Low Temperature Aftertreatment (LTAT) Test Protocol Development

USDRIVE
DRIVING RESEARCH AND INNOVATION FOR VEHICLE EFFICIENCY AND ENERGY SUSTAINABILITY

Why

- Assist DOE and USDRIVE in evaluation and management of solicited projects
- Provide strategy of test standardization for sharing material performance evaluation in open public forum
- Support fundamental materials development and strategy for ***comparative*** evaluation and benchmarking

Aspirations

- General industry consensus
- Consistent with anticipated technologies
- Accurate, Reproducible, Realistic
- Simple, Inexpensive to perform
- Practical, have utility
- Literature citations

Reactor Base-lining

- Ensure reported data dictated solely by material behavior
- Excludes artifacts (e.g., equipment effects)
- Suggest user conduct one-time blank base-lining without catalyst per application (i.e., blank run)
- Characterize/ensure fate, quantify recovery, of reactive species

Considerations

Performance ↕ Modeling | Functionality ↕ Device | Conversion ↕ Passive Adsorption | Combustion Platform

- Typically governed by relative maturity within technology life-cycle
- Early development: screening for performance of material evolutions
- Modeling performed on promising material candidates
- Often dictates complexity of test methodologies employed

- Sometimes synonymous, e.g., oxidation
- Functionality: conversion-based and adsorption-based
- Devices moving towards multi-functionality
- Early material development typically functionality-based

- Conversion: Rate (reaction)
- Adsorption: Rate (ads/des) ***PLUS*** capacity
- (Passive) adsorption characterization more complex

Combustion modes

	low temperature (e.g., RCCI)	dilute gasoline lean	dilute gasoline stoichiometric	clean diesel
NO	25 ppm	475 ppm	1000 ppm	170 ppm
NO_2	15 ppm	25 ppm	0 ppm	30 ppm
NOx	40 ppm	500 ppm	1000 ppm	200 ppm
HC (as C_1)	3000 ppm	2000 ppm	2000 ppm	500 ppm
CO	3000 ppm	2000 ppm	5000 ppm	500 ppm
H_2			2000 ppm	
O_2	14%	9%	0.5%	12%
CO_2	5%	8%	13%	6%
H_2O	5%	8%	13%	6%

Proposed HC Blend
(Final Definition–9/1/14)

- 2 to 3 per combustion mode
- mixed in various magnitudes to accurately represent HC profile
- representatives from each HC class

- **Ethylene**
- **Ethanol**
- **Propane**
- **Toluene**
- **n-Dodecane**

Step 1: Oxidation

Performance | Functionality ***AND*** device | Conversion

Powder ⟺ Core — Degreening ***required*** prior to protocol – ***suggest*** 700°C/4-hrs (10% H_2O/air)

Pre-treatment
- O_2/N_2, H_2O, CO_2
- 20min/550°C

Activity testing
- full exhaust
- 100°C – 550°C

Protocol step description	Temperature	NO	CO	HC	O_2	H_2O	CO_2	Time, min
Pre-treatment	550°C for 20 min	0	0	0	[O_2]	[H_2O]	[CO_2]	20
Cool	550°C – 100°C	0	0	0	[O_2]	[H_2O]	[CO_2]	-
Hold	100°C for 10 min	[NO]	[CO]	[HC]	[O_2]	[H_2O]	[CO_2]	10
Ramp	100-550°C @ 2°C/min	[NO]	[CO]	[HC]	[O_2]	[H_2O]	[CO_2]	225
Hold	550°C for 5 min	[NO]	[CO]	[HC]	[O_2]	[H_2O]	[CO_2]	5
Cool	550°C – 100°C	0	0	0	[O_2]	[H_2O]	[CO_2]	Var*

Constant Parameters
- [O_2], [H_2O], [CO_2], HC make-up
- SV, aged state, poisoning (e.g., S)

Variable Parameters
- [CO], [HC C_1], [NO], [NO_2]

Protocol Detail

- Catalyst aged state, poison state considered constant
- Aging, chemical poisoning should precede protocol
- Temperature ramping employed for simplicity
- Rate of ramping small – ***pseudo-steady state***

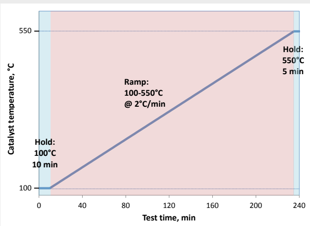
Requirements

Analytical *
- [CO], [CO_2], feed HC
- [NO], [NO_2], [N_2O], [O_2]

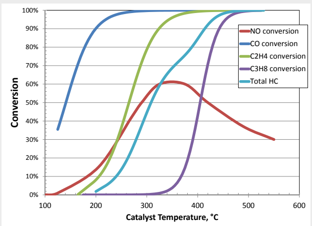
Temperature Measurement
- catalyst inlet
- within catalyst powder
- back face of core

* **Ensure catalyst insensitivity to exhaust modification for analytical capability**

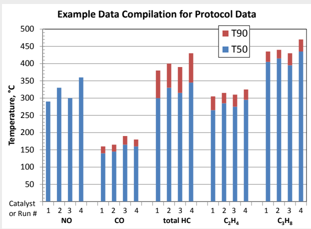
≤ 4-hr test ideal



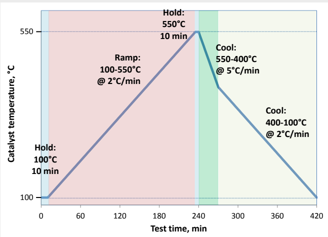
Single run: conversion vs. temp



Multiple runs: T50, T90 data



Characterizing Hysteresis



Rate of cool-down should be ***actively*** controlled
Ensure no axial or radial temperature gradients
Suggest {≤5°C/min > 400°C}, {≤2°C/min < 400°C}

NO Reduction

NO disappearance and NO → NO_2 would diverge
Inclusion of [N_2O] analysis necessary to quantify

$[NO, NO_2]_{IN} - [NO, NO_2, 2{*}N_2O]_{OUT} = NO_X$ *reduction to* N_2

Carbon Balancing – Partial HC Conversion

HC disappearance and HC→CO_2 would diverge
Characterizes HC partial conversion as lump sum
Requires omission of CO_2 from feed **

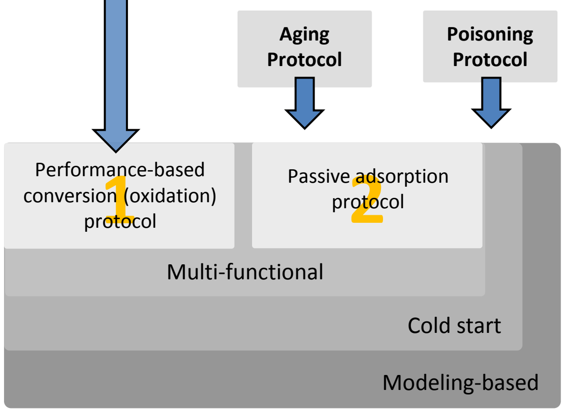
$[CO, HC\ C_1]_{IN} - [CO, CO_2, HC\ C_1]_{OUT} = HC\ C_1$ *partial conversion*

** **Ensure catalyst insensitivity to CO_2 omission from feed for carbon balancing**

Current Considerations

1. Details of HC blend
2. Minimum/peak temperature versus combustion mode
3. Cooling rate for hysteresis characterization
4. Inclusion of sulfur (~2–5 ppm) in simulated exhaust
5. Aging requirement
6. Poisoning requirement
7. Carbon balancing requirement
8. Single versus multiple SV
9. Powder→core SV conversion
10. Repeatability, # of cycles
11. Standardized hardware configuration requirement
12. Catalyst powder particle size requirement

Easily modified to other *CONVERSION-BASED* applications



How many protocols will be required ?
Can we get to 'one-size-fits-all' ?