Progress Report for GCC Strategic Project Grant, July 2002

1. Name of Grantee: T.G. Shepherd, Department of Physics, University of Toronto

2. Project Title: Modelling of Global Chemistry for Climate (GCC), STPGP 235109

3. Co–investigators:

J.P.D. Abbatt, Department of Chemistry, University of Toronto
P.A. Ariya, Departments of Chemistry and Atmospheric & Oceanic Sciences, McGill University
I. Folkins, Department of Physics & Atmospheric Science, Dalhousie University
J. Li, Canadian Centre for Climate Modelling and Analysis, Meteorological Service of Canada, Victoria
U. Lohmann, Department of Physics & Atmospheric Science, Dalhousie University
J.C. McConnell, Department of Earth & Atmospheric Science, York University
N.A. McFarlane, Canadian Centre for Climate Modelling and Analysis, Meteorological Service of Canada, Victoria; also School of Earth & Ocean Sciences, University of Victoria
D.V. Michelangeli, Department of Earth & Atmospheric Science, York University
S.M. Polavarapu, ARMA, Meteorological Service of Canada, Toronto; also Department of Physics, University of Toronto
J.F. Scinocca, Canadian Centre for Climate Modelling and Analysis, Meteorological Service of Canada, Victoria; also School of Earth & Ocean Sciences, University of Victoria
W.E. Ward, Department of Physics, University of New Brunswick

4. Budget:

	NSERC Award	NSERC Spent	Partners Cash	Partners In-kind
Year 1	$431,750	$431,750	$538,005	$803,500
Year 2	$378,250	$269,262	$574,535	$803,500
Year 3	$366,250	$0	$594,665	$803,500
Year 4	$369,250	$0	$169,355 (partial)	$803,500
Year 5	$347,250	$0	not yet known	$803,500

N.B. "Spent" means spent or committed. "Partners Cash" includes GCC funding from CFCAS, which has replaced much of the MSC Climate Research Network funding promised in the original proposal (see more details under item 8 below); at this point we only have commitments until early in 2004 (Year 4), but there is the possibility of obtaining additional funding from CFCAS and CSA through to the end of the project, which we will request in due course.

5. Amount Remaining in the NSERC Grant Account as of 30 June 2002: $108,988.

6. Achievement of Objectives: The broad objectives of the GCC project are the development and use of a capability for modelling the global chemical climate of the atmosphere, both for climate change studies and for the integration of models and measurements. The achievement of our objectives is discussed for each of these aspects in turn. With the exceptions noted below, all tasks are proceeding on schedule.

Climate model development and validation. RA D. Plummer has coordinated the development of the tropospheric chemistry module in CMAM, including improved sources and sinks (Task I). Basic research has been conducted on aerosol properties and formation processes by the Abbatt and Lohmann groups (Task II), and on organic and sulfate oxidation processes by the Ariya group (Tasks I, II). An off-line diagnostic of the chemical transport budget has been developed by RA J. de Grandpré, and used to compare spectral and semi-Lagrangian transport (Task III). Basic research on dynamics and transport has been conducted by the

Shepherd group (Task III). Implementation of the correlated-k radiation scheme in CMAM (Task IV) by Li and RA V.I. Fomichev has been delayed because of problems CCCma had with the scheme, but is proceeding; other aspects of Task IV have progressed in the meantime. RA J.N. Koshyk completed his comparison of CMAM fields with radar measurements, and further comparisons with a variety of in-situ and space-based measurements have been carried out by the Folkins, McConnell, and Ward groups (Task VI). We continued our participation in the SPARC GRIPS middle atmosphere GCM intercomparison activity, sending delegations to the annual GRIPS workshops in Hamburg (2001) and Tsukuba (2002), and we participated (by invitation) in the inaugural SPARC/SCOSTEP workshop on temperature trends in the upper atmosphere (Kuhlungsborn, 2002).

Climate model applications. Scinocca and RA C. McLandress, and post-doc L. Campbell, have investigated the driving of the QBO by parameterized gravity waves in the tropics, and McLandress has examined the QBO's mesospheric effects (Task XII). The sensitivity of the resolved tropical waves to the parameterization of convection has been assessed (Task XIII) within the context of a SPARC GRIPS subproject. RA J. de Grandpré has also considered the effects of increased vertical and horizontal resolution on transport (Task XIII). In the fall of 2001 we were asked to participate in an intercomparison of five fully interactive chemistry-climate models for the 2002 WMO/UNEP Ozone Assessment (falling within Task VII, although not specifically anticipated). (These Assessments, now conducted every four years, form the scientific basis for the Montréal Protocol and its amendments.) The latest generation of models — one from the UK, one from Japan, two from Germany, and CMAM — was to be used to provide the current best estimate of future ozone changes, focusing on the coupling between the ozone layer and climate change. For this intercomparison we chose to perform three special-purpose "timeslice" experiments describing the 1980, 2000 and 2045 time periods. (CFCs are expected to return to 1980 levels in about 2045.) This was a significant effort in terms of both human and computational resources (mainly by RA S.R. Beagley and Shepherd, though many others also contributed), but we felt it was important for Canada to contribute to this activity. The results are described in Austin *et al.* (2002), and had a major impact on the conclusions of the 2002 Assessment. Taken together, the new simulations predict that there will *not* be a severe Arctic ozone hole (resulting from climate change) rivalling that of the Antarctic in the coming decades; this is in contrast to simpler calculations considered in the 1998 Assessment. This underscores the importance of participating in international assessments, because the collective result was much stronger than an individual model result could ever be. We will publish more detailed analyses of our own simulations in due course.

Data assimilation development and validation (Task V). After having coupled CMAM to MSC's 3D variational (3DVAR) data assimilation scheme, efforts focused on improving this system by adapting it to the new version of CMAM with T47L65 resolution and interactive chemistry. Statistics had to be defined that were appropriate for this model, and the 3DVAR scheme had to be adapted for a generalized vertical coordinate. This system was then validated for a one-month period (January 1994), and compared against the UKMO analysis. An assessment of data availability has however precluded the proposed reanalysis of the early UARS period; it is moreover essential to take advantage of the efforts of the MSC ARMA group for the operational weather forecast. The result has been a recent decision to focus efforts on the current time period. This also has the significant advantage of making the CMAM data assimilation product useful for current activities (see item 11). First results from the CMAM stratospheric assimilation have been presented at AGU and AMS conferences in December 2001 and January 2002 respectively, as well as at the first of what are expected to become annual SPARC stratospheric data assimilation workshops (Washington, D.C., June 2002).

Interpretation and analysis of measurements (Task X). RA C. McLandress has used CMAM data to construct synthetic measurements of stratospheric winds and ozone fluxes, in order to assess the measurement requirements (especially accuracy) needed to achieve the science goals of the Canadian SWIFT instrument, which is scheduled for launch in about five years' time on the Japanese GCOM-A1 satellite. These calculations have formed the basis of the SWIFT "Mission Requirements Document" being put together by the European Space Agency, which is managing the mission. Before he left the project, RA D. Chartrand began work on developing a trajectory model to facilitate comparison between CMAM fields and retrievals from the Canadian OSIRIS, ACE and MAESTRO instruments. In his absence, this work was carried forward by RA D. Sankey and by members of the McConnell group, and has now been picked up by RA K. Semeniuk. We will use synthetic chemical measurements from CMAM to determine the range of validity in space and time (as a function of altitude, latitude, and time of year) of trajectory methods for propagating chemical information. In related work, Sankey has assessed the validity of using chemical correlations to infer missing species.

Technology transfer (Task XIV), which is the responsibility of Scinocca and RA S.R. Beagley, is described in item 11. The highly collaborative nature of our project is reflected in various ways: in our active Scientific Steering Committee (which met in person to coordinate the research for at least one full day three times in 2001, and in March 2002, with the next meeting scheduled for early August 2002); in the CMAM data assimilation subgroup (see further discussion in item 8); and in the many research collaborations between different members of the project. These collaborations have yet to be reflected in many publications in item 10, as by their very nature they take longer to bear fruit, but we anticipate many such publications involving multiple members of the project to result over the next few years.

7. Problems Encountered: The only problems encountered have had to do with personnel, and the effects on the project have overall been limited. Highly experienced RAs J.N. Koshyk and D. Chartrand left their positions early in the project to work in the private sector. (In both cases, the reasons included both salary and the lack of perceived permanent opportunities within the academic or government research sectors.) Koshyk was replaced quickly with D. Sankey, while Chartrand left, then returned for a few months, then left again, and has recently been replaced with K. Semeniuk. Unfortunately, it takes a long time to replace the expertise that is lost when an experienced researcher leaves for the private sector.

8. Partnerships and Collaboration: Our non-academic partners are the Meteorological Service of Canada (MSC) and the Canadian Space Agency (CSA). From the MSC, Drs. Li, McFarlane, Polavarapu and Scinocca are involved as co-Investigators, and Drs. R. Ménard, Y. Rochon and K. von Salzen are involved as Collaborators. MSC provides considerable in-kind support of the GCC project, consisting of the time of its scientists as well as supercomputing time on the MSC computing system. At the time of the original proposal, the MSC had also promised very considerable cash support through its Climate Research Network (CRN). Severe cuts to MSC in the 2000 Federal budget subsequently led to a phasing-out of the CRN, and the GCC project received phase-out awards of $325,000 and $150,000 from the CRN in FY 2001-2 and 2002-3, respectively, following its transitional award of $344,300 in FY 2000-01. Fortunately, this phase-out coincided with the formation of the Canadian Foundation for Climate and Atmospheric Sciences (CFCAS), which has replaced the CRN in many respects — not just for our project. We successfully applied for CFCAS funding to replace the lost CRN funding, and took the opportunity to shore up a few gaps in our support. (In particular, MSC had intended to support Dr. S. Ren's participation in the GCC project from its own resources, but the same budget cuts that led to the demise of the CRN made this impossible, so we sought and obtained CFCAS funding for Ren as a GCC RA. We also obtained CFCAS funding for an RA devoted solely to tropospheric chemistry, D. Plummer.) This GCC application to CFCAS consisted of the original NSERC GCC application, together with a brief justification for the (relatively minor) budget changes, and was made in the context of the existing NSERC, MSC/CRN and CSA support for GCC. Our CFCAS support has been phasing in while our CRN support has been phasing out, with awards of \$155,105, \$352,125, and \$521,625 in FY 2001-2, 2002-3, and 2003-4, respectively. Meanwhile, CSA has delivered on its promised support of one RA equivalent, worth approximately \$78,000 per annum. The result is that our cash support from MSC, CFCAS, and CSA together has been both healthy and stable, as reflected in item 4. Our CFCAS support is presently assured until 31 March 2004, and our CSA support until 30 June 2004. Beyond that point, we have the possibility to apply for additional funding from both sources to take us to the end of the project timeline; we will make such applications in due course.

To supplement the interactions at our thrice-yearly Scientific Steering Committee meetings and annual workshops, the university-based RAs in our project have had the opportunity to spend extended periods of time at the MSC (CCCma) lab in Victoria. This past year, C. McLandress, D. Plummer, and S.R. Beagley have visited Victoria, and V.I. Fomichev will be making a visit later this year. Toronto-based S. Ren, Y. Yang and D. Sankey spend significant amounts of their time each week at the MSC (ARMA) lab in Toronto, including a biweekly meeting of the CMAM data assimilation subgroup (Task V) attended by Ren, Yang, Sankey and now Semeniuk from the university side, and by Rochon and Polavarapu from the MSC side. This CMAM data assimilation subgroup receives guidance from an Advisory Committee consisting of Shepherd and McConnell from the university side, and McFarlane, Ménard, and ARMA Chief D. Steenbergen from the MSC side, which meets three times per year.

Interaction with CSA occurs on an ongoing basis through the specification of our workplan each year, by which we focus our efforts to most effectively meet the needs of CSA's space science program. The most pressing such need at the present time is the definition of the science measurement requirements for the CSA-supported SWIFT instrument, as described in item 6 above. Since SWIFT's effectiveness will be assessed against these requirements, this is a crucial activity with far-reaching implications for CSA.

9. Training of Research Personnel: "NSERC" means the person's stipend was paid (at least in part) from the NSERC GCC Strategic Project Grant; "MSC", "CFCAS" and "CSA" mean it was paid from the direct GCC cash support from these agencies listed in item 4; and "other" means it was paid from supervisors' other sources.

J. Anstey, Ph.D. student, Toronto: Task VII [other]
S.R. Beagley, Research Associate, York: Tasks VII, XIV [MSC/CFCAS]
C. Braban, Ph.D. student, Toronto: Task II [NSERC]
C. Braun, Research Assistant, Dalhousie: Task VI [NSERC]
L. Campbell, Post-doctoral fellow, Toronto: Task XII [NSERC]
B. Carlin, Ph.D. student, Dalhousie: Task II [NSERC]
D. Chartrand, Research Associate, York: Tasks IX, X [NSERC/MSC/CFCAS/CSA]; now with Jacques Whitford Environmental Consultants
S. Codoban, Ph.D. student, Toronto: Task III [NSERC]
J. de Grandpré, Research Assistant, York: Tasks III, XIII [MSC/CFCAS]
V.I. Fomichev, Research Associate, York: Tasks IV, VIII, X [NSERC/MSC/CFCAS]
M. Fruman, Ph.D. student, Toronto: Task III [other]
C. Fu, Ph.D. student, York: Task VI [other]

A. Jonsson, Ph.D. student, Stockholm (long-term visitor at York): Task VI [NSERC]
J.N. Koshyk, Research Associate, Toronto: Tasks V, VI [MSC]; now with TD Bank
J.V. Lukovich, Ph.D. student, Toronto: Task III [NSERC]; now an RA at York
D. Matthews, M.Sc. student, McGill: Task II [NSERC]
C. McLandress, Research Associate, Toronto: Tasks X, XII [NSERC/MSC/CFCAS/CSA]
L. Neef, M.Sc. student, Toronto: Task V [other]
D. Pendlebury, Ph.D. student, Toronto: Task III [NSERC]; now a post-doc at Northwest Research Associates, Bellevue, WA
D. Plummer, Research Associate, York: Task I [CFCAS]
G. Probst, M.Sc. student, McGill: Task I [NSERC]
C. Reader, Research Associate, Victoria: Task II [MSC/CFCAS]
S. Ren, Research Associate, Toronto: Task V [CFCAS]
B. Revenaz, M.Sc. student, McGill: Task I [NSERC]; now with an environmental consulting company in the US
J. Russell, Post-doctoral fellow, UNB: Task VI [NSERC]
A. Ryzhkov, Post-doctoral fellow, McGill: Task I [NSERC]
D. Sankey, Research Associate, Toronto: Tasks III, V, X, XI [NSERC/MSC/CFCAS]
K. Semeniuk, Research Associate, York: Task IX, X [NSERC/MSC/CFCAS/CSA]
A. Tang, Ph.D. student, York: Task X [other]
J. Taylor, undergrad summer student, UNB: Task X [NSERC]; now a grad student at Toronto
X. Wang, Post-doctoral fellow, York: Task IX [NSERC]
Y. Yang, Research Associate, Toronto: Task V [NSERC]
X. Zhang, M.Sc. student, York: Task VI [other]; now an RA at York

10. Accessibility of Results to the Supporting Organizations:

• GCC Scientific Workshop, 5–6 November 2001, University of Toronto

This was our first workshop of the project, and will be followed by annual workshops every year in the late fall. These are basically internal workshops, to which all GCC participants (including students and post-docs) come and present their work. Other interested researchers within the Canadian community are also invited, and we bring in three renowned international experts for longer invited talks.

• T.G. Shepherd represented the GCC project at the MSC/CFCAS Climate Research Workshop in Ottawa on 5 March 2002, and at the CSA/MSC Atmospheric Environment Workshop in London, Ontario on 15-17 May 2002. These two workshops addressed respectively the climate modelling and models/measurements aspects of GCC, from the perspective of establishing the partners' research priorities.

• The project has so far resulted in 44 papers presented at national and international conferences, of which 16 were invited. (Our annual workshop is not included in this total.)

• Publications and theses arising directly from the project (*not* included here, so as not to double-count, are 10 papers written by GCC members and published in this time period which were listed as submitted or accepted in the final report for the MAM Phase 2 Strategic Grant):

Austin, J., Shindell, D., Beagley, S.R., Brühl, C., Dameris, M., Manzini, E., Nagashima, T., Newman, P., Pawson, S., Pitari, G., Rozanov, E., Schnadt, C. and T.G. Shepherd, 2002: Uncertainties and assessments of chemistry-climate models of the stratosphere. *Atmos. Chem. Phys.*, submitted.

Avzyanova, E. and P.A. Ariya, 2002: Kinetic studies of ozonolysis of selected terminal and internal alkenes: evaluation of HO yield. *Int. J. Chem. Kinet.*, in press.

Folkins, I., 2002: Origin of lapse rate changes in the upper tropical troposphere. *J. Atmos. Sci.*, **59**, 992–1005.

Folkins, I. and C. Braun, 2002: Tropical ozone as an indicator of deep convection. *J. Geophys. Res.*, in press.

Folkins, I. and C. Braun, 2002: Tropical rainfall and boundary layer convective mass. *J. Clim.*, submitted.

Folkins, I., Hintsa, E.J., Kelly, K.K. and E.M. Weinstock, 2002: Simple explanation for the 11 to 15 km increase in tropical relative humidity. *J. Geophys. Res.*, submitted.

Fu, C., McLandress, C., McConnell, J.C. and V.I. Fomichev, 2002: Impact of the diurnal tide on the seasonal and vertical variation of ozone in the equatorial upper mesosphere. *Geophys. Res. Lett.*, submitted.

Haynes, P.H. and T.G. Shepherd, 2001: Report on the SPARC Tropopause Workshop. *SPARC Newsletter*, No. 17, 3–10.

Jonsson, A., de Grandpré, J. and J.C. McConnell, 2002: A comparison of mesospheric temperatures from the Canadian Middle Atmosphere Model and HALOE observations: zonal mean and signature of the solar diurnal tide. *Geophys. Res. Lett.*, in press.

Kaercher, B. and U. Lohmann, 2002: A parameterization of cirrus cloud formation: homogeneous freezing of supercooled aerosols. *J. Geophys. Res.*, **107**, 10.1029/2001JD000470.

Kaercher, B. and U. Lohmann, 2002: A parameterization of cirrus cloud formation: homogeneous freezing including effects of aerosol size. *J. Geophys. Res.*, in press.

Lesins, G. and U. Lohmann, 2002: GCM aerosol forcing estimates using geographically varying aerosol sizes deduced from AERONET measurements. *J. Atmos. Sci.*, submitted.

Lohmann, U., 2002: Possible aerosol effects on ice clouds via contact nucleation. *J. Atmos. Sci.*, **59**, 647–656.

Lohmann, U., 2002: A glaciation indirect aerosol effect caused by soot aerosols. *Geophys. Res. Lett.*, **29**, 10.1029/2001GL014357.

Lohmann, U. and B. Kaercher, 2002: First interactive simulations of cirrus clouds formed by homogeneous freezing in the ECHAM GCM. *J. Geophys. Res.*, **107**, 10.1029/2001JD000767.

Manson, A.H., Meek, C.E., Hagan, M., Koshyk, J.N. *et al.*, 2002: Seasonal variations of the semi-diurnal and diurnal tides in the MLT: multi-year MF radar observations from 2-70°N, modelled tides (GSWM, CMAM). *Ann. Geophys.*, **20**, 661–677.

Manson, A.H., Meek, C.E., Koshyk, J.N. *et al.*, 2002: Gravity-wave activity and dynamical effects in the middle atmosphere (60-90 km): observations from an MF/MLT radar network and results from the Canadian Middle Atmosphere Model (CMAM). *J. Atmos. Sol.-Terr. Phys.*, **64**, 65–90.

Matthews, D. and P.A. Ariya, 2002: Reactions of DMS in the marine boundary layer. *Atmos. Env.*, submitted.

McLandress, C., 2002: Interannual variations of the diurnal tide in the mesosphere induced by zonal-mean wind oscillations in the tropics. *Geophys. Res. Lett.*, in press.

Pendlebury, D. and T.G. Shepherd, 2002: Planetary-wave-induced transport in the stratosphere. *J. Atmos. Sci.*, submitted.

Ryzhkov, A., Leighton, H.G. and P.A. Ariya, 2002: Formation pathways for peroxides upon reactions of Criegee biradical. *J. Phys. Chem.*, submitted.

Sankey, D. and T.G. Shepherd, 2002: Correlations of long-lived chemical species in a middle atmosphere general circulation model. *J. Geophys. Res.*, submitted.

Scinocca, J.F., 2002: Nonhydrostatic effects in the parameterization of non-orographic gravity-wave drag. *J. Meteor. Soc. Japan*, in press.

Scinocca, J.F., 2002: An accurate spectral non-orographic gravity wave parameterization for general circulation models. *J. Atmos. Sci.*, submitted.

Shepherd, T.G., 2002: Issues in stratosphere-troposphere coupling. *J. Meteor. Soc. Japan*, in press.

Theses:

Lukovich, J.V.: Large-scale mixing in the middle atmosphere. Ph.D. thesis, Department of Physics, University of Toronto, 2001.

Pendlebury, D.: Planetary-wave-induced transport in the stratosphere. Ph.D. thesis, Department of Physics, University of Toronto, 2001.

Revenaz, B.: Box modelling of HO_x formation upon ozonolysis of alkenes. M.Sc. thesis, Department of Chemistry, McGill University, 2001.

Zhang, X.: A comparison of CMAM and HALOE mesospheric data. M.Sc. thesis, Department of Earth and Atmospheric Science, York University, 2002.

11. Potential Benefits: We have completed the technology transfer of the gas-phase stratospheric chemistry module of CMAM to MSC, and the code is now being run and further optimized within the CCCma environment. Because of the large number of advected chemical species, the treatment of advected tracers in the CCCma GCM had to be completely modified. Transfer of the heterogeneous chemistry module is now underway. When complete, CCCma will be in a position to perform climate simulations addressing the interaction between ozone depletion and climate change. Later in the project, the tropospheric chemistry module being developed by GCC will also be transferred to MSC, and will be designed to extend its existing sulfate chemistry in a natural fashion. When coupled with other modules (land-surface, biogenic emission/uptake, ocean), this will provide CCCma with the capability of simulating chemical climate in a fully interactive fashion, thereby helping it to stay at the leading edge of the IPCC assessment activity.

The development of a stratospheric data assimilation capability based on CMAM is now essentially complete, and CMAM will soon be running in a continuous data assimilation cycle using current data. This development has led to some spin-off benefits for the operational NWP assimilation activities at MSC. Because CMAM is being run with stratospheric chemistry, the stratospheric analyses will include chemical as well as dynamical fields. (Unlike with dynamical fields, it is not necessary to assimilate chemical fields in order to produce a useful chemical analysis; this fact underlies the use of Chemical Transport Models.) As a first application, it is anticipated that MSC may soon be able to use the CMAM ozone analyses. CMAM chemical analyses should also be useful for direct comparison with current Canadian stratospheric chemistry measurement programs such as MANTRA (balloon), OSIRIS, ACE and MAESTRO (satellite), and Eureka (ground-based). The CMAM middle atmosphere data assimilation capability (both dynamical and chemical) will be a unique tool within the international context, which will enable CSA to assess proposed new measurement strategies in a sophisticated fashion.

The CSA has recently made a commitment to invest heavily in research into planetary atmospheres, with a particular focus on Mars. It turns out that CMAM is ideally suited for development as a model of the Martian atmosphere. Although this development has yet to begin, it represents a clear potential benefit of the GCC activity to the burgeoning Canadian research community in planetary atmospheres, both experimental and theoretical.