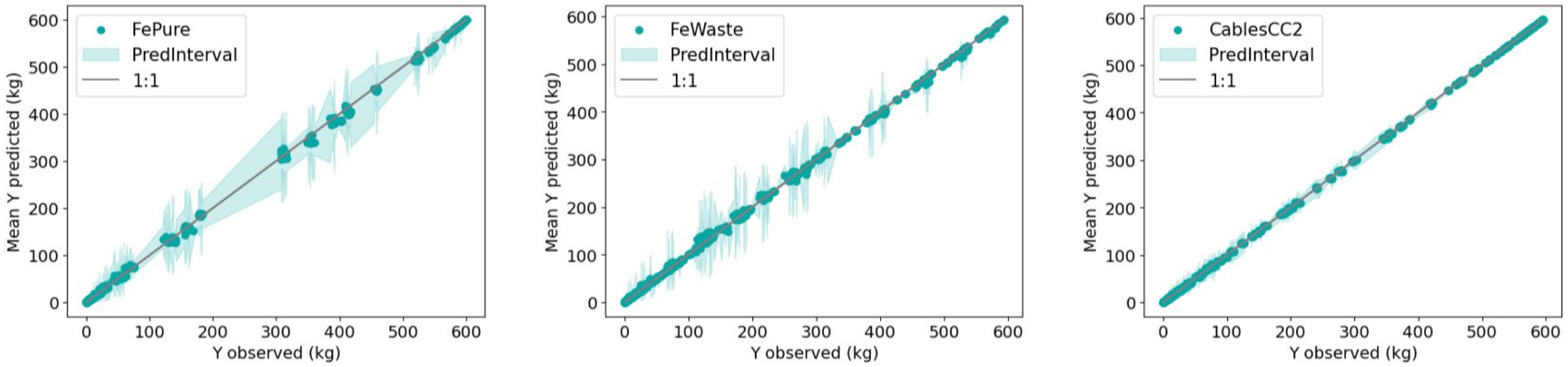






Overview of prediction performance

> Model 3: Linear functions and all conditional models



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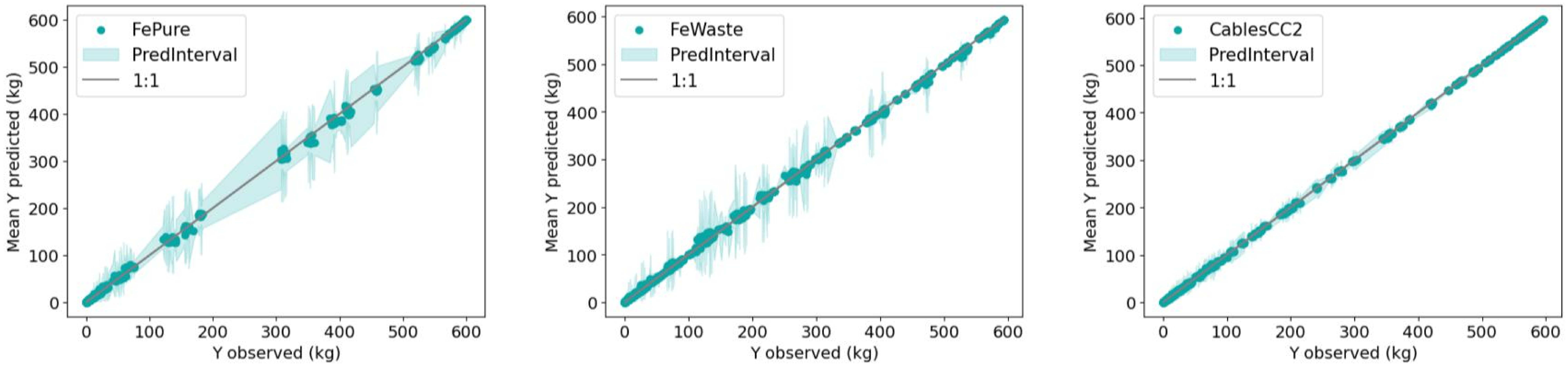

What can this model tell us that Model 1 does not?

First steps in Explainable AI in this framework

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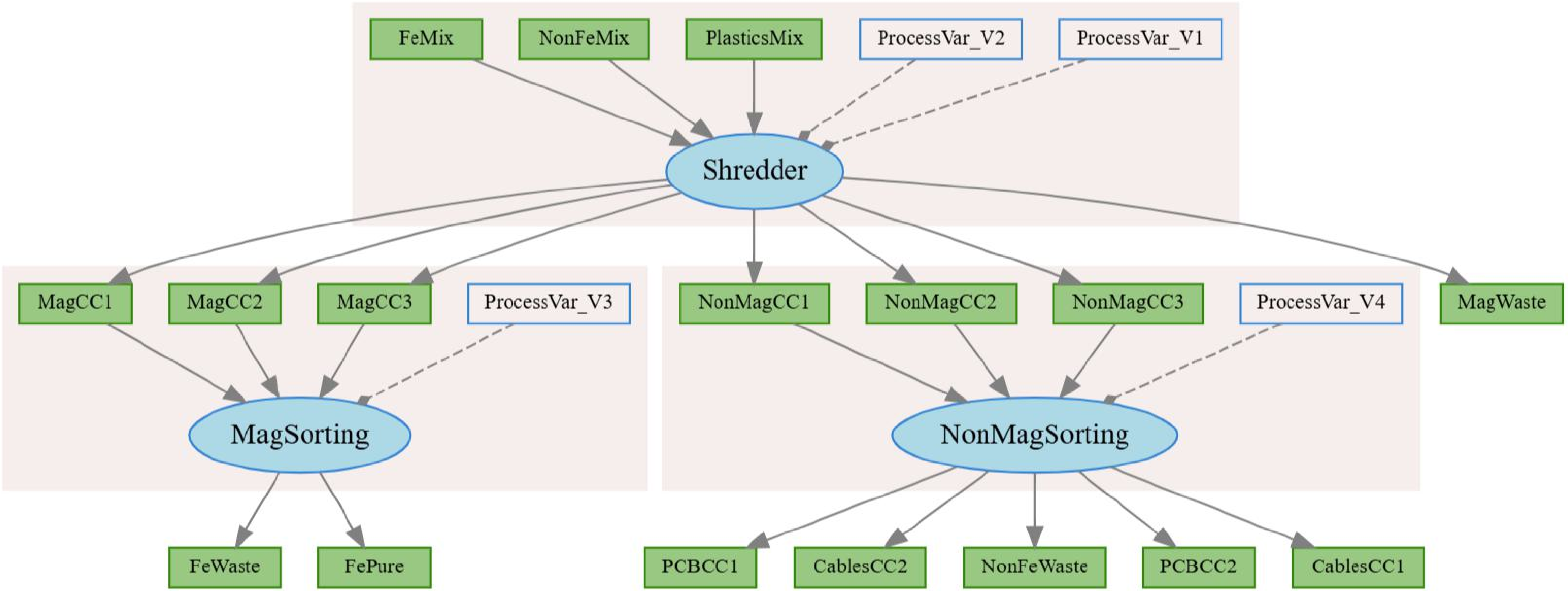
Process model



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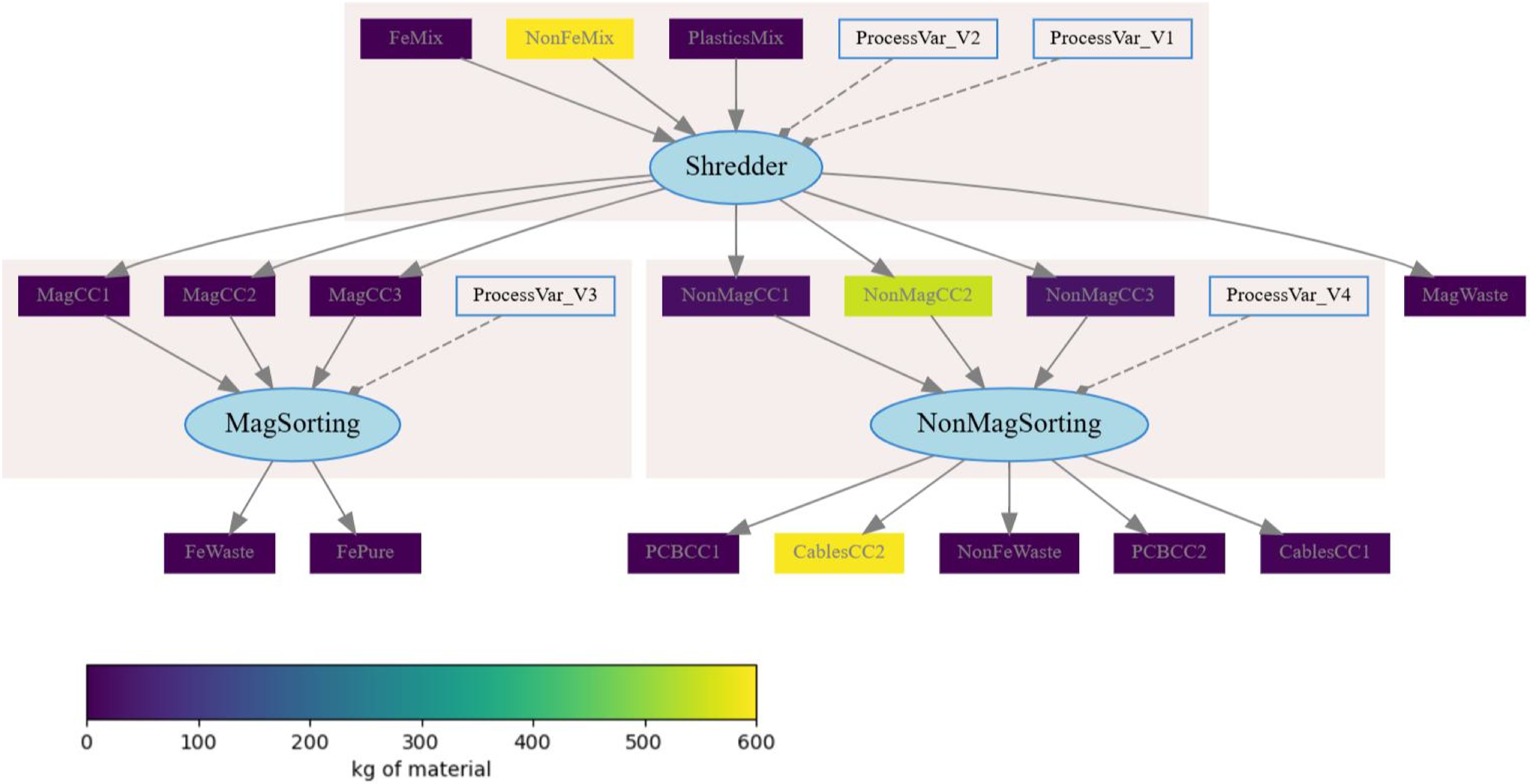
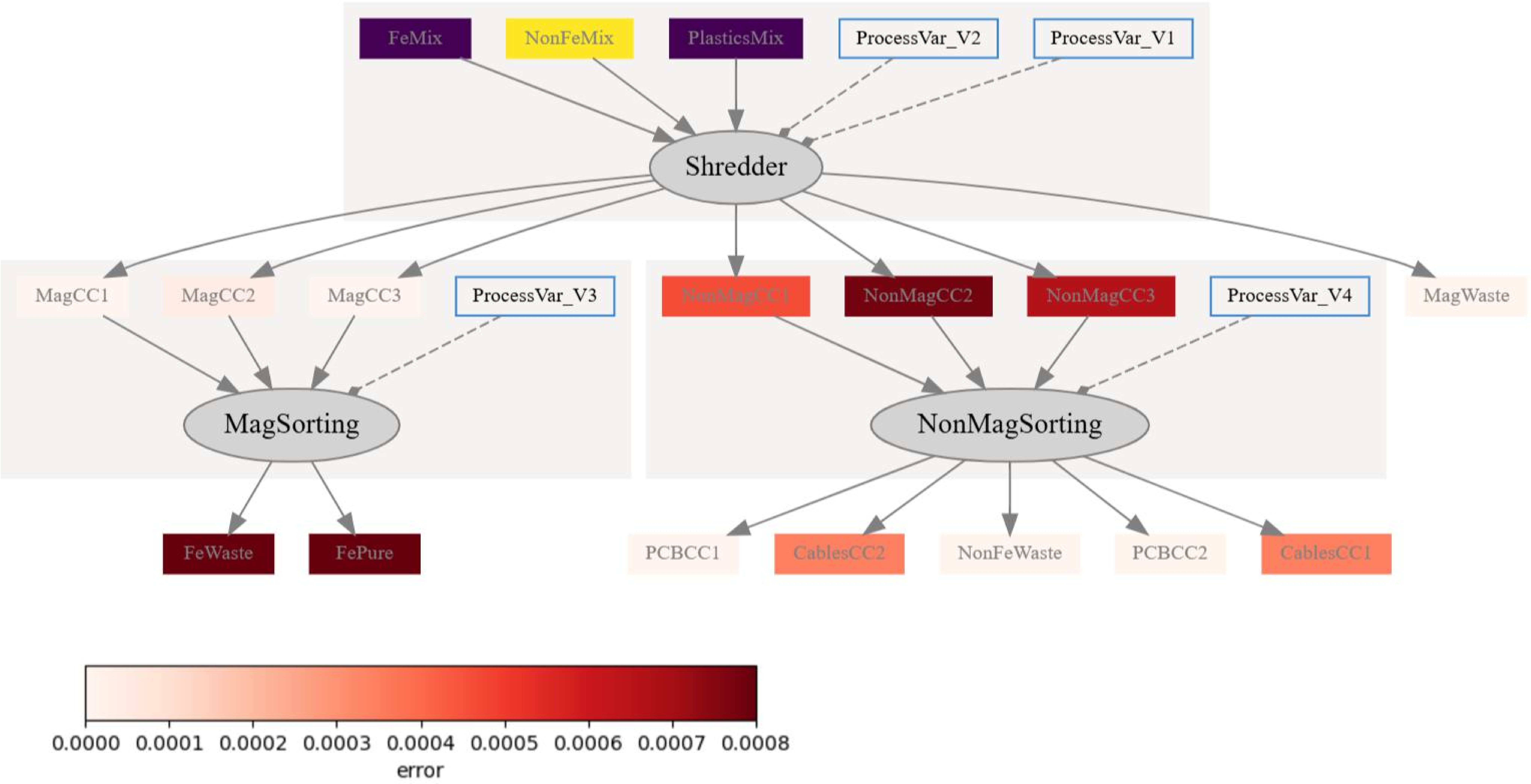
Material flow



Error propagation



Takeaways

Conclusions

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- It supports strong non-linear relationships from input to output stages
- We are able to quantify not only the predicted output of the process but also the prediction error, **at every process stage**
- Combining elements of conditional relationships and non-linear relationships sets a solid basis for XAI

What’s next?

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- Use this framework to fully exploit conditional deep models for XAI

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- Use this framework to fully exploit conditional deep models for XAI
- With this basis for XAI, we will be able to build systems where humans have full control and understanding of process behavior
- We need to implement process optimization in the framework, i.e., best process settings for optimal output
- In a further future, we would need to use this framework for optimal experimental design. There are still so many processes that need to be digitalized where data is completely absent.

Thank you for your attention!

Time for questions

KIRAMET project FFG No.899661

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This work is part of the KIRAMET project

KIRAMET project FFG No.: 899661

SCCH is an initiative of

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