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Comparisons of spectrally resolved nightglow emission locally simulated with space and ground level observations.

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ABSTRACT

A mesospheric model of the airglow emission is developed to recover the night variations observed at ground level. The model is based on a 1D vertical photochemical model, including the photodissociation and heating processes. The spectral radiation is calculated at high altitude and propagated through the atmosphere to the ground. We also include short scale vertical dynamic such as turbulences and the molecular diffusion. Simulations reveal realistic emissions when compared with space observations. In addition, we estimate the impact of changes associated with parameterized atmospheric tides. The comparison with observations is performed over high altitude and ground level. We confront the model outputs at high altitude with satellite observations (SABER and GOMOS) and the simulations propagated at ground level are compared to local measurements campaigns performed in France and India. Biases between observed and simulated radiances and volume emission rates are suspected to be due to the impact of gravity waves or the large scale dynamic.

Key words. nightglow emission – modeling – mesosphere

1. Introduction

The night airglow is the radiation emitted over a wide spectrum originating from the chemical de-excitation of molecules in the mesosphere and thermosphere. Discovered by Meinel (1950), it has been studied for decades. First investigations were made by ground-based observations (Chamberlain and Roesler, 1955) and rocket measurements (Baker and Stair, 1988). Satellites allowed direct observation of the nightglow outside the atmosphere with a large spatial and temporal coverage. Among them, WINDII (Shepherd et al., 2012), SABER (Marsh et al., 2006), HRDI (Burrage et al., 1994) or more recently GOMOS (Bellisario et al., 2014) built the main climatology of the various sources of the nightglow.

33 The main feature of the emission comes from the infrared emission of the rovibrationally excited
34 OH (Leinert et al., 1997) created by the reaction of H and O₃. Many factors have an effect on the
35 variations of the signal. For example, gravity waves increase locally the intensity of the emission,
36 tides induces diurnal variations, atomic oxygen controls the ozone recombination and therefore the
37 airglow intensity. The observation of the emission can then be a useful signature for the understand-
38 ing of the various physical and chemical phenomena occurring at high altitude such as the role of
39 the gravity waves (Hines, 1960) and atmospheric tides (Petitdidier and Teitelbaum, 1977).

40 Both imaging systems and spectrometers enable the observation of the airglow. The first ones,
41 with a large field of view, measure the photon quantity emitted by the airglow layer (Takahashi and
42 Batista, 1981; Lowe et al., 1991), and retrieve the structures at high altitude such as gravity waves
43 (Taylor et al., 1995b,a; Pautet et al., 2014) and tides (Mulligan and Nallen, 1998). The second ones
44 allow the studies of the rovibrational population of OH, the retrieval of temperature (Takahashi and
45 Batista, 1981), and the wind velocity (Didebulidze et al., 2011).

46 Many studies used an analytical approach for the estimation of the airglow emission. For exam-
47 ple, Le Texier et al. (1987) use a two-dimensional dynamical and photochemical coupled numerical
48 model to estimate the annual variations of the OH emission layer for various latitudes. McDade
49 (1991) investigates vertical variations of the OH vibrational distributions, in particular the impact
50 of quenching and vibrational deactivation processes. Altitude of the OH nightglow layer is also
51 predicted by Liu and Shepherd (2006) using a multiple linear regression analysis of six years of
52 WINDII records. Relations between gravity waves and O₂ and OH airglows perturbations are high-
53 lighted by Liu and Swenson (2003) with the help of a one-dimensional model. Grygalashvyly et al.
54 (2014) show the mean state and trends of the hydroxyl layer during the period 1961-2009 by cou-
55 pling an OH*-model with a chemistry-transport model.

56 However, these studies do not spectrally resolve the emission as they only produce global -or
57 transition specific- volume emission rate (VER). In order to simulate the emission spectrum at
58 the various altitudes concerned, it is mandatory to include in the model the various excited states
59 implicated in the emission as reactive species. Very few models able to simulate the full spectrum
60 observed at high altitude were developed and none are available for ground-based analyses. Moreels
61 et al. (1977) describe a 1D chemical model with eddy diffusion but without dynamical effects or
62 heating and suffers from instability. Rodrigo et al. (1991) also include O(¹D) and O₂(¹Δ) to discuss
63 the Eddy diffusion coefficient. Makhlof et al. (1995) look at the atomic oxygen green line at 557.7
64 nm and OH emission in a diurnal 1D model which pairs up with a simple gravity wave model to
65 study their perturbations (Makhlof et al., 1998). Yee et al. (1997) model is based on TIME, im-
66 plemented with OH, O₂ and O emission reactions and comparisons with satellite observations from
67 HRDI. More recently, Fytterer et al. (2019) derive night-time atomic oxygen and atomic hydrogen
68 in the mesopause region by extending a chemistry box model with several chemical reactions and
69 physical quenching processes involving OH(*v*), providing in addition transitional VER. It is worth
70 noting that these models listed above are not implemented with a radiative transfer model, required
71 in order to propagate the spectrum simulated at high altitude down to the ground.

72 The objective of this study consist in simulating nightglow that can be observed at ground level.
73 Therefore a local photochemical model was developed based on the most up-to-date coefficients.
74 On the contrary to other models, various excited states along with a radiative transfer module are in-
75 cluded in order to obtain the OH spectral emission emitted at high altitude, and propagate it down to
76 the ground through interaction with the neutral atmosphere for comparison to local measurements.

77 To include the various dynamical processes on the 1D model, temperature and wind fluctuations
78 over short timescales are forced and simulated externally.

79 Interests of such a study are manifold. Right below the boundary between Earth's atmosphere
80 and outer space, the knowledge of the energy exchange such as gravity waves breaking are impor-
81 tant to better constrain climate models. Temperature, wind velocity or molecule concentrations are
82 variables that can be retrieved with the observation of the airglow (Khomich et al., 2008). Seen from
83 the ground, the airglow layer is also important. In the case of infrared astronomy, H band included
84 between 1.45 and 1.8 μm is polluted by OH emission. A flat field is commonly used to estimate this
85 pollution over integration time of few hours, not taking into account its short time variability. Other
86 spectral bands can also be impacted (Slanger et al., 2003). Finally, passive night vision system are
87 interested in using the airglow emission layer propagated down to the ground and reflected by the
88 surface (Derelle et al., 2012).

89 In the following section, we describe the various parts of the model, including the photodisso-
90 ciation processes, the heating, the emission calculation and propagation. Local dynamic in 1D is
91 implemented and a tide parameterization is used. Then we present the first results of the model
92 and a short sensitivity test on the tidal effects. Finally, we compare the outputs of the model at
93 high altitude with observations from space using SABER instrument and GOMOS spectrometer,
94 and ground-based IR camera obtained during successive measurement campaigns to test the model
95 output and suggest the next steps required to improve the model.

96 2. Description of the model

97 2.1. The photochemical code

98 Since we aim to build a model simulating the photochemical reactions at high altitude, 24 species
99 are taken into account in the model (Table 1), including the calculation of all the vibrational states
100 of OH and excited states of molecular and atomic oxygen. The stable species are used as inputs
101 producing as outputs the excited states listed in Table 1, distributed on a vertical 1D grid. Then,
102 these excited species lead to the computation of atmospheric spectral emission or integrated volume
103 emission rate (see section 2.4). Tables A.1, A.2 and A.3 list the chemical reactions used in the
104 model, following the numbering from Moreels et al. (1977). 81 reactions are taken into account and
105 the reaction coefficients are mostly taken from the JPL atmospheric data (Sander et al., 2011). We
106 use the backward Euler method based on the Taylor series to resolve the chemical system Jacobson
107 (2005). This method brings a positive solution regardless the selected time step and the solution is
108 also iterated in order to insure the stability and precision of the system.

109 Initial data originate from MSISE-90 data (Hedin, 1991) for local comparison. MSISE-90 model
110 intends to provide the neutral temperature and densities (O, N₂, O₂ and H for example) up to ther-
111 mospheric heights. For other cases, standard atmospheric profiles are interpolated over a vertical
112 grid ranging from 25 to 125 km with a 500 m altitude resolution. Chemistry of NO_x, ClO_x and CO_x
113 have been left out to alleviate the system since their contributions are mostly prominent below 25
114 km (Brasseur and Solomon, 2005).

Table 1. List of the species used in the present model. Excited states are used for OH (all vibrational, from 1 to 9), and also $O_2(^1\Delta)$, $O_2(^1\Sigma)$, $O(^1D)$ and $O(^1S)$.

Stable species	Name	Excited states
O_3	Ozone	
H	Hydrogen	
OH	Hydroxyl	Vibrational states: $OH_{v,v=1..9}$
$O_2(^3\Sigma_g)$	Molecular Oxygen	$O_2(^1\Delta), O_2(^1\Sigma)$
$O(^3P)$	Atomic Oxygen	$O(^1D), O(^1S)$
HO_2	Hydroperoxyl radical	
N_2	Dinitrogen	
H_2	Dihydrogen	
H_2O	Water vapour	
H_2O_2	Hydrogen peroxide	
$M=H_2+N_2+O_2$		

115 2.2. Chemical photodissociation

116 The OH vibrational states originate from the reaction 8 between H and O_3 (Table A.1). As the
 117 ozone photodissociates during the day, the model runs starting from the previous night to reproduce
 118 a realistic ozone profile. In order to compute photodissociation effects, we use a combination of
 119 high resolution SOLSPEC solar spectrum (Thuillier et al., 2009) and SOLSTICE experiment for
 120 UV range (Rottman et al., 2001) based on SUSIM instrument (Floyd et al., 2002). Interpolations
 121 have been operated down to 0.05 nm in the UV region to take into account the Lyman- α line, the
 122 Schumann-Runge and the Huggins bands. Above 3 μm , data are derived from Thekaekara (1974).
 123 The solar zenith angle is calculated using the Chapman function (Smith and Smith, 1972) to esti-
 124 mate the optical depth. The solar irradiance is propagated through the Beer-Lambert law at each
 125 altitude level. The induced photolysis acts on several molecules: O_2 , O_3 , H_2O , H_2O_2 and HO_2 .
 126 Cross sections of the molecules are taken from the Max-Planck Institute and Harvard CfA. For the
 127 Rayleigh diffusion, we use Nicolet’s formula (Nicolet, 1984). Since the cross sections of O_2 and O_3
 128 display large variations in some spectral band, a fine resolution of 10^{-4} μm is used to simulate the
 129 spectral details in the Schumann-Runge band, the Chappuis band and around the Lyman- α wave-
 130 length. The spectral quantum yields for the produced species are summarized on tables A.4 and A.5
 131 and are taken from Moreels et al. (1977). For the visible and IR region, the resolution is from 10^{-2}
 132 up to 1 μm in order to avoid long computation time.

133 2.3. Heating effects

134 The mesopause is subject to strong energy exchanges (Mlynczak, 1997). The importance of the
 135 heating has been noticed by Mlynczak (2000). We consider in the model the solar heating, the
 136 chemical heating and also the radiation cooling (by CO_2). The solar irradiance is absorbed by the
 137 O_2 and O_3 molecules between 50 and 110 km (Brasseur and Solomon, 2005). The energy is enough
 138 to break the chemical bounds of the molecules. The difference of energy between the initial and final
 139 states is converted into kinetic energy. We apply here the formulation from Brasseur and Solomon

140 (2005) that expresses the difference of absorbed solar radiation at a specific layer i , between two
141 vertical levels:

$$142 \frac{dT(i)}{dt} = \frac{\cos(Z)}{\rho(i)C_p} \int_{\lambda} \frac{I(z, \lambda)}{dz} d\lambda \quad (1)$$

143 with dT/dt the heating rate, *i.e.* the variation of the temperature T with time t at the layer i , the
144 solar zenith angle Z , the density ρ , the calorific capacity C_p , and $I(z, \lambda)$ the incident solar intensity
145 at a wavelength λ and an altitude z . The formulation is valid for middle atmosphere, in the absence
146 of clouds. The correction of C_p with the range of temperature is assumed to be small and therefore
147 neglected. This leads to heating up to 10 Kelvins per day.

148 Exothermic reactions in the middle atmosphere have been listed by Mlynczak and Solomon
149 (1993) (table A.7). We apply their formulation for the calculation of the temperature variation in-
150 duced by the exothermic reactions:

$$151 \frac{dT(i)}{dt} = \frac{2}{7} \sum_r \frac{k_r \rho_{r,1}(i) \rho_{r,2}(i) dH}{k_b N_A \rho(i)} \quad (2)$$

152 With k_r the rate of the considered reaction, the density of the reactants considered $\rho(1, 2)$ and air ρ ,
153 the reaction enthalpy H , the Boltzmann constant k_b and the Avogadro number N_A .

154 The radiative cooling tallies with the CO₂ infrared radiation around 15 μm . We use here
155 the Fomichev parametrisation (Fomichev et al., 1998) which takes into account LTE (Local
156 Thermodynamic Equilibrium) and non-LTE effect at high altitude.

157 These heating rates, encompassing the solar heating, the chemical heating and the radiative cool-
158 ing are multiplied by the time step of the model, providing a temperature perturbation within the
159 layer. The profiles of the different heating rate profiles shows that, in the stratosphere, chemical
160 heating and radiative cooling have a similar amplitude. Around the mesopause, the chemical heat-
161 ing exhibits the strongest effect. At higher altitude, the solar heating gets more important together
162 with the radiative cooling.

163 2.4. Emission calculation

164 Since we aim to compare the model results with ground based observations, we compute the fully
165 resolved spectrum of the airglow. The intensity of an emission line is written according to:

$$166 I_{(j', \nu' \rightarrow j'', \nu'')} = N_{(j', \nu')} A_{(j', \nu' \rightarrow j'', \nu'')} \quad (3)$$

167 Where $I_{(j', \nu' \rightarrow j'', \nu'')}$ is the transition intensity between the rovibrational state (j', ν') and (j'', ν'') , j and
168 ν are respectively the rotational and vibrational quantum numbers, $N_{(j', \nu')}$ is the population of the
169 rovibrational state, and $A_{(j', \nu' \rightarrow j'', \nu'')}$ is the Einstein coefficient of the transition taken from Turnbull
170 and Lowe (1989) (see tables A.6 and A.4). The photochemical part of the model calculates the
171 populations of the various vibrational excited states of OH. And then, the rotational population of
172 each vibrational state is computed using the Boltzmann distribution.

173 At this stage, it is also possible to compute the Volume Emission Rate (VER) ϵ based on the
174 vibrational excited states of $[OH]_v$ and the Einstein coefficients A_v from Turnbull and Lowe (1989).
175 The VER for a specific vibrational transition is given by:

$$176 \epsilon = \frac{[OH]_v}{A_v} \quad (4)$$

177 It is also worthily to mention that because of the low temperature at this altitude, the local thermal
 178 emission of the atmosphere is spectrally located in the mid and far infrared and does not interfere
 179 with the emission.

180 2.5. Emission propagation

181 The emission propagation is insured by the model RAYJN developed by ONERA (Simoneau et al.,
 182 2011). It calculates the radiation at the ground including the solar radiation (in daily conditions),
 183 the thermal radiation of the atmosphere and the nightglow emission. The diffusion through the
 184 atmospheric layers follows the discrete-ordinate method developed by Nakajima and Tanaka (1986).
 185 The radiative transfer equation is written hereafter:

$$186 \frac{dL(\tau, \Omega)}{d\tau} = -L(\tau, \Omega) + J_{th} + J_{ds} + J_{dm} + J_{glow} \quad (5)$$

187 With $L(\tau, \Omega)$, the radiance for the optical depth τ , which propagates in the direction Ω . J_{th} , J_{ds} ,
 188 J_{dm} and J_{glow} are the different sources functions, respectively from the thermal emission, the simple
 189 scattering, the multiple scattering and the nightglow emission. The expressions of the various
 190 sources follow:

$$191 J_{th} = k_a(s, \sigma)B(T) \quad (6)$$

$$192 J_{ds} = k_d(s, \sigma)F_0(s, \sigma)p(s, \sigma, \Omega, \Omega_0) \quad (7)$$

$$193 J_{dm} = k_d(s, \sigma) \int_{4\pi} L(s, \sigma, \Omega, \Omega')p(s, \sigma, \Omega, \Omega')d\Omega' \quad (8)$$

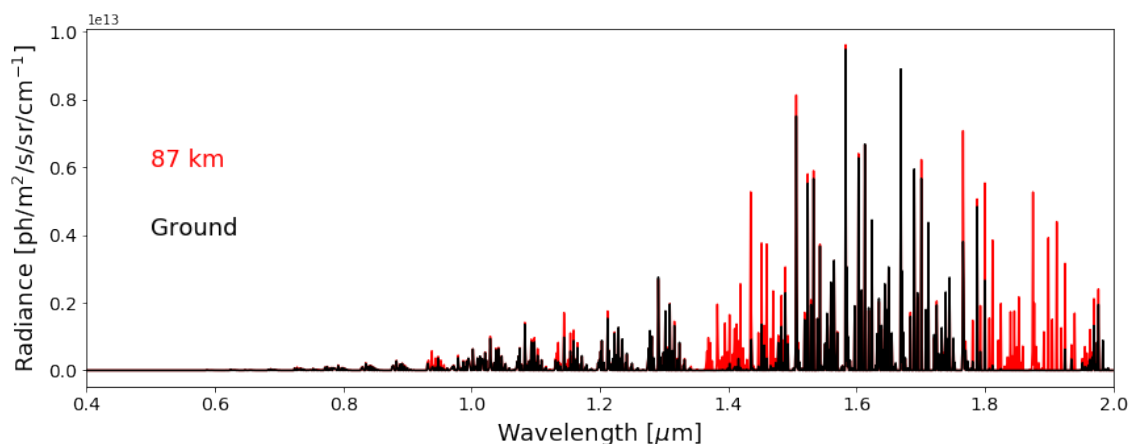
$$194 J_{glow} = \frac{I(s, \Omega)}{4\pi} \quad (9)$$

195 with s denoting the position, σ the wavenumber, $B(T)$ the Planck function, k_a and k_d the absorption
 196 and diffusion coefficient, F_0 the solar radiance, p the phase function associated to the angle (Ω, Ω') ,
 197 L the radiance, I the intensity of the nightglow emission. An example of the spectrum modeled at
 198 high altitude (in red) and the result at the ground level (in black) is given in Figure 1. We observe
 199 the strong absorption band around $1.4 \mu\text{m}$ originating from the water vapor absorption.

203 2.6. Vertical dynamic

204 Local vertical dynamic responsible for the chemical components transport is induced by the Eddy
 205 diffusion, the molecular diffusion and the wind advection. The turbulence (Eddy) diffusion starts
 206 with the Eddy diffusion coefficient, calculated with the formula from Lindzen (1981). At the same
 207 time, the diffusion coefficient is calculated with the formula from Jacobson (2005). We verify that
 208 turbulences are prevailing below 100 km and then diffusion overtakes the vertical dynamic. We use
 209 the Crank-Nicolson forward implicit Euler Scheme, which is in second order in time to resolve the
 210 turbulence-diffusion equation.

211 The wind advection presents two components, the vertical drift velocity, calculated with the
 212 molecular diffusion coefficient, and the tidal wind, which is described in the next paragraph. We
 213 use here a semi-Lagrangian scheme to resolve the advection.



200

201 **Fig. 1.** Example of a spectrum at 87 km (in red) and the same spectrum propagated at the ground level (in
 202 black). We notice the strong water vapor absorption band around 1.4 μm .

214 The dynamic dominates long-lived species loss rates. For example, $\text{O}(^1\text{D})$ is driven by the dy-
 215 namic up to 90 km. Above, the emission dominates the loss rate. On the other side, the excited states
 216 of OH are short-lived and therefore the emission dominates the loss rates. Nonetheless, because of
 217 the dependance of the OH excited states on the concentration of species such as O_3 , the dynamic
 218 remains important to properly simulate the emission rates.

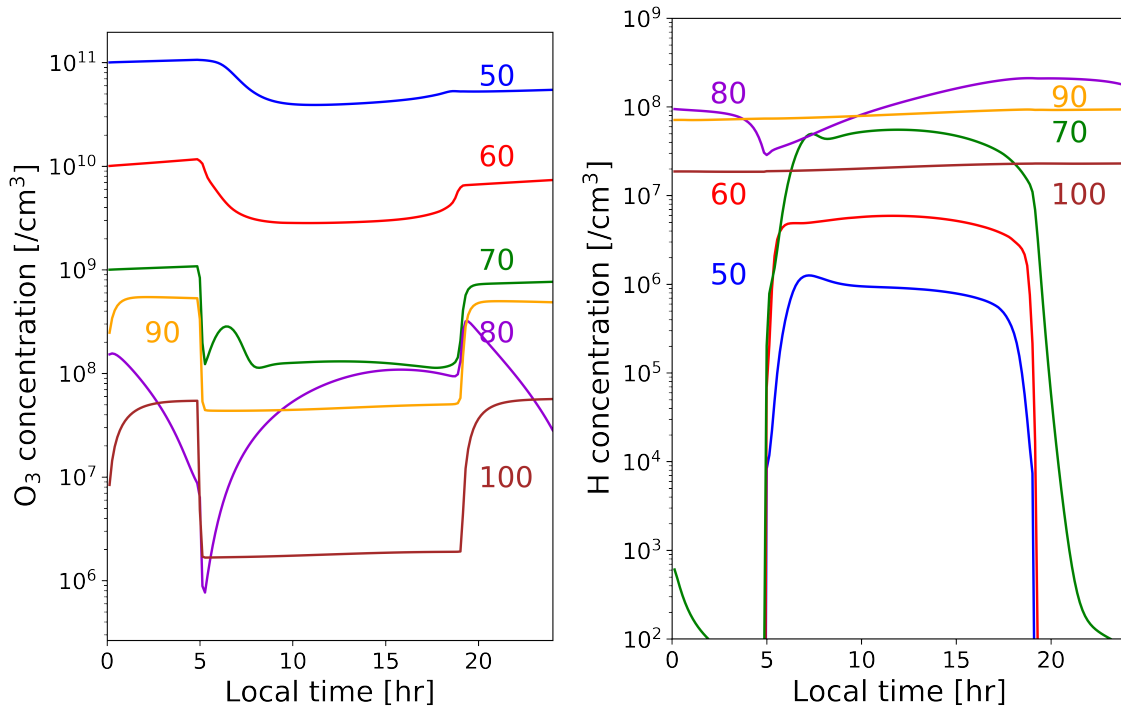
219 2.7. Tides parameterization

220 To ensure a fair representation of the migrating tides in the timescale of a night, we use simulations
 221 performed by the Global-Scale Wave Model (GSWM) (Hagan et al., 1999). It solves the linearized
 222 Navier-Stokes equations to provide the wind speed and temperature perturbations. The vertical
 223 wind, which is solved by the advection, is implemented and the temperature perturbation acts on
 224 the photochemical system.

225 3. Description of the model outputs

226 In this section, chemical compositions and emissions computed by the model are presented. We first
 227 briefly analyze the outputs of the photochemical model on a 1D grid. The variations of the species
 228 allow comparisons with other high altitude 1D studies such as Allen et al. (1981) and Rodrigo et al.
 229 (1986) although we do not detain the various models. The evolutions of H and O_3 concentrations,
 230 sources of the excited OH, are presented in Figure 2. Ozone is strongly affected at high altitude by
 231 the photodissociation showing a strong diurnal change. Its production originates from the recombi-
 232 nation between O and O_2 . H is also strongly dependent on the photodissociation of H_2O that leads
 233 to the increase of H during the day below 80 km (Haefele et al., 2008).

237 The filling of the OH vibrational states from the photochemical resolution shows that the lower
 238 energy populations are preferred (Figure 3) which is consistent with the Maxwell-Boltzmann dis-
 239 tribution law although OH is in NLTE. Others studies such as Pickett et al. (2006) or von Savigny
 240 et al. (2012) present similar results. We also observe that the altitude of the emission maximum



234

235 **Fig. 2.** Examples of molecules concentration evolution, O_3 on the left and H on the right. Ozone is strongly
 236 dependent on the solar cycle above 60 km. Below 80 km, H originates from the water vapor dissociation.

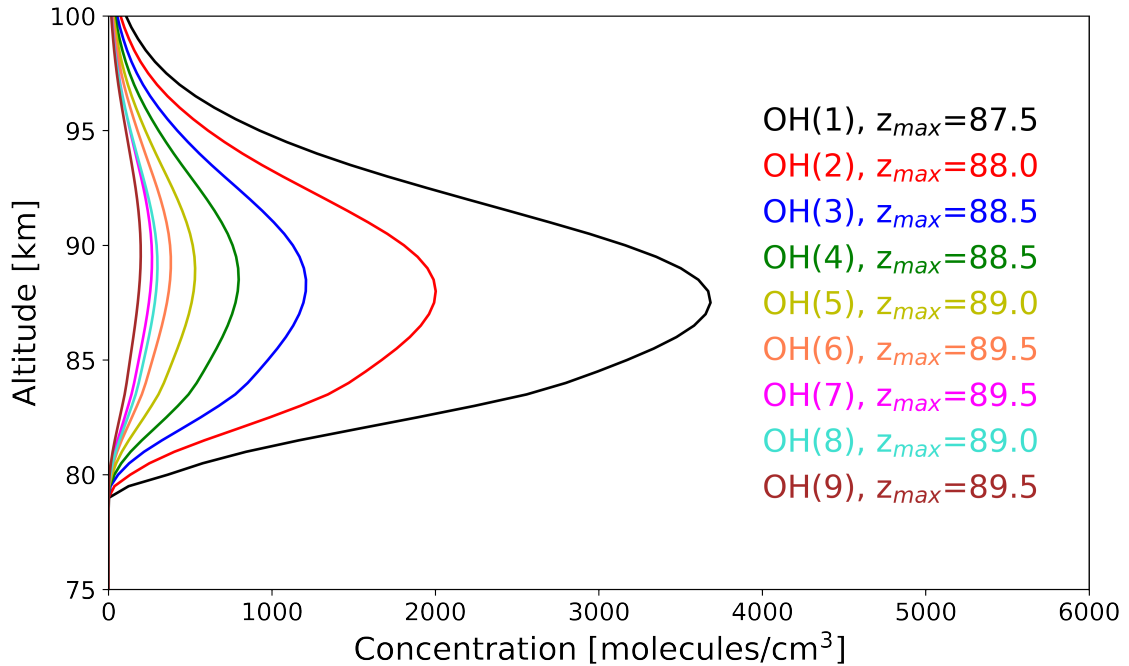
241 depends on the vibrational level. Higher levels have their maximum at higher altitudes (Moreels
 242 et al., 1976).

244 The temporal VER evolution of the global OH vibrationally excited states along the altitude is
 245 represented in Figure 4 (top panel). The airglow emission grows when the night starts, to reach its
 246 maximum during the middle of the night. The altitude of the maximum decreases during the night
 247 of a few kilometers. We also notice that the airglow layer width decreases as well.

248 In order to investigate the effect of the tidal parameterization and the model sensitivity, the model
 249 by doubling the amplitude of the tides. The result is shown in Figure 4 (bottom panel). The max-
 250 imum occurs in the second part of the night, supported by the compression of the airglow layer.
 251 Tides have an effect on the time evolution of the emission, and specifically on the time of the max-
 252 imum of the emission, on the thickness of the emitted layer, and on the variation of the altitude of
 253 the maximum of the emission.

259 4. Discussions

260 In this section, we discuss the results by comparing model simulations with past observations re-
 261 ported in the literature, starting with the WINDII instrument observing the OH(8-3) transition, or
 262 the P1(3) line (Melo et al., 2000). Since the atmospheric profiles corresponding to these measure-
 263 ments are not available, we cannot reproduce the emission profiles but only obtain a quantitative
 264 estimation. Uncertainties through a bootstrap analysis would require in addition uncertainties on



243

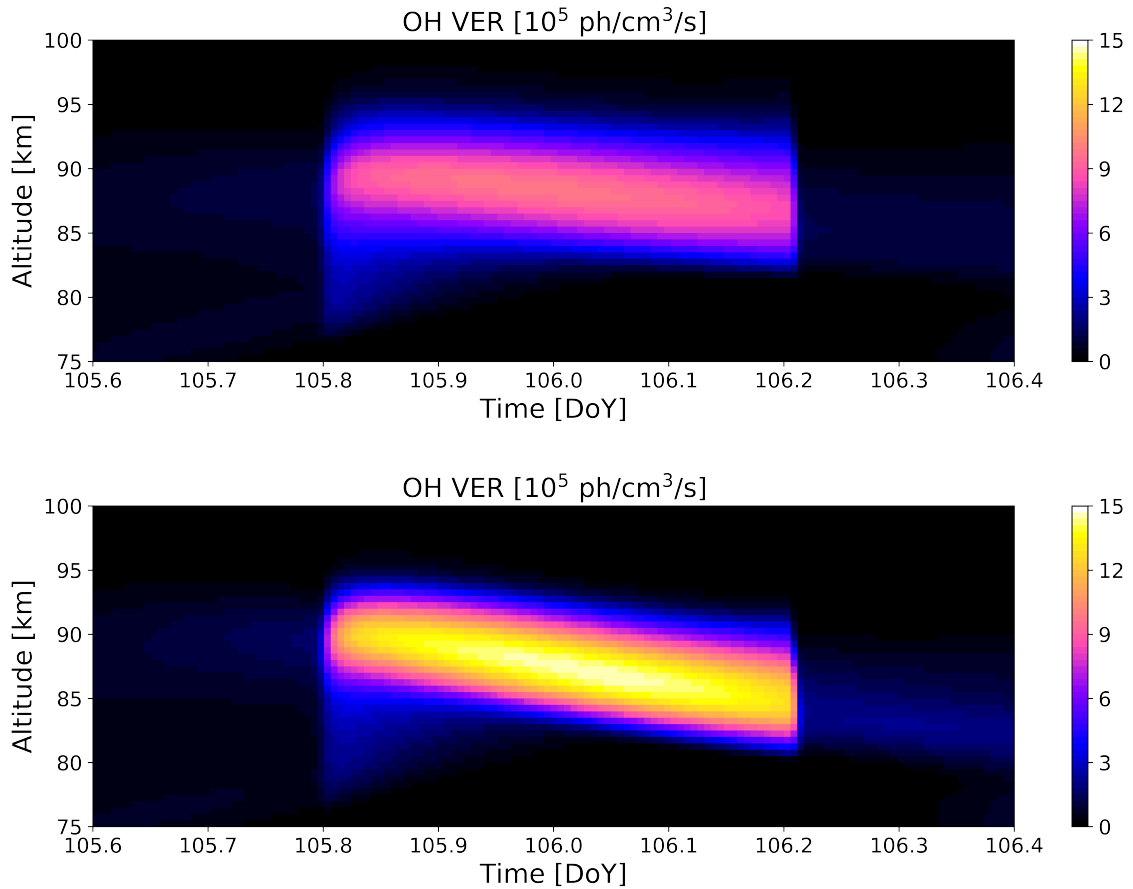
Fig. 3. Examples of OH vibrational states concentration as function of altitude.

265 the atmospheric profiles and a full line-by-line computation of the spectral emission with its propa-
 266 gation at short temporal intervals.

267 The model outputs have been filtered to take into account the WINDII instrumental characteristic,
 268 centered at 734.6 nm with a spectral width of 1.2 nm. The emission profiles observed and modeled
 269 are look-alike, with a maximum for the first at 55 ph/cm³/s and for the second at 80 ph/cm³/s.
 270 Analogously, the Visible Airglow Experiment (VAE) (Hays et al., 1973) has observed the OH(8-3)
 271 band around 731.6 nm with a spectral width of 1.58 nm. Emission profiles used for the comparison
 272 are provided by Abreu and Yee (1989). The maximum has been found at 72 ph/cm³/s for the obser-
 273 vation and we established a profile for the same condition of observations with a maximum at 79
 274 ph/cm³/s. The study reported a layer thickness of 12.5 km and our model shows a layer thickness
 275 of 10.5 km.

276 Measurements provided by the SABER instrument aboard the Timed platform are compared with
 277 the model. SABER is a satellite instrument dedicated to the nightglow observation. The spectral
 278 bandwidth ranges between 1575 and 1725 nm, and also between 1930 and 2170 nm corresponding
 279 to $\Delta\nu = 2$ transitions (Mlynczak et al., 2013). We present in Figure 5 (a) and (b) (red solid line)
 280 the Volume Emission Rate profiles of the airglow emission observed around 1.6 μm and around 2.0
 281 μm respectively for a concordant choice of space and time (orbit 67574 for the 29th of May 2014).
 282 Because SABER data does not provide uncertainty, we selected a time interval of \pm one month
 283 around the 29th of May to estimate the mean VER profile (in black) and the standard deviation (in
 284 grey) associated to all the profiles included in $\pm 30^\circ$ in latitude and longitude. The seasonal varia-
 285 tions is filtered by a running window of 2 months to keep informations about temporal variability.

292 Our simulations underestimate the observations albeit they belong to the range of the standard
 293 deviation. In the case of the 1.6 μm VER, the altitude of the peak is consistent with the closest profile

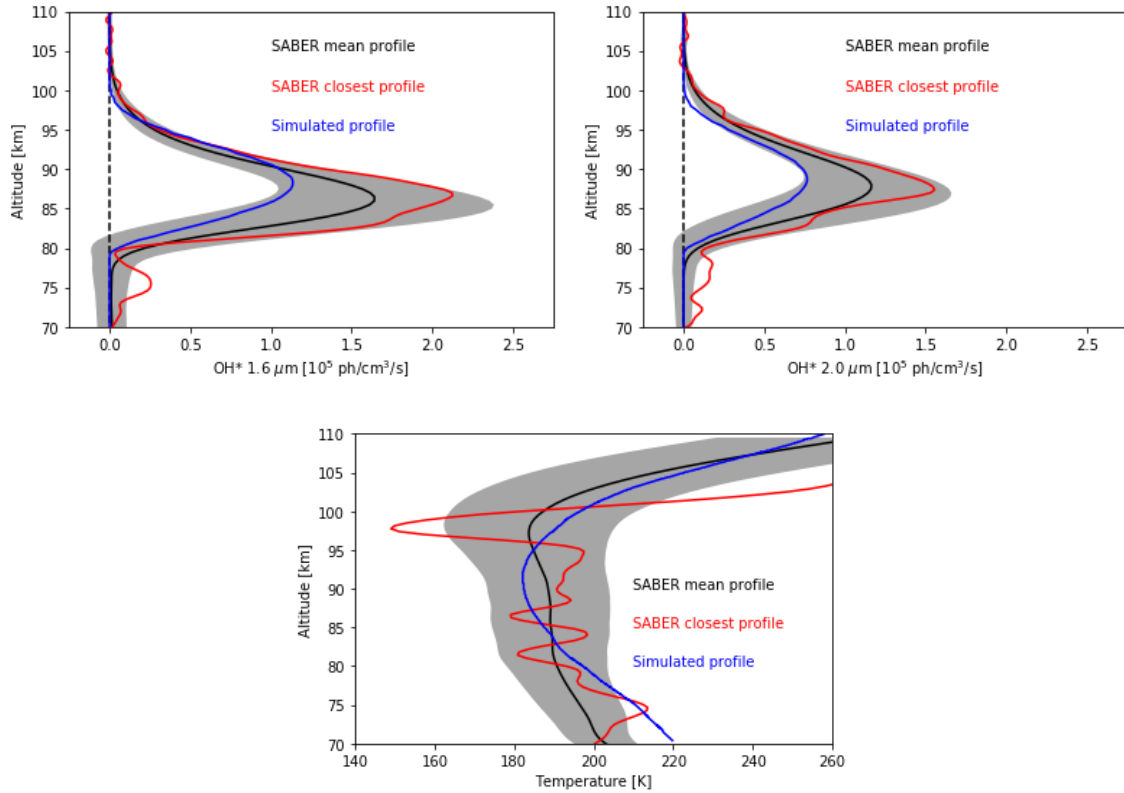


254
255

256 **Fig. 4.** Top panel: example of the OH Volume Emission Rate (in 10^5 $\text{ph}/\text{cm}^3/\text{s}$) between 80 and 95 km for
257 one night (starting at Day of Year 105.8 and ending at DoY 106.2). Bottom panel: same example but with the
258 tidal amplitude doubled.

294 but is higher than the mean profile peak. The consistency is increased for the $2.0 \mu\text{m}$ peak altitude.
295 The difference in the profile-to-profile comparison is useful to highlight the limits of the model.
296 To understand this, the temperature profiles are displayed in Figure 5 (c). The SABER (mean and
297 closest) and modeled (coming from MSIS data) temperature profiles are represented in black, red
298 and blue respectively. SABER closest temperature profile highlights strong perturbations induced
299 by the presence of gravity waves.

300 The impact of gravity waves (GW) on the airglow is subject of numerous studies (Pautet et al.,
301 2005, 2014; Taylor et al., 1995a). They act on both the temperature and density of the area where
302 they propagate and they are able to transport energy and momentum up to the mesospheric region.
303 Therefore, changes in temperature and concentrations will lead to changes in emission. For ex-
304 ample, a local increase in density can induce a local increase in the observed VER. A change in
305 temperature will imply changes in chemical rates and therefore in OH excited states sources. In this
306 particular case where the simulated VER is lower than observed, we assume that the GW increases
307 the temperature as seen in Figure 5 (c) and modify the density, leading to changes in the chemistry
308 of the nightglow production. Not shown here, the oxygen profile is also larger for the observation



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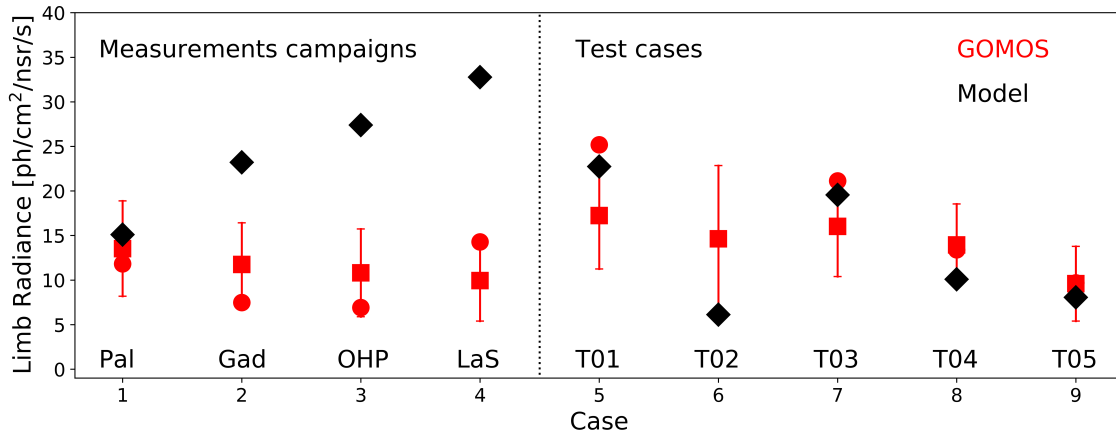
288 **Fig. 5.** (a): OH $1.6 \mu\text{m}$ profiles from simulation (in blue), and observations (mean profile in black and closest
289 profile in red). The ± 1 standard deviation from the mean is represented with the grey shade. (b): Same as (a)
290 but for OH $2.0 \mu\text{m}$. (c): Associated temperature profiles. The simulated temperature profile originate from
291 MSIS data.

309 in comparison to the observation. This comparison implies that a proper representation of the GW
310 effects in the model is required to recover a more realistic profile of the observed nightglow.

311 4.1. Comparison with GOMOS data

312 GOMOS was an instrument on board ENVISAT dedicated to the observation of ozone using the
313 stellar occultation (Bertaux et al., 2010). Airglow data have been obtained by two spectrometers
314 looking at, below and above the star. The complete method is described on Bellisario et al. (2014).
315 GOMOS allowed the recovery of the OH airglow between 925 and 955 nm, corresponding to a part
316 of the OH(8-4) band. Chen et al. (2019) uses the R branch between 930 and 935 nm to retrieve
317 global nighttime atomic oxygen abundances.

318 We compare the limb view from GOMOS to the model for several cases (mixing local mea-
319 surements campaigns with specific locations). Averaged OH(8-4) radiation observed between years
320 2002 and 2010 over all longitudes have shown a semi-annual variation at the Equator, with maxima
321 at the solstices (Bellisario, 2015). Due to the geometry of the occultation observations, the compar-
322 ison is not straightforward. We would require the spatial evolution of OH emission profiles along
323 the line of sight to estimate the limb radiance by simulation. As a first approximation, we use an



341

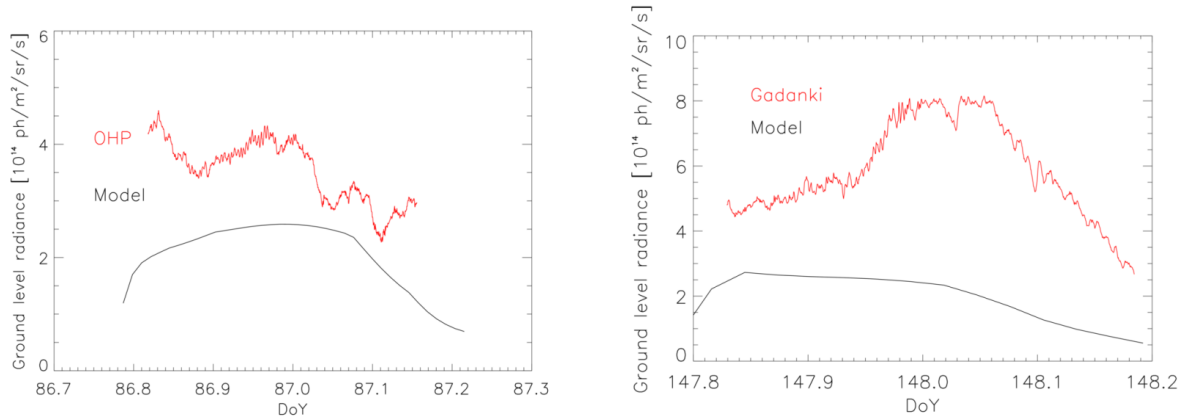
342 **Fig. 6.** In red squares are represented OH(8-4) integrated limb radiances from GOMOS between 925 and 955
 343 nm averaged within a month and $\pm 15^\circ$ latitude for several cases. Corresponding simulations are associated
 344 with the black diamonds and the closest observations are in red circles.

324 homogeneous emission layer and geometrical assumptions for the line of sight limb radiance. The
 325 geometrical line of sight is estimated of about 508 km for a layer at 87 km with a width of 10 km. In
 326 Figure 6 are represented in red the GOMOS limb radiances and in black the corresponding model
 327 simulation limb radiances. For a specific date and location, GOMOS data are averaged (red squares)
 328 within the month (to avoid seasonal variations), within a $\pm 15^\circ$ latitude interval over all longitudes
 329 for full dark conditions in most cases (i.e. no light contaminations). The standard deviations of the
 330 available spectra within these conditions are represented with the error bars. In addition, the closest
 331 observations is added with the red circles.

332 The cases representing the measurements campaigns (detailed in the next section) are shown on
 333 the left-hand side and other test cases for specific locations in latitude and time on the right. Overall,
 334 the range of simulated limb radiances matches the GOMOS observations. The measurements cam-
 335 paigns do not show a consistent behaviour, with simulated limb radiances increasing for decreasing
 336 observations. On the other side, the test cases show consistency with two high cases matching sea-
 337 sonal maxima (T01 and T03 at 0°N , respectively on March the 1st, 2014 and October the 1st, 2014).
 338 T02 (70°N on November the 11th) shows a strong decrease in the simulation whereas the observa-
 339 tions decrease is fainter. The standard deviation is however higher in this case. T04 and T05 both at
 340 60°S , but respectively on April the 15th and July the 1st also show consistency with a small decrease.

345 4.2. Comparison with ground-based observation campaign

346 During the measurement campaigns performed by ONERA, the main camera used is a Short-Wave
 347 InfraRed (SWIR) camera. It is based on a thermoelectric cooled InGaAs detector and its spectral
 348 bandwidth ranges from 0.9 to 1.7 μm (vibrational transitions $\Delta\nu = 2$ and 3 of the OH Meinel
 349 band system). The integration time is of about 400 ms, for a night with a typical luminosity. The
 350 camera is radiometrically calibrated in laboratory in order to get absolute integrated radiance, in
 351 photons/s/m²/sr. For the comparison, we integrate the spectral radiance modeled at the ground level
 352 between 0.9 and 1.7 μm for a zenithal line of sight.



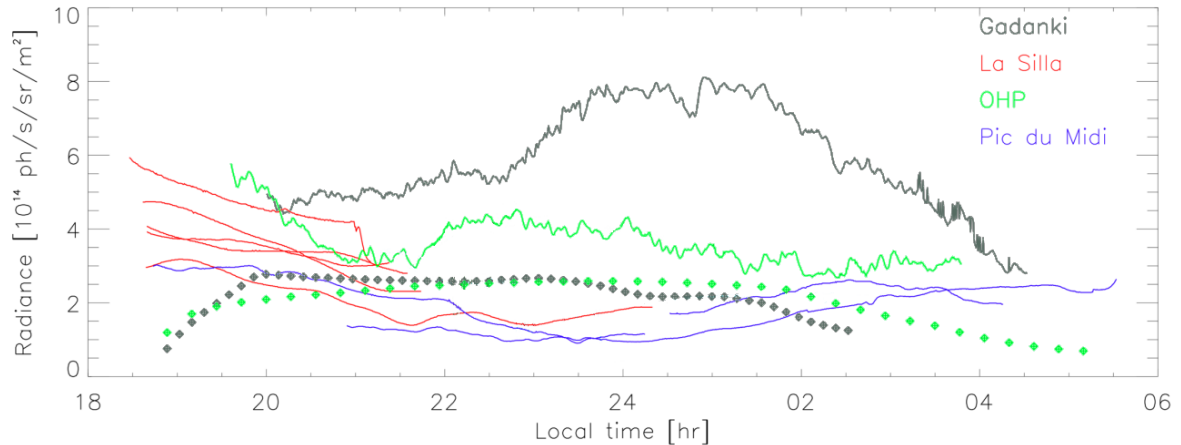
357

358 **Fig. 7.** (a): Comparisons between the measurement campaign at OHP, France in red and and the model in
 359 black. (b): Same but for Gadanki, India. The model underestimates in both case the intensity of the nightglow
 360 measured on the ground level, especially at Gadanki, where the night showed a strong activity of gravity
 361 waves.

353 We present the result for 2 nights, in Figure 7. They correspond to the Observatoire de Haute
 354 Provence (OHP, France), 43.93°N, 5.71°O, on March, the 28th, 2014 and the NARL at Gadanki
 355 in India, 13.46°N, 79.18°E on May the 29th, 2014. In red are represented the observed radiance at
 356 ground level and in black are represented the output of the model.

362 In the case of OHP, the level of radiation observed varies from 4 to 2 x10¹⁴ ph/s/m²/sr with a
 363 stair-like evolution whereas the model presents an evolution around 2 x10¹⁴ ph/s/m²/sr. In the case
 364 of Gadanki (Figure 7), the model presents also variations around 2 x10¹⁴ ph/s/m²/sr whereas the
 365 evolution observed presents a strong grow from 4 to 8 x10¹⁴ ph/s/m²/sr and then it decreases until it
 366 reaches 3 x10¹⁴ ph/s/m²/sr. These differences may be due to a strong gravity wave activity that were
 367 observed during the campaign and which are not taken into account yet in the model. Specially at
 368 Gadanki, we observed the beginning of a strong GW activity temporally correlated with the sharp
 369 increase of the radiance at DOY 147.94. A following study will focus on the ground observations
 370 performed in Gadanki and the impact of the gravity wave activity seen in the airglow layer.

371 Several campaigns have been carried at different locations with the same instrument. We present
 372 in Figure 8 the evolution of these measurement campaigns (in solid lines) that took places respec-
 373 tively in La Silla (29°15'S, 70°44'O, Chile), Pic du Midi (43°55'N, 5°42'E, France). The evolutions
 374 of most of the nights correspond to a decrease from the beginning of the night and during the second
 375 part of the night, we can notice small increases that might originate from tidal effects in Pic du Midi
 376 observations. The intensity of the simulated airglow is presented in diamonds and corresponds to
 377 the range of observations, between 1 and 4 x10¹⁴ ph/s/m²/sr. We relate these differences in intensity
 378 and evolution to dynamical effects such as gravity waves and tides. These effects need to be better
 379 taken into account in the model to retrieve correctly the evolution of the night airglow.



380

381 **Fig. 8.** Summary of the measurement campaigns (in solid lines) carried out by ONERA. Besides Gadanki
 382 and OHP (Figure 7), campaigns have been performed at La Silla (Chile) and Pic du Midi (France). The
 383 crosses represent the evolution of the nightglow modeled at the ground level.

384 5. Conclusion

385 We have developed a numerical model that allows the estimation of the night airglow radiation at
 386 ground level. A photochemical model with dynamic modules calculates the evolution of the vibra-
 387 tionally excited OH species. Comparisons with emission and OH density already estimated in past
 388 studies show a fairly good overall agreement despite the various uncertainties in the model and the
 389 diversified datasets. When confronting the model outputs to SABER data, we relate the differences
 390 to the impact of local gravity waves that lead to an increase of the VER at high altitude. Comparisons
 391 between the model and high altitude limb observations from space using GOMOS measurements
 392 present similar evolution for test cases although local cases require further investigations. To do
 393 so, the simulated emission at high altitude is propagated down to the surface for comparison with
 394 ground-based observations carried out by ONERA. Night time evolution of the VER shows similar
 395 level of intensity with a factor of 2 except over Gadanki where larger differences are reported. In ad-
 396 dition, discrepancies in the time evolution can be noted. We suspect that these discrepancies could
 397 be due to the large scale dynamic or effects of gravity waves. At this step nor large scale dynamic or
 398 gravity waves were explicitly included in the model and should be implemented in further studies
 399 (see Swenson and Gardner (1998); Faivre et al. (2003) or Vargas et al. (2007) for parameterization
 400 of gravity waves). An example of anomalies generated by atmospheric tides has shown to perform
 401 a significant effect on the evolution and structures of the airglow layer. Nocturnal evolutions with
 402 model and observations do not show yet a perfect agreement. To overcome these problems, the in-
 403 clusion of the present model in a global atmospheric model would allow the simulation to be feed
 404 with proper 3D dynamic and atmospheric state.

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413 cess: 1st December 2019) and MSIS model output data are available at [https://ccmc.gsfc.nasa.gov/
414 modelweb/models/msis_vitmo.php](https://ccmc.gsfc.nasa.gov/modelweb/models/msis_vitmo.php) (last access: 11th February 2020). The editor thanks two anonymous
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646 **Appendix A: Reactions tables**

Table A.1. List of the reactions used in the model. Most of the references of the reaction coefficients are taken from [Sander et al. \(2011\)](#).

N ^o	Reaction	Reaction rate	Reference
01	$O_2+h\nu \rightarrow O+O$	Photolysis	Sander et al. (2011)
02	$O_3+h\nu \rightarrow O+O_2$	Photolysis	Sander et al. (2011)
03	$O+O_2+M \rightarrow O_3+M$	$(6E-34)*(t/300)^{-2.4}$ $t \in [100;268]$ K	Sander et al. (2011)
04	$O+O_3 \rightarrow O_2+O_2$	$(8E-12)*\exp(-2060/t)$ $t \in [200;409]$ K	Sander et al. (2011)
05	$O+O+M \rightarrow O_2+M$	$(4.23E-28)/(t^2)$	Schmidt et al. (2006)
06	$O+O+M \rightarrow O_2(^1\Delta)+M$	$(0.04)*(4.7E-33)*(300/t)^2$	Makhlouf et al. (1998)
07	$O+O+M \rightarrow O_2(^1\Sigma)+M$	$(1.7E-37)$	Young and Black (1966)
08	$O(^1D)+O_3 \rightarrow O_2+O_2$	$(1.2E-10)$ $t \in [103;393]$ K	Sander et al. (2011)
09	$O(^1D)+O_3 \rightarrow O_2+O+O$	$(1.2E-10)$ $t \in [103;393]$ K	Sander et al. (2011)
10	$O(^1D)+O_2 \rightarrow O+O_2$	$(3.2E-11)*\exp(70/t)$	Schmidt et al. (2006)
11	$O(^1D)+N_2 \rightarrow O+N_2$	$(1.8E-11)*\exp(107/t)$	Schmidt et al. (2006)
12	$O(^1D)+O \rightarrow O+O$	$(2.5E-11)$	Kalogerakis et al. (2006)
13	$H+O_3 \rightarrow OH^*+O_2$	$(1.4E-10)*\exp(-470/t)$ $t \in [196;424]$ K	Sander et al. (2011)
14	$OH+O \rightarrow H+O_2$	$(1.8E-11)*\exp(180/t)$ $t \in [136;515]$ K	Sander et al. (2011)
15	$OH+O_3 \rightarrow HO_2+O_2$	$(1.7E-12)*\exp(-940/t)$ $t \in [190;357]$ K	Sander et al. (2011)
16	$OH+OH \rightarrow H_2O+O$	$(1.8E-12)$ $t \in [233;580]$ K	Sander et al. (2011)
17	$OH+HO_2 \rightarrow H_2O+O_2$	$(4.8E-11)*\exp(250/t)$ $t \in [252;420]$ K	Sander et al. (2011)
18	$H+HO_2 \rightarrow H_2+O_2$	$(6.9E-12)$ $t \in [245;300]$ K	Sander et al. (2011)
19	$H+HO_2 \rightarrow 2OH$	$(7.2E-11)$ $t \in [245;300]$ K	Sander et al. (2011)
20	$O+HO_2 \rightarrow OH+O_2$	$(3E-11)*\exp(200/t)$ $t \in [229;391]$ K	Sander et al. (2011)
21	$H+O_2+M \rightarrow HO_2+M$	$k_0=(4.4E-32)*(t/300)^{-1.3}$ $k_\infty=(7.5E-32)*(t/300)^{0.2}$ $t \in [298;1500]$ K	Sander et al. (2011) Sander et al. (2011)
22	$H+OH+M \rightarrow H_2O+M$	$(2.5E-31)$	Schott (1960)
23	$H+H+M \rightarrow H_2+M$	$(2E-32)*(273/t)^{0.81}$	Trainor et al. (1973)
24	$HO_2+HO_2 \rightarrow H_2O_2+O_2$	$(3E-13)*\exp(460/t)$ $t \in [222;1120]$ K	Sander et al. (2011)
25	$OH+H_2O_2 \rightarrow H_2O+HO_2$	$(1.8E-12)$ $t \in [283;386]$ K	Sander et al. (2011)
26	$O+H_2O_2 \rightarrow OH+HO_2$	$(1.4E-12)*\exp(-2000/t)$	Sander et al. (2011)
27	$O+H_2O_2 \rightarrow O_2+H_2O$	$(1.5E-13)*\exp(-2000/t)$	Gattinger and Vallance Jones (1973)
28	$H+H_2O_2 \rightarrow H_2+HO_2$	$(1E-13)$	Gattinger and Vallance Jones (1973)

Table A.2. List of the reactions used in the model (continuation).

N°	Reaction	Reaction rate	Reference
29	$\text{H}+\text{H}_2\text{O}_2\rightarrow\text{OH}+\text{H}_2\text{O}$	$(5\text{E}-12)*\exp(-3000/t)*\text{sqrt}(t)$	Gattinger and Vallance Jones (1973)
30	$\text{O}(^1\text{D})+\text{H}_2\rightarrow\text{OH}+\text{H}$	$(1.2\text{E}-10)$ $t \in [204;420] \text{ K}$	Sander et al. (2011)
31	$\text{O}(^1\text{D})+\text{H}_2\text{O}\rightarrow\text{OH}+\text{OH}$	$(1.63\text{E}-10)$ $t \in [217;453] \text{ K}$	Sander et al. (2011)
32	$\text{O}+\text{OH}+\text{M}\rightarrow\text{HO}_2+\text{M}$	$(1.4\text{E}-31)$	Thomas and Bowman (1972)
33	$\text{HO}_2+\text{O}_3\rightarrow\text{OH}+2\text{O}_2$	$(1\text{E}-14)*\exp(-490/t)$ $t \in [197;413] \text{ K}$	Sander et al. (2011)
34	$\text{H}_2\text{O}+h\nu\rightarrow\text{OH}+\text{H}$	Photolysis	Sander et al. (2011)
35	$\text{H}_2\text{O}_2+h\nu\rightarrow 2\text{OH}$	Photolysis	Sander et al. (2011)
36	$\text{HO}_2+h\nu\rightarrow\text{OH}+\text{O}$	Photolysis	Sander et al. (2011)
37	$\text{H}+\text{O}_2\rightarrow\text{OH}+\text{O}$	$(3.4\text{E}-10)*\exp(-8250/t)$	Day et al. (1972)
38	$\text{H}_2+\text{OH}\rightarrow\text{H}_2\text{O}+\text{H}$	$(2.8\text{E}-12)*\exp(-1800/t)$ $t \in [200;1050] \text{ K}$	Sander et al. (2011)
39	$\text{H}+\text{OH}\rightarrow\text{H}_2+\text{O}$	$(2\text{E}-13)*\exp(-3400/t)*\text{sqrt}(t)$	Nicolet (1971)
40	$\text{H}+\text{O}_3\rightarrow\text{HO}_2+\text{O}$	$(1.5\text{E}-11)*\exp(-2000/t)*\text{sqrt}(t)$	Gattinger and Vallance Jones (1973)
41	$\text{H}_2+\text{O}\rightarrow\text{OH}+\text{H}$	$(1.66\text{E}-11)*\exp(-4400/t)$	Hochanadel et al. (1972)
42	$\text{O}_2(^1\Delta)+\text{O}_3\rightarrow 2\text{O}_2+\text{O}$	$(5.2\text{E}-11)*\exp(-2840/t)$ $t \in [283;360] \text{ K}$	Sander et al. (2011)
43	$\text{O}_2(^1\Sigma)+\text{O}_3\rightarrow 2\text{O}_2+\text{O}$	$(3.5\text{E}-11)*\exp(-135/t)$ $t \in [210;310] \text{ K}$	Sander et al. (2011)
44	$\text{O}_2(^1\Delta)+\text{O}_2\rightarrow\text{O}_2+\text{O}_2$	$(3.6\text{E}-18)*\exp(-220/t)$	Atkinson and Welge (1972)
45	$\text{O}_2(^1\Delta)+\text{N}_2\rightarrow\text{O}_2+\text{N}_2$	$(1\text{E}-20)$	Becker et al. (1971)
46	$\text{O}_2(^1\Delta)+\text{O}\rightarrow\text{O}_2+\text{O}$	$(1.3\text{E}-16)$	Atkinson and Welge (1972)
47	$\text{O}_2(^1\Delta)+\text{H}_2\text{O}\rightarrow\text{O}_2+\text{H}_2\text{O}$	$(4.8\text{E}-18)$	Sander et al. (2011)
48	$\text{O}_2(^1\Delta)+\text{O}_2(^1\Delta)\rightarrow\text{O}_2(^1\Sigma)+\text{O}_2$	$(2.3\text{E}-18)$	Izod and Wayne (1968)
49	$\text{O}+\text{HO}_2\rightarrow\text{OH}^*+\text{O}_2$	$(3\text{E}-11)$	Makhlouf et al. (1995)
50	$\text{OH}^*+\text{M}\rightarrow\text{OH}+\text{M}$	$(5\text{E}-14)$	Moreels et al. (1977)
51	$\text{OH}^*+\text{O}_2\rightarrow\text{OH}+\text{O}_2$	$(4.4\text{E}-12)*P\nu^{\Delta\nu}$	Adler-Golden (1997)
52	$\text{OH}^*+\text{N}_2\rightarrow\text{OH}+\text{N}_2$	$(1\text{E}-13)$	Adler-Golden (1997)
53	$\text{O}(^1\text{D})+\text{O}_2\rightarrow\text{O}_2(^1\Delta)+\text{O}$	$(5\text{E}-13)$	Moreels et al. (1977)
54	$\text{O}(^1\text{D})+\text{O}_2\rightarrow\text{O}_2(^1\Sigma)+\text{O}$	$(3\text{E}-11)$	Noxon (1970)
55	$\text{OH}^*+\text{O}\rightarrow\text{H}+\text{O}_2$	$(8\text{E}-12)$	Moreels et al. (1977)
56	$\text{OH}^*+\text{O}\rightarrow\text{OH}+\text{O}$	$(2\text{E}-11)$	von Savigny et al. (2012)
57	$\text{O}_2(^1\Sigma)+\text{O}_2\rightarrow\text{O}_2+\text{O}_2$	$(1.5\text{E}-16)$	Becker et al. (1971)
58	$\text{O}_2(^1\Sigma)+\text{N}_2\rightarrow\text{O}_2+\text{N}_2$	$(2.2\text{E}-15)$	Becker et al. (1971)
59	$\text{O}_2(^1\Sigma)+\text{H}_2\text{O}\rightarrow\text{O}_2+\text{H}_2\text{O}$	$(5\text{E}-12)$	Becker et al. (1971)
60	$\text{O}+\text{O}+\text{O}\rightarrow\text{O}(^1\text{S})+\text{O}_2$	$(4.8\text{E}-33)$	Moreels et al. (1977)
61	$\text{O}(^1\text{S})+\text{O}_2\rightarrow\text{O}+\text{O}_2$	$(4.9\text{E}-12)*\exp(-580/t)$	Atkinson and Welge (1972)
62	$\text{O}(^1\text{S})+\text{N}_2\rightarrow\text{O}+\text{N}_2$	$(5\text{E}-17)$	Atkinson and Welge (1972)
63	$\text{O}(^1\text{S})+\text{O}\rightarrow\text{O}+\text{O}$	$(7.5\text{E}-12)$	Atkinson and Welge (1972)
64	$\text{O}_2(^1\Sigma)\rightarrow\text{O}_2+h\nu$	(0.0758)	Chabrilat (2001)
65	$\text{O}_2(^1\Delta)\rightarrow\text{O}_2+h\nu(1.27 \mu\text{m})$	$(2.58\text{E}-4)$	Chabrilat (2001)
66	$\text{H}+\text{HO}_2\rightarrow\text{H}_2\text{O}+\text{O}$	$(1.6\text{E}-12)$ $t \in [245;300] \text{ K}$	Sander et al. (2011)

Table A.3. List of the reactions used in the model (continuation).

N°	Reaction	Reaction rate	Reference
67	$2\text{OH}+\text{M}\rightarrow\text{H}_2\text{O}_2+\text{M}$	$k_0=(6.9\text{E}-31)(t/300)^{-1}$ $k_\infty=(2.6\text{E}-11)$	Sander et al. (2011) Sander et al. (2011)
68	$\text{O}+\text{O}_2+\text{O}\rightarrow\text{O}_3+\text{O}$	$(2.15\text{E}-34)*\exp(345/t)$	Allen et al. (1984)
69	$\text{O}(^1\text{S})\rightarrow\text{O}+h\nu(297\text{ nm})$	(0.134)	Slanger et al. (2006)
70	$\text{O}(^1\text{D})\rightarrow\text{O}+h\nu(630\text{ nm})$	(6.478E-3)	Fischer and Tachiev (2004)
71	$\text{O}(^1\text{D})\rightarrow\text{O}+h\nu(636.4\text{ nm})$	(2.097E-3)	Fischer and Tachiev (2004)
72	$\text{O}(^1\text{S})\rightarrow\text{O}(^1\text{D})+h\nu(557.7\text{ nm})$	(1.26)	Wiese et al. (1996)

Table A.4. List of the emissions used in the model and the corresponding radiative lifetimes.

Reaction	Radiative lifetime (ms)	Reference
$\text{OH}_{\nu=1}\rightarrow\text{OH}+h\nu$	44	Turnbull and Lowe (1989)
$\text{OH}_{\nu=2}\rightarrow\text{OH}+h\nu$	21.8	Turnbull and Lowe (1989)
$\text{OH}_{\nu=3}\rightarrow\text{OH}+h\nu$	14.2	Turnbull and Lowe (1989)
$\text{OH}_{\nu=4}\rightarrow\text{OH}+h\nu$	10.3	Turnbull and Lowe (1989)
$\text{OH}_{\nu=5}\rightarrow\text{OH}+h\nu$	7.83	Turnbull and Lowe (1989)
$\text{OH}_{\nu=6}\rightarrow\text{OH}+h\nu$	6.2	Turnbull and Lowe (1989)
$\text{OH}_{\nu=7}\rightarrow\text{OH}+h\nu$	5.04	Turnbull and Lowe (1989)
$\text{OH}_{\nu=8}\rightarrow\text{OH}+h\nu$	4.21	Turnbull and Lowe (1989)
$\text{OH}_{\nu=9}\rightarrow\text{OH}+h\nu$	3.62	Turnbull and Lowe (1989)
$\text{O}_2(^1\Sigma)\rightarrow\text{O}_2+h\nu$	13.192612E3	Chabrillat (2001)
$\text{O}_2(^1\Delta)\rightarrow\text{O}_2+h\nu$	3875.969E3	Chabrillat (2001)
$\text{O}(^1\text{D})\rightarrow\text{O}+h\nu$	116618.08	Fischer and Tachiev (2004)
$\text{O}(^1\text{S})\rightarrow\text{O}+h\nu$	7462.68	Slanger et al. (2006)
$\text{O}(^1\text{S})\rightarrow\text{O}(^1\text{D})+h\nu$	793.65	Wiese et al. (1996)

Table A.5. Quantum yields selected for the O_2 photodissociation (from [Moreels et al. \(1977\)](#)).

$\lambda[\text{nm}]$	O_2	O	$\text{O}(^1\text{D})$	$\text{O}(^1\text{S})$
<102.5	1	0.99	0	0.01
[102.5;110[1	0.91	0	0.09
[110;134[1	0.99	0	0.01
[134;175[1	0	1	0
[175;197.34[1	1	0	0
[197.34;242.4[1	0.91	0	0.09
≥ 242.4	0	0	0	0

Table A.6. Einstein coefficients used in the model to express the reaction coefficients between the excited states of OH (from [Turnbull and Lowe \(1989\)](#)).

ν'	$\nu''=$									Total
	$\nu'-1$	$\nu'-2$	$\nu'-3$	$\nu'-4$	$\nu'-5$	$\nu'-6$	$\nu'-7$	$\nu'-8$	$\nu'-9$	
1	22.74									22.74
2	30.43	15.42								45.85
3	28.12	40.33	2.032							70.48
4	20.30	69.77	7.191	0.299						97.56
5	11.05	99.42	15.88	1.315	0.051					127.7
6	4.00	125.6	27.94	3.479	0.274	0.010				161.3
7	2.34	145.1	42.91	7.165	0.847	0.063	2.85E-4			198.4
8	8.60	154.3	59.98	12.68	2.007	0.23	1.92E-4	4.5E-3		237.8
9	23.72	148.9	78.64	19.94	4.053	0.62	7.24E-3	3.42E-4	7.67E-6	275.9

Table A.7. List of the reactions used for the chemical heating.

N ^o	Reaction	ΔH (kcal/mol)
03	$O+O_2+M \rightarrow O_3+M$	-25.47
04	$O+O_3 \rightarrow O_2+O_2$	-93.65
05	$O+O+M \rightarrow O_2+M$	-119.40
13	$H+O_3 \rightarrow OH^*+O_2$	-76.90
14	$OH+O \rightarrow H+O_2$	-16.77
15	$OH+O_3 \rightarrow HO_2+O_2$	-39.91
17	$OH+HO_2 \rightarrow H_2O+O_2$	-70.61
18	$H+HO_2 \rightarrow H_2+O_2$	-55.68
20	$O+HO_2 \rightarrow OH+O_2$	-53.27
21	$H+O_2+M \rightarrow HO_2+M$	-49.10
24	$HO_2+HO_2 \rightarrow H_2O_2+O_2$	-39.58
33	$HO_2+O_3 \rightarrow OH+2O_2$	-28.29