NOx Absorber Workshop Objectives

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for the CLEERS (Diesel Cross-Cut Lean Exhaust Emissions Reduction Simulation) Committee

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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 Proceedure (FTP) driving cycles

Advantages of System Modeling

- Reduced cost and time for system optimization
- Identification of bottlenecks and opportunites
- 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.

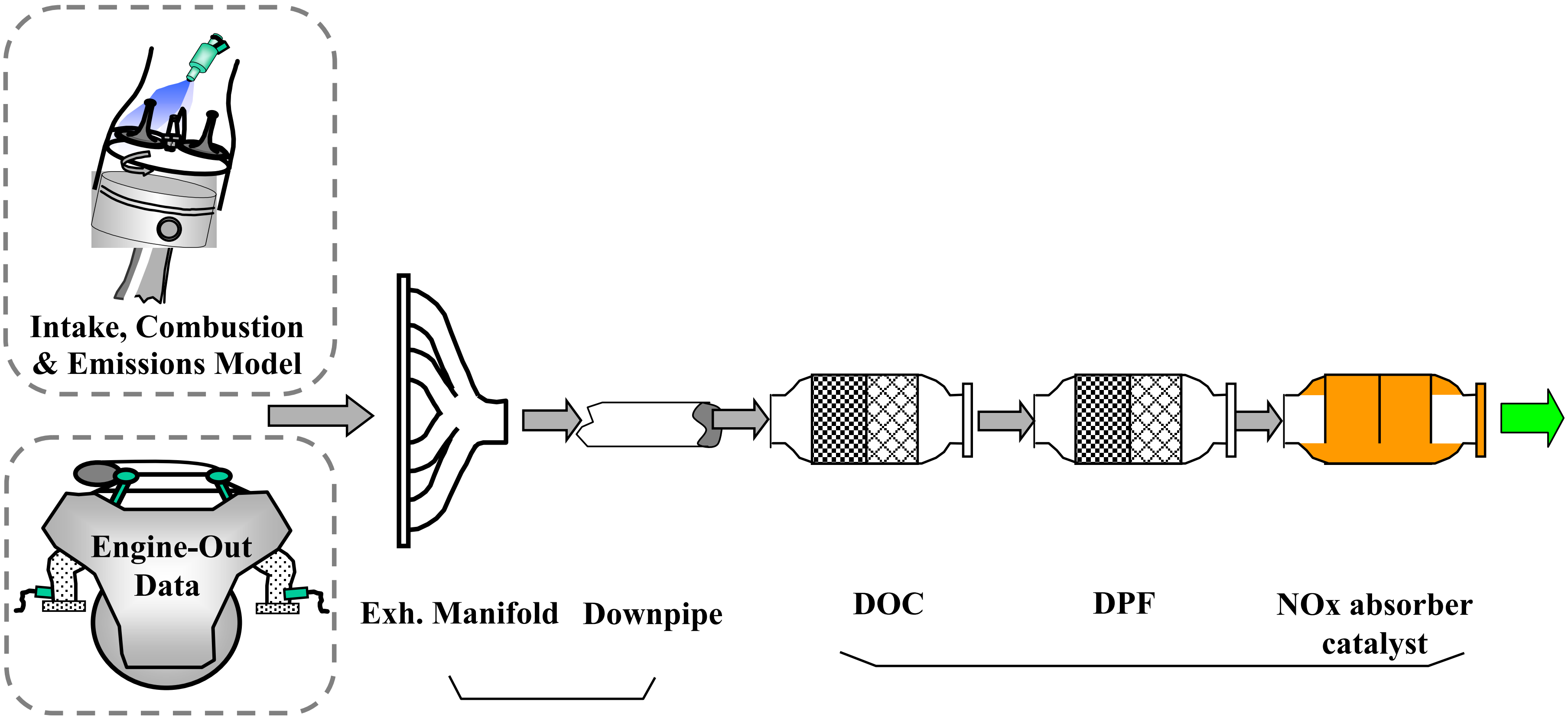
Specific Aftertreatment Component Models

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.

NOx Adsorber



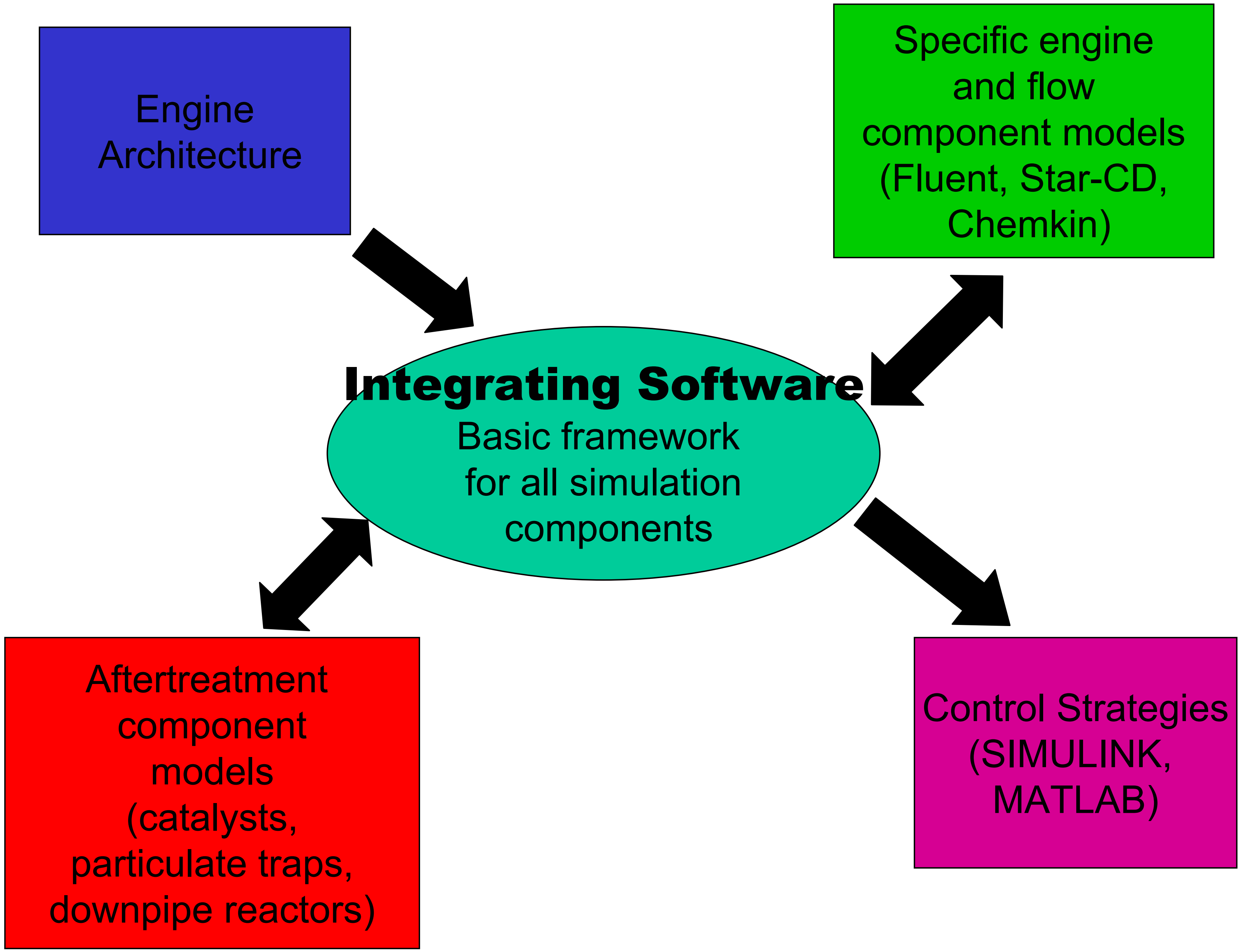
Realistic 1 second or better data over the FTP

Mixing, heat loss and gas phase reactions

Component architecture

Key requirements for realistic simulations

- Accurate measurement or prediction of engine-out conditions
  - Variable flow, composition, temperature
  - Normal operation (cold start, acceleration, load change)
  - Anomalous operation (misfire, cylinder cut-out)
- Predict component response under engine conditions
  - Use reactor measurements to develop simulation parameters
  - Correlate/refine reactor response to component engine response over the range of conditions
- Federal Test Procedure (FTP) prediction
  - Ultimate standard for the simulation
  - Evaluate engine control algorithm for effect on catalyst efficiency


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)

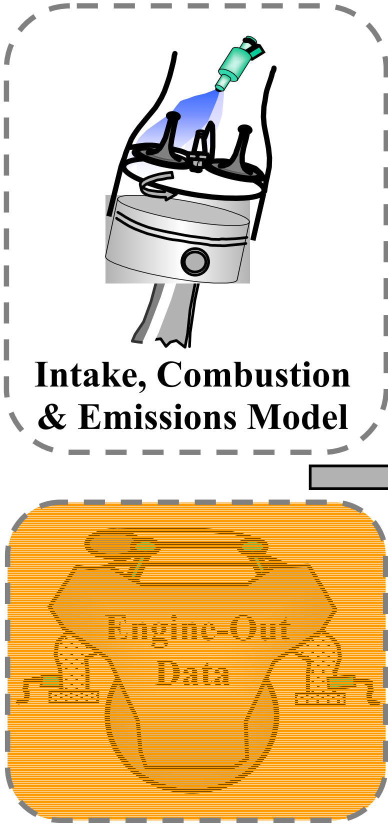
- ORNL Home (Stuart Daw, Coordinator)
- Central system for evaluating aftertreatment models with a complete set of aftertreatment model
- Suite of baseline models for comparison Library of benchmark case inputs (e.g., OEM engine out data and catalyst out if possible)
- Library of benchmark case results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

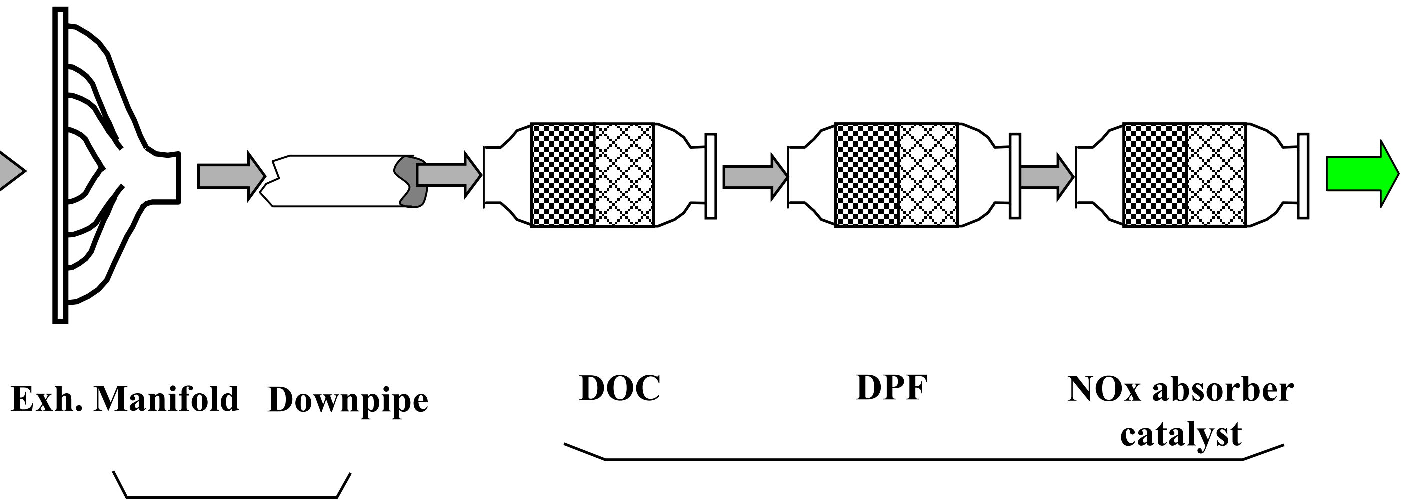
Engine out Issues for NOx Absorbers

- Integrated engine out compositions (i.e.; how much NOx has gone into the absorber)
- Variation of engine out compositions with the FTP cycle (e.g.; prediction of engine transients)
- Engine out compositional variations with NOx and possibly SOx regeneration strategy/strategies

Measured Engine-out parameters

- *Advantage-correct values*
- *Disadvantage-difficult to extrapolate to other conditions*





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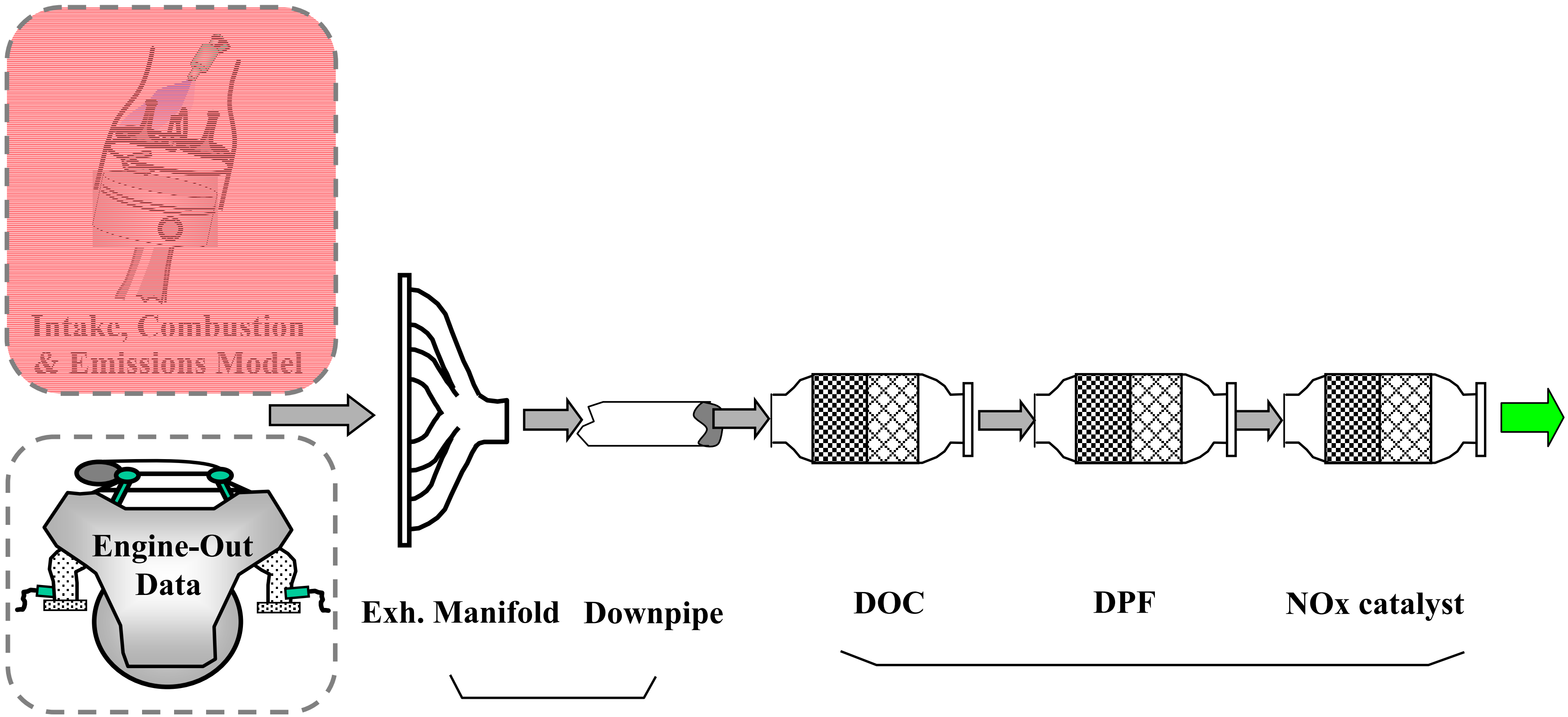
Component architecture

Engine/Aftertreatment Integration Strategy

- Software
  - **GT Power** (low dimensional engine simulation, generally poor emission predictions, good integration of aftertreatment component models)
  - **Matlab/Simulink** (good integration of all component models including outside engine simulations)
  - **Advisor/PSAT** (can integrate aftertreatment models, can estimate transient emissions from steady state dyno data)
  - **Chad/Kiva or CFD engine code** (would have to integrate through other code, best chance of ab initio emissions predictions)

Elements of the System



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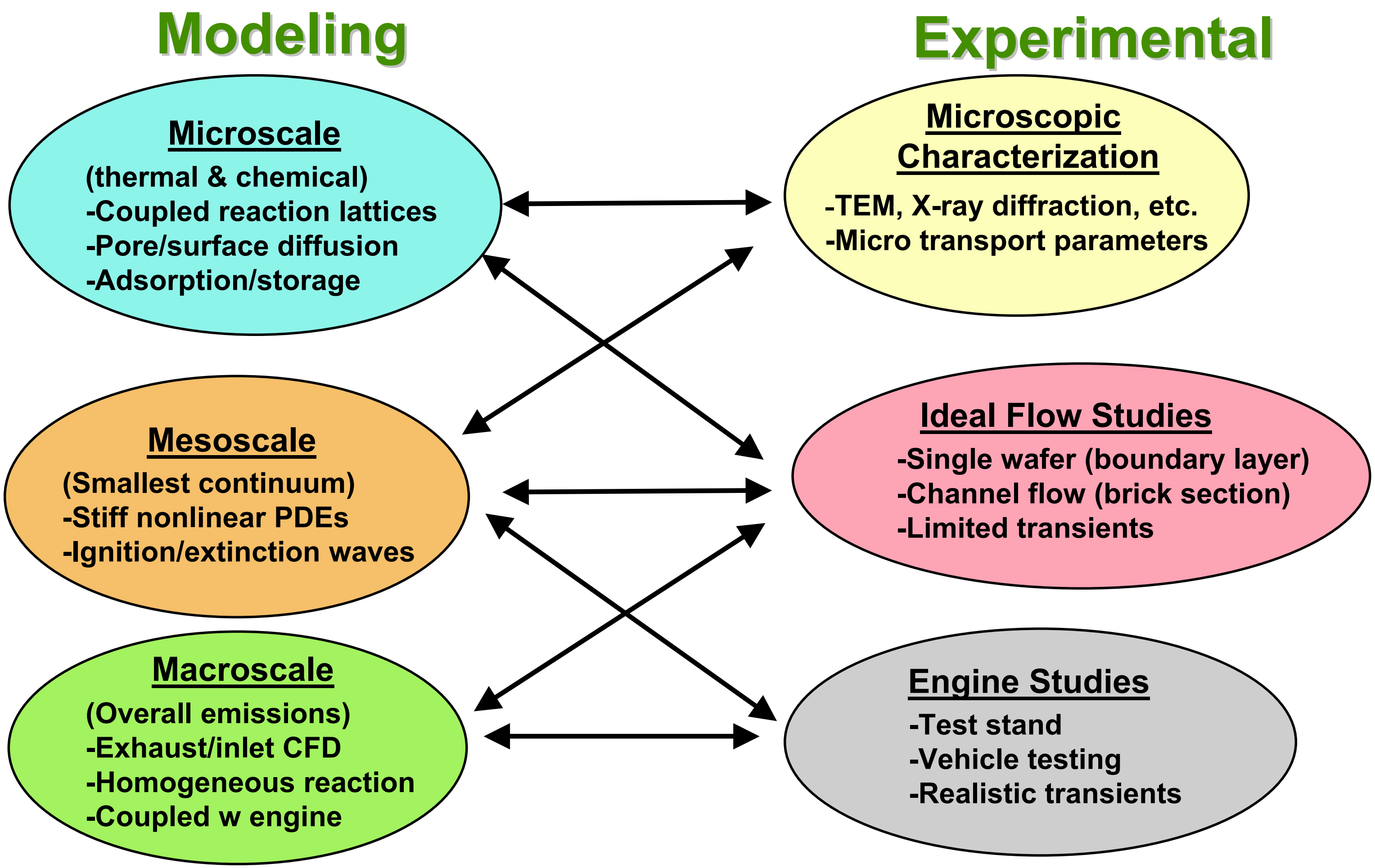
Component architecture

Composition Data Bases for Benchmarking and Testing
(Chris Rutland's talk)

- <u>Engine data base 1</u>: Excel spread sheets of exhaust valve out for an FTP cycle. This would include temperature, mass flow rate, composition and also any temperature measurements at the catalyst position.
- <u>Engine data base 2:</u> Constant speed runs with composition, flow rate, temperature at the exhaust valve. This data should be in a format amenable for input to ADVISOR/PSAT
- <u>Engine data base 3:</u> GT-Power input files for various engines
- <u>Reactor data base:</u> Catalytic reactor runs on monolith wafer or catalytic powders. Included in this database would be some designation of the catalyst material (even just a known serial number and aging history), temperature, composition, space velocity.

Multidisciplinary Projects Can Provide Faster Track to Improved Catalysts



Goals for LNT Workshop

- Define and prioritize the surface and reaction kinetic information needed to develop both detailed and global LNT models
- Identify and prioritize the reactor data need to develop the models
- Identify and prioritize the engine data needed to both develop and verify the LNT catalyst models