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Department of Energy
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Germantown, MD 20874-1290
ATTN: Dr. Peter W. Lunn

Submitted by:

Mission Research Corporation
One Tara Blvd., Suite 302
Nashua, NH 03062

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Introduction:

The activities in this contract effort were aimed at developing sensitivity analysis techniques and "Fully Equivalent Operational Models" (FEOMs) for applications in the Department of Energy Atmospheric Chemistry Program (ACP). Accurate and reliable chemistry models are required to assess the effects of anthropogenic activities on the Earth's environment and to form a basis for informed regulatory actions. A potential impact of the current and projected anthropogenic activities is modification of the chemical trace-gas composition in the atmosphere, which determine the character of the environment. Trace gases are important due to their possible influence on processes such as UV shielding ozone and radiative forcing. Modifications to trace gas concentrations could result from significant exhaust emissions. The impact of such emissions are not currently well known, but the potential for important effects is large. Accurate and reliable three-dimensional (3-D) chemistry transport models (CTMs) are required for quantitative assessments. A significant bottleneck in the development of 3-D CTMs is the computational cost of detailed evaluation of the chemical evolution of the atmosphere. Integration of atmospheric chemical kinetics can take up to 90% of the total CPU time for current models. [Peters *et al.*, 1995; Sandilands and McConnel, 1997; and Sandu *et al.*, 1997] Furthermore, it is becoming ever more apparent that heterogeneous, aqueous phase, and non-methane hydrocarbon chemistry is important for evaluation of emission impacts. [Harrison *et al.* (1996); Ravishankara (1997); Finlayson-Pitts and Pitts (1997)] These factors increase the numbers of chemical species and reactions required in the models. Increased chemical complexity yields a slower CTM, at least to the extent that traditional chemical equation solution algorithms are used.

Empirical representations are one alternative to traditional chemical kinetic ODE (ordinary differential equation) solvers. These representations do not solve the chemical equations directly; rather, they rely on a pre-calculated knowledge database that describes a chemical model's input-output relationships. Via these quantitative input-output relationships, a representation of the model can be used directly to calculate species concentrations and related chemical properties from inputs that characterize an initial photochemical state. For example, a representation technique might take species concentrations at time t_1 and directly calculate concentrations at time t_2 based on functional input-output relationships. Evaluation can be extremely fast because often only a limited set of additions and multiplications need be used. In contrast, a traditional model would numerically integrate a series of differential equations, often taking many operationally complex steps to march forward from t_1 to t_2 . Output quality from different representation approaches can vary greatly depending on (a) the type of expansions used (exact model representations versus model approximations) and (b) the expansion-function evaluation methods used (explicit calculation of the functions versus evaluation through non-linear curve-fitting techniques).

In this contract effort, we have developed a new model representation algorithm that uses a hierarchical, correlated function expansion containing a finite number of terms [Shorter *et al.*, 1999]. A full expansion of this type is an exact representation of the original model and each of the expansion functions is explicitly calculated using the original model. After calculating the expansion functions, they are assembled into a Fully Equivalent Operational Model (FEOM) that can directly replace the original model. Reductions in computing time can be enormous. For

example, a diurnal chemistry model based on a Gear integrator was replaced by its FEOM equivalent for a factor of 10^4 reduction in computing time. Even with this dramatic acceleration factor, sufficient accuracy was maintained to achieve stable integration of the chemistry for a simulated period of over 30 years (see Figure 6 below). In a different application, the FEOM technique was applied to a two-stream radiation transfer model for atmospheric heating rate profiles. The resulting FEOM was $\sim 10^3$ times faster than the original model (Shorter et al., 1999).

The FEOM representation technique has several key features that make it a superior approach to increasing the efficiency of computations without degrading accuracy. Among them are:

- Exact representation of the original model
- Independent evaluation of the expansion functions due to orthogonality
- Explicit calculation of the expansion functions, thus eliminating fitting errors
- Rapid convergence behavior of the expansion
- Implicitly enforced conservation properties (e.g., mass conservation)

We have applied the FEOM technology to develop an ultra-fast atmospheric chemistry algorithm for the analysis of atmospheric chemistry issues under the DOE/ACP program. The FEOMs have been constructed using chemical mechanisms in coordination with the ACP program. Our research has provided DOE/ACP with ultra-fast FEOM chemistry solvers for inclusion in their core models. These FEOMs encapsulate complex tropospheric chemistry identified by the ACP science team.

In addition to the specific applications developed in this program, there are additional advantages of the FEOM technology. FEOMs could accelerate Global Circulation Models (GCMs) through accurate yet rapid calculations of radiation transfer and heating rates (c.f., Figure 7 below). With extremely fast chemistry and radiation transfer modules, development of computationally efficient integrated GCM-CTM may become feasible. Such development, however, was beyond the scope of the current effort.

Definition of the FEOM approach:

The integration of chemical kinetics is computationally very expensive and can take more than 90% of the CPU runtime of an atmospheric chemical transport model [Peters *et al.*, 1995; Sandilands and McConnel, 1997; and Sandu *et al.*, 1997]. There are a number of methods for solving the kinetic equations in atmospheric models. These include implicit numerical stiff ODE solvers, explicit solvers, and model representations. Tremendous effort has been expended to reduce the computational cost of solving chemical kinetics. Two types of approaches have been taken: (1) improving implicit and explicit ODE solving techniques to exploit some of the characteristics of chemical systems, such as sparse matrixes; (2) developing accurate representations that capture the input-output relationships of chemical mechanisms and use this information to rapidly predict the chemical evolution. The latter approach has the greatest potential for reducing the computational costs, since complex computations are not required. However, the level of accuracy required for stable chemical integration of kinetics is very high and puts very stringent requirements on prediction quality.

There are several approaches for model representations of a chemistry solver. Some of the more notable includes Spivakovsky *et al.* [1990] who used a curve fitting parameterization method to express the input-output chemical model response as an expansion function approximation; Turanyi [1994] who extended the approach of Spivakovsky *et al.* by converting the expansion functions into orthogonal functions, thus allowing easier independent evaluation; and Shorter *et al.* [1999], who use an *exact* finite order hierarchical function expansion that exploits the natural input parameter correlation to generate FEOMs.

The Fully Equivalent Operational Model (FEOM). A FEOM addresses the perceived difficult problem of mapping the input-output relationship behavior of complex systems. A traditional approach to mapping the behavior of a system with n input variables $x_1, \dots, x_n$ would consist of sampling each variable at s points to assemble an interpolated lookup table of computational effort s^n . Realistically one may expect s to be approximately 5 or 10 and n can be 10 - 10^2 or larger. Viewed from this perspective, attempts at creating a lookup table would be prohibitive. Furthermore, the interpolation for a point in n -dimensional space would be exceedingly difficult. However, this analysis implicitly assumes that all n variables are important and, most significantly, that there are correlations among variables to all orders (i.e., independently, in pairs, ..., up to all n variables acting in a tightly correlated fashion).

The fundamental principle underlying the FEOM representation is that output correlations between independent variables diminish very rapidly in a time sequence. This assertion does not eliminate strong variable dependence or even the possibility that all the variables are important. Various sources of information support this point. First, variables in most physical models enter as simple functions, often as additive sums of low-order multiplicative terms. This kinematic simplicity tends to survive in the output, although often scrambled in a complex fashion. Second, traditional statistical analyses of model behavior have revealed that a variance and covariance analysis of the output in relation to the input variables often adequately describes the physics (i.e., only low-order correlations describe the dynamics). Finally, these statements are also familiar from many-body physics where rarely do interactions higher than two-body play a significant role. These general observations lead to a dramatically reduced computational scaling when one seeks to map input-output relationships of complex systems. Considering this analysis, one may show that only power-law scaling in the number of variables suffices to learn the input-output behavior, such as $\sim n^l$. Here, l is the highest order of significant correlation and, typically $l \leq 3$ has been found to be quite adequate. Such polynomial growth poses a far more tractable algorithm than the often-accepted view of exponential growth (s^n) indicated above with traditional algorithms.

The approach to generating a FEOM is to first evaluate the input-output response of the model. This is achieved by performing a hierarchical, correlated function expansion on the model using a special mathematical structure and evaluating each term of the expansion independently. This expansion is then used as the FEOM. One may show that a function, $g(\mathbf{x}) \equiv g(x_1, x_2, \dots, x_n)$ can uniquely be decomposed into summands of different dimensions:

$$g(x_1, x_2, \dots, x_n) = f_0 + \sum_{i=1}^n f_i(x_i) + \sum_{1 \leq i < j \leq n} f_{ij}(x_i, x_j) + \dots + f_{1,2,3,\dots,n}(x_1, x_2, \dots, x_n) \quad (1)$$

where f_0 is a constant, $f_i(x_i)$ is a function of one variable x_i ; $f_{ij}(x_i, x_j)$ is a function of two variables, x_i, x_j ; and the higher dimensions follow until $f_{1,2,3,\dots,n}(x_1, x_2, x_3, \dots, x_n)$ which is a function of all the variables. The function $f_i(x_i)$ describes the independent action of the variable x_i on the output, while $f_{ij}(x_i, x_j)$ gives the pair-correlated impact on the output, etc. Finally the last term $f_{1,2,3,\dots,n}(x_1, x_2, x_3, \dots, x_n)$ contains any residual correlated behavior over all of the system parameters. It is important to note that this expansion is of finite order and is always an exact representation of the model output.

Since the change in many input variables, either independent or cooperative with other parameters, has little impact on the model output, the expansion functions that describe the negligible impact can be removed from the expansion. Their relative magnitudes identifies these functions. The ability to remove these functions comes from the special mathematical structure of the expansion and the function definitions that makes them orthogonal to all other functions. Most approaches which use empirical curve fitting techniques cannot remove functions, since the effects of all the input parameters impacts on the model output are mutually convolved and represented by a high dimensional function. The FEOM's ability to remove these functions is a key feature permitting the reduction in the runtime of the FEOM. Furthermore, this model representation makes interpolating between input parameter changes trivial since their impact is represented with low dimensional functions. Importantly, no constraining forms are applied to the expansion functions; they are numerically represented as an interpolative look-up table. Other attempts at casting analogous model look-up table replacements largely have not been successful as they have relied on fitting functions or complete sets of mathematical functions. The FEOM procedure introduces the critical component of hierarchical variable correlations in natural synchronization with system behavior, and then admits arbitrary correlated behavior. The individual functions are explicitly calculated by running the model a number of times with a series of judiciously chosen input sets. Special care is taken to ensure that the entire phase space of the model input is covered when generating the FEOM. The FEOM generation process is shown schematically in Figure 1.

Mass Conservation: An inherent property of a closed chemical system is conservation of mass. Although the chemical species can change in quantity, the total amount of each element must stay constant. This fact provides a very strong constraint on chemical solvers, which must be implicitly built into the chemistry FEOM. The orthogonal FEOM expansion functions are defined such that mass conservation is true for each expansion function. This property can be understood conceptually on the basis that each expansion function describes the impact on the output through set of coupled interactions over a fixed number of model variables (i.e., independent interactions, binary interactions, etc.). Thus, if an interaction produces a chemical species, that same interaction must also destroy species with the elements that form the new species. For example, an increase in NO concentration, in the example below, will increase the ClONO₂ concentration and also decrease the ClO concentration. This maintains the mass balance on the Cl atoms.

Prototype FEOMs:

Here we describe the application of the FEOM algorithm to two very different models of interest to DOE/ACP during our contract period - a chemistry solver and a radiation transfer model. The chemistry FEOM demonstrates the ability of this technique to generate a stable chemical solver. Although the example is for a stratospheric air parcel, the mechanism for developing a tropospheric FEOM is identical. The radiation transfer FEOM is described here to illustrate the breadth of the applicability of the FEOM algorithms. Furthermore, it shows that accurate radiative transfer calculations can be performed extremely fast. Thus, this technology can also be used for calculating photolysis rates for the CTM and heating rates for GCMs. However, these latter applications are beyond the scope of the contract effort.

Chemistry FEOM: A chemistry FEOM developed under this contract yields the rapid modeling of ozone and its related species. The FEOM “learned” the chemical evolution of a parcel at 20 km and 45 N latitude with a fixed input-output interval of 24 hours. The FEOM takes species concentrations at a known time t_i and predicts the concentration of ozone (and all additional species) at $t_{i+1} = t_i + 24$ hours. Then the FEOM can be reapplied using the concentrations predicted for t_{i+1} to obtain values for $t_{i+2} = t_i + 48$ hours. By repeated application of the FEOM, the chemical evolution over the course of several years can be evaluated. The chemical mechanism encapsulated in the FEOM contains 39 species and 106 reactions. The diurnal cycle was

approximated with a square wave and no chemical correlation assumptions were made. The FEOM application is shown schematically in Figure 2.

The input variables to the chemistry FEOM are the species concentrations at t_i , the length of daylight, temperature, and six radiation parameters for the photolysis rates. The input variable phase space was based on the extreme minimum and maximum values calculated in an annual cycle. To ensure that the input phase space would be appropriate for future applications of the FEOM, the minimum values for each variable were reduced by 50% and the maximum values were doubled. The FEOM outputs were the species concentrations at $t_i + 24$ hours.

The first and second order functions of Equation (1) were calculated for each of the output species. This was achieved by evaluating a number of input parameter sets with a Gear-based chemical integrator. There are 46 first order expansion functions for each output species. The 12 largest magnitude first order functions for ozone are shown in Figure 3. It is seen that while most of the functions are linear, several have curvature. This clearly demonstrates the importance of using a non-linear technique, as well as the benefit of numerically representing the functions.

First order expansion functions for predicting ozone

Figure 3. The numerical representation of the 12 largest magnitude first order expansion functions for the calculation of ozone. Each function represents the impact of a single input variable on the output ozone concentration. In the FEOM, values between the points are interpolated.

There are $N(N-1)/2$ second order functions, which are two dimensional surfaces, for each output species. This equates to 1035 functions in this 46 input variable problem. The four highest magnitude functions represent the synergistic impact on output ozone concentrations due to input changes in (1) ozone and water; (2) ozone and a photolysis parameter; (3) ozone and length of daylight; and (4) ozone and methane.

There are $N[(N-1)/2](N-2)/3$ third order functions, which are three dimensional surfaces, for each output species. This equates to 15180 functions in this 46 input parameter problem. The results presented here only contain first and second order expansion functions. However, preliminary work has shown that incorporation of a small number of selected third order terms further improves the output prediction quality.

Once all the zeroth, first, and second order functions in Equation 1 were calculated for each of the output species, a FEOM for each species was assembled from the functions. A substantial number of the first and second order functions were small in magnitude relative to f_0 . This is due to the lack of importance of particular parameters acting individually or cooperatively upon the final output. Since these functions would not significantly contribute to the final summation, they were removed from the FEOM expansion. Their removal leads to an overall increase in the FEOM prediction speed since fewer interpolations and additions are required. The number of first and second order terms retained for each output species are shown in Table I.

Table I. The number of first and second order terms that were retained for each output species. Note that all 39 species are calculated with the FEOM.

Species	# of 1 st Order Terms	# of 2 nd Order Terms	Species	# of 1 st Order Terms	# of 2 nd Order Terms
O	9	63	CH ₃ O	28	234
O(¹ D)	6	24	CH ₂ O	28	228
O ₂	1	0	HCO	29	256
O ₃	4	11	HOCl	31	304
NO	28	226	CH ₃ OO	30	301
NO ₂	27	211	H		
NO ₃	27	187	Cl	24	209
N ₂ O ₅	22	122	ClO	28	242
HNO ₃	17	60	HCl	14	76
N ₂ O	3	0	ClONO ₂	22	150
H	27	254	HO ₂ NO ₂	27	202
OH	27	212	CO ₂	1	0
HO ₂	28	226	BrO	30	220
H ₂ O	1	1	Br	31	232
H ₂ O ₂	28	224	HBr	27	270
H ₂	1	0	BrONO ₂	30	223
CH ₄	2	2	BrCl	34	333
CO	8	37	Cl ₂ O ₂	32	301
CH ₃	28	241	N ₂	1	0
CH ₃ O ₂	30	283	OCIO	34	339

The quality of the FEOM predictions was assessed with three methods (1) comparison with a Gear-based model calculated output for 1000 Monte Carlo generated input variable sets; (2) comparison of a Gear-based model to a sequentially applied FEOM for integration over a full year, and (3) comparing two multi-year FEOM runs in which one is a background calculation and the other is a perturbed calculation.

The Monte Carlo input sets for the 1000 runs were generated by randomly picking values for all 39 species, temperature, length of day light, and the six radiation parameters all over their respective annual variation range. (Note: This test did not explicitly build in the known atmospheric correlations between species concentrations and as a result is a very stringent test.) The quality metric was the standard deviation of the difference between the FEOM predictions and the Gear-based model-calculated output for the 1000 runs (Table II). The FEOM requires about 5×10^{-4} seconds to predict all 39 species concentrations while the Gear based model required 6 seconds. Thus the computational savings between the FEOM and the Gear based model is a factor of 10^4 .

The FEOM's ability to integrate chemistry in a stable manner was demonstrated by sequentially applying the FEOM and comparing the output to a Gear-based model. This involves initializing the FEOM at $t=0$ with parameter values consistent with January 1, and using the FEOM to predict all 39 species concentrations at $t=24$ hours (January 2), then reapplying the FEOM to the output predictions to once again predict the species concentrations at $t=48$ hours (January 3), and so on through time. Figure 4 shows 6 of the 39 output species concentrations predicted during the 360 sequential FEOM calculations covering one year, along with the six corresponding species output calculated with the Gear model. Each time, the previous output was used as input and the physical variables (temperature, daylight length, and photolysis rates) were updated to correspond to an annual cycle. It is anticipated that the inclusion of stabilization algorithms will improve the sequential prediction. This includes an error estimation capability that would call a chemical integrator if the estimated FEOM output error were too large for safe application.

Table II. The percent error of the FEOM predictions relative to model calculations for one 24 hour period. The FEOM used in this evaluation included first and second order expansion functions. It is expected that the addition of third order expansions will further improve the quality of the output.

Species	% Error in the Prediction
Ozone	0.001
NO ₂	1
ClONO ₂	0.2
NO	0.9
HNO ₃	0.05
N ₂ O ₅	3.0
BrONO ₂	0.06
BrO	0.4
ClO	1

Comparison of FEOM and Gear Output

Figure 4. Comparison of six species concentrations in a one year chemistry calculation with a Gear Based solver (blue) and a Chemistry FEOM (magenta). The FEOM calculation used 360 sequential 24 hour predictions and was constructed with first and second order expansion functions only. The deviation is due to accumulated error in the FEOM predictions. This can be corrected by the addition of third order terms. Preliminary results indicate that incorporating third order terms significantly reduce the deviations. Furthermore, since the FEOM is implicitly mass conserving, these initial deviations will not cause the system to “blow up”. This is demonstrated in Figure 5 with a 7 year simulation.

Two long-term FEOM integrations were performed to test the sensitivity of the differential equation solvers to small perturbations. The first run was a background case and the second was perturbed by adding a constant flux of NO_2 as a simple simulation for aircraft emissions. At the beginning of each simulated day, 1×10^6 molecules/ cm^3 of NO_2 , less than 1% of ambient, was added to the simulated "box". The ozone concentrations are plotted in Figure 5 for each run. It is clearly seen that the FEOM responded to the small perturbation in a regular and stable fashion.

A key requirement of chemical solvers is stability over very long time periods. The FEOM developed under this contract is stable and has been run to simulate a 30-year duration, shown in Figure 6. This required 10,800 re-applications of the FEOM. The FEOM output concentrations of O_3 , NO_2 and N_2O are shown in Figure 6. The steady decrease in N_2O is due to its photolysis and the lack of replenishment in the box model. The increase in NO_2 occurs due to the NO_y production from the N_2O photolysis. The change in the O_3 is in response to the NO_2 variations. This NO_x source is about five times the external NO_2 flux.

Figure 5. Comparison of chemistry FEOM predictions for an unperturbed (red solid line) and perturbed (blue dashed line) air parcels. The perturbation was a constant flux of 1×10^6 molecules $\text{cm}^{-3} \text{ day}^{-1}$ of NO_2 (over one day, less than 1% of the ambient NO_2 concentration). This demonstrates the chemistry FEOM ability to (a) respond to small chemical perturbations and (b) integrate chemistry in a stable manner for long periods of time.

Figure 6. Output for a 30-year simulation using the FEOM chemical solver. The FEOM was re-applied 10,800 times to achieve the temporal range. This demonstrates both the accuracy and the stability of the FEOM solver and the approach in general.

Radiative Transfer FEOM: A second illustration of FEOM for radiative transfer further demonstrates the FEOM capabilities. The calculation of radiative transfer in atmospheric mass transport models is computationally very intense. Radiative transfer modules (RTM) are used to calculate altitude dependent photolysis rates and atmospheric heating rates (HR) due to absorption and emission of light. The HR is used by other modules to calculate atmospheric temperature profiles and atmospheric dynamics. Here we present our results of an ultra-fast FEOM for directly calculating atmospheric heating rates.

The evolution of atmospheric dynamics is very sensitive to the atmospheric heating rate profiles. As such, a first-principles approach has historically been used. This involves separating the radiation into many different wavelength bands, calculating wavelength-dependent absorption coefficients for each trace gas absorber, and coupling the downward and upward radiation fluxes. As a result, RTMs are computationally very intensive. The two-stream model used to generate the FEOM calculates radiative fluxes in eight optical bands covering both the short and long wave regions. Each band can be segmented into 5 sub-bands. The fast exponential sum-fitting technique [Ritter and Geleyn, 1992] was used to combine the effects from multiple gases (H_2O , O_3 , and CO_2). The atmospheric trace gas concentrations were either prescribed by McLatchy soundings (O_3 and CO_2) or varied as input parameters (H_2O). The heating rate was determined by the difference in the flux into and out of each level. This FEOM was developed for clear air.

The input to the FEOM consists of the water and air temperature profiles, the surface temperature, and the surface albedo. The output is the heating rate at each of the 30 atmospheric layers. This is shown schematically in Figure 7. The H_2O and air temperature profiles are represented as deviations from a reference mid-latitude summer profile. The profiles are broken into 30 discrete layers spaced 0.67 km apart and span an altitude from 0 to 20 km. In each layer, the H_2O value can vary from 10% to 160% of the reference value. The temperature can vary from 90% to 110% of the reference values. We emphasize that the H_2O and temperature values in each layer are treated independently from all other layers and thus the profiles can be very structured. The surface temperature can vary from -8 to 50°C and the surface albedo can vary from 0 to 1.0. Table III summarizes the description of the parameters as well as the minimum and maximum variation.

The RTM calculates the altitude-dependent atmospheric heating rate in degrees per second. The heating rate can be either positive, indicating that the atmospheric layer is absorbing more energy than it is emitting, or negative, indicating more optical emission than absorption. The values are typically in the range $\pm 4 \times 10^{-5}$ K/sec (± 3.5 K/day).

Table III. List of Input Parameters for the FEOM.

<i>Parameter</i>	<i>Description</i>	<i>Minimum</i>	<i>Maximum</i>
1-30	H_2O for Level 1 to 30	0.1 x ref	1.6 x ref
31-60	Air Temperature for Level 1 to 30	0.9 x ref	1.1 x ref
61	Surface Temperature (°C)	-8	50
62	Surface Albedo	0.0	1.0

The FEOM actually consists of a set of sub-FEOMs. Each sub-FEOM predicts the heating rate for a specified atmospheric layer. Although each sub-FEOM only predicts the heating rate for a specified layer, it uses information from all other layers to make the prediction. This information is contained in the input variables: 30 H₂O values (one for each layer), 30 air temperatures (one for each layer), the surface temperature, and the surface albedo.

For each of the sub-FEOMs, the first and second order expansion functions (Equation 1) were calculated. There are one zeroth order term (e.g., determined by a run with the nominal values of the model), 62 first order term, and 1891 second order terms. This is a total of 1954 functions for each sub-FEOM, which equates to 58,620 functions for all levels, although most of them are not significant. After calculating and evaluating all first and second order functions, only 304 first order functions and 138 second order functions for *all 30 sub-FEOMS* were found to be important. ***That is only 0.8% of all the functions!***

The completed FEOM was evaluated for prediction accuracy and runtime relative to the original two-stream RTM. The evaluation was performed by running both models over a range of input conditions and comparing output results and the time required to attain the results. The input sets were generated using Monte Carlo methods such that each input variable was assigned a random value within its phase space. This procedure produced very structured H₂O and temperature profiles and provided a rigorous test of the FEOM algorithm. Three sample H₂O and temperature profiles and their resulting heating rates are shown in Figure 8. The FEOM prediction agrees well

Figure 8. Input H₂O and temperature profiles from three of the Monte Carlo - generated input sets (left) and the corresponding heating rate (right) calculated with the RTM (lines) and the FEOM (symbols).

with the model output. A quantitative assessment of the FEOM accuracy was calculated as the root mean square average of the absolute difference between the two-stream RTM-calculated heating rate and the FEOM-predicted heating rate for all 1000 input sets. This was performed for each atmospheric layer represented in the model. *The largest magnitude RMS error at any altitude was 4% of the RMS output value.*

The runtime was assessed by observing the execution time for the RTM and FEOM calculations over 1000 input sets. The RTM required 0.48 seconds per calculation while the FEOM required only 0.11 milliseconds per calculation. *Thus the FEOM provides heating rate predictions 10^3 times faster than the two-stream RTM with comparable output fidelity.* This work clearly demonstrates the ability to accurately represent a radiate transfer model with a FEOM.

Conclusion: The work performed under this contract clearly shows the value of the FEOM approach to large-scale calculations of atmospheric chemical dynamics and radiative transfer. We have published several papers under this contractual effort, which are appended to this report.

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**APPENDIX – COPIES OF REPORTS AND PAPERS PUBLISHED UNDER THIS
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