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Reduced Cost & Complexity for Off-Highway Aftertreatment

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Project Overview

Timeline

- Start – Oct 2020
- Finish – June 2024
- Project Kickoff – Dec 2020
- 40% complete

Barriers

- **Lack of cost-effective emission control** for meeting EPA NOx/PM standards
- **Cost of emission control** devices
- **Durability** of the emission control system

Budget

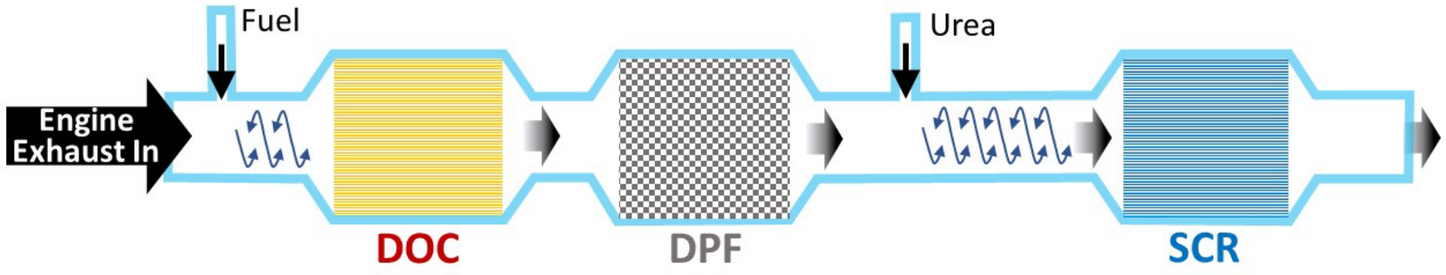
- Contract value – $3.193M
  - $2.5M DOE share
  - $0.693M partner share
- Funding received from DOE
  - $2.5M

Project Team

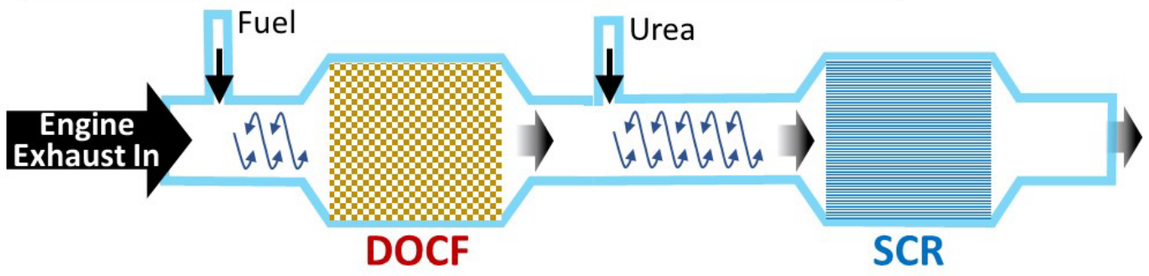
- Pacific Northwest National Laboratory
- John Deere Power Systems
- Michigan Technological University
- Kymanetics, Inc.
- Carus Corporation

Relevance

Current John Deere Off-road Aftertreatment Configuration



Future Off-road Aftertreatment Configuration



Goal

Develop combined DOC and DPF technology (i.e., DOCF) for simultaneous CO, HC, and PM emissions control in a single device

- **Advanced DOC-catalyzed DPFs offer a highly promising strategy of aftertreatment integration**
  - Reduced total thermal mass
    - ✓ Faster warm-up
    - ✓ Reduced cold-start emissions
  - Reduced cost and space requirements
  - Improved performance, reduced total PGM, greater responsiveness
    - ✓ Faster NO_2 yield for downstream SCR
    - ✓ Faster NO_2 production for NO_2-assisted soot oxidation
    - ✓ Reduced PGM usage by reducing redundant functions in separate DOC & DPF

Milestones

#	Milestone	Assigned	Type	Mo. into Project	Description
M1.1	Baseline system definition complete	John Deere	Technical	3	Evaluation of baseline T4-S5 system and first- generation DOCF complete, testing protocols established
M1.2	Advanced imaging of catalyst in baseline system complete	Kymanetics	Technical	6	Advanced imaging (e.g., X-ray CT) and materials characterization of baseline DOCF technology including washcoat location/chemistry, and ash location, chemistry and morphology
M1.3	DOCF model structure development complete	MTU	Technical	9	2D structure of DOCF model complete for characterizing axial and wall mass transfer, reaction, and heat transfer
M1.4	Spaci-MS demonstration complete	PNNL	Technical	12	Specially resolved testing of first-generation DOCF complete
M1.5	Technology road-mapping complete	MTU	SMART	15	Front-zone catalyst design for second-generation DOCF devices is completed with pathway identified to 20% PGM reduction
GNG-1	Pathway identified to 20% reduced PGM in front-zone washcoat	**PNNL**, MTU, John Deere	Go/No-Go	15	Assessment of first-generation DOCF complete, pathway identified to 20% reduction in front-zone PGM

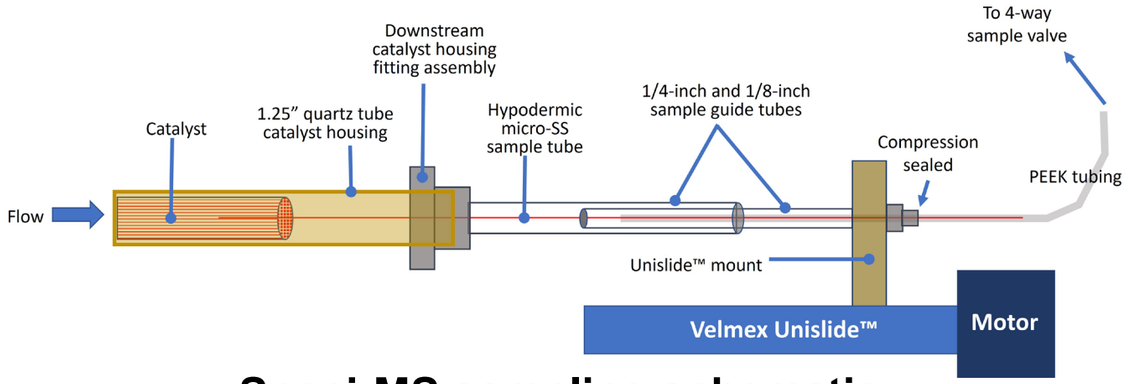
Complete

Nearing completion

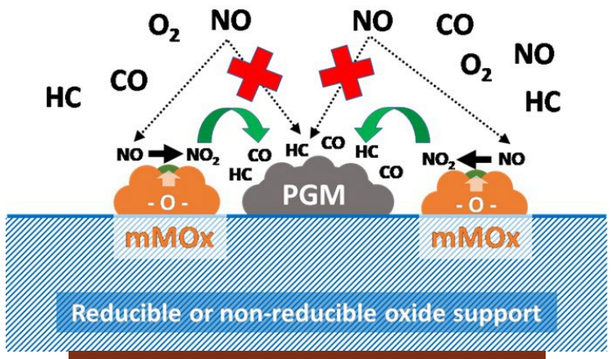
Approach

Cost Reduction Targets	Substrate + PGM Cost	Canning Cost
DOCF PGM only	16–30%	5–20%
DOCF with PGM and non-PGM (i.e., mMOx) materials	24–44%	5–20%

- Targets
  - A washcoat design and device architecture that enables:
    - ✓ Cost effective soot management – efficient active regen and sufficient passive regen
    - ✓ Fast CO and HC light-off with minimum PGM usage
  - Prediction and mitigation of the adverse impacts of ash deposits on device performance
- How
  - Custom predictive model development with high accuracy for modeling DOCF performance
  - Accuracy supported by
    - ✓ Spatially resolved intra-channel gaseous analysis (i.e., Spaci-MS)
    - ✓ Engine testing & validation
  - Advanced device aging characterization imaging techniques for clarification of wall, catalyst, and ash
  - Pursue opportunities to augment PGM performance & versatility through active & durable mixed metal-oxide catalysts



Spaci-MS sampling schematic



Enhanced reactivity of mMOx structures through cooperative interaction with PGM

Approach – DOCF Modeling

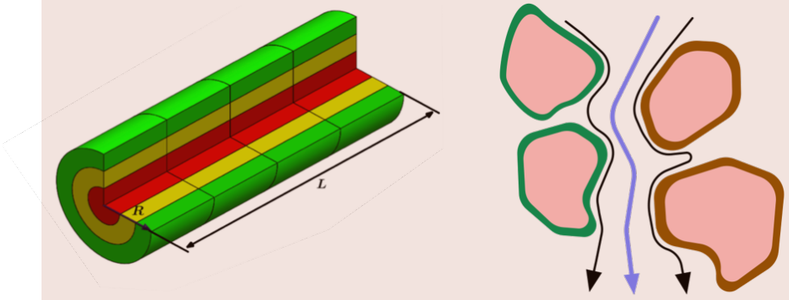
- **Purpose** – Predict axial-specific CO, HC, NOx and PM emission control performance with high accuracy as a ***f(X)*** of *local* washcoat loading, washcoat formulation, and device structure
- **Impact** – Enable optimization of *local* washcoat loading, washcoat chemistry, and device design (e.g., permeability) to target soot management, and pollutant reduction, and cost goals
- **Approach**

SUB-MODELS

Gas State	Reaction Kinetics	Particulate Matter	Thermal

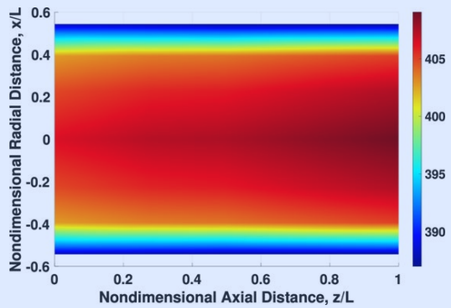
Implemented in both axial and radial domains, i.e., 2D model

Extend and use existing literature on DPF and SCRF models



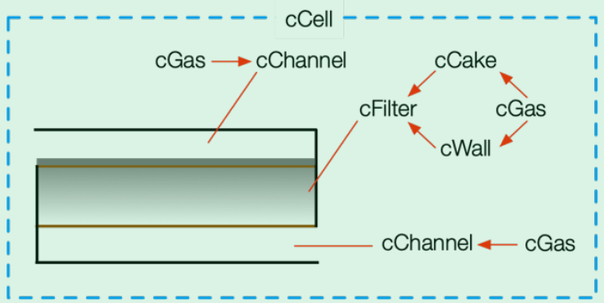
Axial - Radial domains

Exploit Mich Tech SCRF thermal and PM submodels



SCRF temperature example

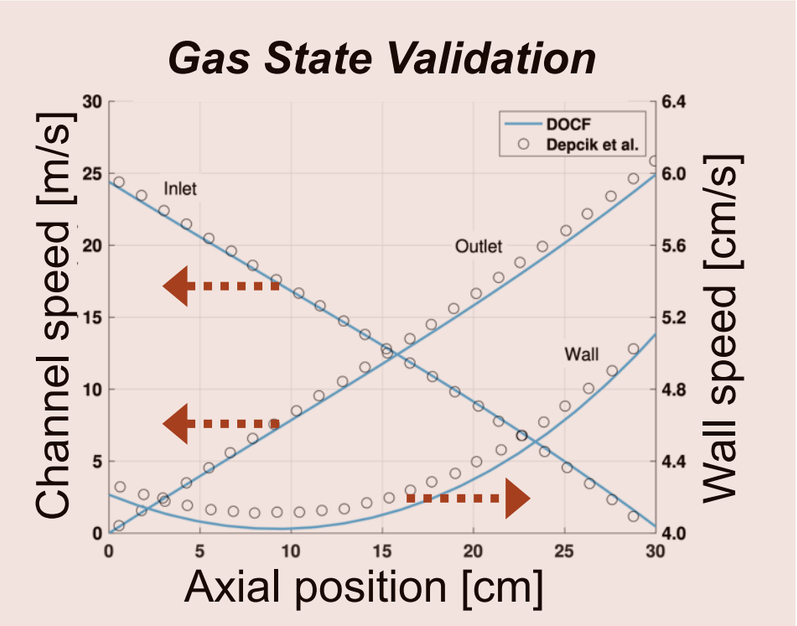
MATLAB, classes with auto-code generation

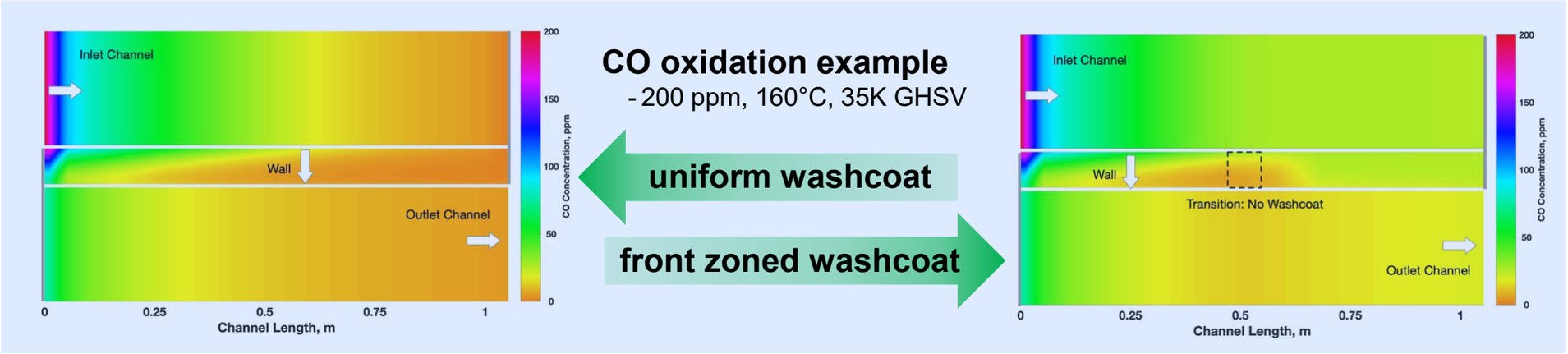


Axial cCell object using several other classes

Technical Accomplishments – DOCF Modeling

- **Architecture** – 19 classes implemented, 6 reused from the existing SCRF model (thermal and PM **[1]**)
  - Exploits MATLAB solvers
    - ✓ *Adaptive mesh boundary-value solutions* for gas state & wall rxns
    - ✓ *Selectable time domain solvers* for PM and thermal responses.
    - ✓ *MATLAB "Fit Objects"* retains complete solution information.
- **Gas State** – Channel & wall state (pressure, velocity)
  - Solved in all domains based on temp field
  - Validated to published data **[2]** shown at right
- **Channel Flow and Wall Reactions**
  - 1st-order channel and 2nd-order wall equations (diff + rxn) complete
  - Bulk and surface flow with spatially-varying washcoats is complete
- **Thermal and PM**
  - Radial-Axial SCRF "zone" and filtration models are implemented in the DOCF model **[1]**.





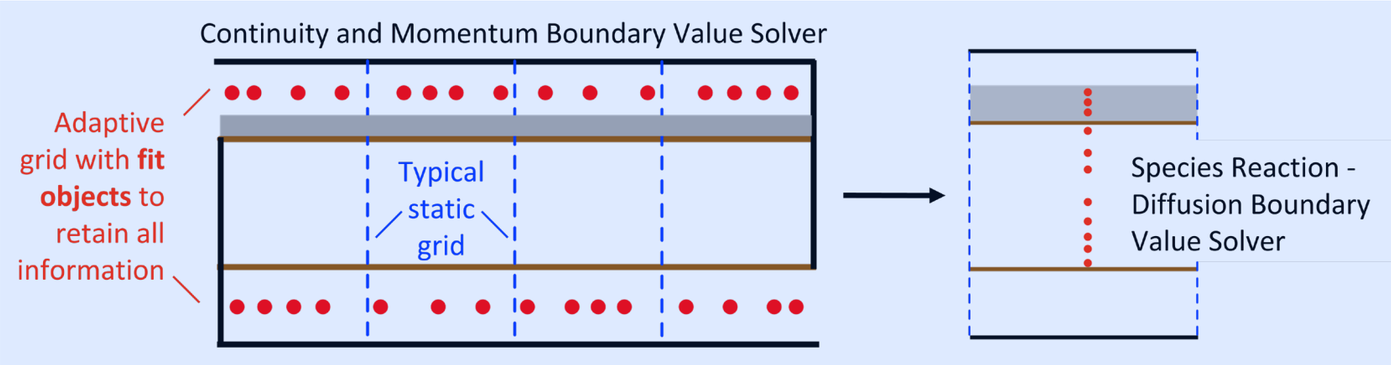
[1] Mahadevan, Johnson, Shahbakhti, 2015, *Emission Control Science and Technology,* V. 1(2) pp. 183-202.

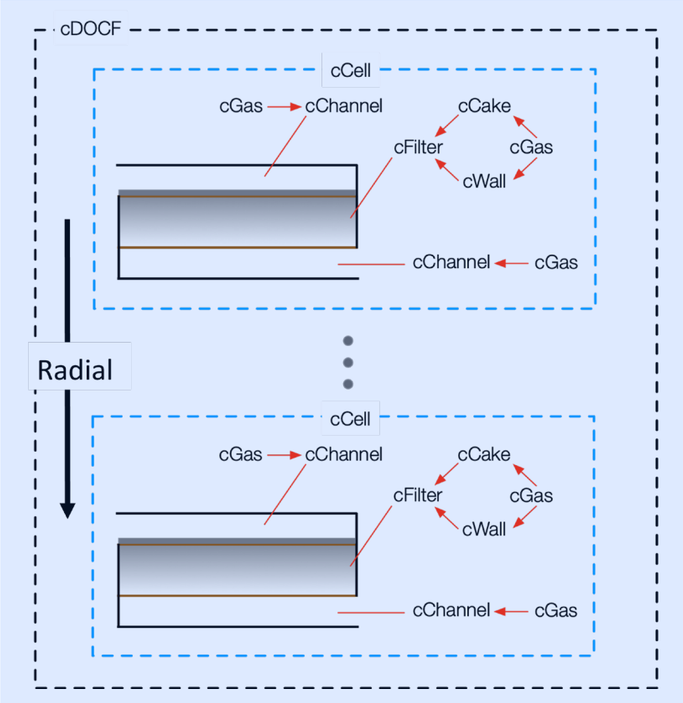
[2] Depcik, Assanis, 2008. Journal of Engineering for Gas Turbines and Power, 130(6).

Technical Accomplishments – DOCF Modeling

Novel DOCF model architecture aids management of physical domains (channels and walls) and solution of the relevant physics (kinetics, thermal, transport)

- *MATLAB object-oriented syntax*
  - Boundary value solvers (species, gas states)
  - Time-stepping solvers (temperature, PM)
- *Combined static and adaptive grids*
  - Static (temperature); Adaptive (wall species)
  - Improved accuracy versus static-only grid approach.
- *Data encoded using fit objects*
  - Retain all information generated during adaptive grid boundary value solutions
  - Fast & accurate operations (e.g., differentiation, integration grid evaluation)
- *Classes (e.g., methods and properties) used to build model*
  - Uses fundamental components - channels, cake, cells, etc.
  - Enables code reuse and makes adding new features easy
- *Live Scripts*
  - Human-readable equations → symbolic expressions
  - Automates code generation → reduces errors, incr. transparency
- *Customization functions*
  - e.g., the radial temperature distribution function,
  - Installed at run-time to avoid users "touching" the code.





Technical Accomplishments – Engine Testing

Engine is carted and operation has been verified in the test cell

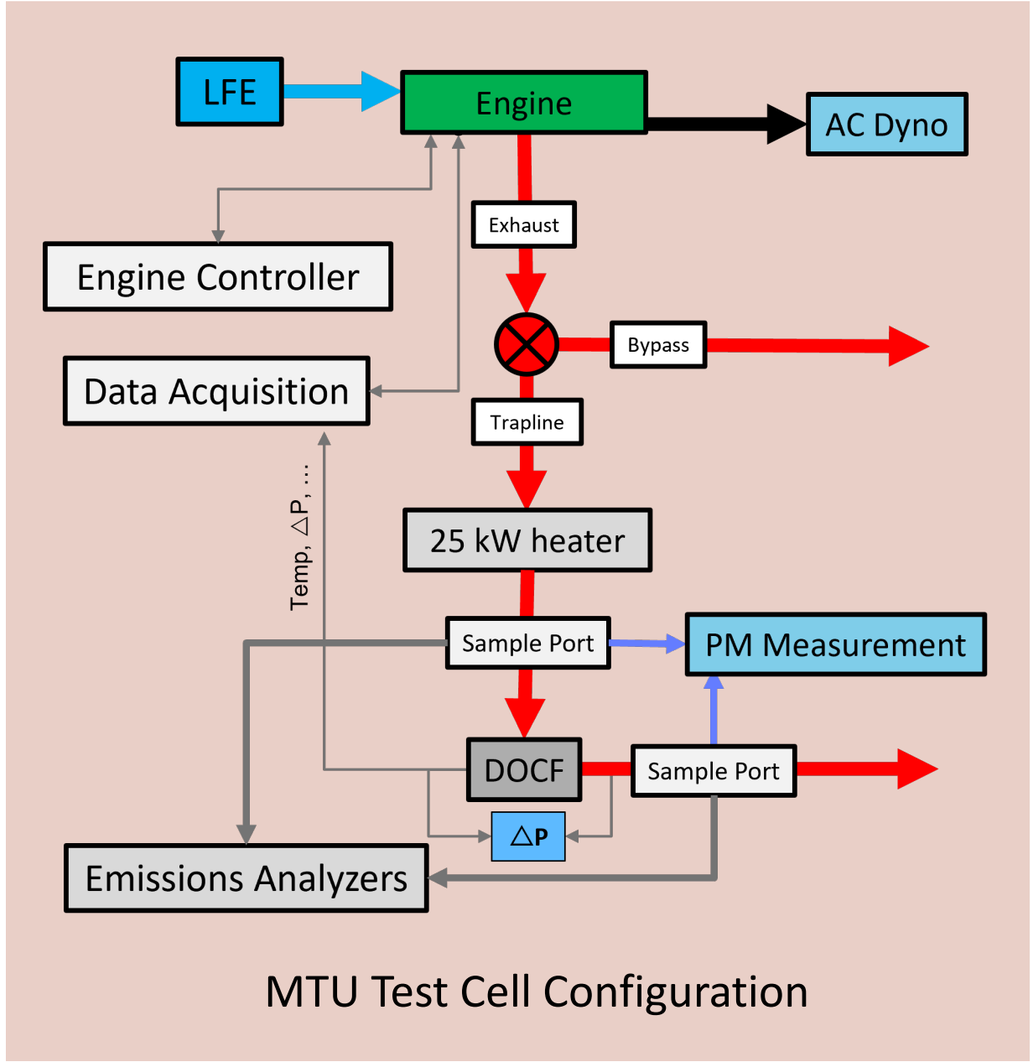
Exhaust temperature management system configured

Exhaust sampling system configured

Instrumentation for exhaust canister sourced

Deere 6.8L Engine Test Bed @ MTU

DOCF

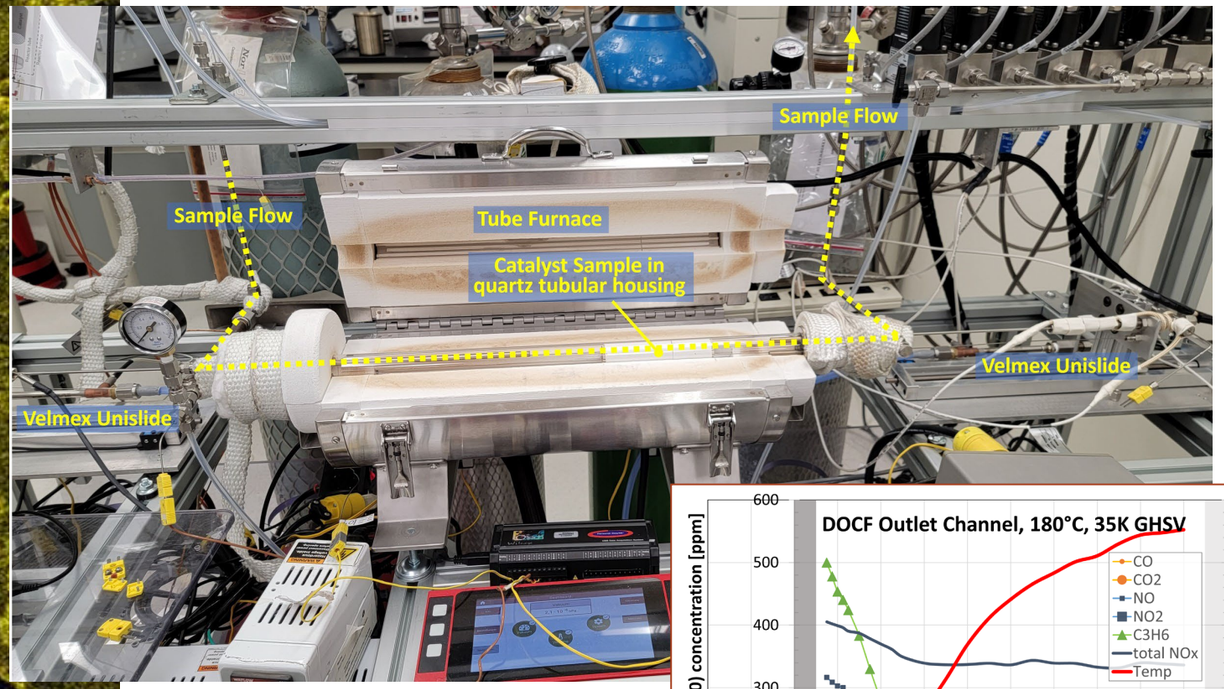


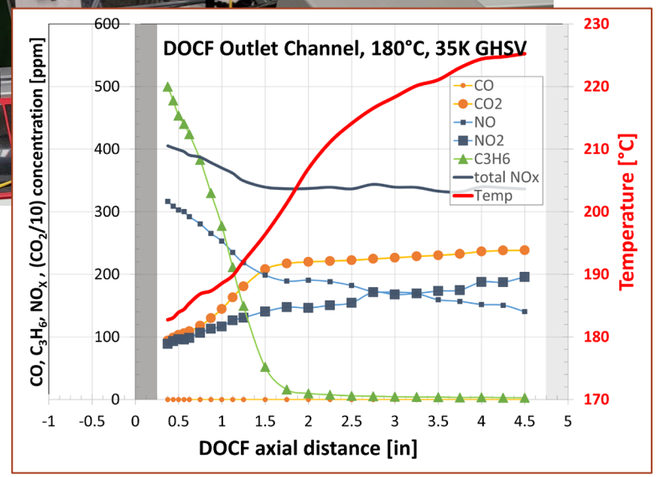
MTU Test Cell Configuration

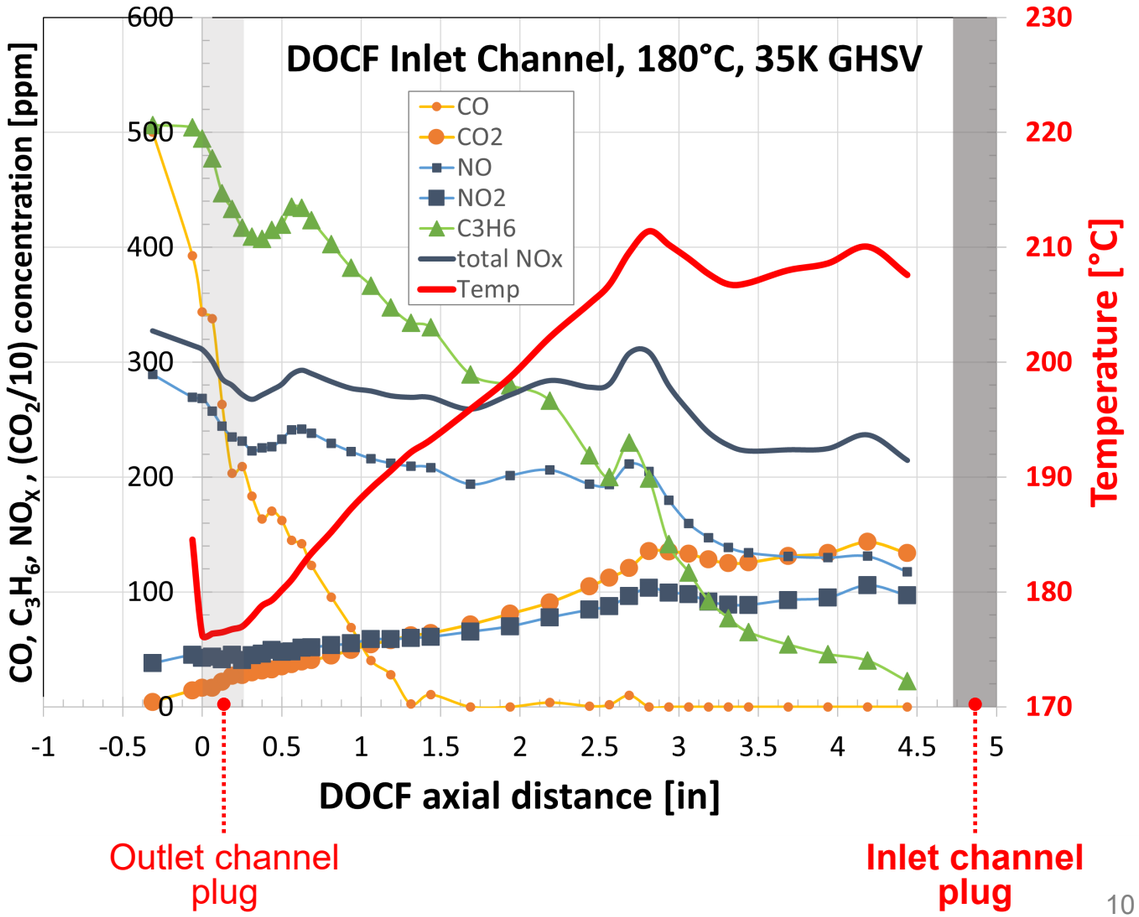
Technical Accomplishments – Spaci-MS SGB

Spaci-MS synthetic gas bench (SGB) elucidating unreported DOCF dynamics and enabling spatially-resolved testing of DOCF structures

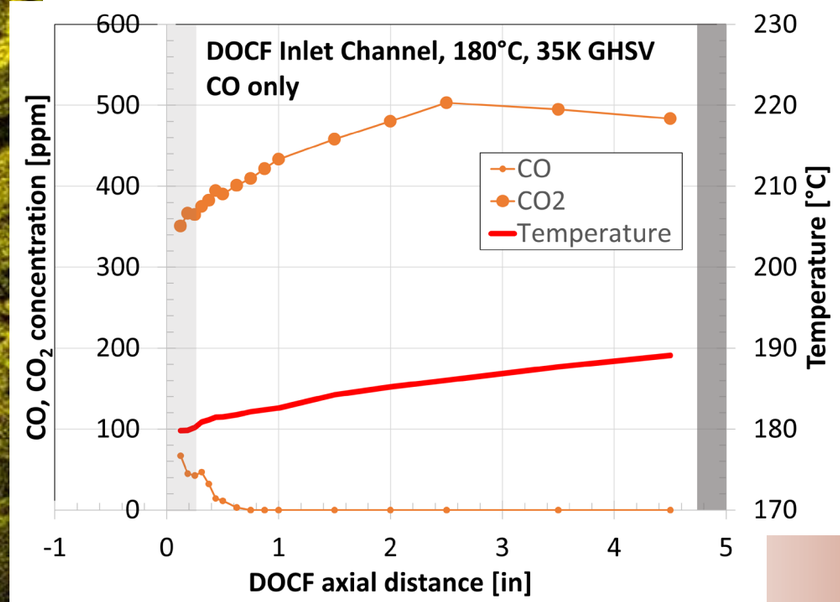
Providing unprecedented insight into DOCF chemical and thermal dynamics

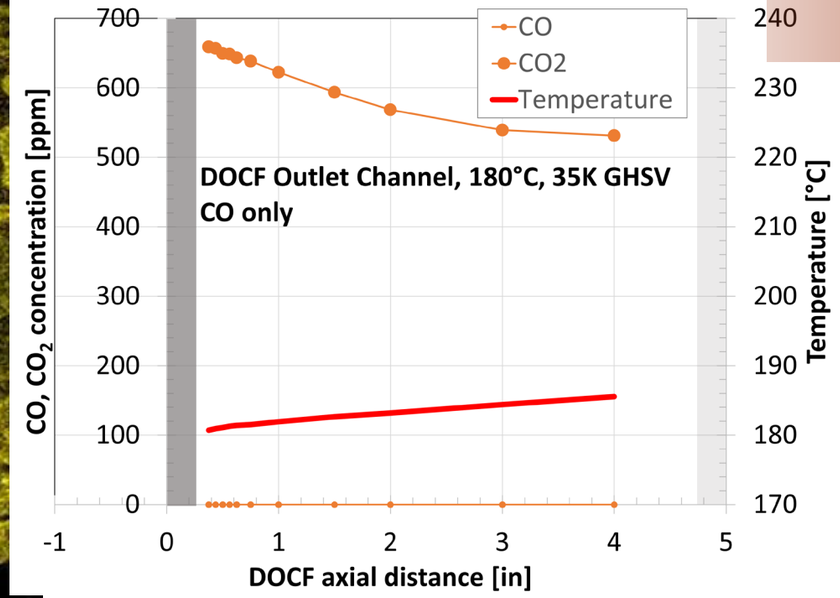






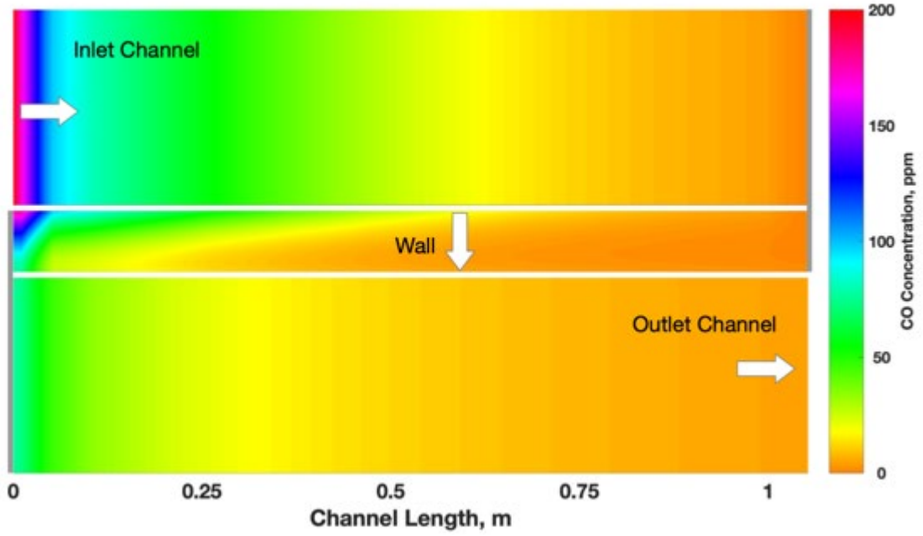
Technical Accomplishments – Spaci-MS SGB





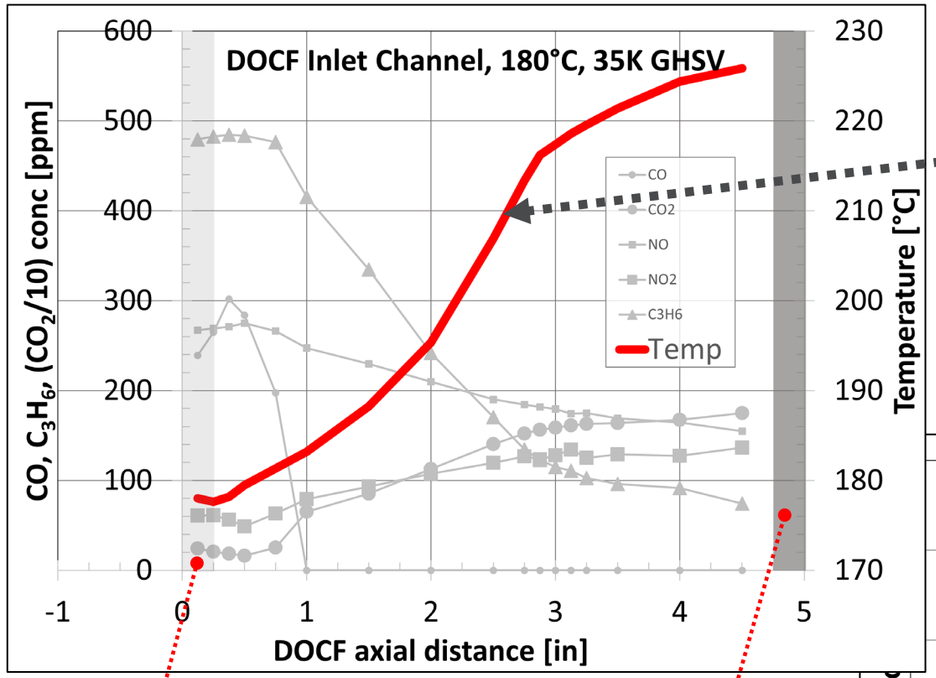
Currently using Spaci-MS data for DOCF model calibration

Ensure highly accurate mass transfer, heat transfer, reaction and species inhibition predictions



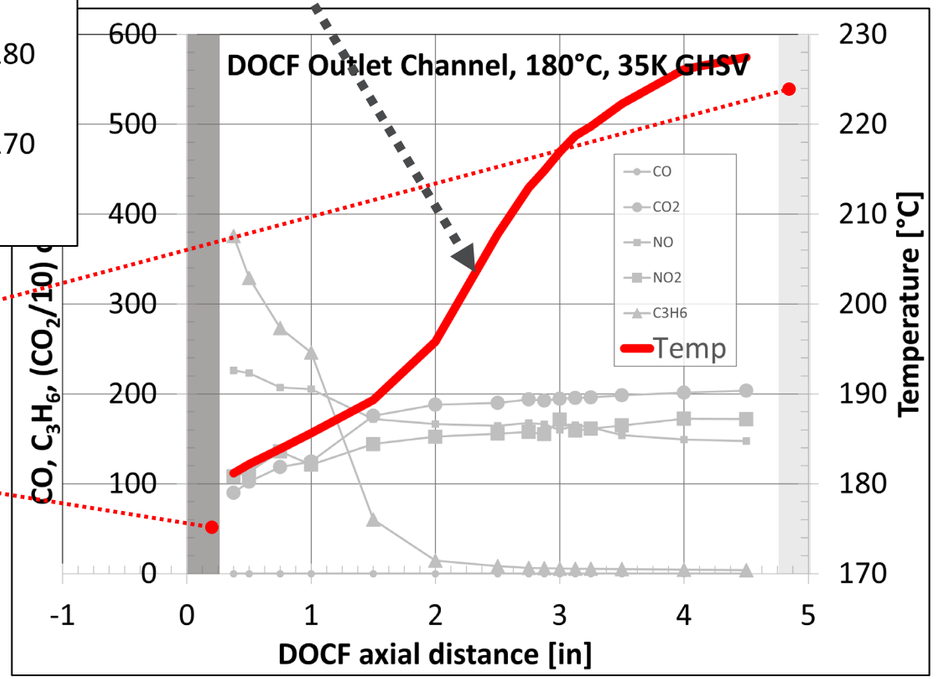
Simplified surrogate reaction(s) testing and modeling to ensure accuracy for targeted specific mass transfer and reaction mechanisms

Technical Accomplishments – Spaci-MS SGB



Heat release dynamics effectively characterized with Spaci-MS bench

- Coupled with HC conversion, will be a key metric in optimizing washcoat distributions for effective soot management



Inlet channel plug

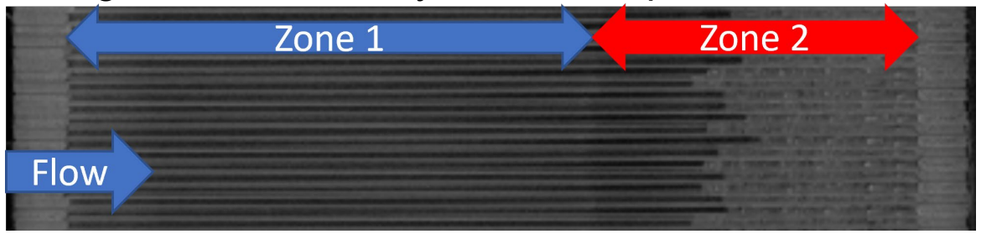
Outlet channel plug

Technical Accomplishments – Advanced Imaging

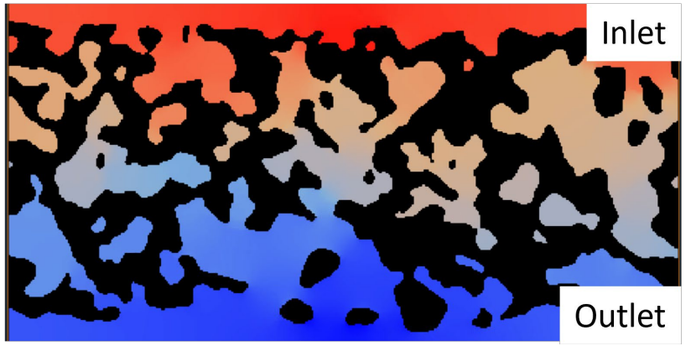
Spatial *substrate + washcoat characterization* and *flow simulation* enabling accurate in-wall predictions of key properties

- Mass transport resistances = catalyst use efficiency
- Ash interactions

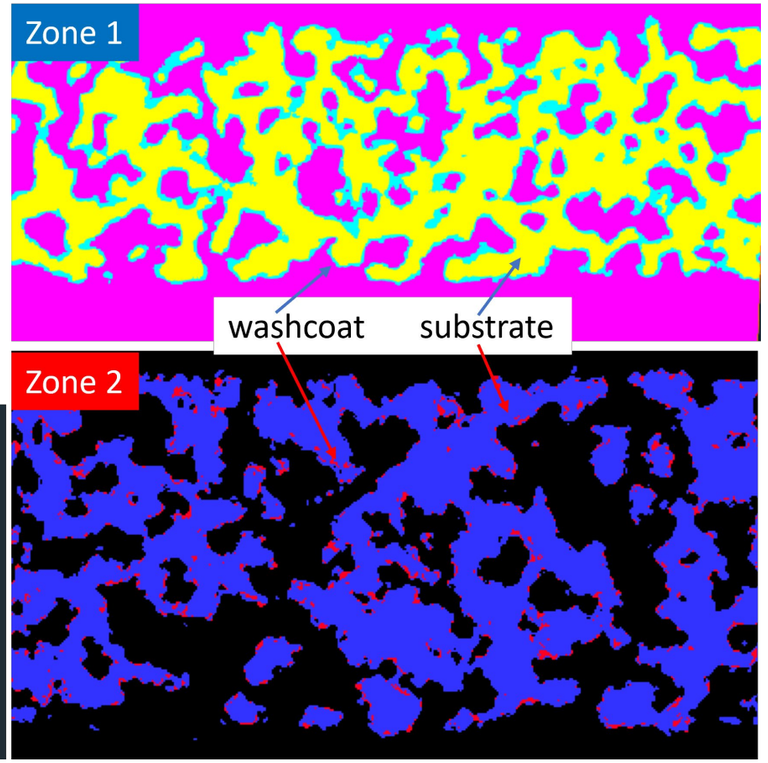
High-resolution X-ray CT data ~1µm voxel size



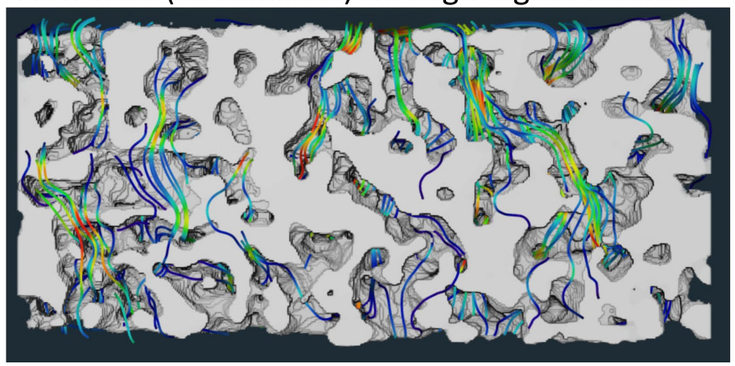
Pressure magnitude



3-phase segmentation=air+washcoat+substrate

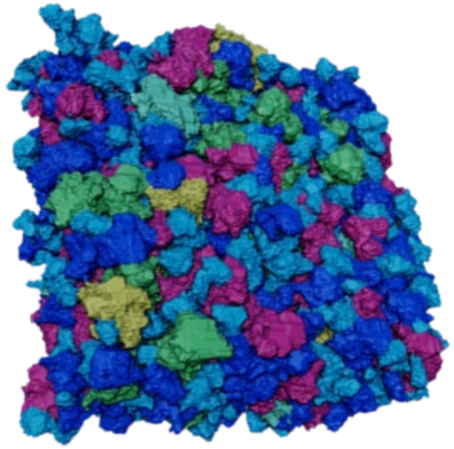


Flow field (streamlines) through digital volume



Outputs

- Multi-scale CT analysis
- Washcoat visualization
- Ash density
- Ash-substrate interactions
- Ash particle characteristics
- Ash profile, plug length
- Permeability
- Porosity
- Pose size & geometry
- Washcoat location
- 3D pressure visualization
- 3D flow field



3D pore histogram (pore size)

Responses to Previous Year Reviewer's Comments

Comment	Response
"… it was not clear to the reviewer how much work will be done on evaluating regeneration under various conditions."	- Soot management is a core focus of the effort. The reviewers are correct in identifying this. - Significant soot work will be performed in the project, including bench-scale and on-engine. - The Spaci-MS bench is will suited to characterize dynamics heat release axially across the DOCF device under various conditions, which we feel will be imperative in optimizing DOCF performance.
"The soot is a known inhibiting agent … little discussion of this issue, and … no plan to study on the bench reactor."	- It is not clear to the project team the nature of the 'inhibitions' that are referenced in relation to DOCF. - To our knowledge there are no known chemical inhibitions between C-NO_2 or C-O_2 reactions in solid phase. - SAE 2020-01-2201 indicates better soot oxidation light-off with catalyzed filter vs. bare filter. SAE 2019-01-0583 give strong indication of the feasibility of DOCF technology.
"… not clear how this is differentiated from the CRADA and why the results from the CRADA could not be used here to indicate the direction of the research."	- The CRADA was tasked with identification of gaps in current knowledge regarding DOCF modeling and current understanding. - Specific take-aways from the CRADA are being implemented in work.

Collaboration & Coordination with Other Institutions

Institution	Contact	DOE funds	Cost Share	Key Role(s)
Pacific Northwest National Laboratory	Ken Rappé	√		Project management, Spaci-MS and bench-scale testing and measurement, modeling
John Deere	Eric Hruby	√	√	Formulated/re-formulated DOC and DOCF catalysts
Michigan Tech	Jeff Naber Gordon Parker	√	√	Wall-scale and device-level modeling, engine dyno testing
Kymanetics	Justin Kamp	√		Catalyst characterization, aging mechanisms
Carus®	Seth Schugars		√	Non-PGM oxidation catalysts

Remaining Challenges and Barriers

- DOCF model
  - Channel flow and wall reactions
    - ✓ Complete model calibration and validation with Spaci-MS data (simple → complex)
  - Thermal and PM
    - ✓ Data mapping, unit testing, and validation
- GNG-1 – Sensitivity study to identify pathway to 20% reduced PGM
- Gen-2 DOCF device production
- DOCF model refinement and *validation on engine*
- Ensuring efficient and cost-effective soot management
  - Heat release sufficiently far forward in device – guidance from Spaci-MS testing and DOCF modeling
  - Sufficient NO_2 availability and make.
  - Soot testing on engine, supported by testing on bench (if warranted).

Proposed Future Research

Baselining Performance & Quantifying Catalyst Performance Targets

1. Define baseline systems & performance targets; characterize catalyst & ash distribution
2. Performance characterization capability development
3. DOCF Model development, validation, and road-mapping
4. Advanced DOCF active-phase development

Budget Period 1

Current Status

Optimizing Front-Zone Washcoat Design in DOCF Technology

1. DOCF device production and characterization
2. Bench-scale performance of advanced DOCF devices
3. Engine baseline testing, DOCF model update/validation & road-mapping
4. Advanced DOCF active-phase technology transfer & evaluation

Budget Period 2

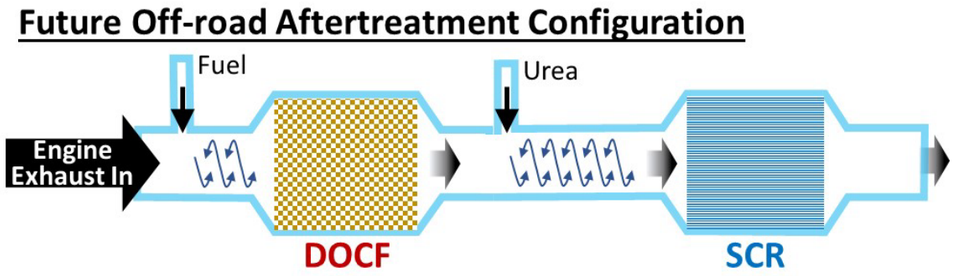
Optimizing DOCF Device Performance

1. Third-generation optimized DOCF device production
2. Engine testing and model validation
3. Bench testing and characterization
4. Evaluating advanced mMOx structures in DOCF washcoat design

Budget Period 3

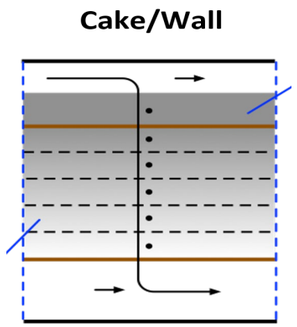
Any proposed future work is subject to change based on funding levels.

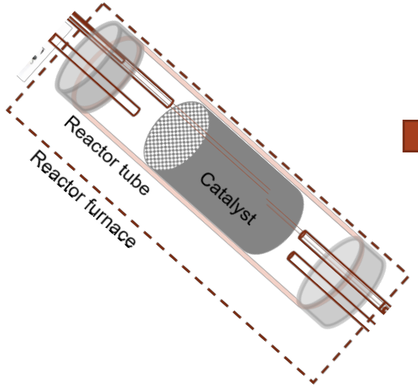
Summary

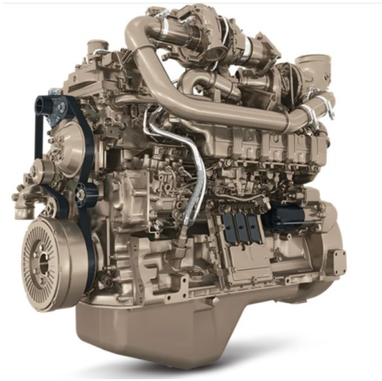


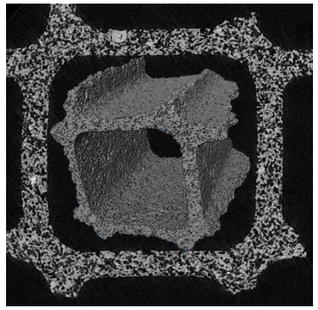
DOCF is being developed for off-road emission control for attractive aftertreatment integration that can reduce cost and space requirements on vehicle, reduce PGM use, and improve system responsiveness

- A DOCF modeling strategy is being developed
  - Will predict axial-specific gas and soot reaction performance and heat release as a function of local washcoat loading, washcoat formulation, and device structure
  - Will enable optimization of local washcoat loading, washcoat chemistry, and device design to target soot management, pollutant reduction, and cost goals
- Spaci-MS testing, engine testing, and advanced imaging capabilities are being developed
  - To measure and characterize key performance, dynamics, and characteristics of DOCF.
  - To support highly accurate modeling of DOCF structures for their efficient and cost-effective iterative development.









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Thank you

Acknowledgements

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Gurpreet Singh

Siddiq Khan

Pacific Northwest NATIONAL LABORATORY · JOHN DEERE · Michigan Tech · CARUS · KYMANETICS

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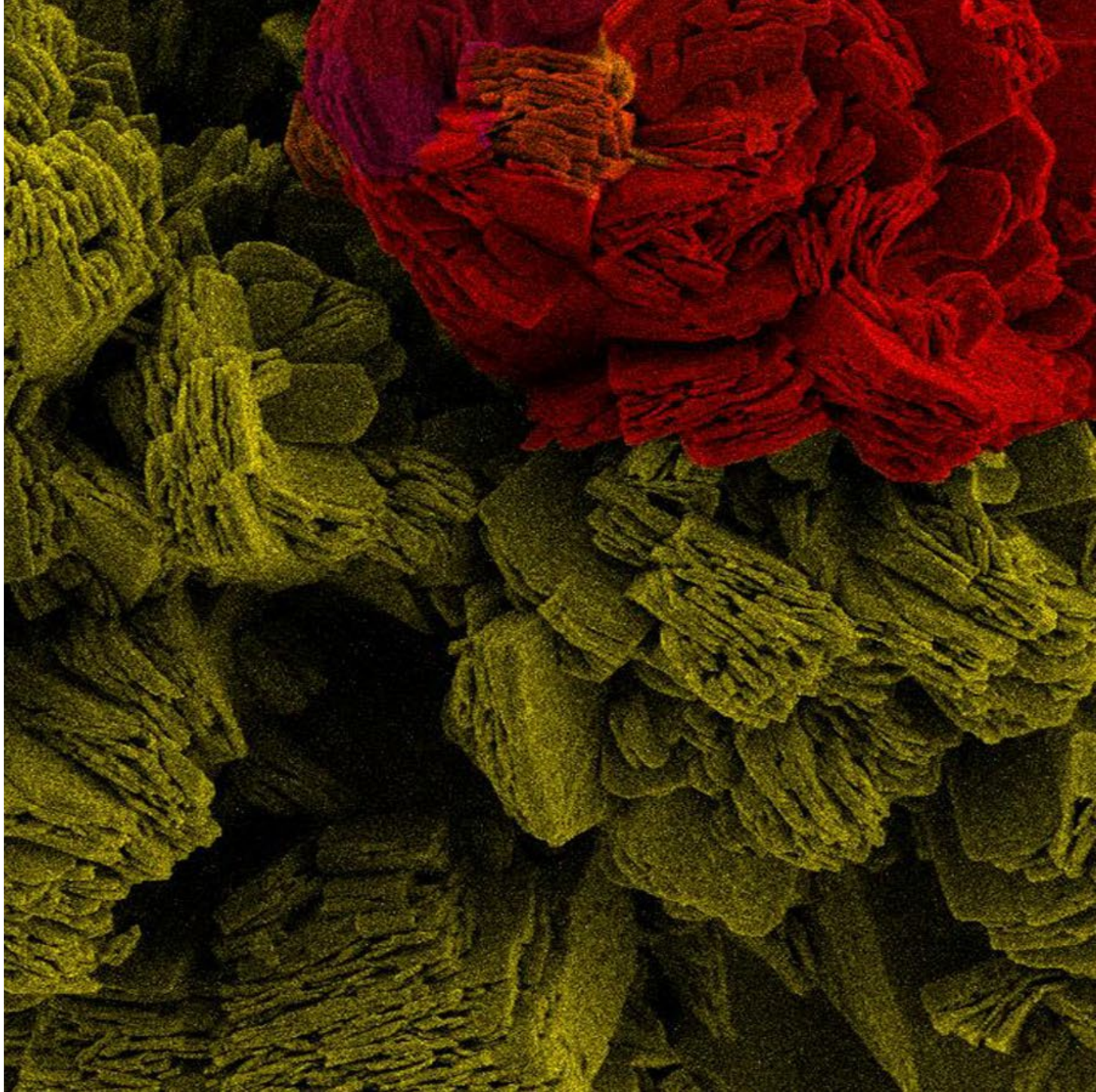
Back-up Slides



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Milestones

	#	Milestone	Type	Mo. into Project
Budget Period 1 Baselining Performance and Quantifying Catalyst Performance Targets	M1.1	Baseline system definition complete	Technical	3
	M1.2	Advanced imaging of catalyst in baseline system complete	Technical	6
	M1.3	DOCF model structure development complete	Technical	9
	M1.4	Spaci-MS demonstration complete	Technical	12
	M1.5	Technology road-mapping complete	SMART	15
	GNG-1	Pathway identified to 20% reduced PGM in front-zone washcoat	Go/No-Go	15
Budget Period 2 Optimizing Front-Zone Washcoat Design in DOCF Technology	M2.1	Second-generation DOCF production complete	Technical	18
	M2.2	Pathway identified for incorporation of advanced mMOx structures	SMART	21
	M2.3	Spaci-MS testing of second-generation DOCF complete	Technical	24

Technical Accomplishments – Active Phase Development

- Conclusion of development for sodium aluminate/alumina routes
  - Changes made to processing agents and process conditions in order to affect pore volume, surface area, and support structures
- New variations have resulted in performance changes to NO_x adsorption, sulfur resistivity, and temperature of NO_x desorption
  - Capable of maintaining >60% activity after multiple heavy sulfation cycles
  - Adsorbing and holding NO_x during low-temperature operation until catalysts have reached sufficient operating temperatures
- New steady state program being designed based on John Deere feedback to evaluate best performing Carus materials for NO oxidation and desorption within ideal temperature range

Technical Accomplishments – DOCF Modeling

- DOCF *Reaction Kinetics* sub-model complete & implemented with both the Thermal and Particulate Matter sub-models.
  - ✓ **This facilitates one of the leading project objectives - determining the effect of washcoat spatial distribution and formulation.**
  - Model applicable amenable to both Spaci-MS and engine calibration
  - Predicts species concentrations axially in both channels and radially through the soot cake & wall with spatially varying kinetics.
  - Reaction rate routine modified to permit spatially varying washcoats including overlapping.
  - Two reaction rate sub-models implemented:
    - ✓ Using bulk wall concentrations
    - ✓ Using catalyst surface concentrations.
  - The latter is potentially more accurate but more complicated and slower than the former; requires iterative solution at each wall gas-solid boundary.
  - Model validation will determine if the latter approach is necessary. Additional model development may take place when assumptions are tested during model validation.

Technical Accomplishments – DOCF Modeling

- Merging of the *Thermal* and *Particulate Matter* routines into the DOCF model is complete, including mapping its data structures.
  - Leverage existing 2D SCRF sub-models previously developed at MTU
  - Uses a different approach than the SCRF model. Thus, unit testing of the sub-model features is needed.
  - Time-domain solver for computing temperature & particulate matter states is implemented; user can select from any of the built-in MATLAB integration methods
  - Sub-models contain time-integrated temperatures of the wall, inlet channel, outlet channel, and PM in the cake and wall.
    - ✓ This contrasts with the gas state and wall reaction sub-models which are steady-state boundary value problem solutions.
  - Sub-model solution approaches structured such that any of the MATLAB built-in integration methods could be selected. This will be important (later) when variable-time step methods may yield considerable execution time savings.
  - Technique developed to allow critical first approximations of wall species solutions to be made from previous solutions to find future solutions.
    - ✓ **This solves a long-standing challenge of the dependency of dynamic modeling sensitivity and accuracy on initial approximations and will improve execution time.**

Publications and Presentations

- Publications
  - None yet.
- Presentations
  - Kenneth G. Rappe “Impact of zoning & permeability on DOC-filter performance through device scale modeling”, 2021 CLEERS Virtual Workshop (oral), September 13–17, 2021.