The role of molecular ions in the overall ionic composition of polar wind outflow

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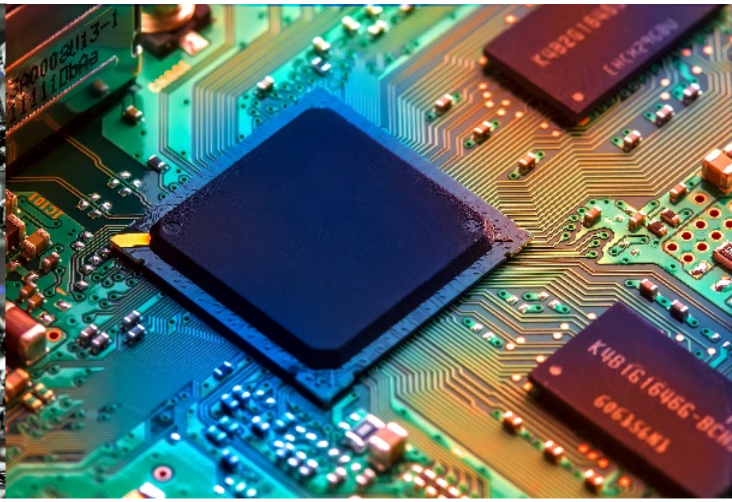

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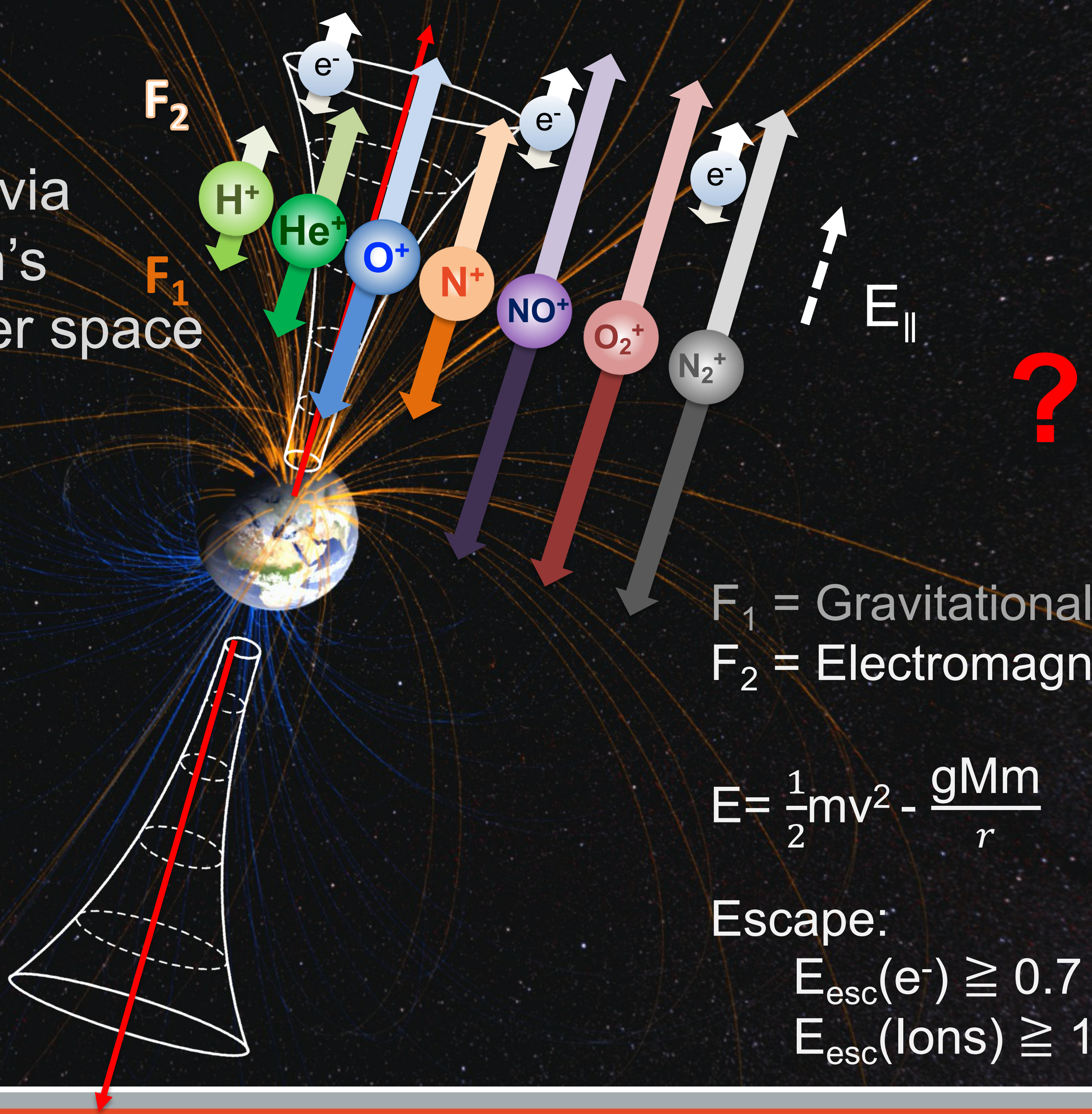
Ions and electrons escape via open field lines to the Earth's magnetosphere and to outer space

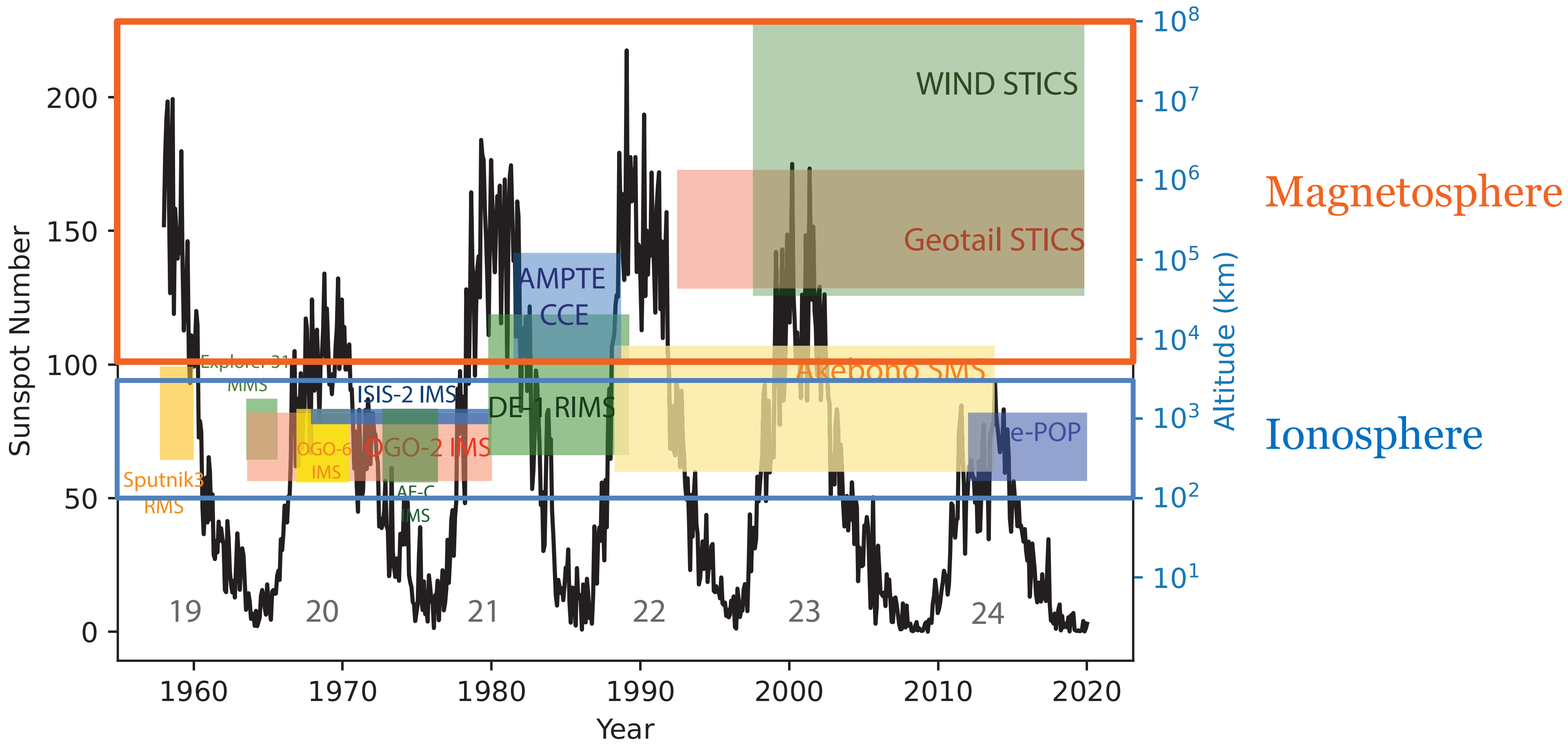


F_1 = Gravitational
F_2 = Electromagnetic

$$E = \frac{1}{2}mv^2 - \frac{gMm}{r}$$

Escape:
$E_{esc}(e^-) \geqq 0.7$ eV
$E_{esc}(\text{Ions}) \geqq 10$ eV

60 Years of N^+ observation



- The presence of N^+ ions could change plasma characteristics in the inner magnetosphere.

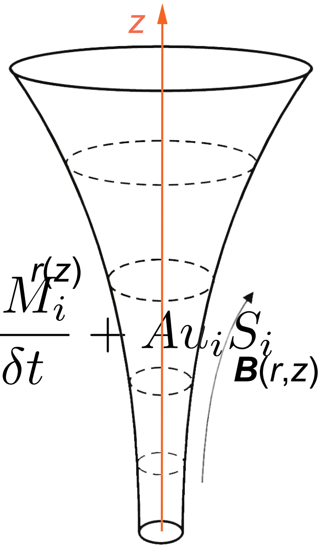
(*Ilie et al.*, [2020], submitted to JASTP)

Polar Wind Outflow Model (referred to as 3iPWOM)

- Chemical & Collisional Scheme
- Suprathermal Electron: GLOW
- Neutral Density: NRLMSISE-90

At each time step, solves for the n, T, v, and $E_\parallel$

Solves for the **transport** and $\mathbf{E}_\parallel$ equations for H^+, He^+, O^+



$$\frac{\partial}{\partial t}(A\rho_i) + \frac{\partial}{\partial r}(A\rho_i u_i) = AS_i$$

$$\frac{\partial}{\partial t}(A\rho_i u_i) + \frac{\partial}{\partial r}(A\rho_i u_i^2) + A\frac{\partial p_i}{\partial r} = A\rho_i(\frac{e}{m_i}E_\parallel - g) + A\frac{\delta M_i}{\delta t} + Au_iS_i$$

$$\frac{\partial}{\partial t}(\frac{1}{2}A\rho_i u_i^2 + \frac{1}{\gamma_i - 1}Ap_i) + \frac{\partial}{\partial r}(\frac{1}{2}A\rho_i u_i^3 + \frac{\gamma_i}{\gamma_i - 1}Au_ip_i)$$
$$= A\rho_i u_i(\frac{e}{m_i}E_\parallel - g) + \frac{\partial}{\partial r}(A\kappa_i\frac{\partial T_i}{\partial r}) + A\frac{\delta E_i}{\delta_t} + Au_i\frac{\delta M_i}{\delta t} + \frac{1}{2}Au_i^2S_i$$

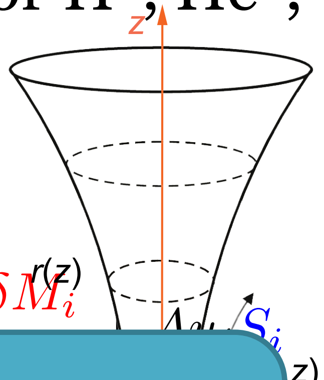
$$E_\parallel = -\frac{1}{en_e}[\frac{\partial}{\partial r}(p_e + \rho_e u_e^2) + \frac{A'}{A}\rho_e u_e^2] + \frac{1}{en_e}\frac{\partial}{\partial r}(\sum_i \frac{m_e}{m_i}[(u_e - u_i)S_i - \frac{\delta M_i}{\delta t}] + \frac{\delta M_e}{\delta t})$$

Seven Ion Polar Wind Outflow Model :7iPWOM

- New **Chemical** & **Collisional** Scheme
- **Suprathermal Electron: GLOW**
- Neutral Density: NRLMSISE-00

At each time step, solves for the n, T, v, and $E_\parallel$

Developed from PWOM (Glocer et al., 2018), 7iPWOM solves Transport Equations and $E_\parallel$ equation for H^+, He^+, N^+, O^+, N_2^+, NO^+, O_2^+



$$\frac{\partial}{\partial t}(A\rho_i) + \frac{\partial}{\partial r}(A\rho_i u_i) = AS_i \quad [1]$$

Source term

$$\frac{\partial}{\partial t}(A\rho_i u_i) + \frac{\partial}{\partial r}(A\rho_i u_i^2) + A\frac{\partial p_i}{\partial r} = A\rho_i(\frac{e}{m_i}E_\parallel \ldots \delta M_i \ldots A \ldots S_i \quad [2]$$

$$\frac{\partial}{\partial t}(\frac{1}{2}A\rho_i u_i^2 + \frac{1}{\gamma_i - 1}Ap_i) + \frac{\partial}{\partial r}(\frac{1}{2}A\rho_i u_i^3 + \ldots$$
$$= A\rho_i u_i(\frac{e}{m_i}E_\parallel - g) + \frac{\partial}{\partial r}(A\kappa_i\frac{\partial T_i}{\partial r}) + A \ldots \delta t \ldots \delta t \ldots 2$$

Energy Change [3]

$$E_\parallel = -\frac{1}{en_e}[\frac{\partial}{\partial r}(p_e + \rho_e u_e^2) + \frac{A'}{A}\rho_e u_e^2] + \frac{1}{en_e}(\sum_i \frac{m_e}{m_i}[(u_e - u_i)S_i - \frac{\delta M_i}{\delta t}] + \frac{\delta M_e}{\delta t})$$

Static molecular ions (zero v and constant T)

Blue: Chemistry Related; Red: Collision Related

Correct Equation

(*Lin et al.*, [2020], GRL)

Chemistry and Collisions

3iPWOM
H^+, He^+, O^+

Chemistry process	Reaction rate($cm^3 s^{-1}$)	Reference
$O + h\nu \longrightarrow O^+ + e^-$	see text	
$O_2 + h\nu \longrightarrow O^+ + O + e^-$	see text	
$He + h\nu \longrightarrow He^+ + e^-$	see text	
$H + h\nu \longrightarrow H^+ + e^-$	see text	
$O + e^* \longrightarrow O^+ + 2e^-$	see text	
$O_2 + e^* \longrightarrow O^+ + O + 2e^-$	see text	
$He + e^* \longrightarrow He^+ + 2e^-$	see text	
$H + e^* \longrightarrow H^+ + 2e^-$	see text	
$O^+ + N_2 \longrightarrow N + NO^+$	1.2×10^{-12}	[R. Schunk & Nagy, 2009]
$O^+ + O_2 \longrightarrow {O_2}^+ + O$	2.1×10^{-11}	[R. Schunk & Nagy, 2009]
$He^+ + O_2 \longrightarrow O^+ + O + He$	9.7×10^{-10}	[R. Schunk & Nagy, 2009]
$He^+ + N_2 \longrightarrow {N_2}^+ + He$	5.2×10^{-10}	[R. Schunk & Nagy, 2009]
$He^+ + N_2 \longrightarrow N^+ + N + He$	7.8×10^{-10}	[R. Schunk & Nagy, 2009]
$H^+ + O \longrightarrow H + O^+$	$2.2 \times 10^{-11} \times T_e^{0.5}$	[R. Schunk & Nagy, 2009]
$H + O^+ \longrightarrow H^+ + O$	$2.5 \times 10^{-11} \times T_e^{0.5}$	[R. Schunk & Nagy, 2009]

Chemistry and Collisions

3iPWOM
H^+, He^+, O^+

7iPWOM
H^+, He^+, N^+, O^+,
N_2^+, NO^+, O_2^+

Chemistry process	Reaction rate$(cm^3 s^{-1})$	Reference
$O + h\nu \longrightarrow O^+ + e^-$	see text	
$O_2 + h\nu \longrightarrow O^+ + O + e^-$	see text	
$He + h\nu \longrightarrow He^+ + e^-$	see text	
$H + h\nu \longrightarrow H^+ + e^-$	see text	
$O + e^* \longrightarrow O^+ + 2e^-$	see text	
$O_2 + e^* \longrightarrow O^+ + O + 2e^-$	see text	
$He + e^* \longrightarrow He^+ + 2e^-$	see text	
$H + e^* \longrightarrow H^+ + 2e^-$	see text	
$O^+ + N_2 \longrightarrow N + NO^+$	1.2×10^{-12}	[R. Schunk & Nagy, 2009]
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$H^+ + O \longrightarrow H + O^+$	$2.2 \times 10^{-11} \times T_e^{0.5}$	[R. Schunk & Nagy, 2009]
$H + O^+ \longrightarrow H^+ + O$	$2.5 \times 10^{-11} \times T_e^{0.5}$	[R. Schunk & Nagy, 2009]
$N + h\nu \longrightarrow N^+ + e^-$	see text	
$N_2 + h\nu \longrightarrow N^+ + N + e^-$	see text	
$N_2 + h\nu \longrightarrow N_2^+ + e^-$	see text	
$O_2 + h\nu \longrightarrow O_2^+ + e^-$	see text	
$NO + h\nu \longrightarrow N^+ + O + e^-$	see text	
$NO + h\nu \longrightarrow NO^+ + e^-$	see text	
$NO + h\nu \longrightarrow O^+ + N + e^-$	see text	
$N_2 + e^* \longrightarrow N_2^+ + 2e^-$	see text	
$O_2 + e^* \longrightarrow O_2^+ + 2e^-$	see text	
$N_2 + e^* \longrightarrow 2N^+ + 3e^-$	see text	
$N_2 + e^* \longrightarrow N^+ + N + 2e^-$	see text	
$N^+ + O_2 \longrightarrow NO^+ + O$	3.07×10^{-10}	[R. Schunk & Nagy, 2009]
$N^+ + O_2 \longrightarrow O_2^+ + N$	2.32×10^{-10}	[R. Schunk & Nagy, 2009]
$N^+ + O_2 \longrightarrow O^+ + NO$	4.6×10^{-11}	[R. Schunk & Nagy, 2009]
$N^+ + NO \longrightarrow NO^+ + N$	2×10^{-11}	[Lindinger et al., 1974]
$N^+ + O \longrightarrow N + O^+$	2.2×10^{-12}	[Richards & Voglozin, 2011]
$N^+ + H \longrightarrow N + H^+$	3.6×10^{-12}	[Harada et al., 2010]
$N_2^+ + N \longrightarrow N^+ + N_2$	10^{-11}	[Richards & Voglozin, 2011]
$N_2^+ + NO \longrightarrow NO^+ + N_2$	4.1×10^{-10}	[R. Schunk & Nagy, 2009]
$N_2^+ + O \longrightarrow NO^+ + N$	1.3×10^{-10}	[R. Schunk & Nagy, 2009]
$N_2^+ + O \longrightarrow O^+ + N_2$	1.0×10^{-11}	[R. Schunk & Nagy, 2009]
$N_2^+ + O_2 \longrightarrow O_2^+ + N_2$	5.0×10^{-11}	[R. Schunk & Nagy, 2009]
$O^+ + NO \longrightarrow NO^+ + O$	8.0×10^{-13}	[R. Schunk & Nagy, 2009]
$N^+ + e^- \longrightarrow N$	$3.6 \times 10^{-12} \times (\frac{250}{T_e})^{0.7}$	[R. Schunk & Nagy, 2009]
$N_2^+ + e^- \longrightarrow N + N$	$2.2 \times 10^{-7} \times (\frac{300}{T_e})^{0.39}$	[R. Schunk & Nagy, 2009]
$NO^+ + e^- \longrightarrow N + O$	$4.0 \times 10^{-7} \times (\frac{300}{T_e})^{0.5}$	[R. Schunk & Nagy, 2009]
$O_2^+ + e^- \longrightarrow O + O$	$2.4 \times 10^{-7} \times (\frac{300}{T_e})^{0.7}$	[R. Schunk & Nagy, 2009]

Chemistry and Collisions

New sources/losses for O^+

3iPWOM
H^+, He^+, O^+

7iPWOM
H^+, He^+, N^+, O^+, N_2^+, NO^+, O_2^+

Chemistry process	Reaction rate$(cm^3 s^{-1})$	Reference
$O + h\nu \longrightarrow O^+ + e^-$	see text	
$O_2 + h\nu \longrightarrow O^+ + O + e^-$	see text	
$He + h\nu \longrightarrow He^+ + e^-$	see text	
$H + h\nu \longrightarrow H^+ + e^-$	see text	
$O + e^* \longrightarrow O^+ + 2e^-$	see text	
$O_2 + e^* \longrightarrow O^+ + O + 2e^-$	see text	
$He + e^* \longrightarrow He^+ + 2e^-$	see text	
$H + e^* \longrightarrow H^+ + 2e^-$	see text	
$O^+ + N_2 \longrightarrow N + NO^+$	1.2×10^{-12}	[R. Schunk & Nagy, 2009]
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$N + h\nu \longrightarrow N^+ + e^-$	see text	
$N_2 + h\nu \longrightarrow N^+ + N + e^-$	see text	
$N_2 + h\nu \longrightarrow N_2^+ + e^-$	see text	
$O_2 + h\nu \longrightarrow O_2^+ + e^-$	see text	
$NO + h\nu \longrightarrow N^+ + O + e^-$	see text	
$NO + h\nu \longrightarrow NO^+ + e^-$	see text	
$NO + h\nu \longrightarrow O^+ + N + e^-$	see text	
$N_2 + e^* \longrightarrow N_2^+ + 2e^-$	see text	
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$N_2^+ + O_2 \longrightarrow O_2^+ + N_2$	5.0×10^{-11}	[R. Schunk & Nagy, 2009]
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Chemistry and Collisions

New sources/losses for O^+

New sources for H^+

3iPWOM
H^+, He^+, O^+

7iPWOM
H^+, He^+, N^+, O^+, N_2^+, NO^+, O_2^+

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$O_2 + e^* \longrightarrow O^+ + O + 2e^-$	see text	
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$N_2 + h\nu \longrightarrow N^+ + N + e^-$	see text	
$N_2 + h\nu \longrightarrow N_2^+ + e^-$	see text	
$O_2 + h\nu \longrightarrow O_2^+ + e^-$	see text	
$NO + h\nu \longrightarrow N^+ + O + e^-$	see text	
$NO + h\nu \longrightarrow NO^+ + e^-$	see text	
$NO + h\nu \longrightarrow O^+ + N + e^-$	see text	
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Chemistry and Collisions

New sources/losses for O^+

Suprathermal Electron (SE) Production

New sources for H^+

3iPWOM
H^+, He^+, O^+

7iPWOM
H^+, He^+, N^+, O^+, N_2^+, NO^+, O_2^+

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$N + h\nu \longrightarrow N^+ + e^-$	see text	
$N_2 + h\nu \longrightarrow N^+ + N + e^-$	see text	
$N_2 + h\nu \longrightarrow N_2^+ + e^-$	see text	
$O_2 + h\nu \longrightarrow O_2^+ + e^-$	see text	
$NO + h\nu \longrightarrow N^+ + O + e^-$	see text	
$NO + h\nu \longrightarrow NO^+ + e^-$	see text	
$NO + h\nu \longrightarrow O^+ + N + e^-$	see text	
$N_2 + e^* \longrightarrow N_2^+ + 2e^-$	see text	
$O_2 + e^* \longrightarrow O_2^+ + 2e^-$	see text	
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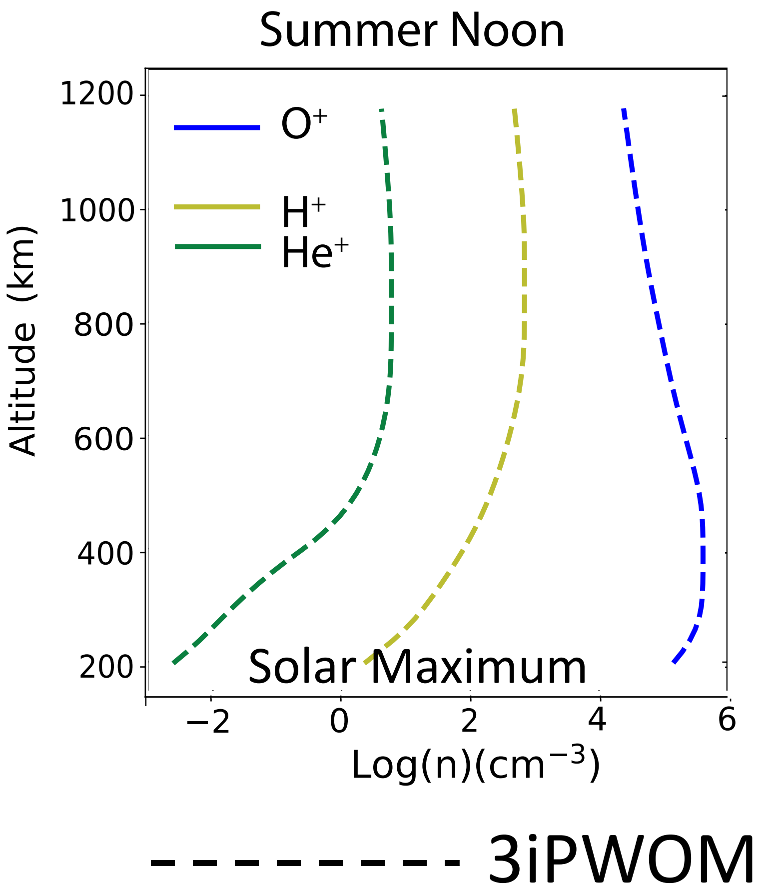
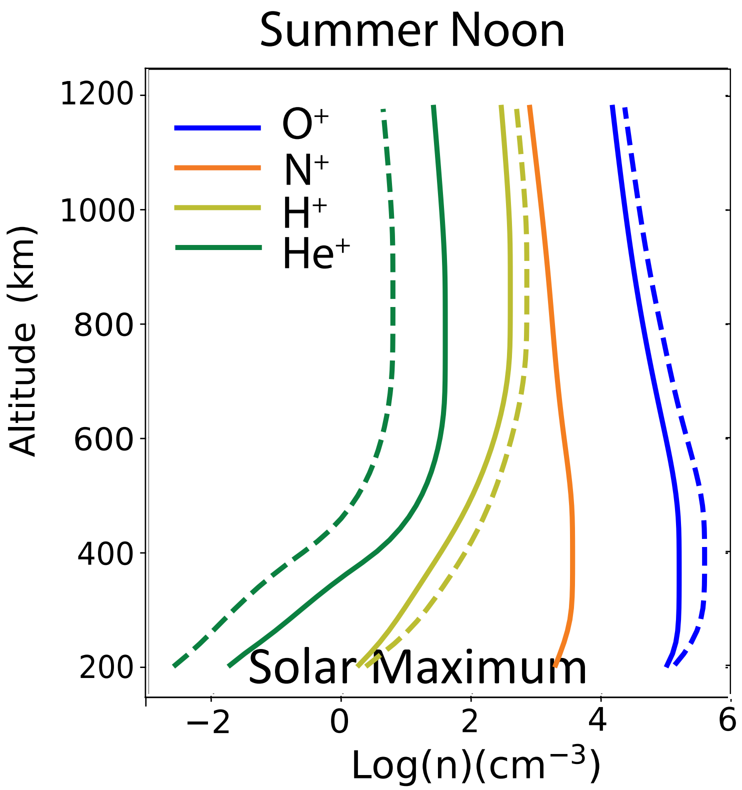
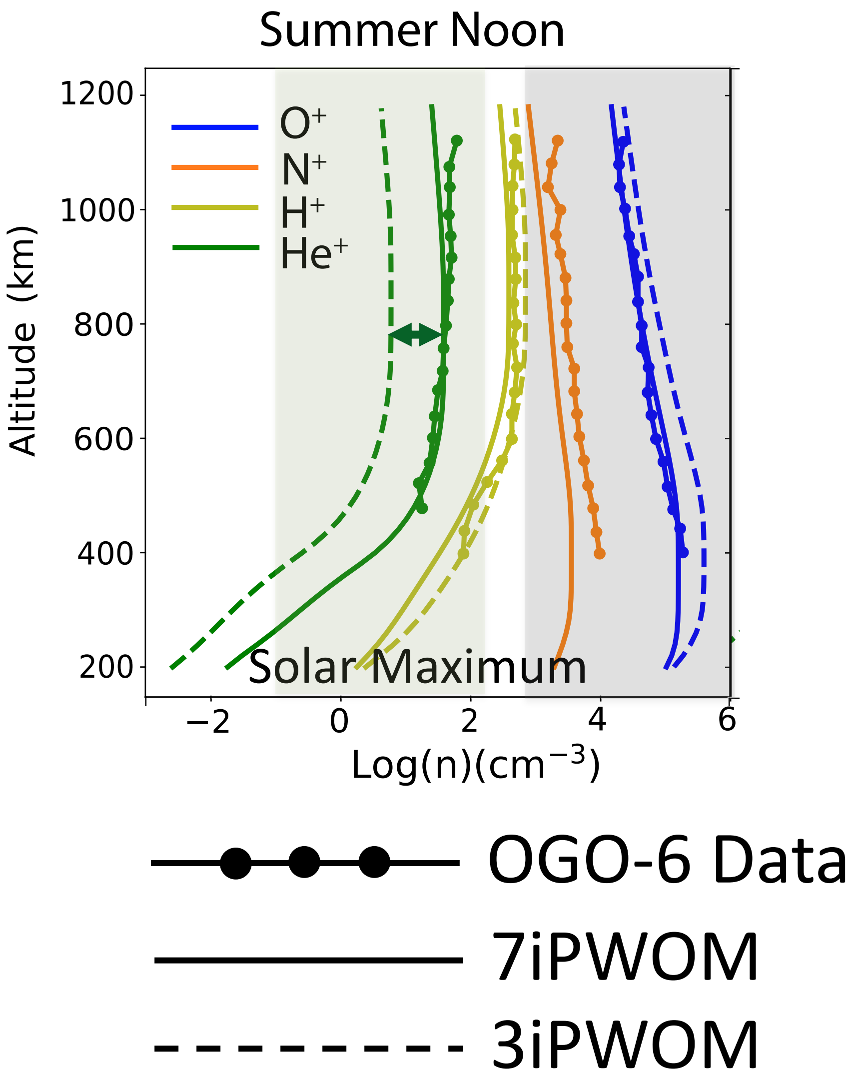

Summer Noon
O+
H+
He+
Solar Maximum
Altitude (km)
1200
1000
800
600
400
200
−2
0
2
4
6
Log(n)(cm−3)
3iPWOM



7iPWOM

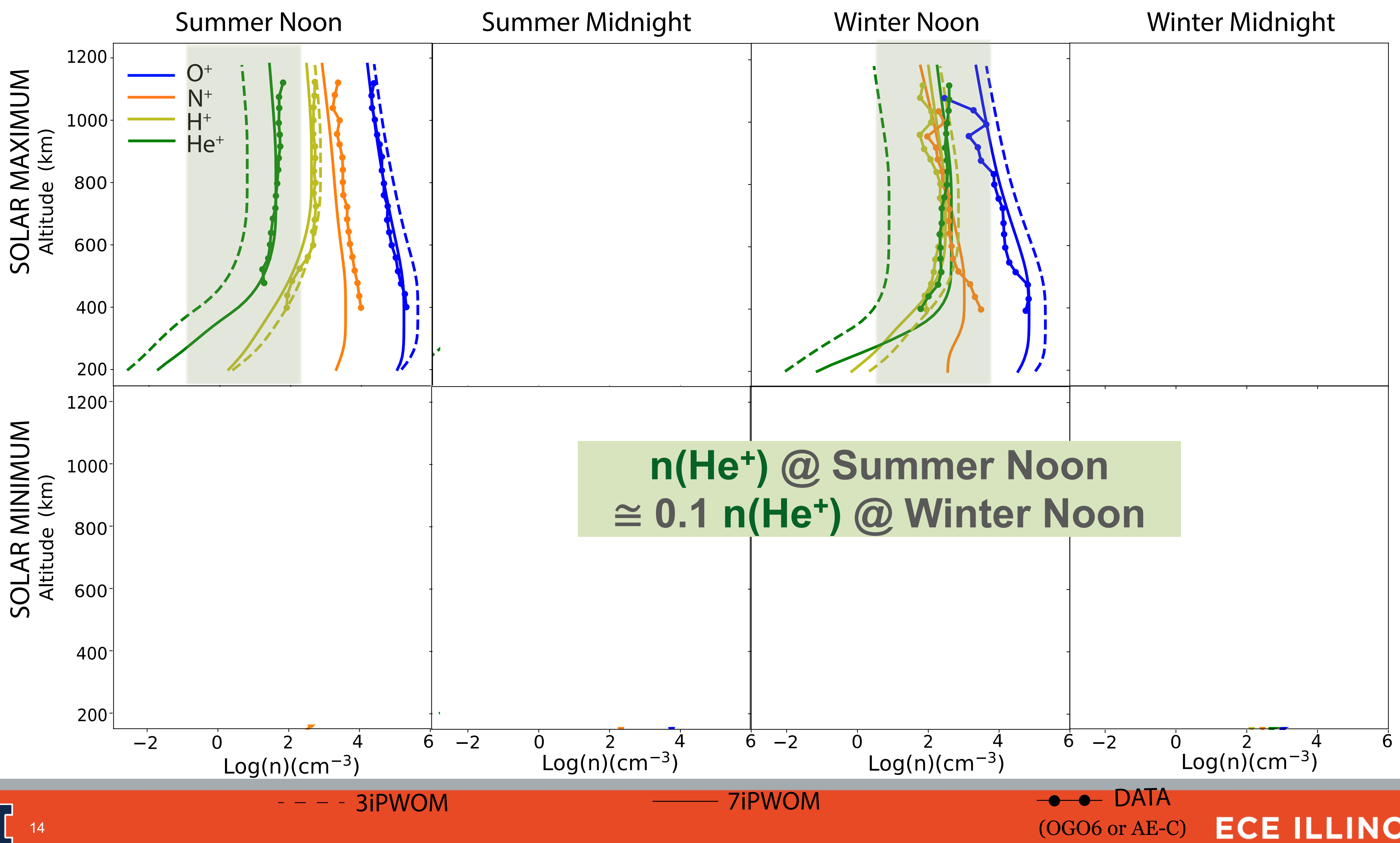
3iPWOM



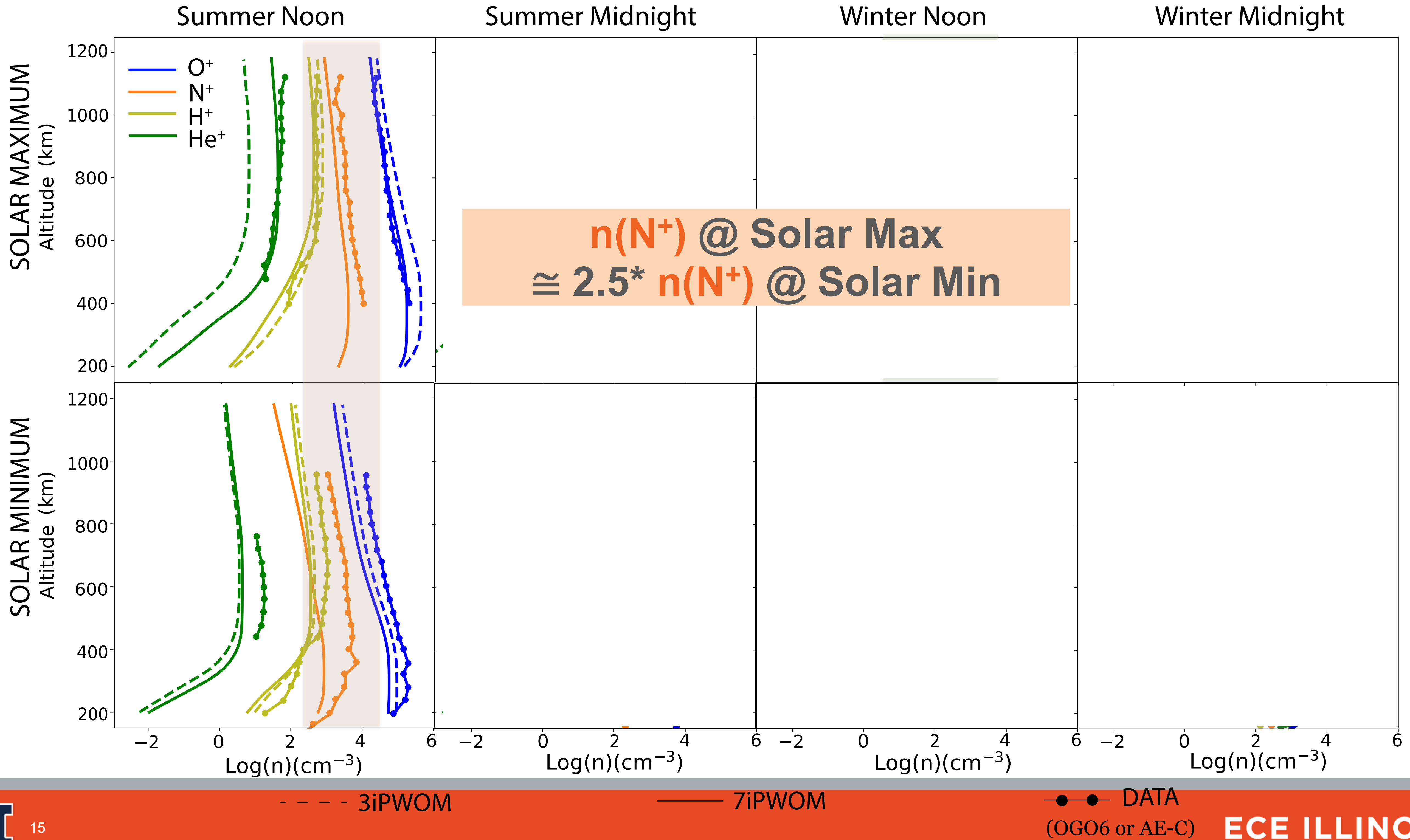
- Comparison with observations shows that the presence of **N^+** improves the outflow solution for ***all species.***

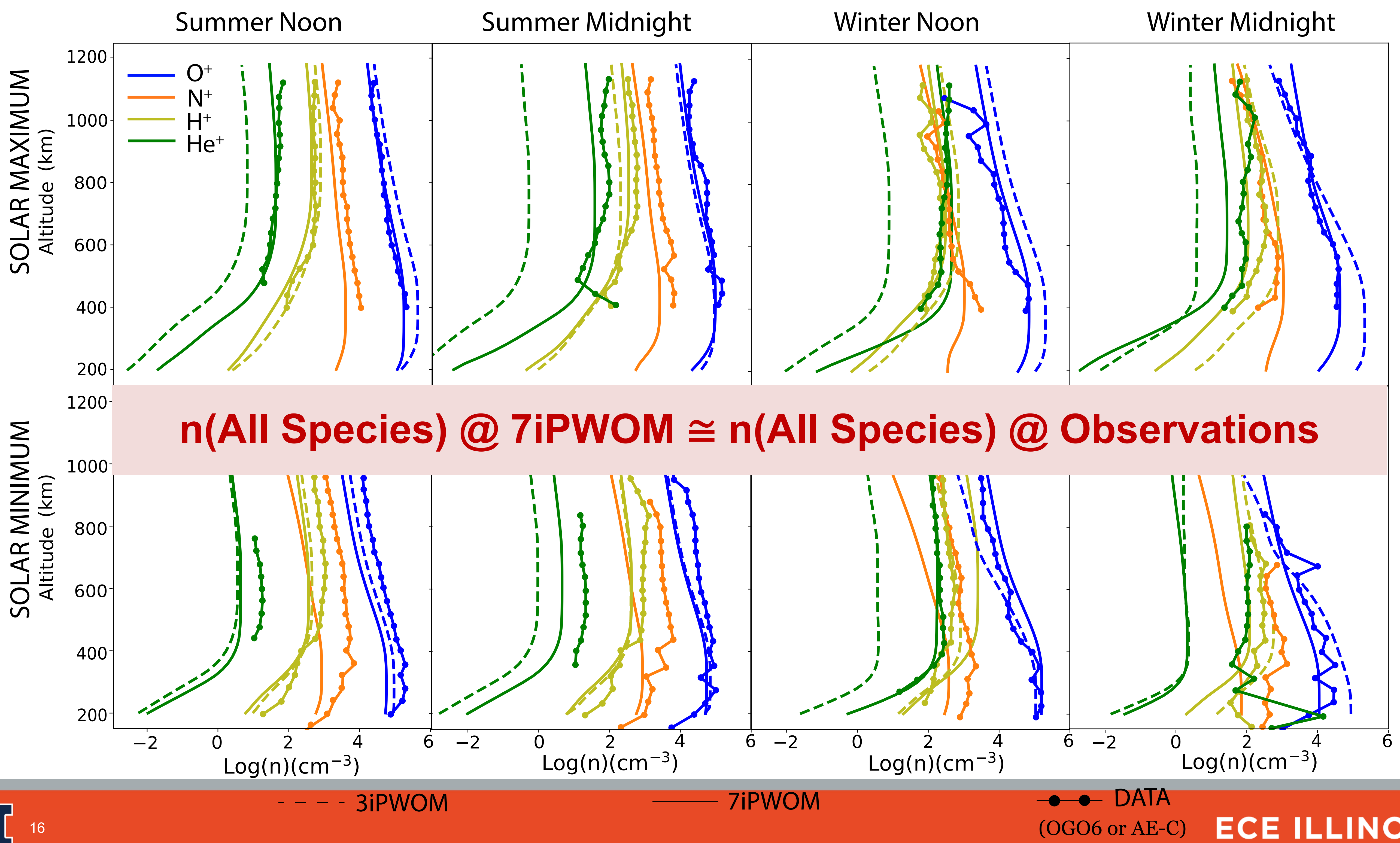
- **He^+ solution shows the biggest improvement, as 7iPWOM predicts a density one order of magnitude higher than 3iPWOM, aligned with observations.**

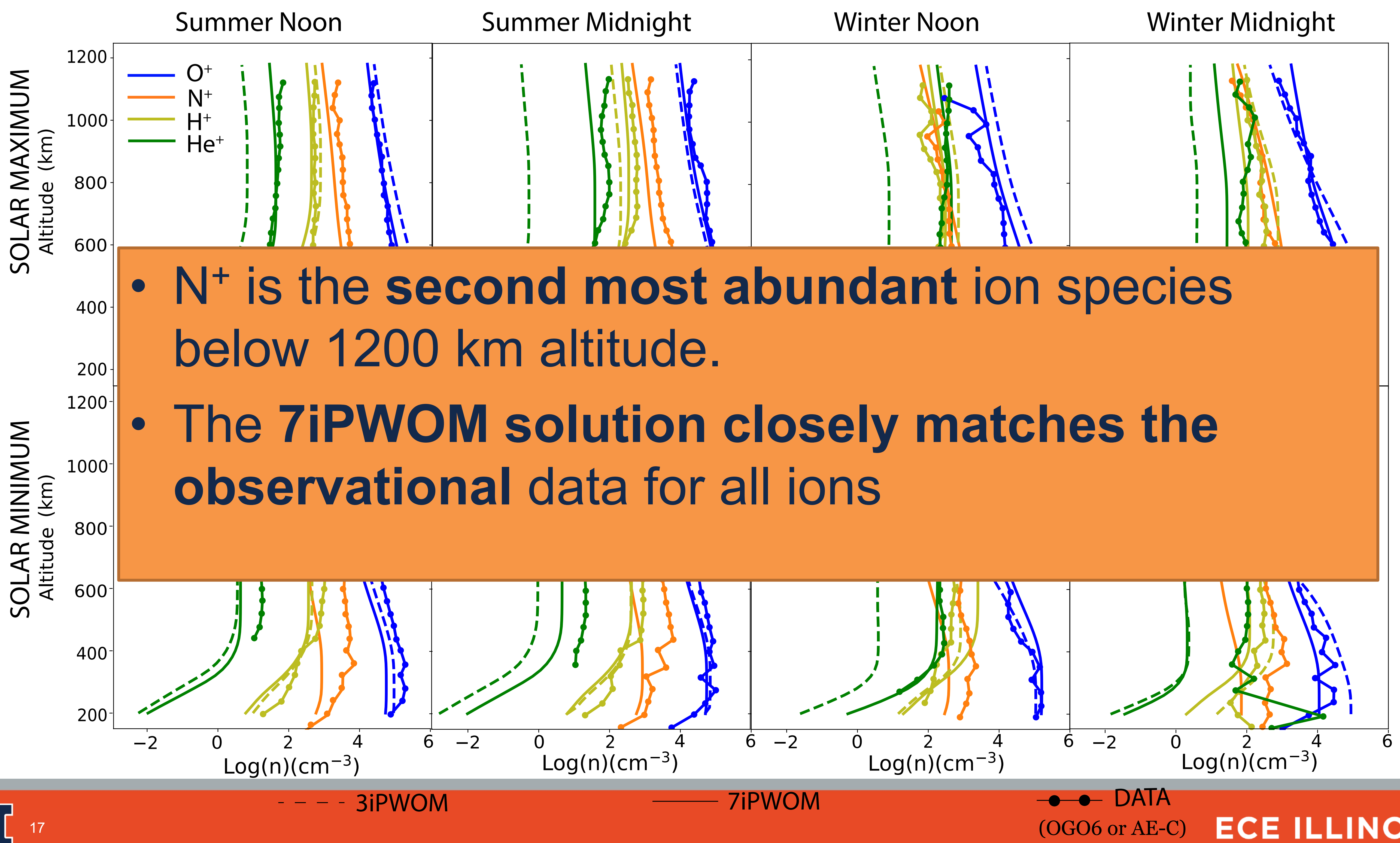
$n(N^+) \cong 10\%$ of $n(O^+)$



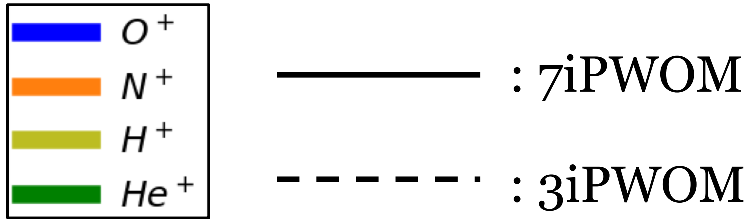
Summer Noon
Summer Midnight
Winter Noon
Winter Midnight
SOLAR MAXIMUM
Altitude (km)
SOLAR MINIMUM
Altitude (km)
O+
N+
H+
He+
Log(n)(cm−3)
n(He+) @ Summer Noon
≅ 0.1 n(He+) @ Winter Noon
3iPWOM
7iPWOM
DATA
(OGO6 or AE-C)


Summer Noon
Summer Midnight
Winter Noon
Winter Midnight
SOLAR MAXIMUM
SOLAR MINIMUM
Altitude (km)
O+
N+
H+
He+
Log(n)(cm−3)
n(N+) @ Solar Max
≅ 2.5* n(N+) @ Solar Min
3iPWOM
7iPWOM
DATA
(OGO6 or AE-C)

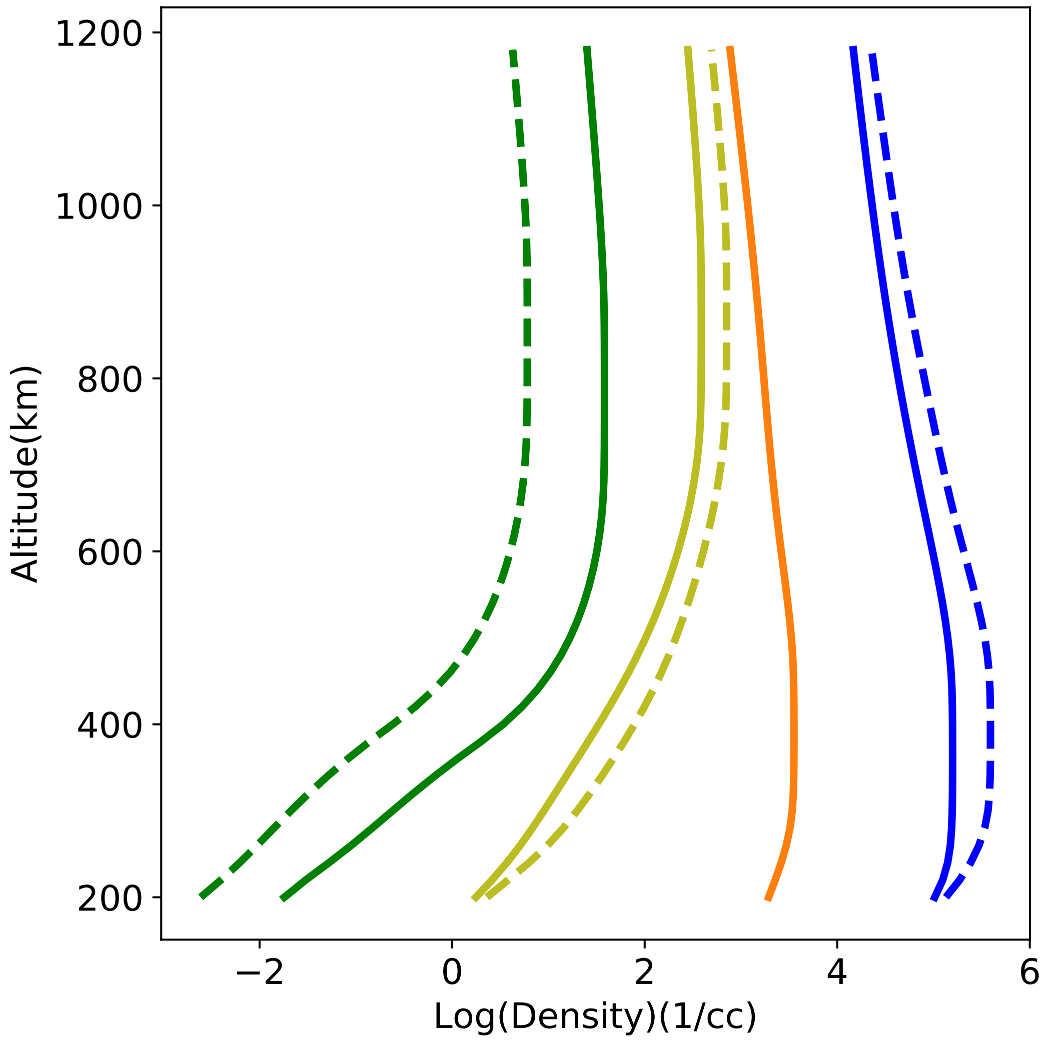

Summer Noon
Summer Midnight
Winter Noon
Winter Midnight
SOLAR MAXIMUM
Altitude (km)
SOLAR MINIMUM
Altitude (km)
O+
N+
H+
He+
Log(n)(cm−3)
n(All Species) @ 7iPWOM ≅ n(All Species) @ Observations
3iPWOM
7iPWOM
DATA
(OGO6 or AE-C)



- N^+ is the **second most abundant** ion species below 1200 km altitude.
- The **7iPWOM solution closely matches the observational** data for all ions



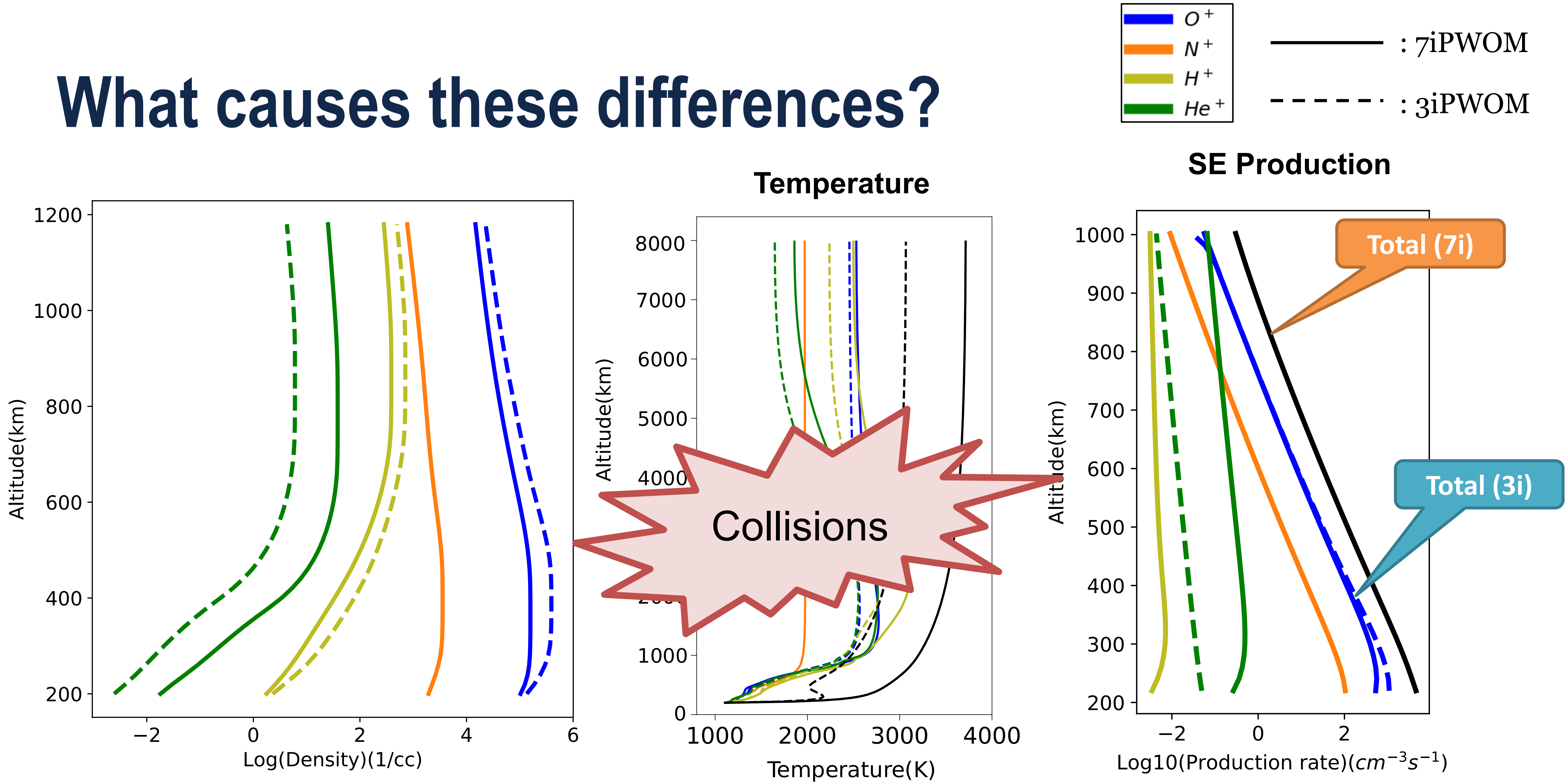
What causes these differences?



Presence of N^+ and molecular species leads to :

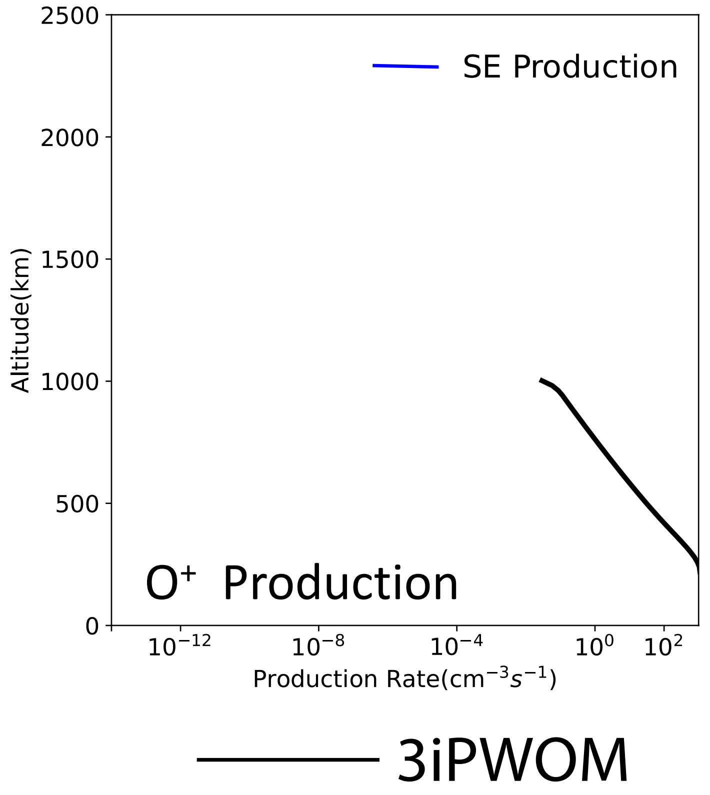
- A significant increase (~1 an order of magnitude) in He^+ density.
- H^+ solution improves as compared with measurements
- O^+ density profile better matches the data, and the density is a factor 2 larger.
- N^+ profile matches observations
- ***All species show an increase in temperature/energy.***

What causes these differences?



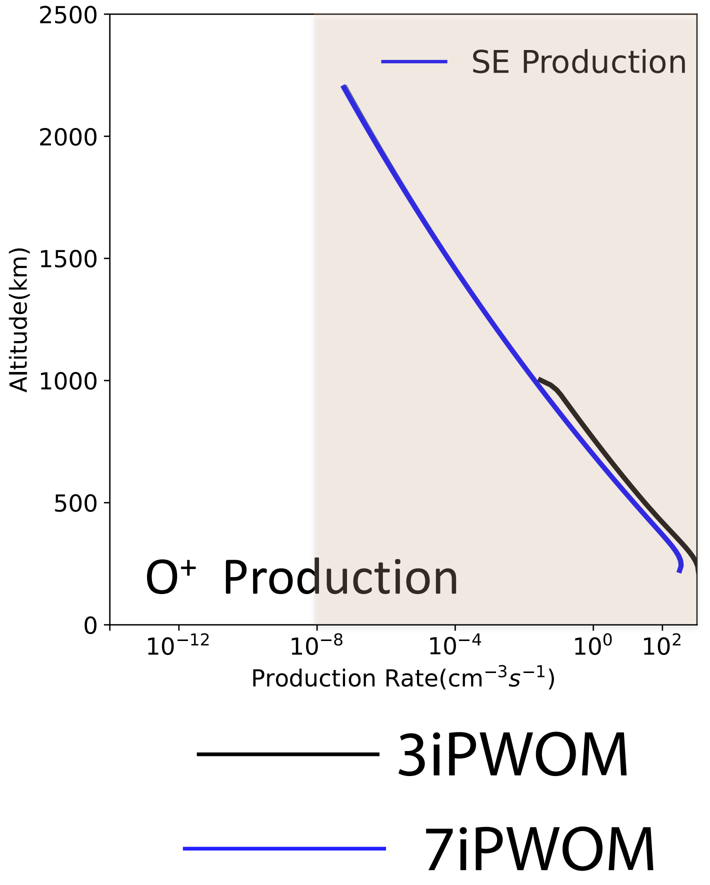
Chemistry?

SE production



Chemistry?

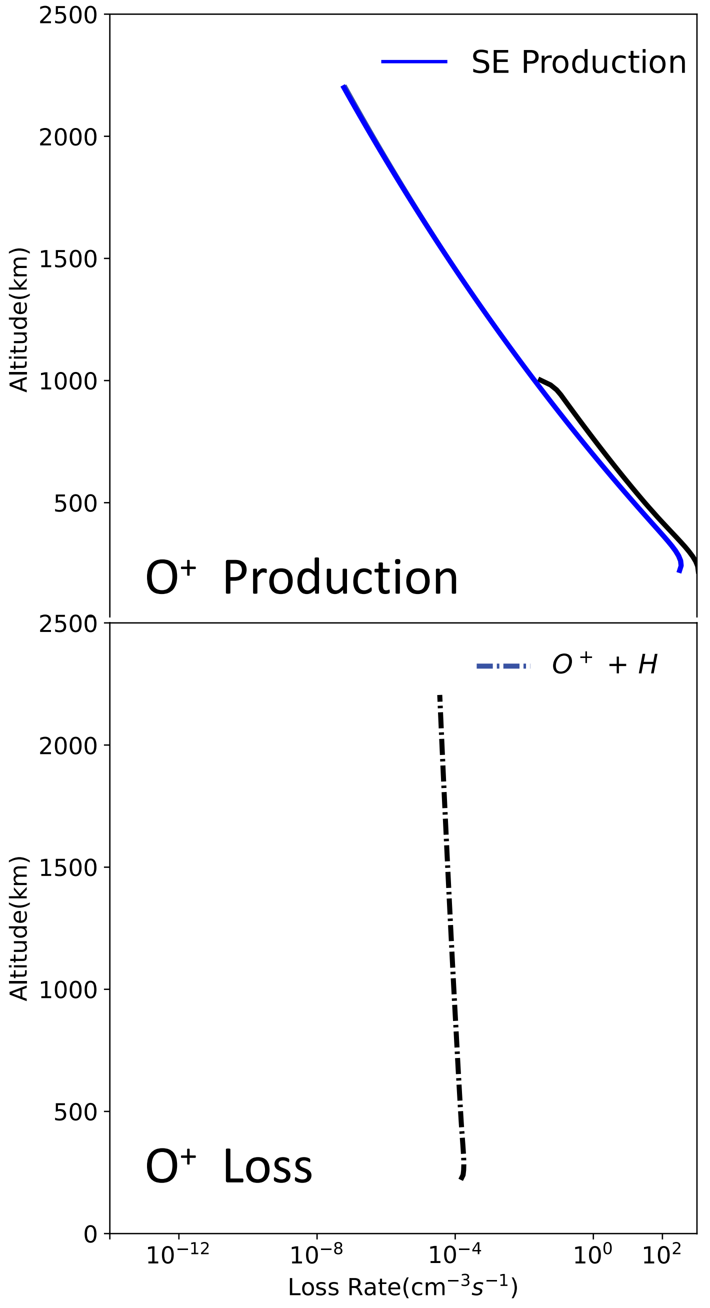
SE production



Chemistry?

SE production

Charge exchange
with H^+



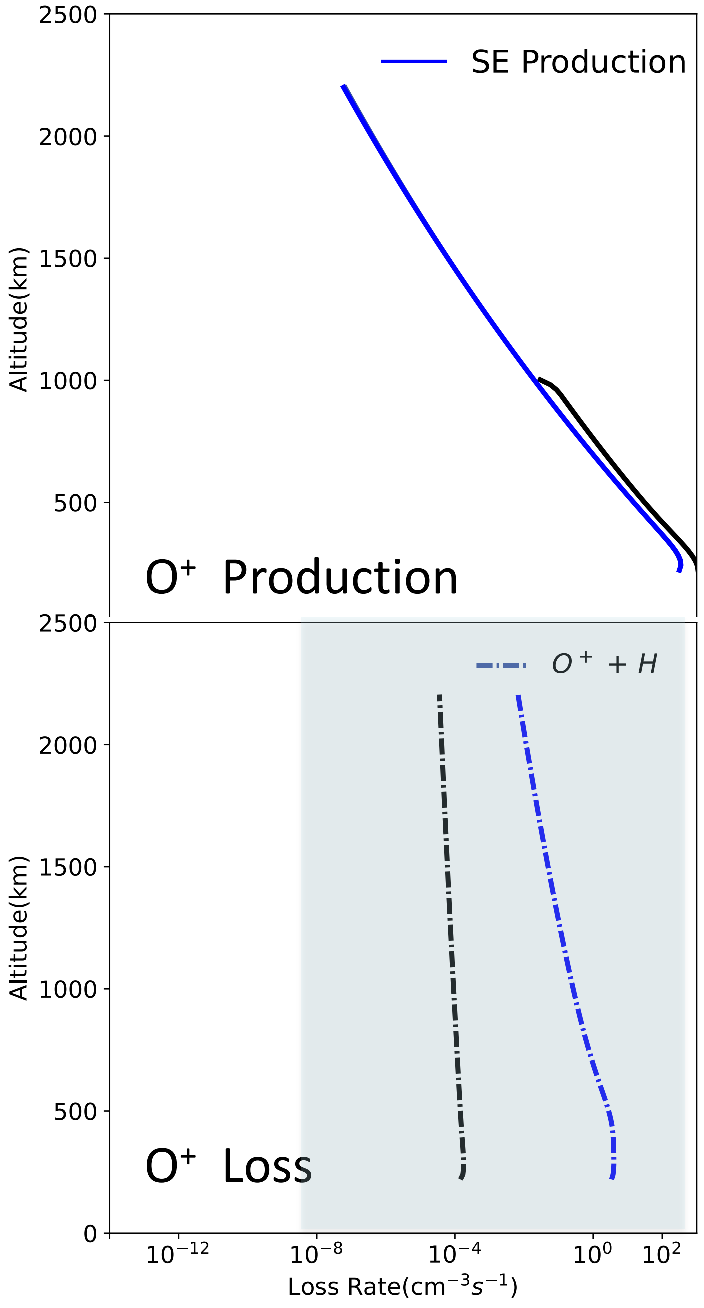
7iPWOM

3iPWOM

Chemistry?

SE production

Charge exchange with H^+



7iPWOM

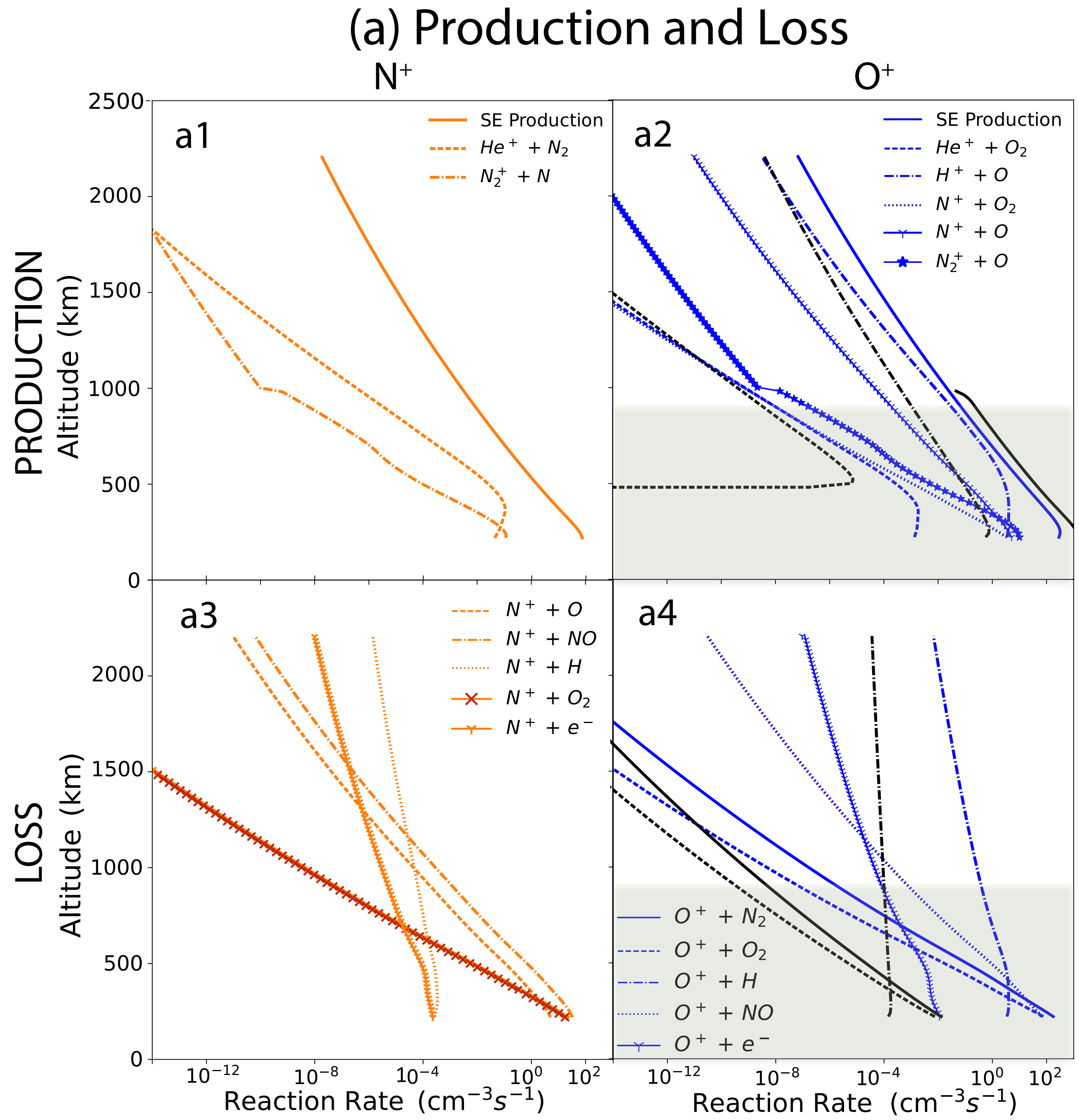
3iPWOM

Chemistry?

Different Chemistry at low altitude

SE production

Charge exchange with H^+



7iPWOM

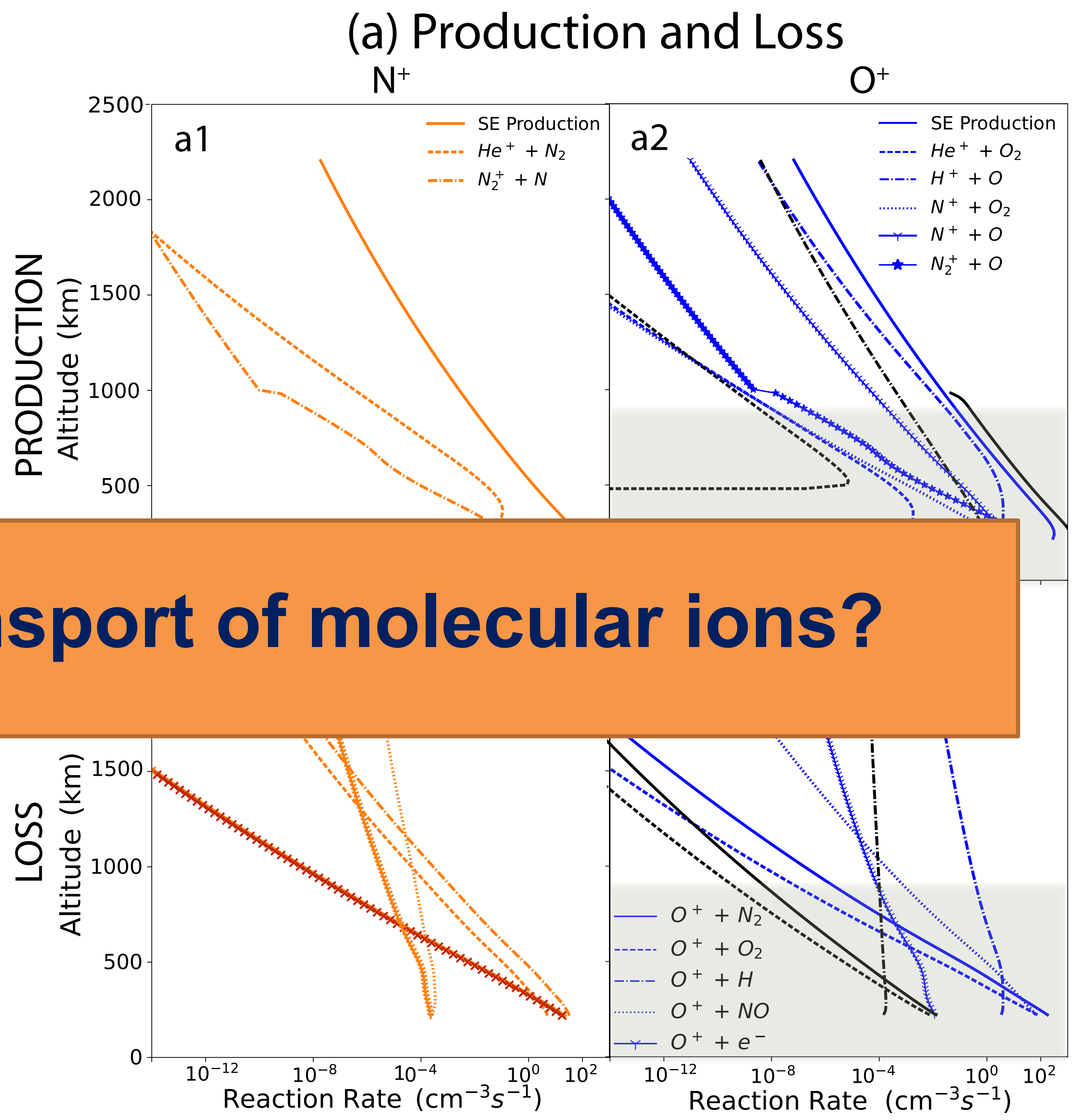
3iPWOM

Chemistry?

Different Chemistry at low altitude

How about the transport of molecular ions?

Charge exchange with H^+

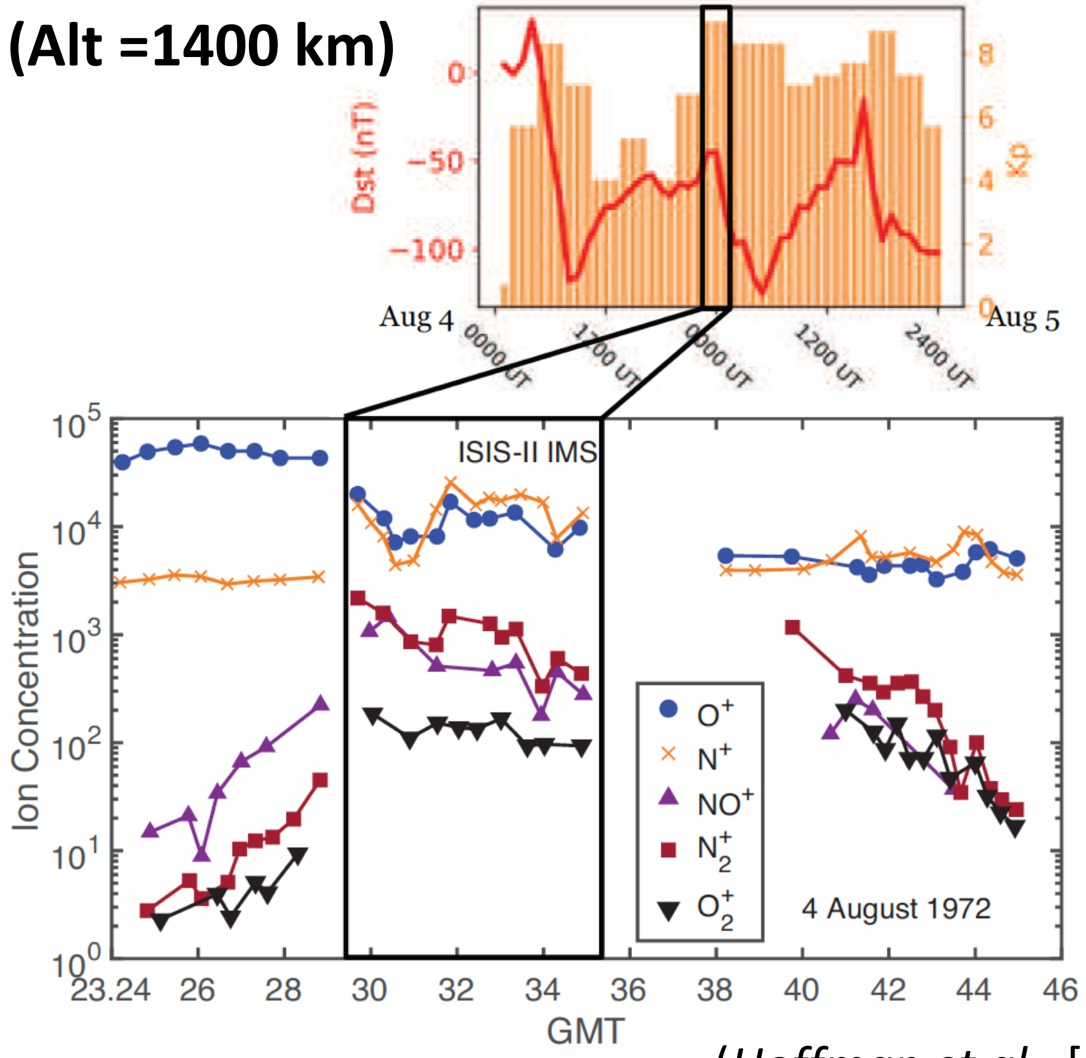


7iPWOM

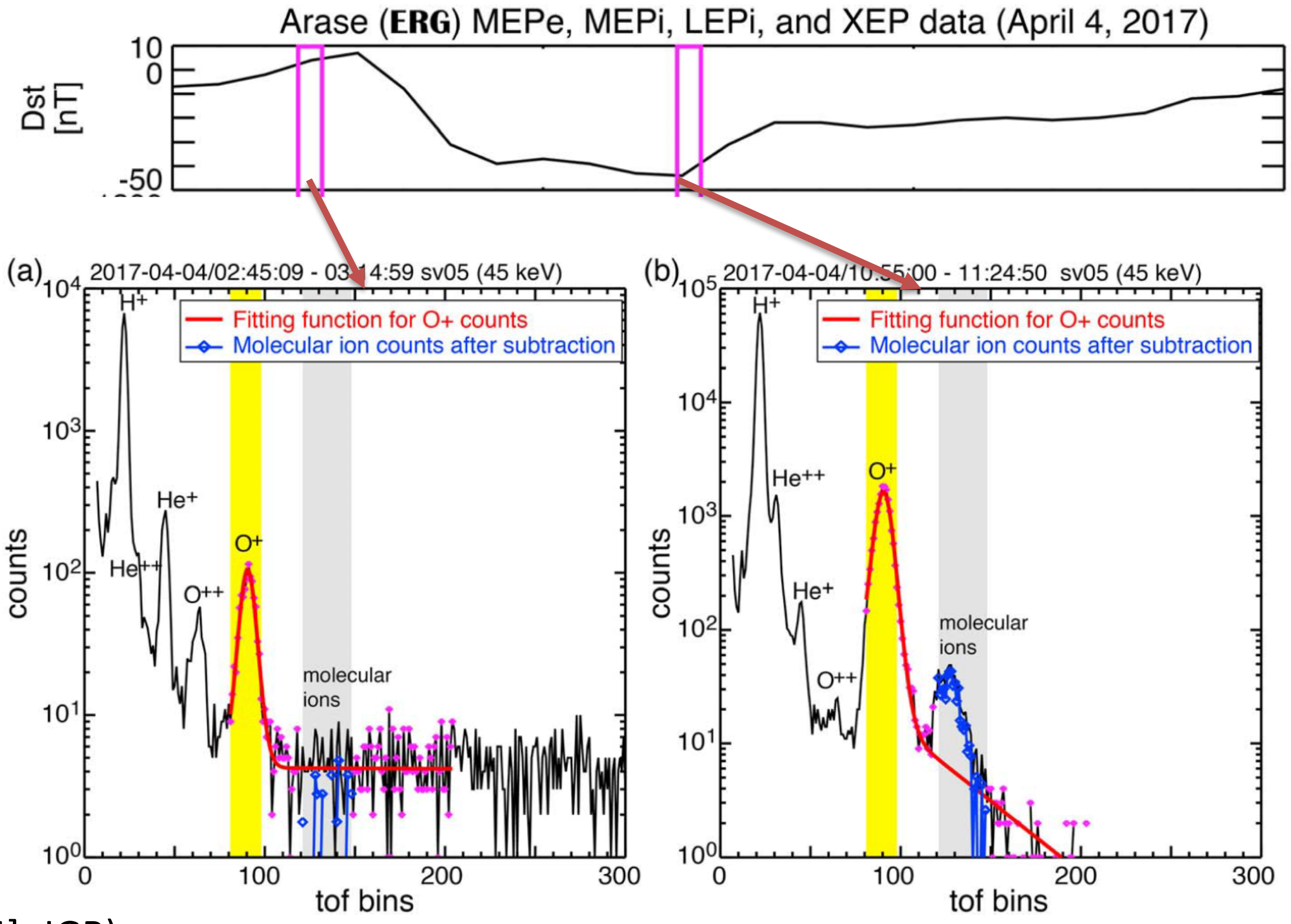
3iPWOM

Observations of Molecular Ions

Ionosphere
(Alt =1400 km)



(*Hoffman et al.*, [1974], JGR)

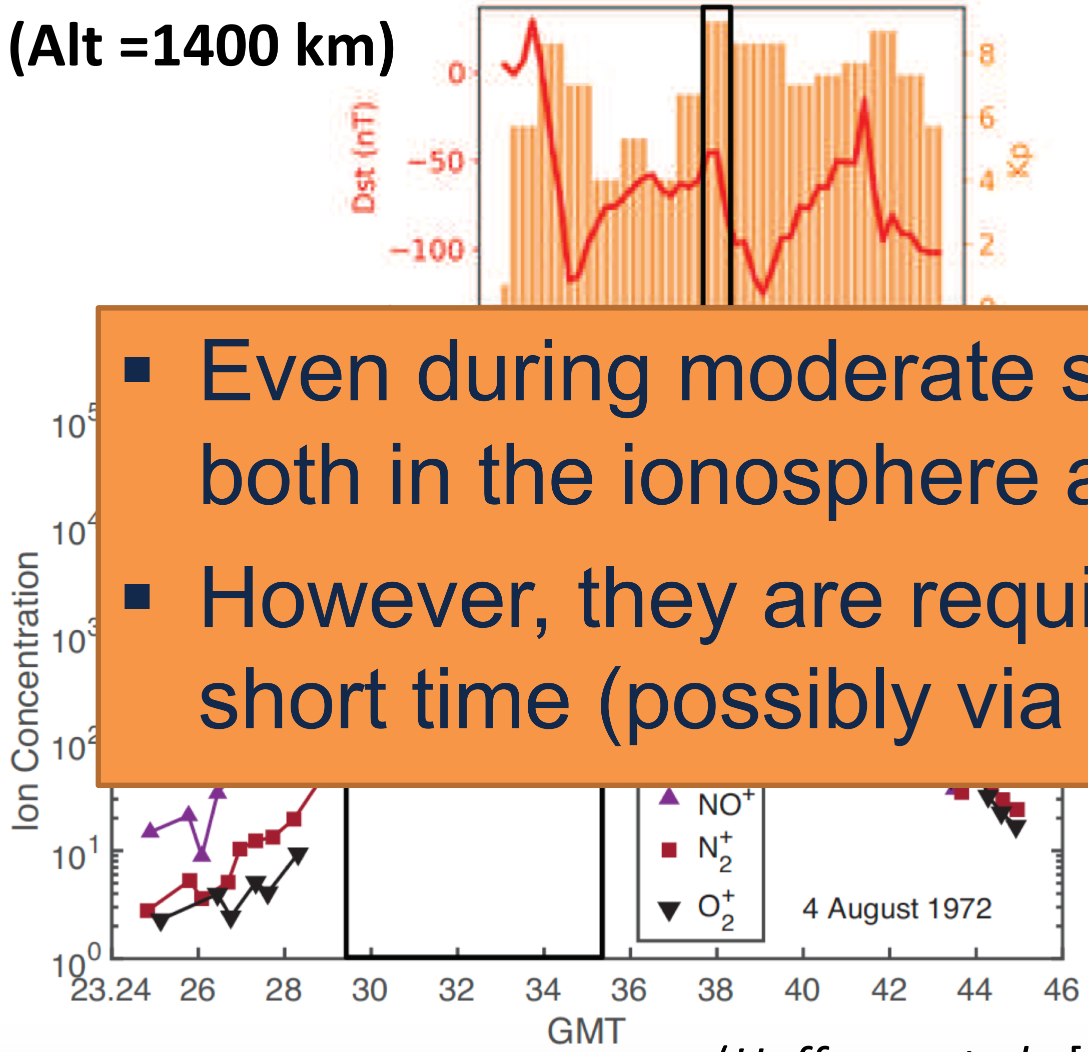


(*Seki et al.*, [2019], GRL)

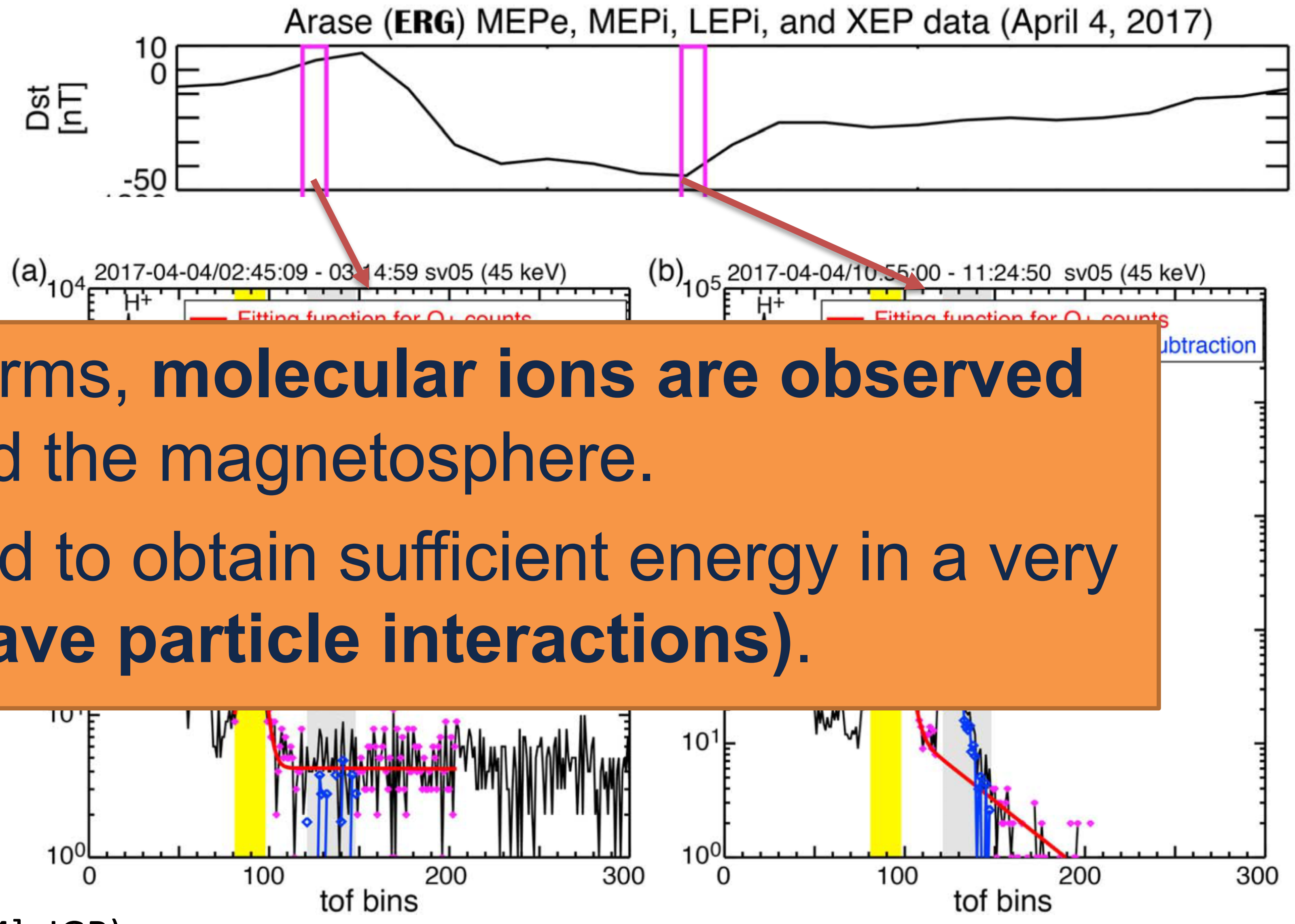
Observations of Molecular Ions

Inner Magnetosphere

Ionosphere
(Alt =1400 km)



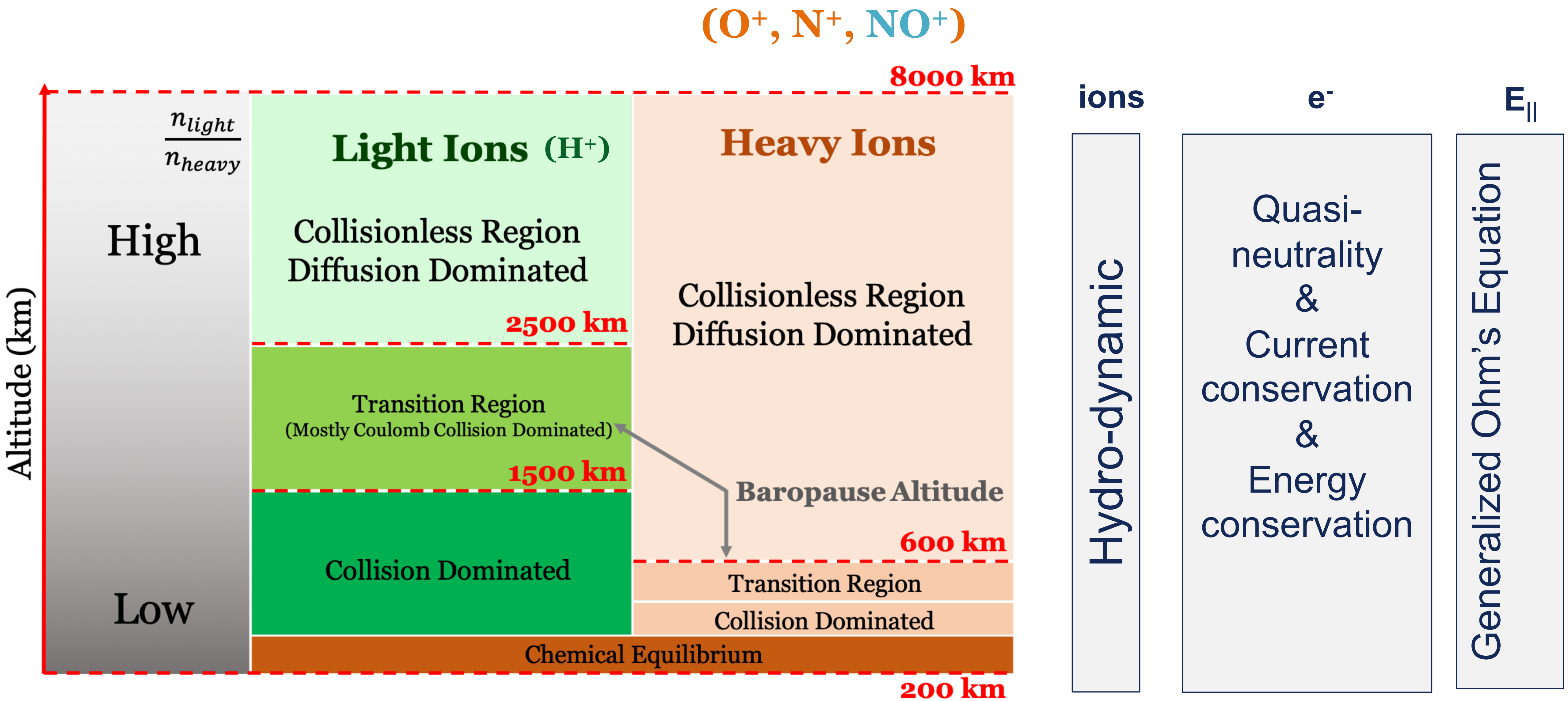
(*Hoffman et al.,* [1974], JGR)



(*Seki et al.,* [2019], GRL)

- Even during moderate storms, **molecular ions are observed** both in the ionosphere and the magnetosphere.
- However, they are required to obtain sufficient energy in a very short time (possibly via **wave particle interactions**).

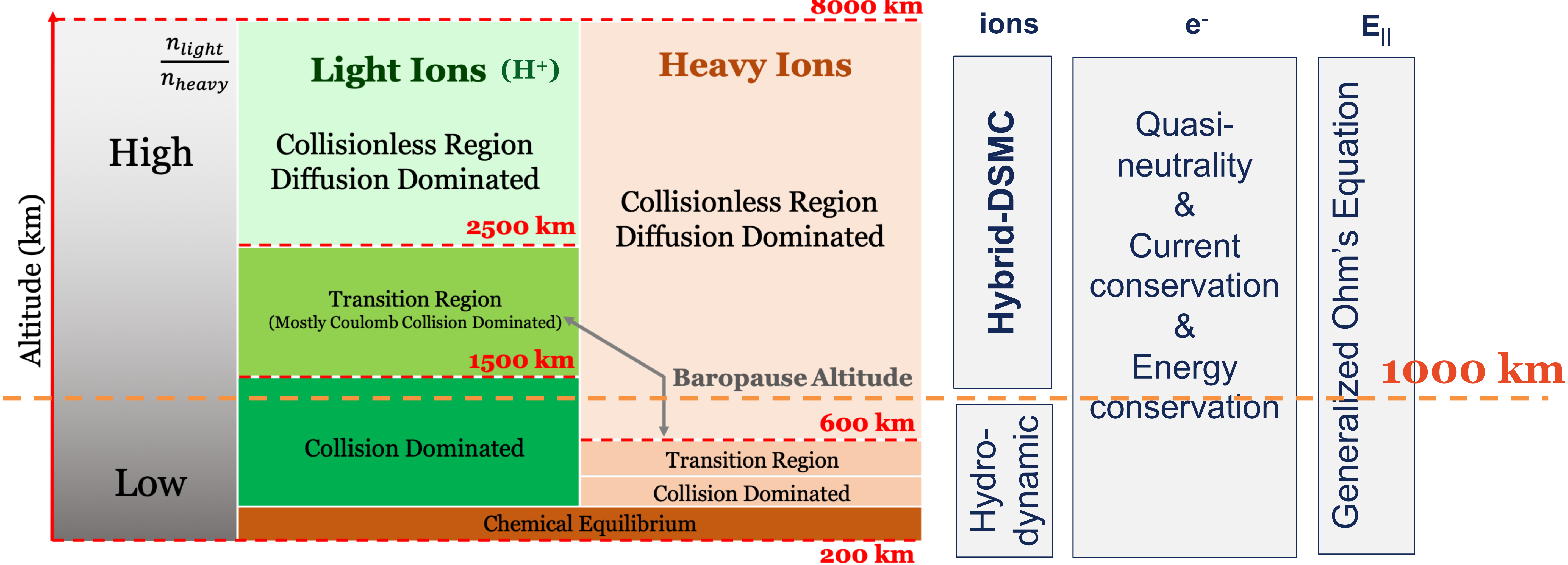
Our approach: 7iPWOM



Our approach: 7iPWOM

$$m\frac{\partial v_\parallel}{\partial t} - qE_\parallel + \frac{GmM_{planet}}{r^2} + \mu\frac{\partial B}{\partial s} = 0$$

(O^+, N^+, NO^+)



Our approach: 7iPWOM

$$m\frac{\partial v_{\parallel}}{\partial t} - qE_{\parallel} + \frac{GmM_{planet}}{r^2} + \mu\frac{\partial B}{\partial s} = 0$$

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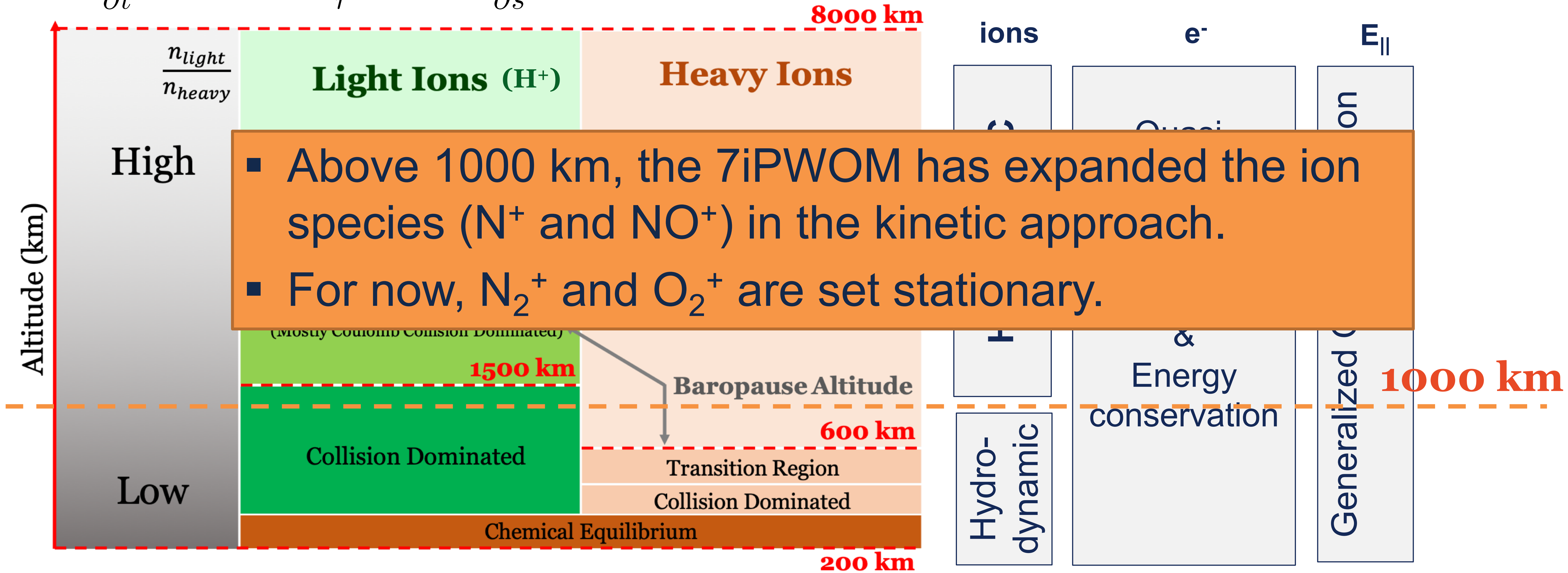
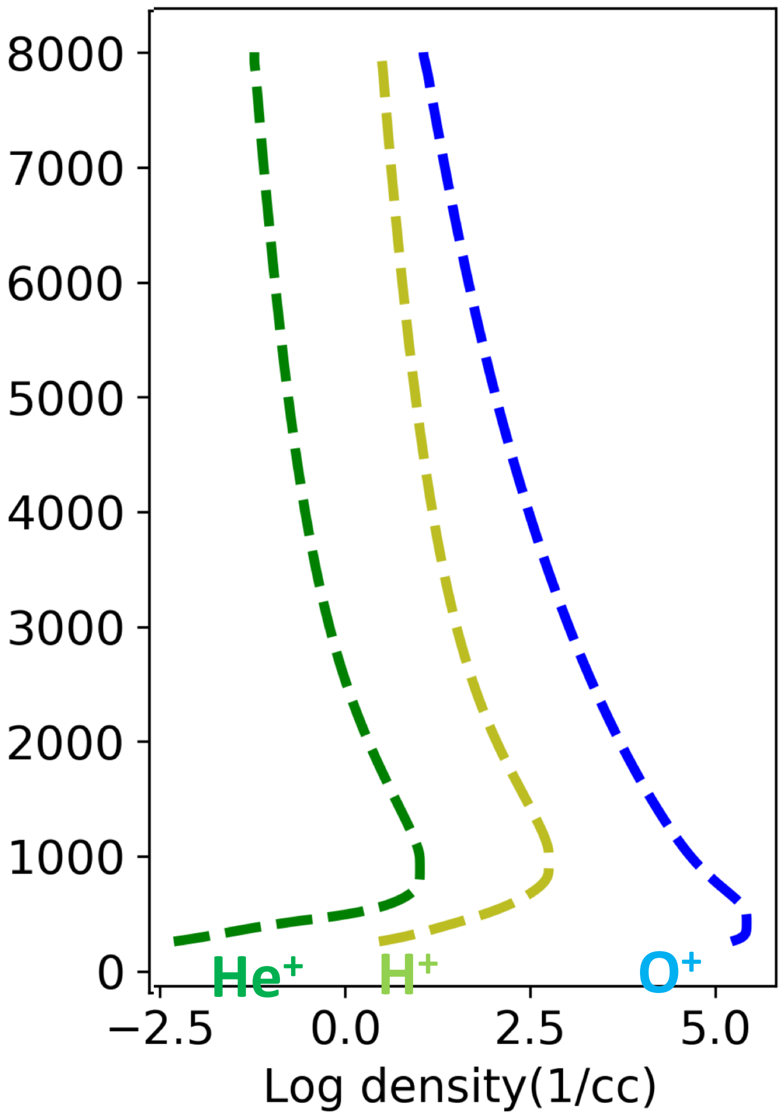


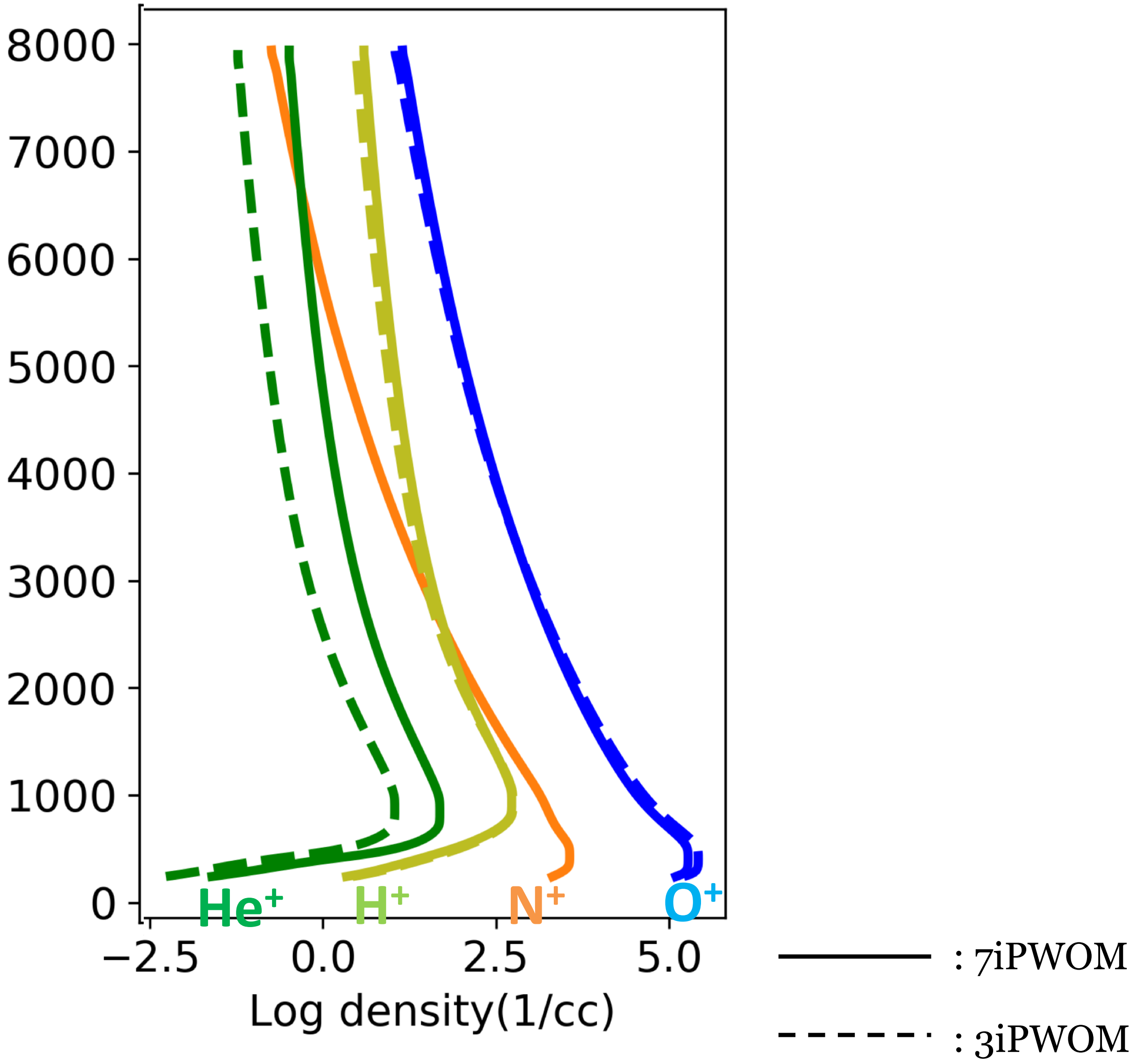
- Above 1000 km, the 7iPWOM has expanded the ion species (N^+ and NO^+) in the kinetic approach.
- For now, N_2^+ and O_2^+ are set stationary.

Steady State: 3iPWOM Fluid Solution

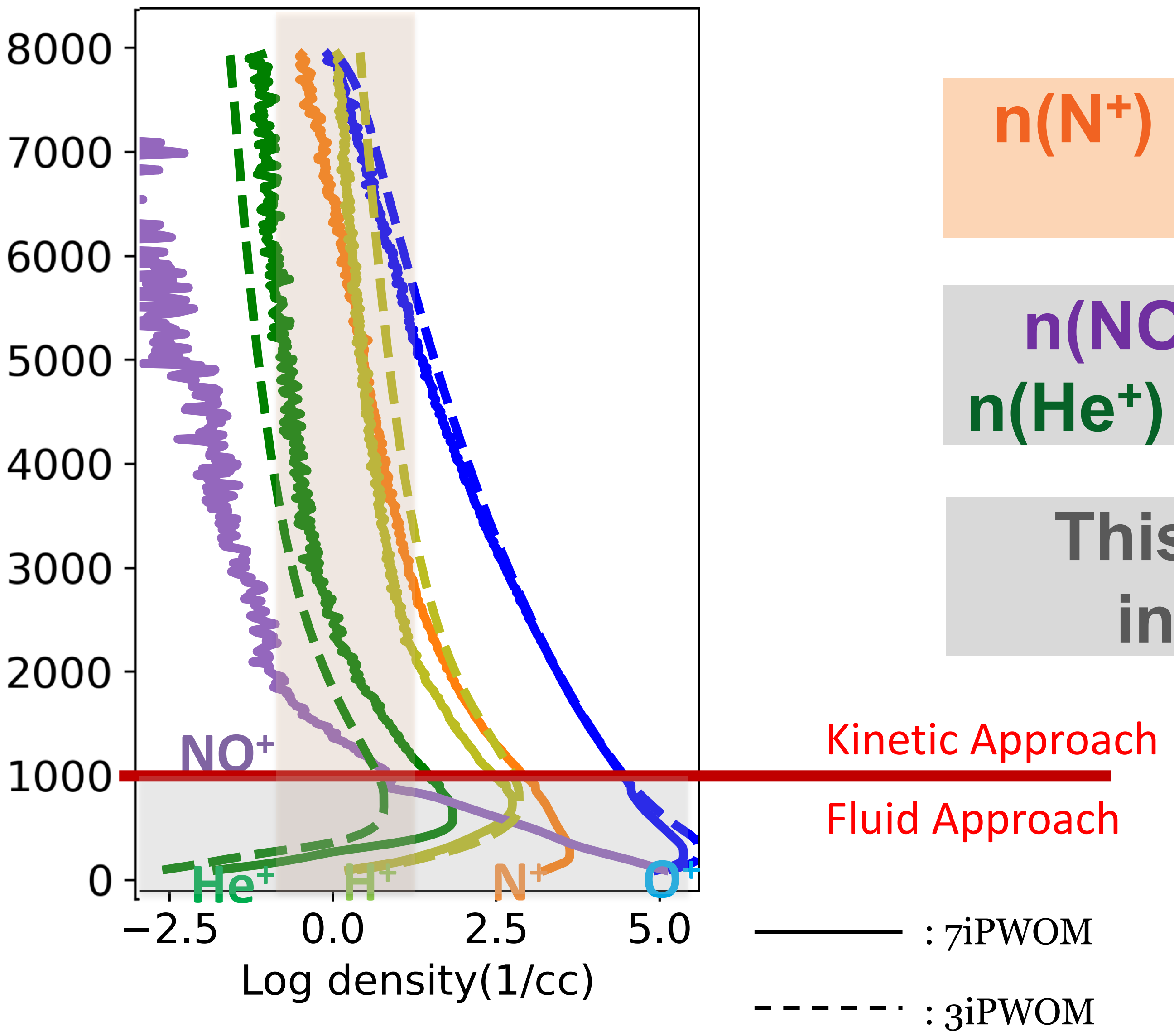


- - - - - : 3iPWOM

Steady State: 7iPWOM Fluid Solution (static NO^+)



7iPWOM Fluid + Kinetic Solution (Dynamic NO^+)

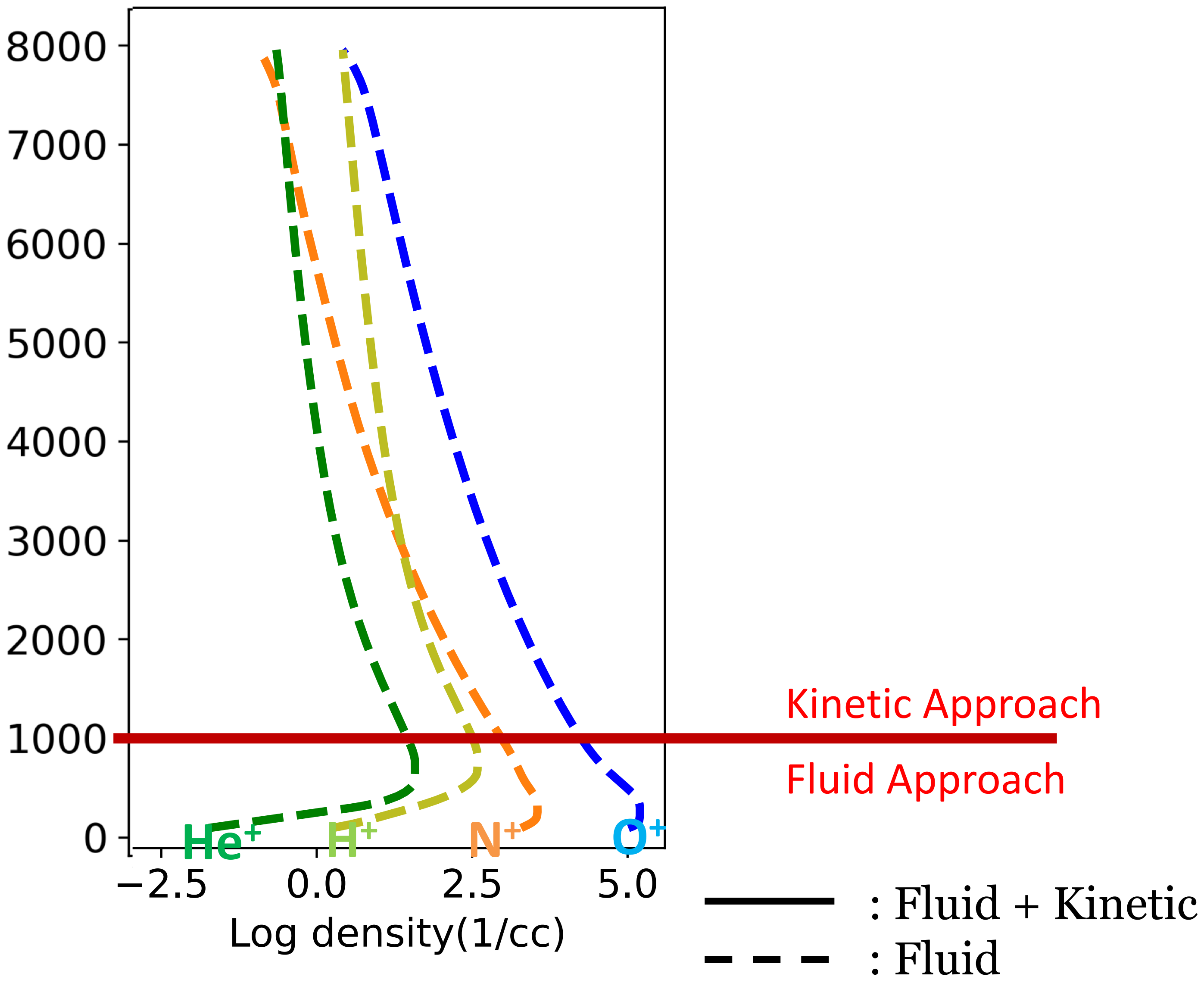


n(N^+) is still important in the kinetic solution

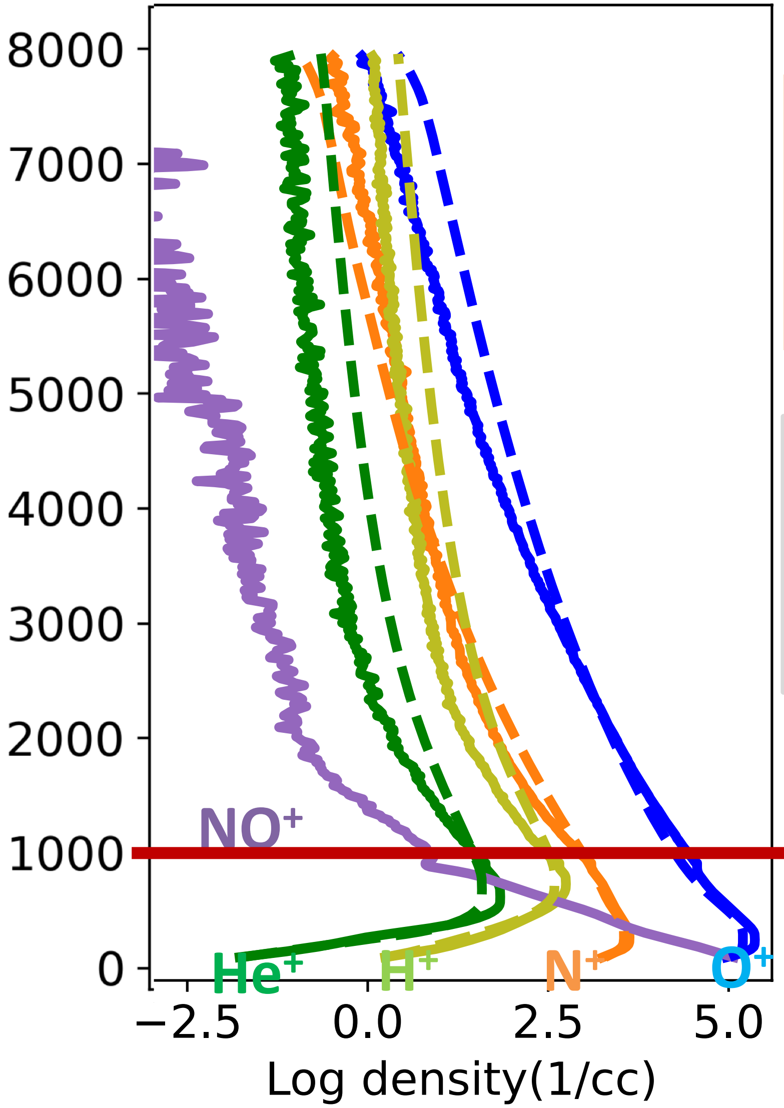
n(NO^+) is comparable with n(He^+) below 1000 km altitude

This simulation required increased resolution

Compare (Fluid + Kinetic) vs (Fluid) Solution



Compare (Fluid + Kinetic) vs (Fluid) Solution



$n(N^+)$ seems to behave differently when the kinetic model is employed above 1000 km.

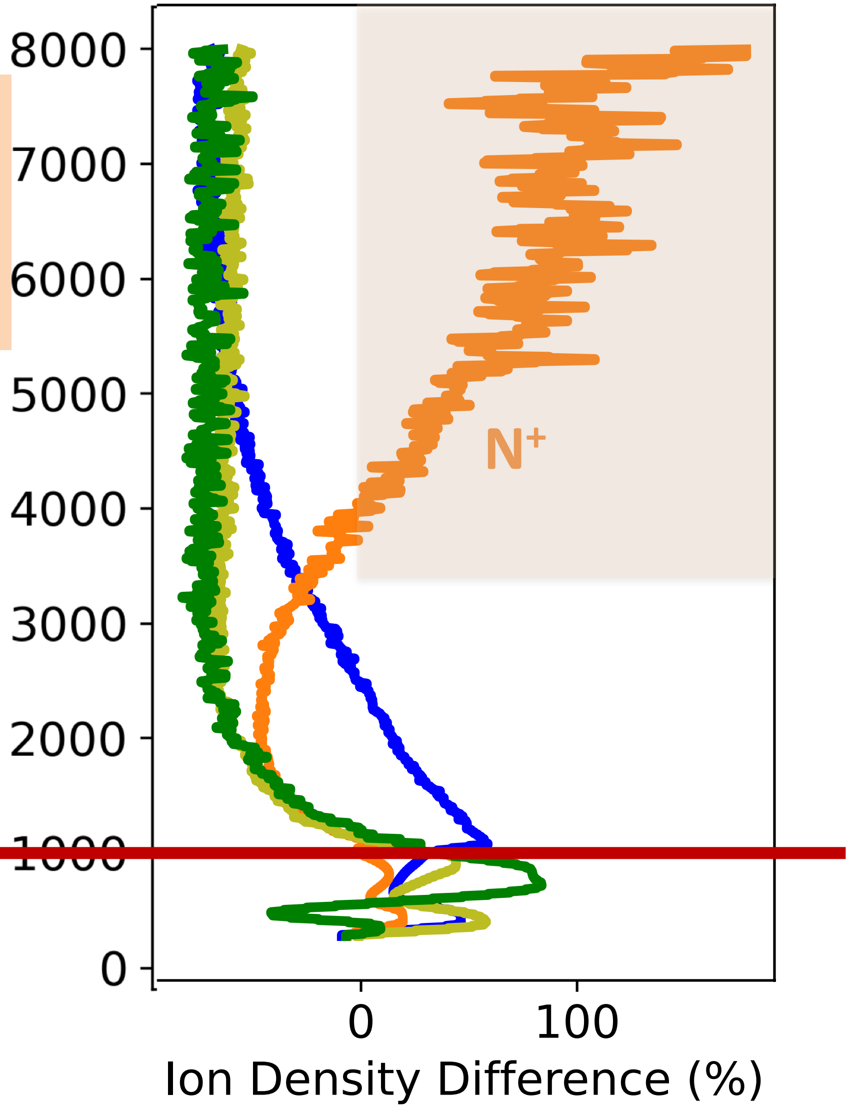
More work is required to examine solution

Kinetic Approach

Fluid Approach

: Fluid + Kinetic

: Fluid



Summary and Future work

- **N^+ ions are a key species** in the ionosphere and their presence alter the outflow for all conditions.
- Comparison with **available data below 1200km**, 7iPWOM shows **tremendous improvement** of the outflow solution when N^+ is included.
- Preliminary simulations using the kinetic 7iPWOM suggest that **molecular ions could also play an important role** in the local transport of all species [*more work to be done here*].
- The molecular ions, such as NO^+, need to acquire sufficient energy in a very short time to escape from the ionosphere, and the energization of molecular ions, via wave particle interaction, are still under investigation.