Knowledge Graph Approach to Automation of Combustion Mechanism Development

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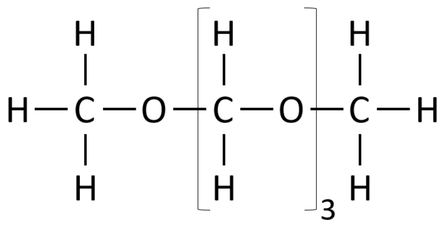


In this work, a knowledge graph based framework for automatic calibration of combustion mechanism has been developed to facilitate assessing alternative fuels. The calibrated mechanism of polyoxymethylene dimethyl ether (PODE3) was able to accurately predict combustion characteristics in engines.

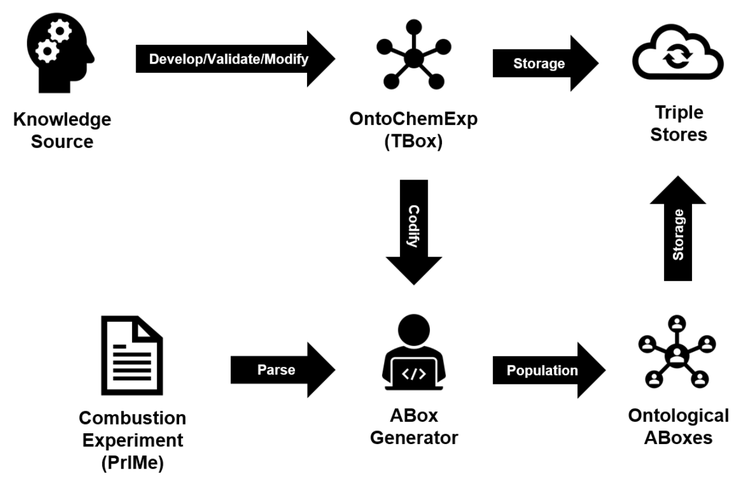
INTRODUCTION

J-Park Simulator (JPS) [1] is an integration of real-time linked-data and autonomous agents. JPS implements ideas of intelligent operations thus offering new ways of solving the climate change problem. The development of accurate combustion mechanism plays a vital role in promoting an energy transition towards sustainable resources. Presently, this work is manually undertaken by researchers with heavily borrowed sub-mechanism from each other. It is not only time consuming but also prone to errors. To improve this process, a knowledge graph that captures the combustion experimental data was constructed in this work based on PrIMe database [2]. Taking existing mechanism [3] as a starting point, MoDS [4] agent, utilizing *k*inetics [5], was developed to tune the model against various sources of experimental data that were retrieved from the knowledge graph. With a good agreement with experimental data, such a combination was demonstrated as an additional component of JPS to facilitate its overall aim of decarbonisation.

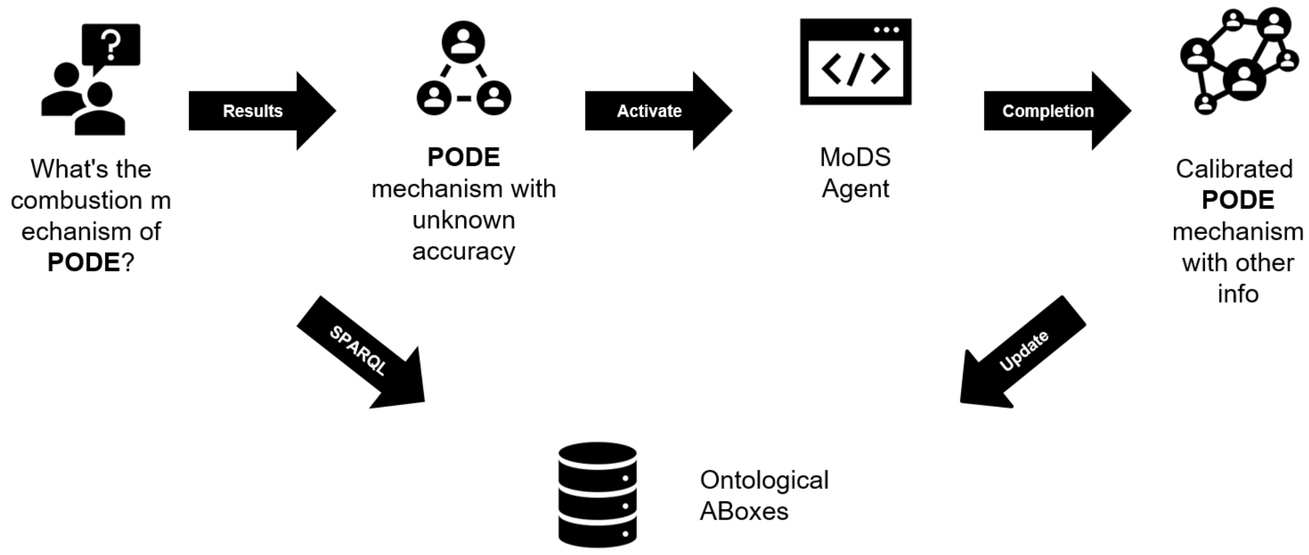
METHODOLOGY

There are two major steps involved:

- knowledge graph construction



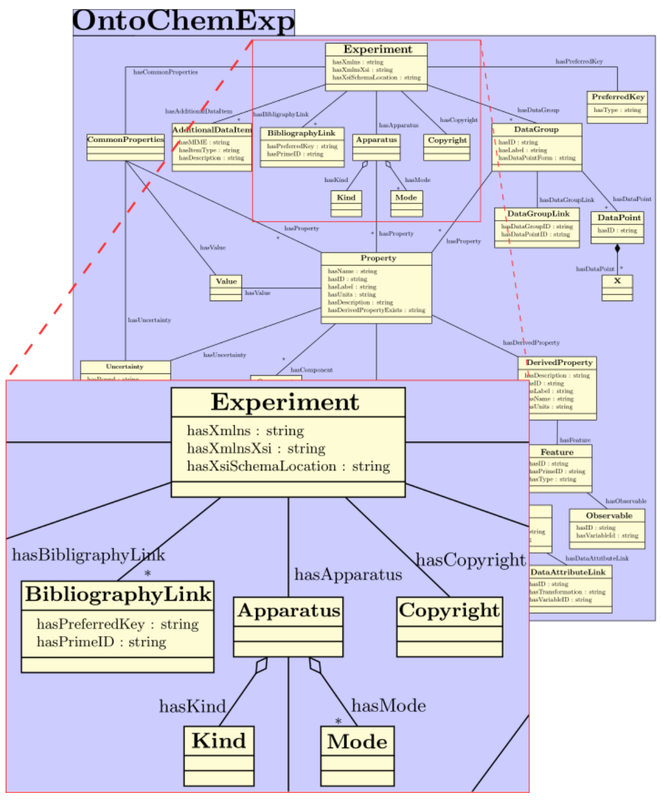
- autonomous agent development



RESULTS AND DISCUSSION

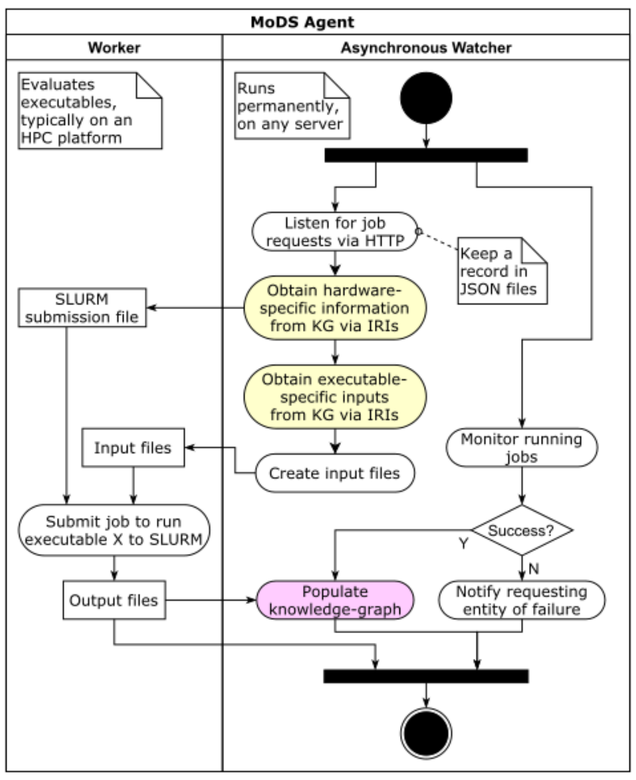
Constructed knowledge graph in UML

- Logical description of combustion
- Graphical representation of data



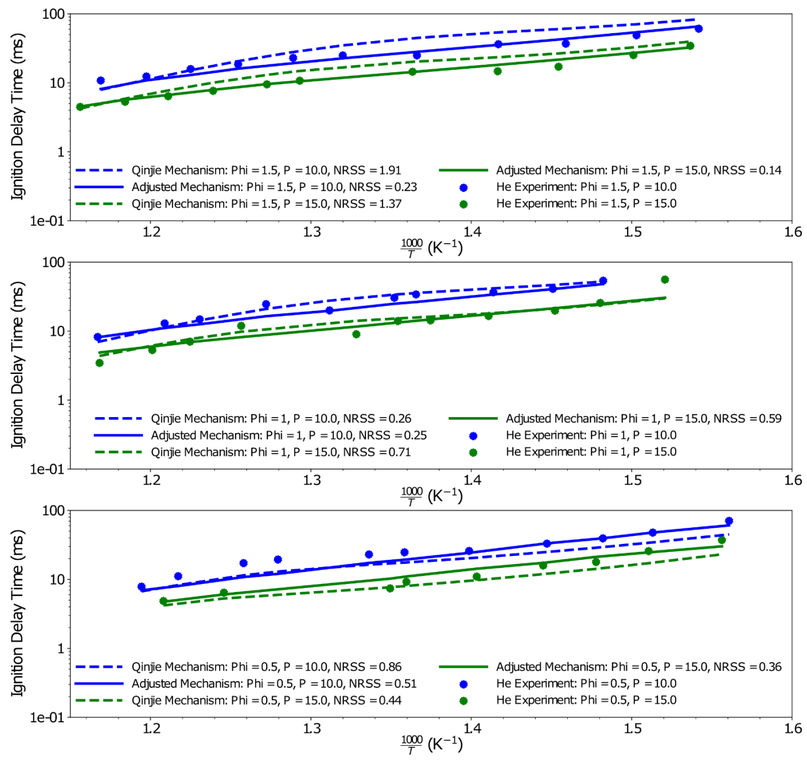
MoDS agent conceptual workflow

- Automated model calibration
- Easy response to HTTP request



Performance of calibrated mechanism

- Improved accuracy in simulation
- Better understanding of mechanism



CONCLUSIONS AND FURTHER WORK

This work presents a knowledge graph approach to automate the process of developing chemical mechanisms. The combination of knowledge graph and the autonomous agent promotes the JPS towards an intelligent operation. Future development of the JPS ecosystem will offer a better understanding of energy problem and play a vital role in tackling climate change.

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KEY REFERENCES

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