Simulating Integrated Engine-Emissions-DOC-DPF Performance

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Acknowledgements

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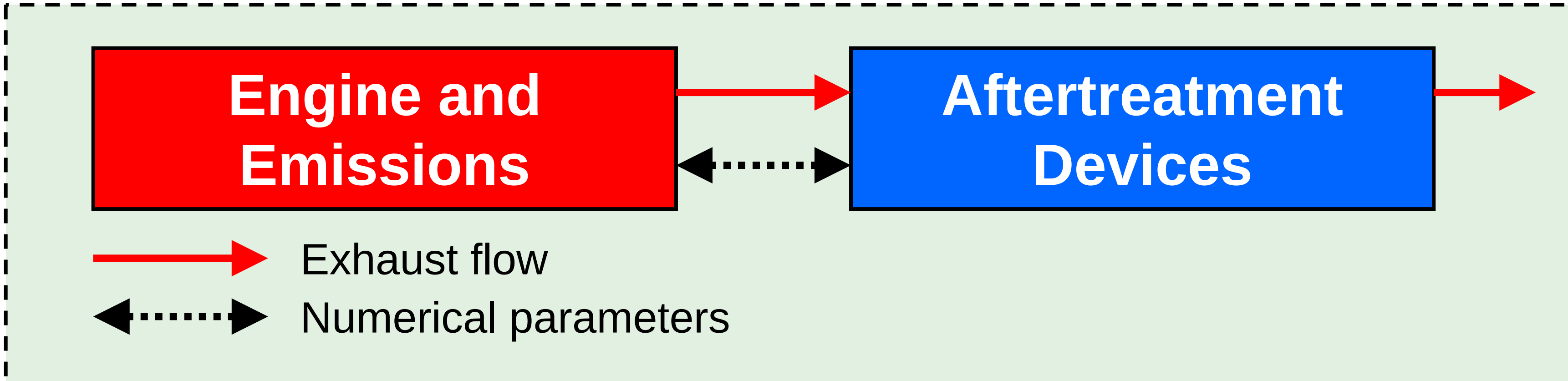
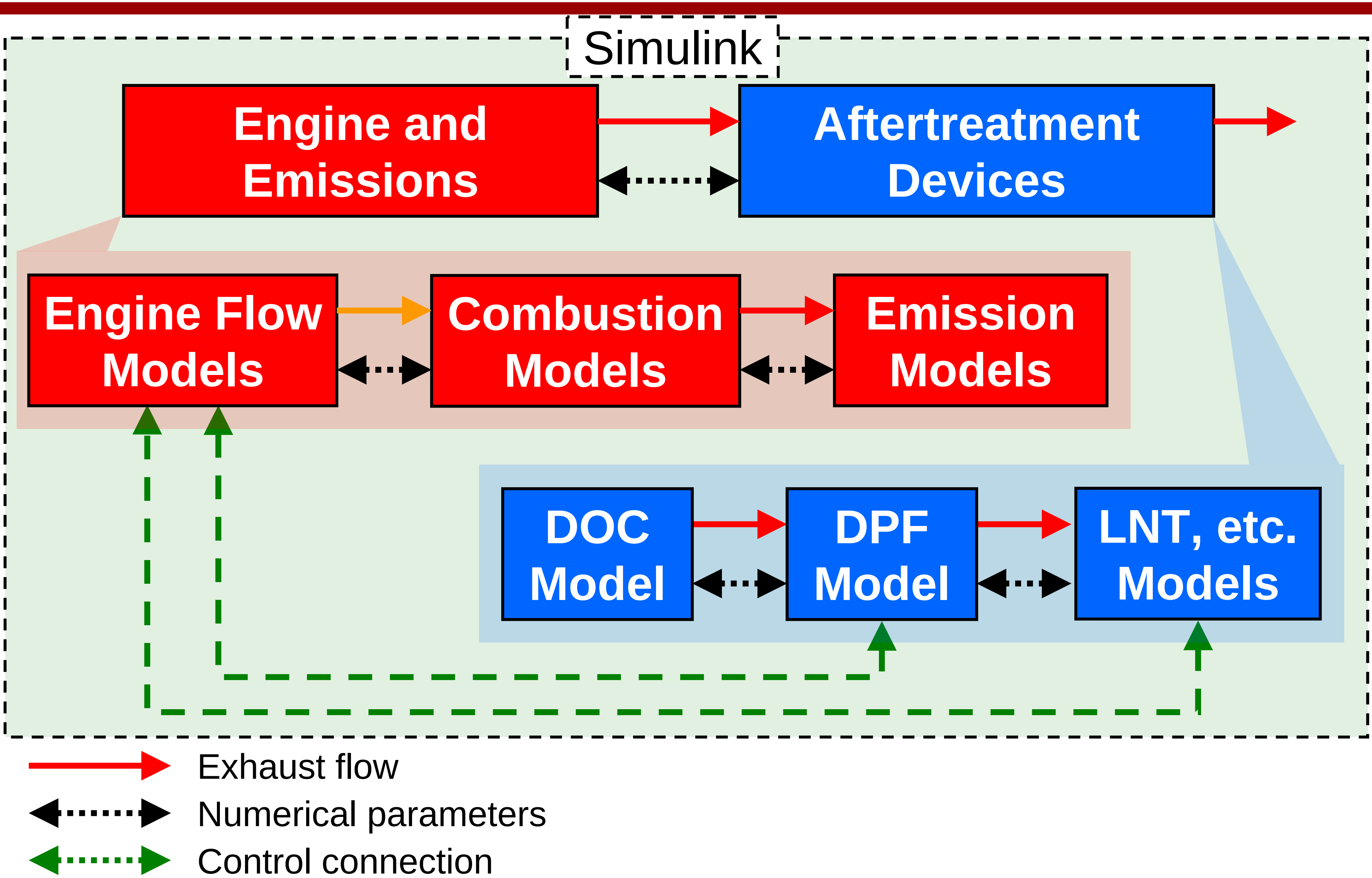
System Models: Current Literature



- He, GM R&D (SAE 2007-01-1138)
  - Integrated in Simulink
- Pischlinger, et al., FEV (SAE 2007-01-1128)
  - In-house integration environment
- Guthenke, et al., DaimlerChrysler (SAE 2007-01-1117)
  - GUI based in-house integration environment
- Piscaglia, et al., Polt. Di Milano (SAE 2007-01-1133)
  - Simulink
  - DPF model to test ECU model

- Detailed physics based AT models
- Primary use: evaluate AT configurations
- No engine or emissions models
  - Driven by laboratory data

ERC Work: Integrated System Level Model



System Modeling Approach

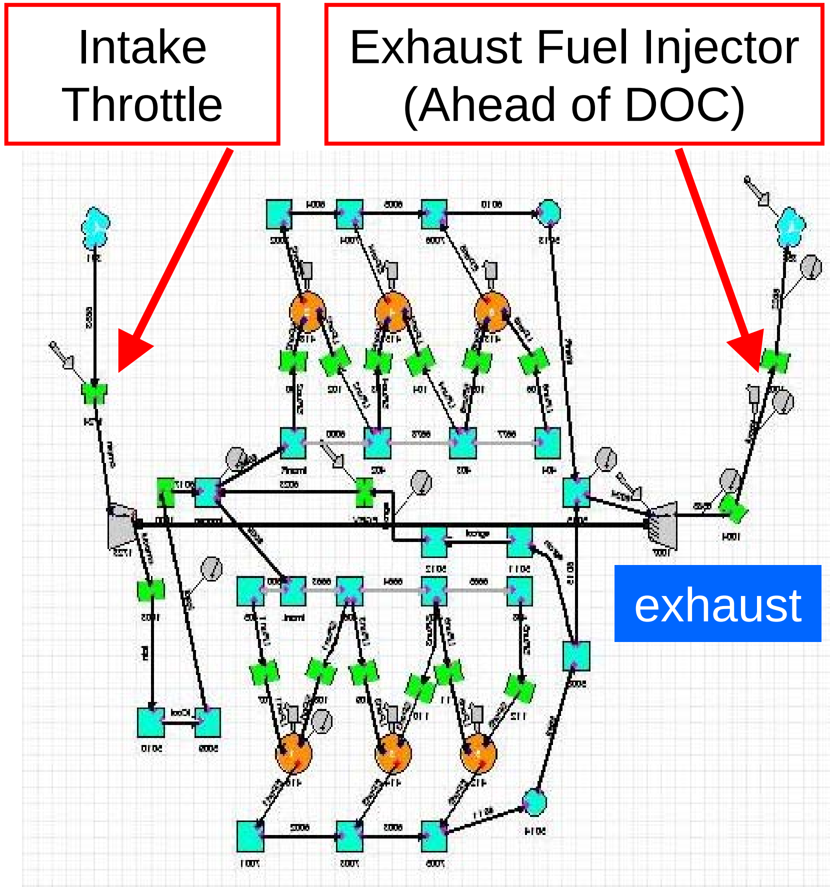
- Develop an integrated system level computer model
  - Capture interactions:
    - Device – Device
    - Device - Engine
  - Transient
  - Conventional and LTC (HCCI, PCCI, etc.) diesel combustion
- Develop new component models as needed
  - Examples: LTC heat release, emissions, heat transfer
- Incorporate existing models/modules
  - Examples: DPF, DOC, LNT, …
- Integrate components as modules in an overall system level environment
  - Environment: Matlab-Simulink
    - Also allows controllers
  - Develop modular approach for efficiency and ease-of-use
- Validation
  - Component level: experimental data
  - System level: experimental data (when available) and “sense checks”

Objectives and Results

- Explore steady state and transient scenarios
  - Examine and help explain device interactions
  - Suggest 'guidelines' of operation
    - Based on model results and analysis

- Recent results
  - LTC combustion under load transients
  - Effect of DPF loading and regeneration on engine operation
  - Compare different DPF regeneration techniques
  - Model prevention and control of runaway DPF regenerations

Diesel Engine Model



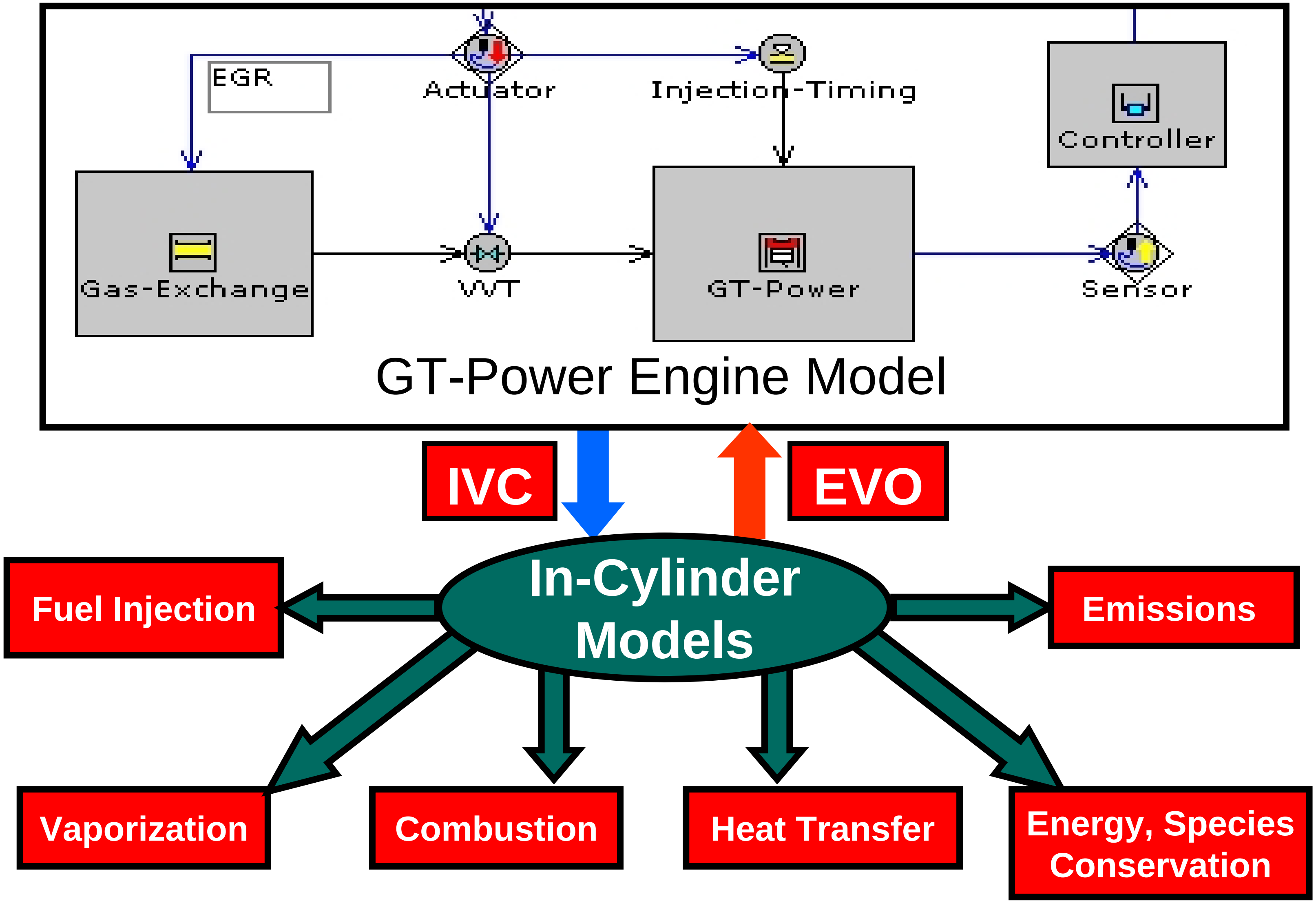
Example of a WAVE engine model with sensors and actuators

- WAVE or GT-Power
- Industry standard
- Includes:
  - Heat transfer models
  - Flow models
  - Turbocharger model (VGT)
  - Simple Combustion model
    - Heat release rates from experimental pressure
    - Could also use built in heat release models
    - Calibration required
- Communicate with Simulink using sensors and actuators

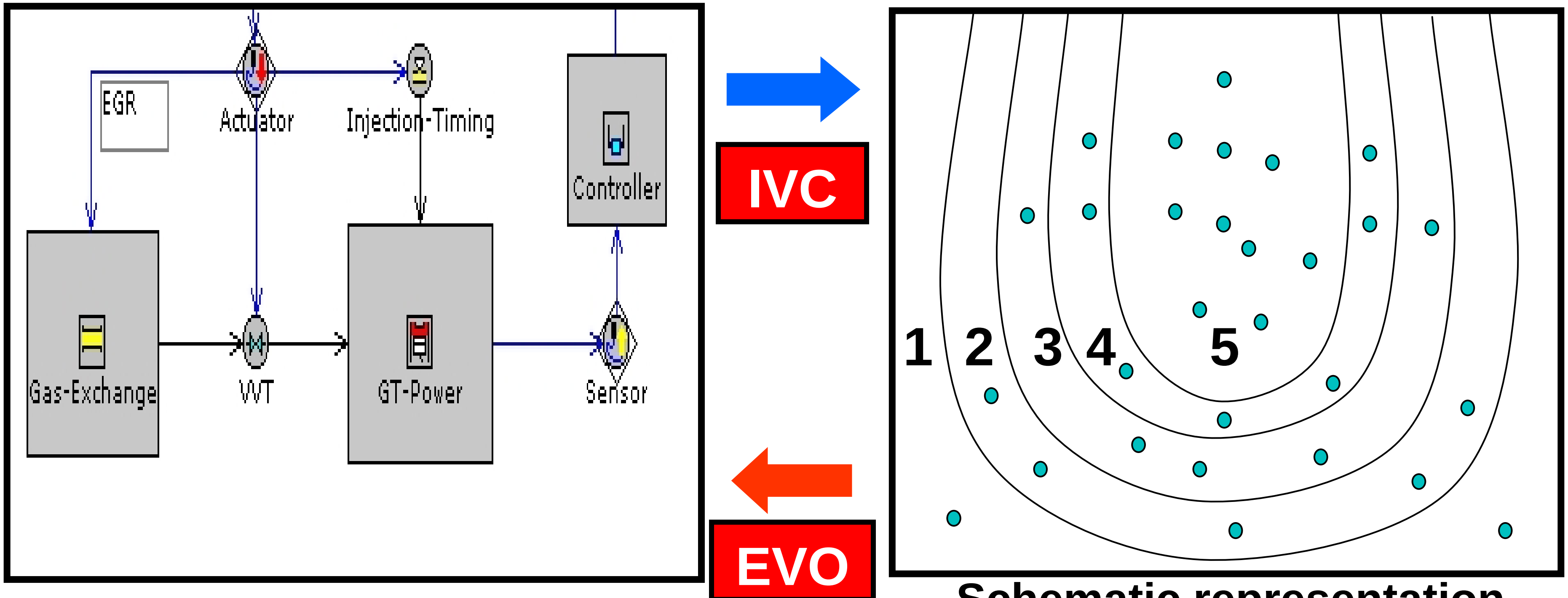
Traditional Diesel Engine Model - Disadvantages

- Simple combustion (heat release) model
  - Prescribed function, calibrated with engine data
  - Simple spray models
- Simple emissions models
- Sufficient for conventional diesel operation but not for new LTC type combustion technologies
- Need improved combustion / heat-release models and emissions models for current application

User Defined Cylinder Models



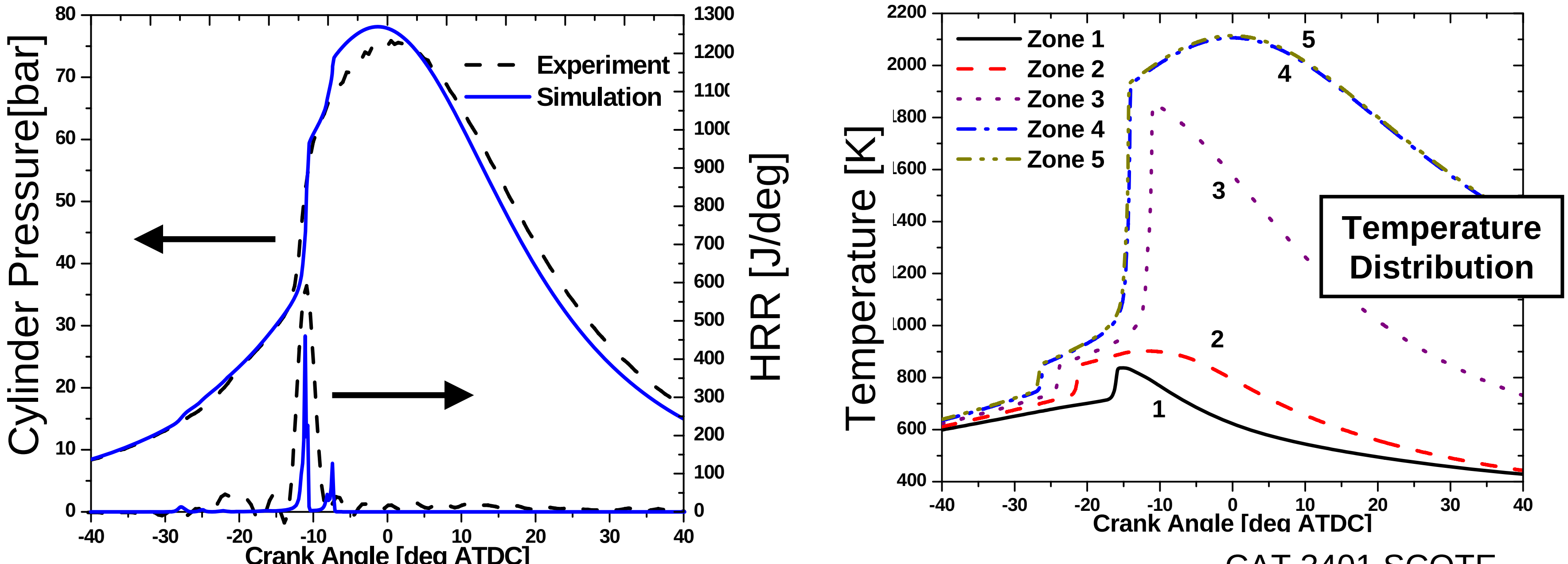
Multi-Zone Combustion Model



Schematic representation of zones

- Combustion chamber initialized with multiple zones
- The zones include sub-models for vaporization, chemical kinetics (CHEMKIN), heat transfer, energy/species conservation

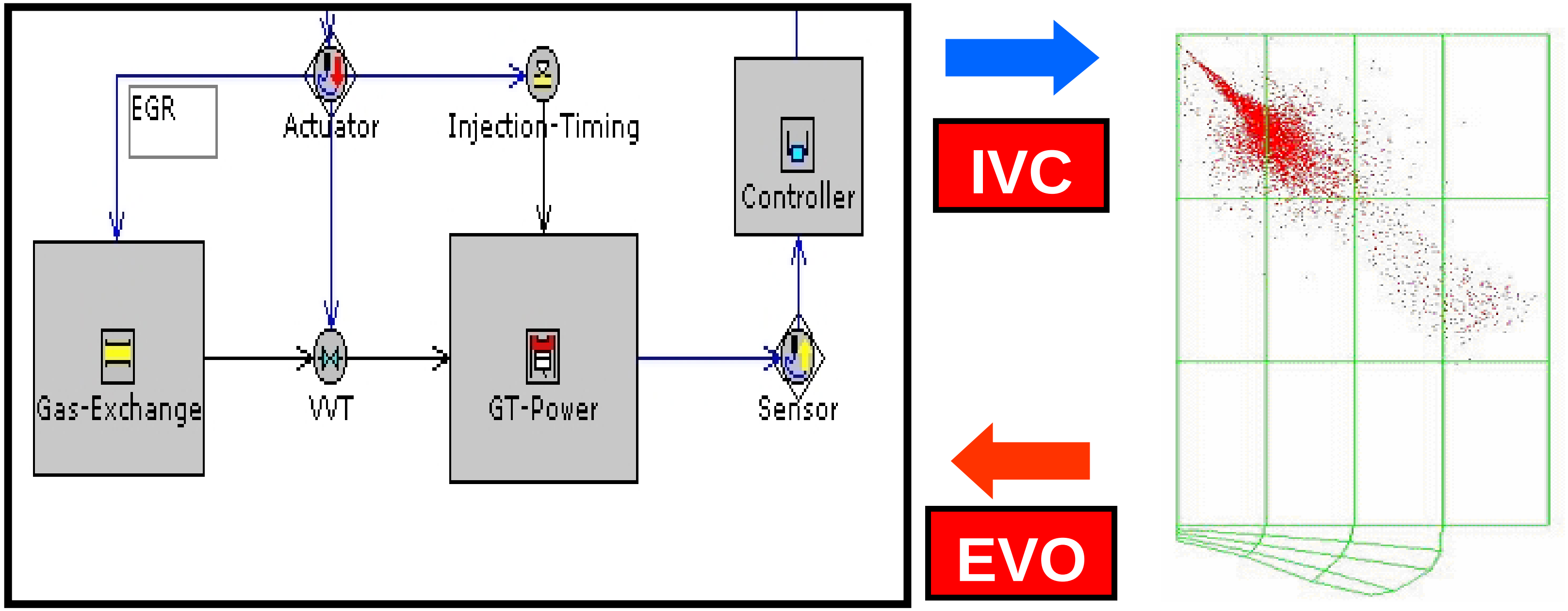
Multi- Zone Model Validation



CAT 3401 SCOTE,
821 rpm, 25% Load

- SOI = -128 ATDC; Injection Duration = 32.5CAD
- Start of combustion predicted accurately
- Capture variations in combustion phasing due to thermal and charge stratifications: Useful for parametric LTC studies
- Limitations: Requires specified fuel distribution (e.g. no spray)
  No mixing between zones

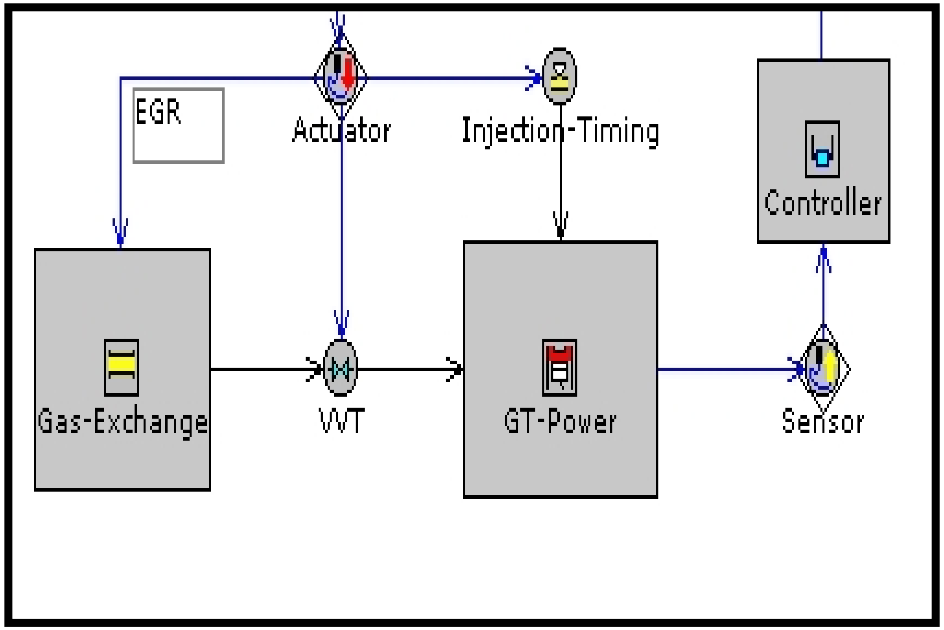
CFD In-Cylinder Model

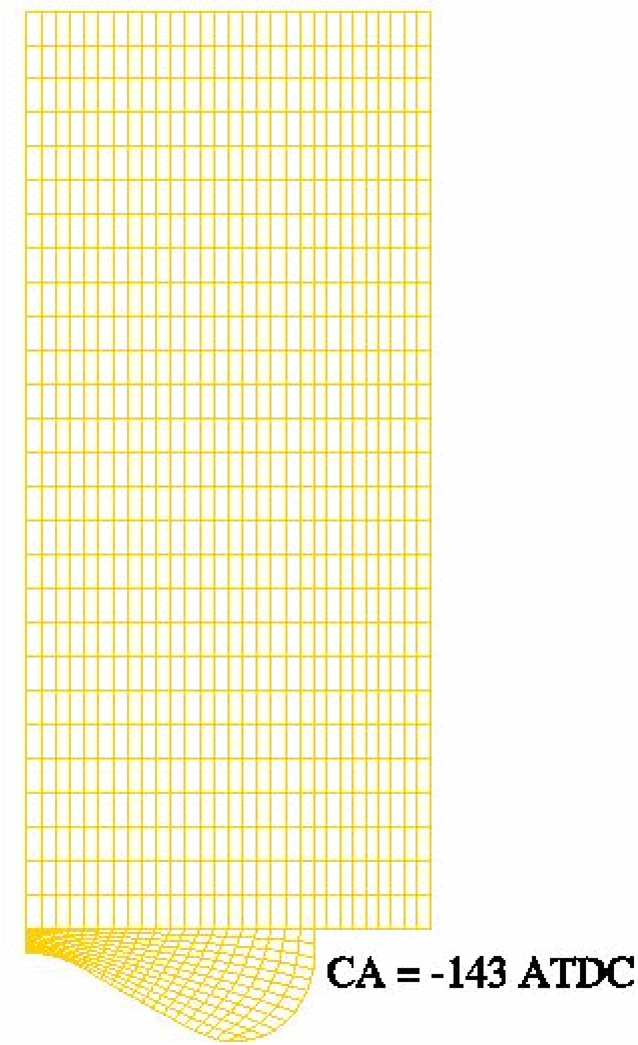


Detailed in-cylinder CFD model (KIVA-Chemkin)

- Accurate modeling of fuel injection, spray dynamics, mixing, vaporization, chemistry and emissions calculations
- Fine – coarse mapped grid

CFD In-Cylinder Model





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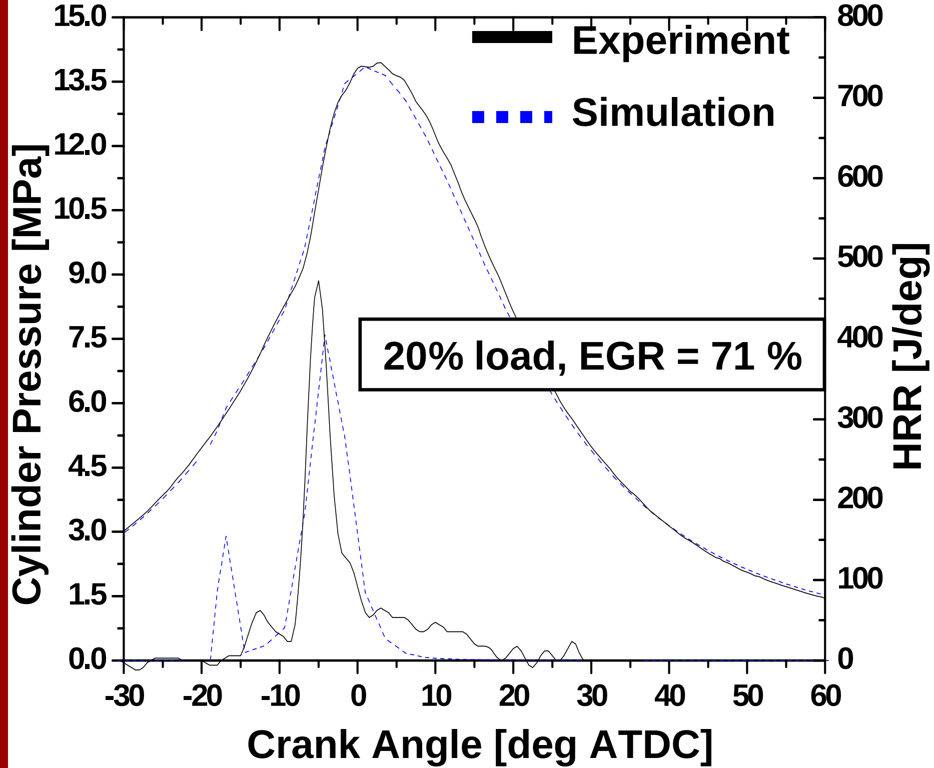
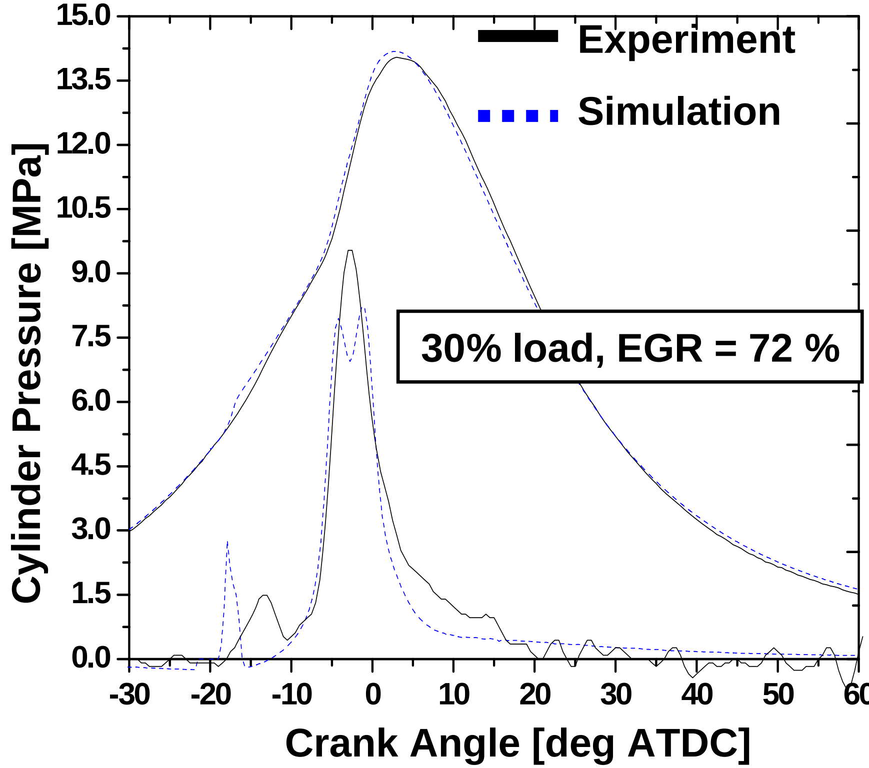
Model Validation



SOI = -50 ATDC



SOI = -50 ATDC

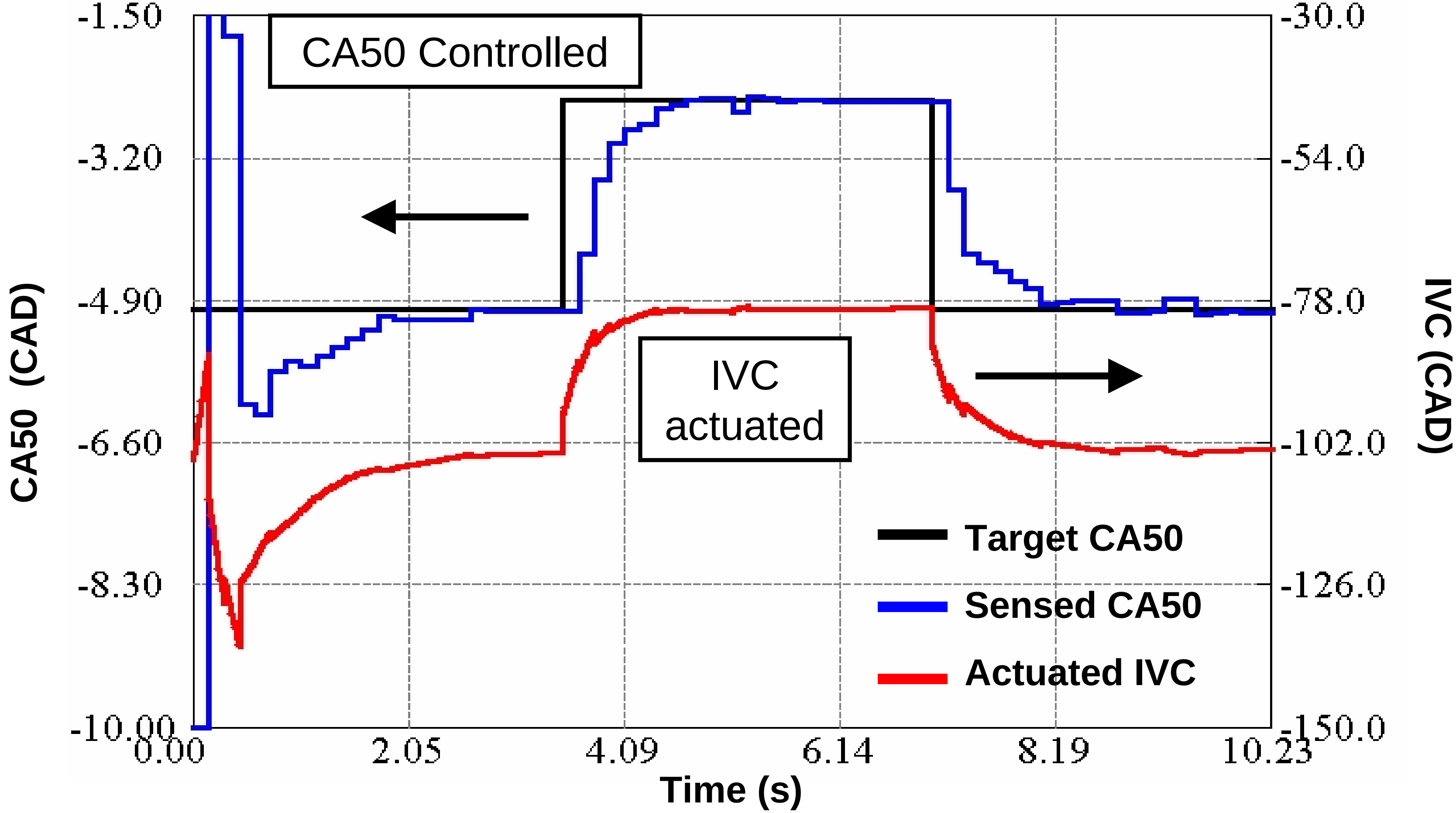
- Simulation results agree very well for lower loads
- Captures cool flame ignition and main combustion for early injection operation

Run Times for Different Approaches

Single Zone user combustion model	4 minutes
5 zone external cylinder model	17 minutes
GT-Power with mapped grid approach in 2-D	~70 minutes
GT-Power with refined grid in 2-D (1052 cells at BDC)	~ 9 hours
GT-Power with mapped grid using 3-D sector grids	~90 minutes
GT-Power with refined 3-D sector grids (5460 cells at BDC)	~ 1 day

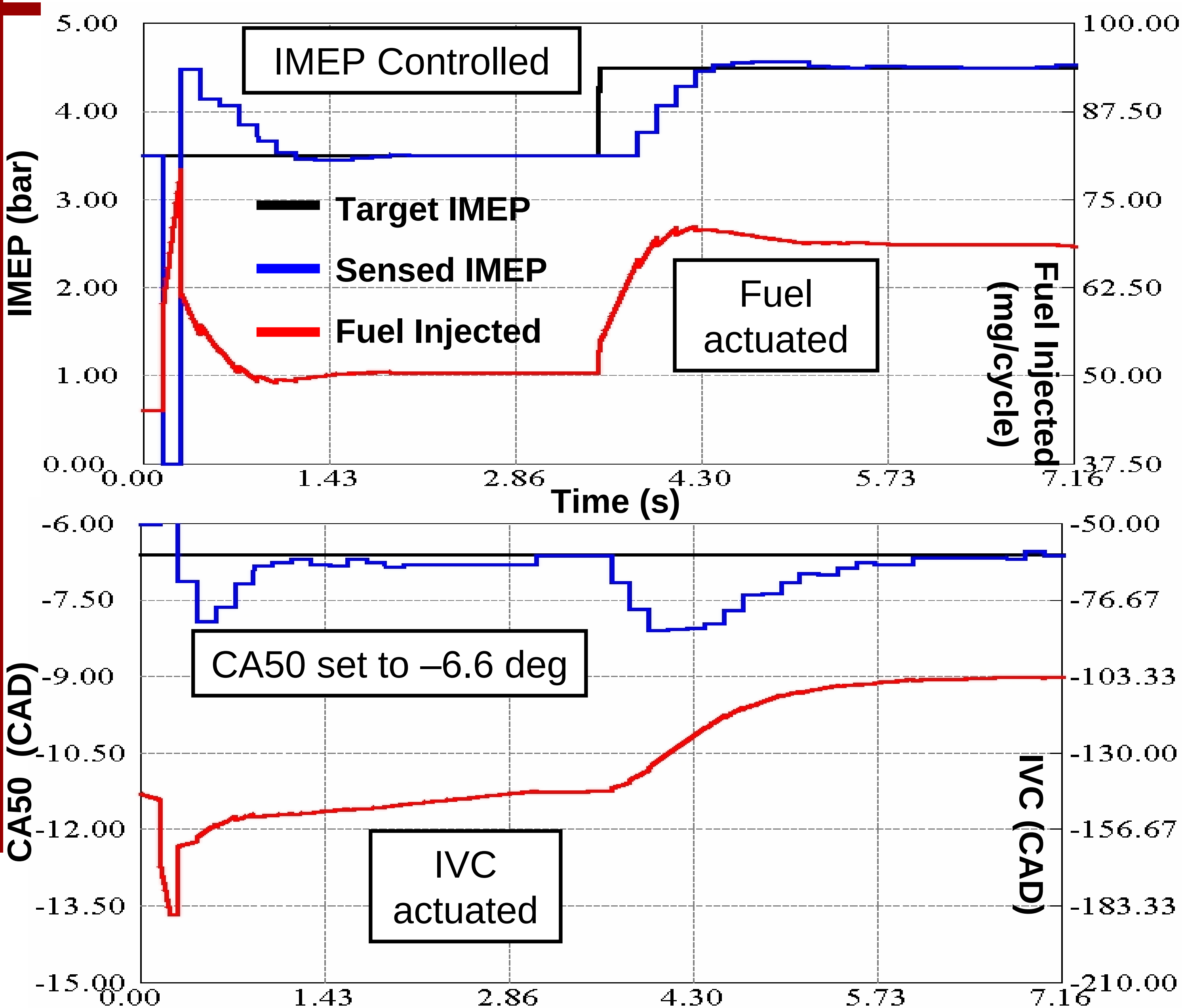
- The modeling approaches can be used in multiple cycle, transient simulations

CA50 Controlled by Actuating IVC



- Step transient induced in CA50
- Controller forces a delay in intake valve closure

Dual Control – Control CA50 During Load Increase



Step change in load

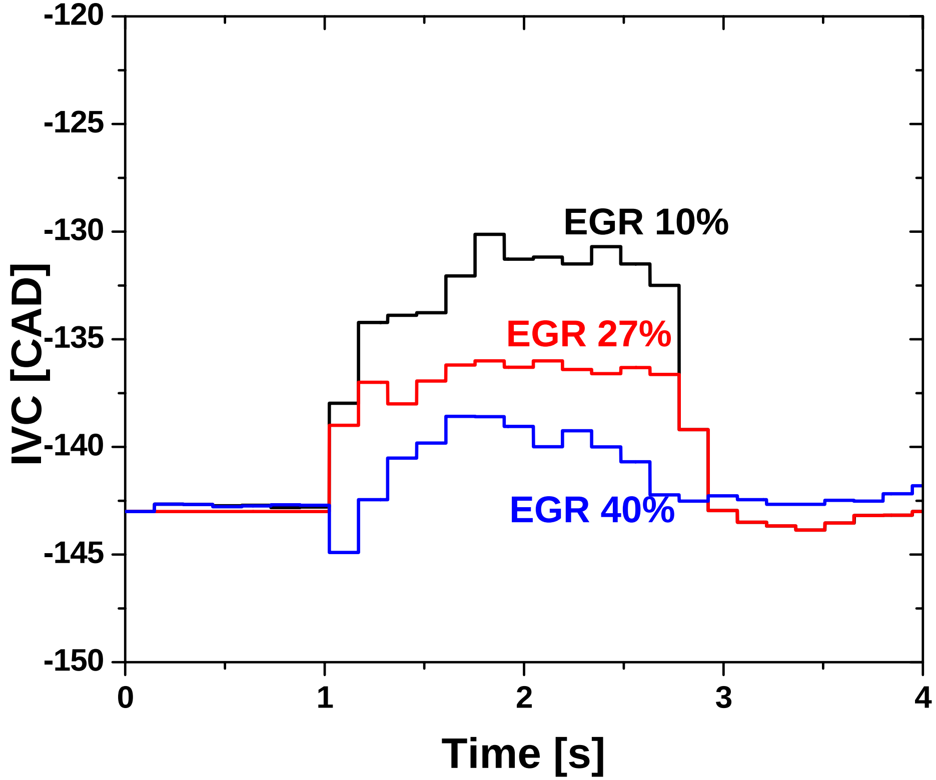
IVC actuated to maintain combustion phasing

Diesel-PCCI Mode Change: Cooled EGR and IVC

- Model transition: conventional – PCCI – conventional
- Conventional SOI:
  –12 deg ATDC
- PCCI mode SOI:
  IVC + 5CAD

- IVC response for PCCI under different EGR conditions
  - IVC actuation during the mode transition decreases with increase in EGR

Intake valve closes early with increase in cooled EGR



CA50 set to - 5.7 ATDC
IMEP set to 5.3 bar

Emissions Models

- Need accurate, fast emissions models to drive the aftertreatment device models
- Focus: Simpler, faster engine combustion models (for now)
  Long run times for DPF filling
- General approach:
  - Use good physically based phenomenological model as starting point
  - Improve model using neural networks to replace model coefficients
- Models required
  - Soot
  - NOx

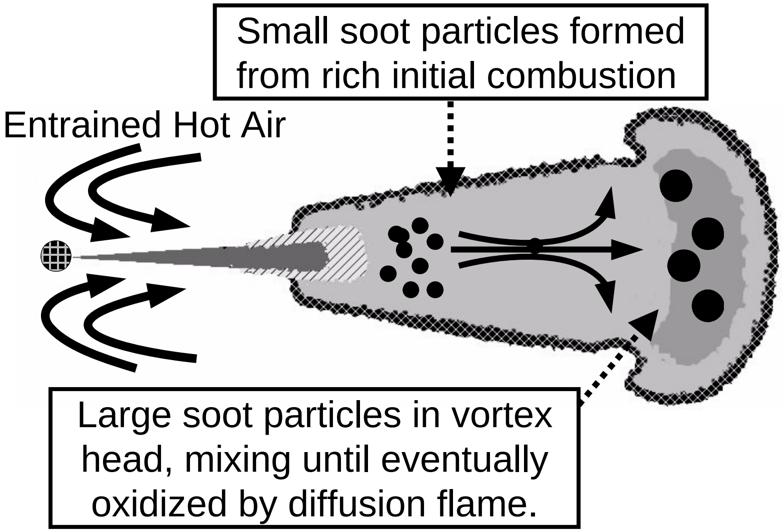
  } completed

  - CO2
  - HC

  } under development

Soot Emissions Model

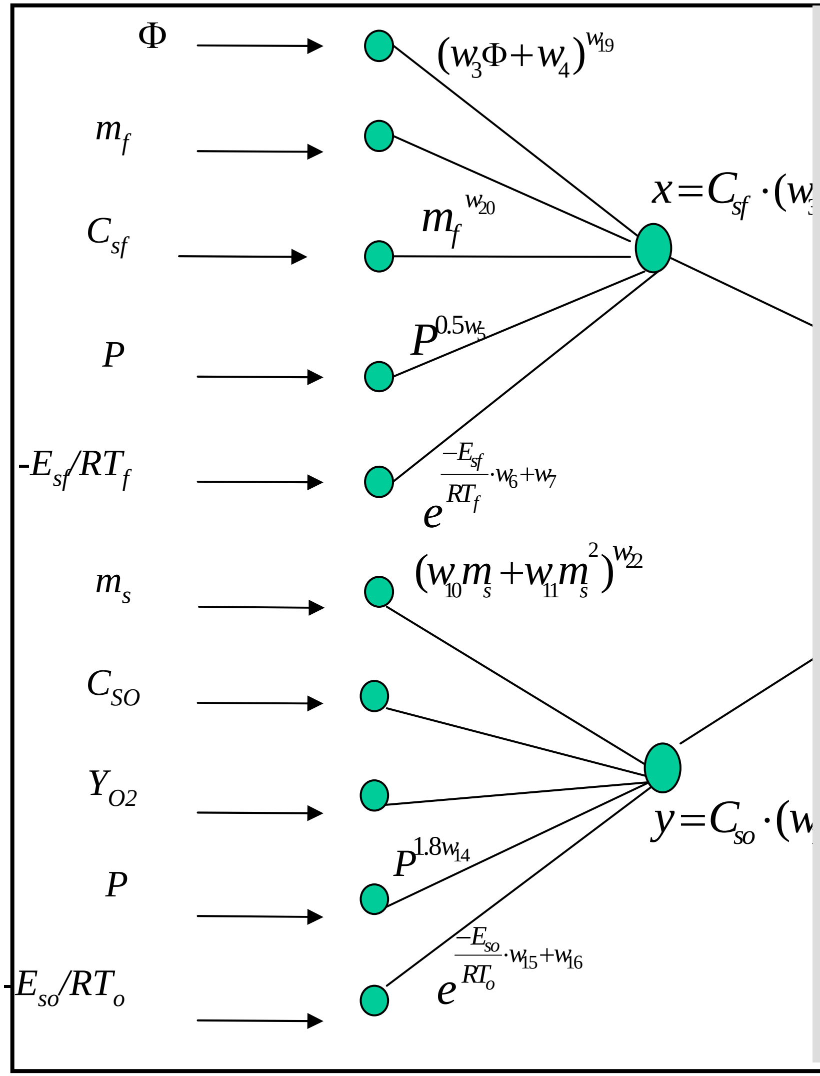
- Physically based neural network model
- Physical model: Bayer and Foster, SAE 2003-01-1070
- Phenomenological models for
  - Injection spray
    - Predicts spray angle, liquid penetration, liftoff length, local equivalence ratio, temperatures, etc.
  - Particulate formation and oxidation



$$\frac{dm_s}{dt} = C_{sf}\ \phi\, m_f\ P^{0.5} e^{\frac{-E_{sf}}{RT}} - C_{so}\ m_s\ P^{1.8}\ e^{\frac{-E_{so}}{RT}}$$

- Inputs are obtained from the engine model
  - Profiles of in-cylinder pressure, in-cylinder mean temperature, mass flow rate of fuel through injector, heat release rate
  - Engine speed, percent EGR, global equivalence ratio

Neural Net Soot Emissions Model



- Neural network weights added to the physical model
- Neural network weights trained using experimental engine data for 8 modes of operation
  - Approximately 57% reduction in error of predicted soot
- Converted into an M-file
  - M-file version runs in 1/3 the time of the original Simulink version
  - Small time steps are no longer propagated to other component models

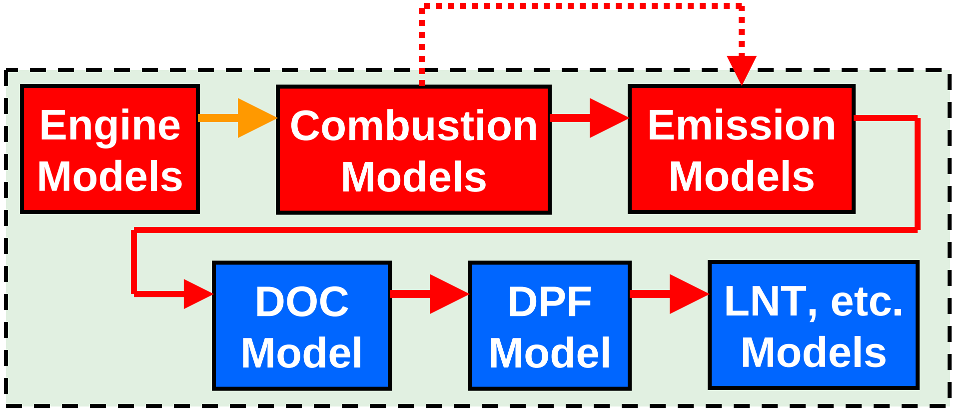
Brahma et. at., SAE 2005-01-1122

Soot Model and Time Steps

- Each component / module in integrated system requires a certain time step, Δt
- Overall system runs at ~2.5ms Δt (primarily set by engine model)
- Soot requires 0.5 CA data (~ 0.05 ms Δt)
  - Model requires crank-angle resolved spray and heat release profiles
- Simulink manages time stepping
  - Probes models to determine required times
  - Adjusts overall simulation to smallest Δt in system
- Soot model Δt requirement can severely limit overall system speed

Solutions for Managing Disparate Time Scales

- Hide inner workings of model from Simulink
  - Use self-contained Matlab or Fortran/C routines
  - Use sub-cycling time integration inside routines
  - Use level 2 S-functions
    - These can specify their own hit time
- Use external file for data transfer
  - Pass small Δt data outside of Simulink



- Implement periodic ‘triggering’
  - Skip calculation in model except every ‘n’ engine cycles
  - Use most recent solution until next calculation

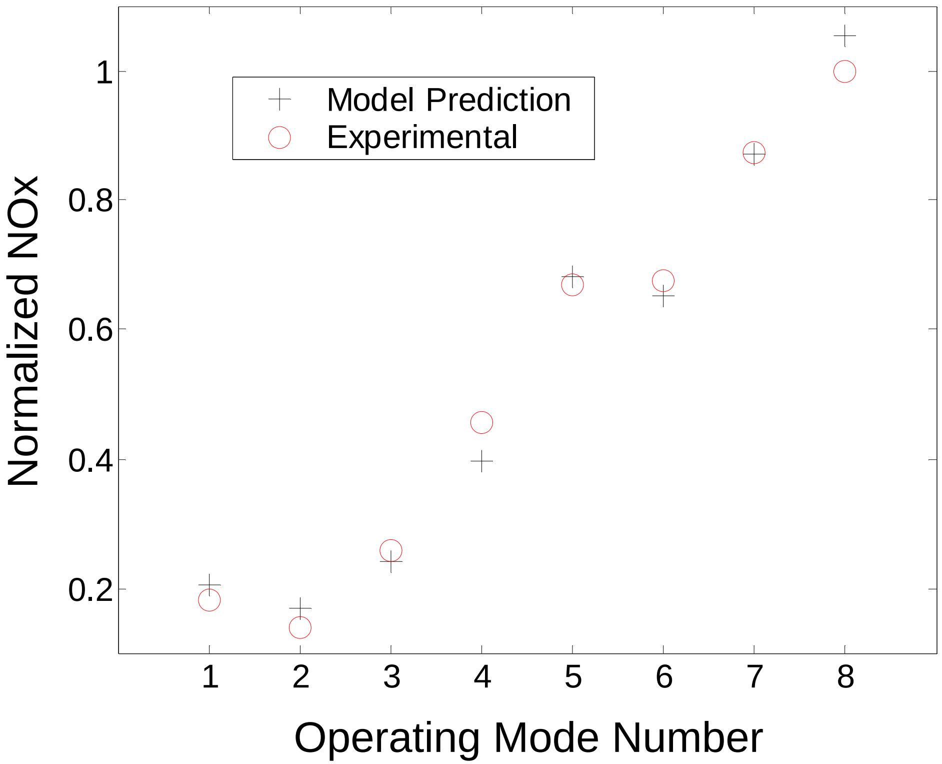
NOx Emissions Model

- Physically based neural network model (Brahma and appendix of England et. al., SAE 2006-01-0263)
- Implemented as an M-file
- Inputs are obtained from the engine and soot models
- NOx prediction is based on maximum rate of formation

$$NO_X = K_1 \max \left[\frac{\exp\left(\frac{-K_2}{T_{Diffusion\_Flame}}\right)[O_2]^{1/2}[N_2]}{T_{Diffusion\_Flame}^{1/2}} \right]$$

- Trained using experimental engine data for 8 modes of operation

Experimental NOx Compared to Model Prediction

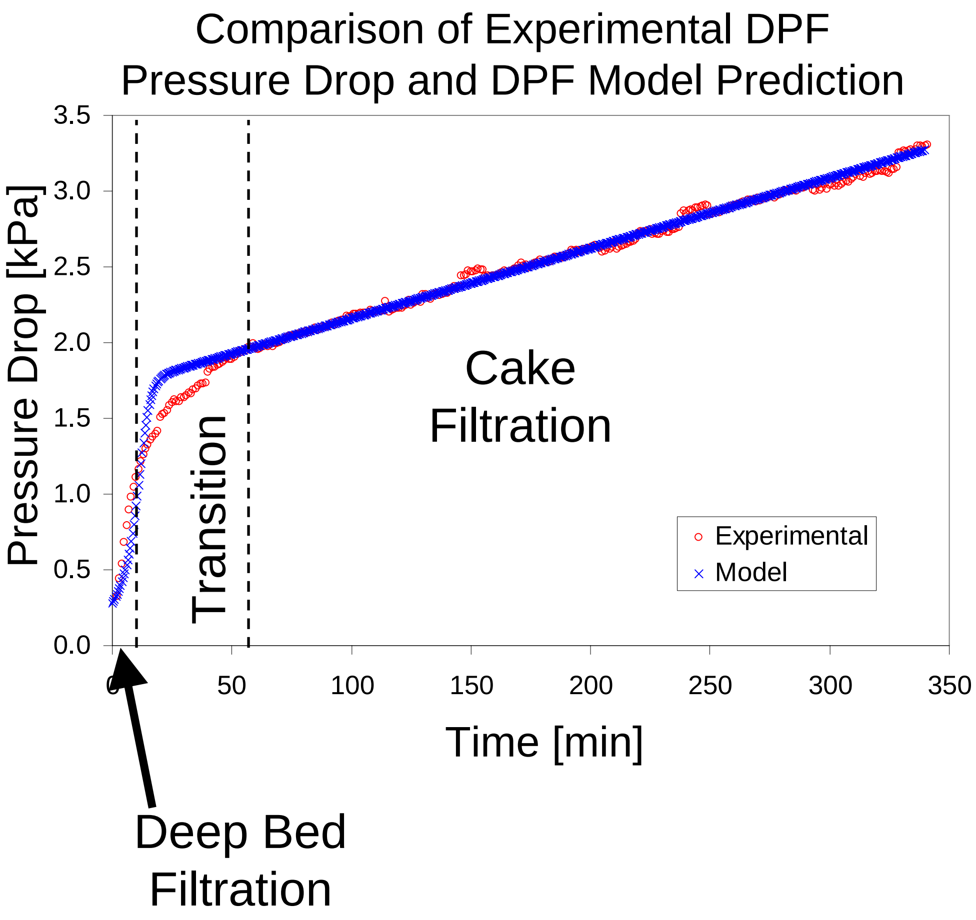


DOC Model

- Proprietary GM model (Bissett)
  - Includes kinetics for oxidation of CO, HC, and NO to NO2
- Implemented as a Fortran version
  - Faster than Simulink version
- Fortran allows decoupling of integration time
  - DOC model can operate at large time steps (10 ms or longer)

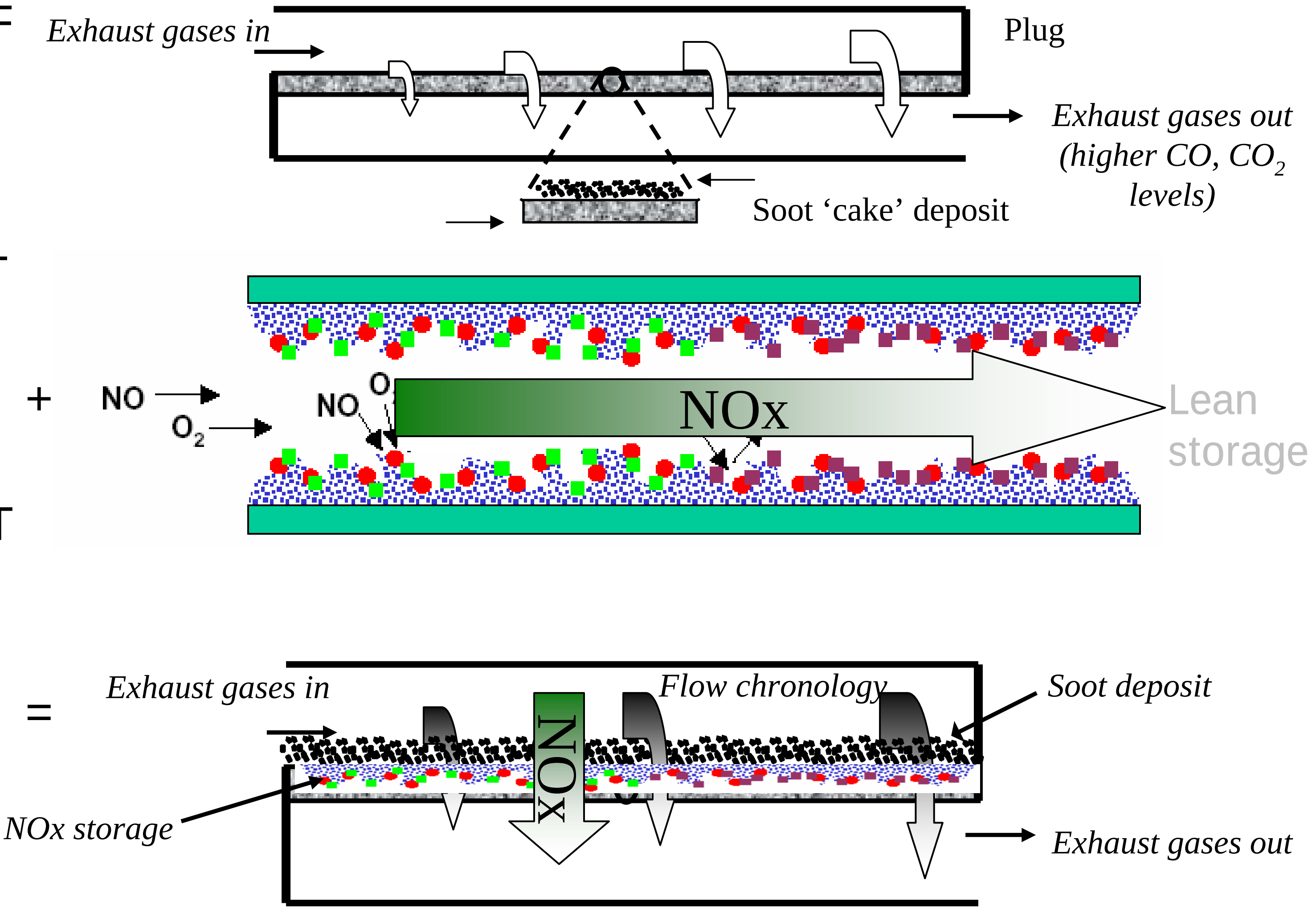
DPF Model

- Modified version of the MTU 1-D model (based on work of Konstandopoulos and Johnson)
- Fortran code linked to Simulink using an S-function (level 2)
- Input and output modified for dynamic use in Simulink and time integration improved
- Calibrated against experimental data
- Darcy law pressure drop for the wall and soot layer
- Device sub models describe:
  - Particle deposition inside wall and on wall surface
  - Flow and temperature fields
  - Catalytic and thermal oxidation of soot



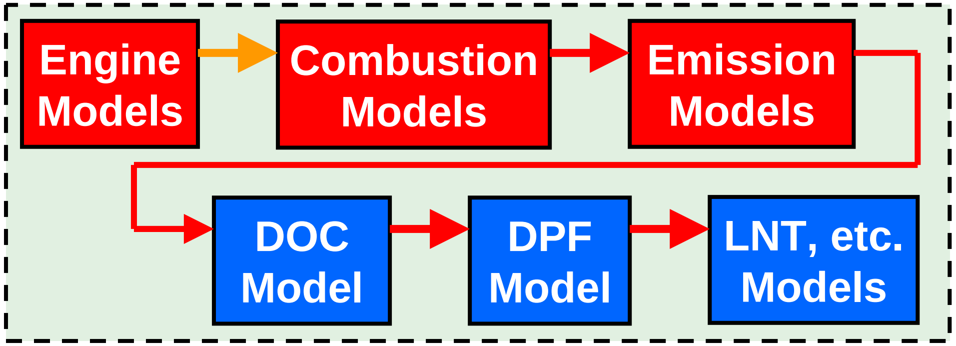
Combined DPF-LNT

- DPF
- LNT
- SNT



Controllers and Validation

- Controllers implemented in Simulink for:
  - Engine load (fueling)
  - Engine speed
  - EGR
  - Turbo boost
  - DPF regeneration



- The component models tested and validated individually

- The integrated model is tested to verify proper component interaction
  - DPF loading and regeneration simulations to test the model and component interaction
  - The simulation results are consistent with experimental results presented by Singh et. al. (SAE 2006-01-0879)

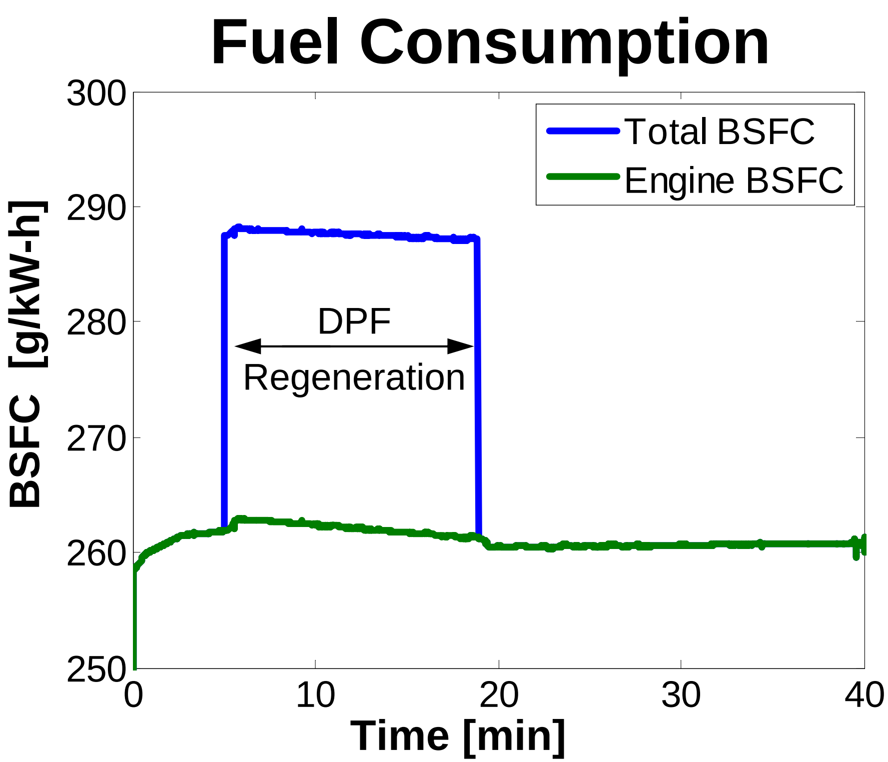
DPF Loading and Regeneration

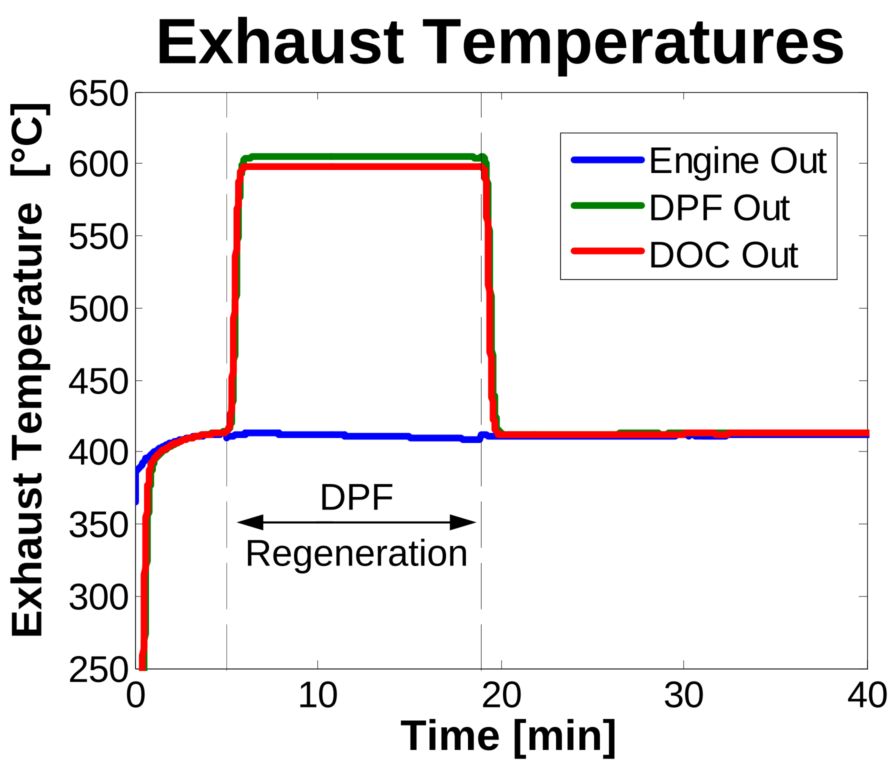
- Simulate a light duty, turbo charged, CIDI engine
  - Common rail direct fuel injection
  - Variable geometry turbine
- Regeneration: modes 3 and 5
  - DPF initially loaded to 3 [g/l] of soot and regeneration starts at 3.2 [g/l]
  - Mode 5: Fuel injected ahead of the DOC
  - Mode 3: Fuel injected ahead of the DOC with intake throttling assistance
- Regeneration tests were done with mode switching (mode 5 to 2) during regeneration to investigate prevention/control of regeneration runaway

Mode Number	Load	Engine Speed [RPM]	Approximate Fueling Rate [kg/hr]	EGR [mass %]
2	Very Low	970	1.42	62.14
3	Low	1120	4.035	37.96
5	Moderate-Low	1520	9.365	19.15
8	Moderate	2320	18.85	10.50

DPF Regeneration (Mode 5)

- Fuel injected in exhaust before DOC
- Increases reactions in DOC and exhaust T
- Controlled to achieve a desired DPF inlet temperature of 600 °C





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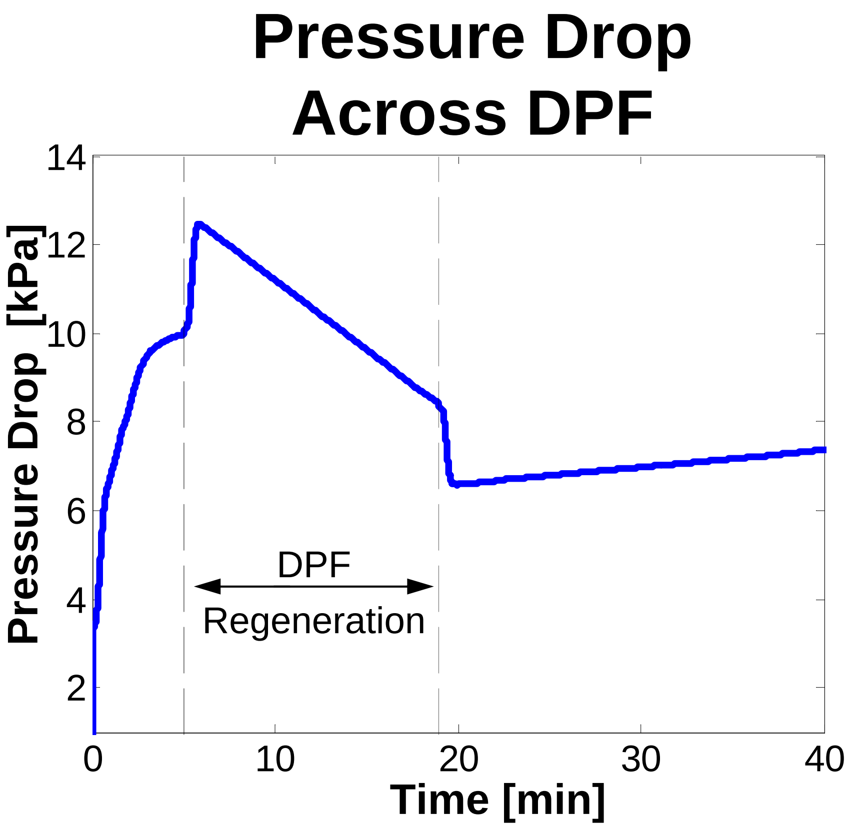
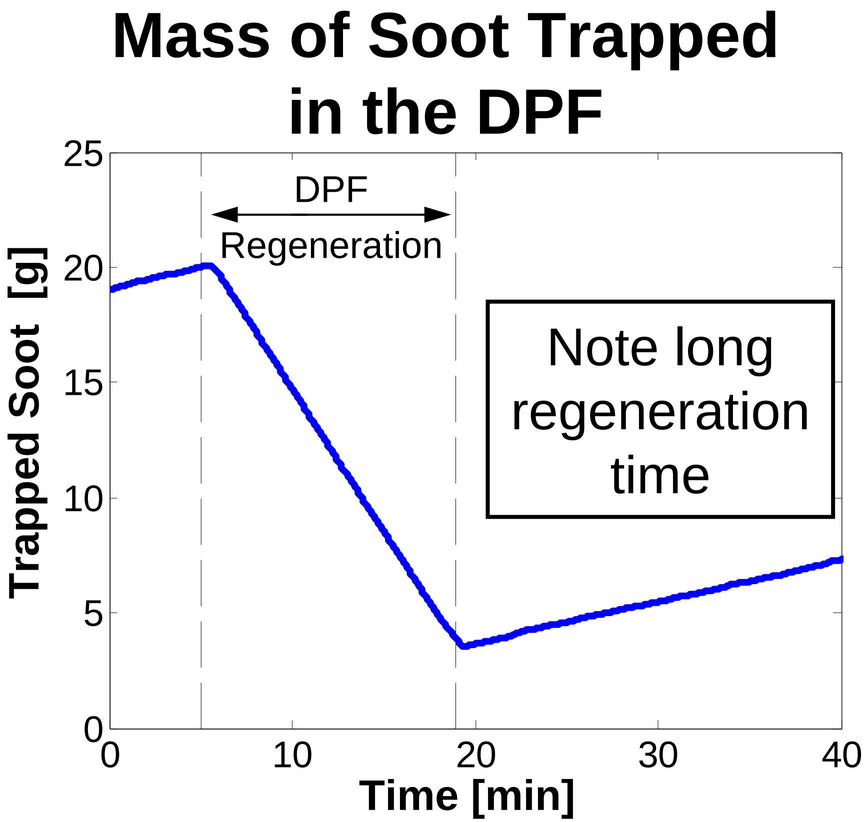
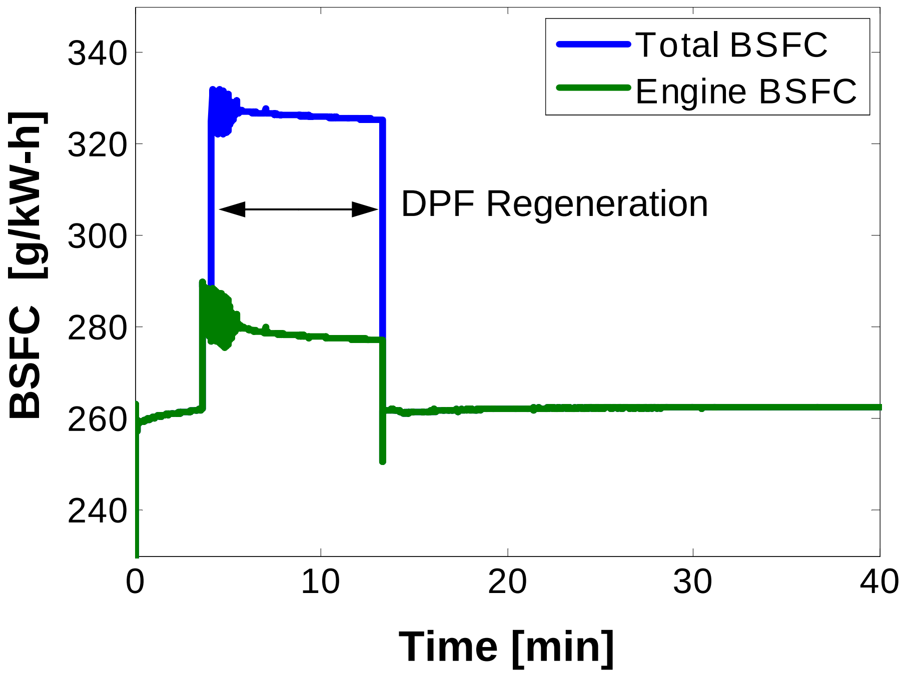




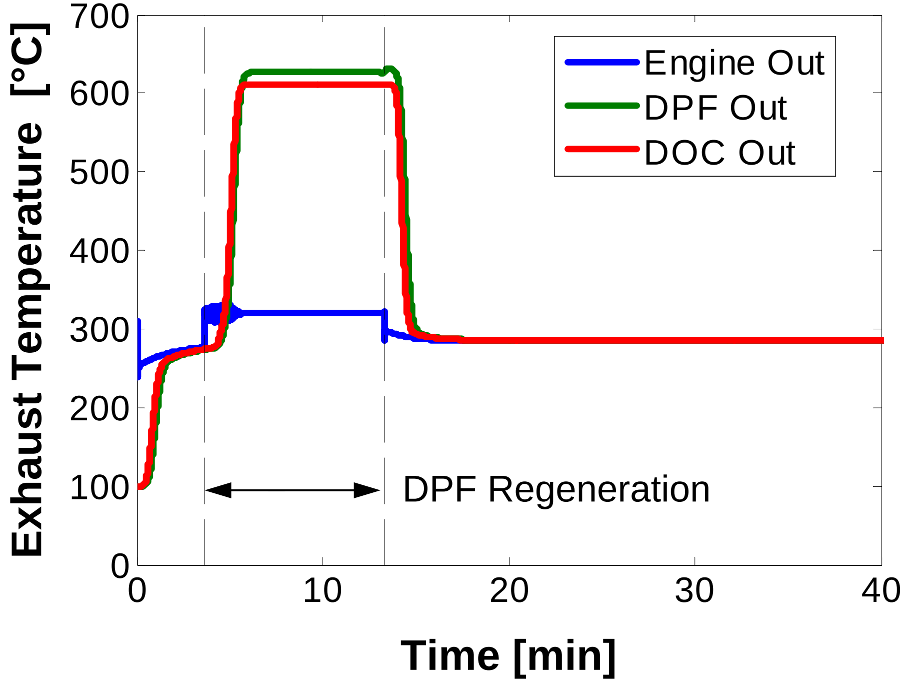
Throttle Assisted Regeneration (Mode 3)

- Engine exhaust temperatures too low for fuel injection before DOC (> 300 C required)
- Throttle engine intake air flow
  - Increases equivalence ratio and engine exhaust T (ΔT = 44 °C)
- Higher exhaust T allows fuel injection in exhaust before DOC

Fuel Consumption



Exhaust Temperatures



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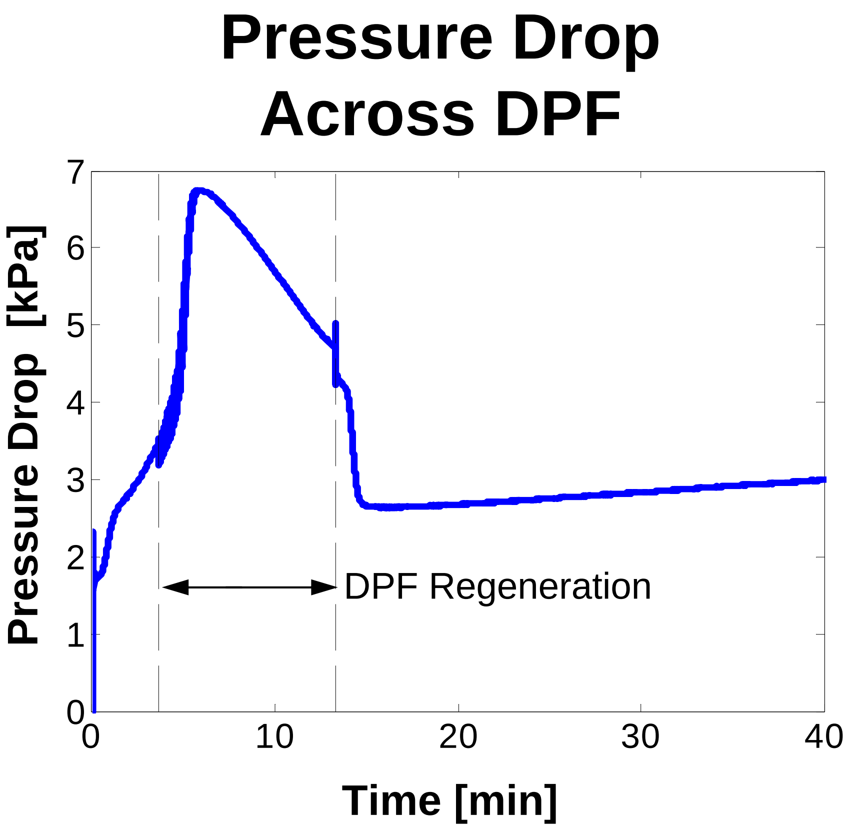
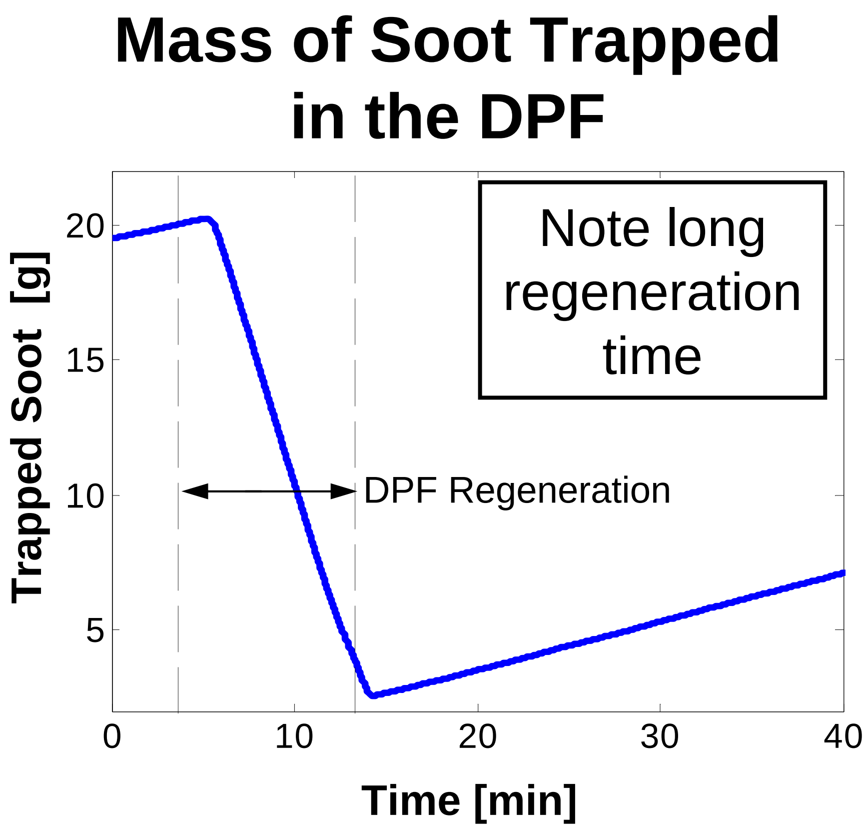
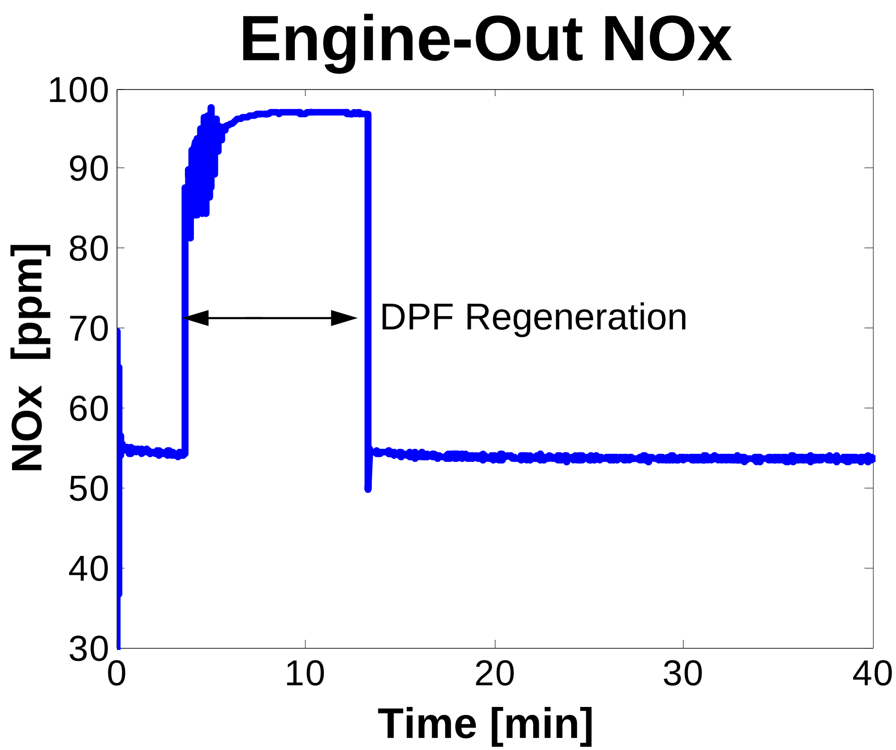




Throttle Assisted Regeneration (Mode 3)

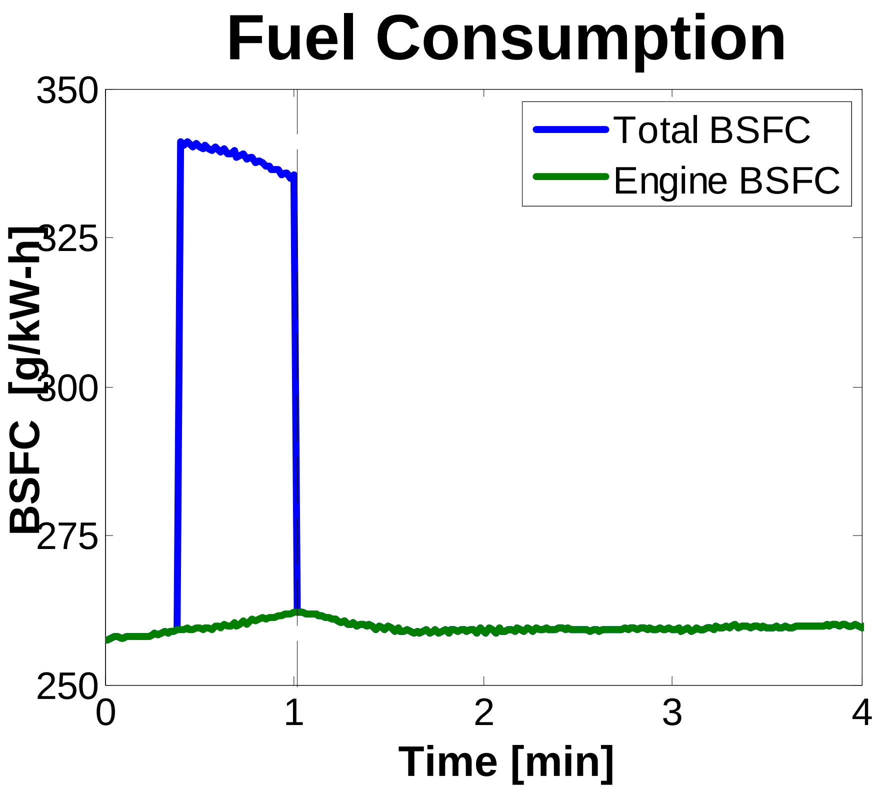
- Engine out NOx increased significantly during DPF regeneration
- Intake throttling required reducing EGR to maintain sufficient O2 for given load
- Reduced EGR resulted in higher engine out NOx

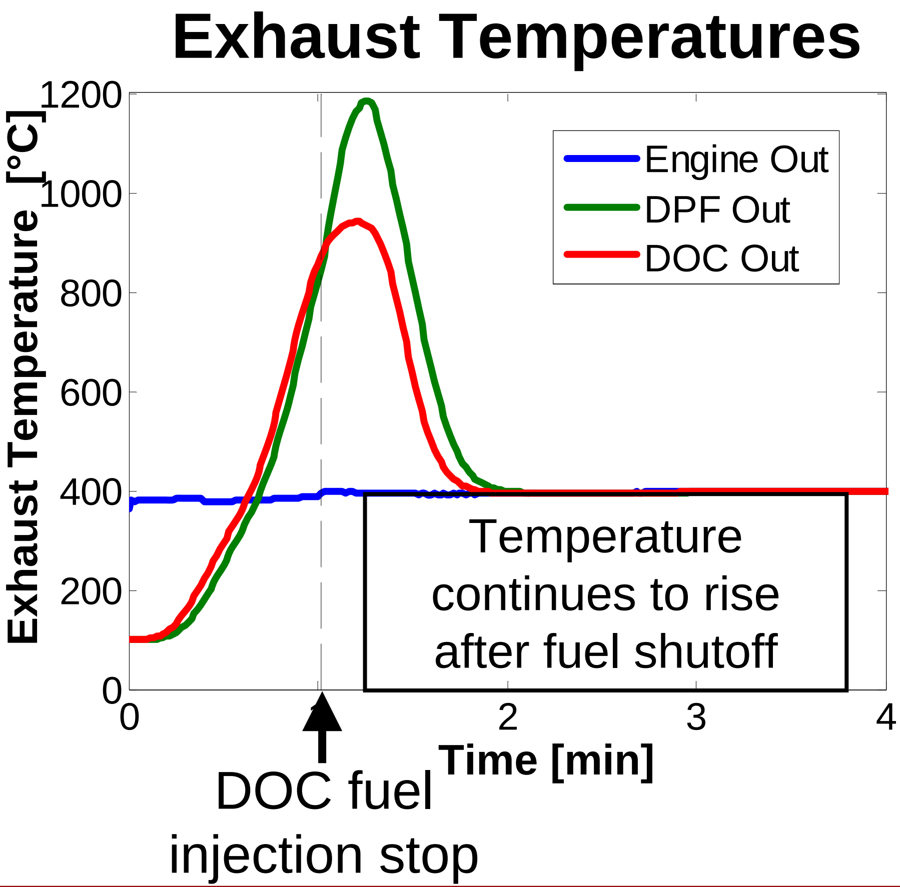


Good Device Gone Bad

Runaway Regeneration (Mode 5)

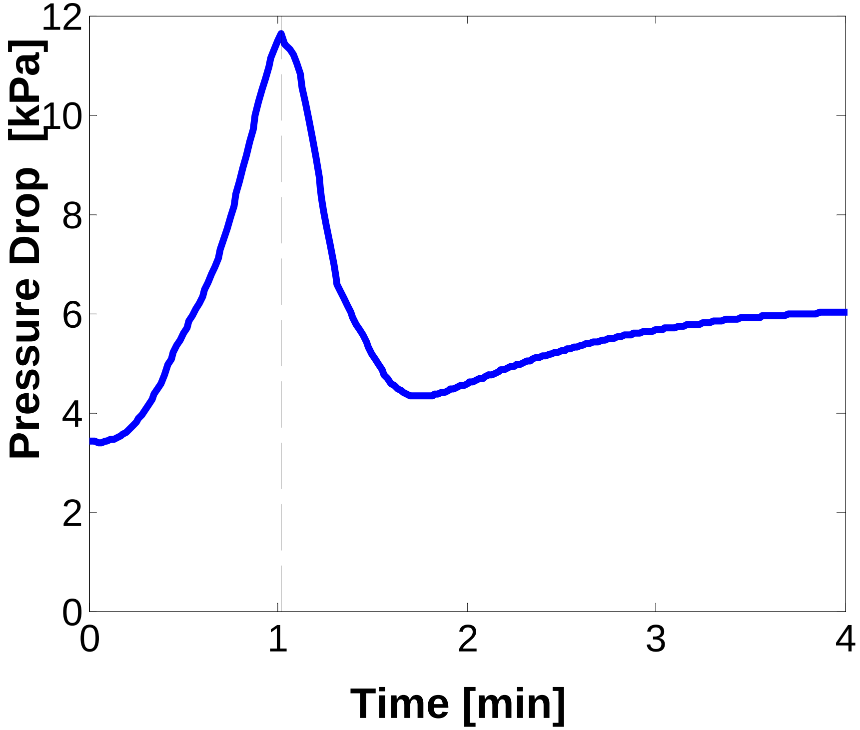
- Regeneration by fuel injection before DOC
- Try to reduce regeneration time by injecting more fuel
- Results in runaway regeneration



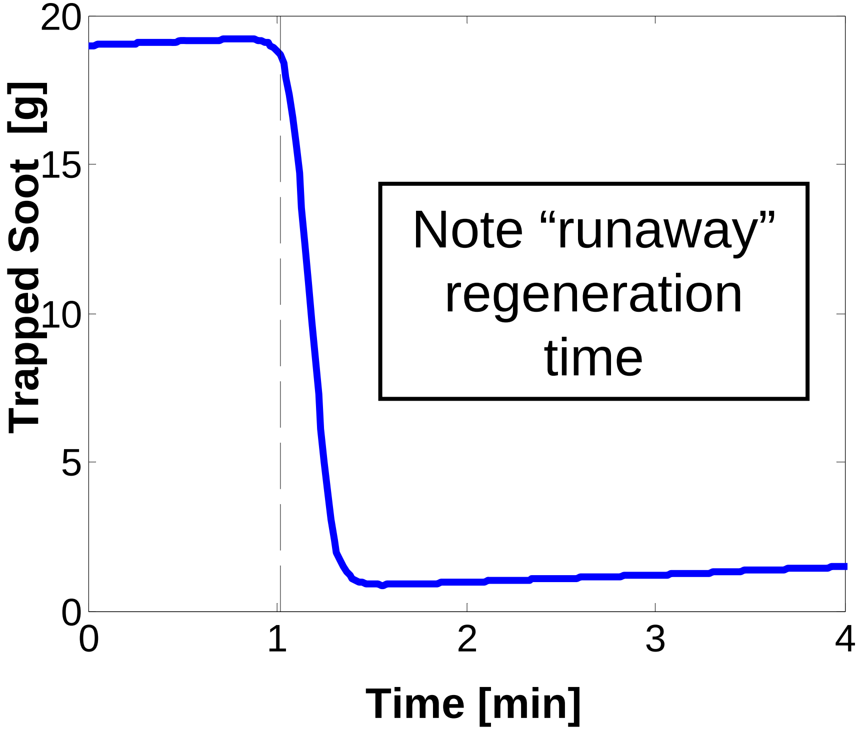


Runaway Regeneration (Mode 5)

Pressure Drop Across DPF



Mass of Soot Trapped in the DPF



Preventing Runaway Regenerations

- Use ΔT predictive capability in the regeneration controller via simple energy balance:

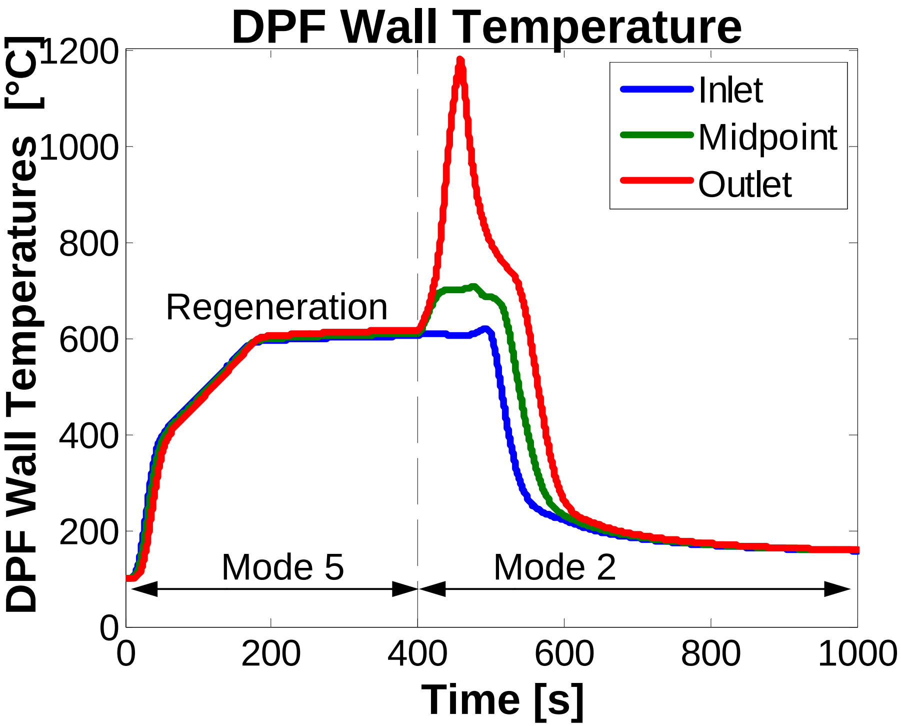
$$\dot{m}_{fuel} = \frac{\dot{m}_{exh} Cp_{exh} \Delta T_{exh}}{LHV_{fuel}}$$

- Very simple energy balance will get the DPF inlet temperature within 10 [°C] of the target value
- Use PI feedback control to adjust the predicted exhaust fuel injection rate to obtain the target DPF inlet temperature
- Feedback PI controller alone (without predictive capability) is not recommended

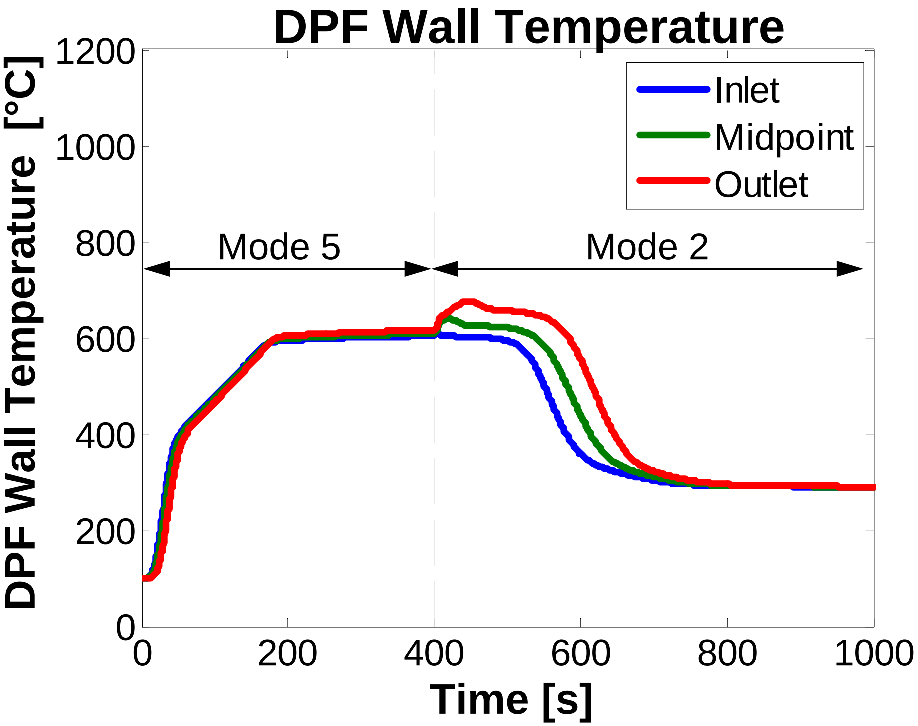
Regeneration During Mode 5-2 Transient

- Runaway regeneration occurs when DPF is very hot and:
  - Exhaust flow rate is suddenly lowered in mode transitions
  - Excess O2 is available in exhaust
  - Consistent with results from Koltsakis, et al. (SAE 2007-01-1127)
- Prevent runaway regeneration by intake throttling to reduce available O2 in exhaust

Regeneration: Runaway after Mode Switch



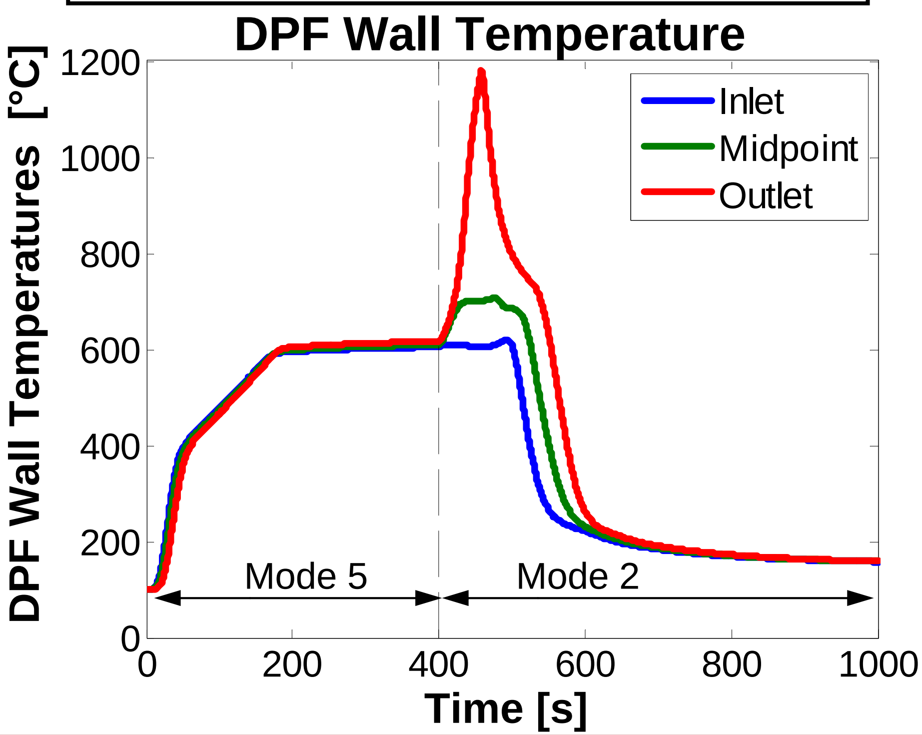
Prevent Runaway with Intake Throttling



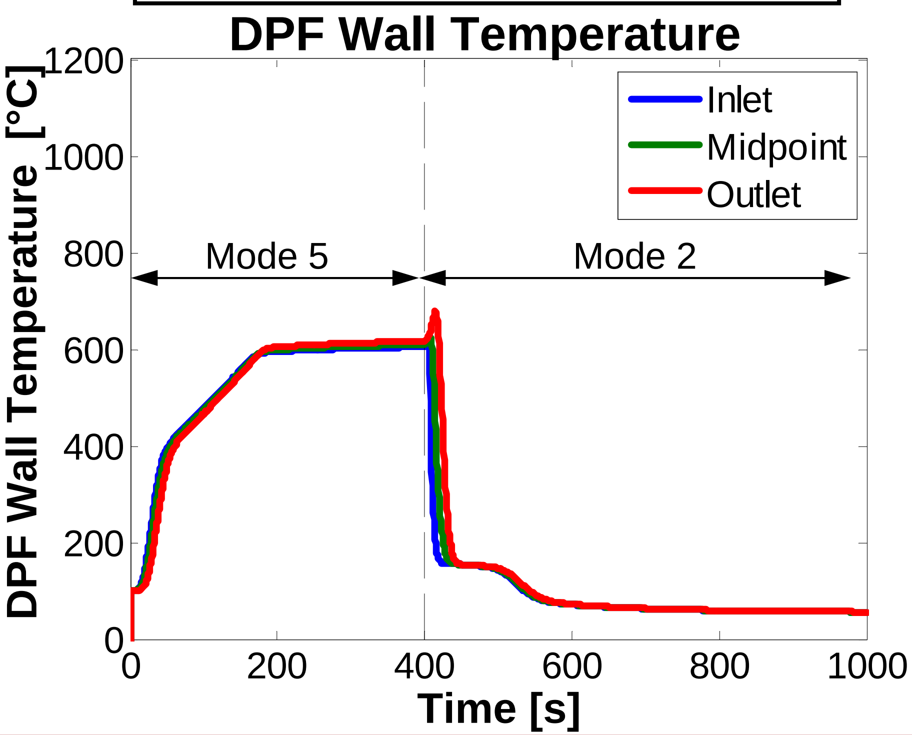
Regeneration During Mode 5-2 Transient

- Alternative method to prevent runaway:
  - Air injection into exhaust
- Cool air removes heat from soot oxidation reactions

Regeneration: Runaway after Mode Switch



Prevent Runaway with Air Injection into DPF

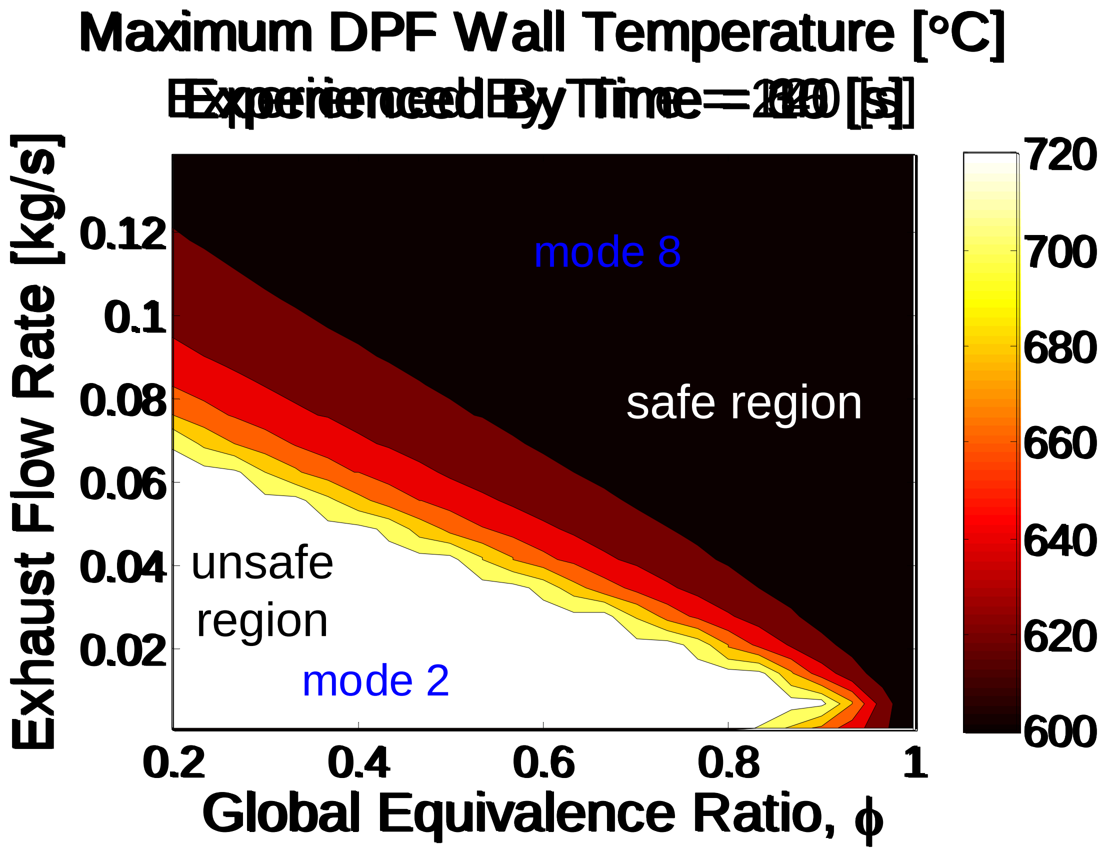


Controlling Runaway Regenerations

- The integrated model has been used to simulate how a runaway regeneration can be detected and controlled
  - Reactive control
- Can the integrated model be used to detect unfavorable conditions before a runaway regeneration starts to prevent runaway proactively?
  - To investigate this possibility phase diagrams have been generated

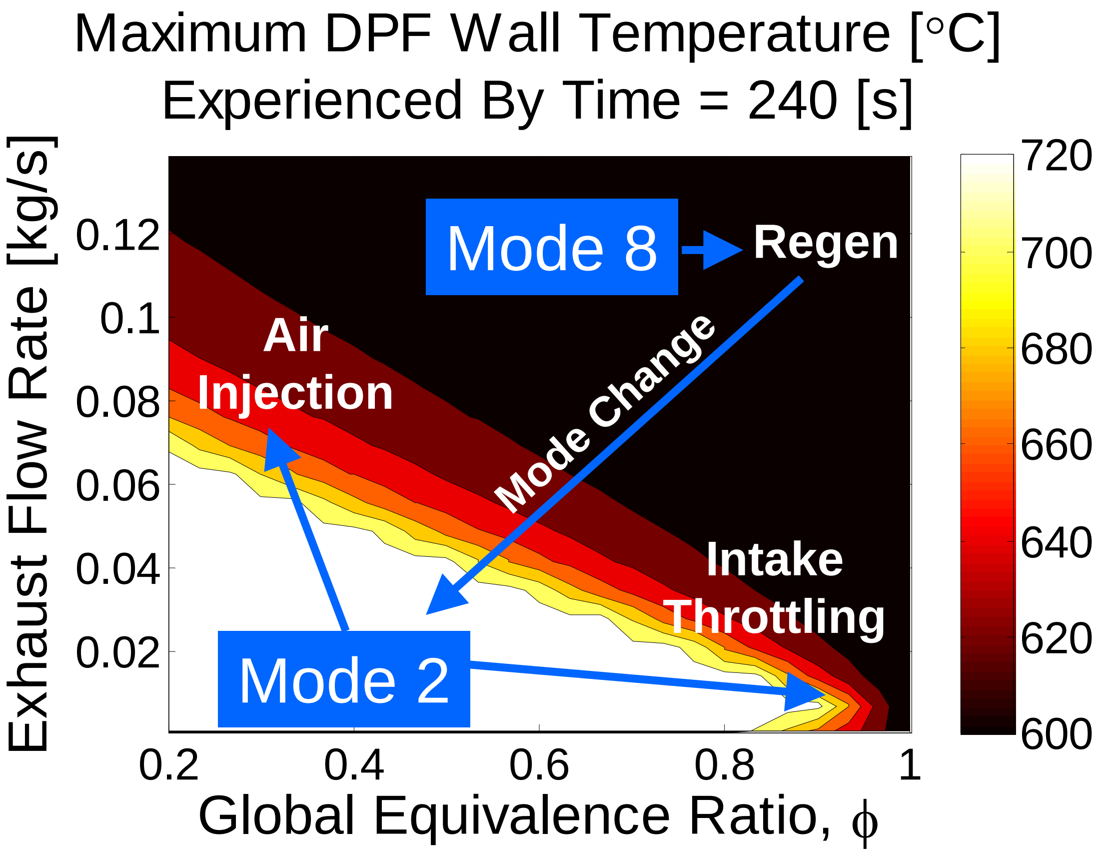
DPF Phase Diagrams

- Phase Diagrams:
  - Max DPF wall T
  - Function of:
    - Equivalence ratio (e.g. available O2)
    - Exhaust flow rate
- Example:
  - Mode 8 to mode 2 transient during regeneration
- Conditions:
  - Initial DPF wall temperature = 600 °C
  - Soot loading = 4 g/l
  - Inlet temperature = 162 °C (after switch to mode 2)



Using the Phase Diagrams

- Runaway regeneration occurs when DPF is very hot and:
  - Exhaust flow rate is low
  - Excess O2 is available
- By using the phase diagram unsafe operating conditions can be identified and avoided by:
  - Intake throttling
  - Air injection into DPF inlet



Summary

- Integrated system model for diesel aftertreatment studies
- Advanced engine combustion model for LTC studies
- Accurate emissions models to drive the aftertreatment devices
- Accurate, modular aftertreatment devices models
- Implemented in Simulink for controls and numerical management
- Integrated model used to explore DPF regeneration
  - Phase maps to explore runaway regeneration recovery

Ongoing Activities

- Development of additional submodels
  - CO and HC emissions models
  - Incorporation of an SCR device model
- Continue improvements to integrated system
  - Improve computer run times
  - Improve modularity and ease-of-use
- Continue to use the system model to study device interactions and appropriate operation for transient and regeneration scenarios
  - Develop ‘guidelines for operation’

Thank You