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A chemical-dynamical model of wave-driven sodium fluctuations

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Abstract. A comprehensive chemical-dynamical model is used to investigate the interaction of gravity waves with twenty minor species involved in the atomic sodium chemistry in the mesopause region. We find that chemistry becomes important on the underside of the sodium layer, primarily below 85 km altitude, where the relative importance of chemistry in wave-driven sodium fluctuations increases with increasing wave period and increasing horizontal wavelength. We also find that for altitudes below 80 km an adequate determination of the effects of chemistry in these fluctuations requires the inclusion of several reactions related to ozone chemistry. However, the atomic Na density is too low this region to be routinely observed by current sodium lidars. Importantly, we find that above 85 km altitude sodium can be treated as a passive tracer of gravity wave motions.

1. Introduction

Sodium lidar observations have been used with great success to characterize gravity wave dynamics of the mesopause region [e.g., Shelton et al., 1980; Avery and Tetenbaum, 1983; Gardner and Voelz, 1987; She et al., 1991; Senft and Gardner, 1991; Bills and Gardner, 1993]. The interpretation of these observations has relied on the assumption that Na is a passive tracer of dynamics, tacitly assuming that the effects of chemistry are unimportant. However, the validity of this assumption has never been thoroughly tested. Here, we examine in some detail gravity wave-driven Na fluctuations with the objectives of determining the importance of chemistry in these fluctuations and assessing whether Na behaves as a passive tracer of gravity wave motions.

These objectives are accomplished by utilizing a model that describes the interaction of gravity waves with chemically active minor species. Here, our model of wave-driven minor species fluctuations [e.g., Hickey, 1988] is extended to include the chemistry relevant to Na. This has been facilitated by the recent development of a detailed model of Na chemistry that predicts a seasonal variation of the Na layer in excellent agreement with lidar observations [Plane, 1991; Helmer and Plane, 1993], and has been tested against the results from combined lidar and rocket-borne photometric observations of the atomic sodium and air-glow layers [Clemesha et al., 1995]. Additionally, the model of Helmer and Plane has been run in a time-dependent mode in order to study the response of the Na concentration to the effects of temperature perturbations having gravity wave periods. Their results showed that Na will not be a conserved quantity below about 87 km when the passage of a wave causes adiabatic temperature fluctuations, and that the chemical response should be

considered when using time-resolved lidar observations of the Na layer as a tracer of gravity wave motions. However, Helmer and Plane did not model the gravity waves comprehensively, and the effect of neglecting the complete dynamics has remained uncertain. We now explicitly tackle this problem by not only accounting for the temperature fluctuations due to a gravity wave, but also by including the dynamical effects of vertical advection and compression. We rigorously demonstrate for the first time that by accounting for these complete dynamical effects the chemical response can be neglected when interpreting time-resolved observations of gravity waves in the Na layer above 85 km altitude.

2. Theory

The model solves a system of chemically coupled, linearized continuity equations for the minor species, including temperature perturbations and the dynamical effects of advection and divergence. The method of solution has been described before [e.g., Walterscheid et al., 1987; Hickey, 1988]. The model employs the WKB approximation (i.e., atmospheric quantities vary little over a vertical wavelength) and includes the effects of the diffusion of heat and momentum in the gravity wave dynamics [Hickey, 1988; Schubert et al., 1991].

The model of the Na chemistry and the chemical reactions employed here are described by Helmer and Plane [1993]. Briefly, the model output is representative for winter conditions at 70°N. Given concentrations of minor species (such as O, H and O₃) and major ions (NO⁺ and O₂⁺), it provides mean state densities of the following Na-containing species: Na, NaO, NaO₂, NaO₃, NaOH, NaCO₃, NaHCO₃, Na⁺, and Na.X⁺ (X = N₂, H₂O or CO₂). Here, least-squares polynomials were fit to the mean temperature and to the logarithms of mean number densities provided by their model.

The perturbations in these species due to gravity waves are calculated by solving a system of coupled, linear, algebraic continuity equations. Assuming plane, monochromatic linear waves, each of these equations is written as

$$i\omega \delta n = \delta P - \delta L + \bar{n} \{ f_2 / \bar{H}_n - f_1 \} \delta T / \bar{T} \quad (1)$$

where ω is the wave angular frequency; δT and δn are the perturbed temperature and minor species density about their mean state values (bearing an overbar); f_1 and f_2 are dynamical factors relating the velocity divergence and vertical velocity to the temperature perturbation through the relations $\nabla \cdot \mathbf{v}' = f_1 T' / \bar{T}$ and $w' = f_2 T' / \bar{T}$, respectively; δP and δL are the perturbed chemical production and loss, respectively, of species n ; and \bar{H}_n is the scale height of species n .

Examination of the set of chemical reactions provided by Helmer and Plane [1993] reveals that O₃ is lost only through reactions involving the trace species Na and NaO. If these were the

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Table 1. Reactions Related to OH Chemistry [after *DeMore et al.*, 1994]

Reaction	Rate Coefficient*
$O+OH \rightarrow H+O_2$	$2.2 \times 10^{-11} \exp(120/T)$
$H+O_2+M \rightarrow HO_2+M$	$5.7 \times 10^{-32} (T/300)^{-6}$
$H+O_2 \rightarrow OH+O$	$1.4 \times 10^{-10} \exp(-470/T)$
$O+HO_2 \rightarrow OH+O_2$	$3 \times 10^{-11} \exp(200/T)$
$O+O+M \rightarrow O_2+M$	$4.7 \times 10^{-33} (T/300)^{-2}$
$O+O_2+M \rightarrow O_3+M$	$6.0 \times 10^{-34} (T/300)^{-2.3}$

* Rate constants are in units of $\text{cm}^6 \text{s}^{-1}$ for termolecular reactions and $\text{cm}^3 \text{s}^{-1}$ for bimolecular reactions

only chemical losses, the chemical lifetime for O_3 would exceed two days between 75 and 100 km altitude, and O_3 would behave as a passive, chemically inert tracer of gravity wave motions. However, O_3 reacts with other significantly more abundant species than either Na or NaO, such as atomic hydrogen. The chemical lifetime of O_3 due to reaction with H is only a few minutes, so that chemistry is important to gravity wave-driven O_3 fluctuations if the $H+O_3$ reaction is included. Although Na perturbations are strongly coupled to O_3 perturbations through the reaction $Na+O_3 \rightarrow NaO+O_2$, the reverse is not true because the Na density is significantly less than the O_3 density. Therefore, correct modeling of gravity wave-driven Na fluctuations requires incorporation of additional chemical reactions to those provided by *Helmer and Plane* [1993]. These additional reactions, provided in Table 1, introduce two minor species (OH and HO_2) into our model that are additional to those of *Helmer and Plane* [1993]. Mean number densities for OH and HO_2 are calculated using the reactions of Table 1 assuming that these species are in steady-state (reaction rates are from *DeMore et al.* [1994]). Altogether, we solve a total of twenty simultaneous continuity equations for the minor and trace species included in the model.

If the effects of chemistry are neglected in Equation (1) and we assume that wave motions occur adiabatically with horizontal phase trace speeds much less than the local sound speed (which implies that the vertical wavelength, $\lambda_z \ll 2\pi\bar{H}$) then the major gas density perturbations are exactly out of phase with those of the temperature perturbations [see, for example, equations (A25) and (A26) of *Schubert et al.*, 1991]. Under such conditions, and for an isothermal atmosphere, Equation (1) becomes

$$\delta n = \frac{\bar{n}}{(\gamma - 1)} \left\{ 1 - \frac{\gamma \bar{H}}{H_n} \right\} \delta T / \bar{T} \quad (2)$$

where \bar{H} is the local scale-height of the major gas, and $\gamma (=1.4)$ is the usual ratio of specific heats. If the further assumption is made that the unperturbed sodium layer can be approximated by a Gaussian profile [e.g., *Gardner and Voelz*, 1987] with centroid height z_0 and rms thickness σ_0 , then Equation (2) becomes [see Equation (4) of *Bills and Gardner*, 1993]

$$\delta n = \frac{\bar{n}}{(\gamma - 1)} \left\{ 1 - \frac{\gamma \bar{H}_m}{\sigma_0^2} (z - z_0) \right\} \delta T / \bar{T} \quad (3)$$

where \bar{H}_m is the major gas scale-height at the peak of the undisturbed Na layer. Equations (2) and (3) imply that the Na response to a given temperature perturbation is independent of all wave parameters, depending only on the parameters of the mean, undisturbed state. The appropriateness of these two equations will be subsequently evaluated by comparing them numerically to Equation (1). According to (3), Na and temperature perturba-

tions should be 180° out of phase on the top side of the Na layer and in phase on the bottom side [*Bills and Gardner*, 1993]. This phase change occurs at an altitude of $z = z_0 + \sigma_0^2 / \gamma \bar{H}_m$, which is about 92.3 km for the parameters adopted here ($\sigma_0 = 4.37$ km, $z_0 = 90.1$ km and $\bar{H}_m = 6.29$ km). This change in phase between δn and δT is also predicted by equations (1) and (2). The three equations also predict that at the peak of the undisturbed Na layer (~90 km), relative Na fluctuations should be 2.5 times greater than relative temperature fluctuations.

3. Results

In order to assess the importance of chemistry in the Na fluctuations we have performed calculations with just dynamics and with dynamics and chemistry coupled together. Results are presented in terms of a complex, amplitude-independent parameter $\eta(z)$, defined by

$$\eta = (\delta n / \bar{n}) / (\delta T / \bar{T}) \quad (4)$$

where all symbols are as previously defined, and n refers to Na number density. We primarily discuss $|\eta|$, and present results for several combinations of horizontal wavelength and wave period. Note that the wave dynamics includes the effects of the diffusion of heat and momentum [e.g., *Hickey*, 1988; *Schubert et al.*, 1991] using a Prandtl number of two and a nominal kinematic viscosity of $100 \text{ m}^2 \text{ s}^{-1}$. Results are presented primarily for the region between 77 and 100 km altitude because this is the principal region within which sodium lidar measurements are obtained, but they are displayed down to 75 km altitude in Figure 2 to more clearly show the effects of the OH chemistry.

Figure 1 shows the mean, undisturbed Na, Na^+ and $NaHCO_3$ number densities as a function of altitude as produced from the model of *Helmer and Plane* [1993]. Na is more abundant than its sources (Na^+ and $NaHCO_3$) over much of the altitude range, and consequently dominates there. Its density peaks near 90.1 km altitude and its profile has a full-width, half maximum of about 10.3 km. The profiles of the other major sodium-species are provided in *Helmer and Plane* [1993], and are not repeated here.

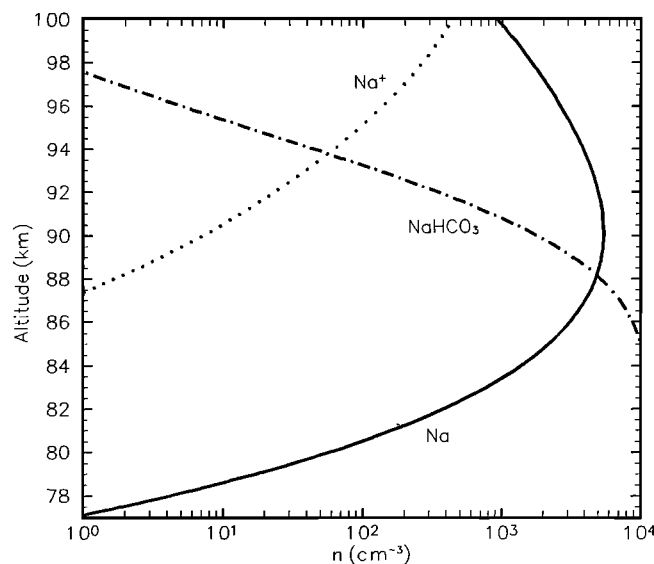


Figure 1. Mean undisturbed Na (solid line), Na^+ (dotted line) and $NaHCO_3$ (dashed-dotted line) profiles derived from the model of *Helmer and Plane* [1993].

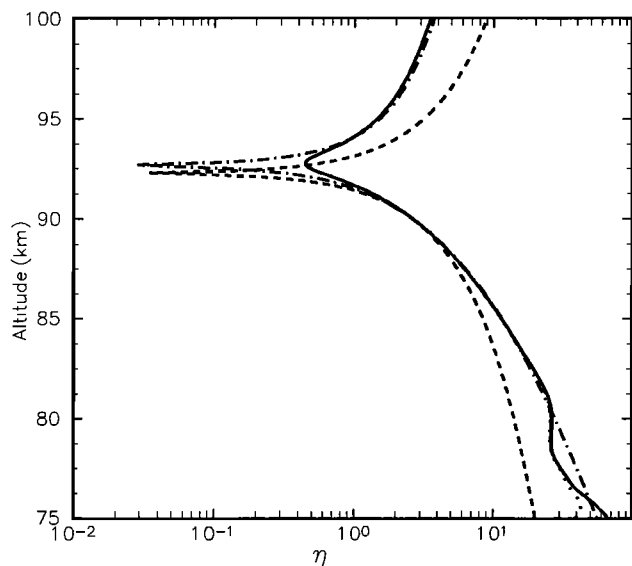


Figure 2. $|\eta|$ for a gravity wave with $\lambda_x = 100$ km, $T = 20$ minutes, and using equation (1) without OH chemistry (solid line) and with OH chemistry (dotted line); using equation (2) (dashed-dotted line); or using equation (3) (dashed line).

Figure 2 shows $|\eta|$ plotted as a function of altitude for a wave period of 20 minutes and a horizontal wavelength (λ_x) of 100 km ($\lambda_z \approx 27$ km). Two of the curves represent results obtained using Equation (1) either with or without the inclusion of the $H+O_3$ reaction. The differences in these two sets of results are only appreciable at the lowest altitudes in the model, below 82 km. In this region, Na is controlled by both O_3 and H, through reactions (R1), (R8), (R9a), (R16) and (R17). Its short chemical lifetime at these altitudes suggests that it will be strongly affected by O_3 and H fluctuations. Because H fluctuations are also affected by the $H+O_3$ reaction, the resulting affects on Na are large. However, below 77 km the Na density falls below 1 cm^{-3} and Na is no longer observable by current Na lidars.

The other two curves in Figure 2 are derived from Equations (2) and (3). Equation (2) describes the Na perturbations exceptionally well except within a narrow region centered about 2 km above the peak of the Na layer. Equation (3), which has been derived by *Bills and Gardner* [1993], does not appear to describe the Na response to gravity wave forcing as well as Equation (2) due, in this case, to the apparently inadequate representation of the undisturbed Na layer by a Gaussian profile at high latitudes. Note that we employed a fourth-degree least-squares polynomial to represent the logarithm of the mean Na density, while a Gaussian profile assumes a quadratic representation. The former representation was required to fit the model output of *Helmer and Plane* [1993] over a 35-km height range, which, being based on the observations of *Tilgner and von Zahn* [1988], is appropriate for winter conditions at 70°N . The Gaussian representation gives a good fit to the monthly-averaged Na profiles of *Senft and Gardner* [1991] at Illinois over a height range of approximately 20 km and centered on the Na peak, and is therefore appropriate for a latitude of 40°N . The minimum in $|\eta|$ ($|\eta|_{\min}$) is associated with a change in sign of η due to the first-order perturbations vanishing just above the undisturbed Na peak, and occurs near 92.3 km for Equation (3) and near 92.8 and 92.7 km for Equations (1) and (2), respectively. This ~ 0.5 km altitude difference is primarily due to the difference between the polynomial representations of the logarithms of Na density in equations (2) and

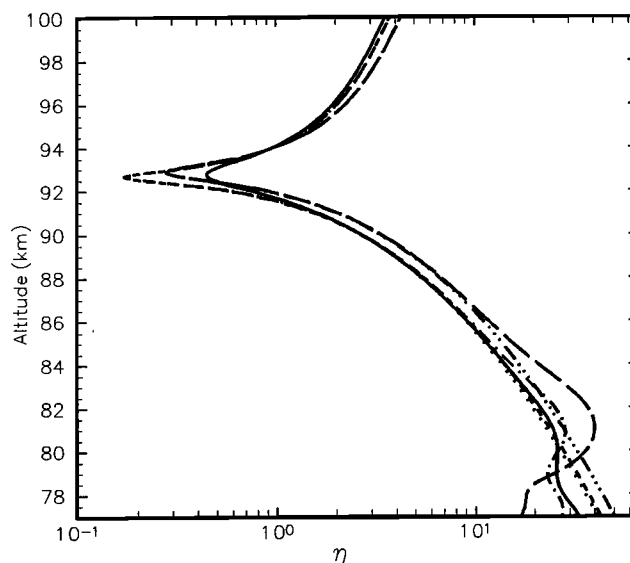


Figure 3. $|\eta|$ for gravity wave with $\lambda_x = 100$ km, and a period of 20 minutes with dynamics and chemistry (solid line) or dynamics alone (dotted); a period of 1 hour with dynamics and chemistry (dashed-dotted) or dynamics alone (short dashed); and a period of 3 hours with dynamics and chemistry (long dashed) or dynamics alone (dash-triple dotted).

(3). All three minima are different in magnitude, each being the small difference between two large, approximately equal magnitude numbers of opposite sign, demonstrating the sensitivity of $|\eta|_{\min}$ to the approximations employed in deriving Equations (2) and (3). Results derived from these equations are independent of wave parameters and so are not repeated in subsequent figures.

Figure 3 shows the parameter $|\eta|$ plotted as a function of altitude for a single horizontal wavelength of 100 km and for three waves of period 20 minutes, 1 hour and 3 hours ($\lambda_z \approx 27$, 8.7, and 2.7 km, respectively). For each wave there are two sets

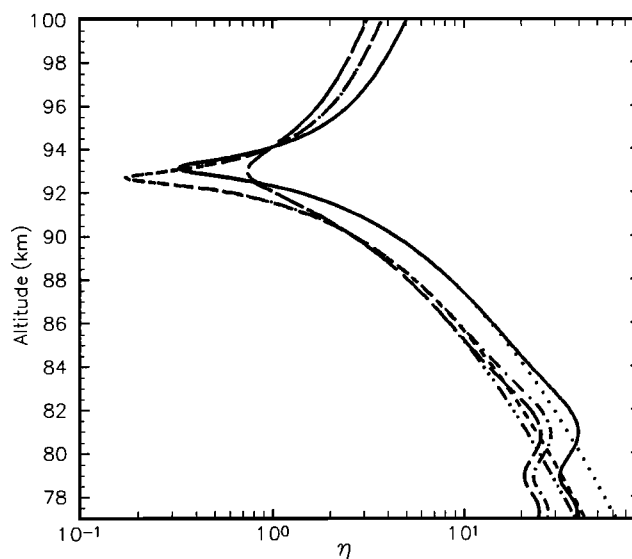


Figure 4. $|\eta|$ for gravity wave with a period of 1 hour, and $\lambda_x = 10$ km with dynamics and chemistry (solid line) or dynamics alone (dotted); $\lambda_x = 100$ km with dynamics and chemistry (dashed-dotted) or dynamics alone (short dashed); and $\lambda_x = 500$ km with dynamics and chemistry (long dashed) or dynamics alone (dash-triple dotted).

of results corresponding to either the inclusion or the exclusion of chemistry in the dynamical fluctuations. Note that the "complete" ozone chemistry is employed whenever chemistry is included. For a given wave, differences between the two sets of results obtained with and without chemistry become significant only below about 85 km altitude. $|\eta|$ displays a weak dependence on wave period that is not predicted by Equations (2) or (3). Above about 85 km altitude the Na fluctuations are purely dynamically controlled.

Figure 4 shows the parameter $|\eta|$ plotted as a function of altitude for a single wave period of 1 hour and for three waves of horizontal wavelength 10, 100 and 500 km ($\lambda_x \approx 1.6, 8.7$ and 52 km, respectively). Above about 85 km altitude the Na fluctuations are purely dynamically controlled, and display a strong dependence on λ_x compared to the dependence on wave period. Differences between results obtained with and without chemistry are slightly larger for the larger wavelength waves between about 77 and 85 km altitude. The results for $\lambda_x = 500$ km are probably not in fact appropriate for sodium lidar observations, because these observations are biased towards waves having vertical wavelengths that are comparable to the thickness of the atomic sodium layer which is always much smaller than 52 km.

4. Discussion and Summary

For the first time a comprehensive model describing the dynamical interaction of linear internal gravity waves with the mesospheric Na chemistry has been used to demonstrate that above about 85 km altitude (i.e., above 5 km below the Na peak) Na fluctuations due to gravity waves are primarily dynamical, with the Na behaving as a passive, chemically inert tracer of gravity wave motions. In this region, the bottom-side source of Na (NaHCO_3) is generally much less abundant than Na (see Figure 1), with the result that chemical coupling between these two species does not significantly affect wave-driven Na fluctuations. However, below this altitude the effects of chemistry can be important for some of the larger scale waves and should be considered in their interpretation. The response of Na to gravity wave forcing, as described through the parameter η , generally increases towards the lower altitudes. Importantly, the response calculated here with the complete gravity wave dynamics is much greater, by about a factor of 5, than the response due to temperature variations alone [Helmer and Plane, 1993].

Some of the reaction rates adopted here are uncertain, and the model may be sensitive to some of their values. In particular, at mesospheric temperatures (~ 200 K), k_{17} describing the reaction $\text{NaHCO}_3 + \text{H} \rightarrow \text{Na} + \text{H}_2\text{CO}_3$ is uncertain within a factor of 5 [Helmer and Plane, 1993]. However, since the pre-exponential factor of k_{17} has been set at the collision number and is therefore an upper limit, the activation energy must also be an upper limit. Hence, the possible chemical response of Na to wave-induced temperature fluctuations should also be at a maximum in this model. If the response were in fact less, our overall conclusions would be unchanged. We also believe that our conclusions would not be significantly different if we were to employ a different mean state using, for example, the number densities of minor species for summer rather than winter.

The assumption of small horizontal phase trace speed relative to the local sound speed that validates the use of equations (2) and (3) also implies small vertical wavelengths. Gravity waves

having short vertical wavelengths, less than about 15 km, and periods greater than about 25 minutes, are most easily measured using sodium lidars [e.g., Gardner and Voelz, 1987]. Therefore, the wave parameters adopted in the present study are applicable to sodium lidar investigations of gravity waves.

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