Geoscientific Model Development Discussions

Implementation of the chemistry module MECCA (v2.5) in the modal aerosol version of the Community Atmosphere Model component (v3.6.33) of the Community Earth System Model

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Implementation of the chemistry module MECCA (v2.5)

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Abstract

A coupled atmospheric chemistry and climate system model was developed using the modal aerosol version of the National Center for Atmospheric Research Community Atmosphere Model (modal-CAM) and the Max Planck Institute for Chemistry's Module Efficiently Calculating the Chemistry of the Atmosphere (MECCA) to provide enhanced resolution of multiphase processes, particularly those involving inorganic halogens, and associated impacts on atmospheric composition and climate. Three Rosenbrock solvers (Ros-2, Ros-3, RODAS-3) were tested in conjunction with the basic load balancing options available to modal CAM (1) to establish an optimal configuration of the implicitly-solved multiphase chemistry module that maximizes both computational speed and repeatability of Ros-2 and RODAS-3 results versus Ros-3, and (2) to identify potential implementation strategies for future versions of this and similar coupled systems. RODAS-3 was faster than Ros-2 and Ros-3 with good reproduction of Ros-3 results, while Ros-2 was both slower and substantially less reproducible relative to Ros-3 results. Modal-CAM with MECCA chemistry was a factor of 15 slower than modal-CAM using standard chemistry. MECCA chemistry integration times demonstrated a systematic frequency distribution for all three solvers, and revealed that the change in run-time performance was due to a change in the frequency distribution chemical integration times; the peak frequency was similar for all solvers. This suggests that efficient chemistry-focused load-balancing schemes can be developed that rely on the parameters of this frequency distribution.

1 Introduction

The spatial and temporal resolutions of geophysical modeling systems used to diagnose impacts of anthropogenic perturbations are increasing rapidly. As a result, the need to more explicitly resolve many of the physical and chemical processes that previously operated below the resolution and within the uncertainty ranges of these

modeling systems is increasing accordingly. Individually, the computational skill of physical and chemical systems is high. But, the computational needs of these systems in combination with dynamical and geophysical models has made coupled investigations prohibitive. The capabilities of current high-performance computing platforms available to geoscientific modeling are beginning to permit the coupling of these systems for scientific research. Of particular interest are the interactions between atmospheric chemistry and climate, particularly with respect to multiphase processes and their interactions with tropospheric composition, clouds, precipitation, and radiative transfer.

Multiphase interactions, primarily between gases, aerosols and cloud droplets, represent a highly non-linear set of processes that significantly impact the processing and lifetimes of many important tropospheric species. Of increasing interest are chemical transformations involving inorganic, halogenated (Cl and Br) compounds and associated influences on the cycling of NO_x, HO_x, sulfur, O_3, CH_4 and non-methane hydrocarbons, Hg, and other compounds of both natural and anthropogenic origin.

Accurately resolving interactions that control multiphase processes requires they be dealt with explicitly. The computationally difficult solution of the stiff system of ordinary differential equations (ODEs) derives from multiphase processes (e.g. mass transfer). Computational speed must be optimized in order to execute simulations of sufficient duration to provide time for model equilibration (spin-up) and generation of a sufficient sample size for analysis.

This manuscript outlines a coupled atmospheric chemistry and climate modeling system that leverages an efficient multiphase atmospheric chemistry mechanism, MECCA (Module Efficiently Calculating the Chemistry of the Atmosphere; version 2.5; Sander et al., 2005, 2011) within a 3-mode size-resolving aerosol module (Modal Aerosol Module) version of the National Center for Atmospheric Research's (NCAR) Community Atmosphere Model (version 3.6.33; Gent et al., 2009; Liu et al., 2011; hereafter referred to as modal-CAM). Modal-CAM is embedded as the atmosphere component of the NCAR Community Climate System Model (CCSM3.0; Collins et al., 2006). (Note:

Since completion of the work presented here, CCSM has been renamed the Community Earth System Model, CESM). The coupled modeling system was designed to investigate the role of aqueous processes and inorganic halogen cycling through use of their explicit representation in MECCA combined with the size-resolving modal aerosol

5 physics and atmospheric coupling of modal-CAM. Chemistry and climate results will be validated and interpreted in detail in forthcoming manuscripts.

2 MECCA model description

MECCA version 2.5 contains a comprehensive atmospheric reaction mechanism that includes transformations involving O_3, CH_4, HO_x, and NO_x, non-methane hydrocar-

10 bons (NMHCs), halogens (Cl, Br, I), and sulfur. In addition to gas-phase reactions, the scheme includes fully integrated multiphase transformations (both aqueous-phase and heterogeneous pathways) involving aerosols and cloud droplets. Mass transfer is calculated dynamically per Schwartz (1986). Photochemical reaction rates vary as a function of solar zenith angle under clear-sky and cloudy conditions based on Land-

15 graf and Crutzen (1998). See Table S1 in the Supplement for a complete description of the chemical scheme. Also see Sander et al. (2011) for a complete description of the MECCA system.

MECCA uses the Kinetics PreProcessor (KPP, Sandu and Sander, 2006) to build a solution based on a choice of several predefined numerical methods. KPP was de-

20 signed to facilitate programming fast and accurate solutions to chemical reaction mechanisms based on user-defined implicit solvers and solver configurations. It relies on sparse linear algebra routines to optimize serial computational performance, and is therefore well suited for atmospheric chemistry problems over a wide range of complexities.

25 The tropospheric chemical mechanism used in the coupled model was based on a subset of the full MECCA mechanism. Other than the addition of gas-phase reactions for non-methane hydrocarbons (NMHCs; based on von Kuhlmann et al., 2003),

the mechanism was identical to that used in Keene et al. (2009) configured for three aerosol size bins. Photochemical rates were calculated using MECCA's JVAL sub-model.

3 Modal-CAM atmosphere model

Atmospheric processes were simulated in 3 dimensions using CAM at 1.9° × 2.5° lat-long resolution with 26 vertical levels (Gent et al., 2009). CAM is built upon an extensive set of high-performance computational routines to preserve scalability and performance of the model across changes in resolution and model physics. The high-performance structure relies upon message passing interface (MPI), or, at the user's discretion, a combination of MPI and shared-memory process routines.

The dynamical core (approximation of the equations of motion on a discrete, spherical grid) is based on a flux-form semi-Lagrangian method (see Lin and Rood, 1996) that is better suited for tracer transport. This permits grid-wide stability of the chemistry solution, in contrast to discrete methods that introduce large dispersion and diffusion errors in their approximation of the equations of motion which propagate into and destabilize the chemistry solver.

Modal-CAM incorporates a comprehensive set of processes that control the evolution and coupling of three fixed-width log-normally distributed aerosol modes (Aitken, accumulation and coarse). The modal aerosol treatment is described in detail in Liu et al. (2011). Each mode consists of internally mixed populations of non-sea-salt (nss) SO_4, organic matter from primary sources (OM), secondary organic aerosol (SOA) from volatile organic precursors, black carbon (BC), inorganic sea salt, and mineral dust. The nss-SO_4 is assumed to be in the form of NH_4HSO_4. OM and BC are only treated in the accumulation mode. SOA is only in the Aitken and accumulation modes, and mineral dust is only in the accumulation and coarse modes. Aerosol number and aerosol water are also calculated for each mode. Aerosol mass and number associated with stratiform cloud droplets are treated explicitly.

The following processes affect aerosols in the model: Grid-resolved transport, sub-grid vertical transport by turbulence and convective clouds, emissions (surface and elevated), sedimentation and dry deposition, activation and resuspension, wet removal (in- and below-cloud by stratiform and convective clouds), condensation of $H_2SO_4(g)$ and condensation/evaporation of semi-volatile organics and water, cloud chemistry (which produces sulfate in cloud droplets), transfer (renaming) of particles from Aitken to accumulation mode due to condensation and cloud chemistry, aerosol nucleation, and aerosol coagulation (Aitken and accumulation modes only). Trace gas processes include transport, emission, and dry and wet deposition.

4   MECCA/Modal-CAM coupling

The coupling involves (1) adding MECCA chemical species to CAM, (2) interfacing MECCA gas, aerosol and cloud chemistry routines within CAM (and disabling the corresponding CAM routines), and (3) as needed, modifications to CAM routines for processes that affect MECCA and modal-CAM species (e.g. emission of sea-salt species). This initial implementation is not a complete two-way coupling between MECCA and modal-CAM (some MECCA aerosol species do not influence all of the modal-CAM physics). This was done to minimize unnecessary modifications to processes that have little impact from one system to another.

The coupling interfaces bulk inorganic aerosol species in modal-CAM for microphysical routines and accurate speciation in MECCA necessary to constrain the multiphase chemistry. Sea salt (NaCl) in modal-CAM was speciated as Na^+, Cl^-, SO_4^{2-}, CO_3^{2-}, and Br^- in MECCA. SO_4 in modal-CAM was speciated as $H_2SO_4(aq)$, HSO_4^-, and SO_4^{2-} in MECCA. Online tropospheric O_3 calculated by MECCA was used in CAM's radiation routines. Total overhead stratospheric O_3 necessary for photochemical rate calculations was prescribed.

All chemical species in MECCA were added as dynamically-active trace species in CAM and, thus, were included in aerosol and cloud-water composition and affected

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by advection, turbulent diffusion, transport, dry deposition, wet removal, and emissions (species specific). For the 3-mode chemical mechanism, 189 MECCA-specific chemical species (96 gas, 31 per aqueous mode), and 16 CAM-specific species were included as dynamically-enabled tracers (aerosol liquid water was shared between CAM and MECCA). Since impacts on aerosol physical properties due to small changes in abundance of inorganic aerosol species other than Na^+, NO_3^-, NH_4^+ and SO_4^{2-} are limited, and to simplify the modal-CAM aerosol size and inter-modal exchange routines, mass and density of any species specific to MECCA only were not considered in calculations of particle mass and size (i.e. density of aged and fresh sea salt are the same). As a result, they only interacted with particle dry diameter through changes in $nss-SO_4$, NH_4^+, and NO_3^-. As well, hygroscopicity and refractive index values of aerosol species were controlled by bulk NaCl, NH_4^+, NO_3^- and $nss-SO_4$ in modal-CAM. NH_4^+ and NO_3^- are only considered in 7-mode modal-CAM bulk speciation scheme. Aerosol and cloud droplet liquid water in MECCA was coupled directly to that calculated by modal-CAM's water uptake routine. To ensure that sea-salt sulfate in MECCA was not included in the modal-CAM $nss-SO_4$ bulk species, only the net change in SO_4 due to MECCA chemistry ($\Delta SO_{4,Chemistry}$) was considered where

$$nss\text{-}SO_4(t + \Delta t) = nss\text{-}SO_4(t) + \Delta SO_{4,Chemistry} \tag{1}$$

Cloud properties (cloud fraction, liquid water, and droplet number) were controlled by modal-CAM routines, and cloud chemistry was only activated above a grid-box cloud-fraction threshold of 1×10^{-5}. Since the system uses redundant chemical species, it was necessary to ensure the impact of emissions, scavenging, and deposition on both the bulk (e.g. NaCl in modal-CAM), and analog species (e.g. Na^+ and Cl^- in MECCA) are proportional. Modal-CAM stores information about both sets of species throughout a timestep, and changes are updated accordingly – either from MECCA to CAM or CAM to MECCA.

Since mass-transfer from the gas to aqueous phase is included in the MECCA chemical ODE, modal-CAM gas-aerosol exchange and condensation routines are switched

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off. Mass and particle size calculations were controlled by modal-CAM. With the exception of that involving SOA, all gas-aerosol exchange was calculated by MECCA. Nss-SO_4 for each mode, H_2SO_4 vapor, and corresponding net changes per timestep were calculated by MECCA and passed to modal-CAM for calculation of nucleation and Aitken-to-accumulation mode transfer. Since the only new source of nss-SO_4^{2-} in the modal aerosol routines was through nucleation of $H_2SO_4(g)$, any addition (or loss) of nss-SO_4^{2-} due to modal aerosol processing was passed to MECCA as addition (or loss) of $H_2SO_4$to (from) each phase. In this configuration, both total nss-SO_4^{2-} and $[H^+]$ are conserved.

Emissions of sea-salt constituents (Cl^-, Br^-, SO_4^{2-}, and HCO_3^-) were calculated within CAM's emission routine proportional to the sea-salt particle number emissions based on the inorganic composition of bulk seawater. All aerosol species in MECCA were coupled to CAM's dry and wet deposition and scavenging. Ion balance is maintained in MECCA by adjusting an inert dummy cation tracer representing the combined charges of Na^+, Ca^+, and Mg^+, which was not coupled to modal-CAM NaCl mass.

5 Computational configuration and performance

In a global simulation grid that includes the breadth of atmospheric chemical scenarios at any one time-point in the simulation, the use of implicit methods for the multiphase chemistry solution disrupts the scalability of the MPI-based parallel system. In particular, the stiffness of the chemical mechanism, and thus the time and resources needed to reach a solution for a given grid-box, varies geographically in the 3-D domain (e.g., see Fig. 2 of Kerkweg et al., 2007). Proximity to large sources and sinks of highly-reactive species or large gradients in physical or chemical conditions complicate the implicit solution. In CAM, systematic, non-random decomposition and allocation of column-subsets of the 3-D grid to the available computational processes segregates a disproportionately large chemical-solution burden into a small subset of processes. Since CAM's time-stepping routines rely on an MPI AllGather routine,

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model performance is limited by the speed of the slowest column-subset. Model load-balancing optimizations (available since CAM version 3.6) permit the building of MPI column-subsets and allocating them to processes in ways which enhances the distribution of "difficult" columns across available computational process units (see Mirin and Worley, 2011). The option used for this study (phys_loadbalance = 2) builds column-subsets from north/day-south/night grid-point pairs. For example, a grid-point at 45° N, 0° E is paired with the point at 45° S and 180° E. Consequently, since most land area is in the northern hemisphere, this procedure load-balances based across day/night, season, and, to a large extent land/ocean. The set of paired points are then combined into column-subsets and assigned to processes. The maximum number of column-subsets that can be obtained (thus, the number of independent computational processes that can be used simultaneously) is controlled by dynamic limitations and the horizontal grid size. CAM has been designed to permit allocating additional processes to solve model physics separately from the dynamics routines, which allows a much faster computation of the coupled system.

To test the computational performance of the coupled system, decomposed as described, three positive-definite, adjustable-timestep Rosenbrock methods were tested for accuracy and performance metrics. Sander et al. (2005) found that 2nd and 3rd order solvers performed best in terms of both stability and computational speed. For stability reasons, the Ros-3 (3-stage, order 3(2), L-stable) solver was employed preferentially in past MECCA simulations (e.g. Keene et al., 2009). As such, for these tests, coupled simulation results using Ros-3 are considered the benchmark against which results using Ros-2 (2-stage, order 2(1), L-stable) and RODAS-3 (4-stage, order 3(2), stiffly accurate) solvers are compared (see Hairer and Wanner, 1991). The coupled system was run at 1.9×2.5 degree lat/lon resolution for 5 years with the Ros-3 solver to stabilize chemistry in the troposphere – defined as a net change in year-to-year total global O_3 mass of less than 1 % (actual net O_3 change between years 4 and 5 was 0.16 % versus 4.7 % between years 3 and 4 of the equilibration period). One-month (January) simulations were then executed using the three solvers. Ros-2

and RODAS-3 were compared to Ros-3 for computational speed and reproducibility of several species. Absolute and relative tolerances were set to $10\,cm^{-3}$ and 0.01, respectively.

Figure 1 compares mass mixing ratio results of the one-month benchmark for O_3, OH, Br_2, and coarse-mode aqueous H^+ for all model layers between the surface and 900 mb. These species were selected to reflect climate relevance, source of stiffness, halogen cycle reproducibility, and relevant aqueous processes. Regression statistics are given in Table 1. Ros-2 is able to reproduce O_3 and OH with reasonable confidence, whereas Br_2 and to a much greater extent, H^+ were less precisely reproduced. The reason for the systematic over-prediction of H^+ by Ros-2 is not clear, but may reflect stiffness associated with the aqueous (acid-base) reactions and mass transfer. Conversely, results based on RODAS-3 were more similar to those based on Ros-3 in terms of both absolute (regression slope near 1) and relative differences (higher correlation coefficient; Table 1). The H^+ root mean square error (RMSE; normalized against mean Ros-3 mixing ratios) was still high for the RODAS-3 results. The scatter at higher H^+ mixing ratios generally corresponded to continental regions where sources of atmospheric acids are relatively greater and sea-salt Cl^- and associated regulation of aerosol acidity via HCl phase partitioning is relatively less important. H^+ is highly sensitive to changes in chemistry and circulation in these regions. Circulation changes may also be reflected in the other species due to radiative forcing by O_3 over the benchmark time period. The comparisons demonstrate that RODAS-3 performs markedly better than Ros-2 for all four species.

Completion of the one-month benchmark simulation with RODAS-3 was 9 % faster than Ros-3, and Ros-2 was 18 % slower. This is in agreement with a study of KPP solvers in the GEOS-Chem chemistry transport model (Eller et al., 2008; Henze, 2007), though GEOS-Chem uses KPP for gas-phase only calculations and is driven by offline circulation. The frequency distributions of average integration times (or waiting-time for completion of one chemistry timestep) for all grid cells varied among the solvers tested (Fig. 2). Relative to RODAS-3, Ros-2 and, to a lesser extent, Ros-3 were skewed

towards relatively longer integration times, though there was no systematic change in the peak integration time frequency. These results indicate that the performance gain is due primarily to reduction in frequency of large waiting times and suggest that chemistry-centric grid decomposition and column subsetting that leverages this fre-
5 quency distribution may yield better model performance. The distribution of waiting times across the global grid demonstrates a physical dependence. While not shown here, chemistry waiting times are inversely dependent upon altitude – the maxima occur in the model surface layer. Further, data show a weak but positive correlation to a combination of total aerosol liquid water and solar zenith angle (as a measure of pho-
10 tochemistry). Based on the benchmark simulation intercomparison, MECCA chemistry for the fully-coupled simulations was solved using the RODAS-3 solver.

MECCA, as the chemical operator in CAM, had a substantial impact on model runtime prohibiting the use of this configuration for long-term (century-scale) simulations without a large cost in computational resources. Incorporation of the MECCA species
15 and chemistry routines increased CAM's runtime by a factor of 15 relative to modal-CAM configured with the standard chemical module. Replacing modal-CAM's chemical module with MECCA chemistry slowed overall computational speed by a factor of 8. The transport routines were a factor of 7 slower due to an increase from 25 to 205 active tracers. Further, the data storage needs of a system this extensive were
20 large enough that considerations of I/O (Input/Output) frequency and number of diagnostic quantities was necessary. Monthly-mean output from a 10-yr simulation of the coupled system required nearly 850 GB storage, which added an additional computational burden due to the system I/O. I/O is often limiting factor in high-performance system scalability, though it was not a large factor in this system.

6   Summary

A coupled atmospheric chemistry and climate system model was developed to investigate the details of multiphase processes and associated impacts on chemistry and

climate. The computational needs of the chemical system required that performance of individual modules be enhanced. Comparison of three implicit Rosenbrock solvers revealed substantial differences in computational performance for coupled simulations that were distinct from similar investigations based on boxmodels alone. This is likely due to the effect of fixed versus variable physical conditions in 0-D versus 3-D global models, combined with the impact of load balancing methods on the net system runtime (solver performance in individual gridboxes was not evaluated). Overall the RODAS-3 solver provided the best performance for the current computational configuration.

In addition to optimizations discussed above, such as chemistry-centric load-balancing, several strategies can be pursued to further increase the coupled system's performance. First, chemical species with atmospheric lifetimes smaller than a residence-time in a given grid box (so called short-lived species such as $O(_1D)$) can be ignored by the dynamics routines. Prior to including MECCA into CAM for this study, the cost of including additional tracers was the largest factor impacting the system's computational burden. Second, reduction of the size of the chemical mechanism in combination with load-balancing will likely have the greatest impact on runtime. A systematic approach to determining the smallest mechanism necessary to constrain the behavior of a specific subset of chemical species (e.g. O_3 and sulfur) is currently being developed using this system. Lastly, the adoption of optimized or parallel-capable linear algebra routines has the potential to significantly speed up the implicit chemistry, but we are not aware of any successful studies showing this. Doing so would require substantial changes to the existing parallelization strategy in CAM. The development of hybrid systems using stream and conventional processors provides a good opportunity to examine this approach.

Both MECCA, CAM, and the CESM are available for download. The code used here can be made available to users upon request.

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Table 1. Comparison of one-month benchmark simulations of the coupled modal-CAM/MECCA system for Ros-2 and RODAS-3 solvers versus Ros-3.

	Species	Regression Line	R^2	RMSE (%)
Ros-2	O_3	$0.98 \times + 0.56$	0.99	6.5 %
	OH	$1.0 \times + 1.5 \times 10^{-4}$	0.98	17 %
	Br_2	$0.91 \times + 0.87$	0.94	42 %
	H^+ (Coarse Mode)	$2.35 \times + 0.048$	0.93	410 %
RODAS-3	O_3	$0.98 \times - 0.36$	0.99	5.1 %
	OH	$0.99 + 7.3 \times 10^{-5}$	0.99	11 %
	Br_2	$0.95 \times + 0.98$	0.97	29 %
	H^+ (Coarse Mode)	$0.92 + 0.011$	0.97	120 %
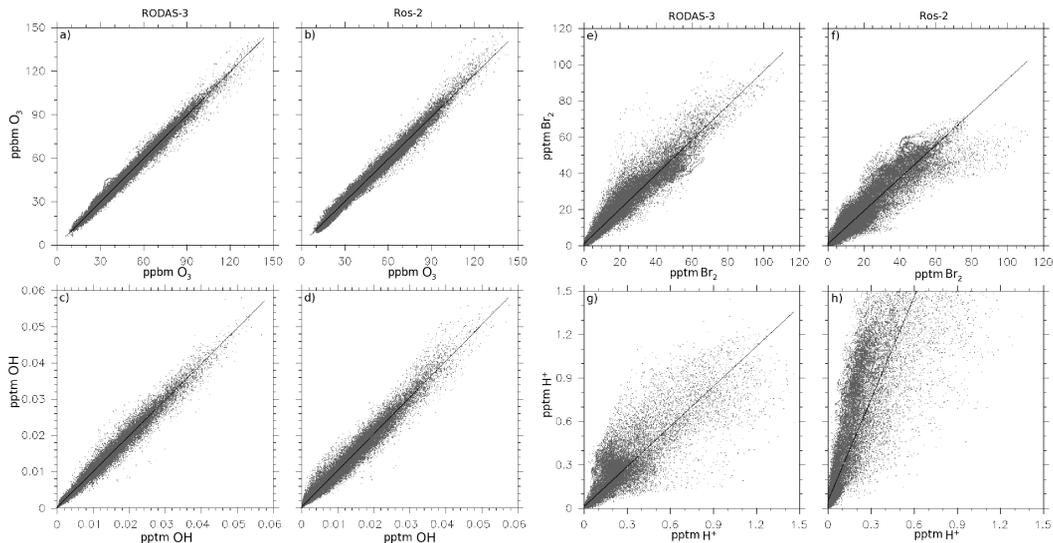
Fig. 1. Comparison of O_3 (**a** and **b**), OH (**c** and **d**), Br_2 (**e** and **f**), and coarse mode H^+ (**g** and **h**) at grid boxes between the surface and 900 mb from one-month benchmark simulations using RODAS-3 and Ros-2 solvers (Y-axes) versus Ros-3 (X-axis) over the same time period. Black lines are least-squares standard linear regressions (see Table 1).
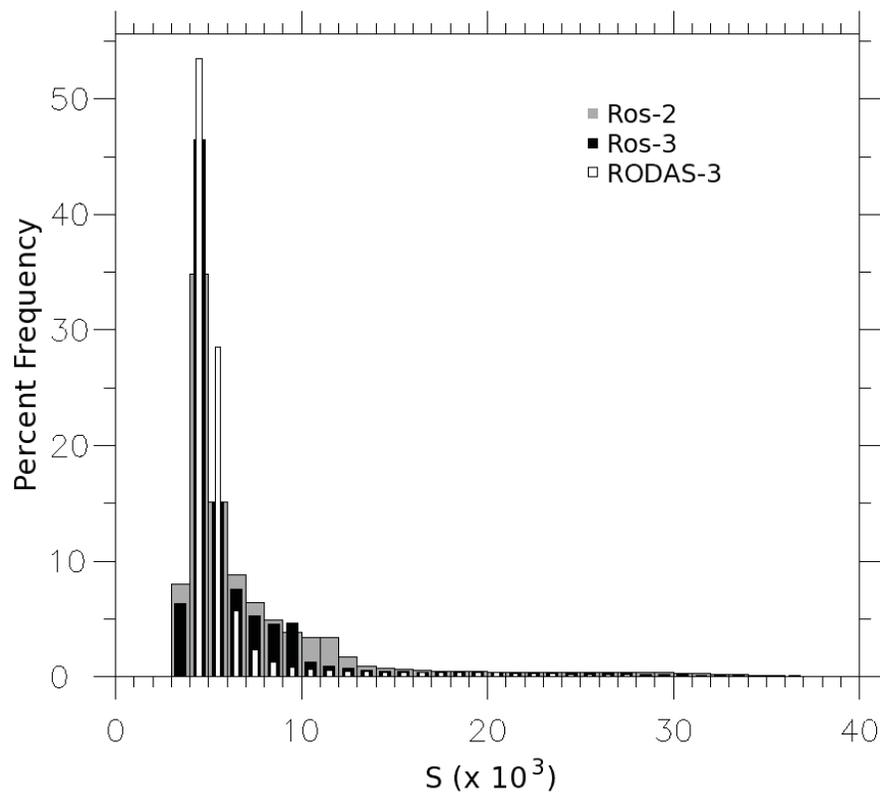
Fig. 2. Histogram of the percent frequency distribution of per grid-box chemistry integration times (in milliseconds) using MECCA in the modal-CAM global atmosphere for the one-month benchmarks using three different Rosenbrock solvers.

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