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# AUTOMATED CREATION AND TESTING OF REDUCED CHEMICAL KINETIC MECHANISMS

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## ABSTRACT

A Computational Problem Solving Environment (PSE) for creating and automatically testing reduced chemical kinetic mechanisms for combustion systems has been developed. The PSE integrates the automatic chemical mechanism reduction code CARM (Computer Aided Reduction Method) and the codes that simulate perfectly stirred reactors (PSR's) and plug flow reactors (PFR's) into a user-friendly computational environment.

The PSE gives the engineer the ability to rapidly set up, run and examine large numbers of problems. The demonstration problem presented here consists of comparing detailed and reduced chemical kinetic calculation results for methane-air combustion including NO<sub>x</sub> formation in a stirred reactor. The PSE gives the combustion engineer the ability to easily test chemical approximations over many hundreds of combinations of inputs in a multidimensional parameter space. This tool allows combustion chemistry approximations to be validated and characterized with a thoroughness and rigor that was not feasible before.

## INTRODUCTION

Computational Fluid Dynamics (CFD) codes aimed at solving practical engineering problems involving chemically reacting flow can presently incorporate only very simplified descriptions of the chemical processes involved. For example, detailed chemical kinetic descriptions of hydrocarbon oxidation may require the tracking of hundreds of chemical species and thousands of reaction steps. CPU and memory limitations prohibit implementation of full detailed chemistry into CFD simulations of practical combustors. Techniques are now available to create red-

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duced chemical kinetic mechanisms that reproduce the results of detailed chemical kinetic descriptions over a range of conditions using many fewer species, and thus less CPU time and memory. However, the range of validity of reduced mechanisms has not often been well characterized in the past.

A promising approach to creating reduced chemical kinetic mechanisms is to use steady-state assumptions for a number of chemical species<sup>1,2</sup>. Chen<sup>3</sup>, has recently automated the mechanism reduction process into a computer code called CARM (Computer Assisted Reduction Method). CARM produces source code for the calculation of the chemical source terms defined by the reduced mechanism that can be linked easily to a combustion simulation code.

Mechanism reduction using steady-state assumptions has been extensively applied to hydrogen and methane combustion<sup>1,2</sup>. Using CARM, these techniques have also been applied to combustion of hydrocarbons such as ethylene and *n*-heptane<sup>4</sup>, NO<sub>x</sub> reduction in coal-fired furnaces<sup>5</sup>, incineration of hazardous chemicals<sup>6</sup>, and recently to a large detailed chemical kinetic mechanism for JP-8 combustion<sup>7</sup>.

In this paper we begin with an overview of the capabilities of the CARM PSE software, followed by a section devoted to the details of the software implementation. Results are then given and discussed for the methane/air test problem followed by a section giving the conclusions of this work.

## OVERVIEW

The new problem-solving environment was created using a combination of existing and emerging software technologies. Specifically, we combined:

- A problem solving environment called SCIRun<sup>8</sup>,
- The CARM software<sup>3</sup> for automatic chemical kinetic mechanism reduction,
- Public domain codes<sup>9,10</sup> for modeling simple, zero-dimensional combustion reactors and
- The Microsoft SQL Server database software.

Combining these technologies resulted in a PSE with the following capabilities:

Multiple Test Case Setup: Easy-to-use Graphical User Interfaces (GUI's) were constructed for the public domain Chemkin combustion simulation codes PSR<sup>9</sup>, which models a well-stirred reactor, and SENKIN<sup>10</sup>, which models which models a plug flow reactor. The input panels allow the user to select all the needed inputs. The user has the option of holding each input constant or varying it over a selected range. The PSE then automatically loops over the selected values of the parameters to be varied. The same setup may be used for detailed chemistry as well as reduced mechanisms created by CARM or any other type of chemical kinetic approximation.

Databasing and Visualization of Results: The results of the runs (which may number hundreds or thousands) are stored in a relational database. Results may be extracted from this database in 1D, 2D, or 3D form allowing a multitude of visualization options including line and carpet plots as well as 3D field visualization. Results of both detailed and approximate chemistry can be simultaneously accessed and compared, allowing calculation of statistical error measures and examination of the conditions under which reduced mechanisms or other approximations fail.

Creation of Improved Reduced Mechanisms: Integration of the CARM automatic mechanism reduction software into the PSE allows the entire reduced mechanism creation and testing process to occur seamlessly within a single computational environment. Test problem inputs may be set up using the PSE's GUI's. Before this project, only PSR cases were allowed as inputs to CARM. A file adapter was written and integrated into the PSE that converts SENKIN output at selected times to PSR format for input to CARM. CARM, which runs within the PSE, will read the results of these cases and automatically create reduced chemical kinetic mechanisms. These are automatically compiled and linked to the PSR and SENKIN codes. Cases for comparison of detailed and reduced chemistry can then be set up and run and the results examined. The results of this comparison allow the engineer to improve the performance of the reduced mechanism for conditions where agreement with detailed chemistry is unsatisfactory.

## **IMPLEMENTATION DETAILS**

### **SCIRun Overview**

SCIRun<sup>8</sup> provides a framework for integrating a variety of computational algorithms using a dataflow

programming paradigm. SCIRun extends the use of the dataflow programming paradigm into the computational pieces of the simulation process. The elements used to construct a SCIRun dataflow network are described below.

1) A module, drawn as a box in the network, represents an algorithm or operation. A set of input ports and a set of output ports define the module's external parameters.

2) A port provides a connecting point for routing data to different stages of the computation. Ports are strongly typed: each datatype has a different color, and datatypes cannot be mixed. Datatypes are quantities such as scalar fields or matrices, but are not the specific representations, such as regular grids, unstructured grids, banded matrices, sparse matrices, etc. In SCIRun, ports can be added to and removed from a module dynamically. Output ports can cache datasets to avoid recomputation. The user can select which datasets should be cached and which should not.

3) A connection links two modules together; the output port of one module is connected to the input port of another module. These connections control where to send data to be computed. Output ports can be connected to multiple input ports, but input ports accept only a single connection. A module that should accept an arbitrary number of inputs can use a callback mechanism to create a new empty port when the other input ports are full.

4) A network consists of a set of modules and the connections between them. This represents a complete dataflow "program". A dataflow library is responsible for deciding which modules need to be executed and when. An executing module will typically read data from the input ports (if any), perform some operation, and then send the results through one or more output ports. A module is typically re-executed when the user changes a module parameter, when new data is available at an input port, or when data is required at its output port.

SCIRun makes use of some features of object-oriented programming to achieve a very high level of code flexibility and thus reusability. In an object-oriented data model, pieces of data are thought of as objects upon which computations are executed. A powerful property of objects is that they can be specialized or derived from a more general object into variants with differing functionality. In SCIRun, a user can easily introduce a new, specialized type of object without having to alter any other part of the system that uses the same general type.

In this project, we used SCIRun's object-oriented features to accomplish two major tasks: 1) implementation of custom datatypes (which are data

structures passed between modules) and 2) implementation of custom modules.

To create the required custom modules, custom software development was coupled with class derivation. Class derivation was used to achieve code reuse and to maintain compatibility with existing and future SCIRun modules. Each custom module was derived from the SCIRun provided base type "Module", which provides the basic functionality and methods required of any SCIRun module. The resulting derived class for each custom module was then specialized to obtain the desired functionality.

### **Automated Setup and Execution of Model Runs**

#### **MPSR (Multi Perfectly Stirred Reactor) Module**

The public domain Chemkin code PSR<sup>9</sup> is a robust and widely used code that models an idealized combustor in which unburned gases enter the combustion chamber, mix instantaneously with the contents of the reactor, which are assumed to be spatially uniform and constant in time, and exit the reactor after a given residence time. This system is governed by a set of coupled nonlinear algebraic equations involving the species concentrations, temperature, and reaction rates. For long residence times the PSR solution approaches a state of complete chemical reaction (chemical equilibrium). As the residence time decreases, the chemical kinetics has less time to reach completion. For a PSR in which the temperature is not fixed, below a certain residence time the chemistry is too slow to release sufficient heat to maintain the reaction and the reactor blows out. The solution for these conditions is the trivial one of gas passing unreacted through the chamber. The laboratory analog of the PSR is the jet-stirred reactor in which a large number of high-speed gas jets create rapid mixing.

MPSR allows the PSE user to quickly set up and run any number of cases. MPSR contains a GUI that allows all of the needed inputs to the PSR code to be specified. Once the inputs are specified, the user has the choice of holding them constant or making them variable. Variable inputs can be specified as equally spaced, hand selected, or with a biased distribution. The number of cases to be run increases exponentially with the number of parameters selected as variable, so the user is notified of the total number of cases currently selected.

The inputs to the PSR code are the type of problem (fixed temperature or temperature determined by solution of an energy equation), the pressure, inlet species composition, the temperature for fixed  $T$  cases, and the inlet temperature, heat loss, and guessed

temperature for energy equation cases. The inlet gas composition may be specified in one of two ways. The user may simply list the species and their concentrations, or the user may define the composition of a fuel and an oxidizer and specify an equivalence ratio. The equivalence ratio is defined as the mass of fuel divided by the mass of fuel needed for stoichiometric combustion. The user may also select the chemical kinetic mechanism (detailed or reduced). For a detailed mechanism, the user points the module to the location of the binary "linking" file specifying the kinetic and thermodynamic information. For reduced chemistry the user specifies the linking file and the FORTRAN subroutine containing the reduced mechanism information. For reduced mechanism cases, MPSR will automatically compile and link this subroutine. Once setup is complete, MPSR loops over the variable inputs, running the PSR code for each set of input conditions.

The MPSR module runs individual PSR cases by spawning separate processes from a control thread in the module's C++ code (inside of SCIRun). The control thread then monitors the case's execution status and watches for completion. Upon completion, data is communicated from the PSR code process to the MPSR module.

#### **MPFR (Multi Plug Flow Reactor) Module**

Like the MPSR module, the MPFR module allows easy setup and execution of multiple cases. The public domain code SENKIN<sup>10</sup> integrates the set of stiff ordinary differential equations governing the initial value problem of "plug" or uniform flow with chemical reactions. A physical plug flow reactor (PFR) is a duct in which gas with uniform composition reacts as it flows with constant velocity. The inputs to SENKIN are similar to those of the PSR code, namely the initial gas composition, temperature, pressure, and length of the calculation. SENKIN allows several problem types: constant temperature and pressure, constant pressure and enthalpy, constant volume and enthalpy, and time varying temperature or volume. The last two are not supported in the present MPFR module. Again, the inputs to MPFR can be constant or variable. The MPFR module is completely analogous to the MPSR module discussed previously.

### **Data Storage and Interrogation**

Collection and organization of results from many hundreds of runs over a multidimensional parameter space is a central feature of the PSE, replacing a tedious and time-consuming task for the engineer. The outputs of the PSR and PFR codes are the chemical species concentrations (from dozens to possibly hundreds) and,

if not specified as an input, the gas temperature. All of the inputs specified in the MPSR or MPFR module must be stored as well. At the completion of each individual run within the MPSR or MPFR module, the results and inputs are stored in a relational database using the Microsoft SQL Server software.

Tools have been created within SCIRun to access the results of multiple runs using varying chemistry models. These tools use SCIRun's inherent visualization capabilities or give the user the option to output data in a form that can be exported to spreadsheets, plotting software, or other visualization packages. The SCIRun GUI for the database query module provides a simple and intuitive means of extracting a given dependent variable as a function of any 1, 2 or 3 independent variables. The information returned by the database is subsequently passed to downstream modules that allow the user to analyze and compare multiple data sets (norm calculations, differences etc.) or to visualize the information in x-y plots, 2D surface plots or as 3D scalar fields using cutting planes, isosurfaces and other sophisticated scientific visualization techniques.

Due to the large volume of data generated by the PSE, the use of a flat-file database structure was not a viable alternative for storage of results. Instead, we chose to design the PSE to work with a modern relational database. Such a database is capable of handling huge amounts of data, providing commit-or-rollback functionality, and the ability to manage information via the powerful SQL language. The relational database used for this project was Microsoft's SQL Server v7.0.

To communicate with the database, the ANSI standard SQL language was used. SQL statements handle all insertions, deletions and queries for the database. To execute the SQL statements on the database, we chose to use ODBC (Open Database Connectivity). This allowed us to build SQL statements inside of C++ (in SCIRun), and run them on the database.

Modules were created to store, retrieve, and analyze data. The `write_psr_db` and `write_pfr_db` modules store the case information for the PSR and PFR modules. The modules are designed to use ODBC to communicate with the relational database. This design allows the user to write to any database that provides an ODBC driver. For testing, a simple Microsoft Access database was used, but for actual operation, Microsoft SQL Server was used to provide more robust database capabilities. This design also allows for simple or more complex implementations, from a single machine using a single database file, to a cluster of machines from all over the world sending

information to a set of dedicated machines running a high performance database server. These database modules store all of the information for a set of cases, one case at a time. Data is stored as the cases are completed, allowing data visualization before all case sets are complete.

These two modules function in the same way. They both create the SQL commands to send to the ODBC driver for all of the data storage and querying operations. These SQL commands can be natively understood and executed by nearly all mid to high-end database servers. Special care was taken to carefully adhere to SQL standards to eliminate the possibility of using SQL server specific extensions to the SQL language that would limit the PSE to using a specific database implementation.

The `query_db` module is used to interrogate and extract information from the relational databases used by the PSE. This module allows a user to query the database to show stored case sets based on criteria such as the date of the run, the mechanism type of the run, problem type, etc. The case sets in the chosen database that match the search criteria are listed for the user. To view detailed information on a given case set, the user simply clicks on a case set name. Details of the case set are then displayed. This information includes case inputs and parameter space definition details. To extract a dataset from a case set, the user selects one, two or three independent variables, and then chooses the dependent variable of interest from a pop-up list. Upon execution of the module, the information is extracted.

The `diff` and `norm` modules are used to compare results from two different mechanisms. The `diff` module computes a straight difference by subtracting the data on one input port from the data on the other. It can also be configured to calculate the percent difference between incoming datasets. The user interface provides the ability to define which port is the base for this calculation.

The `norm` module computes the  $L_1$ ,  $L_2$ ,  $L_3$ , and  $L_\infty$  norms. These quantities are useful for quantifying the differences between detailed and reduced chemistry. The norms are calculated immediately following user selection, so once data has been received, the value is updated.

### **Parallel Computation**

The PSE performed well during trial runs on parallel SMP hardware. On a dual processor Intel machine, a test case using ~3000 PSR runs completed in 65% of the time required to run the same test case serially.

## **Integrated Mechanism Reduction and Testing**

The CARM module encapsulates the CARM software that generates reduced chemical kinetic mechanisms. As a stand-alone application, CARM is configured and run using command-line menus and manually entered data. The CARM SCIRun module removes these limitations, and allows CARM to be tightly integrated in a SCIRun dataflow network.

The CARM module was created by integrating the CARM source code (FORTRAN77) directly into a C++ SCIRun module. CARM was modified to allow the specification of input cases, number and choice of species retained in the reduced mechanism and specification of all configuration options via the SCIRun GUI and graphical programming connections.

The integration of the CARM software into the PSE allows the entire reduced mechanism creation and testing process to take place seamlessly within a single computing environment. The steps for creating and testing a reduced mechanism within the PSE created in Phase I are as follows:

- 1) Using the MPSR and/or MPFR module, select test problems (typically 5-15) to be run using a detailed kinetic mechanism. CARM reads the results of these test problems and attempts to tailor a reduced mechanism to these conditions.

- 2) Use CARM to create a reduced mechanism based on test problem results. The output of CARM is a FORTRAN routine specifying the species source terms as functions of the composition, temperature and pressure or density.

- 3) Again using the MPSR and/or MPFR module, select conditions for which detailed and reduced chemistry results will be compared. These test runs may cover the parameter space of interest much more extensively than did the problems input to CARM, numbering into the hundreds or thousands. The MPSR or MPFR module is connected to a module that writes results to a database.

- 4) Upon completion of the detailed and reduced chemistry runs, the module for querying the database is used to compare the results. The user may take advantage of any of the visualization and analysis tools described previously to gain insight into how well or poorly the reduced mechanism performs.

- 5) Using information gained in Step 4, the user may return to Step 1 and attempt to create an improved reduced mechanism. We plan to close this loop using automatic optimization techniques in future work.

The CARM PSE allows easy examination of how factors such as the number and choice of species retained in the reduced mechanism, the size of the original detailed mechanism, and the choice of input

test problems to CARM affect the range and validity of the reduced mechanism.

## **RESULTS**

This section describes the results of the methane/air combustion demonstration problems. Combustion of methane in air provides an excellent starting point for testing and demonstration of the capabilities of the CARM PSE. Methane, as the principal component of natural gas, is of practical and economic importance. The combustion kinetics of methane, among the simplest of hydrocarbon compounds, have been extensively studied and are in a high state of development compared to those of larger hydrocarbons. The detailed mechanism used for this demonstration is GRI3.0<sup>11</sup>, which contains 53 chemical species and 325 elementary reaction steps.

### **Variation of Three Parameters**

In this demonstration we compared results of the GRI3.0 mechanism with reduced mechanisms created by CARM in which 10 and 15 species are retained for calculation. The 10-species mechanism for methane-air combustion retains the species H<sub>2</sub>, H, O<sub>2</sub>, OH, H<sub>2</sub>O, CH<sub>4</sub>, CO, CO<sub>2</sub>, NO, and N<sub>2</sub> while approximating others with algebraic expressions. The 15-species mechanism includes the additional species CH<sub>2</sub>O, CH<sub>3</sub>, HCN, H<sub>2</sub>CO, and O. These reduced mechanisms were created using input adiabatic PSR cases with inlet temperature of 300 K, pressure of 1.0 atm., equivalence ratio,  $\phi = 1.0$  (stoichiometric conditions) and residence time,  $\tau$  ranging from 0.003 to 0.1 sec. In order to demonstrate the PSE's ability to visualize the comparison of reduced and detailed chemistry, especially reduced mechanism failures, we have compared the 10 and 15 species reduced mechanisms to detailed chemistry for significantly off-design conditions: pressures from 0.5-10 atm. and equivalence ratios from 0.5-2.0. The residence time was varied from 0.001 to 0.1 seconds. Five values of pressure, equivalence ratio, and residence time were selected for a total of 125 cases for each mechanism - 375 in all. Running and comparing this many cases without the PSE would not have been feasible.

Figure 1 shows calculated CO mole fraction in an adiabatic PSR for  $P = 1.0$  atm. as a function of equivalence ratio and residence time for detailed chemistry, and reduced mechanisms with 10 and 15 species. The detailed chemistry results generally show the expected trends of increasing CO with increasing equivalence ratio due to a shortage of O<sub>2</sub> for oxidation of CO to CO<sub>2</sub>, and increasing CO with decreasing residence time due to less time being available for

complete combustion. For the shortest residence time (0.001 sec.) and most fuel-rich ( $\phi = 2.0$ ) case the detailed chemistry model predicts blowout. This means the gas passes unreacted through the chamber and no CO formation is predicted. Prediction of the conditions under which blowout does or does not occur is a stringent test of a reduced mechanism.

It can be seen in Figure 1 that the 15-step reduced mechanism agrees qualitatively with detailed chemistry under all the conditions examined but under-predicts CO formation under rich conditions. The 10-species reduced mechanism behaves similarly, giving slightly larger errors and incorrectly predicting burning conditions rather than blowout at  $\phi = 1.5$ ,  $\tau = 0.001$ .

Figure 2 shows the reduced mechanism error, calculated as  $CO_{\text{detailed}} - CO_{\text{reduced}}$ , as a function of equivalence ratio and residence time for detailed chemistry and reduced mechanisms with 10 and 15 species. Note that in Figure 2 the equivalence ratio axis is reversed from that of Figure 1 to show important features of the solution. Both reduced mechanisms give almost no error for stoichiometric to lean conditions ( $\phi \leq 1.0$ ), with increasingly significant errors under fuel-rich conditions. The largest error occurs where the 10-step mechanism fails to predict PSR blowout. These errors are expected for reduced mechanisms designed to work at stoichiometric conditions.

Figure 3 again shows the CO mole fraction error, this time as functions of equivalence ratio and pressure for a fixed PSR residence time of 0.1 sec. Pressure does not have much effect on the validity of either reduced mechanism over the range tested. As before, increasing errors can be seen under fuel-rich conditions, with somewhat worse errors for the 10-species reduced mechanism.

These results demonstrate the ability of the PSE to provide insight into the range of validity of reduced mechanisms or other approximations over a parameter range of interest.

### **Variation of Two Parameters**

To further highlight the capability of the CARM PSE to run, organize, and compare large numbers of cases we have compared the same two reduced mechanisms for methane-air combustion to detailed chemistry in an adiabatic, atmospheric pressure PSR with a residence time of 0.01 sec. for 50 values each of the fuel-air equivalence ratio and PSR inlet temperature. Equivalence ratio was again varied from 0.5-2.0, while the inlet temperature was varied from 300-700 K. Thus, the total number of runs needed to compare detailed chemistry and the two reduced mechanisms was 7500 - far beyond what would have been thought of without the PSE.

Figure 4 shows detailed chemistry results for temperature and NO mole fraction. As expected, both temperature and NO are highest near stoichiometric conditions and for the highest inlet temperatures. Figure 5 shows the calculated temperature error ( $T_{\text{detailed}} - T_{\text{reduced}}$ ) for the 15- and 10-species reduced mechanisms. While both reduced mechanisms predict temperatures within a few degrees of the detailed calculation, the 15-species mechanism gives almost no error for equivalence ratios less than 1.5. Both reduced mechanisms significantly under-predict the temperature for the highest equivalence ratios and lowest inlet temperatures tested.

Figure 6 shows the difference in predictions of NO mole fraction between detailed chemistry and the two reduced mechanisms. Both reduced mechanisms show complex variations of agreement and disagreement, with the 15-species reduced mechanism performing significantly better over the entire parameter space.

Table 1 contains the error norms for temperature and NO mole fraction calculated for this case set. The improved performance of the 15-species mechanism is clearly demonstrated.

### **Reduction in Human Effort**

The CARM PSE has dramatically reduced the human effort needed to generate a high quality reduced mechanism. For example, to generate a reduced mechanism for methane/air combustion and test it over about 30 parameter combinations without the PSE would take about 3 days. With the PSE, this process would take about 1-2 hours. Testing the reduced mechanism over more than 3000 parameter combinations can be done in half a person-day or less, and 1 day of computer time. Smaller test case sets take proportionately less computer time.

Testing over only a few dozen parameter combinations is sufficient for some applications, but for reduced mechanisms to become reliable engineering tools, more thorough and rigorous testing such as is made possible by the CARM PSE is required. If a reduced mechanism compares well to detailed chemistry over a given parameter range in simple reactors like PSR's and PFR's it is reasonable to assume that it will perform similarly in a more complex calculation like a CFD code. The rigorous and thorough comparison of detailed and reduced chemistry made possible by the CARM PSE allows users of reduced mechanisms to have considerably more confidence in the results obtained.

## CONCLUSIONS

The CARM mechanism reduction code produces reduced chemistry approximations that work well under design conditions and often under off-design conditions. Reduced mechanisms produced using CARM and tested and validated using the PSE created in this project hold great promise for incorporating finite-rate kinetics into simulations of combustion processes that are economically and environmentally important. The databasing capability of the PSE allows the large amount of data generated by hundreds or thousands of runs to be efficiently organized, manipulated, and visualized. The CARM PSE gives the user the ability to rapidly determine the parameter ranges where chemical kinetics approximations work well and where they need improvement. This reduction in effort allows reduced chemical kinetic mechanisms produced by CARM or other chemistry approximations to be characterized and validated, compared to detailed chemistry, with greater thoroughness and rigor. The object-oriented software design methodology used by SCIRun resulted in a high level of code flexibility and reusability.

The extensive class libraries available within SCIRun were heavily used during this project. Of particular note were the OpenGL graphics abstract datatypes and the multiprocessing abstract types. The capabilities of the graphics types were leveraged to create powerful, state-of-the-art, customized visualization components. The capabilities of the multiprocessing types were used to create multiple threads required to maintain control over the FORTRAN software elements.

The computational PSE developed in this work significantly reduced the time and effort required to produce and evaluate reduced chemical kinetic mechanisms over large multidimensional parameter spaces.

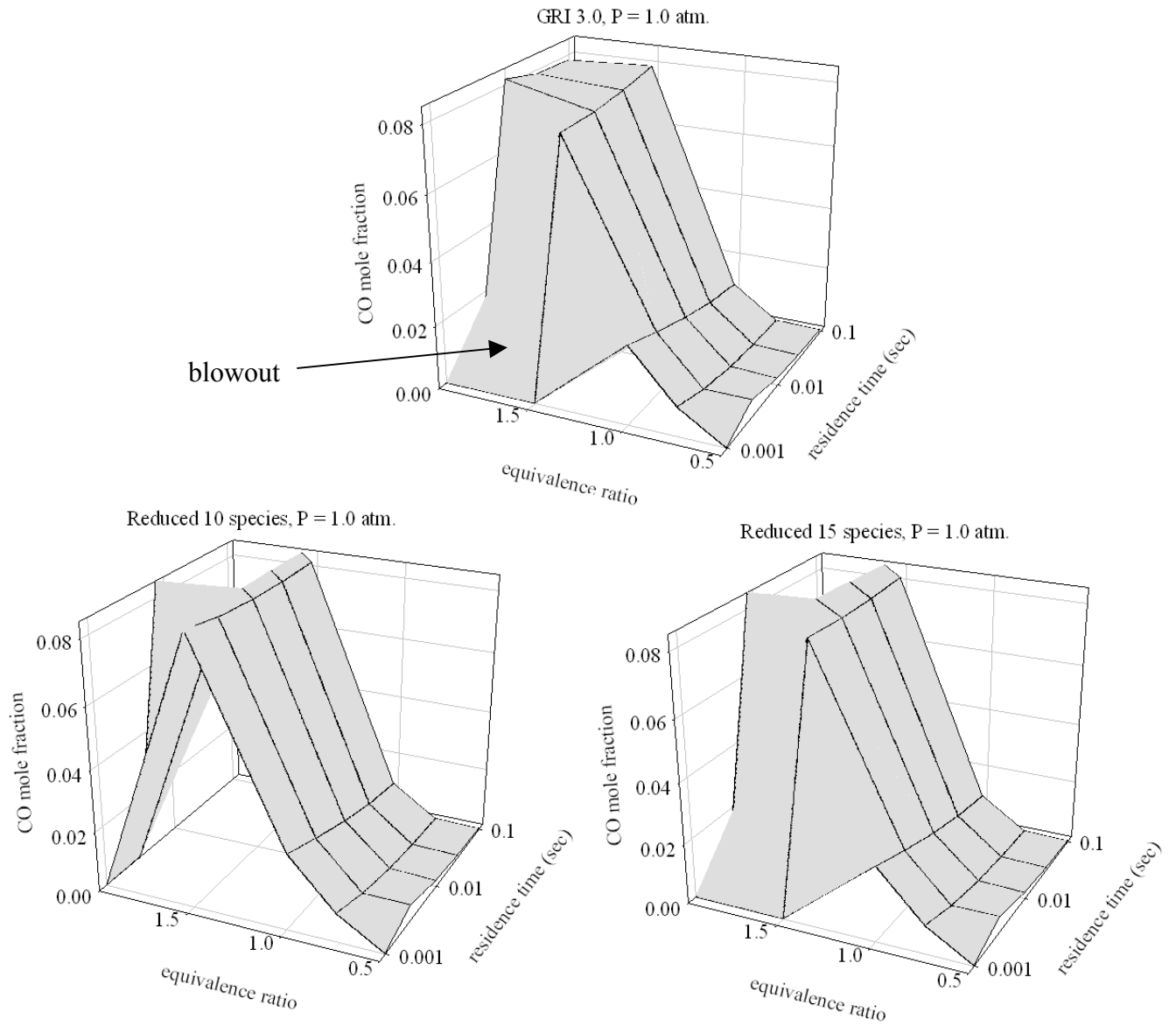
We have striven to create an extensible framework in this project. We believe that the CARM PSE strategy can be extended in a straightforward manner to incorporate reduced mechanism optimization as well as additional modeling capabilities.

## ACKNOWLEDGEMENTS

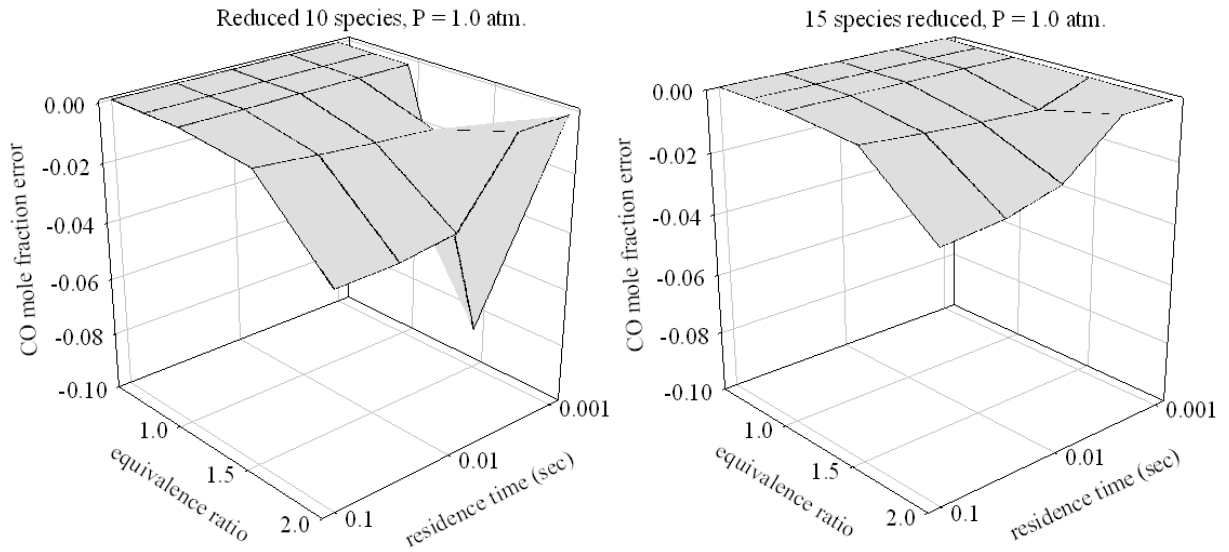
This work was supported by the National Science Foundation under SBIR grant no. DMI-9960841, Program Manager, Jean Bonney.

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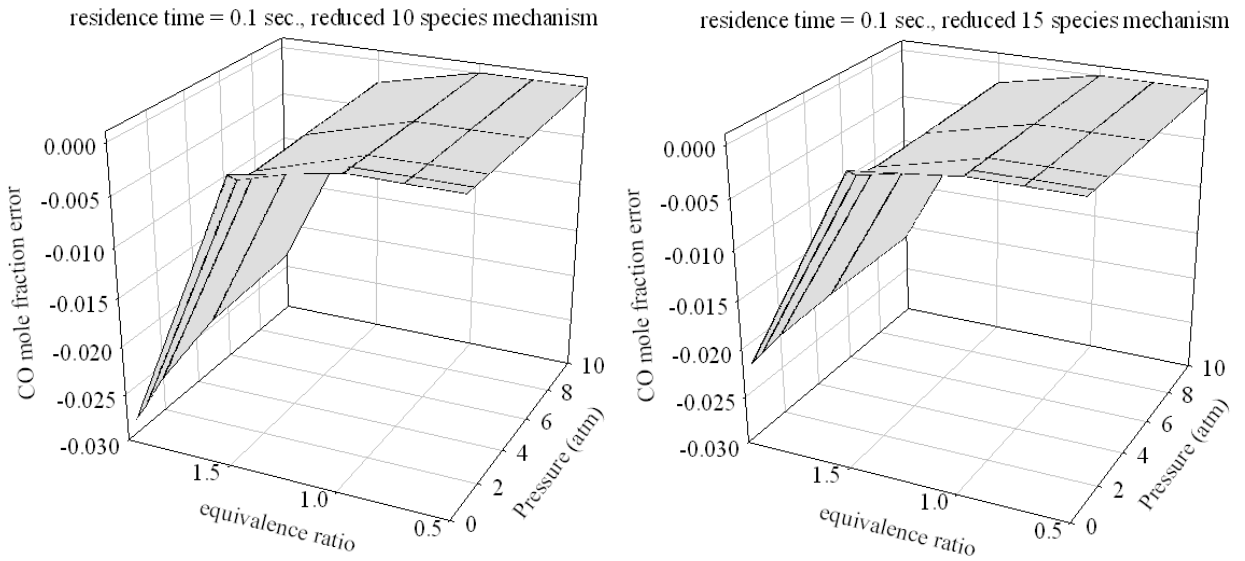
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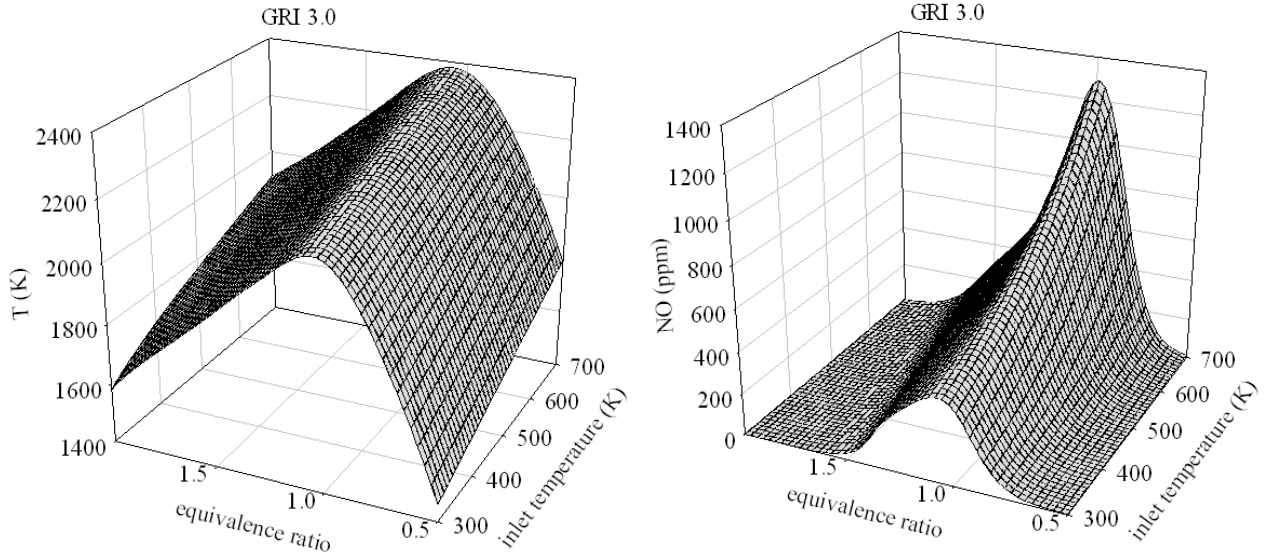
**Figure 1. Adiabatic PSR results for CO mole fraction for detailed and reduced chemistry.**



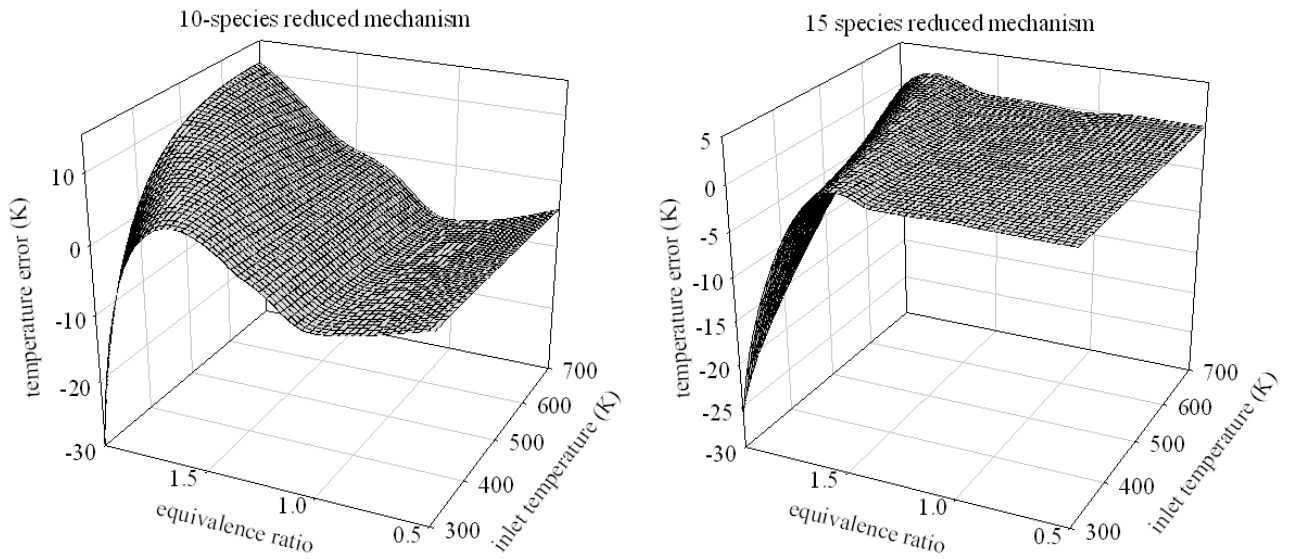
**Figure 2. Calculated CO mole fraction error for two reduced mechanisms as functions of equivalence ratio and residence time.  $P = 1.0$  atm.**



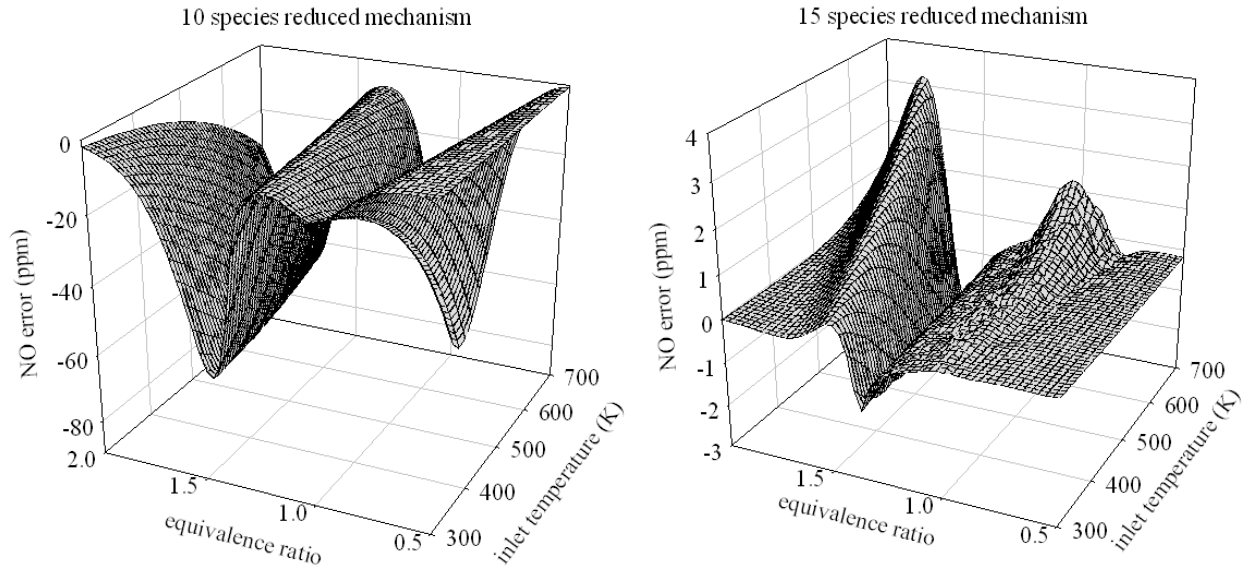
**Figure 3. Calculated CO mole fraction error for two reduced mechanisms as functions of equivalence ratio and pressure. Residence time = 0.1 sec.**



**Figure 4.** Calculated temperature and NO mole fraction for methane/air combustion in an adiabatic PSR,  $P = 1.0$  atm., residence time = 0.01 sec. using detailed chemistry.



**Figure 5.** Calculated temperature error for the 10- and 15-species reduced mechanisms for methane/air combustion in an adiabatic PSR,  $P = 1.0$  atm., residence time = 0.01 sec.



**Figure 6.** Calculated NO mole fraction error for the 10- and 15-species reduced mechanisms for methane/air combustion in an adiabatic PSR,  $P = 1.0$  atm., residence time = 0.01 sec.

**Table 1.** Error norms for temperature and NO mole fraction for the two-dimensional PSR case set.

Reduced Mechanism	Max $T$ error (K)	$L_1$ norm of $T$ error (K)	$L_2$ norm of $T$ error (K)	Max NO error (ppm)	$L_1$ norm of NO error (ppm)	$L_2$ norm of NO error (ppm)
10-species	29.7	1.26e+4	8.12e+4	81.5	5.76e+4	2.36e+6
15-species	26.3	2.88e+3	2.56e+4	3.21	1.37e+3	1.70e+3