SimDOME

User Story: Exhaust after-treatment (EAT) models for vehicular applications

ALMA MATER STUDIORUM UNIVERSITÀ DI BOLOGNA · CMCL · umicore materials for a better life · Fraunhofer IWM · Politecnico di Torino · NIREOS

Aims

- To predict behaviour of EAT devices to comply with ever more stringent emission standard
- To make EAT models accessible via a semantic digital platform

Methodology

- Develop models for catalytic converters and particulate filters
- Ontological descriptions of models, inputs and outputs

Results

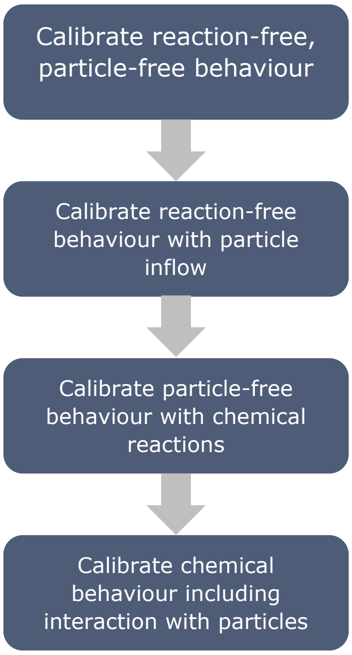
- Capability to capture catalytic converter and filter behaviours
- Developed interoperable workflow of after-treatment models

Summary

Exhaust after-treatment (EAT) devices including catalytic converters and particulate filters are important components of vehicles with Internal Combustion Engines (ICEs). Their role is to mitigate toxic gaseous and particulate emissions in compliance with the legal emission standards.

Optimisation and innovation of EAT technologies are needed to ensure vehicles comply with the latest emission tests. Computational modelling is a key part of such investigations as it enables consideration of a wide range of operating conditions and design parameters in a time- and cost-effective manner.

This example demonstrates the capability of models of catalytic converters and particulate filters, two major types of after-treatment devices, developed within CMCL's *k*inetics™ software.



Case Description

The catalytic converter model is applied to simulate a lab-scale experimental study of a three-way catalyst (TWC) [1]. A one-dimensional flow reactor model is formulated within *k*inetics™ with capabilities to consider detailed heterogeneous chemistry, convective mass transfers and pore diffusion within the catalytic washcoat.

The filter model is applied to model a particulate filter connected with an engine flow bench, with emphasis on its filtration behaviour [2]. The particulate filter model implemented in *k*inetics™ is coupled with a sectional population balance model to consider the impact of particles of various sizes on the internal gas flow of a filter.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement number 814492.

Results

The performance of the catalytic converter model is assessed against literature experimental data. The result for the stoichiometric combustion case is shown here. Qualitative agreements with experimental data can be observed.

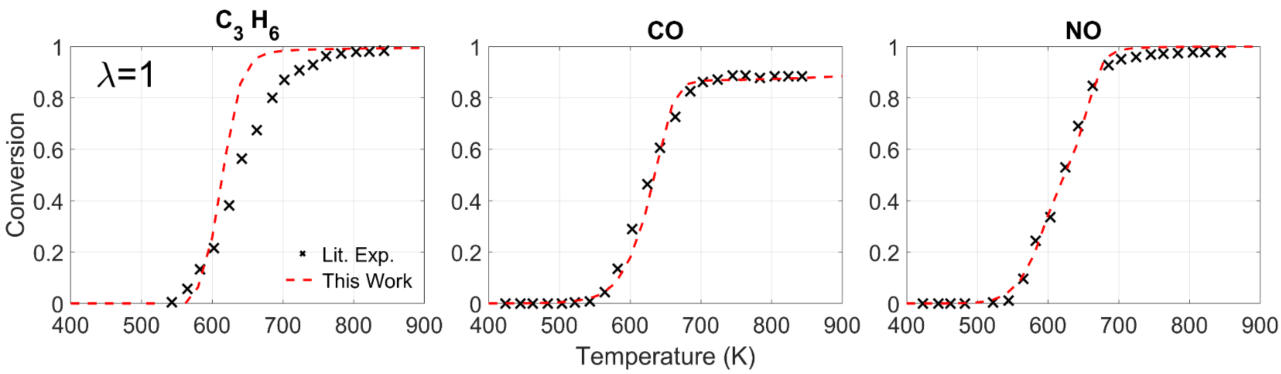


Figure 1: Simulated catalytic pollutant conversions as functions of temperature

The wall permeability of the particulate filter is calibrated against results of particle-free experiments. The filtration model parameters are calibrated against results of particle-loading experiments. The model is shown to be capable of parameterising the particulate filter which enables accurate simulation of its behaviour.

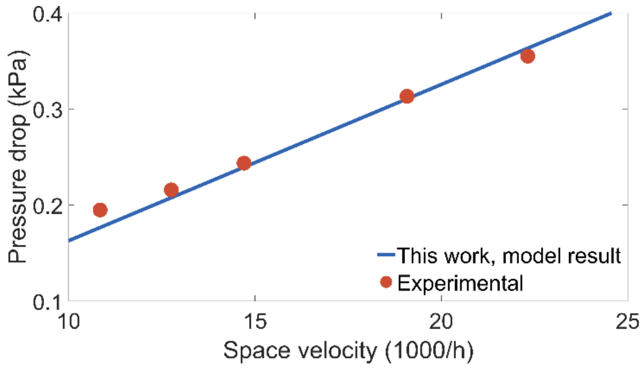


Figure 2: Simulated pressure drop of clean filter as a function of space velocity

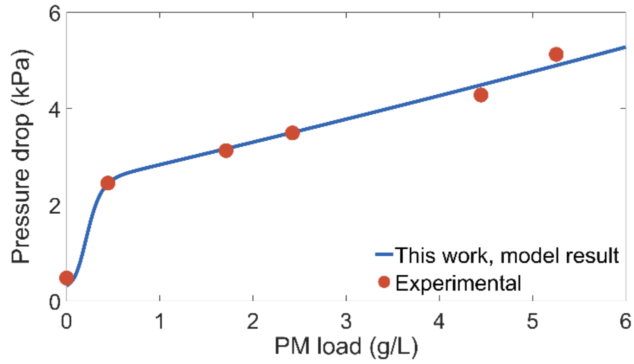


Figure 3: Simulated pressure drop of a filter as it is loaded with engine-out particles

Interoperability solution

Through CMCL's use case, the EAT models have been integrated with the OSP platform, where the inputs, outputs and models are described ontologically to enable interoperability. The workflow of EAT simulations are schematically shown below.

References

[1] D. Chatterjee, O. Deutschmann, and J. Warnatz. Faraday Discussions, 119:371–384, 2002.

[2] A. Sappok, M. Santiago, T. Vianna, and V. W. Wong. SAE 2009-01-1086, 2009.

Contact us:

emanuele.ghedini@unibo.it