Predicting Maximum Temperature Experienced by Pine Biomass Particles in a Takachar Moving Bed Reactor using Machine Learning Models and Thermogravimetric Analysis (TG/DTG)

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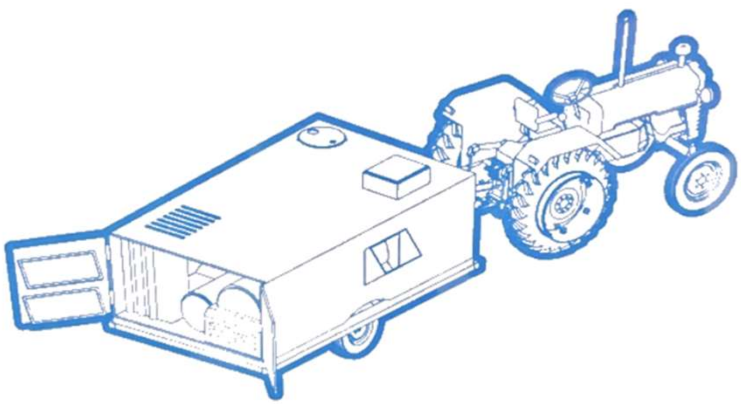
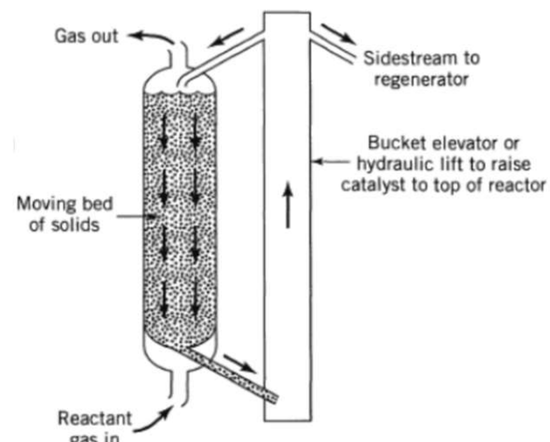
Motivation

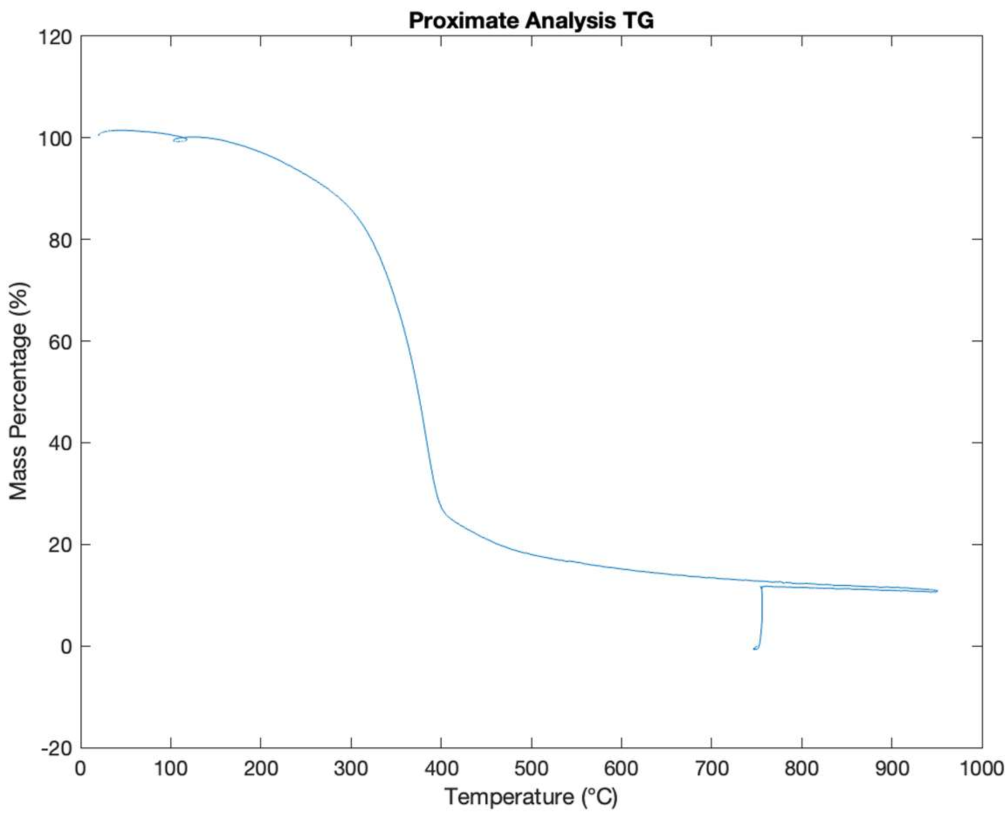
- We want to know the maximum temperature distribution experienced by the biomass particles within the Takachar reactor
    - Not feasible to directly measure for each individual biomass with a thermocouple
- Broader application: issue applies to any moving bed reactor due to inhomogeneous heating, radial temperature gradient





Levenspiel (1999)

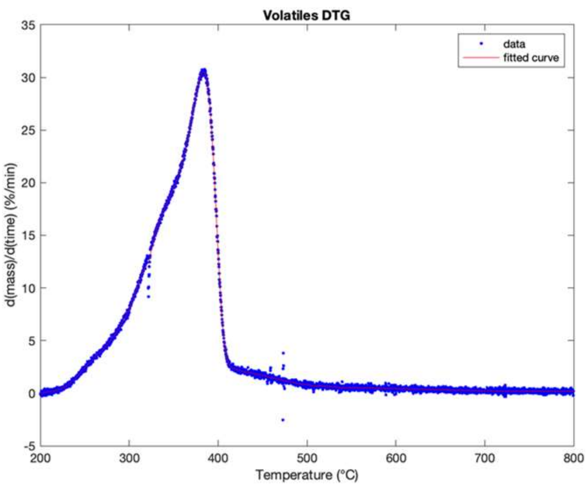
Proximate Analysis/Thermogravimetric Analysis (TG)

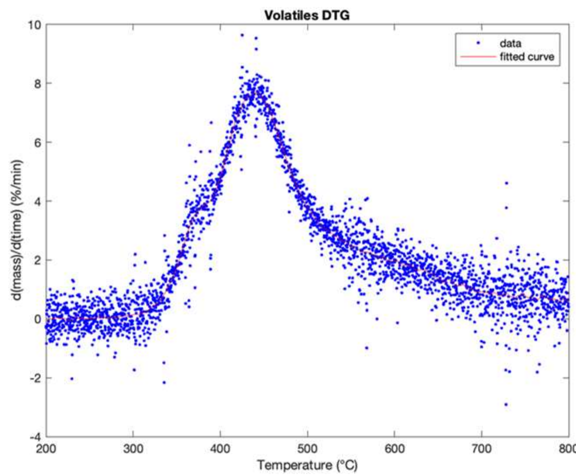


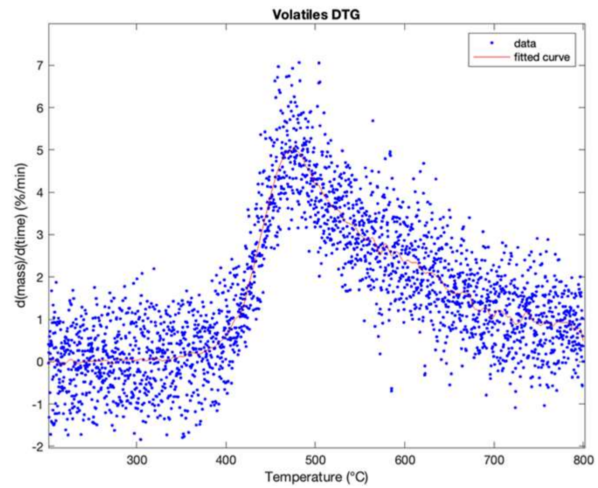
1. 90.00mL/min flow of Nitrogen
2. Ramp 20.00°C/min to 107°C
3. Isothermal for 10.00 min
4. Ramp 28.10°C/min to 950.00°C
5. Isothermal for 7 min
6. Ramp 25.00°C/min to 750°C
7. 90.00mL/min flow of air
8. Isothermal for 5 min

Vasileiadou, et.al.

Derivative Thermogravimetry (DTG)







Vasileiadou, et.al.

Key Thermal Parameters from TG/DTG Analysis

R_{max} = Maximum rate of mass loss (DTG)

T_{max} = Temperature at which R_{max} occurs (DTG)

Dry, Ash free basis

VM = Volatile matter, [wt.%] (TG)

FC = Fixed carbon, [wt.%] (TG)

FCP = Fixed Carbon Proportion (TG)

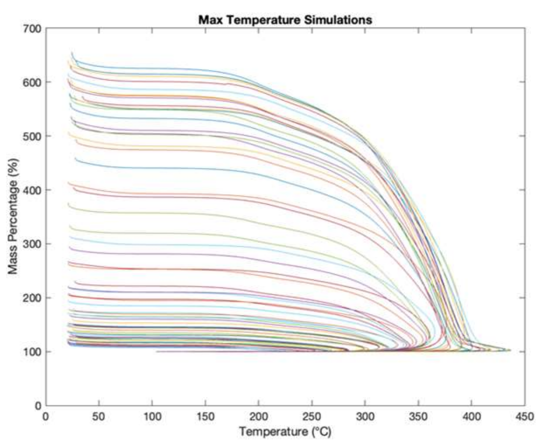
$$FCP = FC/(FC + VM)$$

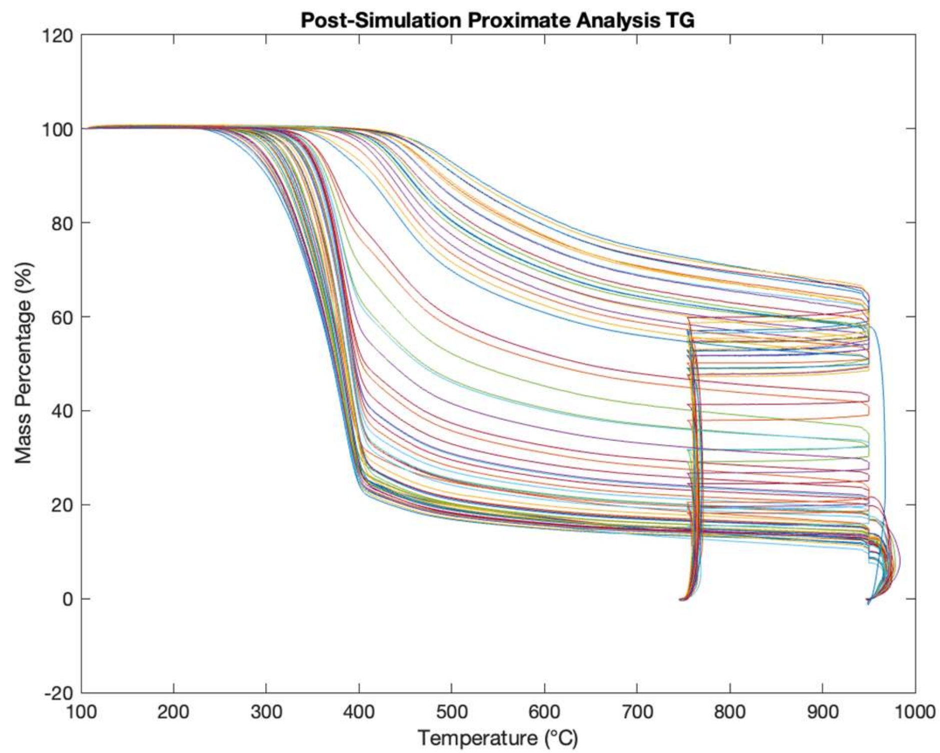
Iordanidis,et.al.

Simulation + Proximate Analysis

1. 90.00mL/min flow of Nitrogen
2. Ramp 6.00°C/min to max temp
3. Equilibrate at 107°C

1. Ramp 28.10°C/min to 950.00°C
2. Isothermal for 7 min
3. 90.00mL/min flow of air
4. Isothermal for 5 min

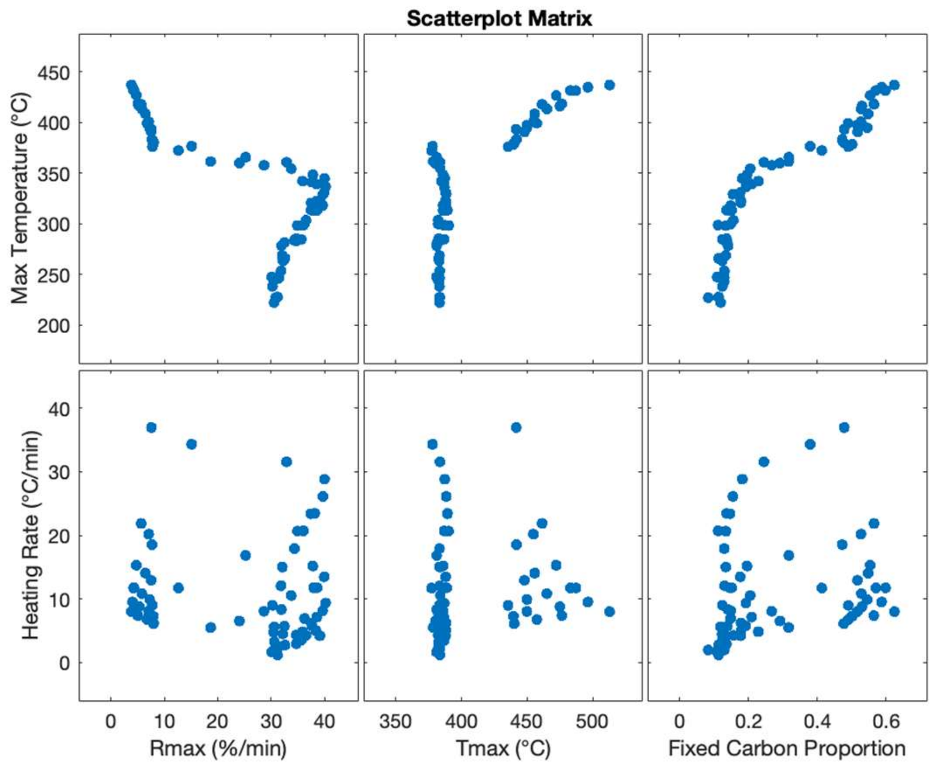




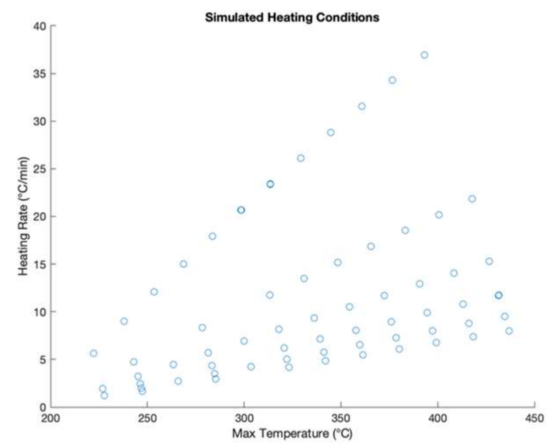
Method

- **Hypothesis:** We can use machine learning algorithms with key features of TG/DTG curves to predict the maximum temperature experienced by individual biomass particles without the need for a thermocouple.
- Simulate field reactor conditions experienced by individual biomass particles in a lab setting with observable maximum temperature. Vary heating rate to intentionally add noise and create a more robust model
- Proximate Analysis can analyze the general composition of a biomass in terms of volatiles and fixed carbon with TG/DTG analysis
- Relate key features of the TG/DTG curves to the known maximum temperature of biomass particles using machine learning models.
- Use Repeated k-fold cross validation to compare and evaluate the predictive strength of the various machine learning models models.

Scatterplot Matrix to Select Response Variable



- Model Boundaries
  - Actual Temperatures range from 222.374 to 436.925°C



Cleveland,et.al.

Matlab Machine Learning Models (1)

Parameters Generated by Regression Learner Application

M1 = Linear Regression

M2 = Interactions Linear Regression

M3 = Robust Linear Regression

M4 = Stepwise Linear Regression

M5 = Fine Tree

M6 = Medium tree

M7 = Coarse Tree

M8 = Linear SVM

M9 = Quadratic SVM

M10 = Cubic SVM

M11 = Fine Gaussian SVM

M12 = Medium gaussian SVM

M13 = Coarse Gaussian SVM

Matlab Machine Learning Models (2)

M14 = Boosted Trees Ensemble

M15 = Bagged Trees Ensemble

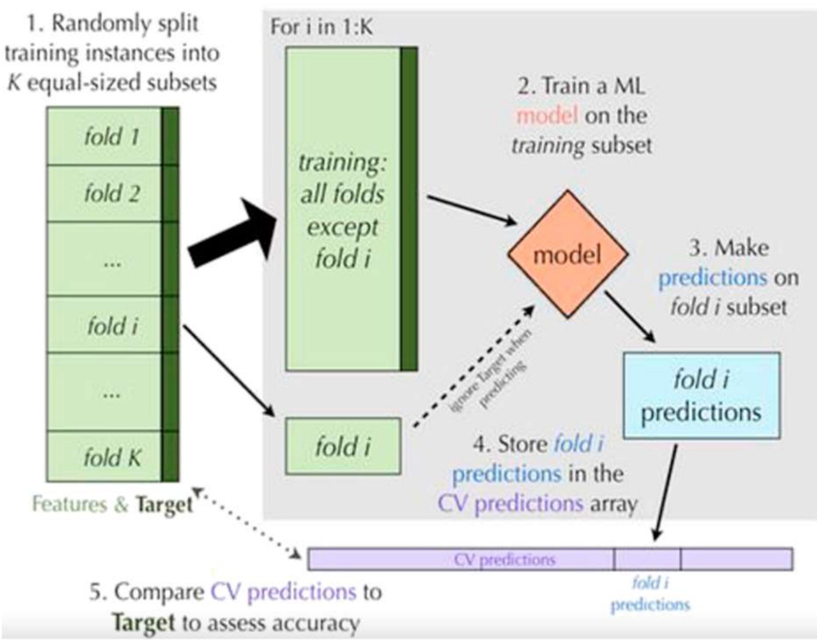
M16 = Squared Exponential Gaussian Process Regression

M17 = Matern 5/2 Gaussian Process Regression

M18 = Exponential Gaussian Process Regression

M19 = Rational Quadratic Gaussian Process Regression

K-Fold Cross Validation



(*Rohani, et.al.)*

Cross Validation can be repeated an arbitrary number of times to provide more robust performance metrics

(Lu, et.al.)

Cross Validation Performance Metrics *(Bouchouicha, et.al.)*

RMSE = $\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\widehat{H}-H\right)^2}$ (°C)

RRMSE = $\frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\widehat{H}-H\right)^2}}{\overline{H}} * 100\%$

MBE = $\frac{\sum_{i=1}^{n}\left(\widehat{H}-H\right)}{n}$ (°C)

MPE = $\frac{1}{n}\sum_{i=1}^{n}\left(\frac{\widehat{H}-H}{H}\right) * 100\%$

$R^2 = 1 - \frac{\sum_{i=1}^{n}\left(\widehat{H}-H\right)^2}{\sum_{i=1}^{n}\left(H-\overline{H}\right)^2}$

- Root mean square error (RMSE, °C) and Mean Bias Error (MBE, °C) provide absolute estimations of the model's random error and bias respectively
- Relative-RMSE (RRMSE, %) and Mean Percentage Error (MPE, %) provide relative estimations of the model's random error and bias respectively
  - Model's performance considered good when RRMSE<10%
- R^2 demonstrates the strength of the relationship between predicted output and true output

Machine Learning Performance Metric Data (1)
10-fold cross validation, 100 iterations

	M1 (LR)	M2 (LR)	M3 (LR)	M4 (LR)	M5 (Tree)	M6(Tree)	M7 (Tree)
RRMSE (%)	4.068 (0.062689)	3.9242 (0.11549)	4.0895 (0.070191)	4.1007 (0.10261)	3.2123 (0.17075)	5.3874 (0.15707)	18.437 (0.11204)
RMSE (°C) 10,15	13.588 (0.20939)	13.108 (0.38577)	13.66 (0.23445)	13.697 (0.34275)	10.73 (0.57034)	17.995 (0.52465)	61.584 (0.37424)
MPE (%), 0.1,0.5	0.20471 (0.039866)	0.087626 (0.079677)	0.22731 (0.053016)	0.18314 (0.049463)	0.1282 (0.22022)	0.21495 (0.25702)	3.6316 (0.026516)
MBE (°C) 0.1,2.5	-0.017805 (0.12912)	-0.34239 (0.29372)	0.028399 (0.17575)	-0.095156 (0.17959)	0.014193 (0.74397)	-0.38617 (0.86976)	-0.0038408 (0.062058)
R^2 0.90,0.95	0.94983 (0.0015507)	0.95328 (0.0028097)	0.94929 (0.001747)	0.949 (0.0025672)	0.96864 (0.0033346)	0.91195 (0.0051559)	-0.030398 (0.012549)

Mean (Standard Deviation) of each performance metric across each iteration

Machine Learning Performance Metric Data (2)

	M8 (SVM)	M9 (SVM)	M10 (SVM)	M11 (SVM)	M12 (SVM)	M13 (SVM)
RRMSE (%)	4.1369 (0.090457)	3.8027 (0.28549)	4.0446 (1.8555)	3.6905 (0.17668)	3.2576 (0.11755)	8.9222 (0.098517)
RMSE (°C) 10,15	13.818 (0.30215)	12.702 (0.95361)	13.51 (6.1978)	12.327 (0.59014)	10.881 (0.39265)	29.802 (0.32907)
MPE (%), 0.1,0.5	0.1228 (0.10834)	-0.05139 (0.15123)	-0.16027 (0.43116)	-0.0011512 (0.088299)	0.28529 (0.10299)	3.0115 (0.075773)
MBE (°C) 0.1,2.5	-0.24574 (0.32373)	-0.25364 (0.51647)	-0.95106 (1.5696)	-1.149 (0.29601)	-0.098814 (0.28771)	5.1567 (0.24404)
R^2 0.90,0.95	0.9481 (0.0022763)	0.95592 (0.0071501)	0.94008 (0.077062)	0.95862 (0.004136)	0.96779 (0.0023425)	0.75868 (0.0053523)

Mean (Standard Deviation) of each performance metric across each iteration

Machine Learning Performance Metric Data (3)

	M14 (TE)	M15 (TE)	M16 (GPR)	M17 (GPR)	M18 (GPR)	M19 (GPR)
RRMSE (%)	5.3143 (0.14786)	4.4055 (0.2426)	2.6042 (0.20987)	2.6124 (0.15187)	2.3035 (0.10146)	2.6445 (0.11934)
RMSE (°C)	17.751 (0.4939)	14.715 (0.81033)	8.6985 (0.70102)	8.7258 (0.50726)	7.6942 (0.33891)	8.8332 (0.39861)
MPE (%)	-4.3059 (0.13412)	0.030781 (0.17748)	0.026875 (0.10445)	-0.050257 (0.095723)	-0.023721 (0.063577)	-0.014602 (0.10081)
MBE (°C)	-14.761 (0.42028)	-1.5232 (0.56807)	-0.18834 (0.35848)	-0.46048 (0.31028)	-0.33669 (0.20031)	-0.37373 (0.31805)
R^2	0.91433 (0.004775)	0.941 (0.0065452)	(0.97931) 0.0041553	0.97925 (0.002528)	0.98389 (0.0014497)	0.97876 (0.0019765)

Mean (Standard Deviation) of each performance metric across each iteration

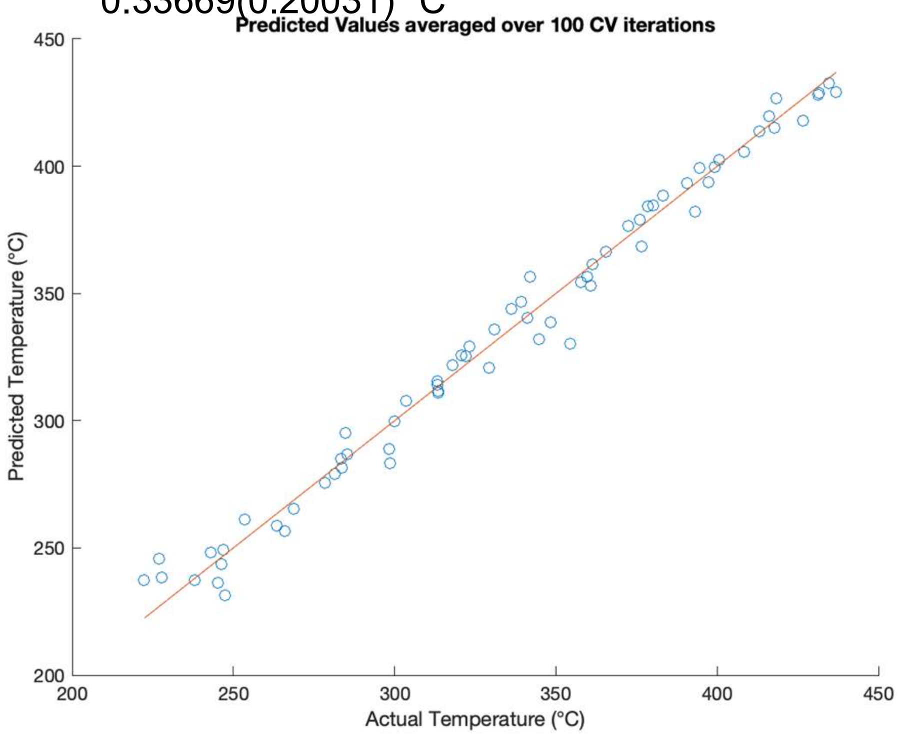
Best Performance Metrics for each ML method

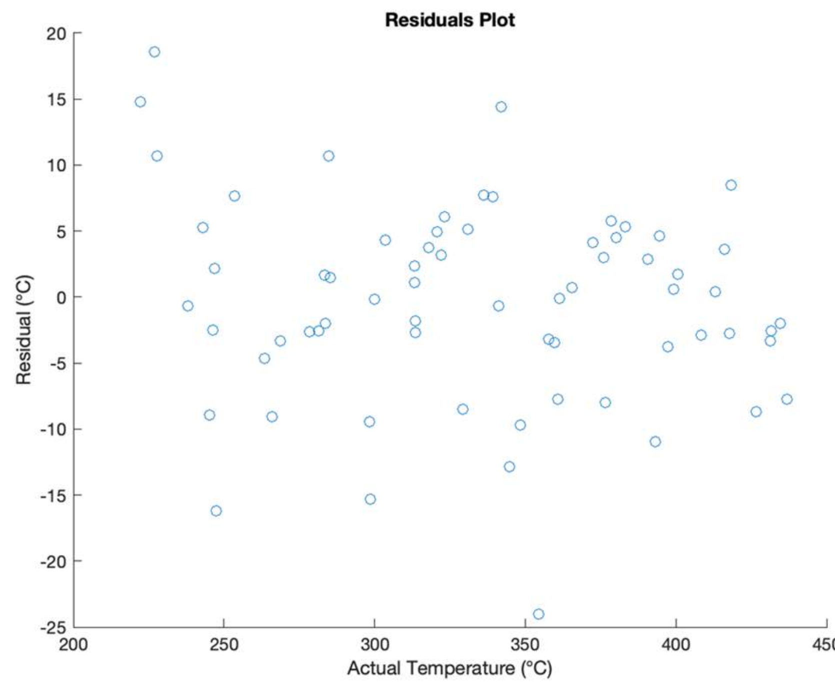
- Linear Regression
  - M1: Linear Regression
- Tree
  - M5: Fine Tree
- Support Vector Machine
  - M12: Medium Gaussian SVM
- Trees Ensemble
  - M15: Bagged Trees Ensemble
- Gaussian Process Regression
  - M18: Exponential GPR

Minimizing RMSE - M18: Exponential GPR

RMSE: 7.6942 (0.33891) °C

MBE: -
0.33669(0.20031) °C

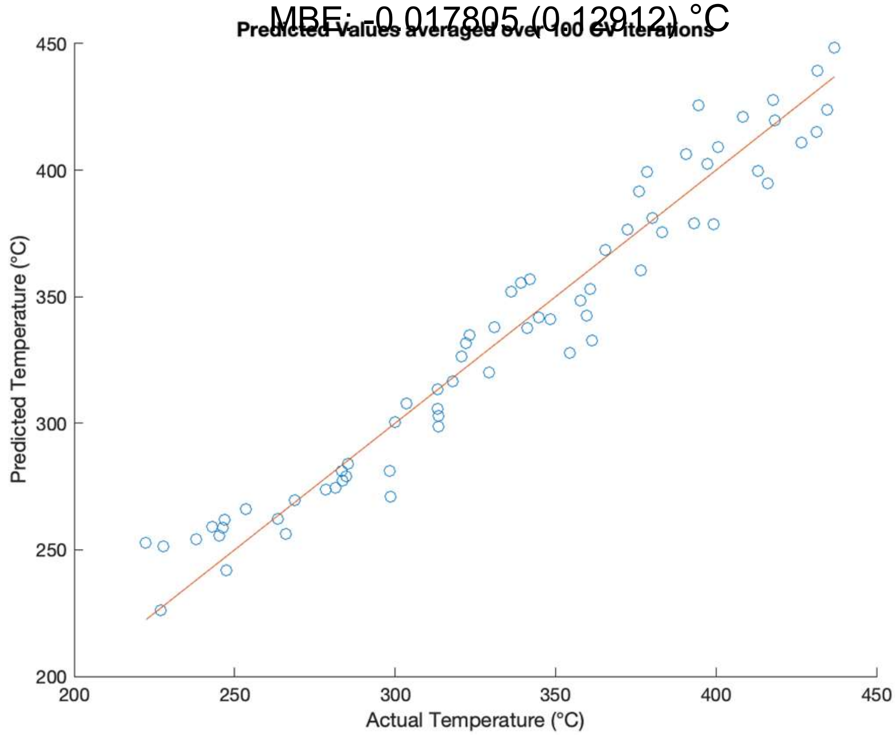


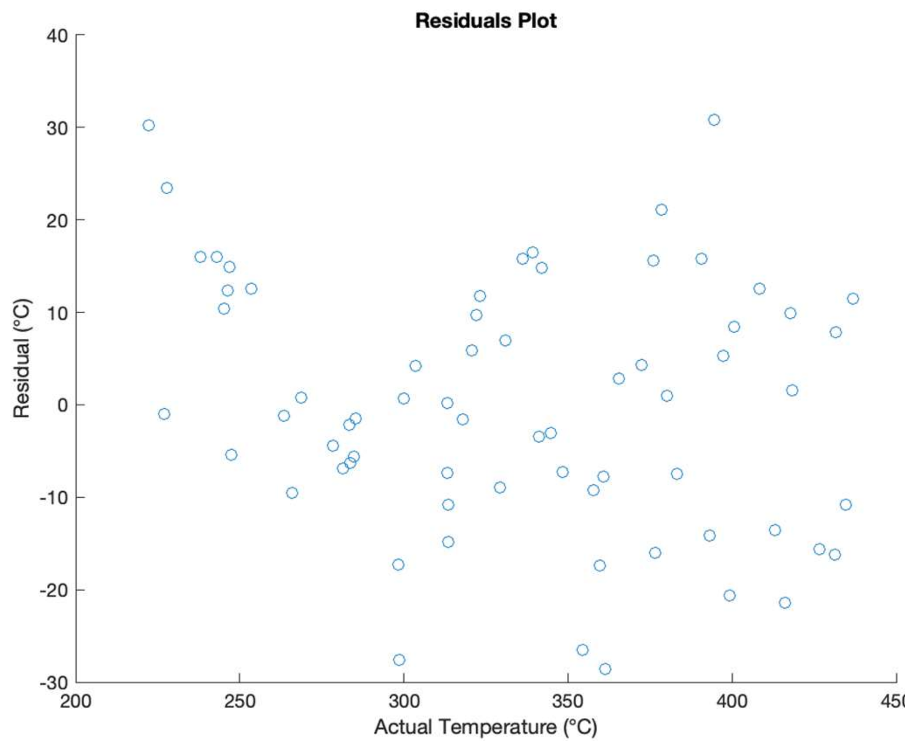


Minimizing MBE - M1: Linear Regression

RMSE: 13.588 (0.20939) °C

MBE: -0.017805 (0.12912) °C

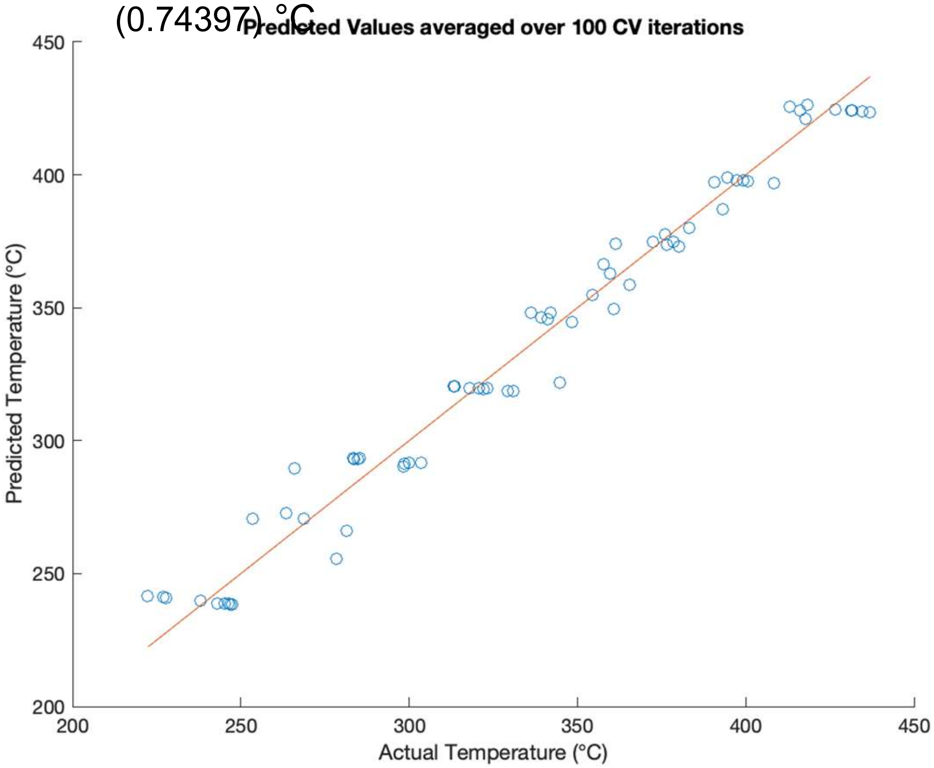


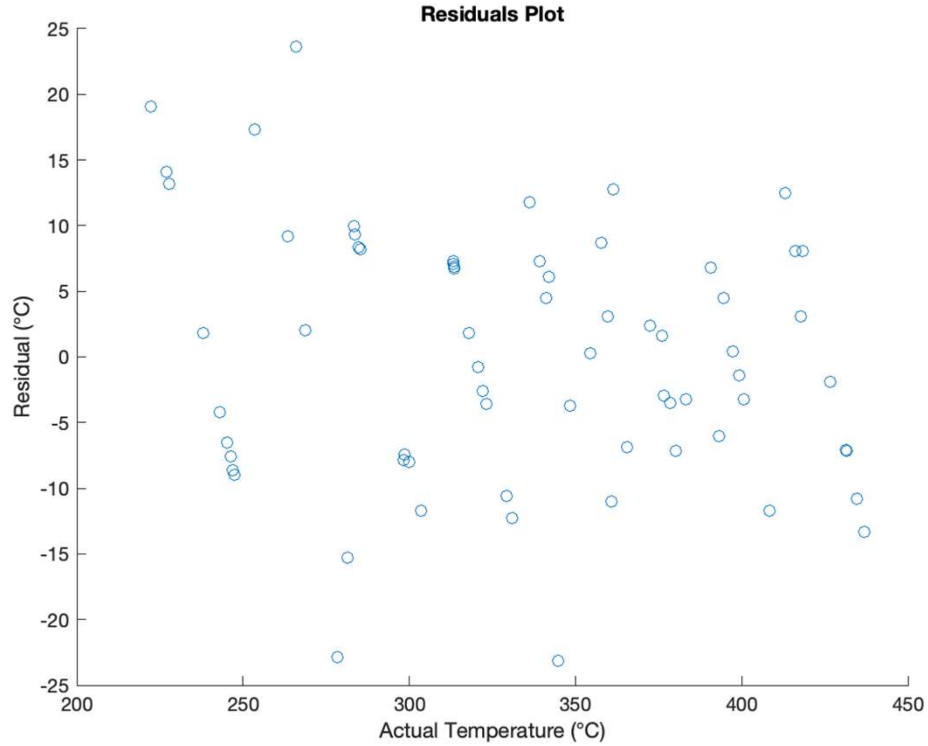


Minimizing MBE - M5: Fine Tree

RMSE: 10.73 (0.57034) °C
(0.74397) °C

MBE: 0.014193

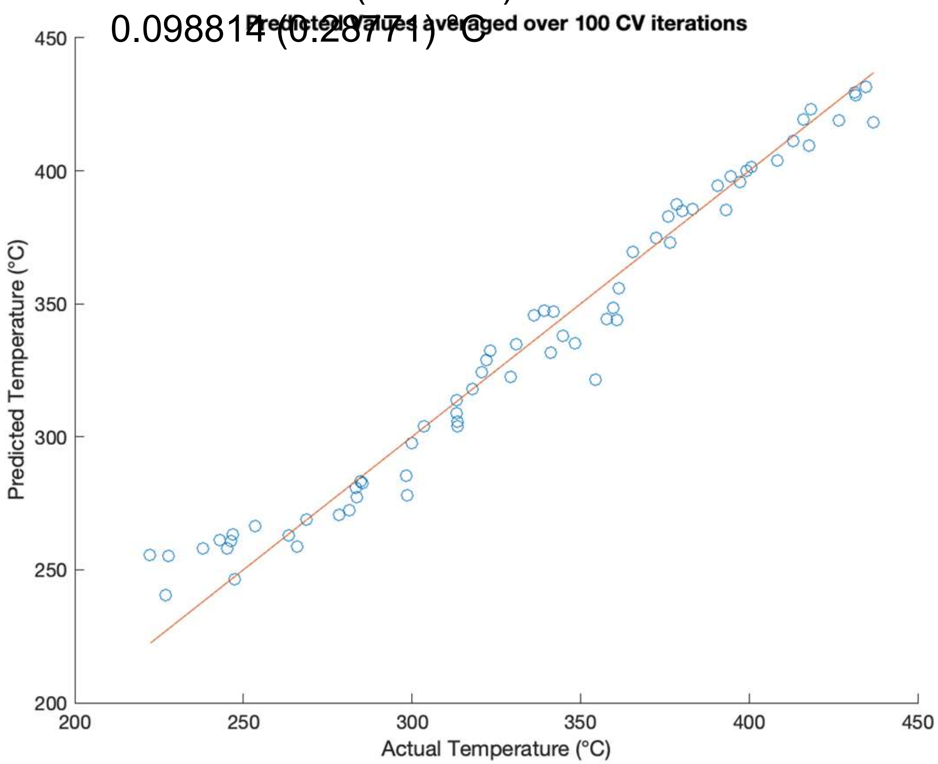


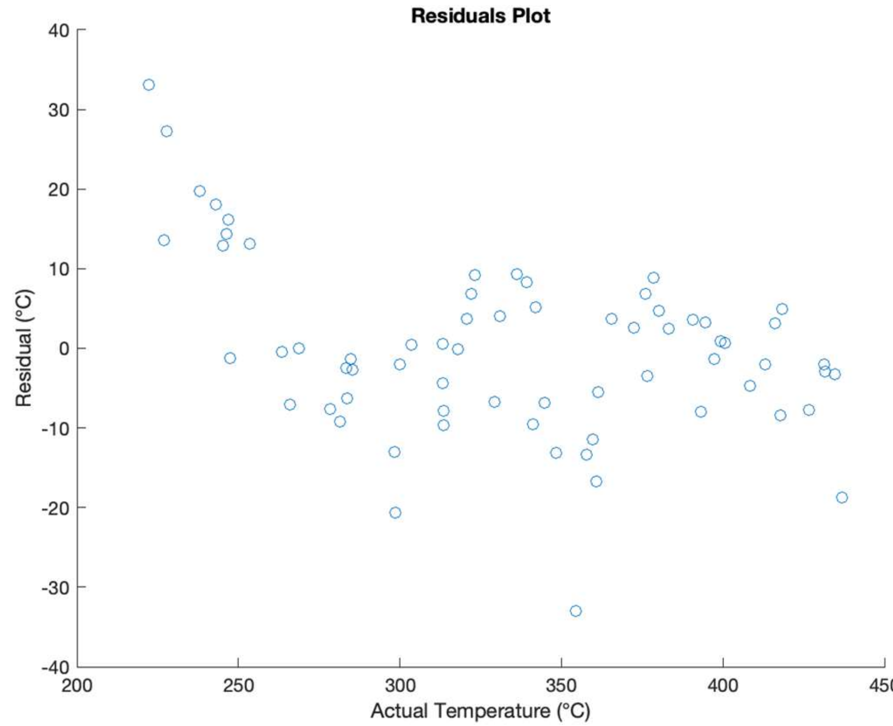


M12: Medium Gaussian SVM

RMSE: 10.881 (0.39265) °C

MBE: -
0.098814 (0.28771) °C

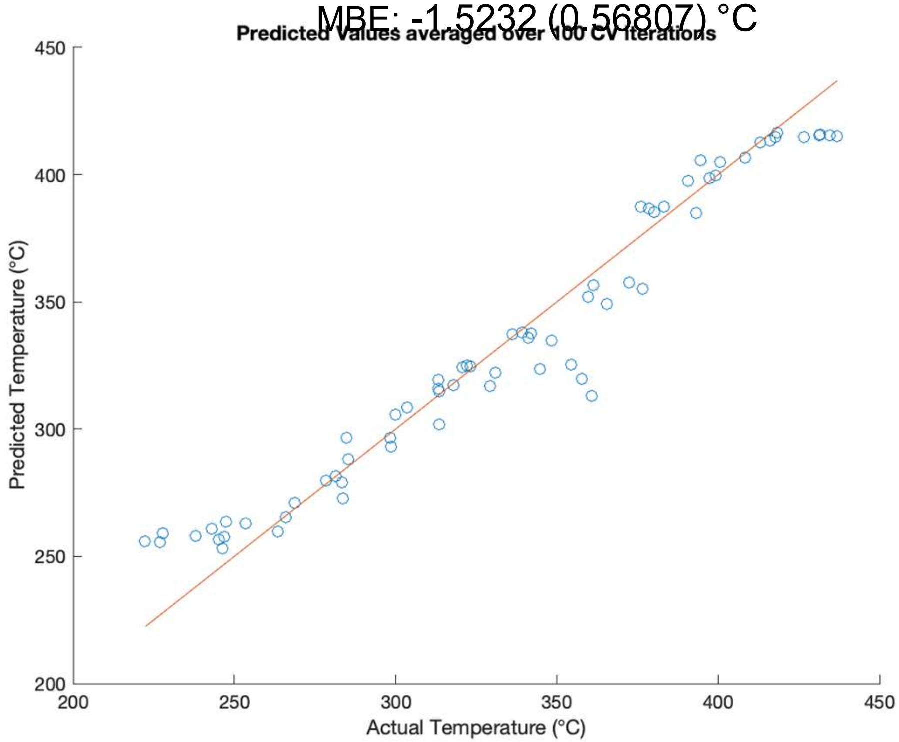


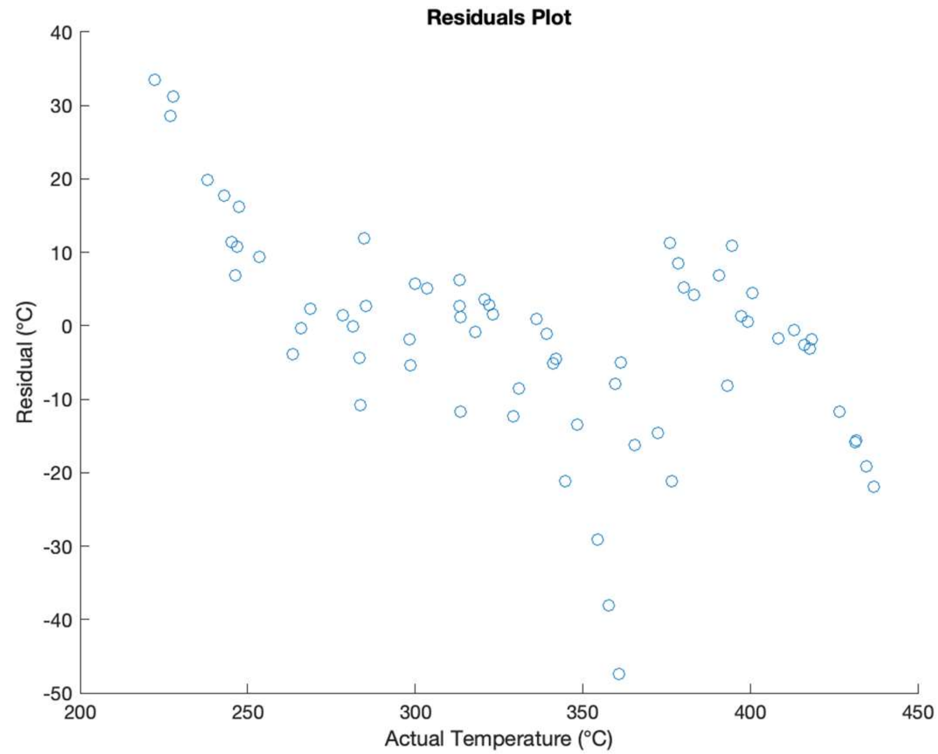


M15: Bagged Trees Ensemble

RMSE: 14.715 (0.81033) °C

MBE: -1.5232 (0.56807) °C





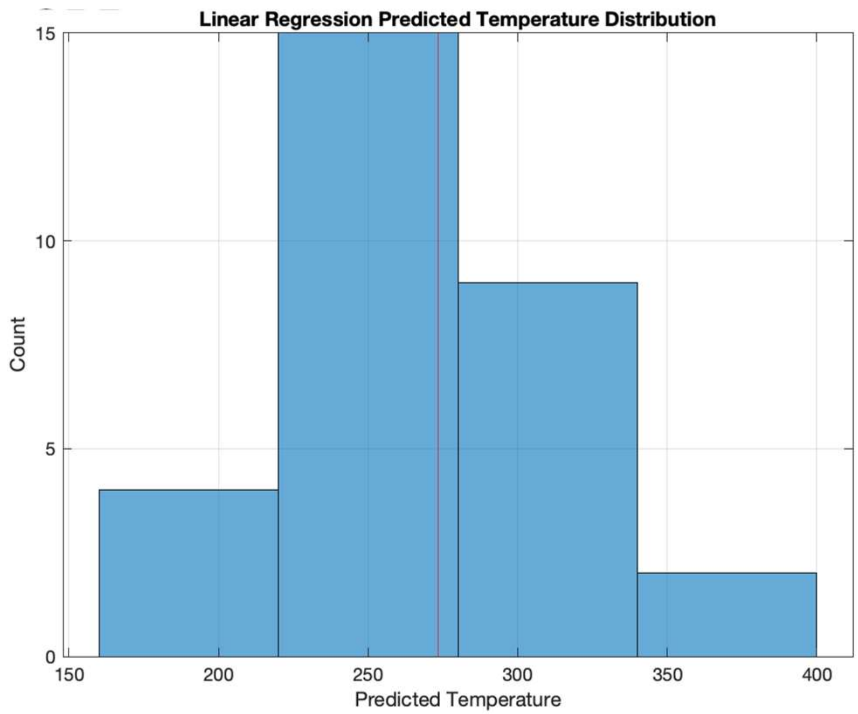
Max Temperature Distribution of Exp. Biomass Particles

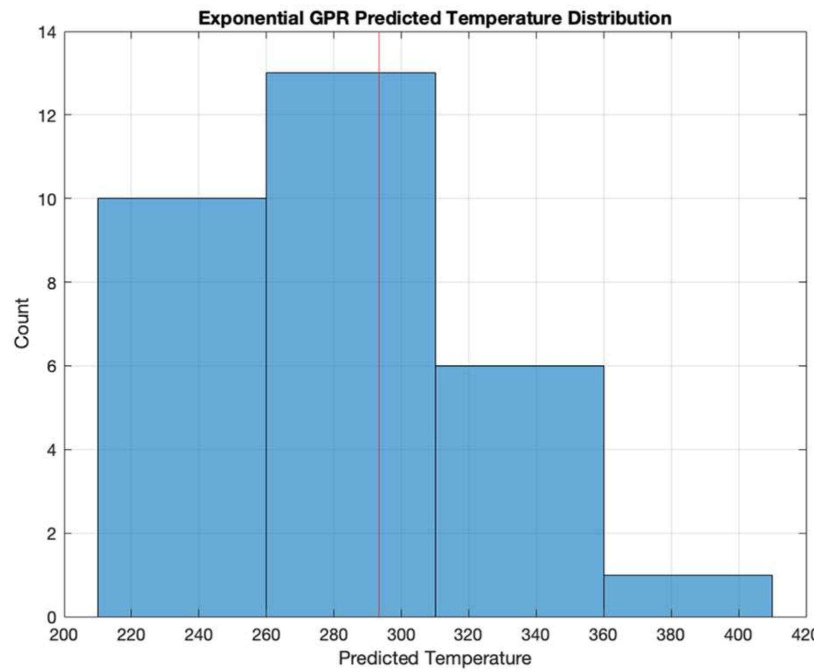
- Focus on M1 (Linear Regression) and M18 (Exponential GPR)
  - Boundaries
- 8 reactor runs
- For each run, 30 biomass sample particles
  - 1 mixed sample, approx. average material properties

1126pine

M1: Linear Regression

M18: Exponential





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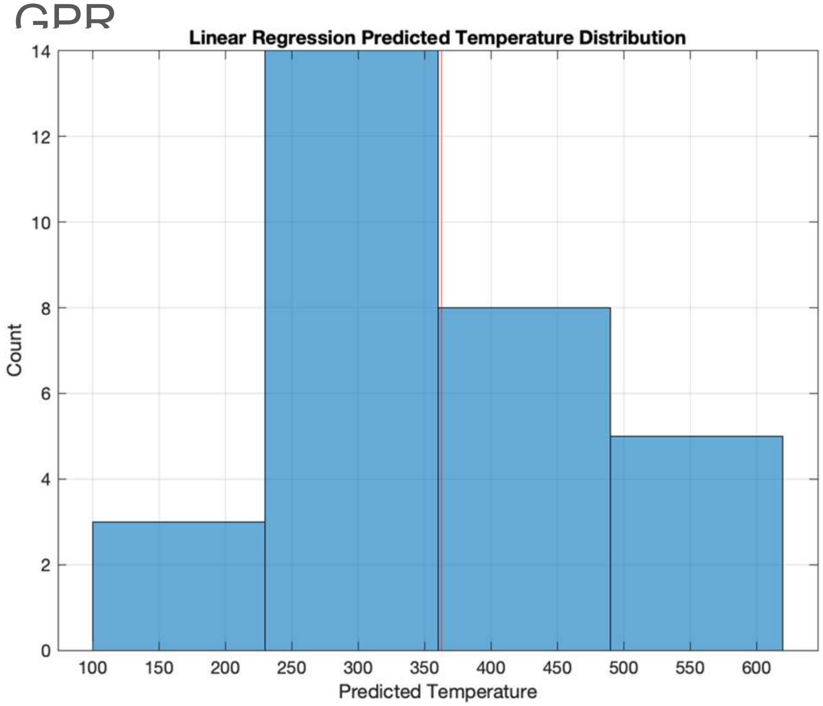
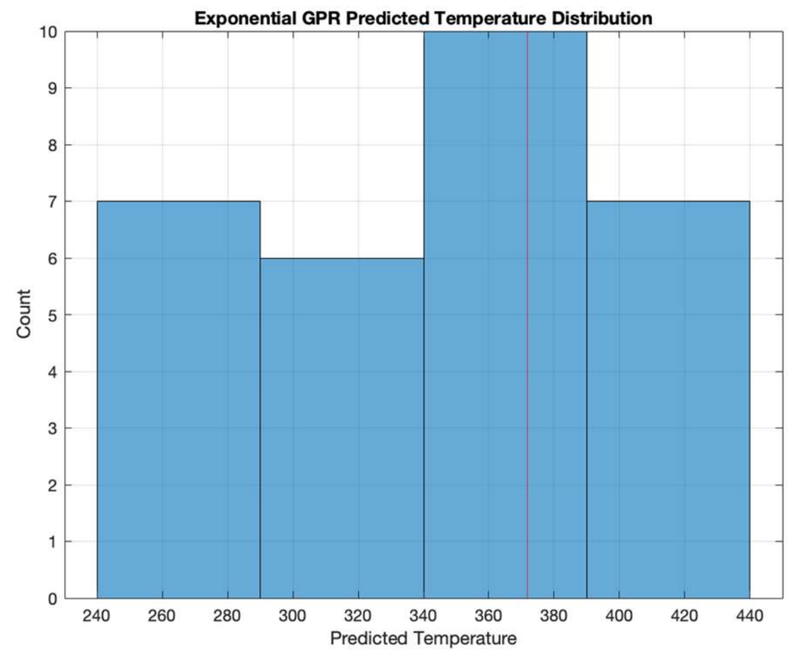
M1: Linear Regression

GPR



M18: Exponential



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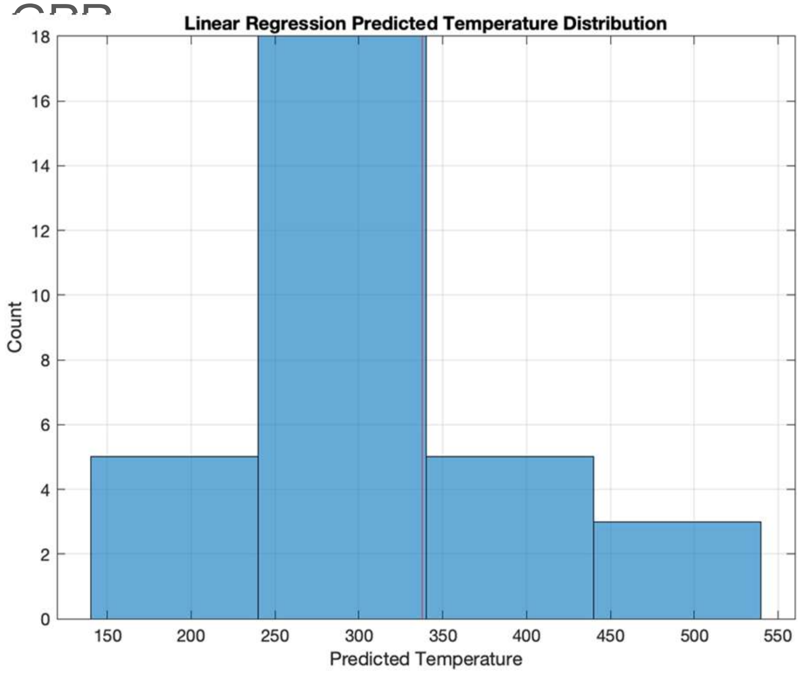
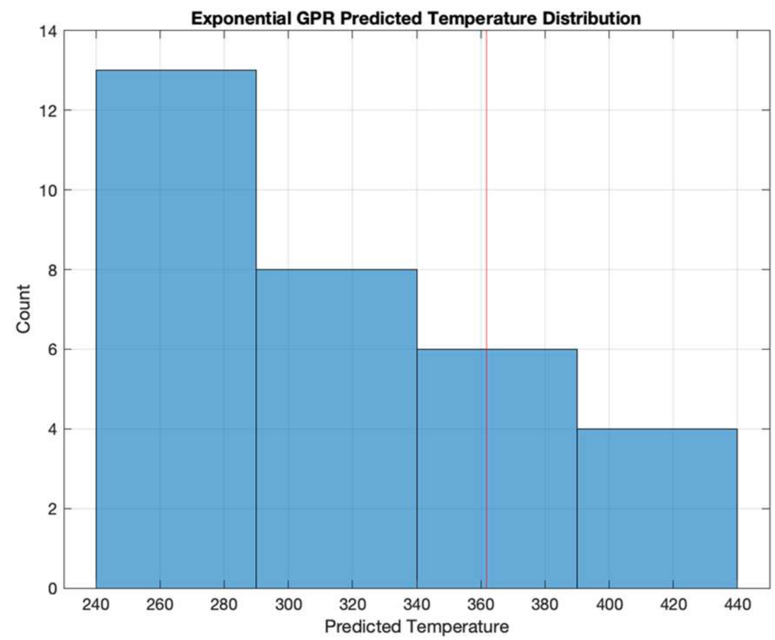
M1: Linear Regression

M18: Exponential GPR





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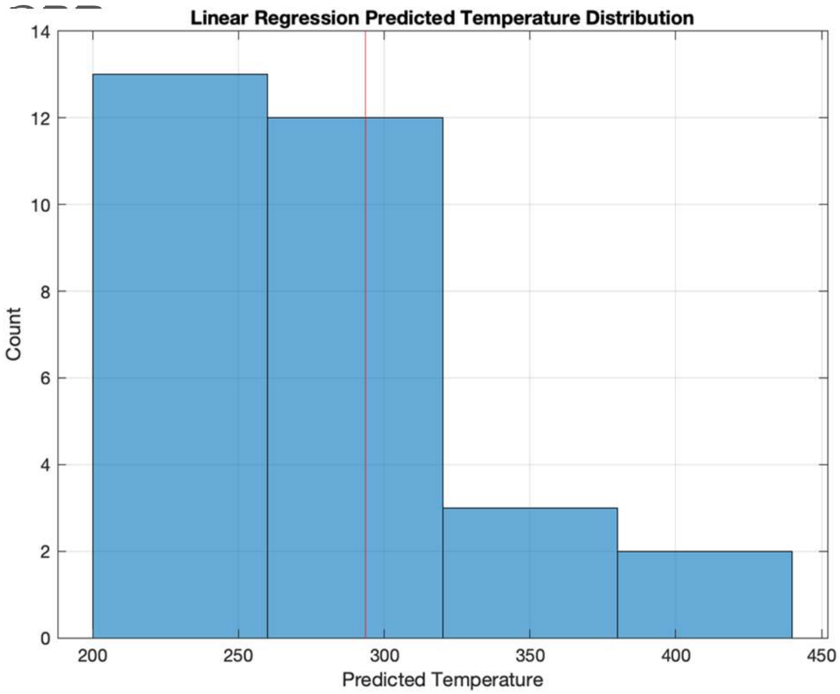
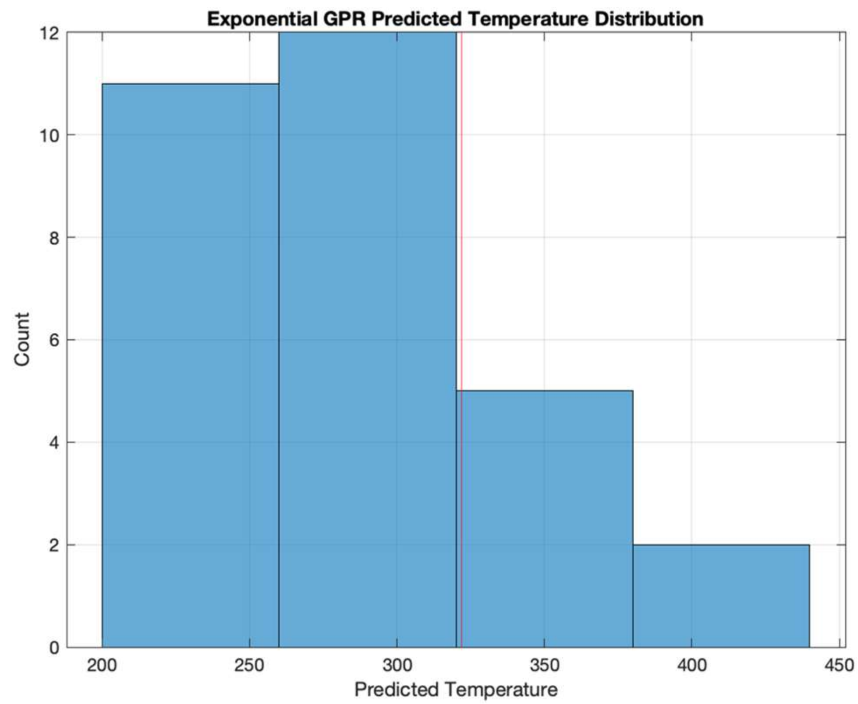
M1: Linear Regression

M18: Exponential





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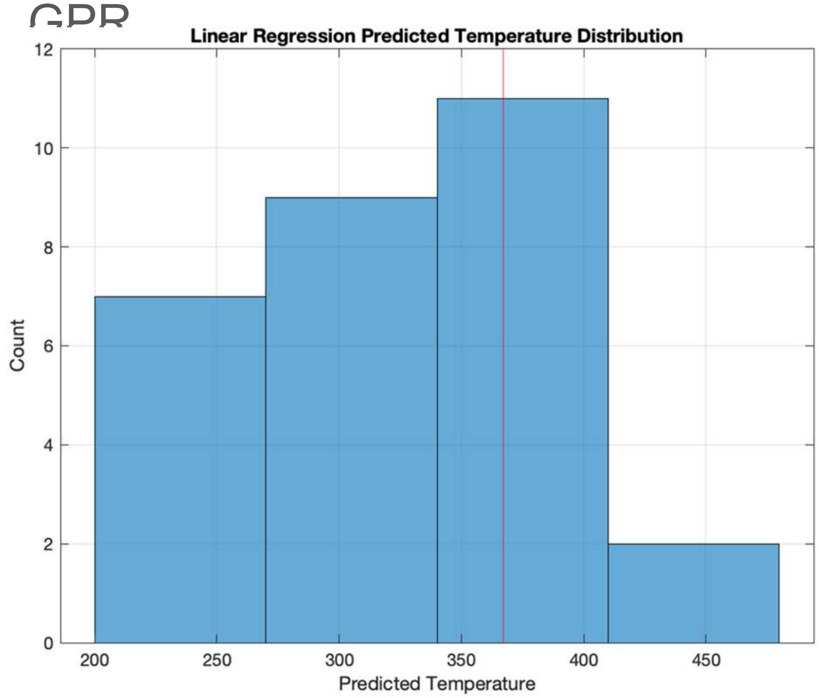
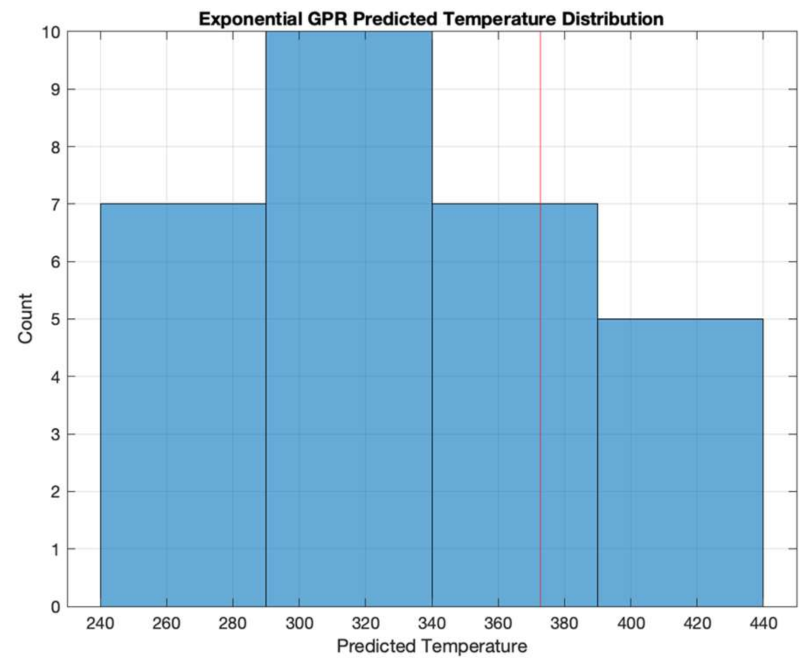
M1: Linear Regression

M18: Exponential GPR





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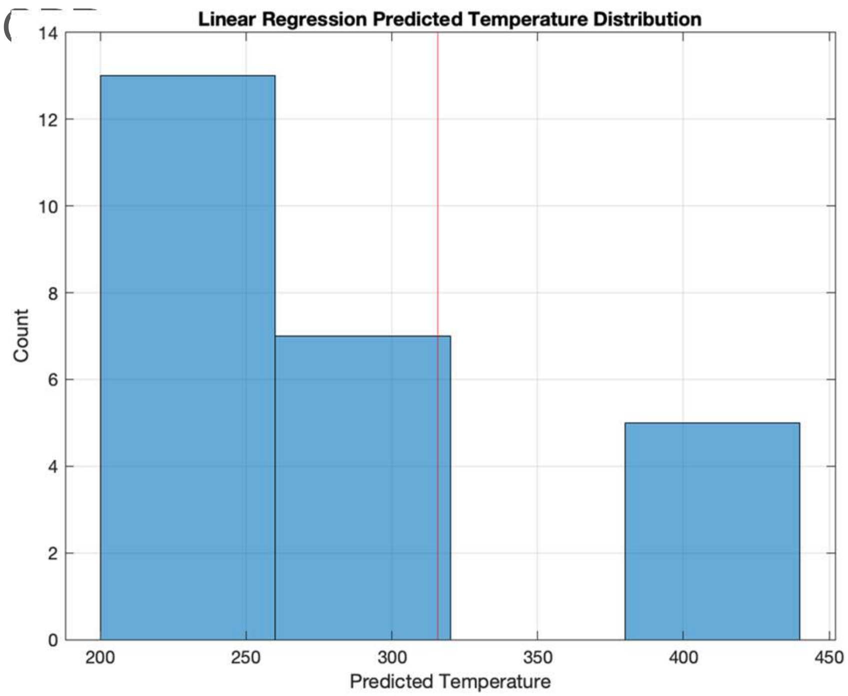
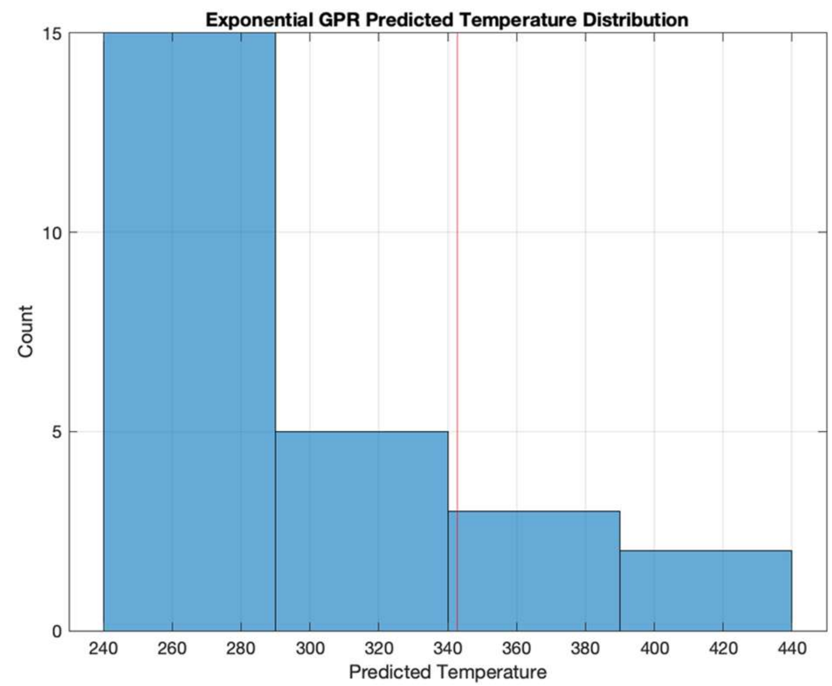
M1: Linear Regression

M18: Exponential





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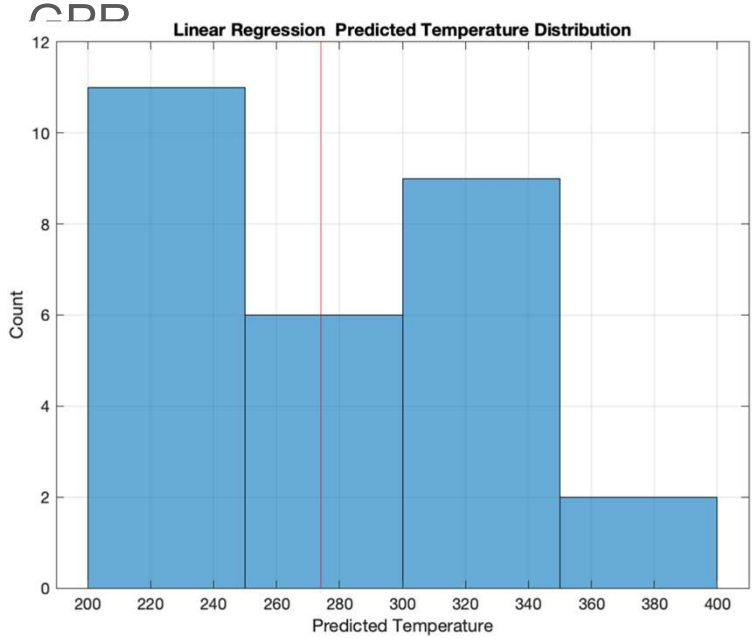
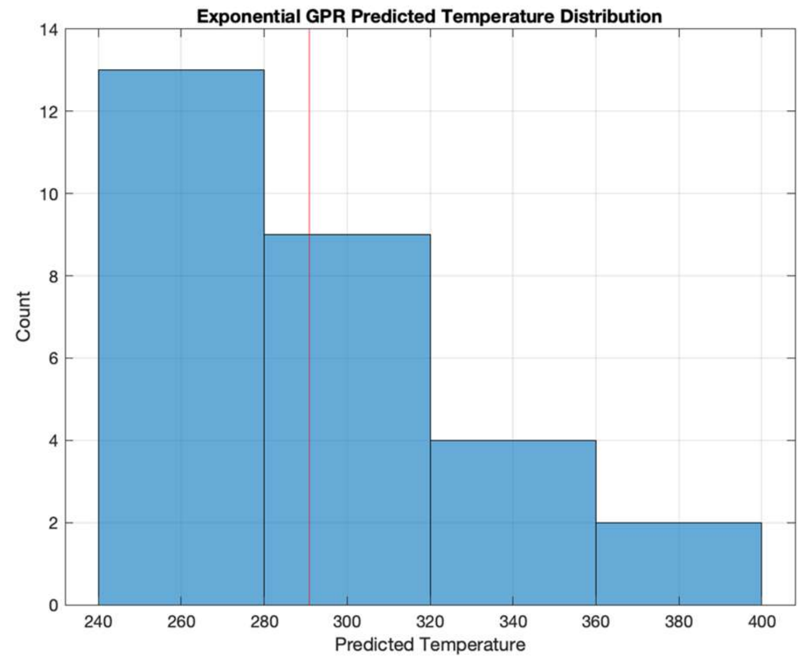
M1: Linear Regression

M18: Exponential GPR





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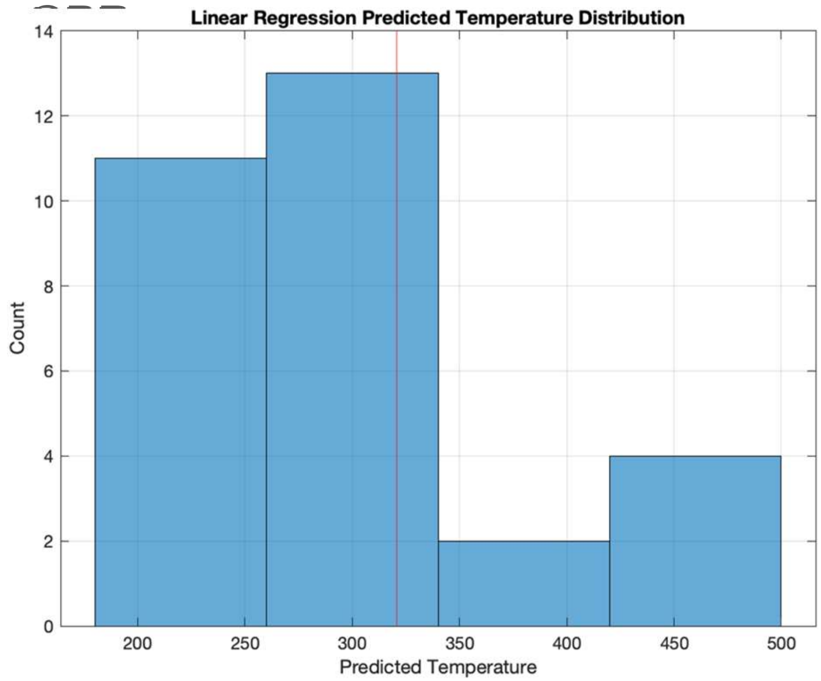
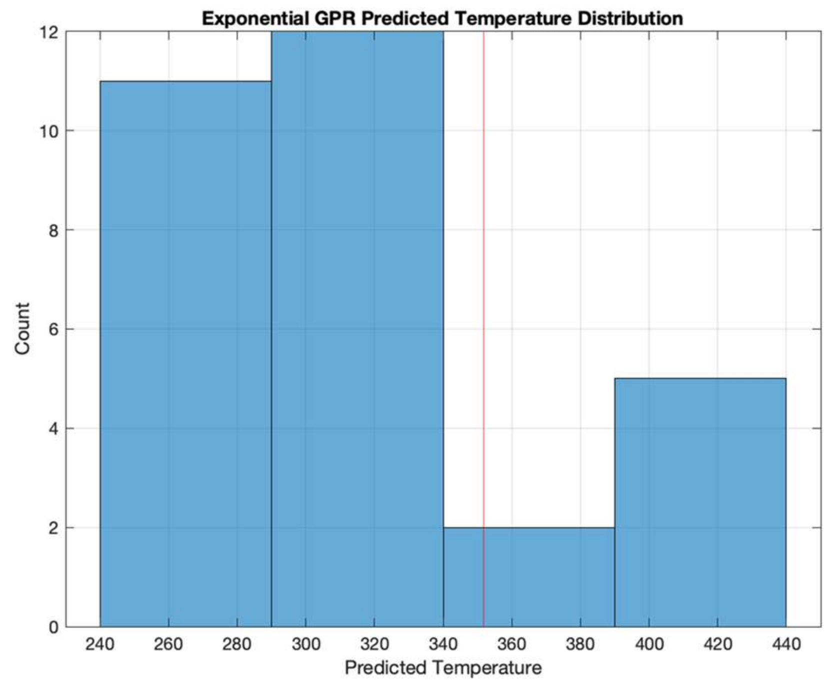
M1: Linear Regression



M18: Exponential



References

IORDANIDIS, A., ASVESTA, A., & VASILEIADOU, A. (2018). Combustion Behaviour of Different Types of Solid Wastes and Their Blends with Lignite. *Thermal Science*, *22*(2), 1077–1088. https://doi-org.revproxy.brown.edu/10.2298/TSCI170704219I

Vasileiadou, A., Zoras, S., & Iordanidis, A. (2021). Fuel Quality Index and Fuel Quality Label: Two versatile tools for the objective evaluation of biomass/wastes with application in sustainable energy practices. *Environmental Technology & Innovation*, *23*. https://doi-org.revproxy.brown.edu/10.1016/j.eti.2021.101739

William S. Cleveland, & Susan J. Devlin. (1988). Locally Weighted Regression: An Approach to Regression Analysis by Local Fitting. *Journal of the American Statistical Association*, *83*(403), 596–610. https://doi-org.revproxy.brown.edu/10.2307/2289282

Rohani, A., Taki, M., & Abdollahpour, M. (2018). A novel soft computing model (Gaussian process regression with K-fold cross validation) for daily and monthly solar radiation forecasting (Part: I). *Renewable Energy: An International Journal*, *115*, 411–422. https://doi-org.revproxy.brown.edu/10.1016/j.renene.2017.08.061

Lu, H.-J., Zou, N., Jacobs, R., Afflerbach, B., Lu, X.-G., & Morgan, D. (2019). Error assessment and optimal cross-validation approaches in machine learning applied to impurity diffusion. *Computational Materials Science*, *169*. https://doi-org.revproxy.brown.edu/10.1016/j.commatsci.2019.06.010

Levenspiel, O. (1999). Part III: Reactions Catalyzed by Solids, Chemical Reaction Engineering (3rd Edition), pp. 367-516, John Wiley & Sons Inc, ISBN 0-471-25424-X, New York