

## NOTES AND CORRESPONDENCE

Effect of Temperature Feedback and Hydrostatic Adjustment  
in a Stratospheric Model

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## ABSTRACT

Calculated perturbations to stratospheric ozone are generally thought to be reduced when temperature feedback is included in the model. We find that when self-consistent hydrostatic adjustment is included with temperature feedback, there can be significant differences in the computed change in local ozone concentration. We present results in two frames of reference (changes in ozone at constant altitude and changes at constant pressure) to illustrate the importance of the frame of reference. Including hydrostatic adjustment is particularly important for calculations of the change in local ozone at constant altitude due to CFM, CO<sub>2</sub> and H<sub>2</sub>O perturbations because large changes in the temperature structure are predicted. Only small differences are computed for increases in N<sub>2</sub>O. Air density adjustment in a constant pressure frame of reference is important when local temperature changes are large.

## 1. Introduction

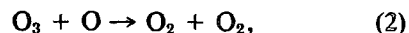
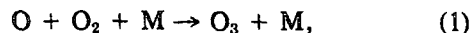
The concentration of ozone in the stratosphere is determined by a complex coupling of chemistry, dynamics and temperature. Most models of the stratosphere that consider perturbations to the chemistry ignore possible changes due to coupling and feedbacks from dynamics and temperature. These models provide a reasonable first-order picture of how the atmosphere might respond to changes in chemistry. A more detailed and accurate picture, however, is obtained with the use of a model capable of also calculating the temperature structure of the atmosphere.

There are three major mechanisms that couple changes in temperature and changes in atmospheric composition. The first mechanism is radiative coupling between temperature and species concentrations. Perturbations to the atmospheric composition affect the temperature profile via the solar and longwave radiation balance. The species O<sub>3</sub>, O<sub>2</sub> and NO<sub>2</sub> are the most effective absorbers of solar radiation in the stratosphere, and O<sub>3</sub>, CO<sub>2</sub> and H<sub>2</sub>O are the most effective absorbers and emitters of longwave radiation in the ambient stratosphere. Large increases in the concentrations of trace species such as CFCl<sub>3</sub>, CF<sub>2</sub>Cl<sub>2</sub> and N<sub>2</sub>O also can significantly affect stratospheric and tropospheric temperatures by their longwave effect (Wang *et al.*, 1976).

The temperature profile in the upper stratosphere

is controlled strongly by the amount of solar absorption by O<sub>3</sub>. Consequently, a decrease in O<sub>3</sub> in the upper stratosphere results in a decrease in the local temperature in that region. In the lower stratosphere the temperature change may have either the same or the opposite sign as the change in ozone depending upon the magnitude of the change to other species and on the structure of the ambient temperature profile (Luther *et al.*, 1977).

The second mechanism is the coupling between temperature and chemical reaction rate coefficients. Changes in temperature may affect species concentrations directly by changing rate coefficients that affect rates of production and destruction of that species or indirectly by changing the concentration of other species upon which production and destruction rates depend (e.g., Blake and Lindzen, 1973). For example, due to the temperature dependence of the reactions



in a fully coupled model, the ozone concentration is not decreased as much as one would calculate when temperature feedback is not included in the model.

The third mechanism is the coupling between changes in air density and changes in rates of reaction. Under conditions of hydrostatic equilibrium and the ideal gas law, changes in the

temperature profile change the air density at a given altitude or pressure level as the atmosphere expands or contracts. Species concentrations at a given level are affected both by changes in density at the level and by changes in rates of reaction due to changes in species concentrations and changes in  $M$ .

The effect of including temperature feedback without hydrostatic adjustment has been included in a number of model calculations (McElroy *et al.*, 1974; Luther *et al.*, 1977; Luther and Duewer, 1978; Boughner, 1978; Groves *et al.*, 1978). These studies considered the effect of temperature feedback on the computed change in ozone due to  $\text{NO}_x$  emissions, releases of chlorofluoromethanes (CFM's), increases in stratospheric  $\text{H}_2\text{O}$ , and doubling of  $\text{CO}_2$ . Chandra *et al.* (1978) included hydrostatic adjustment along with temperature feedback in an assessment of the effect of CFM's on ozone.

During the past several years, our understanding of stratospheric chemistry has improved, leading to significant changes in model chemistry. In this note we examine the effect of temperature feedback and hydrostatic adjustment for several perturbations using updated chemistry. We examine how temperature feedback and hydrostatic adjustment separately affect the calculated change in  $\text{O}_3$  in order to determine when these feedback processes have significant effects on computed changes in either the local concentration or total column of  $\text{O}_3$ .

## 2. Model description

We used the LLL fully coupled one-dimensional transport-kinetics model with radiative equilibrium submodel in this theoretical study. The basic model structure and solution technique are described in Chang *et al.* (1974). A recent general description of the model is included in Luther *et al.* (1979).<sup>1</sup>

Individual species conservation equations are solved simultaneously by means of a variable order multistep implicit method for 34 species [ $\text{O}_3$ ,  $\text{O}(^3\text{P})$ ,  $\text{NO}$ ,  $\text{NO}_2$ ,  $\text{N}_2\text{O}$ ,  $\text{HNO}_3$ ,  $\text{OH}$ ,  $\text{HO}_2$ ,  $\text{H}_2\text{O}_2$ ,  $\text{Cl}$ ,  $\text{ClONO}_2$ ,  $\text{ClO}$ ,  $\text{ClNO}_2$ ,  $\text{HCl}$ ,  $\text{NO}_3$ ,  $\text{N}_2\text{O}_5$ ,  $\text{HONO}_2$ ,  $\text{HNO}_4$ ,  $\text{HOCl}$ ,  $\text{HCO}$ ,  $\text{CH}_2\text{O}$ ,  $\text{CH}_3$ ,  $\text{CH}_3\text{OOH}$ ,  $\text{CH}_3\text{O}$ ,  $\text{CH}_3\text{O}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{CH}_4$ ,  $\text{H}_2$ ,  $\text{CO}$ ,  $\text{CH}_3\text{Cl}$ ,  $\text{CH}_3\text{CCl}_3$ ,  $\text{CCl}_4$ ,  $\text{CF}_2\text{Cl}_2$  and  $\text{CFCl}_3$ ]. Local photochemical equilibrium is assumed for  $\text{O}(^1\text{D})$ ,  $\text{H}$  and  $\text{N}$ . Unless otherwise specified, the vertical distributions of  $\text{N}_2$  and  $\text{O}_2$  are adjusted to satisfy hydrostatic equilibrium at each time step, and the concentrations of the other species are adjusted using interpolation based on the adjustment to  $\text{N}_2$  and  $\text{O}_2$ . The column

abundances of  $\text{O}_2$  and  $\text{O}_3$  at the top boundary are calculated consistent with the calculated temperature and density at that level.

The solar flux, reaction rate coefficients, and absorption coefficients are those recommended in NASA (1979)<sup>2</sup> (see also Luther *et al.*, 1979).<sup>1</sup> Photodissociation rate coefficients are computed at each altitude and time step consistent with all species distributions and the specified solar conditions including multiple scattering (see Luther *et al.*, 1978). The model contains 120 chemical or photochemical reactions.

The model atmosphere extends from the ground to 56.25 km and is divided into 44 layers. Vertical transport in the model is parameterized through an empirically derived "effective" diffusion coefficient (NAS, 1976).<sup>3</sup> The boundary conditions for individual species are either fixed concentrations or fluxes at the surface and flux conditions at the upper boundary. For the long-lived trace species with tropospheric sources, the observed tropospheric mixing ratios in 1977 were used as the boundary conditions. Our ambient atmosphere contains  $\sim 2.0$  ppb  $\text{Cl}_x$  and this atmosphere is used for all comparisons to perturbed atmospheres. The ambient and perturbed atmospheres refer to equilibrium (steady state) conditions.

The temperature is computed using a radiative transfer model assuming radiative equilibrium in the stratosphere. The model includes solar absorption and longwave interaction by  $\text{O}_3$ ,  $\text{CO}_2$  and  $\text{H}_2\text{O}$  and solar absorption by  $\text{NO}_2$  (Luther *et al.*, 1977). The temperature profile is computed above 13 km and is specified below this altitude according to the U.S. Standard Atmosphere (1976). Changes in surface and tropospheric temperatures up to 13 km may be imposed. A full description of current model results for the ambient atmosphere and comparisons with observations are included in Luther *et al.* (1979).<sup>1</sup>

For some of the perturbations that we consider, we assume that the change in surface temperature is negligible. Small temperature changes in the troposphere ( $< 0.5$  K) are expected for perturbations to  $\text{N}_2\text{O}$ ,  $\text{CF}_2\text{Cl}_2$  and  $\text{CFCl}_3$ , and the stratospheric temperature changes due to the infrared properties of these species are also expected to be small (V. Ramanathan, NCAR, private communication, 1979). Based on the work of Manabe and Wetherald (1967), it can be estimated that an increase in the stratospheric water vapor mixing ratio of 2 ppmv will cause an increase in surface temperature

<sup>1</sup> Luther, F. M., J. S. Chang, W. H. Duewer, J. E. Penner, R. L. Tarp and D. J. Wuebbles, 1979: Potential environmental effects of aircraft emissions, Lawrence Livermore Laboratory Report 222 pp. [NTIS UCRL-52861].

<sup>2</sup> NASA Reference Publication 1049, 1979: The stratosphere: Present and future, R. D. Hudson and E. I. Reed, Eds. Washington, DC, 432 pp.

<sup>3</sup> National Academy of Sciences, 1976: Halocarbons: Effects on stratospheric ozone. Washington, DC, 352 pp.

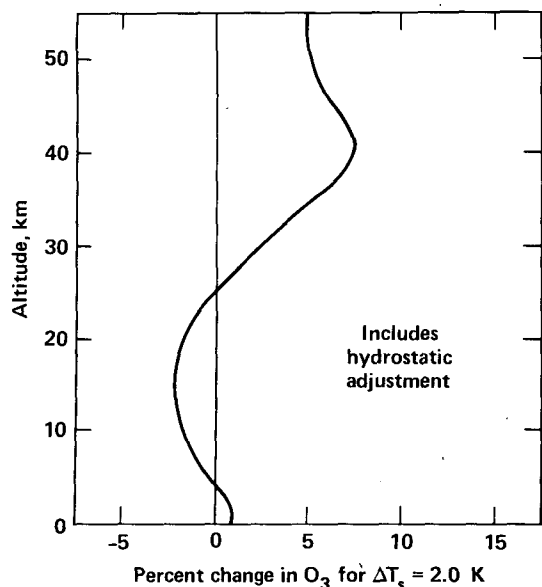


FIG. 1. Percent change in  $O_3$  for a tropospheric temperature increase of 2.0 K.

of  $\leq 0.2$  K. Increasing the surface temperature (and tropospheric temperatures) in our model by 0.5 K causes an increase in total ozone of 0.1%. Neglecting changes in surface temperature of this magnitude has no significant effect on the results. When significant changes in surface temperature are expected, they are imposed in the model.

Imposing a change in tropospheric temperatures has little effect on the stratosphere at a given pressure level because the major effect of hydrostatic adjustment is just to raise or lower the stratosphere as the troposphere expands or contracts. There are slight temperature changes at pressure levels in the lower stratosphere because the upward longwave flux from the troposphere into the stratosphere is changed. When the resulting changes in species concentrations are plotted in a constant altitude frame of reference, the changes in species concentrations may appear significant even though the change in total column is small. This effect is illustrated in Fig. 1, which shows the percent change in  $O_3$  as a function of altitude resulting from an imposed 2.0 K increase in tropospheric temperature. Ozone concentrations decreased slightly below 25 km and increased by as much as 6.5% at 40 km. The apparent changes are caused by a lifting of the ozone profile in the stratosphere due to expansion of the troposphere. Since most studies in the past have presented results in terms of altitude coordinates, we too shall illustrate changes in this frame of reference. However, it is important especially for high-altitude changes that the results be plotted in pressure coordinates because remote sensing tech-

niques provide ozone concentrations as functions of pressure. In the following discussion we illustrate changes in both frames of reference in order to determine the differences and to show when it is important to distinguish between pressure and altitude coordinates.

### 3. Results

We consider four types of perturbations in this paper. Each one is interesting in itself as a possible atmospheric change and illustrates a different sort of change in the temperature structure so that the effects from including or not including temperature feedback and hydrostatic adjustment are quite different.

#### a. Doubling of $N_2O$

A doubling of the surface concentration of  $N_2O$  might be expected if increased land cultivation and fertilizer use or increased disposal of human waste were to stimulate increased bacterial production of  $N_2O$  (NASA, 1979).<sup>2</sup> Increases in atmospheric  $N_2O$  cause an increase in stratospheric  $NO_x$ . The effect on  $O_3$  of increases in  $NO_x$  depends on altitude. At altitudes below  $\sim 24$  km in our model,  $O_3$  is increased when the  $N_2O$  concentration at the ground is doubled primarily because of increased production by a chain of reactions, similar to those that produce  $O_3$  in urban smog (see, e.g., NASA, 1979).<sup>2</sup>

At altitudes above 24 km, catalytic destruction of ozone by the  $NO_x$  destruction cycle, is more efficient, and the net effect is that  $O_3$  (i.e., odd-oxygen) is destroyed. The effect on the temperature structure in a temperature-coupled model, therefore, is also different in the two altitude regions. The temperature is increased in the lower stratosphere and decreased in the upper stratosphere.

The separate effects of including temperature feedback and hydrostatic adjustment in the perturbation calculation for a doubling of the concentration of  $N_2O$  at the ground from 320 to 640 ppb are illustrated in Fig. 2. Fig. 2a shows the percent change in  $O_3$  as a function of altitude for three cases: no temperature feedback, temperature feedback without hydrostatic adjustment and a fully coupled calculation with temperature feedback and hydrostatic adjustment. Including temperature feedback alone acts to lessen the effects of the perturbation locally, as expected from the temperature dependence of reactions (1) and (2). As shown in Fig. 2b, the temperature perturbation is small, less than  $\pm 1.3$  K and of opposite sign at low and high altitudes. Thus, the effects of hydrostatic adjustment are also small and, in fact, cannot be distinguished in the figure from the case of no hydrostatic adjustment. Similar remarks apply for

changes plotted with respect to pressure coordinates. Since the temperature change is small, there is only a small change in the air density. Consequently, the results appear nearly the same when plotted in constant pressure coordinates and are not shown separately for this perturbation.

*b. Releases of CFM's*

Increases in  $CF_2Cl_2$  and  $CFCl_3$  are expected if industrial production and release continue at current rates.  $CF_2Cl_2$  and  $CFCl_3$  are both photolyzed in the stratosphere to produce free chlorine,  $Cl_x$ , which is able to catalytically destroy ozone.

Figs. 3a, 3b and 3c show the calculated percent change in  $O_3$  concentration and the change in temperature when  $CF_2Cl_2$  and  $CFCl_3$  have increased to 1.8 and 0.75 ppb, respectively, compared to an ambient atmosphere which contained 0.22 ppb  $CF_2Cl_2$  and 0.14 ppb  $CFCl_3$  (approximately present day conditions). This represents the expected change at steady state for constant production and release of  $CF_2Cl_2$  and  $CFCl_3$  at 1976 rates. Three cases are again considered: no temperature feedback, temperature feedback without hydrostatic adjustment, and the complete model calculation. The results in Fig. 3a for constant altitude coordinates are similar to those presented by Chandra *et al.* (1978) for this perturbation.

Comparison of Figs. 3a and 3c illustrates the differences caused by viewing changes in constant

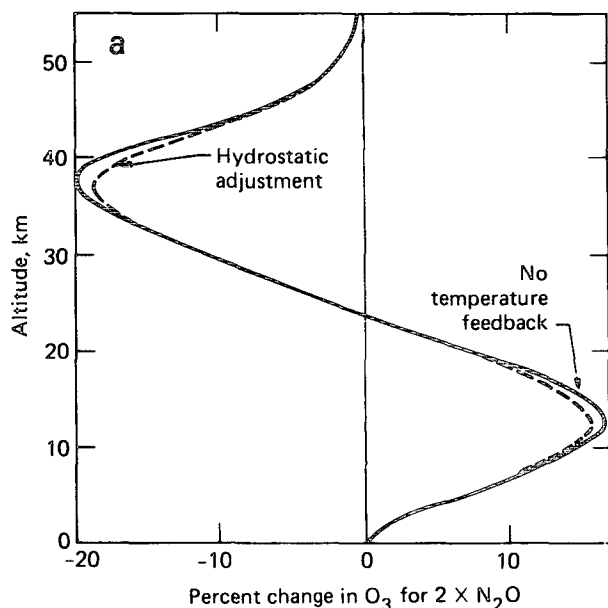


FIG. 2a. Percent change in  $O_3$  for a doubling of the surface  $N_2O$  concentration. The full line shows a calculation which did not include temperature feedback. The dashed line shows the results including temperature feedback only and including temperature feedback and hydrostatic adjustment (same line).

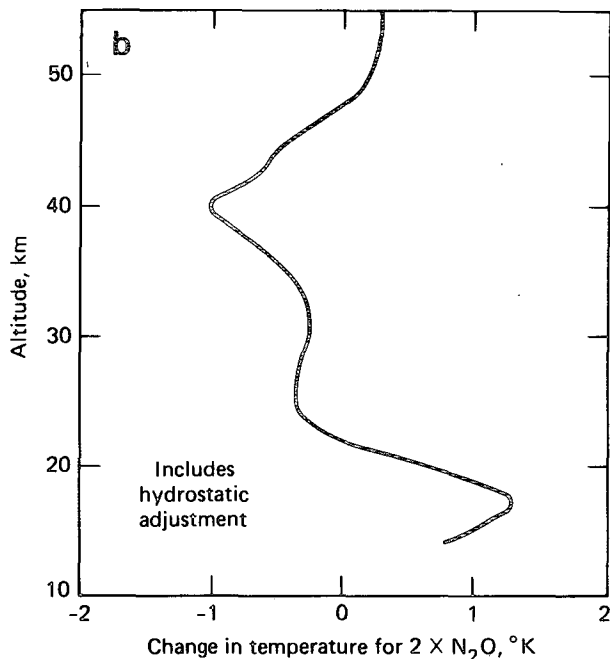


FIG. 2b. Change in temperature for a doubling of the surface  $N_2O$  concentration.

altitude coordinates and constant pressure coordinates. In constant altitude coordinates, the difference between the fully coupled calculation and the calculation that includes hydrostatic adjustment begins to be important at levels above 45 km, due to the cumulative effects of temperature changes below that level. In constant pressure coordinates, only local changes in temperature and therefore air density are able to perturb the chemistry, so that differences between including or not including hydrostatic adjustment are confined to pressure levels where large changes in temperature are calculated (cf. Fig. 3b). In addition, in regions where  $O_3$  is photochemically controlled, negative changes in temperature always have the effect of restoring the ozone concentration in pressure coordinates, but can be associated with a decrease in ozone at high altitude if viewed in constant altitude coordinates.

*c. Doubling of  $CO_2$*

Atmospheric  $CO_2$  is expected to double in 50–100 years assuming the use of fossil fuels continues to grow. Increased atmospheric  $CO_2$  is expected to increase surface and tropospheric temperatures due to the increased greenhouse effect. However, increases in  $CO_2$  should cool the stratosphere where infrared optical depths are small. Reductions in stratospheric temperature cause increases in  $O_3$  due in part to the coupling through temperature-dependent reaction rates for (1) and (2). The changes in

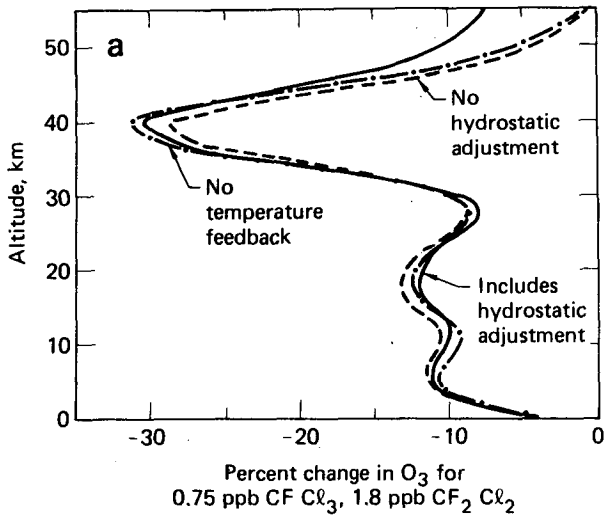


FIG. 3a. Percent change in  $O_3$  for increases in  $CFCl_3$  and  $CF_2Cl_2$  from 0.14 and 0.22 ppb to 0.7 and 1.8 ppb, respectively. The dash-dot line shows a calculation which did not include temperature feedback. The dashed line includes temperature feedback but does not include hydrostatic adjustment, and the full line shows the results of a fully coupled calculation.

ozone concentration and temperature caused by increasing  $CO_2$  from 320 to 640 ppm are shown in Figs. 4a–4c. The calculated temperature change is large (nearly 10 K) near 40 km. Because the temperature change is large, the difference between the calculated change in ozone including hydrostatic adjustment and the change including temperature feedback alone is also large even when viewed in a constant pressure level frame of reference (Fig. 4c). For this perturbation, a significantly larger

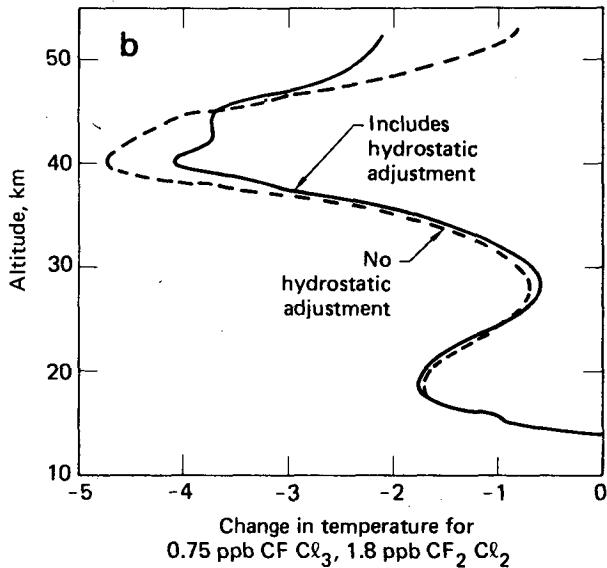


FIG. 3b. Change in temperature for the same calculation as in Fig. 3a (see caption for 3a).

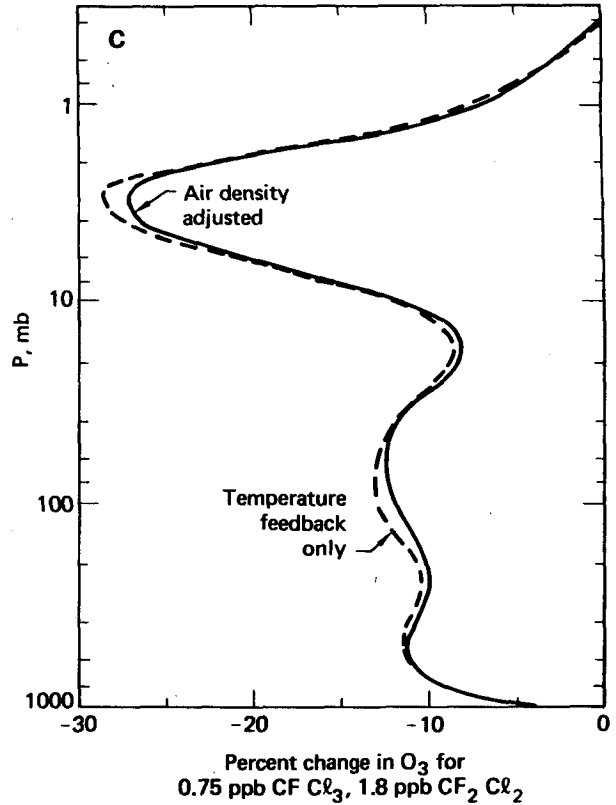


FIG. 3c. Percent change in  $O_3$  at constant pressure levels for the same calculation as Fig. 3a. The full line includes all feedbacks while for the dashed line the background air density was held constant.

increase in local ozone concentration ( $\sim 5\%$  larger at pressure levels near 40 km) is predicted with the fully coupled model.

Fig. 4a also shows the results of a calculation in which we increased the tropospheric temperature by 2.0 K, which is the approximate steady-state surface temperature increase expected for doubled  $CO_2$  (Schneider, 1975). As noted above, tropospheric temperature changes cause changes in air density and concentrations in a constant altitude coordinate system due to hydrostatic adjustment. In this model if the tropospheric temperature is increased 2.0 K, the predicted ozone change at 40 km is increased from 10% to almost 16%. Differences caused by tropospheric temperature changes are negligible, however, if the change in  $O_3$  is plotted as a function of pressure.

d. Doubling of stratospheric  $H_2O$

This perturbation is included to test the model sensitivity to changes in ambient  $H_2O$  levels. This perturbation is also relevant because changes in tropical tropopause temperatures (due perhaps to  $CO_2$  increases) or changes in tropospheric-strato-

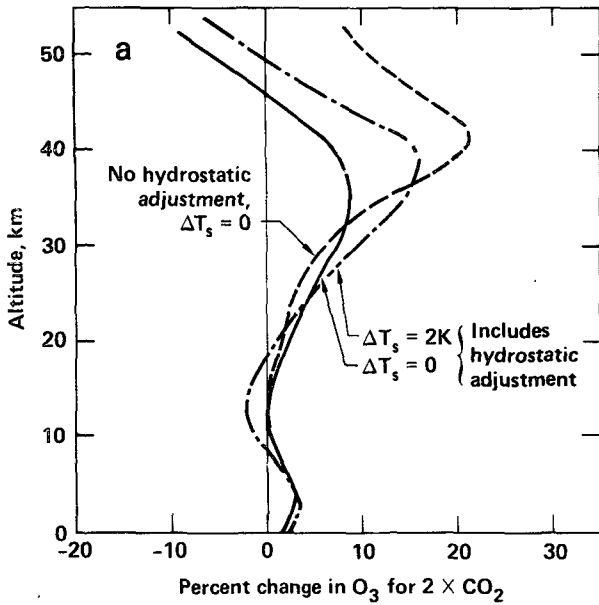


FIG. 4a. Percent change in  $O_3$  for a doubling of the atmospheric  $CO_2$  concentration. The dashed line shows a calculation with temperature feedback but without hydrostatic adjustment. The full and dash-dot curves include hydrostatic adjustment and temperature feedback. For the curve marked  $\Delta T_s = 0$ , the ambient tropospheric temperature was used. For the curve marked  $\Delta T_s = 2\text{ K}$ , the ambient tropospheric temperature was increased by 2.0 K.

spheric exchange rates may lead to increases in stratospheric water vapor.

Figs. 5a and 5b show the calculated change in  $O_3$  and temperature caused by doubling strato-

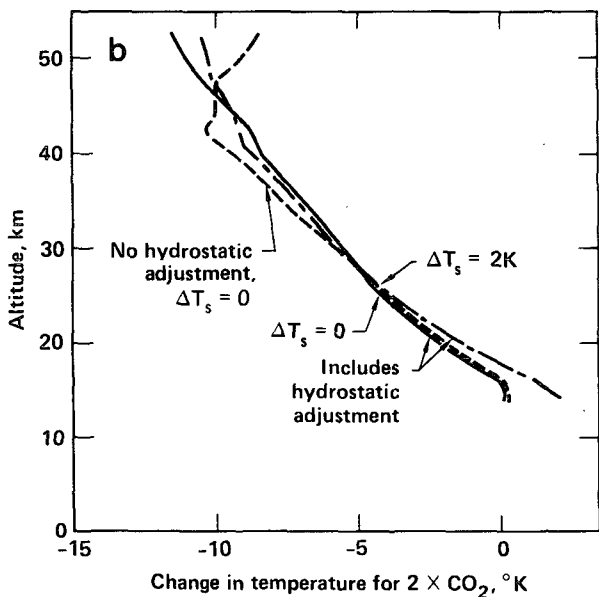


FIG. 4b. Change in temperature for a doubling of the  $CO_2$  concentration (see caption for Fig. 4a).

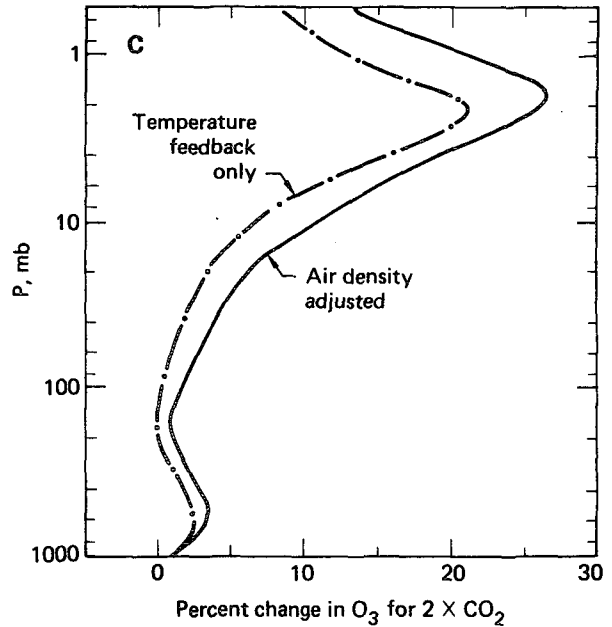


FIG. 4c. Percent change in  $O_3$  at constant pressure levels for the same calculation as Fig. 4a. The full line includes all feedbacks while for the dashed line the background air density was held constant.

spheric water vapor from 3.6 to 7.2 ppm at 14 km. In this case the calculated temperature change results from both increased  $H_2O$  and decreased  $O_3$ . The

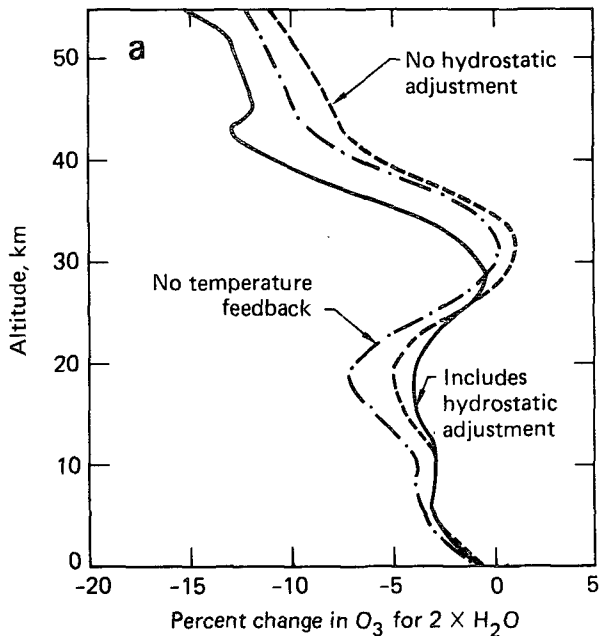


FIG. 5a. Percent change in  $O_3$  for a doubling of the stratospheric  $H_2O$  concentration. The dash-dot line shows a calculation which did not include temperature feedback. The dashed line included temperature feedback but did not include hydrostatic adjustment. The full line was calculated using the fully coupled model.

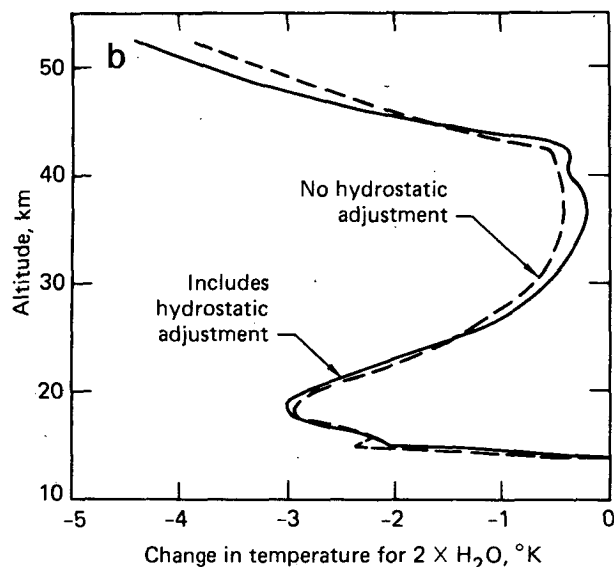


FIG. 5b. Change in temperature for a doubling of the stratospheric  $H_2O$  concentration (see caption for Fig. 5a).

decrease in  $O_3$  is mainly the result of increased  $HO_x$  ( $OH + HO_2 + 2 \times H_2O_2$ ), which is produced from the reaction of  $O(^1D)$  with  $H_2O$ . As was the case for the preceding calculations, when tempera-

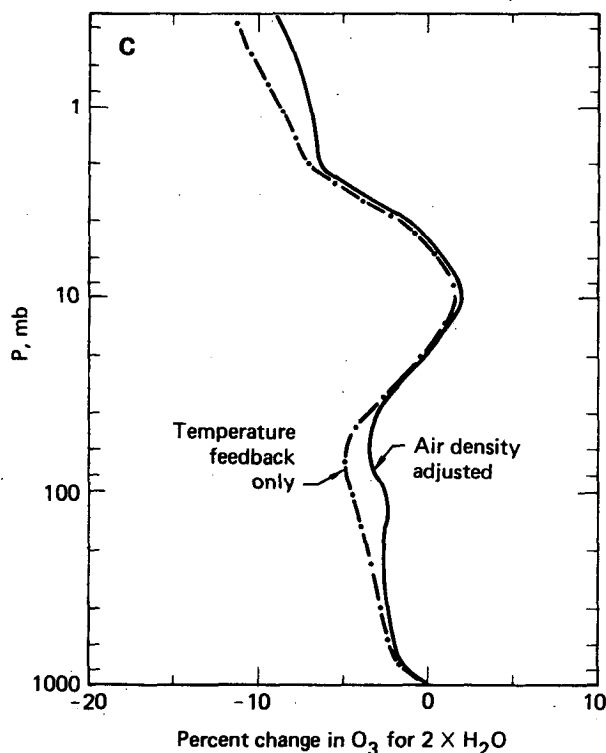


FIG. 5c. Percent change in  $O_3$  at constant pressure levels for the same calculation as Fig. 5a. The full line includes all feedbacks while for the dashed line the air density was held constant.

TABLE 1. The percent change in  $O_3$  concentration at 2 mb.

Perturbation	Percent change in $O_3$ at 2 mb		
	Temperature feedback and hydrostatic adjustment	Temperature feedback only	No temperature feedback
$2 \times N_2O$	-12	-12	-13
0.75 ppb $CFCl_3^*$			
1.8 ppb $CF_2Cl_2$	-23	-23	-27
$2 \times CO_2$ ( $\Delta T_s = 2K$ )	27	21	0.0
$2 \times H_2O$	-7.1	-7.2	-8.8

\* The calculated changes in ozone are with respect to an ambient atmosphere containing 0.22 ppb  $CF_2Cl_2$  and 0.14  $CFCl_3$ .

ture feedback is included, the perturbation is reduced. When hydrostatic adjustment is also included, differences are large throughout the region when viewed in constant altitude coordinates (Fig. 5a), but are confined to pressure levels where temperature changes are significant in constant pressure coordinates (cf. Fig. 5b and 5c).

The results presented here have focused on calculated changes in local ozone concentration as a function of altitude. The altitude structure of predicted changes is important because it may be easier to detect anthropogenic changes to the ozone layer at high altitude (NASA, 1979),<sup>2</sup> where local changes are largest on a percentage basis.

Table 1 summarizes our results for the percent change in  $O_3$  at 2 mb ( $\sim 40$  km) for all perturbations considered. The percent changes in total  $O_3$  are shown in Table 2. In most cases the differences in the predicted change in total  $O_3$  for the three cases (no temperature feedback, temperature feedback without hydrostatic adjustment, and temperature feedback with hydrostatic adjustment) are small—less than 1% in absolute amount.

#### 4. Summary and conclusions

Simulations using the Lawrence Livermore Laboratory one-dimensional stratosphere model show

TABLE 2. Percent change in total ozone column.

Perturbation	Percent change in total $O_3$		
	Temperature feedback and hydrostatic adjustment	Temperature feedback only	No temperature feedback
$2 \times N_2O$	-2.3	-2.2	-1.9
0.75 ppb $CFCl_3^*$			
1.8 ppb $CF_2Cl_2$	-12.4	-12.4	-12.3
$2 \times CO_2$ ( $\Delta T_s = 0$ )	5.4	4.6	0.0
$2 \times CO_2$ ( $\Delta T_s = 2K$ )	5.8		
$2 \times H_2O$	-1.9	-1.8	-3.5

\* The changes in total ozone are with respect to an ambient atmosphere containing 0.22 ppb  $CF_2Cl_2$  and 0.14  $CFCl_3$  (approximately present day conditions). The computed change in total ozone at steady state with no temperature feedback is -14.2% compared to an ambient atmosphere without CFM's.

significant differences in predicted local ozone changes depending on whether or not temperature feedback and hydrostatic adjustment are included. We find that the calculated effects at high altitude are sensitive to tropospheric temperature changes but that differences are minimized when results are plotted in constant pressure coordinates. Because the calculated local ozone changes are largest on a percentage basis at high altitude (for each of the perturbations considered), monitoring high-altitude ozone changes may provide an early warning signal for anthropogenically caused ozone changes and a method for validating models (NASA, 1049). It is important, therefore, to include the effects of temperature feedback and changes in the air density when computing local changes in ozone for comparison with observational data. Including hydrostatic adjustment in a constant altitude frame of reference or air density adjustment in a constant pressure frame of reference is particularly important for calculations of the local ozone depletion due to CFM, CO<sub>2</sub> and H<sub>2</sub>O perturbations because large changes in the temperature structure are predicted.

In the atmosphere there is a complex coupling between chemistry, temperature and dynamics. We have explored in more detail the coupling between chemistry and temperature, but the effect of changes in atmospheric composition and temperature on dynamics was not included. To explore the coupling with dynamics, all of these effects will have to be included in a three-dimensional general circulation model. Because of computational limitations, it is not possible to include all of these effects in a three-dimensional model at this time. The problem is compounded by the fact that the model simulations must cover 10's to 100's of years for these perturbations to reach steady state. In the meantime, considerable insight is gained by the use of one- and two-dimensional models.

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