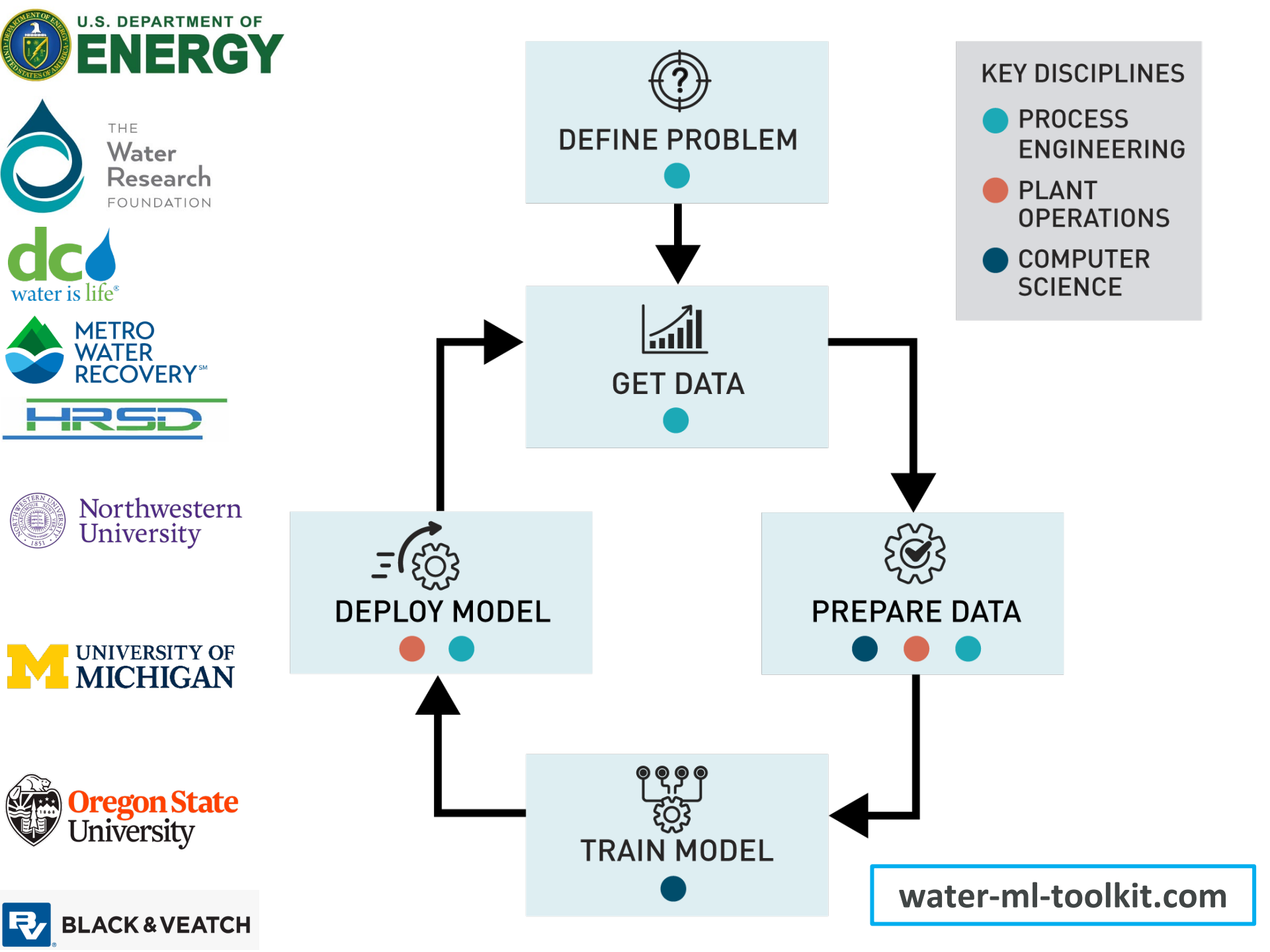
Modeling Phosphorous Removal Using Stakeholder-Centered Problem Solving

Dr. Kate Newhart Oregon State University

inspiring change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DEFINE PROBLEM
GET DATA
PREPARE DATA
TRAIN MODEL
DEPLOY MODEL
KEY DISCIPLINES
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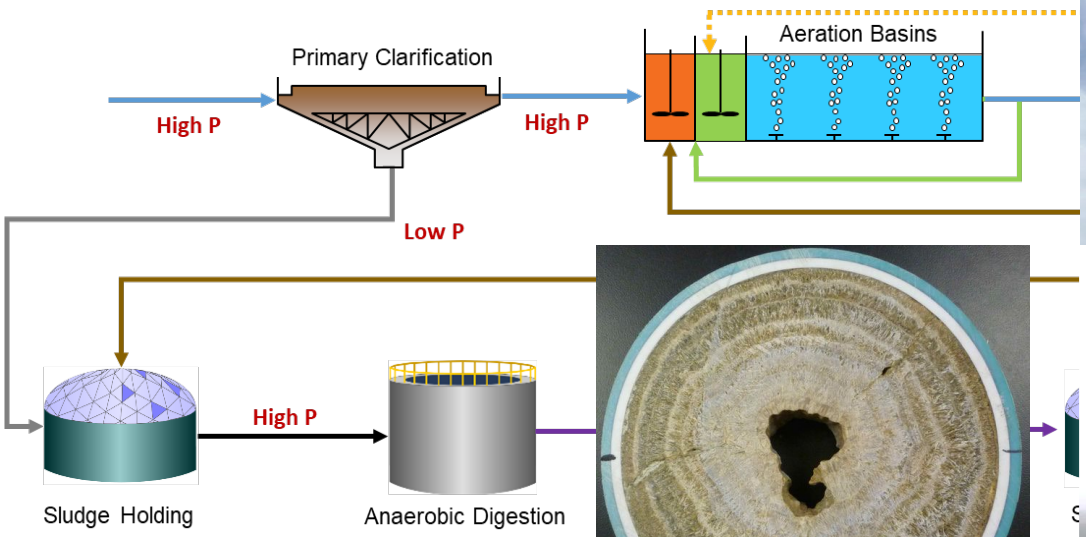
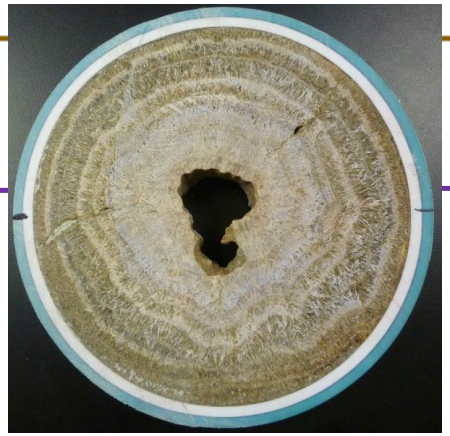
WHAT MAKES A "GOOD" ML PROBLEM?

- Specific to an **ML-appropriate objective**
  - Goal is to minimize energy, not to understand chemical kinetics
- **Measurable** performance criteria
  - X% improvement over status quo
- Implementation is feasible and **integrated into the model design**

Yishi Zuo, 2021

PHOSPHORUS RECOVERY





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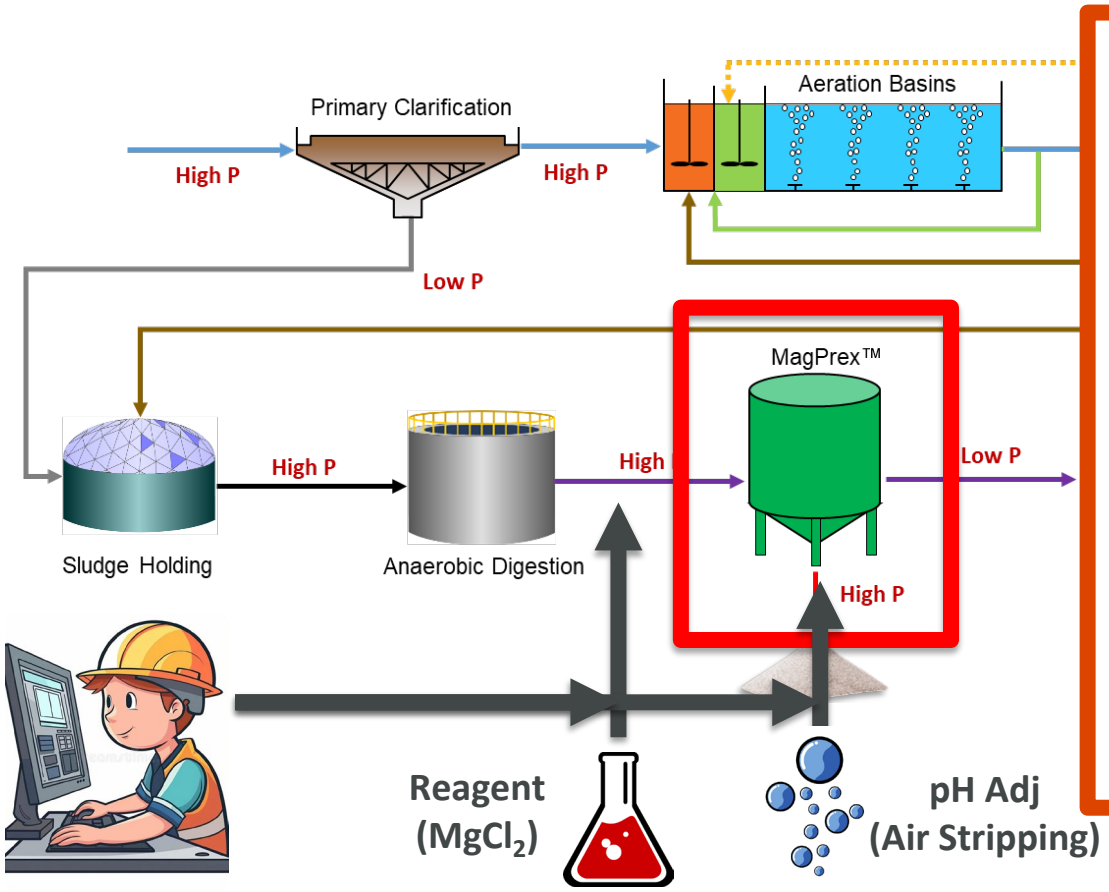
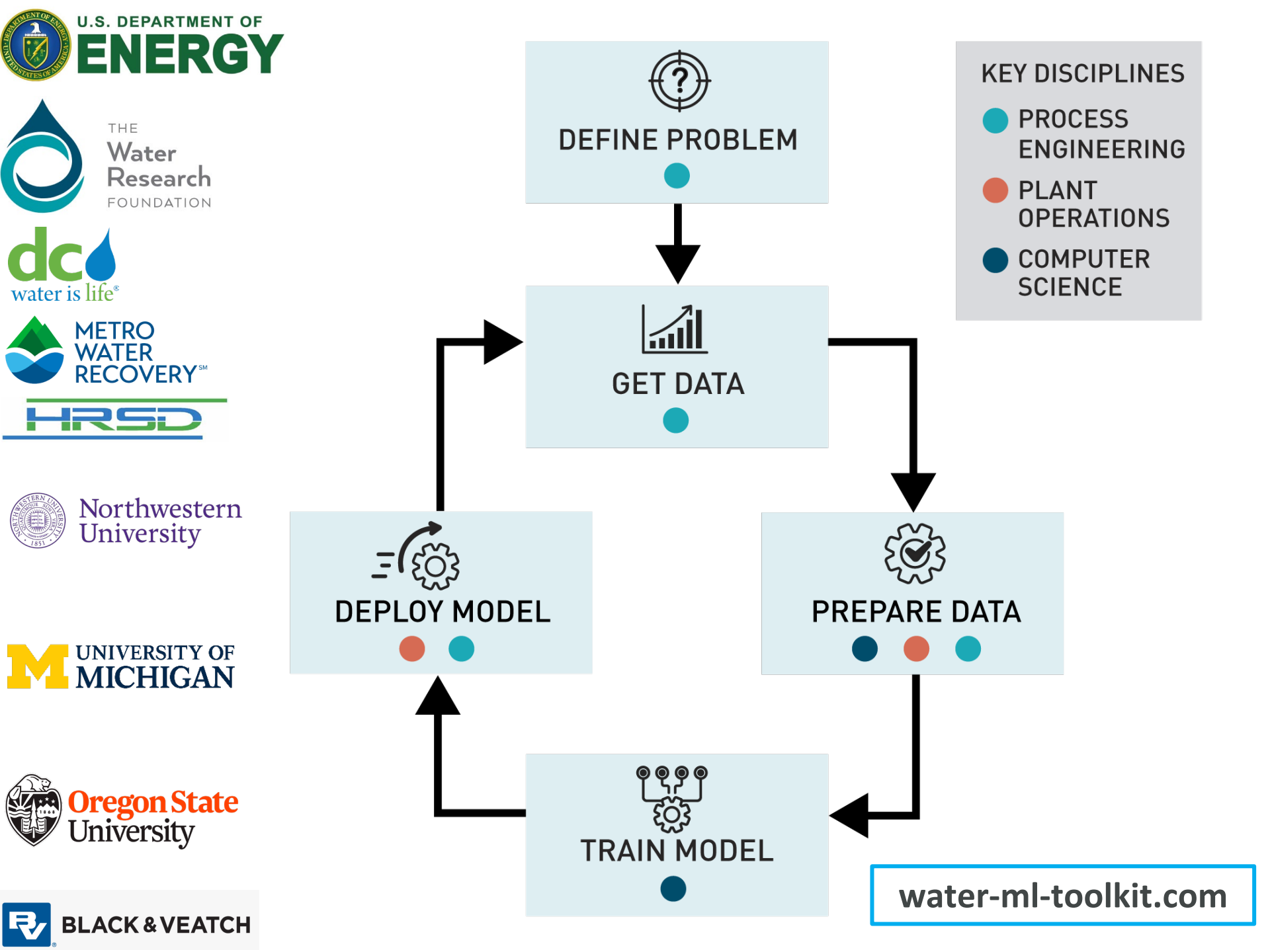


- Mass balance + reaction kinetics model is TERRIBLE
- Anaerobic digestate is NASTY. Sensors don't survive, samples are difficult to analyze
- Operators "guesstimate" reagent and pH setpoints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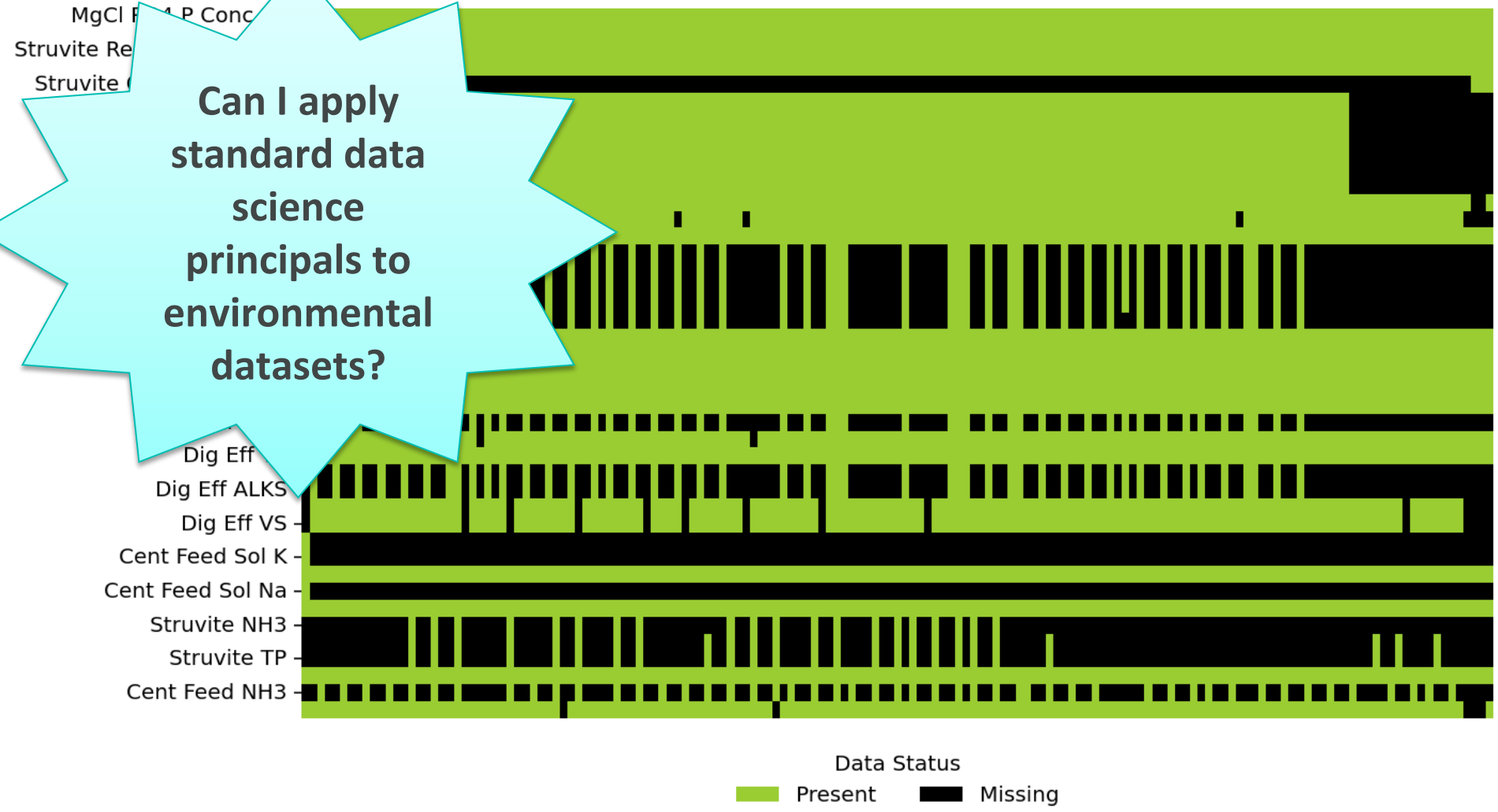
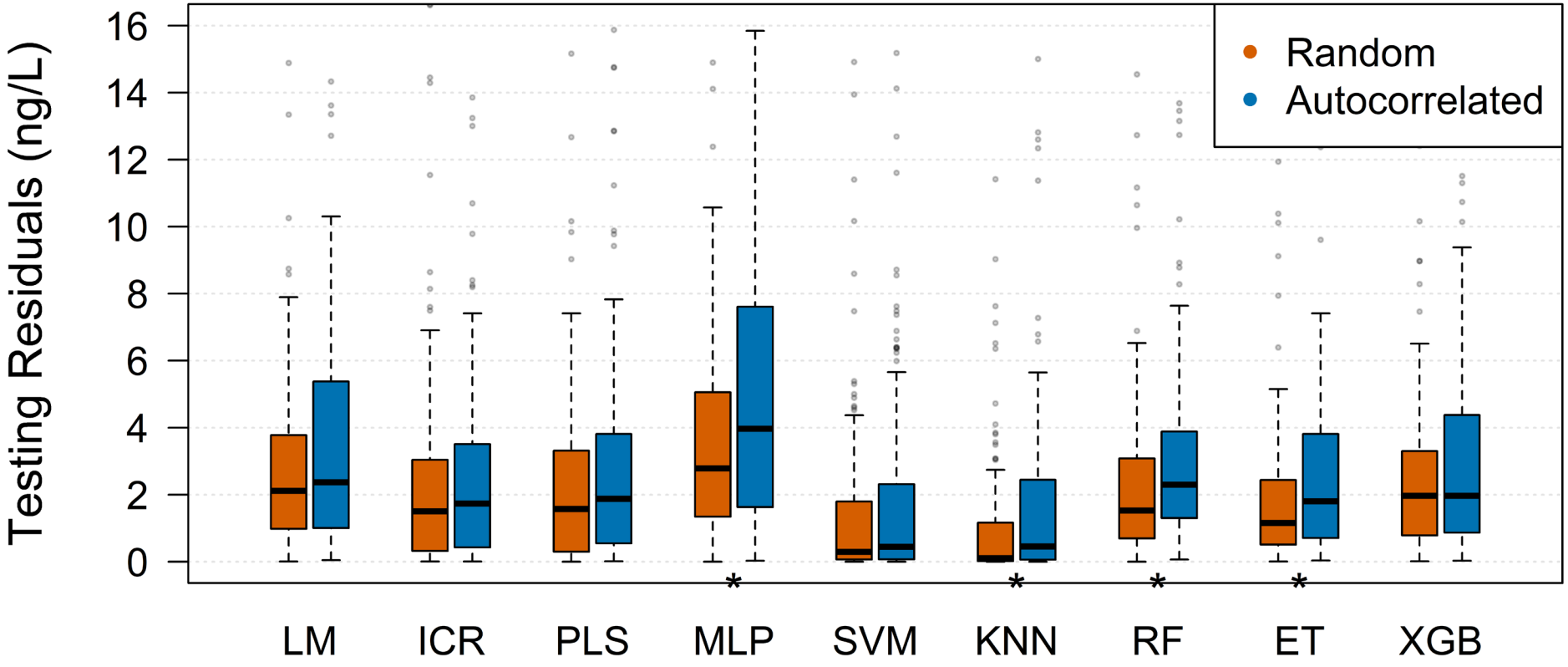
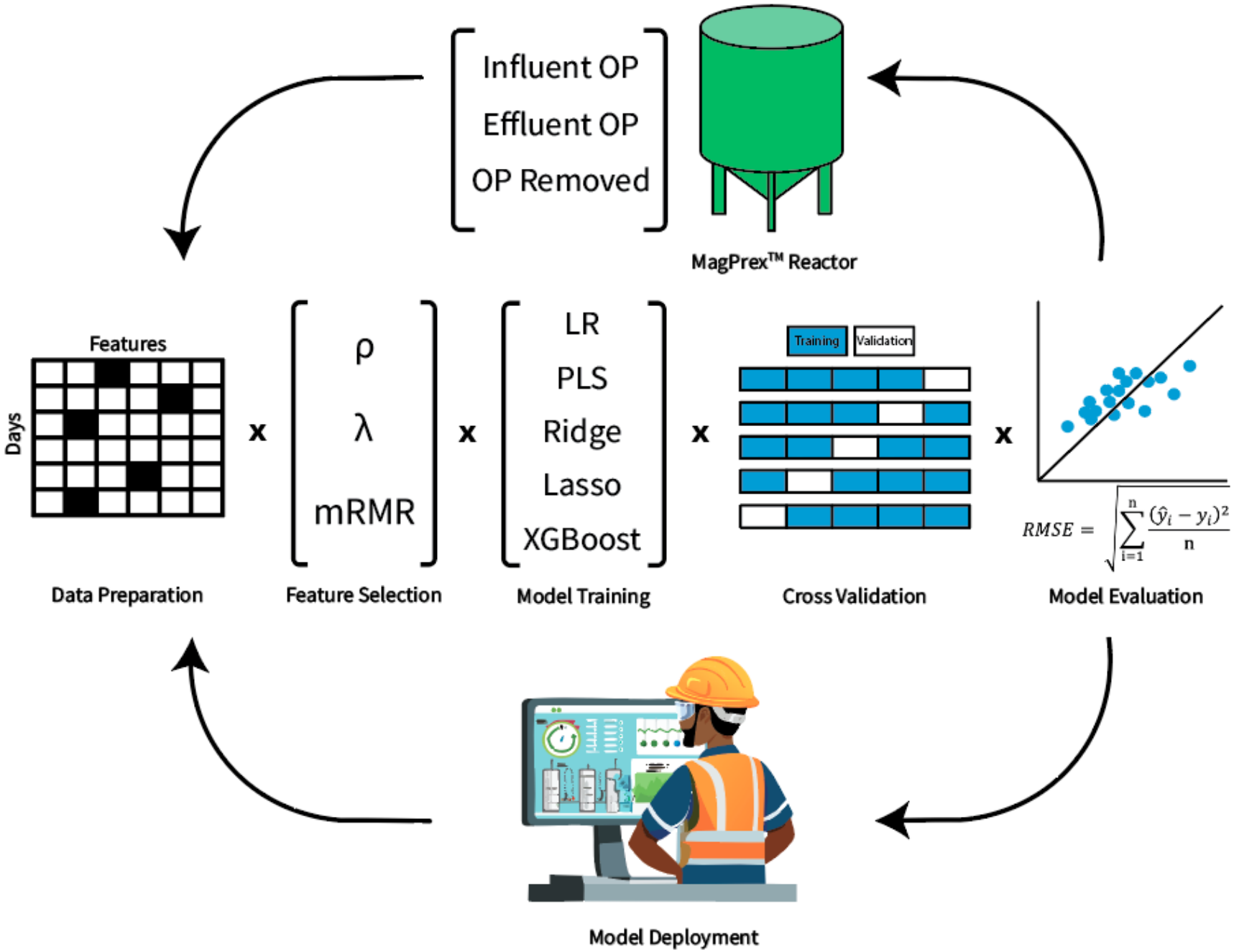
“I HAVE SOOOO MUCH DATA”

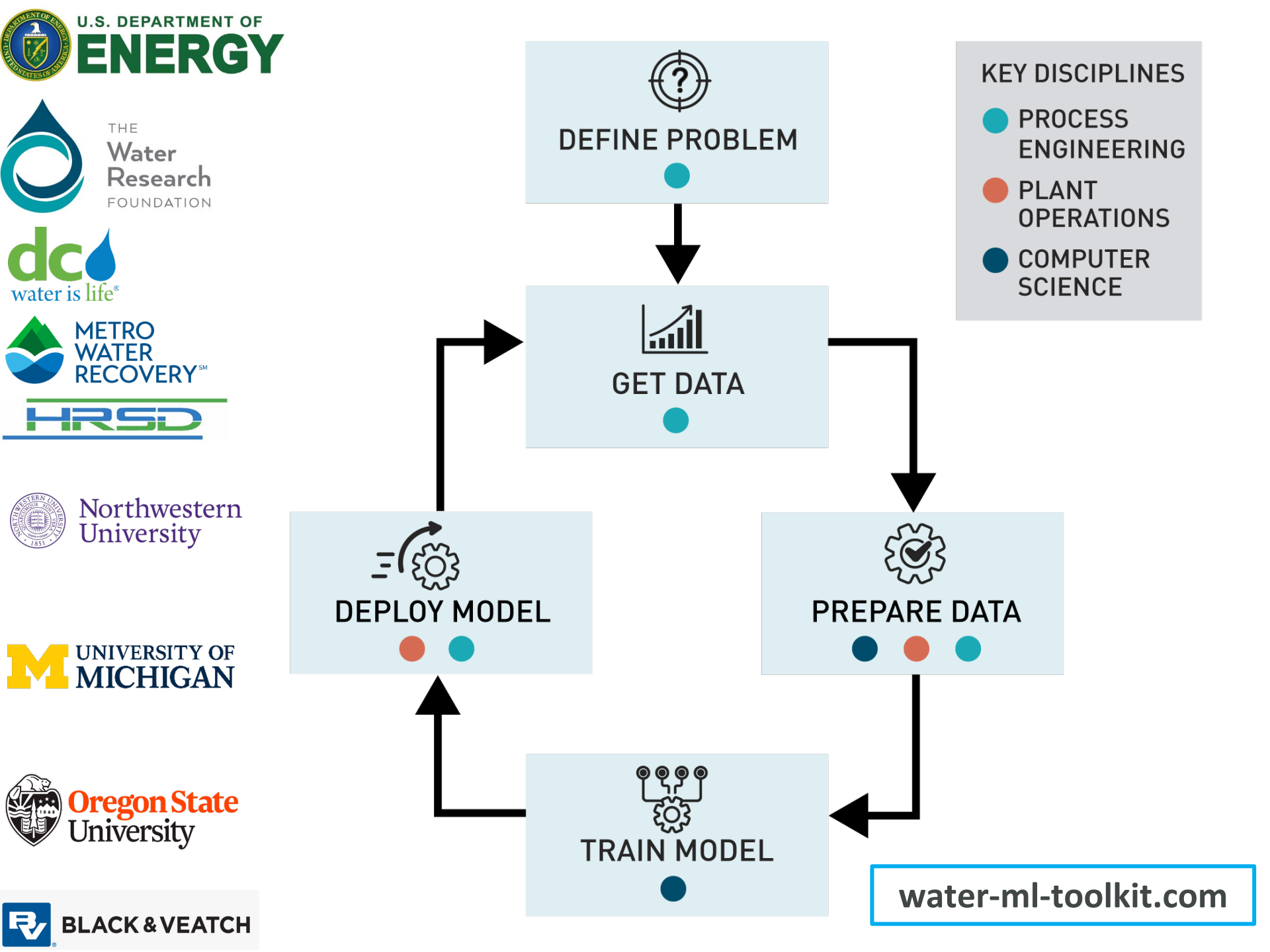


DIFFERENT PROJECT, SAME IDEA

Environmental data is often time-series data. If taken frequently, data could be *autocorrelated* and standard data science practices like random splitting can lead to *data leakage* or artificially low errors.




Influent OP
Effluent OP
OP Removed
MagPrex™ Reactor
Features
Days
x
ρ
λ
mRMR
x
LR
PLS
Ridge
Lasso
XGBoost
x
Training
Validation
x
$RMSE = \sqrt{\sum_{i=1}^{n} \frac{(\hat{y}_i - y_i)^2}{n}}$
Data Preparation
Feature Selection
Model Training
Cross Validation
Model Evaluation
Model Deployment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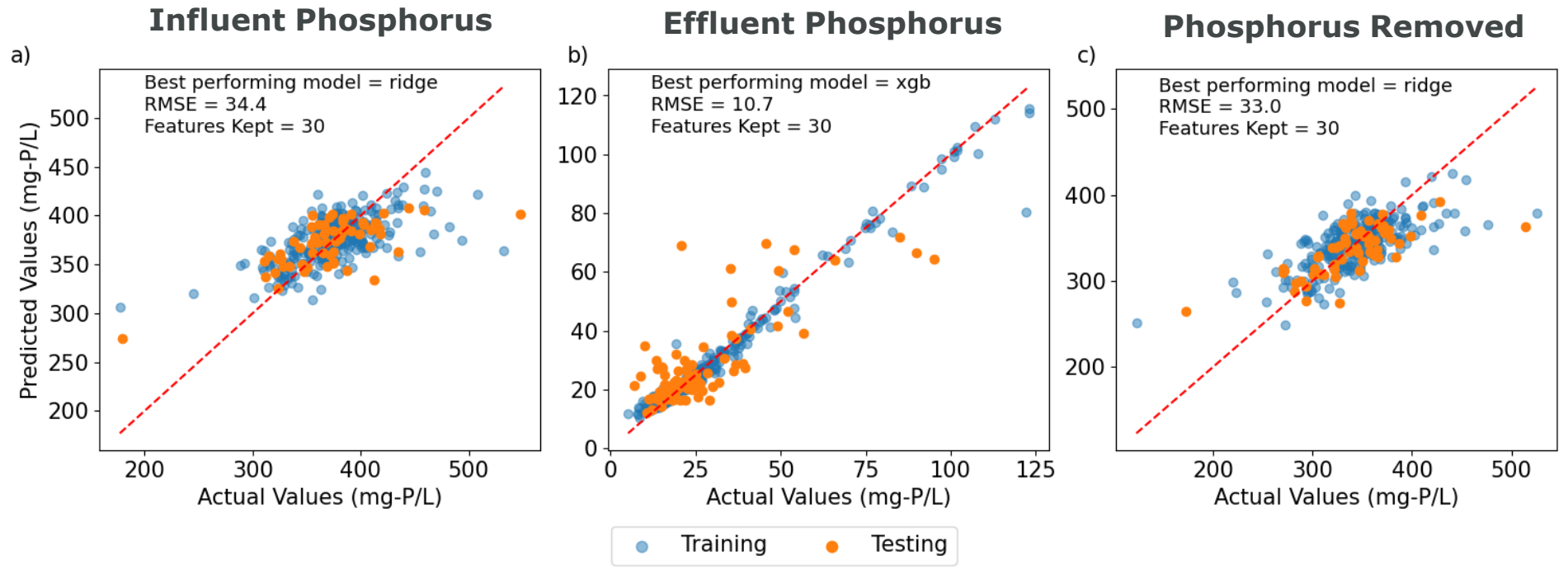
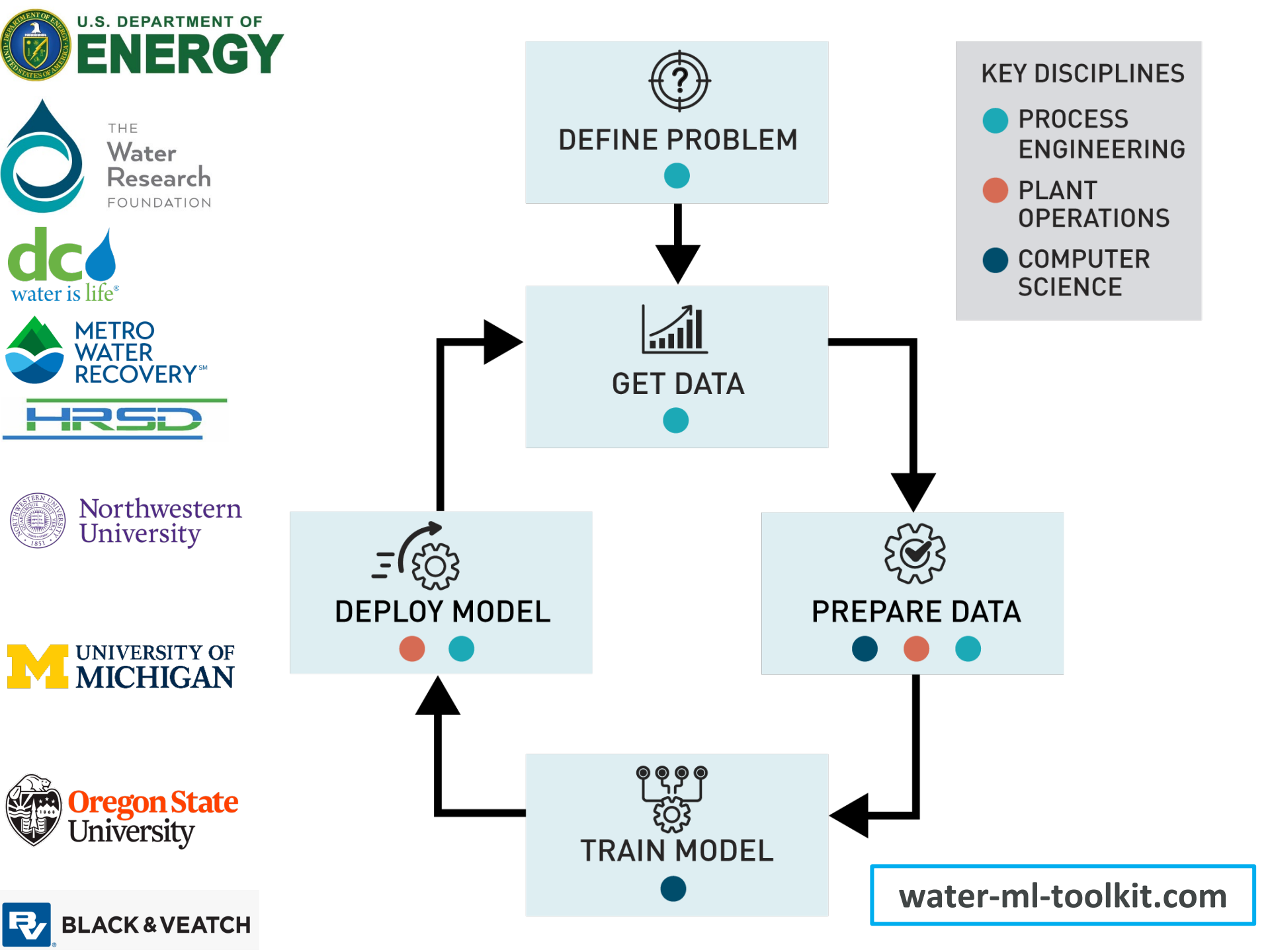
BEST MODELS: 9% NRMSE

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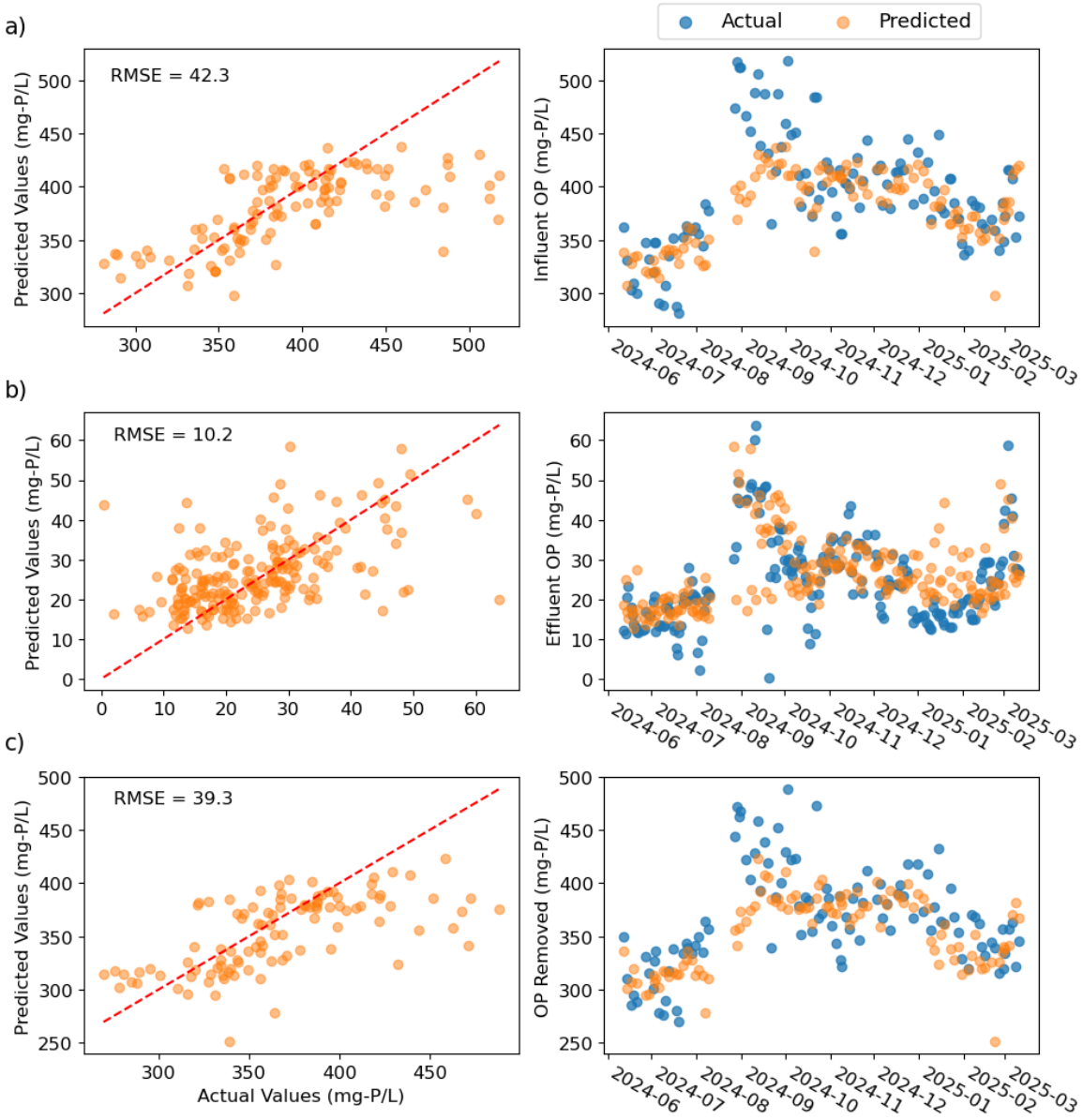


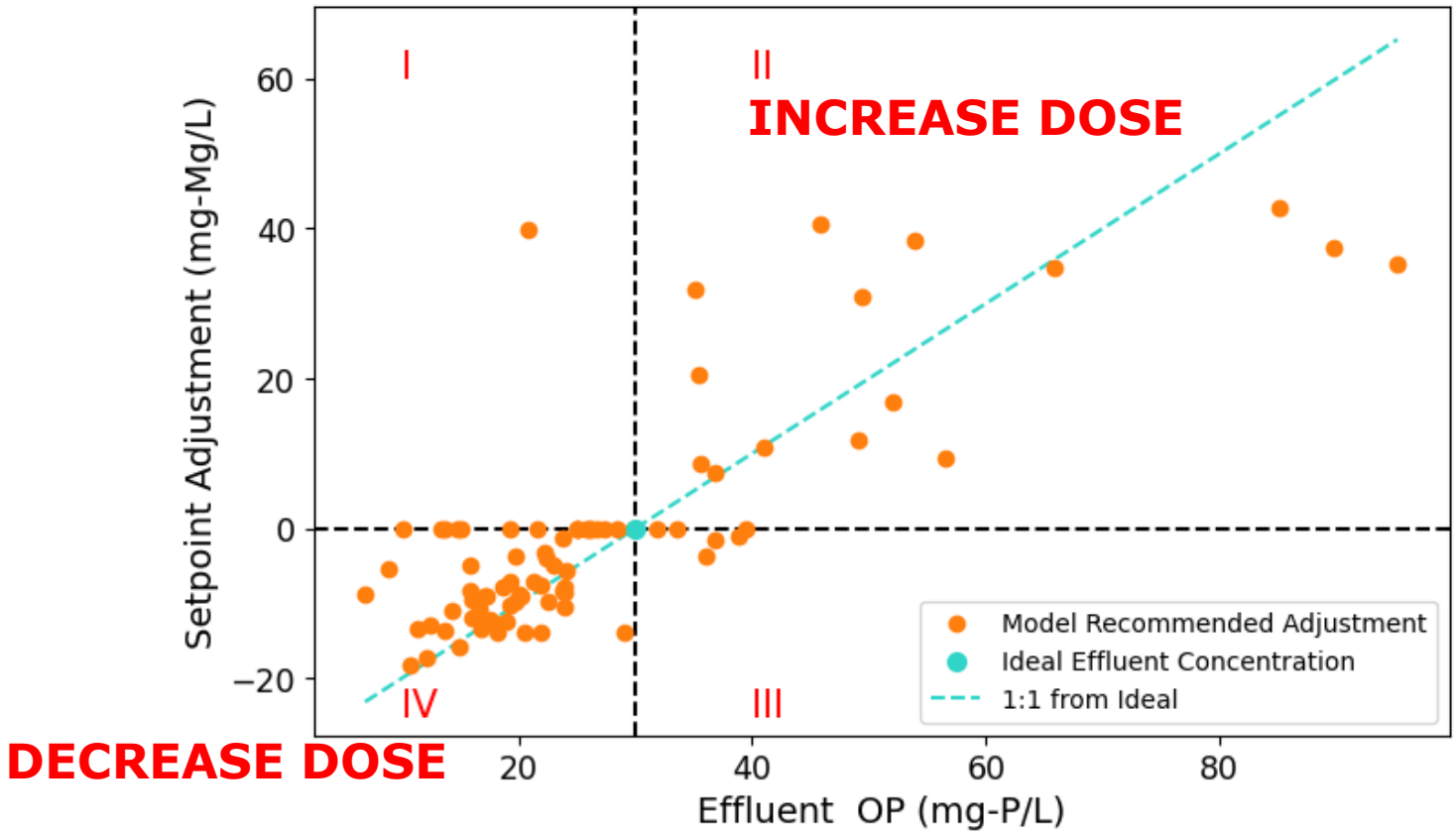
DEPLOY, IRL!

Influent Phosphorus

Effluent Phosphorus

Phosphorus Removed

BASED ON EFFLUENT PHOSPHORUS + INFLUENT CONDITIONS, WHAT SHOULD WE BE DOSING?



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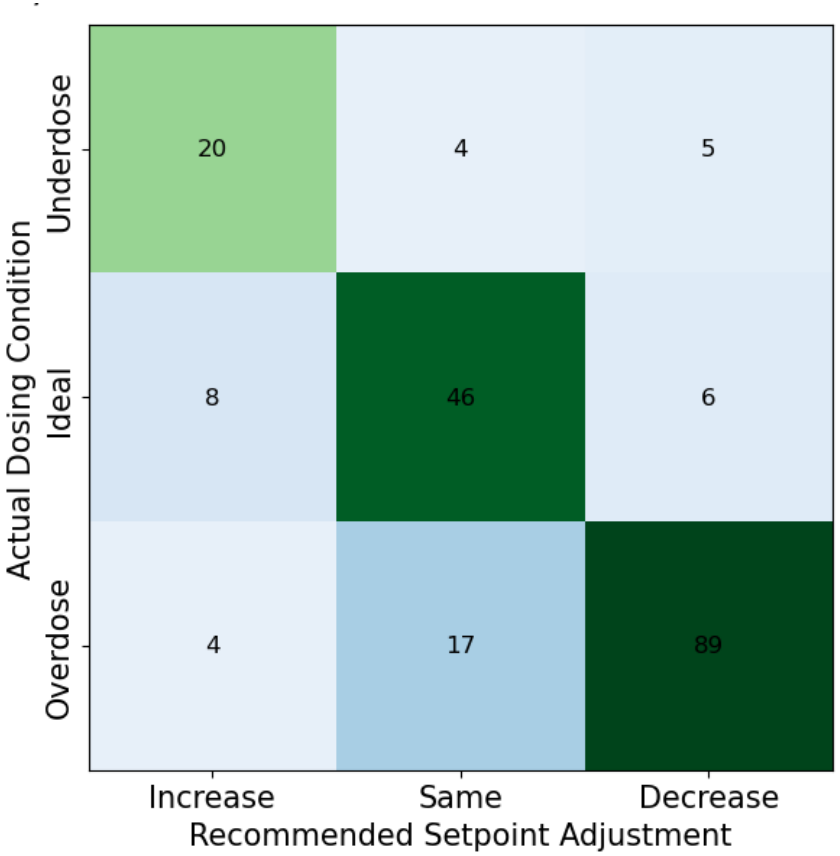
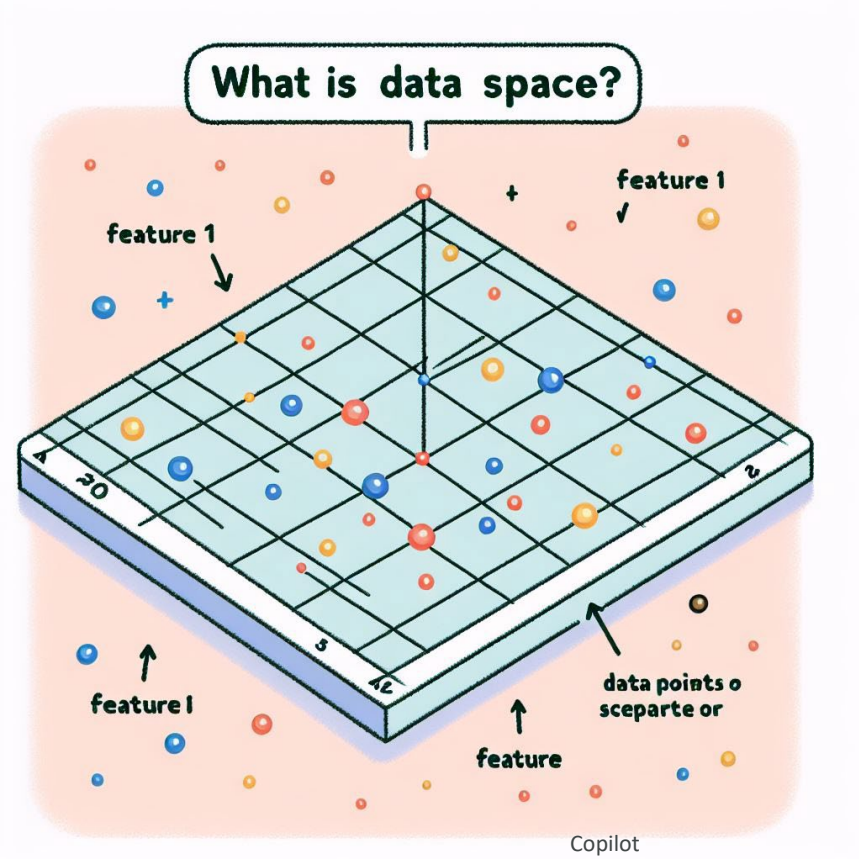
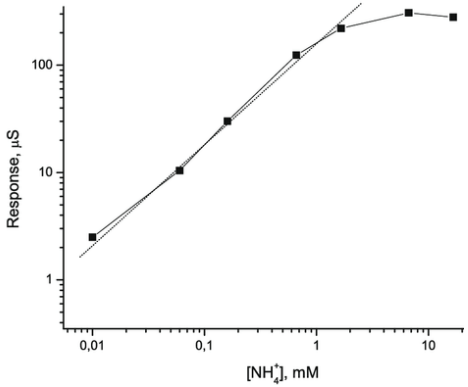


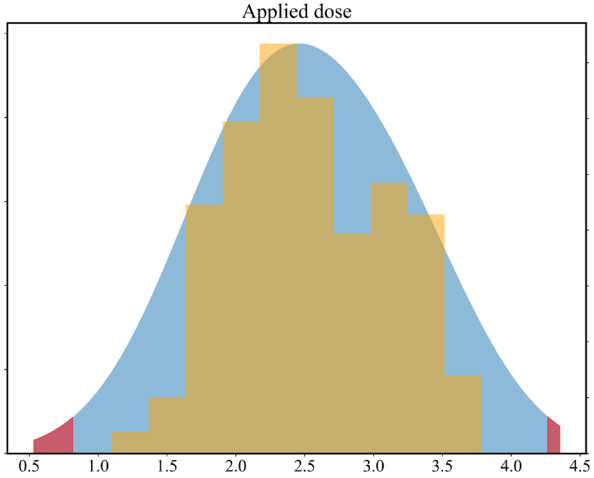
Bin setpoint adjustments: increase, decrease, same

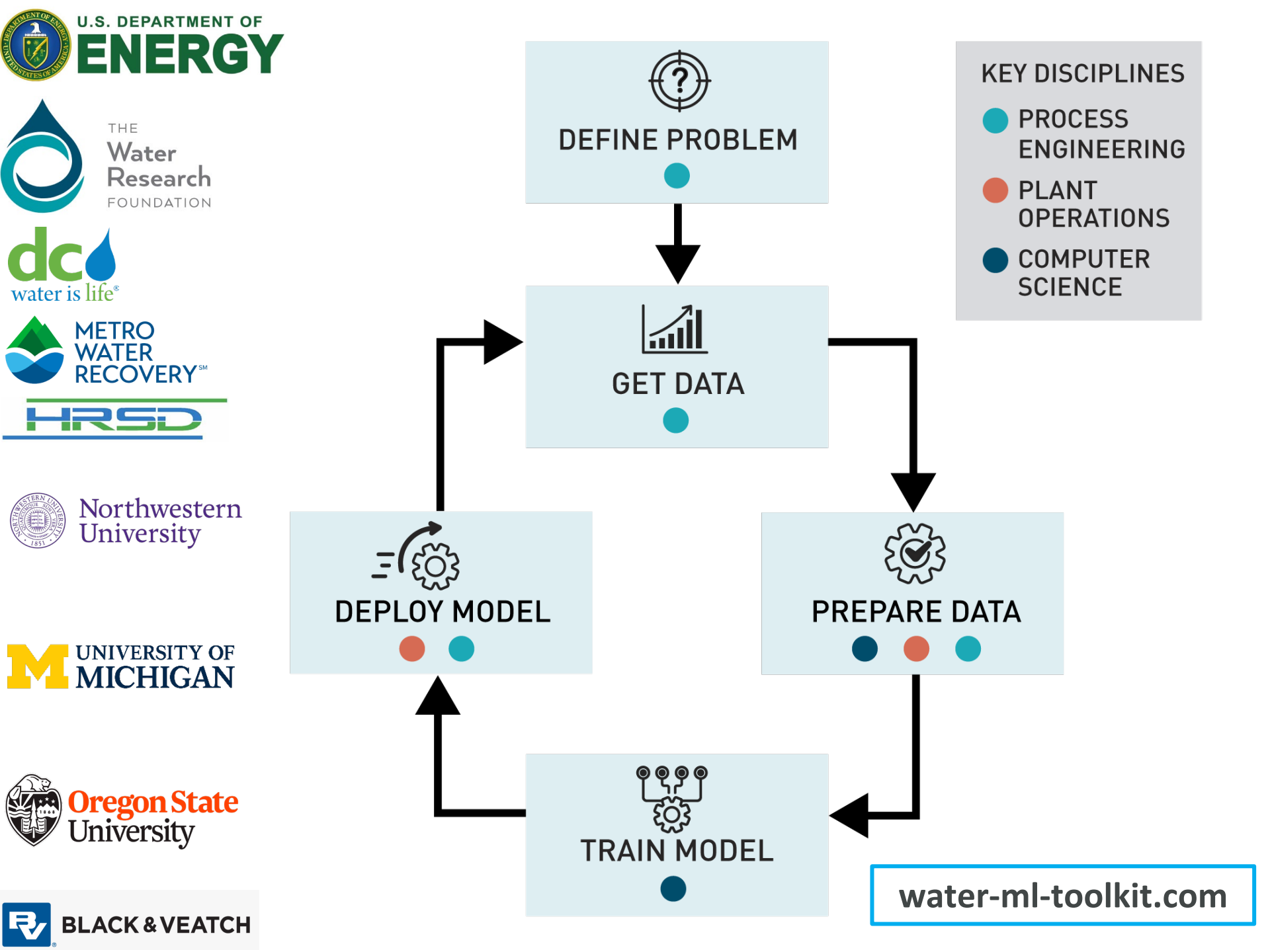
Correct 97% of the time

DATA SPACE


What is data space?
feature 1
feature 1
feature 1
feature
data points o
sceparte or
Copilot


Response, µS
100
10
1
0,01
0,1
1
10
[NH4+], mM


Applied dose
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5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WHAT HAVE WE LEARNED?

- Machine learning models can be used to capture non-ideal / highly non-linear process behavior
- Data are your solution… but also your problem
  - Environmental datasets are smaller than you think!
  - Beware artificially low errors / high accuracy!
- Put on your experimentalist hat!
  - No universal model, data preparation, error metric, etc.
  - Be creative and **user-centric!**

- This could be you!
- Now hiring PhD students!