



Discovery of New NO_x Reduction Catalysts for CIDI Engines Using Combinatorial Techniques

Cooperative agreement DE-FC26-02NT41218 with the United States Department of Energy

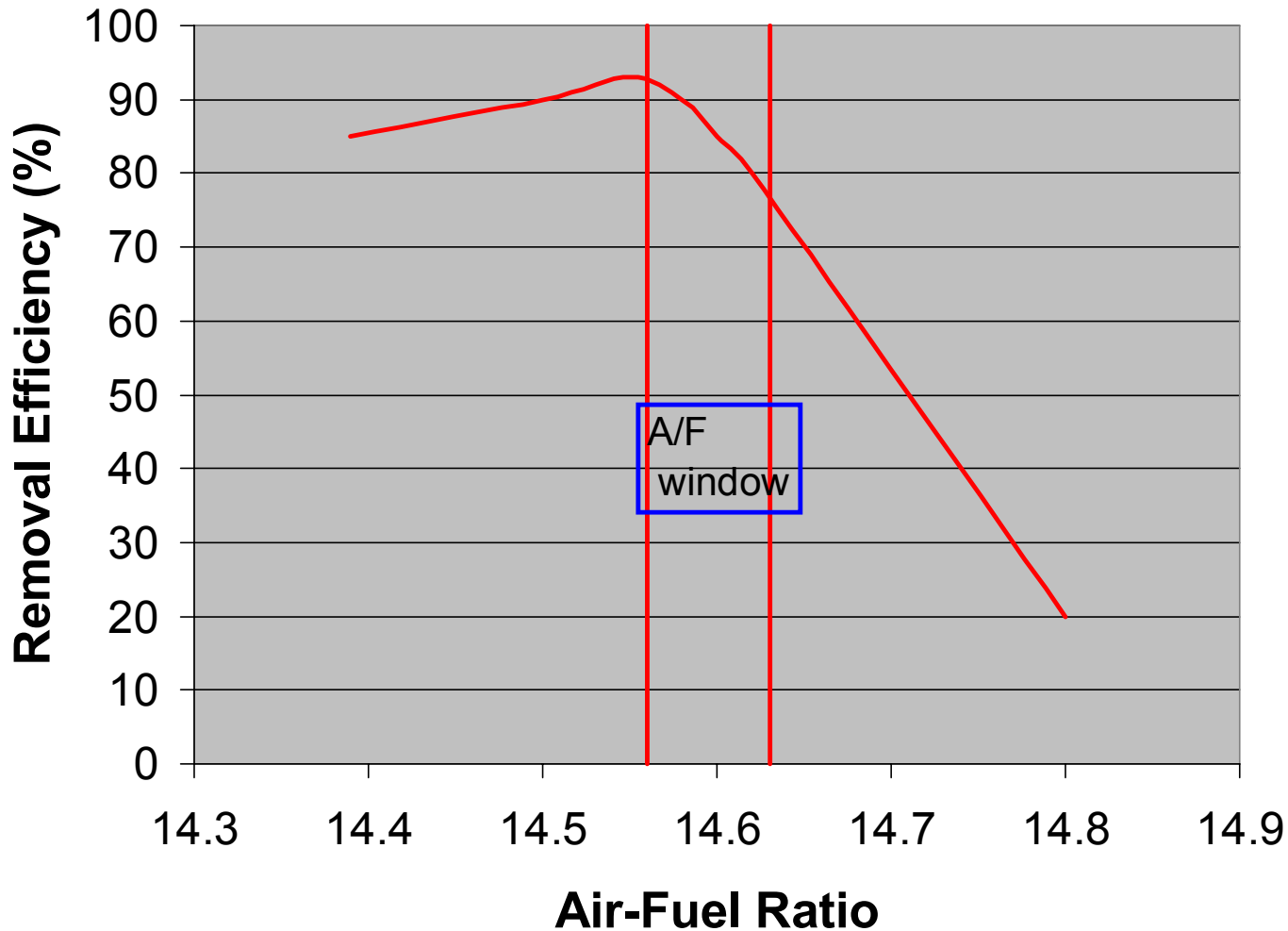
Motor Fuels: Effects on Energy Efficiency & Emissions in the Transportation Sector

Richard Blint

General Motors Corporation

October 9-10, 2002

Traditional Performance of Three-Way Catalysts



Objective

To develop new catalytic materials for NO_x reduction in lean exhaust conditions as occur in diesel exhaust

Combinatorial Catalyst Approach

What are we trying to do?

Discover entire “families” of new NO_x catalysts for lean to stoichiometric exhaust conditions using high throughput (HT, i.e.; combinatorial) techniques

Why combinatorial methods?

There is unexplored compositional space with promise for NO_x reduction. HT methods will let us explore this space.

How is catalyst discovery done today?

Single material analysis at a time: 2-4 weeks, high cost per material, insufficient materials for “data mining”.

DOE Ultra-Clean Solicitation

Proposals aimed at the development of innovative emission control strategies

Proposals REQUIRED the following participants:

- catalyst manufacturer
- Compression Ignition Direct Injection (Diesel) engine manufacturer
- alternative fuels

Program Overview

GM-DOE Ultra Clean Fuels Proposal

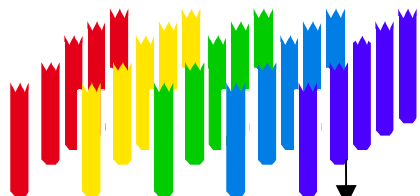
Selection, September 2001

Project value = \$14.4 million

39 month project

- **Start date 8/16/02**
- **Multi-faceted team**

Fast throughput testing



Emission detectors



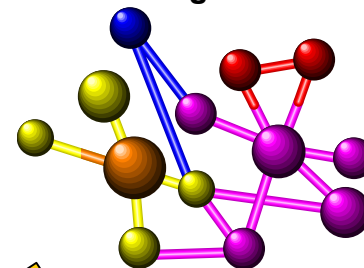
Prediction of new materials



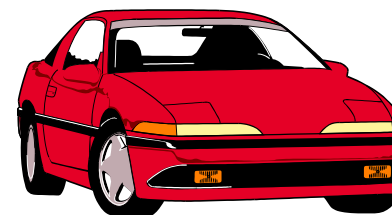
Informatics: A fully correlated library of new materials and experimental results



Structure-activity analysis and data mining



Dyno testing of new catalysts



Program Participants

- **GM** - Diesel engine manufacturer, exhaust system fabrication and utilization. Catalyst validation & emission control strategies. ([Richard Blint, contact](#))
- **Accelrys** –Scientific software provider. Informatics system supplier. ([George Fitzgerald, contact](#))
- **Engelhard** – Surface and materials science company. Supplier of exhaust system catalysts. HT catalytic materials synthesis and testing. ([Gerald Koermer, contact](#))

Automotive Catalyst Discovery Paradigm

Synthesis

Screening

**High Throughput
Experimentation**

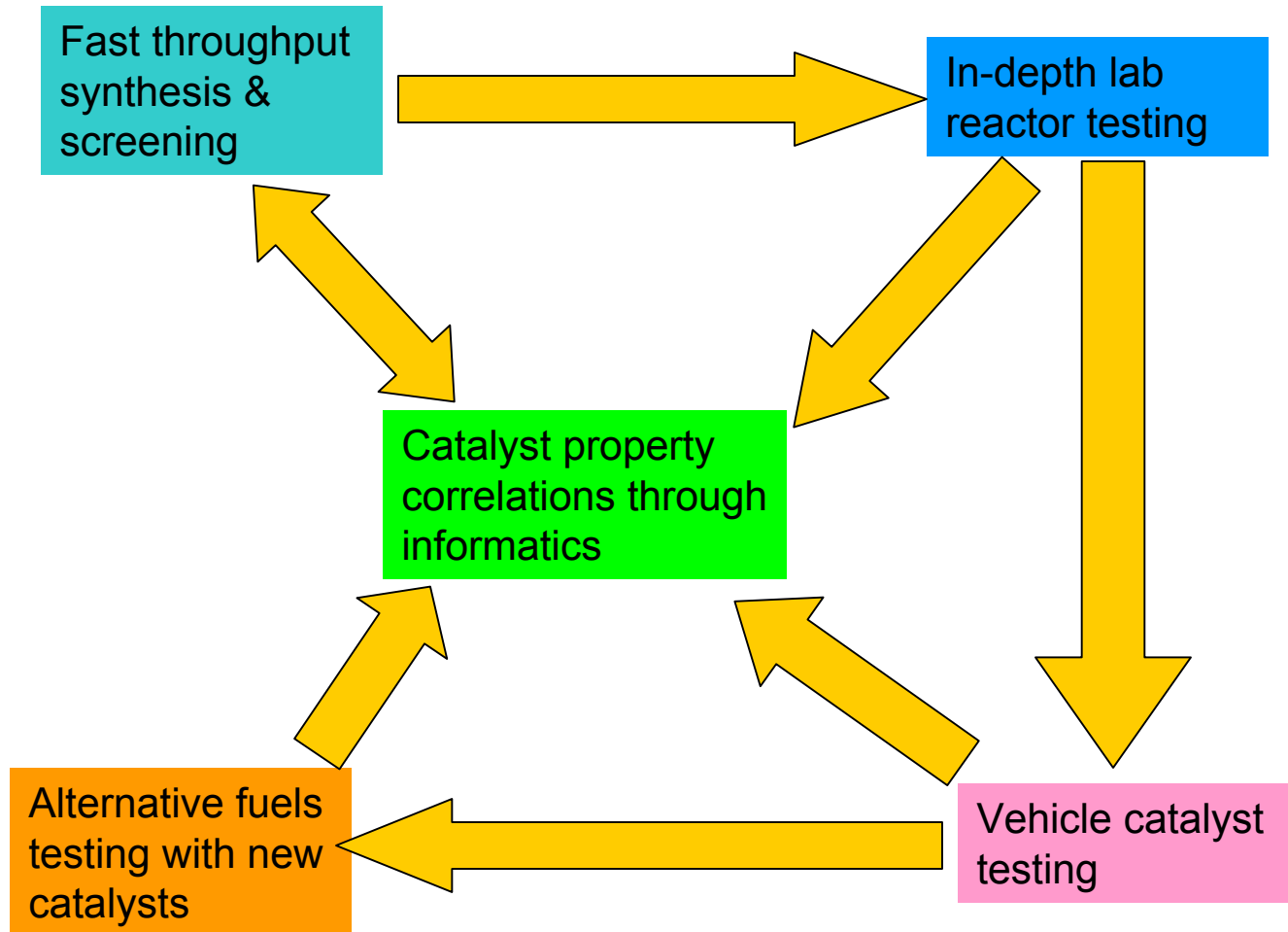
Characterization

Aging

Informatics



Program Process Flow

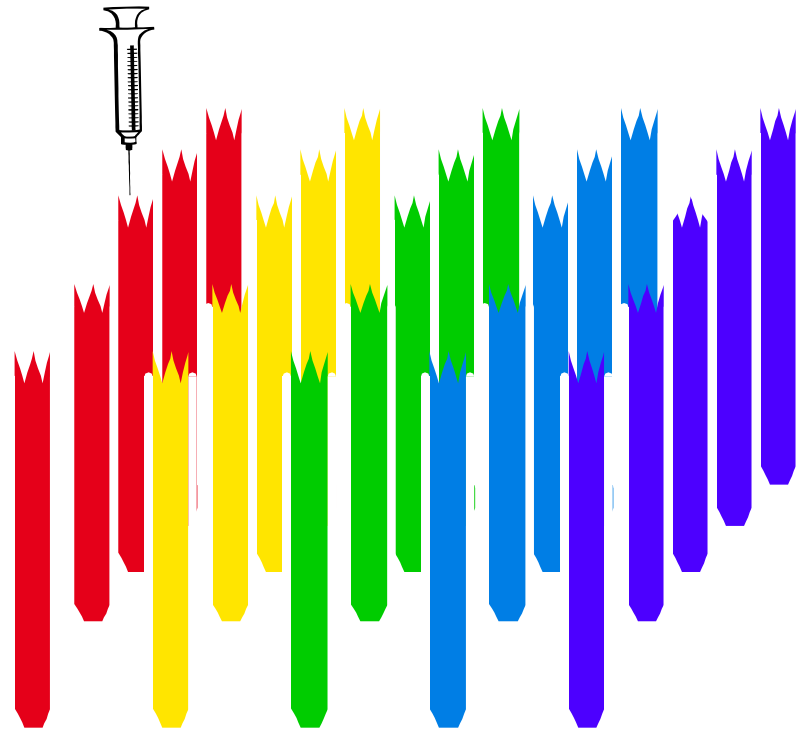


Technical Tasks

- **HT Design and Synthesis of materials/catalysts**
- **HT Screening**
- **Validation and Scale Up**
 - **Traditional lab reactors**
 - **Engine Lab**
- **Tools Development**
 - **Informatics**
 - **Instrumentation**
- **Exhaust Systems Development**
 - **Feasibility analysis**

Robotic Microsynthesis of New Materials

- 300 or more new materials per tray
- automated reagent delivery
- very small test quantities - aspirin tablet vs. bag of marbles



Possible Reactions for Catalytic Material Discovery

- **NOx Reduction**

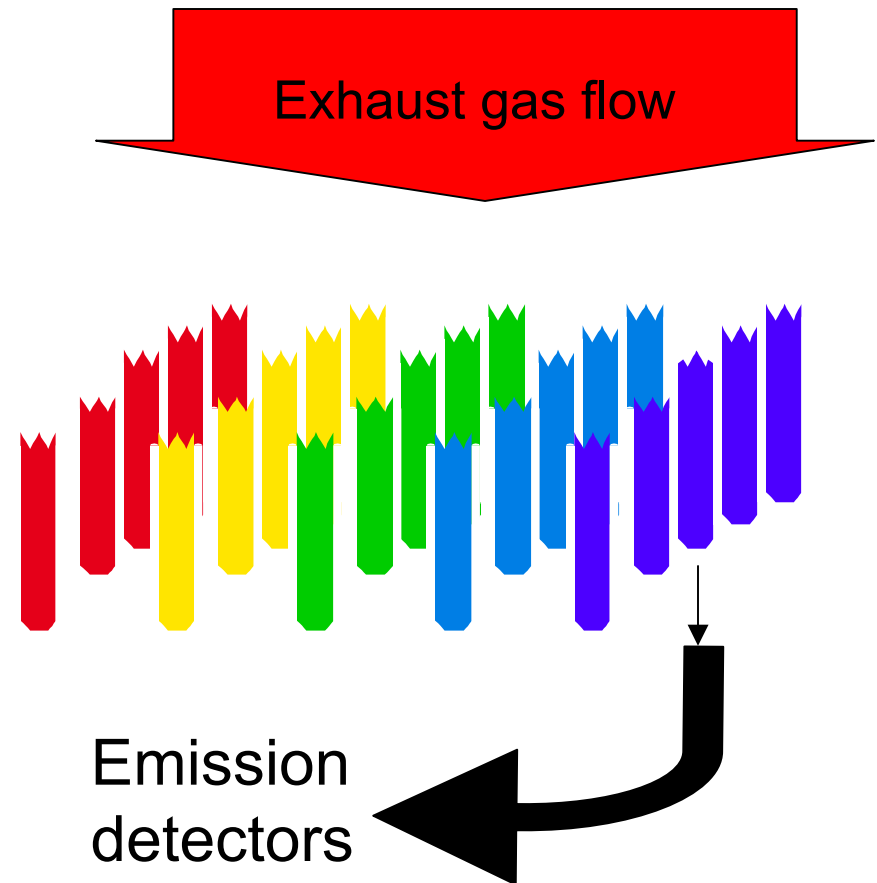


- **NOx Decomposition**



Catalyst Activity Measurements

- All the samples in the same reactor
- Sequential testing of the pollutant conversion of each new material



High Speed Screening Unit

- **Serial Mass Spec Analysis**
- **Steady State Operation**
- **Throughput - ~200 new materials/week for this program**
 - **Increases in the future**

Accelrys - Informatics Development

- Data Acquisition

- Newly developed techniques

- Data Base Development

- Development of CombiMat for materials informatics

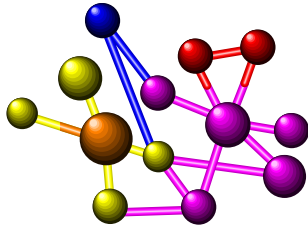
- Data Mining and Analysis

- Based on molecular modeling software

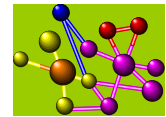
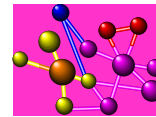
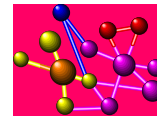
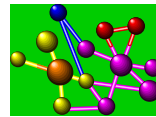
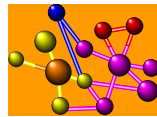
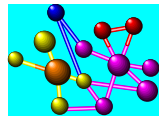
GM Role

- **Prime contractor**
- **Ultimate customer**
- **Classic bench reactor testing of hits from the discovery stage**
- **Feasibility analysis of hits for vehicle application**

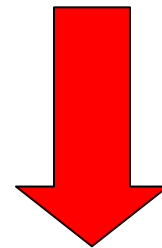
Families of Materials



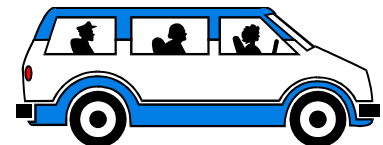
A Hit!!! Works, but properties may not be the best



Cycle through similar materials to optimize the properties including economics



New affordable converter



Combinatorial Catalyst Methods

What is in our approach that can make it succeed?

Use of combinatorial techniques for automotive catalyst discovery

A strategic business partnership with high value for each partner

What difference could it make for the automotive customer?

Enables passenger diesels in the US market

Summary

- Start date (8/16/02)
- Target needs (2007 Tier II and 2010 Emission roll-in requirements)
- New catalyst discovery in 2002-2005 time frame can impact new product rollouts

Project initiation!!!!