Comprehensive Integrated Simulation Methodology for Enabling Near-Zero Emission HD Vehicles

Project ID: ACE173

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- **Cost share partner Marathon Petroleum providing fuels, guidance**
- **Guidance from CRC AVFL Committee**

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Overview

Timeline

Project Start: FY22

Project End: FY24

- **DE-FOA-0002420**
- Develop an enhanced methodology for the integrated simulation of combustion and aftertreatment systems

Budget

	FY 22	FY 23	FY 24	Total
Federal Portion	$ 1,052,362	$ 681,855	$ 870,653	$ 2,604,870
Cost Share	$ 403,675	$ 512,726	$ 512,726	$ 666,818
Total	$ 1,456,037	$ 1,194,581	$ 1,383,379	$ 3,271,688

Any proposed future work is subject to change based on funding levels.

Barriers

- US EPA HD Engine and Vehicle Standards
- "Development of models and simulation tools... to predict performance…"

Partners

- Gamma Technologies
- ORNL
- FEV
- Isuzu North America
- Umicore
- Marathon Petroleum

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Relevance

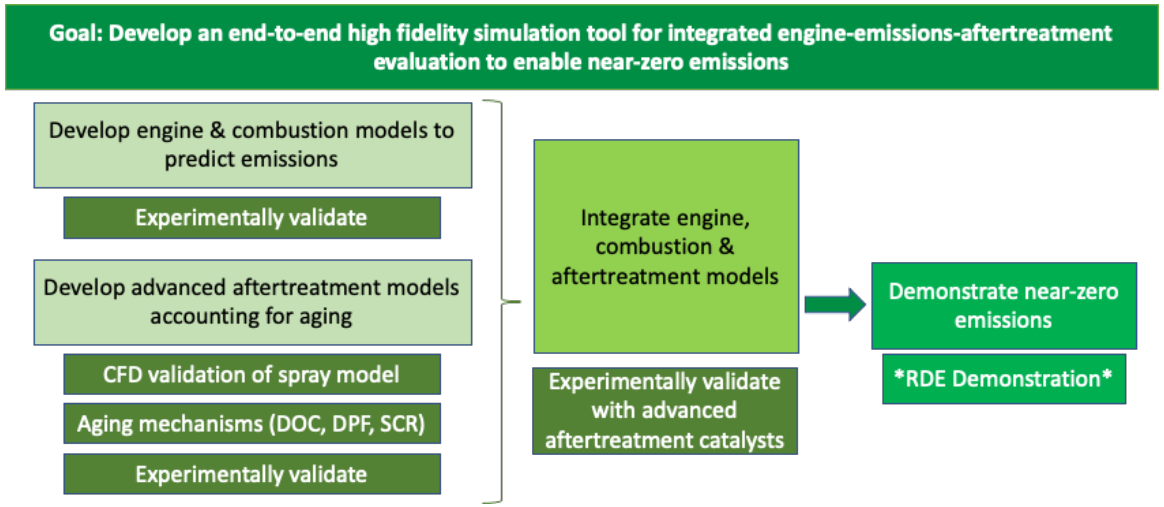
- An integrated simulation platform that can be used to design exhaust system architectures and control strategies that will meet future ultra-low NOx emissions standards over the full useful life of a HD vehicle.

- The key innovations that will be made in this work to create this simulation platform are:
  - Higher fidelity integrated models that can be used to understand the interactions and tradeoffs between the operating strategies for the engine and the aftertreatment
  - Validated emissions control device models that capture catalyst performance over the entire HD vehicle full useful life.
  - Introduction of the VoFLE methodology to provide unprecedented levels of validation to reduced-dimensional aftertreatment models.

- Application of the integrated engine and aftertreatment simulation tool, as proposed in the current submission, will help reduce the time and cost associated with deploying new emission reduction technologies for the heavy-duty market.

Approach

Develop and validate an integrated Reduced-Dimensional (RD) engine, emissions, and aftertreatment system model capable of optimizing controls, thermal management, and insulation strategies while improving component conversion efficiencies to enable near-zero emissions and Virtual Real Driving Emissions (RDE).



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Key Deliverable: integrated engine and aftertreatment simulation tool in GT-SUITE

Technical Accomplishments & Progress

ID	Milestones	Type	Description	
Y1-1	**Baseline aftertreatment system model calibrated**	Technical	The AT system model will be calibrated and verified under the conditions for baseline data	Complete
Y1-2	**Baseine combustion model complete**	Technical	The 0D-VCF-tPDF approach is extended to improve the prediction accuracy of emission quantities and other transient variables in a compression ignition (CI) engine.	Complete
Y1-3	**Baseine combustion model validation complete**	Technical	A comprehensively calibrated combustion model is obtained with respect to prediction of performance	On schedule
GNG1	**Baseline models developed and validated**	Go/No Go	Baseline engine, combustion, and aftertreatment models developed and validated.	On schedule

Collaboration & Coordination with Other Institutions

- Project partners/sub-contractors:
  - Gamma Technologies
  - ORNL
  - FEV
  - Isuzu North America
  - Umicore
  - Marathon Petroleum
- Coordinating Research Council (CRC) Members
  - AVFL Committee Members
    - OEMs
    - Oil & Fuel Companies

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Proposed Future Work

Any proposed future work is subject to change based on funding levels.

ID	Milestones	Type	Description
Y2-1	**ORNL SCR model updated for catalyst aging**	Technical	Revised SCR aging model
Y2-2	**ORNL SCR model integration into GT-SUITE complete**	Technical	Integrated SCR model into GT-Suite
Y2-3	**VoFLE computational campaign complete**	Technical	Prediction of NH3 and NOx distribution maps at the catalyst inlet plane, UWS spray mass histories, and supporting calculations for reduced-order model development.
GNG2	**Integrated model created**	Go/No Go	Engine, combustion, DOC, DPF, and SCR models integrated in GT-SUITE

ID	Milestones	Type	Description
Y3-1	**Engine experiments for validation complete**	Technical	Model validation data collection complete
Y3-2	**Calibration of integrated GT-SUITE model complete**	Technical	A fully integrated and calibrated model of the engine and aftertreatement system will be validated
Y3-3	**Model-optimized engine calibration complete**	Technical	Optimized engine map and AT configuration will be delivered
End of Project Goal	**Near-Zero Emissions Concept demonstrated**	Technical	Near-Zero Emission Concept Demonstrated

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Technical Backup Slides

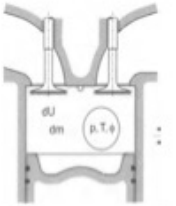
SRM 0D-VCF-tPDF engine model

In order of increasing accuracy and computational time.

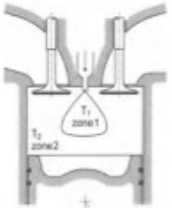
0D combustion

- Single zone model (thermodynamic models)
- Multi zone model (phenomenological models)
- Stochastic reactor model (SRM)

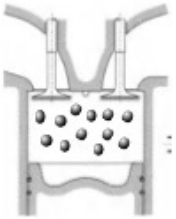
✔ Combustion is based on equilibrium calculation.
✔ Computationally very efficient.
✘ Poor NOx and soot prediction.



✔ Combustion is based on two or more zone calculation.
✔ Moderate computation efficiency.
✘ In-cylinder inhomogeneity is not rigorously modeled.
✘ Accurate NOx and soot prediction may require improved modeling foundation.



✔ Combustion is based on PDF approach.
✔ In-cylinder inhomogeneity is more accurately handled using a mixing model.
✔ Detailed chemistry along with thermal stratification leads to more accurate NOx and soot prediction.
✘ Efficient chemistry solver is required to reduce computational cost.



Fuel Effects on Aftertreatment SOW

- Engine 4.5L 4 cylinder John Deere Engine with production ECU
- Conditions: load sweep at single engine speed
  - Varying SOI timing - limited by misfire, turbine inlet temperature, maximum pressure rise rate or peak cylinder pressure limit
  - Varying EGR - max EGR rate will be determined by the capability of the OEM air system to maintain the intake pressure or an AFR above 20
- Fuels:
  - ULSD
  - 20% Splash blend of Renewable Diesel/ULSD
  - Neat Renewable Diesel
- Aftertreatment (in-kind cost share from Umicore)
  - Current production system
    - De-greened
    - Hydrothermally aged
  - Umicore Advanced Aftertreatment sustem
    - De-greened
    - Hydrothermally aged
- Emissions Measurements:
  - Criteria pollutants, (HC, CO, NOx, CO2) both pre and post AT system
  - Based on discussion at RWE, TSI will loan PM/PN measurement