Diesel Particulate Filter (DPF) Workshop Objectives

Richard J. Blint (GM R & D Center)
for the CLEERS (Diesel Cross-Cut
Lean Exhaust
Emissions Reduction Simulation)
Committee

October 17-18, 2001,
Dearborn, MI

Overall GOAL

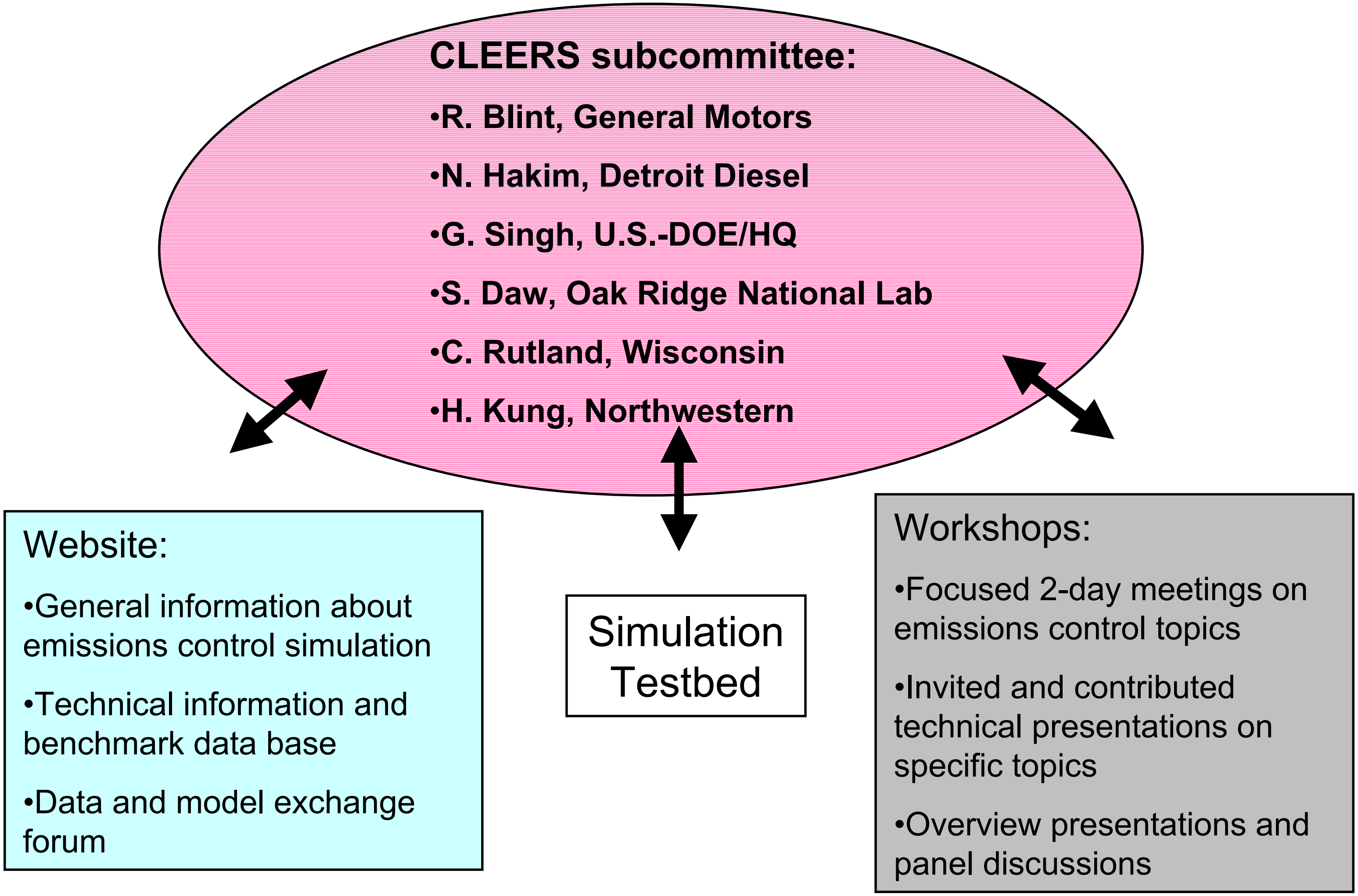
Simulate emission control systems under realistic conditions to optimize the engine/aftertreatment integration

- Issues
  - -Accessible, reliable component submodels
  - Integration of submodels
  - Realistic engine out data for Federal Test Procedure (FTP) driving cycles

Advantages of System Modeling

- Reduced cost and time for system optimization
- Identification of bottlenecks and opportunities
- Improved/tailored component design
  - engines
  - catalysts
  - sensors
  - control strategies
- Vehicle test planning

CLEERS is coordinated by a subcommittee appointed by the Diesel Cross-Cut Team



CLEERS subcommittee:

- **R. Blint, General Motors**
- **N. Hakim, Detroit Diesel**
- **G. Singh, U.S.-DOE/HQ**
- **S. Daw, Oak Ridge National Lab**
- **C. Rutland, Wisconsin**
- **H. Kung, Northwestern**

Website:

- General information about emissions control simulation
- Technical information and benchmark data base
- Data and model exchange forum

Simulation Testbed

Workshops:

- Focused 2-day meetings on emissions control topics
- Invited and contributed technical presentations on specific topics
- Overview presentations and panel discussions

Sponsorship

Diesel Cross Cut Team

(organized by the DOE)

Members

- DaimlerChrysler
- Ford
- GM
- Caterpillar
- Cummins
- DDC
- DOE (OHVT)
- USA TACOM

Technical Workshops

- Overall Concept
  - Promote research collaborations in emission controls simulation
  - Identify state-of-the-art for various technologies and models
  - Identify key unresolved issues, technical paths to solutions
- Approach
  - Sponsor workshops focused on specific simulation topics
  - Workshop parameters
    - 2 days each, 3/yr at accessible locations (e.g., Detroit, Chicago)
    - Participation by industry, academia, national labs
    - Specific topic, 3-4 invited talks, 8-10 contributed talks
    - Published proceedings (Website)

First DOE Crosscut Workshop on Lean Emissions Reduction Simulation

- Title "Addressing the Full-System Context for Lean Exhaust Emissions Control"
- The workshop was held at the National Transportation Research Center (NTRC) in Knoxville, Tennessee, on May 7- 8, 2001
- Sponsored by the Office of Heavy Vehicle Technologies (OHVT)
- The goal of this workshop was to understand how the components fit together globally

Overall Need

Highest priority should be development of more effective predictive tools for emission conversion efficiency and catalyst aging in aftertreatment components.

These new tools should include two types of models:

- 0-D and 1-D component device models for engineering level aftertreatment analysis
- Detailed mechanistic models to understand reaction pathways and rate limiting steps for reactors and catalysts.

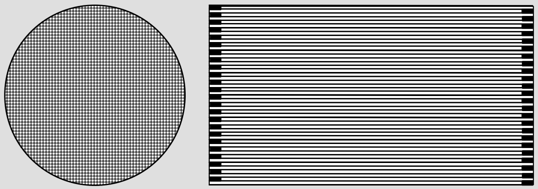
There are important pre-competitive R&D developments needed for both types of models.

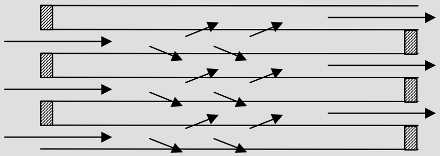
Specific Aftertreatment Component Models

The specific aftertreatment devices that should be modeled first (in approximate order of importance) are:

- Lean-NOx traps
- Diesel particulate filters (especially the regeneration phase)
- Sulfur traps
- Ammonia/urea SCR reactor systems (including the injectors)
- Engine exhaust heaters/conditioners
- Reformers

Sensor performance modeling should also be done at some point, but this should be lower priority than modeling of the above components.

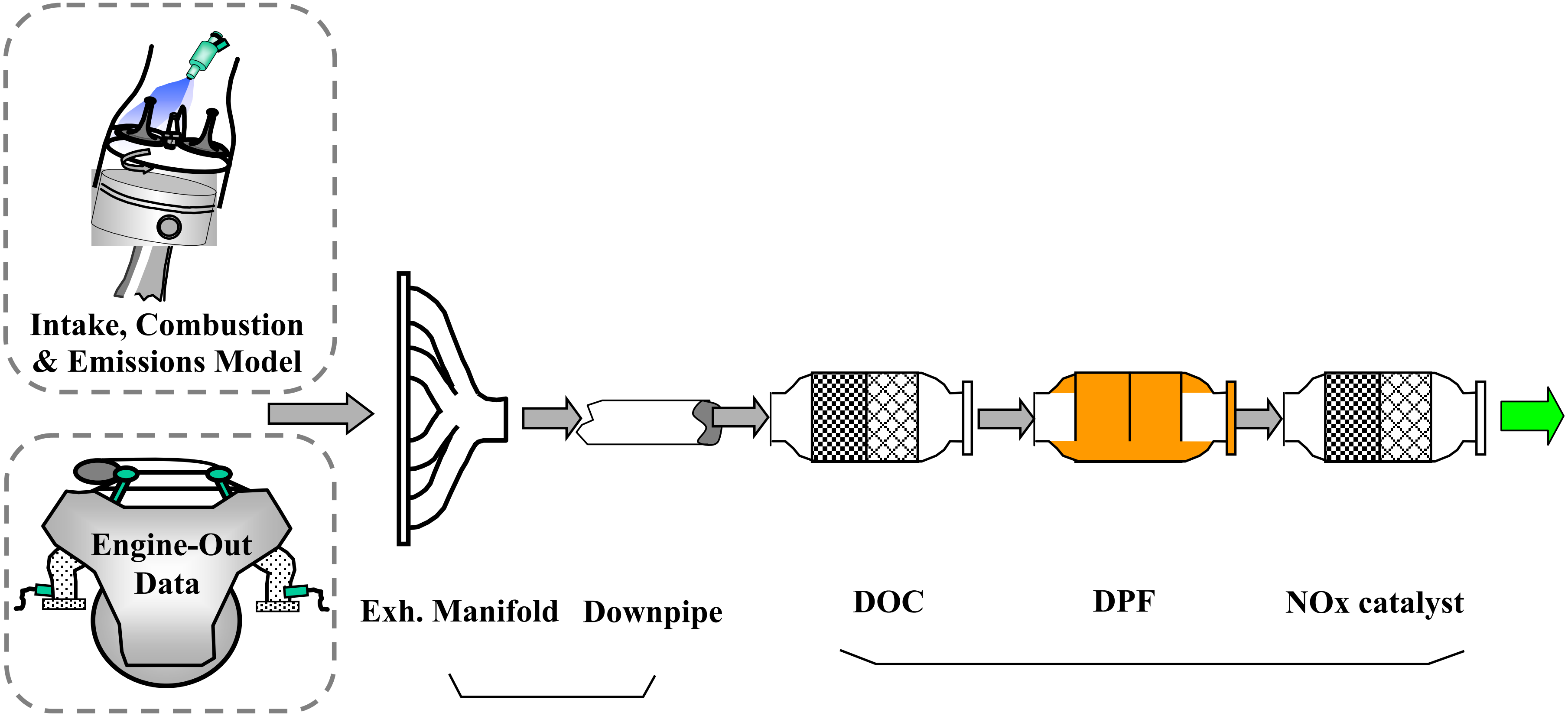




Properties of a typical cordierite monolith used as particulate trap

Cell Density (cells/in^2)	100
Wall Thickness (mm)	0.43
Wall Porosity (%)	48
Mean Pore Size (μm)	13.4
Open Frontal Area (%)	69
Geometric Surface Area (cm^2/cm^3)	13
Hydraulic Channel Diameter (cm)	0.20

DPF Integration Issues

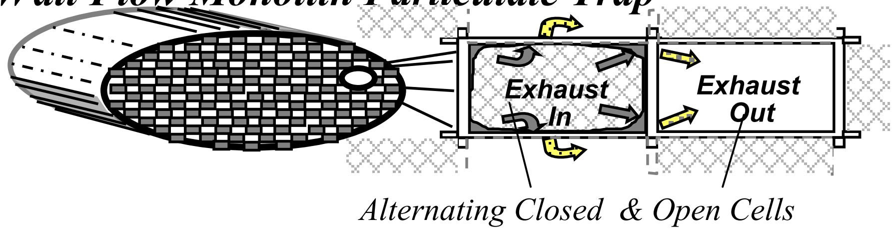


Realistic 1 second or better data over the FTP

Mixing, heat loss and gas phase reactions

Component architecture

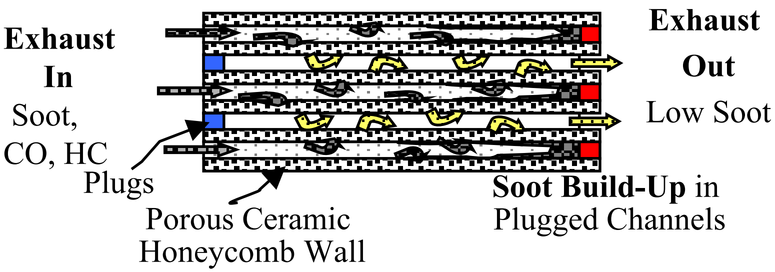
Wall Flow Monolith Particulate Trap



Exhaust In

Exhaust Out

Alternating Closed & Open Cells



Exhaust In

Soot,
CO, HC

Plugs

Porous Ceramic
Honeycomb Wall

Exhaust Out

Low Soot

Soot Build-Up in
Plugged Channels

Typical trap capacity= 5 gm of soot

2 liter trap/liter of engine displacement will require regeneration every 250 miles

DPF Model

Model inputs could include:

- Exhaust mass flow rate and density
- Position along exhaust pipe
- Exhaust emission concentrations at the filter front
- Monolith dimensions, cell density, wall thickness and substrate material
- Monolith substrate porosity and permeability
- PM layer porosity and permeability
- Substrate and PM layer thermal conductivity, heat capacity and density
- Lubricant consumption and ash content

Model outputs may include:

- Pressure drop over DPF as a function of PM build-up
- Prediction of natural regeneration under certain driving conditions
- Heat released during regeneration
- Heat input required to initiate regeneration in a forced regeneration condition
- DPF maximum temperature

DPF Regeneration Issues

- Soot ignition temperature (550 C)
- Soot ignition on catalytic surface (approximately 450 C)
- Typical diesel exhaust temperature (200 C)
- Soot oxidation produces a strong exotherm (i.e.; when started will often combust much of the soot)
- Control the oxidation so that the support is not damaged

Regeneration Strategies (Ignite the soot)

- Engine control & post injection of fuel (i.e.; intentionally raises the engine exhaust temperature)
- Fuel additives
- Electrically heat the DPF
- Non-thermal plasma initiation of oxidation
- Microwave heating of the DPF

CHEMICAL REGENERATION,

- NO is catalytically converted to NO_2
- Chemical regeneration operates at relatively low temperature (250-350°C).
- Problem is contolling the NO/NO_2 ratio.
- A major drawback is the requirement of low sulfur fuel to minimize sulfate formation and to alleviate the sulfur poisoning effect on the NO oxidation reaction.

THERMAL INITIATION FOR REGENERATION

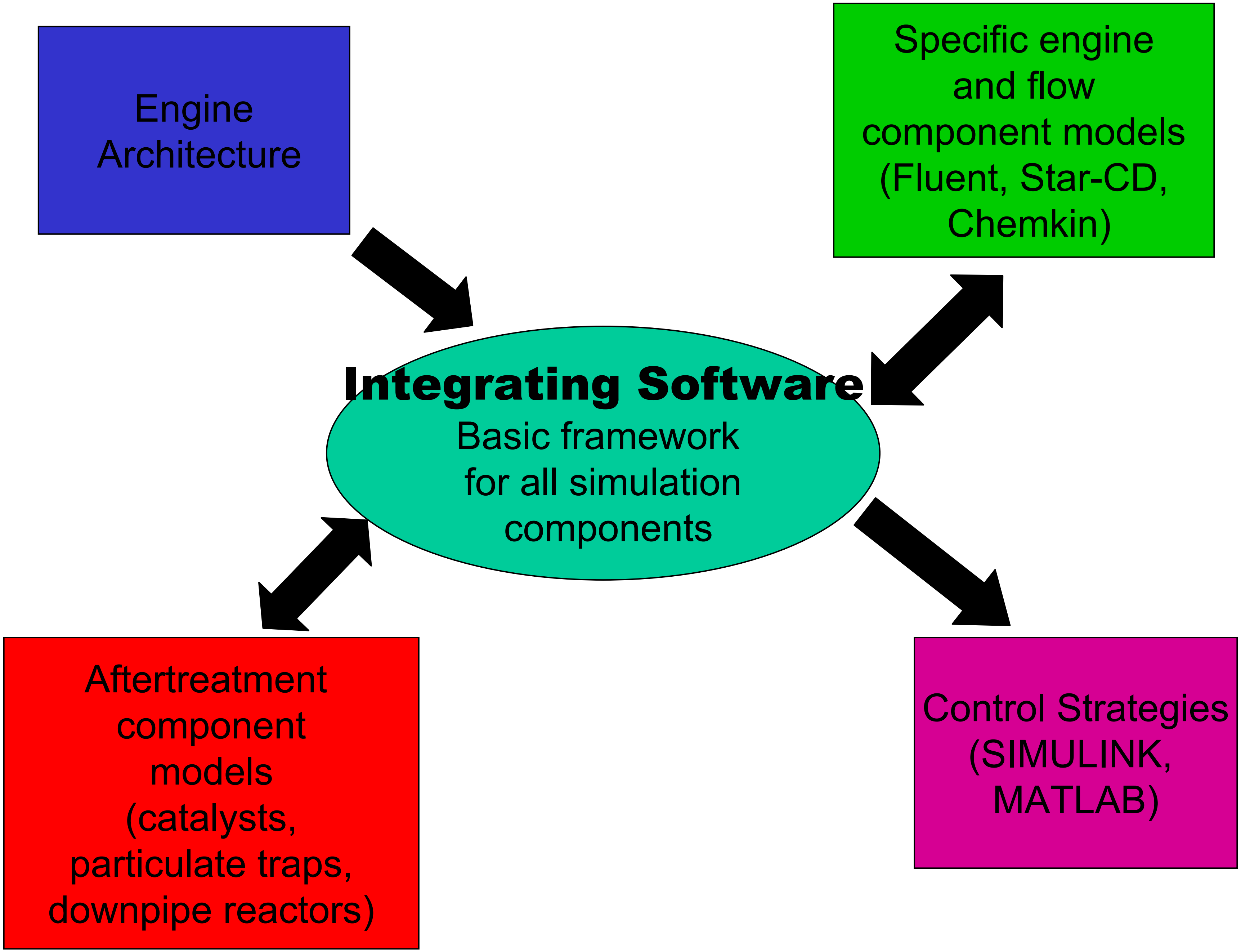
- Has used electrical heaters, gas or oil burners and late injection to elevate the exhaust temperature.
- Burner regeneration system requires a sophisticated fuel metering system, ignition system, and airflow system.
- The heating rate is fast for the burner system which can damage the trap (the burned gas temperature can be as high as 1800 ^{o}C).
- Energy consumption is about 4% of total fuel consumption.
- Throttling the intake or exhaust can increase the exhaust temperature, but not enough to support regeneration.

CATALYST-ASSISTED THERMAL REGENERATION.

- Two types of catalysts have been used for this purpose: surface catalysts and air-borne catalysts
- Since most of the catalysts can only lower the regeneration temperature by 100-200 ^oC, thermal energy is still needed to trigger the regeneration.
- Surface catalysts are coated on the surface of a particulate trap, most commonly, platinum which lowers the particulate ignition temperature to 350-400 ^oC.
- Air-borne catalysts are transition metals (e.g.; cerium, lead, manganese, copper, and iron) added into the fuel which oxidize during combustion and become air-borne. Fresh catalyst has to be continually supplied.

Integration Issues for DPF’s

- Exhaust stream temperature is crucial to the ignition of the soot and is dependent on all the upstream devices.
- NO/NO_2 ratio is important to soot oxidation. How do the upstream devices change this ratio?
- Hydrocarbon content of the exhaust can influence the soot oxidation. How do can we preserve it until it reaches the DPF?



Engine Architecture

Specific engine and flow component models (Fluent, Star-CD, Chemkin)

Integrating Software

Basic framework for all simulation components

Aftertreatment component models (catalysts, particulate traps, downpipe reactors)

Control Strategies (SIMULINK, MATLAB)

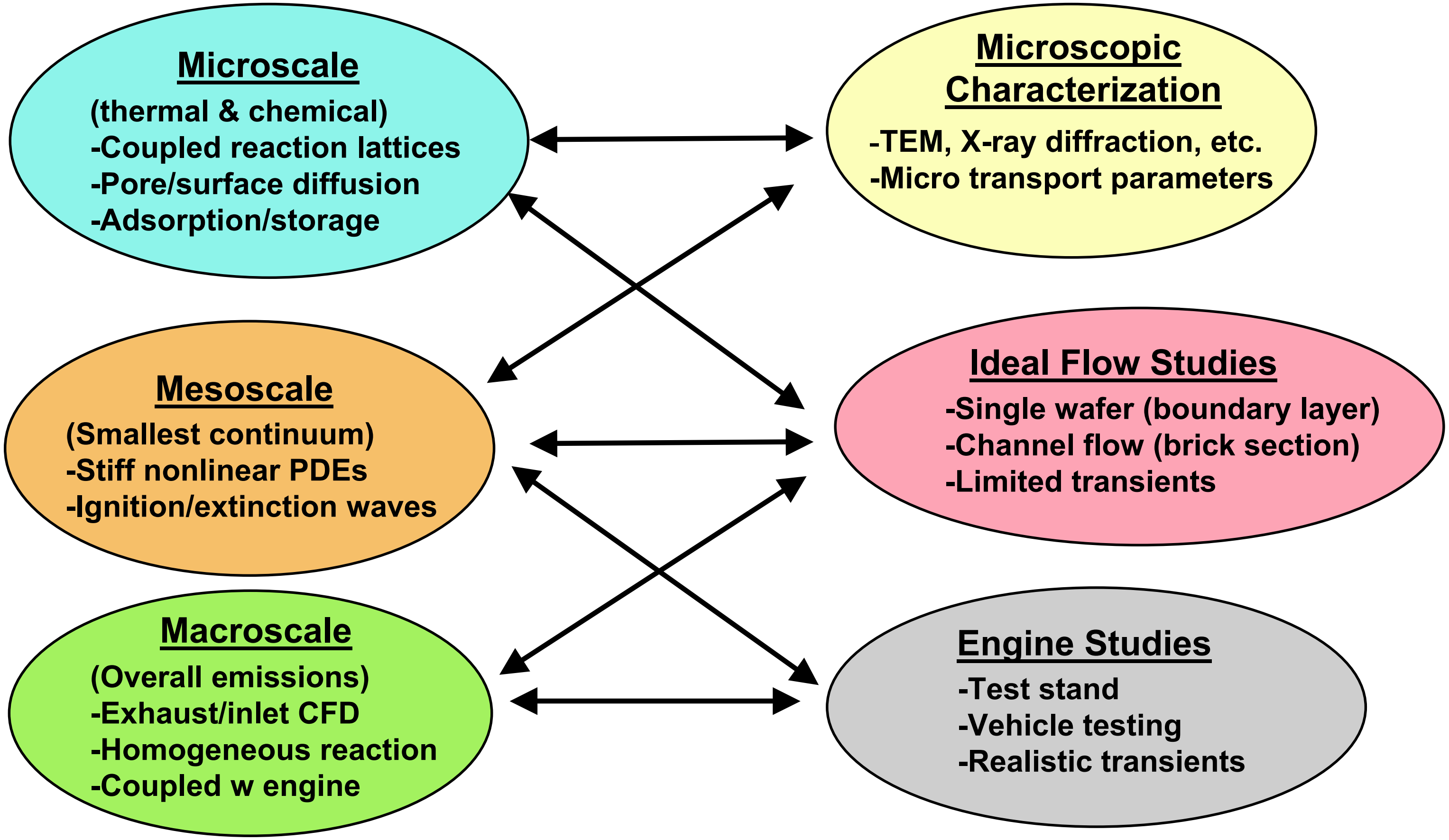
Simulation Center (Goals)

- ORNL Home (Stuart Daw, Coordinator)
- Central system for evaluating aftertreatment models with a complete set of aftertreatment model
- Suite of baseline models for comparison Library of benchmark case inputs (e.g., OEM engine out data and catalyst out if possible)
- Library of benchmark case results for public, private models
- Web-based simulation access

Multidisciplinary Projects Can Provide Faster Track to Improved Catalysts

Modeling

Experimental



Microscale

(thermal & chemical)
-Coupled reaction lattices
-Pore/surface diffusion
-Adsorption/storage

Mesoscale

(Smallest continuum)
-Stiff nonlinear PDEs
-Ignition/extinction waves

Macroscale

(Overall emissions)
-Exhaust/inlet CFD
-Homogeneous reaction
-Coupled w engine

Microscopic Characterization

-TEM, X-ray diffraction, etc.
-Micro transport parameters

Ideal Flow Studies

-Single wafer (boundary layer)
-Channel flow (brick section)
-Limited transients

Engine Studies

-Test stand
-Vehicle testing
-Realistic transients

Goals for DPF Workshop

- Define and prioritize the surface deposition and oxidation experiments to define soot models
- Identify and prioritize the filter data need to develop the models
- Identify and prioritize the engine data needed to both develop and verify the DPF catalyst models