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# A Strategy for Process-Oriented Validation of Coupled Chemistry–Climate Models

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Evaluating CCMs with the presented framework will increase our confidence in predictions of stratospheric ozone change.

The decreasing levels of halogens in the stratosphere should lead to a gradual recovery from the chemical ozone depletion that has occurred over the past decades (WMO 2003). However, climate change resulting from increases in greenhouse gas concentrations will influence the stratosphere through a range of radiative, dynamical, and chemical mechanisms. A schematic diagram showing the principal regions and processes in the stratosphere is displayed in Fig. 1. An improved understanding of these processes and, more generally, of the interaction between chemistry and climate is needed if credible predictions of the future levels of stratospheric ozone, and its impact on climate and surface UV radiation, are to be made. Such predictions are required for the WMO/UNEP and IPCC assessments as part of

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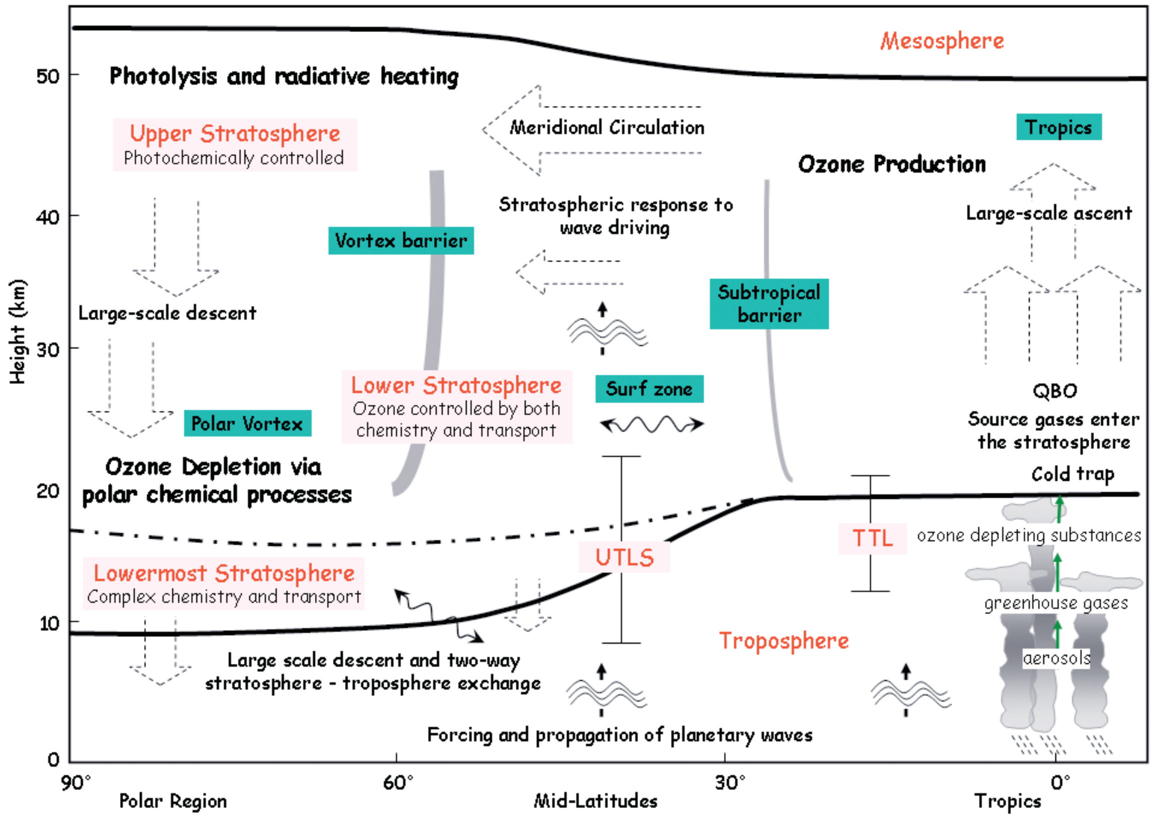


**FIG. 1. Schematic diagram of the principal regions and processes in the upper troposphere and lower stratosphere. Broad arrows denote diabatic circulation and wavy arrows denote transport along isentropic surfaces. The average position of the tropopause is shown by the lower thick-black line, the average position of the stratopause by the upper thick-black line, and the 380-K isentropic surface by the thick-black dot-dashed line. The vertical bars denote the range of the UTLS and TTL.**

the policy formulation processes associated with the Montreal Protocol and the Kyoto Protocol on Climate Change.

A number of CCMs with detailed descriptions of the stratosphere have been developed over the last 5–10 yr in order to provide these predictions. However, the predictions of current CCMs produce a wide range of results concerning the timing and extent of ozone-layer recovery, both in the Arctic and Antarctic winters (WMO 2003). The main features of current CCMs are summarized in Table 1. Figure 2 shows as an example the modeled minimum Antarctic total ozone for the time period 1960–2060 (Austin et al. 2003). In contrast to CTMs, which specify the meteorological conditions, CCMs specify the chemical and dynamical forcings and predict the resulting change in the chemistry–climate system. They simulate a climate that bears a statistical relationship to the real atmosphere, and so a comparison of model results with measurements must be performed in a statistical manner. This is problematic, because it appears to take many decades of observations to define a robust stratospheric climatology, especially in the Arctic winter. While tropospheric climate models can be validated, in part, by their ability to reproduce the climate record over the twentieth century, the paucity of stratospheric climate data prior to the satellite era (post-1979) limits such possibilities for model validation of stratospheric change.

For these reasons, the validation of CCMs requires a process-oriented basis to complement the standard comparison of models with climatologies of observations. By focusing on processes, models can be more directly compared with measurements. In this case, natural variability becomes an aid because it allows dependencies between model fields to be examined in a larger variable space and, thereby, makes identifying cause-and-effect relationships within a model more reliable. An important example is the physically based relationship between planetary wave drag and polar temperatures (see the section labeled "Stratospheric response to wave drag"), which can be quantified by producing a scatterplot of the two quantities with each point representing a different year. In the context

**Table 1. Main features of current CCMs. CCMs are listed alphabetically. The horizontal resolution is given in either degrees latitude x degrees longitude (grid point models), or as T21, T30, etc., which are the resolutions in spectral models corresponding to triangular truncation of the spectral domain with 21, 30, etc., wavenumbers, respectively. All CCMs have a comprehensive range of chemical reactions except that in the UMUCAM model the chemistry is parameterized. The coupling between chemistry and dynamics is represented in all models, but to a different degree. All models include O-GWD schemes, most models additionally include NonO-GWD.**

| Model | Horizontal resolution | No. vertical levels/upper boundary | Coupling chemistry/ dynamics | GWD | Group and location | Reference |
|---|---|---|---|---|---|---|
| AMTRAC | 2° x 2.5° | 48/0.0017 hPa | $O_3$, $H_2O$ | O-GWD + NonO-GWD | GFDL, USA | Anderson et al. (2004), Austin (2002) |
| CCSR/NIES | T21 | 30/0.06 hPa | $O_3$, $H_2O$, $CH_4$, $N_2O$, CFCs | O-GWD + NonO-GWD | NIES, Tsukuba, Japan | Nagashima et al. (2002), Takigawa et al. (1999) |
| CMAM | T32 or T47 | 65/0.0006 hPa | $O_3$, $H_2O$ | O-GWD + NonO-GWD | MSC, University of Toronto, and York University, Canada | Beagley et al. (1997), de Grandpré et al. (2000) |
| E39/C | T30 | 39/10 hPa | $O_3$, $H_2O$, $CH_4$, $N_2O$, CFCs | O-GWD | DLR Oberpfaffen-hofen, Germany | Dameris et al. (2005) |
| ECHAM5/ MESSy | T42 | 90/0.01 hPa | $O_3$, $H_2O$, $CH_4$, $N_2O$, CFCs, $NO_2$, aerosols | O-GWD + NonO-GWD | MPI Mainz, MPI Hamburg, DLR Oberpfaffen-hofen, Germany | Jöckel et al. (2004), Roeckner et al. (2003), Sander et al. (2004) |
| FUB-CMAM-CHEM | T21 | 34/0.0068 hPa | $O_3$, $H_2O$, $CH_4$, $N_2O$, CFCs | O-GWD + NonO-GWD | FU Berlin, MPI Mainz, Germany | Langematz et al. (2005) |
| GCCM | T42 | 18/2.5 hPa | $O_3$ | O-GWD | University of Oslo, Norway; SUNY Albany, USA | Wong et al. (2004) |
| GEOS CCM | 2° x 2.5° | 55/80 km | $O_3$, $H_2O$, CFCs, $CH_4$, $N_2O$ | O-GWD + NonO-GWD | NASA GSFC, USA | S. Pawson, and P. A. Newman 2005, personal communication |
| GISS | 4° x 5° | 23/0.002 hPa | $O_3$, $H_2O$, $N_2O$, $CH_4$, CFCs | O-GWD + NonO-GWD | NASA GISS, USA | Schmidt et al. (2005a, manuscript submitted to *J. Climate*) |
| HAMMONIA | T31 | 67/2.10$^{-7}$ hPa | O, $O_2$, $O_3$, $H_2O$, $N_2O$, $CO_2$, $CH_4$ | O-GWD + NonO-GWD | MPI Hamburg | Schmidt et al. (2005b, manuscript submitted to *J. Climate*) |
| LMDREPRO | 2.5° x 3.75° | 50/0.07 hPa | $O_3$, $H_2O$, $N_2O$, $CH_4$, CFCs | O-GWD + NonO-GWD | IPSL, France | S. Bekki and D. Hauglustaine 2005, personal communication |
| MRI | T42 | 68/0.01 hPa | $O_3$ | O-GWD+ NonO-GWD | MRI, Japan | Shibata and Deushi (2005); Shibata et al. (2005) |
| MAECHAM4/ CHEM | T30 | 39/0.01 hPa | $O_3$, $H_2O$, $CH_4$, $N_2O$, CFCs | O-GWD + NonO-GWD | MPI Mainz, MPI Hamburg, Germany | Manzini et al. (2003), Steil et al. (2003) |
| SOCOL | T30 | 39/0.01 hPa | $O_3$, $H_2O$ | O-GWD + NonO-GWD | PMOD/WRC and ETHZ, Switzerland | Egorova et al. (2005) |
| ULAQ | 10° x 20° | 26/0.04 hPa | $O_3$, $H_2O$, $CH_4$, $N_2O$, CFCs, $NO_2$, aerosols | Rayleigh frict. + vert. diffusion | University of L'Aquila, Italy | Pitari et al. (2002) |
| UMETRAC | 2.5° x 3.75° | 64/0.01 hPa | $O_3$ | O-GWD + NonO-GWD | Met Office, UK | Austin (2002), Austin and Butchart (2003) |
| UMSLIMCAT | 2.5° x 3.75° | 64/0.01 hPa | $O_3$, $N_2O$, $CH_4$, $H_2O$ | O-GWD + NonO-GWD | University of Leeds, UK | Tian and Chipperfield (2005) |
| UMUCAM | 2.5° x 3.75° | 58/0.01 hPa | $O_3$ | O-GWD, Rayleigh friction | University of Cambridge, UK | Braesicke and Pyle (2003 and 2004) |
| WACCM3 | 2° x 2.5°<br>4° x 5° | 66/140 km | $O_3$, $H_2O$, $N_2O$, $CH_4$, CFCs | O-GWD + NonO-GWD | NCAR, USA | Sassi et al. (2005) |

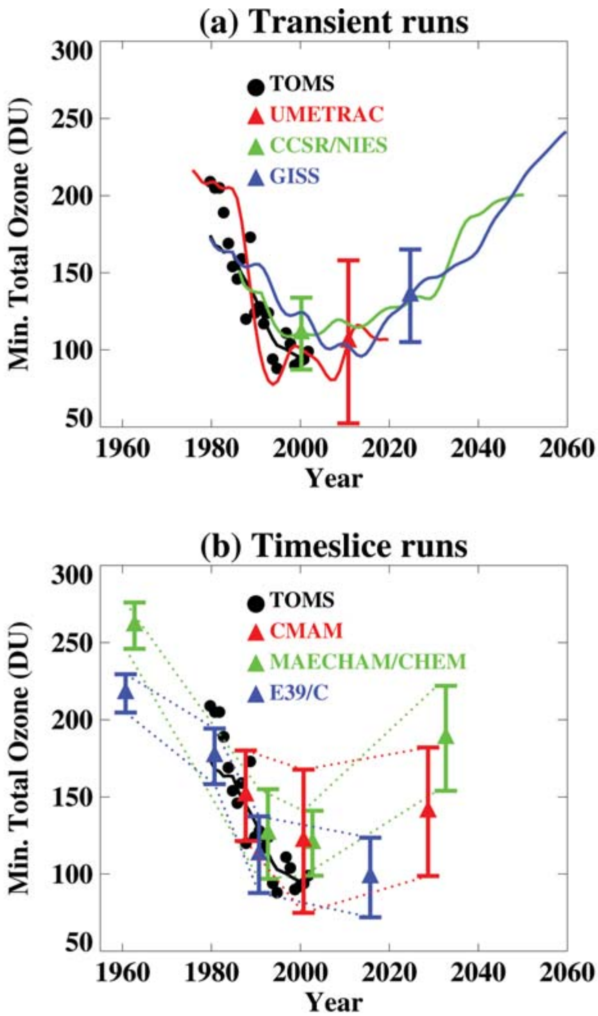


**Fig. 2. Modeled and measured values of minimum total column amounts of ozone in the Antarctic (Sep–Nov). Results are shown for the period 1960–2060 derived from (a) transient runs and (b) time-slice runs of different CCM model experiments in comparison with TOMS satellite data (for the period 1980–2001). The main features of the CCMs identified in the legend are summarized in Table 1. The solid lines in (a) show the results of a Gaussian smoother applied to the results of individual years with vertical bars denoting twice the standard deviation. For the time-slice experiments, the dotted lines are drawn to assist in estimating trends. Transient as well as time-slice experiments show reasonable agreement with TOMS observations. The uncertainty in both experiment types and the differences between CCMs increases significantly for future years. Specifically, the start dates of ozone recovery, defined by when the decadal averaged minimum ozone first begins to increase, vary significantly. Similar CCM experiments for ozone depletion in Arctic winters show poorer agreement with the data and between models (WMO 2003). (Figure from Austin et al. 2003.)**

of stratospheric GCMs (i.e., those without chemistry), process-oriented validation represents the level-II tasks within GRIPS (Pawson et al. 2000). A first attempt at process-oriented validation of stratospheric CCMs is summarized in Park et al. (1999), WMO (2003), and Austin et al. (2003).

Until very recently, the components of the Earth's system (ocean dynamics, marine biogeochemistry, tropospheric and stratospheric chemistry, atmospheric dynamics and physics, terrestrial ecosystems, ecology, etc.) have been investigated separately by different disciplines. As we are moving toward more complex models that include different components of the Earth's system, the strategy of setting up benchmarks and criteria for model validation presented in this paper is also important for other modeling communities in order to consolidate their results and conclusions. Similar efforts are needed for the other components of an Earth System Model to advance our understanding of the various processes and to ensure that employing such complex models would be beneficial.

**LONG-TERM APPROACH TO CCM VALIDATION.** In this work we present a strategy for a more long-term comprehensive approach to CCM validation centered on four main categories: transport, dynamics, radiation, and stratospheric chemistry and microphysics. For each process, Table 2 presents the associated model diagnostics, variables relevant for validation, and sources of observational or other data that can be used for validation. The accompanying text discusses the importance of the selected processes to CCM validation and the utility of the selected diagnostics in a validation study. The relevant time scale for the diagnostic depends on the process and must be borne in mind when comparing models and measurements.

A schematic diagram of the approach to CCM validation is shown in Fig. 3. The strategy resulted from discussions at the workshop on process-oriented validation of CCMs held at Grainau, Germany, in November 2003 (Eyring et al. 2004). Members of the CCM and CTM communities came together with members of the measurement and data analysis communities to develop ideas on this issue. The role of the latter communities was crucial in understanding both the opportunities and the limitations presented by the available data. The size of the task involved with a complete validation exercise quickly became apparent and so the approach taken was to develop a range of diagnostics that can be worked through as time and interest allow. Although the focus of the

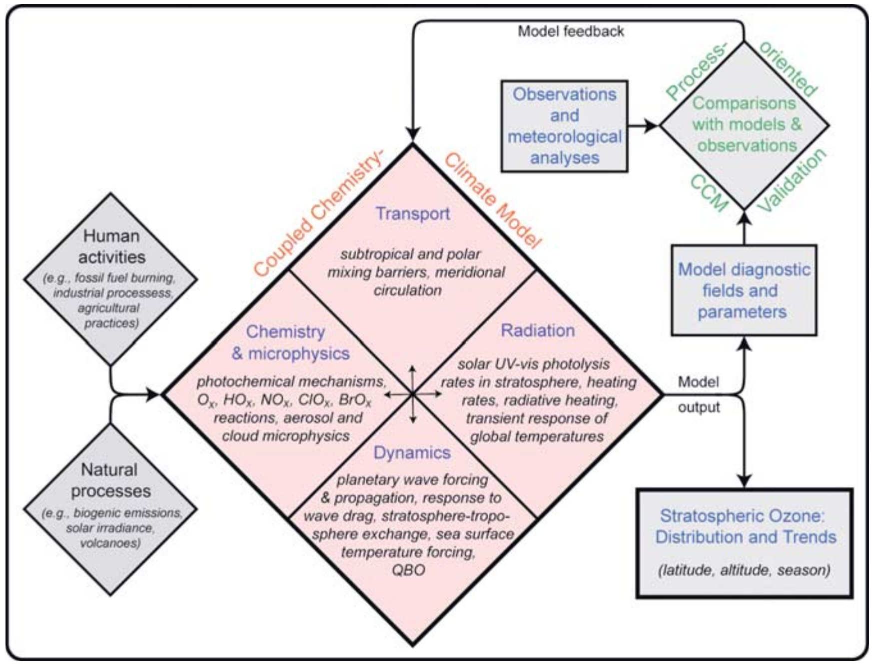


**Fig. 3.** ***Schematic diagram of the presented approach to CCM validation.*** **The centerpiece is a CCM comprised of four basic process categories: transport, dynamics, radiation, and stratospheric chemistry & microphysics. The four categories are fundamentally interdependent and interactive and require as inputs, knowledge of human activities and natural processes. These inputs help quantitatively define processes in the atmosphere and expectations for future changes. Trends in atmospheric constituents and parameters associated with climate forcing are examples of important inputs. The CCM output includes a wide array of parameters and diagnostics associated with the four different categories. The distribution of stratospheric ozone is highlighted separately here because of the strong contemporary interest in halogen-based ozone depletion and the recovery of the ozone loss that has developed over recent decades. The comparisons of model diagnostics and other outputs with atmospheric observations and meteorological analyses are the key to process-oriented CCM validation. In the accompanying Table 2 and discussions, we define the components of these comparisons. Finally, the results of the comparisons can be used to provide feedback to the representation of processes in CCMs in order to improve subsequent CCM validation comparisons. In this way, the uncertainties in future trends in stratospheric ozone and other key model outputs can be reduced.**

present discussion is on defining a methodology for the validation of CCMs, we recognize that observational uncertainties are a potentially important component of CCM evaluation. Observational uncertainties can influence the outcome of model–data consistency tests (see, e.g., Santer et al. 2003a, 2003b) and should be explicitly accounted for in any CCM validation strategy.

*Stratospheric transport.* Transport in the stratosphere involves both meridional overturning (the residual circulation) and mixing, which together represent the Brewer–Dobson circulation. The most important aspects are the vertical (diabatic) mean motion and the horizontal mixing. Horizontal mixing is highly inhomogeneous, with transport barriers in the subtropics and at the edge of the wintertime polar vortex; mixing is most intense in the wintertime "surf zone"—that is, the region surrounding the polar vortex—and is comparatively weak in the summertime extratropics. Accurate representation of this structure in CCMs is important for the ozone distribution itself, as well as for the distribution of chemical families and species that affect ozone chemistry ($NO_y$, $Cl_y$, $H_2O$, $CH_4$; for explanations of chemical formulas used throughout, cf. appendix B). Within both the Tropics and the polar vortex, the key physical quantities to be represented are the degree of isolation and the diabatic ascent or descent, respectively. The impact of diabatic ascent or descent on the actual vertical motion of chemical species depends on the degree of isolation.

Subtropical and vortex-mixing barriers. Useful information can be obtained from instantaneous snapshots of tracer fields, which makes the model–measurement comparison straightforward. For this purpose there is a wealth of high-quality observational data available. A simple check on the degree of isolation is provided by the sharpness of latitudinal gradients of long-lived species ($CH_4$, $N_2O$, CFC-11), while a more detailed diagnosis is obtained from the structure of chemical correlations and from PDFs of such species. Just above the tropical tropopause, where the tropical mixing barrier appears to be fairly leaky, transport into midlatitudes can be quantified by the propagation of the annual cycle in $CO_2$ and $H_2O$, which has been well

**TABLE 2. List of core processes to validate CCMs with a focus on their ability to model future stratospheric ozone.**

| Process | Diagnostic[a] | Variables | Data | References[b] |
|---|---|---|---|---|
| **Stratospheric transport** | | | | |
| **Subtropical and polar mixing barriers** | PDFs of long-lived tracers | $N_2O$, $CH_4$, CFC-11, etc.; potential vorticity (PV) | Satellite and in situ (aircraft, balloons) chemical measurements and meteorological analyses[c] | Strahan and Douglass (2004) |
| | Latitudinal gradients of long-lived tracers | | | Sankey and Shepherd (2003) |
| | Correlations of long-lived tracers | | | Sankey and Shepherd (2003) |
| | Phase and amplitude of tropical $CO_2$ or $H_2O$ annual cycle in lower stratosphere (tape recorder) | $CO_2$, $H_2O$ or idealized annually repeating tracer | Satellite and in situ measurements | Hall et al. (1999), Mote et al. (1996) |
| | Annual cycle of streamer frequency | Daily PV (maybe long-lived tracers) | Meteorological analyses[c] satellite measurements | Eyring et al. (2003), Waugh (1996), Waugh et al. (1997) |
| **Meridional circulation** | Mean age | Conserved tracer with linearly increasing concentration, $SF_6$ or $CO_2$ | In situ measurements | Hall et al. (1999), Waugh and Hall (2002) |
| | Correlation of interannual anomalies of total ozone and Planetary wave flux | Total ozone and heat flux at 100 hPa, zonal and monthly means | Satellite measurements, meteorological analyses[c] | Randel et al. (2002), Weber et al. (2003) |
| | Vertical propagation of tracer isopleths | $H_2O$ or $CO_2$ or idealized annually repeating tracer (tropics), $CH_4$ or $N_2O$ (polar) | In situ and ground-based (polar only) and satellite data | Hall et al. (1999), Kawamoto and Shiotani (2000) |
| | Diabatic velocity, TEM streamfunction | Diabatic velocity, residual velocities | Diabatic velocity inferred from radiative calculation | Eluszkiewicz et al. (1996), Rosenlof (1995) |
| **UTLS transport** | Vertical gradients of, and correlations between, chemical species in the extratropical UTLS | $CO_2$, $SF_6$, $H_2O$, CO, $O_3$, HCl | Balloon, aircraft | Hoor et al. (2002), Marcy et al. (2004) |
| | Relation between meteorological indices (e.g., tropopause height) and total ozone | Daily winds, temperature, geopotential height, total $O_3$ | Meteorological analyses[c] satellite measurements, ozonesondes | Santer et al. (2003a) |
| | Diabatic velocity, vertical $0_3$ profiles in TTL | Diabatic velocity, vertical $O_3$ profiles | Diabatic velocity inferred from radiative calculation, ozonesondes | Thompson et al. (2003) |
| **Dynamics** | | | | |
| **Forcing and propagation of planetary waves** | WFA, PW spectrum (variances and covariances) | Temperature, geopotential height, horizontal winds, High-frequency (daily) data | Meteorological analyses[c] | Hayashi (1982) |
| | Hemispheric ozone variability indices | Total column ozone over several years | Satellite measurements of total ozone (e.g., TOMS, GOME, or SCIAMACHY) | Erbertseder et al. (2005, manuscript submitted to *Atmos. Chem. Phys. Discuss.*) |

[a] In addition to traditional model validation (climatological means, interannual variations etc.).

[b] Listed references only provide examples.

[c] Due to uncertainties use several analyses, not one.

[d] Intercomparison currently not possible because process not included in most CCMs.

observed in aircraft measurements. The ascent rate of tracer isopleths in the Tropics is visible in the "tape recorder" phenomenon seen in altitude-versus-time cross sections of $H_2O$ mixing ratios.

MERIDIONAL CIRCULATION. Both horizontal mixing and the residual circulation are largely driven by the momentum deposition (wave drag) from planetary waves propagating from the troposphere

**Table 2. Continued.**

| Process | Diagnostic[a] | Variables | Data | References[b] |
|---|---|---|---|---|
| **Dynamics (*continued*)** | | | | |
| **Stratospheric response to wave drag** | Annual cycle of temperatures in Tropics and extratropics | Zonal monthly mean temperature, residual streamfunction | Meteorological analyses[c] in situ and space-based observations, profile data | Pawson et al. (2000) |
| | Planetary wave flux vs polar temperature, lagged in time | Heat flux ($v'T'$) at 100 hPa (Jan/Feb), temperature at 50 hPa (Mar), zonal monthly means | | Austin et al. (2003), Newman et al. (2001) |
| | Vortex definition, structure and occurrence of sudden/final warmings | PV, horizontal winds, temperature, area colder than PSC temperature, Vortex area/equivalent latitude; warming statistics; high-frequency (daily) 3D fields | | Limpasuvan et al. (2004), Manney et al. (2005), Nash et al. (1996), Waugh and Randel (1999) |
| | Downward control integral, also scatterplot of planetary wave drag versus gravity wave drag | $w^*$ from model PWD, GWD, other drag zonal and monthly means | Meteorological analyses[c] total drag inferred from diabatic heating calculation | Beagley et al. (1997) |
| | Persistence (e.g., leading empirical orthogonal functions), including Holton-Tan | Geopotential height, temperature, multiyear time series (means, frequency spectra) | Meteorological analyses[c] | Waugh et al. (1999), Zhou et al. (2000) |
| **Stratosphere–troposphere exchange** | Daily mass estimates of the lower-most stratosphere | Daily 380-K isentropic pressure and tropopause pressure | Meteorological analyses[c] | Olsen et al. (2002) |
| **QBO**[d] | Horizontal winds and temperature | Horizontal winds and temperature, zonal and monthly means | Meteorological analyses[c] | Butchart et al. (2003), Giorgetta and Bengtsson (1999) |
| **Radiation** | | | | |
| **Solar UV–visible photolysis in stratosphere** | Radiative transfer of 260–800-nm solar flux, photolysis rates comparison up to 95° solar zenith angle including clouds | Actinic flux (direct and scatter), photolysis rates of $O_3$ and $NO_2$ at local noon pressure, ozone, stratospheric aerosols, tropospheric clouds, aerosols and ozone | Direct flux measurements (balloon, aircraft), inferred photolysis rates (aircraft) | Bais et al. (2003), Hofzumahaus et al. (2004), Kylling et al. (2003) |
| **Heating rates** | Comparison of thermal and solar heating rates in offline runs employing column version of CCM radiation codes | Heating rates and irradiances from CCM radiation code, with a prescribed and standardized set of input atmospheric profiles | Use sophisticated reference radiation models for comparison (line by line) NLTE, discrete-ordinate scattering, etc. | Forster et al. (2001), Oinas et al. (2001) |
| **Radiative heating** | Global average of temperature profile | Annually averaged global trace gas and clouds fields, temperature | Assimilated fields derived from satellite and sonde data, meteorological analyses[c] | Pawson et al. (2000) |
| | Long-term globally averaged transient temperature changes | Changes in ozone, water vapor and high clouds, greenhouse gases, hydrofluorocarbons, aerosols, etc. | SSU/MSU satellite time series | Shine et al. (2003) |

into the stratosphere, with more wave drag leading to a stronger Brewer–Dobson circulation. The relationship between the wave flux and the residual circulation is quantified, through temperature, in the dynamics diagnostics. With regard to chemical transport, the seasonal cycle of $O_3$ in the extratropics exhibits a marked build-up during the winter/spring period due to the Brewer–Dobson circulation. Years with greater planetary wave flux have a greater ozone build-up, a relationship that is well established from

| **Table 2. Continued.** | | | | |
|---|---|---|---|---|
| Process | Diagnostic[a] | Variables | Data | References[b] |
| **Stratospheric chemistry and microphysics** | | | | |
| **Photochemical mechanisms and short-time-scale chemical processes** | Offline box model comparisons of fast chemistry (of order 1 week or less) | Full chemical constituents ($O_3$ loss due to $O_x$, $HO_x$, $NO_x$, $ClO_x$, $BrO_x$, J values) | $HO_x$: balloon, shuttle, aircraft; $NO_x$: satellite, shuttle, balloon, aircraft; $ClO_x$: satellite, shuttle, balloon, aircraft; $BrO_x$: aircraft | Gao et al. (2001), Salawitch et al. (1994) |
| **Long-time-scale chemical processes** | Comparison of abundance of reservoirs and radical precursors | Instantaneous output of all chemical constituents and temperature (one per month) | Satellite measurements of reservoirs and precursors | Millard et al. (2002), Salawitch et al. (2002), Sen et al. (1999) |
| | Tracer–tracer relations | $O_3$, $NO_y$, $CH_4$, $H_2O$, $N_2O$ | | Chang et al. (1996), Fahey et al. (1996), Müller et al. (1996) |
| **Polar processes in winter/spring** | Partitioning of species within the families | Species from families ($ClO_x$, $NO_x$, $HO_x$, $BrO_x$, $Cl_y$, $NO_y$, $Br_y$) temperature, PV from wind fields | Satellite and aircraft measurements | Park et al. (1999), Pierson et al. (2000) |
| | Chemical ozone loss vs PSC activity | $O_3$, passive $O_3$ tracer, $O_3$ production/loss rate, PV from wind fields, temperature | Chemical ozone loss diagnosed from frequent ozone profiles in the vortex over several years, meteorological analyses[c] | Chipperfield et al. (2005), Rex et al. (2004) |
| **Summer processes** | Ozone changes in polar regions | Total ozone, full chemical constituents, temperature | Satellite measurements of total ozone | Fahey and Ravishankara (1999) |
| | Ozone changes in midlatitude regions | | | Koch et al. (2003) |
| **Denitrification and dehydration** | $NO_y$ vs tracer | $NO_y$, $HNO_3$, $N_2O$, $CH_4$, etc. | Satellite measurements of $HNO_3$, $H_2O$, $CH_4$; aircraft observations of $NO_y$, $H_2O$, $CH_4$, $N_2O$; PSC size distributions | Gao et al. (2001), Popp et al. (2001), Santee et al. (2002) |
| | $H_2O + 2\,CH_4$ | $H_2O$ particle-flux rates added to daily polar chemistry, instantaneous output, $CH_4$ | | Nedoluha et al. (2000), Park et al. (2004) |
| **Aerosols and cloud microphysics** | Cirrus cloud frequency of occurrence; $H_2O$ distribution | Ice water content, water vapor, temperature, aerosol size distribution | Aircraft and satellite data; process/cloud-resolving models | Clark et al. (2003), Read et al. (2004), Thomas et al. (2002), Wang et al. (1996) |
| **Stratospheric aerosol processes** | Sulfuric acid size distribution, aerosol optical extinction | Sulfuric acid mass, particle number concentration, water vapor, temperature | Satellite and in situ measurements of aerosols; aerosol climatologies | Thomason and Peter (2005; submitted SPARC report) |
| | Temperature response in the lower stratosphere, chlorine and nitrogen partitioning after major volcanic eruptions | All species from chlorine and nitrogen families, temperature | Satellite and aircraft measurements for temperature response, e.g., MSU data | Dessler et al. (1997), Fahey et al. (1993), Labitzke and McCormick (1992) |

[a] In addition to traditional model validation (climatological means, interannual variations etc.).

[b] Listed references only provide examples.

[c] Due to uncertainties use several analyses, not one.

[d] Intercomparison currently not possible because process not included in most CCMs.

observations and provides a good diagnostic for CCM validation. The Brewer–Dobson circulation also determines the mean age of air, which can be validated from measurements of long-lived species that have increasing concentrations with time (e.g., $SF_6$, $CO_2$). Mean age of air has been found to be a very powerful diagnostic for identifying model deficiencies (Park et al. 1999).

UTLS TRANSPORT. Transport in the UTLS region is complex. The extratropical tropopause "break" is a barrier to quasi-horizontal mixing, causing significant contrasts in chemical species between the extratropical lowermost stratosphere and the tropical upper troposphere. The degree of isolation can be assessed by the sharpness of horizontal or isentropic gradients at the tropopause (because tropopause height changes with latitude), and with chemical correlations (e.g., $O_3$ versus CO). There is a robust relationship between variations in total $O_3$ and in tropopause height, which provides a potentially important diagnostic for CCM validation. The TTL is marked by changes in the vertical stability and in chemical species beginning below the tropical tropopause. Processes in this layer are important for setting chemical boundary conditions for the stratosphere. In addition, convective processes and microphysics affect water vapor and the chemistry of ozone and other minor species. These radiatively active gases can have large impacts on the climate of the UTLS.

*Dynamics.* The basic dynamical state of the stratosphere which controls transport is defined by a number of physical processes. These include the forcing mechanisms and propagation of planetary-scale Rossby and gravity waves, wave–mean flow interaction, and the diabatic circulation. Correct reproduction of the climatological mean state of the stratosphere by CCMs, including interhemispheric differences, and interannual and intraseasonal variability, is important but not sufficient: the basic dynamical mechanisms must be well represented in the underlying GCMs on which the CCMs are based if future changes are to be modeled credibly.

FORCING AND PROPAGATION OF PLANETARY WAVES. The properties of planetary waves (such as their generation, propagation through the stratosphere, and role in the momentum budget of the stratosphere [i.e., the stratospheric response to planetary wave drag (PWD)], can be determined by analyzing planetary wave patterns at different altitudes between the free troposphere and the upper model layers. A WFA can help to resolve transient waves at distinct wavenumbers into standing and eastward- or westward-traveling waves at different frequencies. The amplitudes and phases of the zonal quasi-stationary planetary waves in the lower stratosphere can be found by analyzing total ozone fields using spectral statistical methods. Here, the total ozone column is considered as a conservative tracer to illuminate the variability of wave structures in the lower stratosphere. Spectral harmonic analysis can be applied to derive the wave parameters from the ozone distribution. The spectral properties can further be used to calculate hemispheric ozone variability indices, which are defined as the hemispheric means of the zonal amplitude of the planetary wavenumbers 1 and 2.

STRATOSPHERIC RESPONSE TO WAVE DRAG. Planetary waves can only propagate into the stratosphere when the winds are relatively weak westerlies, and so the Brewer–Dobson circulation is stronger in the winter hemisphere. The wave drag can be quantified from the net planetary wave flux into the stratosphere, normally taken to be $v'T'$ (heat flux) at 100 hPa. Correlations of Eliassen–Palm fluxes (whose meridional and vertical components are respectively proportional to the meridional eddy momentum and eddy heat fluxes) with dynamical fields (e.g., temperature, wind speed) and parameters (e.g., size and persistence of the polar vortex, PSC potential) are necessary to investigate the stratospheric response to wave drag and its consequences for chemical and physical processes in CCMs. Moreover, the ability of CCMs to reproduce correctly the seasonality of the Brewer–Dobson circulation can be checked by comparing the calculated cross sections of the residual circulation mass streamfunction (latitude versus height) with those based on reanalyses (e.g., NCEP, ERA-40). The drag from dissipating gravity waves also plays a significant role in the stratospheric circulation, especially in the Antarctic winter. Here direct observations are not available, but the role of gravity wave drag in different models, and its response to changes in planetary wave drag, can be compared with appropriate diagnostics.

STRATOSPHERE–TROPOSPHERE EXCHANGE. The lowermost stratosphere is the region where isentropic surfaces intersect both the troposphere and stratosphere. The lowermost stratosphere is roughly bounded by the tropopause at the bottom and the 380-K isentropic surface at the top. The month-to-month variation of the mass of this atmospheric layer is sensitive to a number of transport and dynamical processes. Meteorological observations can be used to test this relationship in models.

QBO. CCMs are now just beginning to simulate the QBO, usually through the inclusion of enhanced GWD. It will be important to confirm that the models are obtaining a QBO for the right reasons, and that the extratropics respond in the correct manner. Meteorological reanalyses and radiosonde records can be used for this.

*Radiation.* Radiative calculations are used in CCMs to derive photolysis rates and heating rates. Photolysis rates in the stratosphere control the abundance of many chemical constituents that, in turn, control chemically active constituents, such as ozone. At the same time these trace gases feedback on temperature and, thus, circulation through the radiative heating rates. At present, most models calculate radiative heating rates and photolysis rates in an inconsistent manner. For example, the spherical geometry of the Earth might be included in the photolysis rate calculation, but not in the heating rate calculation. Also, different radiation schemes are usually employed for the two calculations. Such inconsistencies should be avoided. There are currently not enough high-quality measurements that can be used to validate the important radiative processes in global models. Presently, the best radiative models (currently not included in CCMs) provide an important complement to available measurements for CCM validation. Accordingly the approach taken here (unlike the other three categories) is to perform detailed model comparisons between the best radiative models and the radiation modules actually used in CCMs. We evaluate the photolysis and radiative heating rate calculations separately.

Solar UV–visible photolysis in the stratosphere. A photolysis rate generally requires knowledge of the actinic fluxes at solar and UV–visible wavelengths (190–800 nm) as a function of altitude and solar zenith angle. Accurate calculations of these fluxes require accurate representation of scattering, albedo, and refraction. Particular concerns in photolysis rate calculations for the lower stratosphere are the effect of tropospheric cloudiness, which can significantly increase the rates for certain gases and photolysis at solar zenith angles greater than 90°. Diagnostic parameters for photolysis rates in CCM comparisons include the radiative transfer of UV–visible wavelengths and calculated rates for individual gases. The distributions of pressure, ozone, stratospheric aerosols, and tropospheric clouds are important variables in such model comparisons. As a minimum test, the photolysis rates of $O_3$ and $NO_2$ should be stored as three-dimensional fields and compared to observations. In addition, actinic fluxes at the ground in different wavelength intervals should be compared.

Radiative heating rates. Radiative heating is the fundamental link between ozone and climate. As its calculation plays the central part in CCM feedbacks, it is extremely difficult to separate cause and effect in a fully coupled model. Radiative heating rate calculations can only be truly evaluated in an offline comparison of radiation schemes. Currently, the lack of this comparison is one of the most important limitations in understanding CCM differences. A set of standardized background atmospheres and radiation scheme inputs should be compiled, along with a reference set of calculations from several state-of-the-art line-by-line and scattering models. Differences in radiative heating rates and trace gas fields can then be used to evaluate differences between the globally averaged climatological temperature of CCMs and their temperature response to changes in greenhouse gases loadings and other perturbations.

Radiative heating within an online framework. To evaluate radiative heating within an online framework, the long-term global-mean temperature climatology of CCMs can be compared to observations. An online framework allows a combined test of the model's background atmosphere and radiative heating profile. Also, the globally averaged transient temperature changes over both a single year and the past ~25 yr can be compared to SSU and MSU satellite observations. This tests both the evolution of forcing agents, as well as the radiative heating and the radiative relaxation time in the model.

*Stratospheric chemistry and microphysics.* One of the ways in which chemistry and dynamics are coupled is the temperature dependence of many chemical reaction rates. The importance of local control of ozone by chemistry relative to transport varies substantially between various times and places. In the upper stratosphere transport plays a role by controlling the concentrations of long-lived tracers such as inorganic chlorine, but photochemical time scales are so short that transport has a minimal direct impact on ozone. However, in the lower stratosphere, the photochemical time scales are rather longer (typically of the order of months) and interactions with dynamics are complex and more challenging to model accurately. Aerosols have an important role in chemistry in the lower stratosphere, since reactions can take place within or on the particles. Consequently, even though the photochemical lifetime of ozone is typically many months in the lower stratosphere, rapid chemical loss of ozone occurs in the Antarctic lower stratosphere, following exposure of air to polar stratospheric clouds.

Photochemical mechanisms and short-time-scale chemical processes. Validation of chemical processes on time scales of a couple of days can be accomplished by examining the full field of chemical constituents as well as reaction and photolysis rates found by each CCM. The comparisons should focus on times and places where the ozone loss efficiency by each of the catalytic families, as well as ozone production, can be defined from observations of the radical species. Full chemical constituent output from the CCMs (including diurnal variations, if available) would be requested for a handful of times and places of a long-term run, designed to coincide with the availability of atmospheric observations. The offline models would be constrained by abundances of long-lived radical precursors from the CCMs, to provide a meaningful test of the rapid chemistry within each CCM. The offline simulations should include Lagrangian calculations to fully understand the impact of airmass history on radical concentrations for the selected cases. Also, measurements exist for evaluation of CCM photolysis rates.

LONG-TIME-SCALE CHEMICAL PROCESSES. In contrast, the investigation of long-time-scale photochemical processes needs to be done within the CCM itself, as transport has a significant impact. All the model 3D chemical fields need to be output, as well as the appropriate dynamical variables (e.g., temperature). One instantaneous "snapshot" per month should be sufficient for the purpose of comparing the abundances of model reservoirs and radical precursors. The interrelations between long-lived tracers also need to be compared in detail with observations.

POLAR CHEMISTRY IN WINTER/SPRING. The largest chemical $O_3$ losses have occurred in winter/spring, when low temperatures lead to the formation of condensed matter and heterogeneous chemistry becomes important. Some aspects of heterogeneous chemistry can be investigated in box model tests, but because of the possible importance of denitrification and dehydration, as well as transport, 3D simulations are required for a complete analysis. Validating polar processes requires an extensive set of model chemical and particle fields with daily frequency. Measurements from a number of balloon and aircraft campaigns can be used to test the model chemical (and microphysical) schemes. The accumulated winter/spring polar $O_3$ loss is an important contributor to midlatitude trends. A validation of this modeled quantity, including its sensitivity to interannual temperature changes, is crucial for one of the main goals of CCM calculations—the prediction of polar $O_3$ recovery. An empirical relation between chemical $O_3$ loss and temperature can be used for this validation.

SUMMER PROCESSES. In summer, atmospheric chemistry in polar regions is a special case because of the continuous, or near-continuous, daylight. These conditions have revealed some possible discrepancies in $NO_x$ chemistry. This has an impact on ozone amounts directly in the polar regions and also in midlatitudes via transport from the polar regions.

DENITRIFICATION AND DEHYDRATION. These important processes occur in the cold winters of both hemispheres and enhance $O_3$ loss. However, their current representation in CCMs is crude, contributing to uncertainties in polar $O_3$. This is further complicated by a) an incomplete understanding of the mechanism for denitrification and b) CCM polar temperature biases. The CCM representation of denitrification can be investigated by analyzing the key nitrogen containing species, $NO_y$ and $HNO_3$, as a function of well-conserved tracers (e.g., $N_2O$). Similarly, the sum $H_2O + 2\ CH_4$ is approximately conserved in the stratosphere except in the presence of dehydration.

AEROSOLS AND CLOUD MICROPHYSICS. Aerosol and cloud-related processes affect the whole UTLS region through changes in the radiative balance and heterogeneous reactions. Microphysical processes and gas–particle interactions are important to understand dehydration and denitrification in the polar region and the regulation of the overall stratospheric water vapor budget. The required model variables are particle number, mass densities, and relative humidity.

STRATOSPHERIC AEROSOL PROCESSES. Reactions involving sulfate aerosol are known to affect the amount of stratospheric $O_3$. Only a few CCMs currently calculate the sulfur cycle and aerosol processes explicitly. Other CCMs include observed aerosol loadings and prescribed heating rates from major volcanic eruptions. In order to study the effects of these eruptions on stratospheric circulation and chemistry, the temperature response as well as changes in chlorine and nitrogen partitioning have to be examined.

**SUMMARY AND THE WAY AHEAD.** A table of core processes, diagnostics, and datasets for CCM validation has been developed, with a focus on the models' ability to predict future stratospheric ozone amounts and distribution. Of the comprehensive suite of diagnostics for stratospheric CCMs listed in Table 2, several have been applied before to a range of models (Park et al. 1999; Pawson et al. 2000; Austin et al. 2003), but most have not. Some models need further development before the diagnostics can be applied. Thus, while clearly desirable, it is a major task to perform all these diagnoses given the complexity of the CCMs. A step-wise approach is required in the use of the table. In practice, modeling groups need to develop their own priorities among these diagnostics. The choices will depend on the known strengths and weaknesses of each model, the processes and constituents already included, and the existing output from runs already performed. The choices will also depend on the scientific focus of each modeling group and the issue being addressed. For example, predictions of polar ozone loss will have more credibility if a model has been shown to compare well with diagnostics such as ozone loss versus PSC volume, heat flux, and $ClO_x$, $NO_y$, etc. Over time each model will gradually increase the number of tests applied and overall confidence will increase.

The lasting impact and the full benefit will come from concerted validation activities based on the table of processes. In order for these activities to succeed over the next several years, broad support is needed from the atmospheric sciences community and its managers. It is important that the validation procedures and goals defined for these activities are accepted at the start and valued by all participants in this joint exercise.

A new CCM Validation Activity for SPARC (CCMVal) has been established, based on experiences within GRIPS (Pawson et al. 2000) and on the concept that was developed in the workshop on process-oriented CCM validation (Eyring et al. 2004), so that real progress can be expected in the next couple of years in time for the next WMO/UNEP and IPCC assessments.

To facilitate this process-oriented validation of CCMs, we intend to provide all interested scientists with access to diagnostic software packages. These routines will be archived in a central location. The goal in supplying such software is to simplify such activities as quality control of model output, calculation of more complex model diagnostics, statistical evaluation of model/data differences and graphical display of results. Use of this software is not mandatory. Rather, the intent is to make it easier for groups to compute a broad range of calculations in a reasonably consistent way. Centralized software repositories have been of great benefit in other MIPs, such as the AMIP and CMIP. These have freely supplied software for quality control of model output, data visualization, and interpolation of boundary condition datasets to a specific model grid. The CCM community can benefit from the experiences gained during previous model intercomparison exercises, particularly in terms of experimental design, definition of standard model output, and statistical aspects of model–data comparisons. Software developed in the course of previous MIPs, such as "performance portraits" and Taylor diagrams, provide useful means of summarizing many different aspects of climate model performance. In collaboration with groups such as the PCMDI, we intend to modify these diagnostic tools in order to suit the specific needs of the CCM community.

This suite of processes and diagnostics should become a benchmark for validation. Confidence in the performance of CCMs will increase as more model attributes become validated against the whole suite of diagnostics. Further, new models can be evaluated against an acknowledged, benchmark set of diagnostics as the models are developed. At the same time, the diagnostics themselves should develop as experience is gained and as new measurements become available allowing more processes to be diagnosed. It is hoped that this work has laid the groundwork for a more comprehensive approach to CCM validation, which will be further developed by all scientists who become involved. Updated information is available online at www.pa.op.dlr.de/CCMVal/, together with the names of people coordinating the various activities. All scientists interested in participating should contact the coordinating scientists.

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## APPENDIX A: ACRONYMS AND ABBREVIATIONS

| | |
|---|---|
| AMIP | Atmospheric Model Intercomparison Project |
| AMTRAC | Atmospheric Model with Transport and Chemistry |
| CCM | Coupled chemistry–climate model |
| CCMVal | CCM Validation Activity for SPARC |
| CCSR | Center for Climate System Research |
| CFC | Chlorofluorocarbon |
| CMAM | Canadian Middle Atmosphere Model |
| CMIP | Coupled Model Intercomparison Project |
| CTM | Chemical transport model |
| DLR | Deutsches Zentrum für Luft- und Raumfahrt (Germany) |
| E39/C | ECHAM4.L39(DLR)/CHEM |
| ECHAM | European Centre Hamburg Model |
| ECMWF | European Centre for Medium-Range Weather Forecasts (United Kingdom) |
| ERA | ECMWF Re-Analysis |
| EU | European Union |
| FUBCMAM | Freie Universitaet Berlin Climate Middle Atmosphere Model |
| GCCM | Global Tropospheric Climate–Chemistry Model |
| GCM | General circulation model |
| GEOS | Goddard Earth Observing System |
| GFDL | Geophysical Fluid Dynamics Laboratory (NOAA) |
| GISS | Goddard Institute for Space Studies (NASA) |
| GOME | Global Ozone Monitoring Experiment |
| GRIPS | GCM-Reality Intercomparison Project for SPARC |
| GSFC | Goddard Space Flight Center Model |
| GWD | Gravity wave drag |
| HAMMONIA | Hamburg Model of the Neutral and Ionized Atmosphere |
| IPCC | Intergovernmental Panel on Climate Change |
| J | Photolysis rate |
| K | Kelvin |
| LMDREPRO | Modele du Laboratoire de Meteorologie Dynamique-Chimie |
| MAECHAM/CHEM | Middle Atmosphere European Centre Hamburg Model with Chemistry |
| MESSy | Modular Earth Submodel System |
| MIP | Model Intercomparison Program |
| MRI | Meteorological Research Institute |
| MSU | Microwave sounding unit |
| NASA | National Aeronautics and Space Administration (United States) |
| NCAR | National Center for Atmospheric Research (United States) |
| NCEP | National Centers for Environmental Prediction (NOAA) |
| NIES | National Institute for Environmental Studies |
| NLTE | Nonlocal thermodynamical equilibrium |
| NonO-GWD | Nonorographic gravity wave drag |
| NOAA | National Oceanic and Atmospheric Administration (United States) |
| OCLI | Ozone Climate Interactions |
| O-GWD | Orographic gravity wave drag |
| PCMDI | Program for Climate Model Diagnosis and Intercomparison |
| PDF | Probability distribution function |
| PSC | Polar stratospheric cloud |
| PV | Potential vorticity |
| PW | Planetary wave |
| PWD | Planetary wave drag |
| QBO | Quasi-biennial oscillation |
| SOCOL | Solar Climate Ozone Links |
| SCIAMACHY | Scanning Imaging Absorption Spectrometer for Atmospheric Cartography |
| SSU | Stratospheric sounding unit |
| SPARC | Stratospheric Processes and their Role in Climate |
| 3D | Three-dimensional |
| TEM | Transformed Eulerian mean |
| TOMS | Total Ozone Mapping Spectrometer |
| TTL | Tropical tropopause layer |
| ULAQ | University of L'Aquila |
| UMETRAC | Unified Model with Eulerian Transport and Chemistry |
| UMSLIMCAT | Unified Model SLIMCAT |
| UMUCAM | Unified Model University of Cambridge |
| UNEP | United Nations Environment Programme |
| UTLS | Upper troposphere/lower stratosphere |
| UV | Ultravio |
| $v'T'$ | Heat flux |
| WACCM | Whole Atmosphere Community Climate Model |
| WCRP | World Climate Research Programme |
| WMO | World Meteorological Organization |
| WFA | Wavenumber–frequency analysis |

## APPENDIX B: CHEMICAL FORMULAS

| | |
|---|---|
| $BrO_x$ | Bromine radicals |
| $Br_y$ | Inorganic bromine |
| CFCs | Chlorofluorocarbons |
| CFC-11 | $CCl_3F$ |
| $CH_4$ | Methane |
| $ClO_x$ | Chlorine radicals |
| $Cl_y$ | Inorganic chlorine |
| $CO_2$ | Carbon dioxide |
| H | Atomic hydrogen |
| HCl | Hydrogen chloride (hydrochloric acid) |
| $HNO_3$ | Nitric acid |
| $HO_2$ | Hydroperoxyl radical |
| $HO_x$ | Odd hydrogen (H, OH, $HO_2$, $H_2O_2$) |
| $H_2O$ | Water vapor |
| OH | Hydroxyl radical |
| NO | Nitric oxide |
| $NO_2$ | Nitrogen dioxide |
| $NO_x$ | Nitrogen oxides (NO + $NO_2$) |
| $NO_y$ | Total reactive nitrogen (usually $NO_x$, $NO_3$, $N_2O_5$, $ClONO_2$, $HNO_4$, $HNO_3$) |
| $N_2O$ | Nitrous oxide |
| $O_x$ | Odd oxygen (O, O($^1$D), $O_3$) or oxidant ($O_3$ + $NO_2$) |
| $O_3$ | Ozone |
| $SF_6$ | Sulfur hexafluoride |

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