11th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference
6 - 8 September 2006, Portsmouth, Virginia

AIAA 2006-7068

A Modular State-Vector based Modeling Architecture for Diesel Exhaust System Design, Analysis and Optimization

Christopher D. Graff* and Olivier L. de Weck†
Massachusetts Institute of Technology, Cambridge, MA, 02139

Diesel emission regulations for cars and trucks are becoming ever more stringent, and it is important to be able to evaluate the performance of new after-treatment technologies and architectures and their effects on the powertrain and vehicle. This paper presents a new modeling and simulation methodology that treats the entire exhaust system, not just one component. In order to achieve this, a modeling architecture is developed based on a state-vector platform where component sub-models can be easily developed and integrated, forming a larger system which can simulate vehicle operations. The innovation presented in this paper is the modular simulation architecture that allows investigation of a large number of different system architectures without having to manually parameterize each configuration. The system model can then be used as the basis from which multi-disciplinary, multi-objective, system-wide analysis can be performed. The framework is applied to the optimization of a commercial vehicle diesel exhaust treatment system, including a diesel oxidation catalyst and other components.

Nomenclature

x	=	Design vector
q	=	State vector
J	=	Objective function
w_i	=	weight of component i
HC_{emis}	=	Hydrocarbon (HC) emissions
CO_{emis}	=	Carbon Monoxide (CO) emissions
NOx_{emis}	=	Oxides of Nitrogen (NOx) emissions
PM_{emis}	=	Particulate Matter (PM) emissions
HC_{Reg}	=	Hydrocarbon (HC) emissions regulation limit
CO_{Reg}	=	Carbon Monoxide (CO) emissions regulation limit
NOx_{Regs}	=	Oxides of Nitrogen (NOx) emissions regulation limit
PM_{Reg}	=	Particulate Matter (PM) emissions regulation limit

I. Introduction and Motivation

As regulations for vehicle emissions are continuously tightened around the world, manufacturers are forced to comply by developing new technologies in car and truck powertrains. Some of these technologies focus on the internal combustion engine and combustion process directly, while others attempt to remove various components from the exhaust stream such as carbon monoxide (CO), hydrocarbons (HC), oxides of nitrogen (NOx) and particulate matter (PM). Each time the allowable emissions limits are once again lowered, existing system configurations and component technologies are pushed to their achievable limits. In order to further move the constraints, new components and technologies are gradually added to the exhaust aftertreatment system such as oxidation catalysts, particulate filters, thermal regenerators and so forth. With each new added component the complexity of the system increases and thermal, chemical and mechanical interactions between components start to

* Graduate Research Assistant, Department of Aeronautics and Astronautics, 77 Massachusetts Ave., Rm 33-409, Cambridge, MA, 02139, AIAA Student Member
† Associate Professor, Department of Aeronautics and Astronautics and Engineering Systems Division, 77 Massachusetts Ave., Rm 33-410, Cambridge, MA, 02139, AIAA Senior Member.

dominate the response of the system. Different configurations and combinations of the same components might lead to different system performance. Which configurations are most efficient in meeting new emissions regulations? How does each configuration perform over a set of different drive cycles and operating conditions? What is the optimal design of individual components in the context of the overall coupled system?

Rather than having to manually construct a dedicated model for each potential system configuration, we are developing a generic diesel exhaust system modeling and simulation capability to analyze and evaluate new diesel exhaust after-treatment technologies in a multi-disciplinary, multi-objective, system-wide context. The majority of recent research development in diesel exhaust treatment has been in specific technologies which have been targeting certain emission regulations and exhaust species, such as Diesel Particulate Filters, Catalysts, or NOx (oxides of nitrogen) and hydrocarbon traps. So far, there is no clear technological "winner" among the competing technologies that offer to treat similar emissions problems. The purpose of developing this methodology, the models, and tools, is to facilitate simulating the entire after-treatment system in order to better analyze and develop designs, and then optimize those designs for given criteria.

The basis of the methodology is a series of sub-models of after-treatment technologies that integrate into a larger framework of the entire exhaust system. The goal is to be able to obtain the relative performance of different system architectures in objective space given a certain engine/vehicle, assumed operating conditions, and other constraints and parameters. Treating the analysis and optimization in a system-wide model can lead to optimizing the entire exhaust system and achieving better overall performance than simply combining two or more individually optimized components. The information collected from the system analysis can assist designers in identifying design directions during early product development, while building complete diesel emissions treatment solutions.

Section II of the paper summarizes the fundamentals of modeling and simulating exhaust systems, Section III presents the modular state-vector based framework that was developed and Section IV presents initial "proof-of-concept" results. The conclusions are discussed in Section V.

II. Modeling and Simulation Fundamentals

Many exhaust system components can be sufficiently modeled parametrically, or within a one-dimensional geometric description. The majority of critical interactions can be reduced to the chemical conversion process of exhaust gas species, the thermodynamics of reactions, and to heat and mass transfer. The filtration and trap models can be described using simple porous wall, layered filtration models, in some cases even incorporating one-dimensional length geometry. Fundamentally, these technological components can be described in an arrangement of differential equations, with simple geometric variables and other parameters describing the majority of interactions. Given the system-wide analysis viewpoint, there is no need for in-depth finite element modeling when these simpler models can be used to assemble the entire system and give reasonable results for emissions and performance. Additionally, there is the need for the models to reflect varying environmental and operating conditions, and allow for fast computation in order to add-on optimization to the analysis methodology. A complete finite element model would be too complex and detailed for use in these instances. One of the most challenging aspects of modeling and simulating a multi-component exhaust system is that the model should accurately predict not only steady-state conditions, but also transients.

A. Modeling Architecture

Beginning with the realization that the operands of the physical components in the system are the exhaust emission gas species, it is therefore useful to develop the model architecture by investigating this link. The exhaust gas, and certain critical engine operating and performance parameters, can be assigned within a *state vector*, which is then passed through component modules that model certain technologies, such as a particulate filter. The effect of individual components is captured by the way in which they affect the state vector. The state vector becomes the key interface as the input and output of the models. The various performance criteria of the technology being modeled can be then be extracted by examining the differences between the input state vector and output state vector, such as comparing the input emissions level versus output emissions level.

In addition to the state vector describing the conditions pre- and post-component, the operating conditions, vehicle parameters, and exhaust system design are critical to modeling the entire system. In the notional block diagram, Fig. 1, the operating conditions are considered as inputs into the complete exhaust system model. The design of the exhaust system is defined by the modules included within the design space. The system model is then assembled for a particular combination of engine and exhaust system configuration and vehicle operating conditions (drive cycle). Data from the engine exhaust is given at the input and the flow of the exhaust stream through the exhaust system is simulated. The majority of chemical and thermodynamic interactions are modeled within the component modules, and the final output includes the relevant performance data and emissions levels. The "generic" emission module blocks in Fig.1 can be populated by various combinations of component level technologies such as PM filters, NOx traps or oxidation catalysts among others. The entries of the state vector include the mass flow rate, temperature, pressure, amount of particulate matter as well as the density of various chemical species.

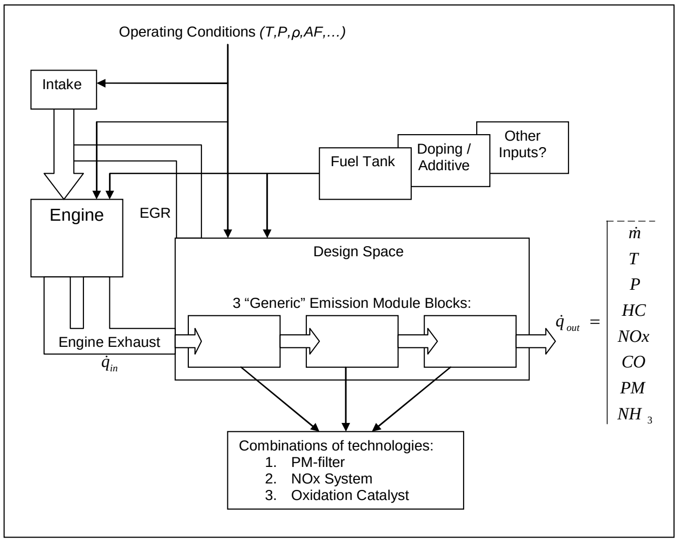

Figure 1. Notional Block Diagram of Engine and Exhaust System.

B. State Vector Platform Concept

Within the exhaust system design space there are clear divisions (or modules) to be used for the sub-models (as shown in Fig. 1). These modules allow us to decompose the design of the entire exhaust system into smaller parts, and recombine the different modules together to form different system architectures. For example, one can have a diesel oxidation catalyst (DOC) model followed by a particulate filter (DPF), or swap the components. This allows us to treat the exhaust system as a linear combination of elements, with the state vector passing through each component. The state vector is not only used to transfer information to and from components, along the length of the exhaust system, *but is used as the platform* from which all the different physical models are built. The state vector defines the key interfaces of data from which all the component models can then perform the appropriate computations.

This is a key point, because without such a clear interface definition, each particular configuration might have to be custom-built as has been done in the past, a potentially very labor-intensive process. Moreover, the state-vector modeling architecture implies that some entries in the state vector will potentially be unaffected by some physical components and be simply fed through directly. Figure 2 shows a 2-module system, with an input data file, two in-line DOC (diesel oxidation catalyst) modules, and a "tailpipe out" emissions output data file.

There is consideration for global feedback, specifically engine operation control from exhaust component feedback. In this case, since the engine emission file is set, the effect of the feedback on the exhaust gas flow has to be characterized, and those effects are implemented as changes to the state vector within the exhaust system model.

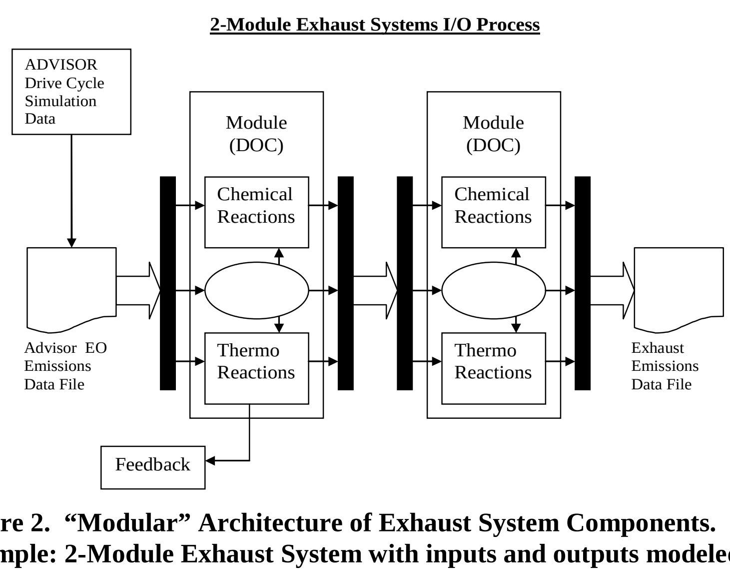

Figure 2. "Modular" Architecture of Exhaust System Components. Example: 2-Module Exhaust System with inputs and outputs modeled.

C. Operation

The exhaust system model will function by using an input file describing the engine exhaust conditions over time. This input file contains all the required information about the exhaust gas flow, given a certain engine/vehicle combination, and its performance over time in a given operating regime. The operating regime, or drive cycle, can reflect steady state conditions or transients, as the input file is a time-based discretization of the state of the exhaust gas flow. The input file data can be based from actual test data or simulation. Particularly, the simulation software package ADVISOR[1] can be used to model different engine/vehicle combinations under different operating regimes or drive cycles. The vehicle model should include all of the relevant engine-out emissions data per time-increment of a specific drive cycle. The input file (shown as the "EO Data File" in Fig. 3) is constructed from a library of engine and drive-cycle files, as required by the user.

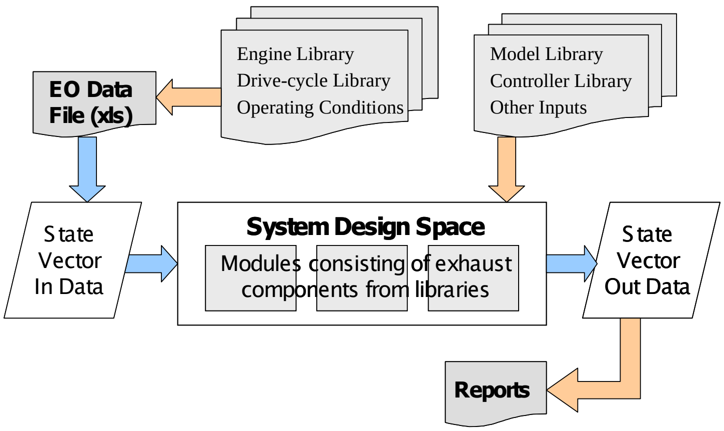

Figure 3. Complete System Model Flow Diagram.

The system program then converts the information from the input data file into the state vector, which is operated on sequentially through the complete exhaust system model. The system model (shown as the System Design Space in Fig. 3), is built from a model and controller library. Different technologies are modeled, along with any required active controllers, and this library is sourced to build the exhaust system model.

After the simulation ends, the program creates an output file, from which reports of performance data can be extracted. The output data, along with data from within the model, can be used to validate and tune the model to the actual components in production or under development.

D. Component Modularity

One of the fundamental concepts behind the state vector platform is that it is possible to develop a number of different models to describe different technologies, and then modularly combine them together to form different architectures[2]. Each model's interface is the strict definition of the state vector and the data that passes to and from the model. This interface allows the user to use the components in a modular way to build different exhaust system architecture from a small library of initial model files.

For example, the user can build any variety of systems, as shown in Fig. 4. System 1, for instance, uses Engine #2, with a DOC (diesel oxidation catalyst) and DPF (diesel particulate filter). The user simply combines the DOC and DPF models from the library in a new system file, and runs the simulation with the Engine #2 data file. In this manner, the user can build a matrix of different architectures run under various drive cycles and engine configurations.

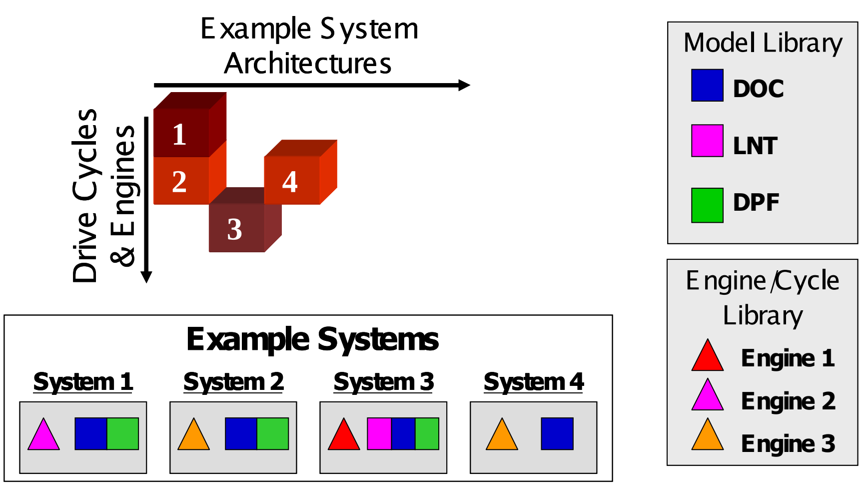

Figure 4. Component Modularity in Exhaust System Model Architecture

The value added is that a wide variety of exhaust system architectures can be simulated under various operating conditions with different engines. The results of these simulations can be analyzed to the engineer's discretion, and well-informed design decisions can be made within early product development. These designs can then be refined using either the same simulation tool or more complex CFD and FEM code, and a baseline design specified for more detailed analysis with much less prototyping, manufacturing, and testing expense.

III. Modeling Framework and Implementation

A software tool was built to implement this *modular state-vector based modeling and simulation architecture* using MATLAB and Simulink, two technical computing languages and interactive environments that allow for computation and multi-domain simulation. Simulink was chosen because it is a robust platform for model-based design of dynamic systems, which matches the time-based requirements imposed by the physical models of the exhaust system components[3]. Another aspect to choosing MATLAB/Simulink is that these programs provide an easy to use graphical environment that allows users to easily and accurately design and run various time-varying systems. These programs also interface readily with a host of other software packages, including stand-alone optimization software.

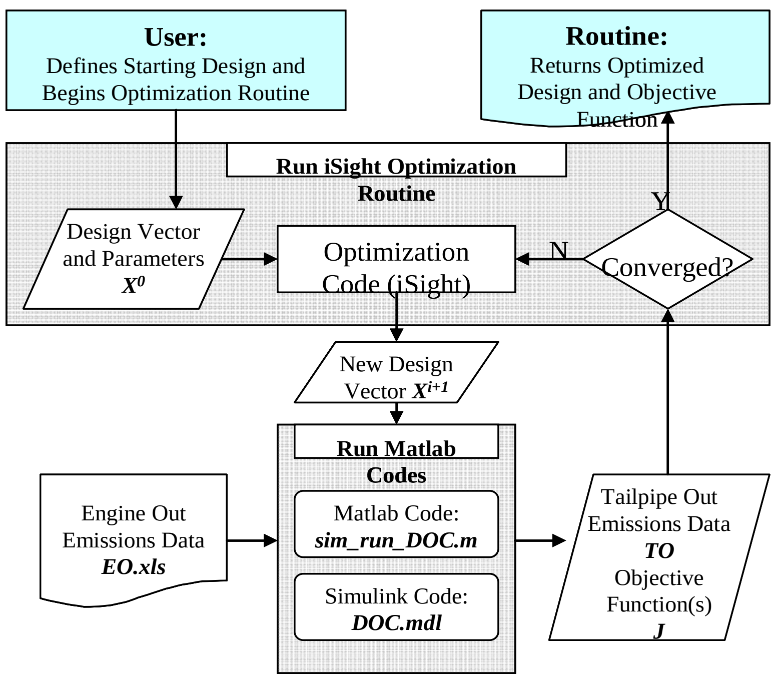

Figure 5. System Simulation Flow Diagram. Included in the diagram are the input and output files, the process (MATLAB and Simulink) files, and the optimization program interface.

Additional benefits of using MATLAB/Simulink within the project are obtained from having available open source, easily updateable system and sub-system models that can help development engineers in their learning and understanding of the behavior of the particular systems. Additionally, the models can be used to help in sizing of particular treatment solutions to a particular vehicle duty cycle.

The basic programming structure (see Fig. 5) of a full exhaust system simulation model includes a MATLAB (.m) file, a Simulink (.mdl) model, and an Engine Out (EO) input file (Microsoft Excel). The MATLAB file contains the main function calls, user defined design variables and parameters, and the file describes the architecture of the exhaust system. The user codes this file using combinations of the various physical model files from a library, or can develop his/her own model files. The Simulink file contains the time-variant physical model and any control algorithm, and effectively mirrors the MATLAB file code.

The optimization portion of the analysis tool was designed to interface with a stand-alone optimization software package to the MATLAB/Simulink simulation tool. The software package chosen for the optimization analysis was iSight, version 9.0, which has a MATLAB interface that allows the user to define the optimization parameters from within the program, allows the optimization routine to run the simulation for each iteration, and then return the appropriate results of the optimized design.

IV. Proof of Concept Results

A. Sizing Optimization Example of a Diesel Oxidation Catalyst

The proof of concept was to implement a relatively standard exhaust system model within the simulation framework previously described, and including optimization by varying some geometric variables. Further work would include adding in more drive cycles and performing a standard design of experiments (DOE) in the manner engineers typically would, and this is included in the next subsection. The first component to consider is a DOC (Diesel Oxidation Catalyst), a catalytic converter specifically formulated to deal with the emissions from a diesel engine[4]. It consists of a monolith honeycomb substrate coated with platinum group metal catalyst, packaged within a (usually) stainless steel container. As the exhaust gas contacts the catalyst, several exhaust pollutants are converted into harmless substances. The four main emissions that are regulated are particulate matter (PM, or organic fraction of diesel particulates), carbon monoxide (CO), hydrocarbons (HC), and oxides of nitrogen (NOx). The DOC specifically controls the CO, and HC emissions, but empirical data shows that it can reduce some NOx emissions as well. Generally, the chemical processes are modeled from first principles[1] or by a conversion efficiency table, where the conversion efficiency percentage reduction of the emissions species is a function of temperature (either gas or catalyst) and potentially of catalyst substrate properties.

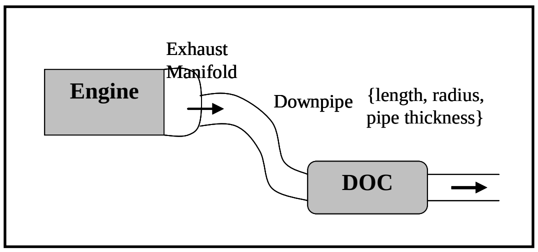

Figure 6. Engine and DOC model

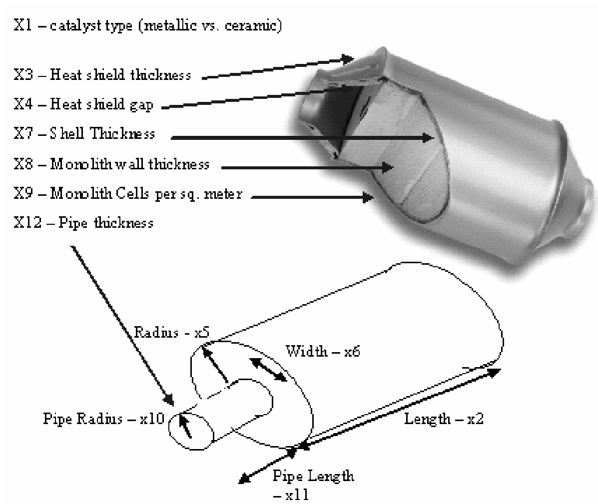

Figure 7. Mapping Design Variables to DOC

Although many variables can be used within the DOC, only a small set were defined as independent variables, with the majority of these variables used for geometric sizing of the catalyst for design purposes. Figure 6 shows an overview of the physical model with respect to the engine, and Fig. 7 shows the detailed mapping of the design variables to the physical implementation of the catalyst design.

The initial simulation also includes a down-pipe between the engine and the catalyst, treated as a standard pipe flow. The geometric sizing variables for the down-pipe are length, radius, and thickness. The constraints of the system are built into the model by bounding the design variables to within a certain range. These ranges can be set within iSIGHT

, and are up to the designer to specify, depending on their constraints within the entire vehicle system. The design variables in the design vector are defined in the next subsection.

1. The Design Vector

The design variables, as partially illustrated in Fig. 7, for the Diesel Oxidation Catalyst are described as follows:

x_1: Describes the type of catalyst; metallic or ceramic catalyst formulation.
x_2: The catalyst overall length. Generally ranges from 10 cm to 80 cm.
x_3: The catalyst's external heat shield thickness.
x_4: The gap distance between the external heat shield and internal shell.
x_5: The radius of the catalyst shell
x_6: This variable models the width between the round ends of the catalyst (if oval in shape)
x_7: The thickness of the catalyst steel shell
x_8: The monolith honeycomb wall thickness
x_9: The cell density, number of honeycomb cells per cross sectional area of monolith
x_{10}: The inlet pipe radius, where the catalyst attaches to other components.
x_{11}: Inlet pipe length, generally short.
x_{12}: Inlet pipe thickness.
x_{13}: Downpipe length
x_{14}: Downpipe radius
x_{15}: Downpipe thickness

The sizing and material constraints are built into the design variable bounds. The designers and users of the models have limited materials to choose from, and are thus limited in the availability and sizes of these materials.

The bounds of the design variables are effectively constraints on the problem. The formulation of the catalyst is the only remaining significant factor. For this example, only the results of a metallic monolith substrate were analyzed with a specific cell density and wall thickness formulation.

2. Objective Function

The initial (performance) objective function is to minimize the tailpipe emissions of the vehicle by incorporating all of the regulated emissions species into the objective function, shown in Eq. (1).

$$\text{Min } [f = HC\_emissions + CO\_emissions + NOx\_emissions + PM\_emissions] \tag{1}$$

The initial objective function was a weighted sum of the normalized emission species. Normalizing the emissions results allows us to directly compare the emissions values, without having to examine the difference in magnitudes of the actual values of exhaust species emissions. In order to normalize the effects of each emissions type, the output of the exhaust system emission species will be divided by a regulatory limit (e.g. issued by the U.S. Government). The values of the normalized emissions contributions (i.e. the summation terms in Eq. 2) will lie between 0 and 1; with any value over 1 effectively making that design infeasible (because it will not meet emissions regulations). This can give the optimizer a direct comparison to evaluate the designs of the exhaust system.

Regulated emissions species are hydrocarbons (HC), carbon monoxide (CO), oxides of nitrogen (NOx), and particulate matter (PM). The regulations allow a certain amount per mile traveled, usually given in grams per mile. These emissions are measured under the US Federal Test Procedure protocol, which puts a vehicle through a specified speed/load drive cycle[1].

The single objective function is thus transformed from Eq. (1) to Eq. (2).

$$\text{Min } [f = w_{HC} \cdot \left(\frac{HC_{emis}}{HC_{\text{Reg}}}\right) + w_{CO} \cdot \left(\frac{CO_{emis}}{CO_{\text{Reg}}}\right) + w_{NOx} \cdot \left(\frac{NOx_{emis}}{NOx_{\text{Reg}}}\right) + w_{PM} \cdot \left(\frac{PM_{emis}}{PM_{\text{Reg}}}\right)] \tag{2}$$

The sum of the individual weights were constrained, Eq. (3), and for the following set of tests, the weights were equal to 0.25.

$$1 = w_{HC} + w_{CO} + w_{NOx} + w_{PM} \tag{3}$$

3. Optimization Set-up

A commercial optimization program, iSIGHT, was used to optimize the DOC and downpipe system. This program was interfaced with the Matlab/Simulink simulation code (see Fig. 5). Each iteration of the simulation took approximately 2 seconds of CPU time. First, the user specifies the initial design point by setting the design vector. The values can be arbitrary (within the bounds) or be sourced elsewhere, for example a DOE (Design of Experiments). Once the optimization algorithm begins, the program outputs the design vector to Matlab/Simulink. The program then runs the simulation model of the exhaust system components, which return the emissions results as the specified performance objective function(s). The optimization algorithm then iterates until the results have converged to a solution, or the termination criteria has been reached.

4. Single Objective Optimization and Sensitivity Analysis

For the single objective optimization case, an initial case of mid-range values for the design variables was used. Other initial design vectors were used to investigate the behavior of gradient based optimization and to verify the global optimum. Afterwards, a sensitivity analysis was performed over the design variables.

The recommended gradient based algorithm for a nonlinear system with continuous design variables is SQP and Newton-based methods, using finite differences to calculate the gradients in our specific case. The recommended heuristic methods are GA (genetic algorithm) and SA (simulated annealing). Within iSIGHT, the recommended optimization scheme is a nonlinear SQP algorithm.

The optimization algorithm converged upon a solution, whose significant sizing design variables are shown in Table 1. These particular design variables were significantly different than the initial starting values, indicating that the optimizer found these to be the most significant changes to the physical design of the exhaust system. However, it took repeated runs to confirm this solution with different starting points. Many times a local optimum design point was found, rather than the global optimum. Oftentimes, it took two optimization runs with the SQP algorithm to converge on the global optimum, due to the adaptive nature of the step. Apparently the program changes the step along the gradient, such that using the optimum point found in the initial optimization routine as the input for the next routine will oftentimes result in a better solution. Illustrations of the convergence histories for successive optimization runs are shown in Fig. 8 and Fig. 9.

Table 1. Results for design variables of example DOC system after single objective optimization.

Design Variables	**Description**	**Converged Solution Value**	**Initial Value**
x_2	DOC Length	0.80 m	0.50 m
x_5	DOC shell radius	0.01 m	0.05 m
x_6	DOC shell width	0.00 m	0.10 m
x_{13}	Downpipe radius	0.049 m	0.05 m
x_{14}	Downpipe length	0.049 m	0.50 m
x_{15}	Downpipe wall thickness	0.0010 m	0.0015 m
Obj		0.286	0.323

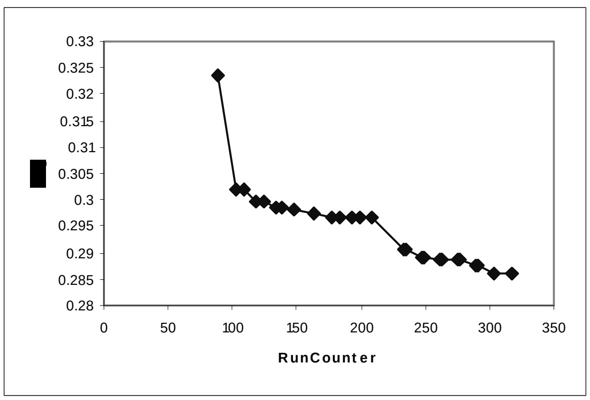

Figure 8. Objective Function Value History of First Pass-Through of SQP Algorithm Routine.

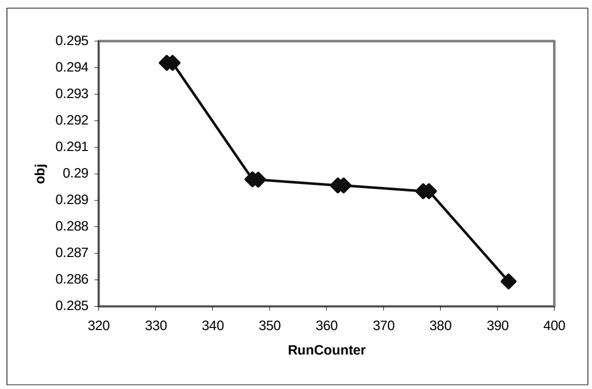

Figure 9. Objective Function Value History of Second Pass-Through of SQP Algorithm Routine

The first optimization run in Fig. 8 took 244 function calls to converge to a solution, with a total CPU time of about 20 minutes. The second optimization routine in Fig. 9 took only 89 runs, and a CPU time of approximately 8 minutes. Evidently the gradient based optimization tends to find local optima, although a global optimum can be found approximately after numerous runs through the optimization routine. A guarantee of global optimality does not exist (KKT optimality criteria) due to the non-convexity of the underlying objective function.

To conduct a sensitivity analysis, a finite difference method was used, where each design variable was perturbed from the optimum, and the corresponding new objective function calculated. The gradient of the objective function was then calculated, and normalized, according to Eq. (4) and Eq. (5).

$$\nabla \bar{J} = \frac{\mathbf{x}^0}{J(\mathbf{x}^0)} \nabla J \qquad (4)$$

where :

$$\nabla J = \frac{\partial P}{\partial \mathbf{x}_i^0} \qquad (5)$$

The normalized sensitivities of the objective function were calculated with respect to the design variables, and are illustrated in Fig. 10.

As can be seen from the figure, the main drivers of the system's emissions performance are the catalyst length and the downpipe length. This makes physical sense, as those physical parameters have the most to do with the thermal characteristics of the catalyst monolith (thermal mass). The sensitivity analysis matches the general intuition of catalyst engineering[5], where the designs have tended toward long, thin tubes, as opposed to boxes or more square cylinders or ovoid shapes. The one aspect of this model that was not tested was the pressure drop across the catalyst. This is one performance influencing parameter that would be worse with a longer catalyst, decreasing engine performance at the expense of better emissions.

For this particular catalyst model, using the FTP city drive cycle, and for the particular engine/chassis combination, we are confident that a near-global optimum was found, given the single objective function defined as in Eq. (2), and the various design parameters that were varied. The reason for this confidence is that multiple simulations from many different initial design points did not result in an improved design. Instead other local minima were found, along with the global minimum results, a summary of which was illustrated Table 1. Similarly, the results of the heuristic (GA) algorithm corroborate those found with the gradient based method.

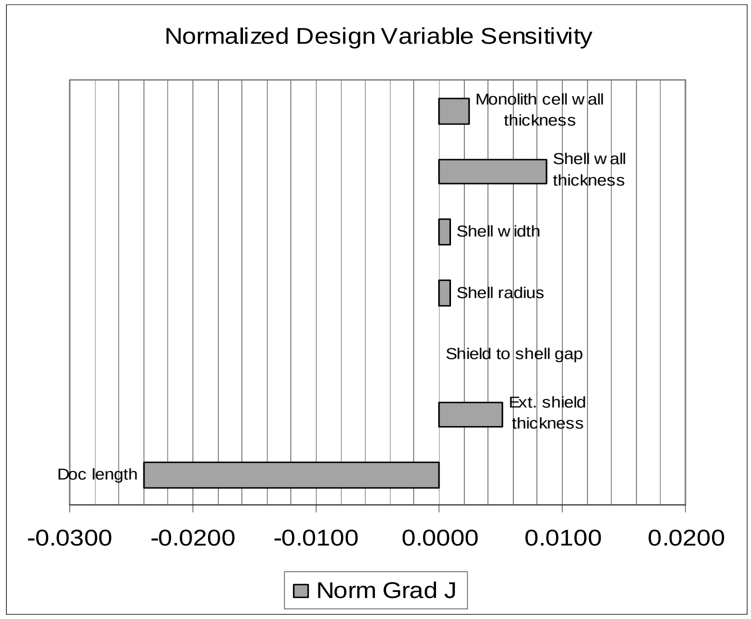

Figure 10. Sensitivity Analysis of Design Variables.

B. Transient and Steady State Design of Experiment Simulation for different Oxidation Catalyst formulations

Upon review of the initial optimization results, it was decided to further investigate the catalyst formulation in detail and include more transient and steady state cycles to test other operating conditions, using the same small diesel engine baseline[1] (Volkswagen 1.9 liter engine). A typical development problem for engineers would be to resolve the catalyst formulation, with regards to cell density and monolith wall thickness, given a certain geometric size, optimized over a variety of different operating points. Using the DOC model previously described and implemented within the modeling framework, a straightforward design of experiments was used to investigation of the thermal mass behavior for the two design variables (monolith wall thickness and cell density).

The initial findings were that there appeared to be areas of the design space in terms of mass of the catalyst (with certain combinations of wall thickness and cell density) that offered the best emission performance level for specific gas species. The results of the study show a few key points also corroborated by other tests[5]:

1. Monolith thermal mass greatly affects the emission performance of the DOC.
2. The general trend for better emissions is lowering thermal mass through use of less cell density and thinner wall thickness, especially in steady state cases.
3. The transient cycle simulations showed that optimal performance of emissions resided within the design space (as given by typical catalyst formulation geometries), albeit close to the boundary. Increasing or decreasing thermal mass from that point led to worse performance, although the vast majority of the design space indicated reducing thermal mass would improve performance.
4. There is a distinct trade-off between light thermal mass that allows for quick warm-up and heavy (large) thermal mass that allows for temperature to remain high during transients. This was evident in the temperature tracking, and the resultant performance of the catalyst due to its temperature.

1. Steady State Case

It can be seen (from Table 2) that the overall objective function is lower with less DOC monolith mass. This was due to the long warm-up time associated with very heavy monoliths, and the resulting poor emission performance.

Table 2. Steady state test case emissions results of typical catalyst configurations.

Steady State			
mon cell wall thk	cell density	200 CPSI	400 CPSI
1 mil	HC [g]	8.6125	8.7046
	CO [g]	9.0546	9.3126
	Nox [g]	2.3822	2.4501
	PM [g]	0.4431	0.453
	Objective	0.7152	0.7263
	mon mass	519 g	734 g
	volume	2.33 liters	2.33 liters
	CS cells	1806	3613
	CSA	9.03 sq in	9.03 sq in
2 mil	HC [g]	8.7558	8.7919
	CO [g]	9.4712	9.6129
	Nox [g]	2.5245	2.5786
	PM [g]	0.4606	0.4678
	Objective	0.734	0.7402
	mon mass	1038 g	1468 g
	volume	2.33 liters	2.33 liters
	CS cells	1806	3613
	CSA	9.03 sq in	9.031 sq in
6 mil	HC [g]	9.095	9.4336
	CO [g]	10.7442	11.9729
	Nox [g]	2.7669	2.9259
	PM [g]	0.5003	0.53
	Objective	0.7779	0.8168
	mon mass	3113 g	4404 g
	volume	2.33 liters	2.33 liters
	CS cells	1806	3613
	CSA	9.031 sq in	9.031 sq in

Table 3. Transient test case emissions results for typical catalyst configurations and low cell density configurations

Transient (FTP)					
mon cell wall thk	cell density	33 CPSI	70 CPSI	200 CPSI	400 CPSI
1 mil	HC [g]	2.9913	2.897	2.8463	2.9822
	CO [g]	10.7892	10.3455	10.0085	10.0528
	Nox [g]	4.1098	4.144	4.1348	4.1192
	PM [g]	0.2552	0.2606	0.272	0.2832
	Objective	0.4023	0.3964	0.3944	0.4
	mon mass	209 g	309 g	519 g	734 g
	volume	2.33 liters	2.33 liters	2.33 liters	2.33 liters
	CS cells	291	640	1806	3613
	CSA	9.03 sq in	9.03 sq in	9.03 sq in	9.03 sq in
2 mil	HC [g]			2.9961	3.2658
	CO [g]			10.2787	10.9635
	Nox [g]			4.1158	4.1626
	PM [g]			0.2963	0.3192
	Objective			0.4109	0.4379
	mon mass			1038 g	1468 g
	volume			2.33 liters	2.33 liters
	CS cells			1806	3613
	CSA			9.03 sq in	9.031 sq in
6 mil	HC [g]			4.0255	4.2781
	CO [g]			12.7871	13.2351
	Nox [g]			4.4813	4.5795
	PM [g]			0.374	0.3921
	Objective			0.5147	0.539
	mon mass			3113 g	4404 g
	volume			2.33 liters	2.33 liters
	CS cells			1806	3613
	CSA			9.031 sq in	9.031 sq in

2. Transient Case

The transient case incorporates the interplay between warm-up time, and heat capacity of the monolith. Table 3 illustrates that within the typical configurations of 200-400 CPSI cell densities and 1 mil to 6 mil thickness walls, it is evident that the lowest thermal mass performed the best in terms of emissions output. However, experimenting with reducing the mass further (in this case by reducing cell density to 1/3, and then 1/6 of the lowest typical cell density), the performance worsened. The overall objective function has a minimum value of just under 0.4 at around 500 g mass (given that the other geometric design variables remained constant).

Each species' performance, though, is different and has different gradients at different thermal masses. It appears that HC and CO emissions are best at or slightly higher values than 500 g of mass. NOx emissions show a non-convex result, where very low NOx emissions were obtained for low thermal mass (under 300 g) and higher (around 1000 g), but performed worse in between and at the extremities. Particulate matter performance clearly was better with lower thermal masses. For differing cycles, there is definite interplay between the requirements of a quick light off of the catalyst and the necessity to hold heat during transient states. This optimum performance point is most likely different for each cycle and engine configuration. However, the ability of the modeling and simulation tool to illustrate this, as well as offering the capability to adjust the architecture and detailed design of the exhaust system, illustrates how valuable the information from the models can be for engineers.

C. Comparison of combined DOC and DPF systems with active controls

1. System Architecture and Base Case Comparison

Expanding on the modeling and simulation tool example cases, a multi-component and multi-objective case study attempted to udevelop a relevant example to illustrate the capabilities of the tool, as well as investigate the optimization results of the comparative architectural systems. The objective is to demonstrate the performance differences both between different component technology designs and their relative arrangement in the overall exhaust system architecture, and examine the hypothesis that it is *more beneficial to examine the system as a whole, rather than optimizing each component separately, and then combine them together into a system configuration*. In particular, a combination of a fuel dosing component, a heat generation device, a DOC, and a DPF (diesel particulate filter) with active regeneration control was modeled and simulated through a set of steady state operating points.

The base case was to take a DOC and DPF unit, and simulate a set of steady state engine operating points over a period of time, to verify what the regeneration capability of a purely passive system (without heat generation device) was. The results showed that the only successful regenerations occurred in high torque / high rpm operating points, where much heat is naturally generated by the engine. The fundamental practical issue involved here is that successful regeneration of DPFs on-board vehicles using passive controls cannot work effectively. There has to be a method to actively control the regeneration to ensure proper emissions performance and complete regeneration. Figure 11 illustrates the engine operating points and regeneration results.

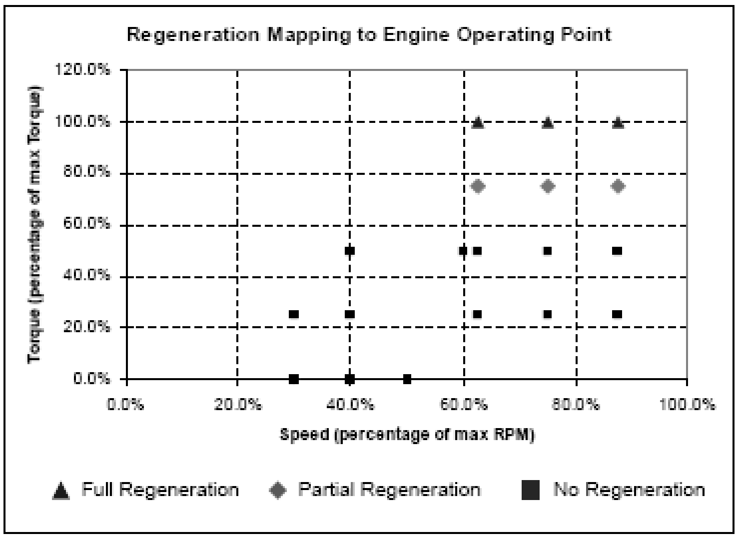

Figure 11: Regeneration Mapping: Engine Operating Point and Regeneration Results for a Passive DOC/DPF System

Three new system architectures were developed to address the regeneration performance issue: a dosing system which injects diesel fuel upstream of the DOC which reacts over the DOC, raising the temperature of the DPF for regeneration; and two thermal heat input systems that combust the exhaust air either upstream of the DOC or upstream of the DPF.

The basic variables included dimensioning variables for the DOC, DPF, and the dosing/heater systems, and the dosing and heating system duration times and fuel flow rates. Four main objectives were also used in the optimization run: minimizing NOx and particulate emissions; minimizing mass of the system; minimizing fuel economy penalty associated with the dosing and heating system; and maximizing the regeneration efficiency. Appropriate algorithms were used to trigger the regeneration system, such that no dosing or combustion attempts were made during engine/exhaust operating conditions that were unfavorable. Further details are available[6].

2. Optimization Results

In order to obtain a valid comparative study between the architectures, a Genetic Algorithm was set-up to perform a trade-off analysis between competing objectives and yield and objective-space optimization. Further refinement was done using a mixed integer gradient based optimization algorithm, for a chosen system architecture. The result of which was then compared with an optimization run done on a component-level basis for the same system. The component-level case optimized each component individually. This comparison was done to validate the hypothesis that a system-wide multi-objective optimization on a complex system such as this can yield better performance than a system that puts together parts from a component level optimization.

The initial objective-space optimization results showed a significant trade-off in all of the system architectures between emission conversion efficiency and system mass, and between fuel economy penalty and regeneration efficiency. Figures 12 and 13 show the results of the GA optimization for the objective trade-offs between the three system architectures. It is evident that while the three systems are relatively similar in their performance trade-off between emissions and mass, the dosing system performs far poorer than the heater systems in the fuel economy and regeneration efficiency. The direction of the utopia point is indicated by a large dot.

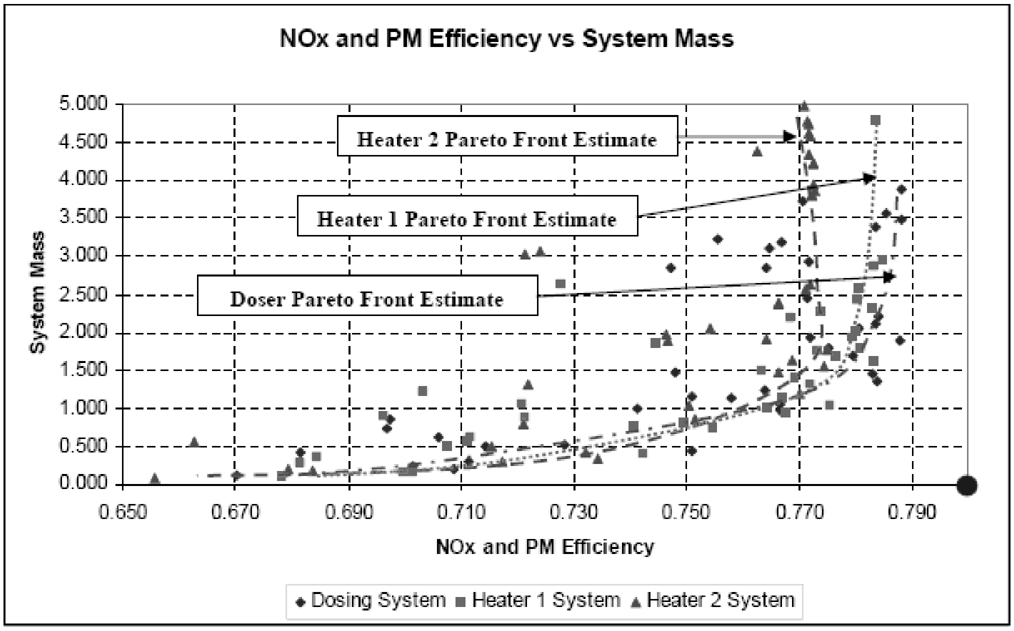

Figure 12: NOx and PM Efficiency vs System Mass Objective Space

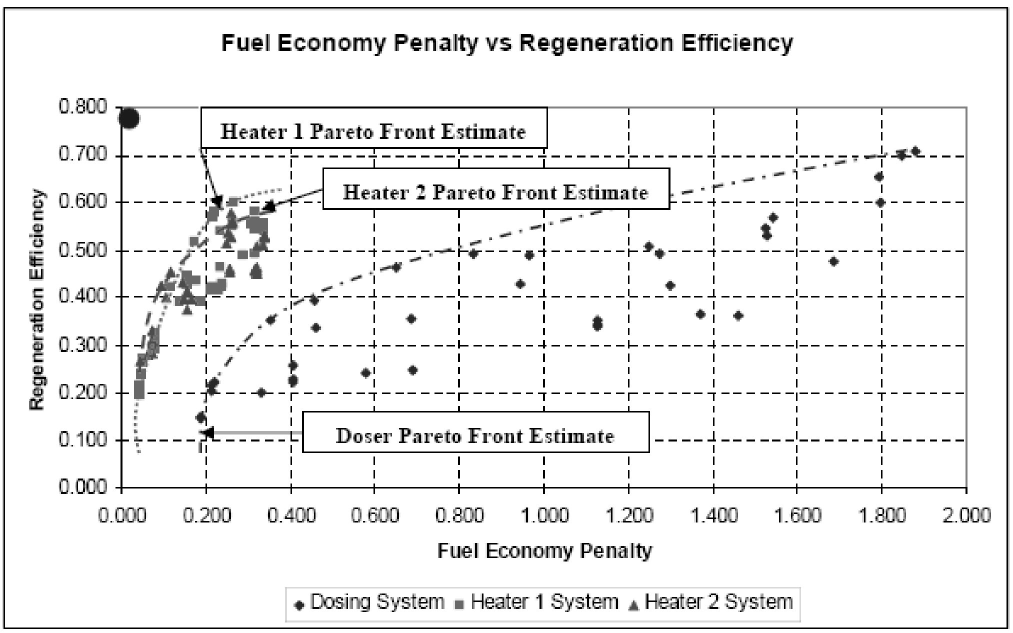

Figure 13: Fuel Economy Penalty vs Regeneration Efficiency Objective Space

The result for the refinement optimization are shown in Table 4. It is evident that while a GA is useful in providing a coarse pass through the objective space, it is still possible for the optimizer to find a better solution (on balance between the competing objectives) using a gradient-based algorithm within a local region identified by the GA.

Table 4: Refinement Optimization Results

Architecture \ Average Objective Result	Avg_eff	NOx & PM Eff	Fuel Econ. Penalty	Regen capable	Regen Eff	DOC Mass	DPF Mass	System Mass
Passive Design (Initial)	0.613	0.742	0	0.150	0.130	0.666	0.667	0.666
Heater 2 Design (Start)	0.478	0.668	0.107	0.714	0.449	0.058	0.045	0.101
Heater 2 Design (Best)	0.512	0.716	0.109	0.785	0.498	0.026	0.009	0.061
Objective Function Improvement	7.1% Better	7.2% Better	1.9% Worse	9.9% Better	10.9% Better	55.1% Better	80.0% Better	39.6% Better

3. Comparison of System Level Optimization with Individual Component Optimization

Once this result was achieved for the heater 2 system, a comparison between an individually optimized case for the heater 2 system was done. In this case, each component of the system (the DOC and the DPF) was optimized for the set of objectives that the particular component can address on a performance basis. The objectives for the DOC were the system mass and emission efficiency, and the DPF objectives were mass, regeneration efficiency, fuel penalty, and emission efficiency. The two individually optimized components were then modeled together and a simulation run to obtain the performance of this new system under the same operational conditions as before.

Table 5: System Level Optimization vs. Individual Component Optimization Comparison

Architecture \ Average Objective Result	Avg_eff	NOx & PM Eff	Fuel Econ. Penalty	Regen capable	Regen Eff	DOC Mass	DPF Mass	System Mass
Passive Design (Initial)	0.613	0.742	0	0.150	0.130	0.666	0.667	0.666
Heater 2 Design (Best Coarse Optimization)	0.478	0.668	0.107	0.714	0.449	0.058	0.045	0.101
Heater 2 Design (Best Refinement Optimization)	0.512	0.716	0.109	0.785	0.498	0.026	0.009	0.061
Heater 2 Design: Individual Component Optimization	0.428	0.669	0.163	0.857	0.488	0.031	0.007	0.063
Percent Difference vs. Coarse System Optimization	10.4% Worse	**0.1% Better**	**52.3% Worse**	20.0% Better	**8.7% Better**	46.5% Better	84.4% Better	**37.6% Better**
Percent Difference vs. Refined System Optimization	16.4% Worse	**6.6% Worse**	**49.5% Worse**	9.2% Better	**2.0% Worse**	19.2% Worse	22.2% Better	**3.3% Worse**

Table 5 shows that the difference between the performance of the individual component result was not significantly better than the coarse system optimization; and was much worse in all objectives versus the refined system optimization. This comparison case study shows that rather than having the optimization algorithm be able to take into account and balance the competing objectives from a system level, the individual optimization with separate components drove a design that may have been very good at the component level, but that did not work as well for the overall system and the entire range of operating points when taking into account the synergies and interactions at the system level. This validates one of the major points of the hypothesis that optimizing components separately in hopes that combining them creates a good system is not as successful in improving objectives when taking the entire system and all of the interactions between components into account.

V. CONCLUSIONS

The significance of developing a modular system modeling methodology for diesel exhaust systems design, analysis, and optimization is that it allows engineers to better analyze and understand the more complex after-treatment technologies that will be implemented in the future. The interactions among components are captured via the state-vector and potential feedback loops between components. This paper presented a new modular state-vector based modeling architecture and framework, as well as the software implementation of the modeling architecture. A proof of concept example was also presented, along with the results for a single objective optimization routine. Further design analysis into the initial results was also illustrated, and a multi-component, multi-objective case study was also presented.

The key point is that optimizing the exhaust system as a whole for a wide variety of operating points and engines during the pre-development design work is more valuable and beneficial than trying to adapt a single point design to be merely acceptable during the testing phase of product development. Being able to compare system components and architectures, as well as design parameters, gives engineers a better understanding of the performance and interactions of the system. This knowledge can be used in the development process to refine designs in preparation for prototyping and testing. Additionally, examining the entire system and its performance over a variety of conditions can lead to building a better overall system than combining single-point optimized components together. Engineers can take advantage of the interactions between components in the system and try to curb the downside effects. This is especially critical when after-treatment technologies are becoming more complex, potentially requiring active control in the future.

Expanding the current simulation model to include other components (such as Lean NOx Traps models or other newer technologies not yet developed) can potentially result in novel system designs that could not have been devised without a systems-wide methodology. Given the architecture and software implementation, engineers can expand the modeling and simulation tool further by adding other performance metrics, such as cost models. Additionally, the architecture of the simulation model is such that new components can be added to a library of models, and system models developed much more quickly from this library. The modularity of the simulation tool allows a flexibility not previously found in flow-based modeling tools, where the entire system model has to be developed from scratch. The methodology presented here supports system level design, analysis, and optimization of diesel after-treatment solutions, but could potentially be extended to other system design problems, particularly those involving various types of internal fluid flow.

Acknowledgments

The authors of the paper would like to thank Rudolph Smaling, Ph.D., for his help and guidance during the project. This research was sponsored by a research grant from ArvinMeritor, Inc. with Mr. Bill Taylor and later Dr. Navin Khadiya serving as contract monitors.

References

[1]ADVISOR2002, NREL's ADvanced VehIcle SimulatOR, Software Package, Version 2002, National Renewable Energy Laboratory, U.S. Department of Energy, Washington D.C., 2002.

[2]Simpson, T. W., Siddique, Z., and Jiao, J., *Product Platform and Product Family Design, Methods and Applications,* Springer Science+Business Media, Inc., New York, 2006, Chap. 10.

[3]Kladopoulou, E. A., Yang, S., Johnson, J. H., Parker, G.G., and Konstandopoulos, A. G., "A Study Describing the Performance of Diesel Particulate Filters During Loading and Regeneration – A Lumped Parameter Model for Control Applications," SAE Technical Paper No. 2003-01-0842.

[4]Heywood, J.B., *Internal Combustion Engine Fundamentals,* McGraw-Hill Book Company, New York, 1988, Chaps. 10,11.

[5]Marsh, P., Acke, F., Konieczny, R., Brück, R., and Hirth, P., "Application Guideline to Define Catalyst Layout for Maximum Catalytic Efficiency," SAE Technical Paper No. 2001-01-0929, 2001.

[6]Graff, C. D., *System Modeling, Analysis and Optimization Methodology for Diesel Exhaust After-treatment Technologies,* S.M. Thesis, Department of Aeronautics & Astronautics, Massachusetts Institute of Technology, June 2006