Physics-informed Prediction of Laminar Burning Velocity of NH_3/H_2/air Mixtures Using Machine Learning

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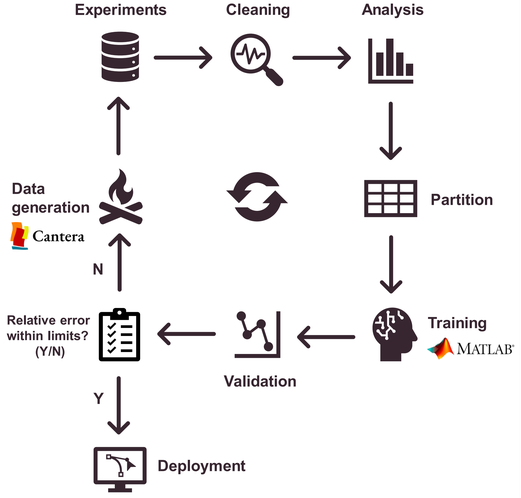
Introduction

- **Laminar burning velocity (LBV)** is a fundamental fuel property that can be experimentally and numerically determined.
- **Computation of LBV** can be time-consuming depending on the mechanism size, stiffness and numerical set-up.
- **Machine learning** can be used to accelerate LBV predictions while preserving accuracy.



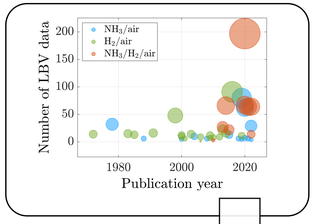
Research Questions

- **Which ML algorithm** would be the best suitable in the prediction of LBV?
- How **accurate** would the ML model be?
- By how much can ML **accelerate** the prediction of LBV compared to 1D numerical simulations?

Methodology

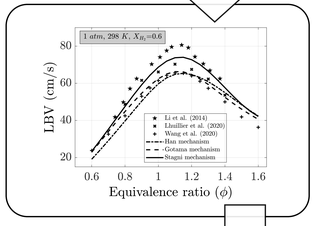
Experimental data collection and analysis

NH_3/air, H_2/air and NH_3/H_2/air LBV data is collected from the literature and analysed.



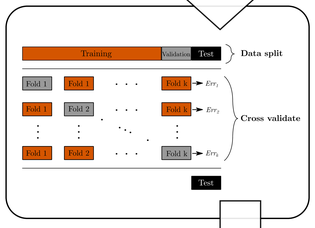
Mechanism selection and LBV data generation

Gotama [1], Stagni [2] and Han [3] mechanisms are tested for LBV computation accuracy. Additional LBV data is generated through 1D simulations on Cantera.



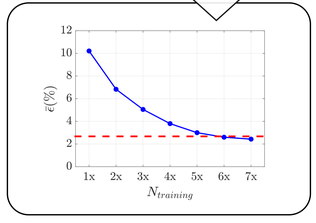
Data partition and k-fold cross validation

The data is partitioned as 70%/15%/15% for training, validation and test datasets, respectively.



ML model selection and optimisation

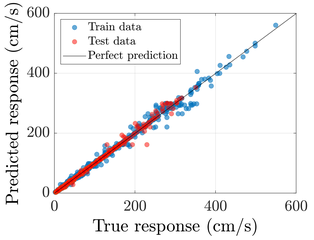
24 different ML algorithms were tested to for the highest accuracy. Chosen model is then optimised based on hyperparameters.



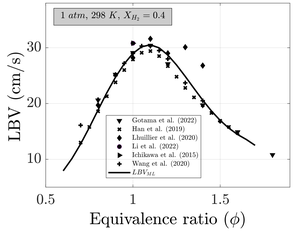
Results

ML algorithms	R^2	MAE	RMSE	Speed-up (t_{1D}/t_{ML})
LR	0.96	12.9	14.6	27000
RT	0.98	9.9	11.5	26000
SVM	0.99	7.5	8.6	24000
GPR	**0.99**	**4.2**	**6.9**	**20000**
ET	0.95	13.1	14.5	26000
NN	0.99	5.4	7.2	9500

ML model evaluation results.



Predictions vs. true values of LBV for GPR algorithm



Application and validation of optimised ML model

Summary

- In this work, **an ML model was developed** to predicts LBV of NH_3/H_2/air mixtures for a wide range of conditions.
- **Gotama mechanism** outperforms the mechanisms by Han and Stagni in the computation accuracy of LBVs for NH_3/H_2/air mixtures.
- The predictive capability of black-box models can be increased via hybrid ML models using **physics-based synthetic data**.
- The model satisfactorily predicts majority of the conditions with reasonable accuracy (R^2**=0.998**).
- ML based predictive models speed up the LBV calculation time from **9500 to 27000 times**.

References

1. Gotama, Gabriel J., et al. "Measurement of the laminar burning velocity and kinetics study of the importance of the hydrogen recovery mechanism of ammonia/hydrogen/air premixed flames." Combustion and Flame 236 (2022): 111753.
2. Stagni, Alessandro, et al. "An experimental, theoretical and kinetic-modeling study of the gas-phase oxidation of ammonia." Reaction Chemistry & Engineering 5.4 (2020): 696-711.
3. Han, Xinlu, Marco Lubrano Lavadera, and Alexander A. Konnov. "An experimental and kinetic modeling study on the laminar burning velocity of NH3+ N2O+ air flames." Combustion and Flame 228 (2021): 13-28.