INFLUENCES OF GRAVITY WAVES THROUGH PHOTOCHEMICAL HEATING IN THE MESOSPHERIC REGION

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ABSTRACT
In this paper, the influence of gravity waves on photochemical heating in the mesospheric region has been studied. The loss of photochemical heating induced by gravity waves is determined by the amplitude of the perturbation, besides the background distributions of temperature and atomic oxygen. Two important results has been investigated, firstly; gravity wave cause a loss of photochemical heating in this region, secondly; as background temperature decreases, or as the background atomic oxygen density increases, the gravity wave induced loss of photochemical heating increases and the ratio between it and the background photochemical heating rate also increases.

I. INTRODUCTION

Atmospheric heating, cooling and energy transportation in the upper mesosphere and the lower thermosphere are very important. The photochemical heating is one of the major heating sources in this region. Gravity waves are one of the most common dynamical fluctuations in the middle atmosphere. The influence gravity waves on the large scale dynamical structure of the middle atmosphere has been thoroughly studied by Lindzen, Fritts, Holton, Tao and Gardner, Lubken, Hickey and Walterscheid, Vohn Zahn and Meyer ,Brasseur and Offermann, Schmidlin, Dickinson and Riese et al.
In this paper, a diabatic gravity wave model including photochemical diabatic processes has been developed. The effects of gravity waves on photochemical heating are analyzed using this model. The results show that gravity waves can cause a reduction in the photochemical heating rate in the mesospheric region. The variations in the reduction of the photochemical heating rate in the mesospheric region, induced by gravity waves with the changes in the background distribution and the atomic oxygen profile, are studied in detail. The accuracy of the results of this paper is obtained by the help of MATLAB Simulation setup.
(The paper has been divided into sections: Introduction, model and the calculation method of the effect of gravity waves on photochemical heating, the method for calculating the effect of gravity waves on photochemical heating, results of calculations, discussion and conclusions and future work).

II. MODEL AND THE CALCULATION METHOD OF THE EFFECT OF GRAVITY WAVES ON PHOTOCHEMICAL HEATING

2.1 Model

Because the middle atmospheric is a system in which radiation, dynamic and chemical reactions are all coupled, the diabatic processes of photochemical heating and atmospheric cooling should be considered in the theory of gravity waves. The model equations for linear inertial internal gravity waves are as follows:

$$\frac{\partial \acute{u}}{\partial t} + \bar{u}\frac{\partial \acute{u}}{\partial x} + \bar{v}\frac{\partial \acute{u}}{\partial y} + \bar{w}\frac{\partial \acute{u}}{\partial z} - f\acute{v} + \frac{\partial \acute{\vartheta}}{\partial x} = 0 \quad (1)$$

$$\frac{\partial \acute{v}}{\partial t} + \bar{u}\frac{\partial \acute{v}}{\partial x} + \bar{v}\frac{\partial \acute{v}}{\partial y} + \bar{w}\frac{\partial \acute{v}}{\partial z} + f\,\acute{u} + \frac{\partial \acute{\vartheta}}{\partial y} = 0 \quad (2)$$

$$\frac{\partial \acute{w}}{\partial t} + \bar{u}\frac{\partial \acute{w}}{\partial x} + \bar{v}\frac{\partial \acute{w}}{\partial y} + \bar{w}\frac{\partial \acute{w}}{\partial z} + f\,\acute{w} + \frac{\partial \acute{\vartheta}}{\partial z} = 0 \quad (3)$$

$$\frac{\partial \acute{u}}{\partial x} + \frac{\partial \acute{v}}{\partial y} + \frac{\partial \acute{w}}{\partial z} + \left(\frac{\partial}{\partial z} - \frac{1}{H}\right)\acute{w} = 0 \quad (4)$$

$$\frac{\partial \acute{\vartheta}_z}{\partial t} + \bar{u}\frac{\partial \acute{\vartheta}_z}{\partial x} + \bar{v}\frac{\partial \acute{\vartheta}_z}{\partial y} + \bar{w}\frac{\partial \acute{\vartheta}_z}{\partial z} + N^2\acute{w} = \frac{R}{HC_p}\left[\frac{\partial Q_o}{\partial T_o}\frac{H}{R}\acute{\vartheta}_z + \sum_{j=1}^{J}\frac{\partial Q_o}{\partial q_j^o} q_j^o \acute{q}_j\right] \quad (5)$$

$$\frac{\partial \acute{q}_i}{\partial t} + \bar{u}\frac{\partial \acute{q}_i}{\partial x} + \bar{v}\frac{\partial \acute{q}_i}{\partial y} + + \bar{w}\frac{\partial \acute{q}_i}{\partial z} + \acute{w}\frac{\partial \ln \bar{q}_i}{\partial z} = \frac{1}{n_i^o}\left[\frac{\partial (P_i^o - L_i^o)}{\partial T_o}\frac{H}{R}\acute{\vartheta}_z + \sum_{j=1}^{J}\frac{\partial (P_i^o - L_i^o)}{\partial q_j^o}\Big|_{\overline{q_J}} q_j^o \acute{q}_j\right] \quad (6)$$

i = 1, 2, 3…….J

Where $\acute{u}, \acute{v}$ *and* $\acute{w}$ the backgrounds are wind in the x, y and z directions, respectively; ϑ is the geopotential; q_i^o (i= 1, 2. . . J) is the background trace gas mixing ratios. They are calculated using a time-dependent one-dimensional photochemical model. f is the Coriolis parameter, H is the scale height, $H_0 = \frac{H}{R}\overline{\vartheta_z}$ .H= $\frac{H}{R}\frac{\partial \bar{\vartheta}}{\partial z}$ is the background temperature, N is the Brunt-Vaisala frequency, Cp is the specific heat at constant pressure, R is the gas constant, and Pi and Li are the rates of photochemical production and loss for species i. The term Q_o represents the background net diabatic heating rate. Eq. (6) is the photochemical reaction continuity equation for species i. u', v', w' and $\acute{\vartheta}$ are perturbations of u, v, w and ϑ, respectively. $\acute{q}_i = \frac{\Delta q_i}{q_i^o}$ is the relative perturbation for species i. This model considers all important photochemical reactions in the middle atmosphere.

The background net diabatic heating term Q_o is composed of a photochemical heating rate H_o and an atmospheric cooling rate C_0, so $Q_o = H_o - C_o$. The calculation of the photochemical heating rate H_o includes solar radiation heating and exothermic chemical reaction heating. The heating effects of all photochemical reactions in Table 1[**appendix**] are considered in the gravity wave model. The calculation of cooling rate C_o considers the cooling by CO_2 , H_2O and O_3 . The atmospheric cooling rate is calculated using the code provided by Fomichev et al. (1996).

2.2 The method for calculating the effect of gravity waves on photochemical heating

In this paper, we study systematically the effect of gravity waves on the photochemical heating rate. We assume existence of wave solution of (1)-(6) of the form

$$\acute{\beta} = \acute{\beta}_0\, e^{\frac{z}{2H}} \mathrm{Cos}(wt - k_x x - k_y y - k_z z) \quad (7)$$

Where $k_x = \frac{2\pi}{l_x}$, $k_y = \frac{2\pi}{l_y}$, $k_z = \frac{2\pi}{z}$ are wave number in x, y and z direction respectively, w is frequency wave. $\acute{\beta}$ Presents any one fluctuation of u, v, w, T and q_i (i =1, 2, 3… J). $\acute{\beta}_0$ is the corresponding amplitude parameter of the wave and $e^{\frac{z}{2H}}$ Express the exponential growth with the height of gravity of wave due to the decreasing atmosphere density.

(a) Equation (7) is substituted into eqs. (1)– (6).Then it's become coupled equations which are composed of J +4 equations. After eliminating the $\acute{w}_o$ the equation becomes

$$i\acute{w}_o\vec{y} = A\vec{y}$$

Where A is a square matrix with dimension equal to J +3 =19, y is a vector which elements are $\acute{u}_0$, $\acute{v}_0$, $\acute{\vartheta}_0$ and $\acute{q}_{0i}$ (i = 1, 2, . . . , J). Here $w_o = w - k\bar{u}$-l$\bar{v}$ is the Doppler shifted frequency. The unknown quantity w_o of the coupled equations can be solved by calculating the Eigen values of matrix A.

(b)

We assume that the temperature perturbation of a gravity wave is

$$\acute{T} = \acute{T}_0\, e^{\frac{z}{2H}} \mathrm{Cos}(wt - k_x x - k_y y - k_z z) \quad (8)$$

Where T_o is the amplitude of the temperature perturbation. Eq. (8) and the wave frequency o calculated in the first step are substituted into Eqs. (1)- (6). The equations become linear algebraic coupled equations with J+2 unknown quantities, u', v' and $\acute{q}_i$ (i=1, 2. . . J). these perturbations can be calculated by solving these linear algebraic coupled equations. The perturbation of vertical wind w' can then be found by solving Eq. (3).

Finally, we can use Eq. (8) to calculate the influence of gravity waves on the time-averaged photochemical heating $\overline{\mathcal{H}''}$. $\overline{x_i' x_j'}$ is calculated as follows[jiyao Xu et.al]:

$$\overline{x_i' x_j'} = \frac{w}{2\pi}\int_0^{\frac{2\pi}{w}} Re[x_i']\mathrm{Re}\,[x_j']dt = \frac{1}{2}|x_{io}'||x_{jo}'|\cos\theta_{ij}$$

$\cos\theta_{ij}$ is the phase difference between the x_i' and x_j' .Re $[x_i']$ means real part of x_i' $|x_{id}'|$ is the magnitude of x_i'.

III. RESULTS OF CALCULATIONS

In this paper, the time-averaged second-order perturbation of photochemical heating rates $\overline{\mathcal{H}''}$, caused by gravity waves for different background temperature and atomic oxygen profiles, are analyzed. A large number of observations of the middle atmosphere show that the variation of temperature induced by the gravity waves is from some degrees to several tens of degrees.

In the above calculation, the background trace gas profiles at noon are taken from the results of the one-dimensional time-dependent middle atmospheric photochemical model for the condition of the summer solstice at latitude of 708N.

3.1. The influence of background temperature variation

Four mesospheric temperature profiles are used in these calculations. The temperature at the mesopause is 190, 140, 130 and 120 K, respectively. The background profiles of various species at noon are calculated for the four temperature profiles using the time-dependent one-dimensional photochemical model for the condition of the summer solstice at latitude of 70^0N. The time-averaged second-order perturbations of photochemical heating $\overline{\mathcal{H}''}$ caused by gravity waves are calculated for the four temperature profiles. It is clear that the effect of gravity waves on photochemical heating $\overline{\mathcal{H}''}$ is concentrated in the range of 80-90 km near the mesopause, and that the effect of gravity waves is to reduce the photochemical heating rate. In the mesosphere, one of the most obvious seasonal variations is that of the temperature distribution. The temperature of the polar mesopause is more than 200 K in winter. In summer, the temperature of the polar mesopause is very low and the mean temperature is in the range 120-140 K (Steven M. Smith, Stubenrauch, C. J, Von Zahn and Meyer, 1989; Lubken et al., 1990).

3.2. The influence of the background distribution of atomic oxygen variation

The changes in photochemical heating loss, induced by gravity waves for several different distributions of atomic oxygen, are analyzed. It indicates that $\mathcal{H}_0$ increases with increasing atomic oxygen density. Atomic oxygen is doubled, the mesopause atomic oxygen density increases to $5.96 \times 10^{11}\ cm^{-3}$ from the original $2.98 \times 10^{11}\ cm^{-3}$.

IV. DISCUSSION AND CONCLUSIONS

The effect of gravity waves on the large scale dynamical structure of the middle atmosphere has been studied. The ratio between the loss of photochemical heating $\overline{\mathcal{H}''}$, caused by gravity waves and the background photochemical heating $\mathcal{H}_0$ increases as background temperature decreases. Therefore, this mechanism should not be neglected at the summer polar mesopause. The peak loss is at about 84 km altitude. Our study indicates that the loss of photochemical heating induced by gravity waves is mainly concentrated in the region of 80-90 km. The effects of gravity waves on photochemical heating are analyzed.

V. FUTURE WORK

(1) Because of the atmospheric radiation, energy from reactions cannot be converted to thermal energy completely. So, the calculation of photochemical heating is very important for the study of the energy budget in the upper mesosphere. This is future work.
(2) The accurate measurements of the background distribution of atomic oxygen are very important to evaluate process correctly. This is future work.

Appendix

Table1

Model Reaction

Photodissociate Reaction

A1. O_4 + hγ → O_2 + O_2
A2. O_4 + hγ → O_3 + O
A3. O_2 + hγ → $O(3_P)$+ $O(1_D)$
A4. O_2 + hγ → $O(3_P)$+ $O(3_P)$
A5. O_3 + hγ → O_2 + $O(1_D)$
A6. O_3 + hγ → O_2 + $O(3_P)$
A7. HO_4 + hγ → $O(3_P)$ +HO_3
A8. HO_3 + hγ → $O(3_P)$ +HO_2
A9. HO_2 + hγ → $O(3_P)$ +OH
A10. OH + hγ → $O(3_P)$ +H
A11. NO_4 + hγ → NO +O_3
A12. NO + hγ → N + $O(3_P)$
A13. NO_4 + hγ → NO_2 +O_2
A14. NO_2 + hγ → NO + $O(3_P)$
A15. NO_4 + hγ → NO_3 + $O(3_P)$
A16. NO_3 + hγ → NO_2 + $O(3_P)$
A17. NO_2 + hγ → NO +O_2
A18. CO_4 + hγ → CO_3 + $O(3_P)$
A19. CO_3 + hγ → CO_2 + $O(3_P)$
A20. CO_2 + hγ → CO + $O(3_P)$
A21. CO + hγ → C + $O(3_P)$
A22. $CH_3\,O_2$ + hγ → $CH_2\,O + OH$
A23. $CH_2\,O$+ hγ → $CO + H_2$
A24. HOCl + hγ → $OH + Cl$
A25. HCl + hγ → $H + Cl$
A26. Cl_2+ hγ → Cl+ Cl
A27. ClO + hγ → Cl+ $O(3_P)$
A28. OClO + hγ → ClO + $O(3_P)$
A29. ClOO + hγ → ClO + $O(3_P)$
A30. ClO NO_2 + hγ → Cl + NO_3
A31. CFCl_3+ hγ → $3Cl + fragment$
A32. CF_2Cl_2+ hγ → $2Cl + fragment$

Three -body Reactions

B1. $O_2\,+\,O_2$ +M→ $O_4\,+M$
B2. $O_3\,+\,O$ +M→ $O_4\,+M$
B3. $O(3_P)+\,O(3_P)$ + M → $O_2\,+M$
B4. $O(3_P)+\,O_2$ + M → $O_3\,+M$
B5. $O(1_D)+\,N_2$ + M → $N_2\,O+M$
B6. H + O_2 +M→ $HO_2\,+M$
B7. OH + NO +M → $HONO+M$
B8. OH + NO_2 +M → $HNO_3\,+M$
B9. HO_2 + NO_2 +M → $HO_2\,NO_2\,+M$
B10. OH + OH +M → $H_2\,O_2\,+M$

B11. $O(3_P) + NO_2 + \mathrm{M} \rightarrow NO_3 + M$
B12. $O(3_P) + NO + \mathrm{M} \rightarrow NO_2 + M$
B13. $Cl + NO_2 + \mathrm{M} \rightarrow ClONO + M$
B14. $Cl + NO_2 + \mathrm{M} \rightarrow ClNO_2 + M$
B15. $NO_2 + NO_3 + \mathrm{M} \rightarrow N_2O_5 + M$
B16. $Cl + NO + \mathrm{M} \rightarrow NOCl + M$
B17. $ClO + NO_2 + \mathrm{M} \rightarrow ClONO_2 + M$
B18. $Cl + O_2 + \mathrm{M} \rightarrow ClOO + M$

Second-order Reactions

C1. $O(3_P) + O_4 \rightarrow O_2 + O_3$
C2. $O(1_D) + O_3 \rightarrow O_2 + O_2$
C3. $O(3_P) + O(3_P) \rightarrow O_2 + O_2$
C4. $O(1_D) + O_3 \rightarrow O_2 + 2O(3_P)$
C5. $O(1_D) + H_2O \rightarrow 2OH$
C6. $O(1_D) + H_2 \rightarrow OH + H$
C7. $O(1_D) + NO_4 \rightarrow NO_3 + O_2$
C8. $O(1_D) + N_2O \rightarrow NO + NO$
C9. $O(1_D) + NO_3 \rightarrow NO_2 + O_2$
C10. $O(3_P) + OH \rightarrow O_2 + H$
C11. $H + O_4 \rightarrow HO_2 + O_2$
C12. $H + O_3 \rightarrow OH + O_2$
C13. $HO_2 + O(3_P) \rightarrow OH + O_2$
C14. $OH + O_4 \rightarrow HO_2 + O_3$
C15. $OH + O_3 \rightarrow HO_2 + O_2$
C16. $HO_2 + O_3 \rightarrow OH + 2O_2$
C17. $OH + OH \rightarrow H_2O + O(3_P)$
C18. $OH + HO_2 \rightarrow H_2O + O_2$
C19. $OH + H_3 \rightarrow H_2O + 2H$
C20. $OH + H_2 \rightarrow H_2O + H$
C21. $H + HO_2 \rightarrow 2OH$
C22. $H + HO_2 \rightarrow H_2 + O_2$
C23. $H + HO_2 \rightarrow H_2O + O(3_P)$
C24. $NO + HO_2 \rightarrow OH + NO_2$
C25. $HO_2 + HO_2 \rightarrow H_2O_2 + O_2$
C26. $H_2O_2 + OH \rightarrow H_2O + HO_2$
C27. $H_2O_2 + O(3_P) \rightarrow OH + HO_2$
C28. $OH + HCl \rightarrow Cl + H_2O$
C29. $OH + ClO \rightarrow Cl + HO_2$
C30. $Cl + HO_2 \rightarrow HCl + O_2$
C31. $Cl + HO_2 \rightarrow OH + ClO$
C32. $ClO + HO_2 \rightarrow HOCl + O_2$
C33. $Cl + O_3 \rightarrow O_2 + ClO$
C34. $ClO + O(3_P) \rightarrow O_2 + Cl$
C35. $HCl + O(3_P) \rightarrow OH + Cl$
C36. $HOCl + O(3_P) \rightarrow OH + ClO$
C37. $NO_2 + O(3_P) \rightarrow NO + O_2$
C38. $NO + O_4 \rightarrow NO_2 + O_3$
C39. $NO + O_3 \rightarrow NO_2 + O_2$
C40. $N + O_2 \rightarrow NO + O(3_P)$
C41. $NO_2 + O_4 \rightarrow NO_3 + O_3$
C42. $NO_2 + O_3 \rightarrow NO_3 + O_2$
C43. $N + NO \rightarrow N_2 + O(3_P)$
C44. $N + NO_2 \rightarrow N_2O + O(3_P)$

C45. $NO_4 + O(3_P) \rightarrow NO_2 + O_3$
C46. $NO_4 + O(3_P) \rightarrow NO_2 + O_3$
C47. $NO_3 + O(3_P) \rightarrow 2NO_2$
C48. $NO_4 + Cl \rightarrow NO_3 + ClO$
C49. $NO_3 + Cl \rightarrow NO_2 + ClO$
C50. $NO + ClO \rightarrow NO_2 + Cl$
C51. $NO_4 + ClO \rightarrow Products$
C52. $NO_3 + ClO \rightarrow Products$
C53. $H_2O_2 + + Cl \rightarrow HO_2 + HCl$
C54. $O_4 + ClO \rightarrow O_3 + ClO$O
C55. $O_3 + ClO \rightarrow O_2 + ClO$O
C56. $O_4 + ClO \rightarrow O_3 + OClO$
C57. $O_3 + ClO \rightarrow O_2 + OClO$
C58. $HCl + O(1_D) \rightarrow Products$
C59. $O_4 + N \rightarrow O_3 + NO$
C60. $O_3 + N \rightarrow O_2 + NO$
C61. $OH + HOCl \rightarrow H_2O + ClO$
C62. $N_2O_5 + M \rightarrow NO_2 + M$
C63.CH_4 + $O(1_D)$ →.CH_3 + OH (90%)
C64. CH_4 + $O(1_D)$ →.CH_2 O+ H_2 (10%)
C65. CH_4 + OH →.CH_3 + H_2O
C66. CH_4 + Cl →CH_3 + HCl
C67. HNO_3 + $O(3_P)$ → OH + NO_3
C68. $N_2O_5 + H_2O$ → 2HNO_3
C69.Cl + $H_3 \rightarrow HCl + H_2$
C70. Cl + $H_2 \rightarrow HCl + H$
C71. Cl + $HOCl \rightarrow Cl_2 + OH$
C72. Cl + HNO_3 → $Products$
C73.ClO + CH_4 → $Products$
C74. ClO + H_3 → $Products$
C75. ClO + H_2 → $Products$
C76. ClO + CO → $Products$
C77. ClO + N_2O → $Products$
C78.OH + $Cl_2 \rightarrow Cl + HOCl$
C79. OH +ClONO_2 → NO_3 + $HOCl$
C80. OH +ClONO_2 → $O(3_P) + ClO$
C81. CFCl_3 +$O(1_D) \rightarrow 2Cl + ClO$ + Fragment
C82. CF_2Cl_2 +$O(1_D) \rightarrow Cl + ClO$ + Fragment
C83. OH + HNO_3 → H_2O + NO_3
C84.CO + OH → H + CO_2

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