Inferring Limitations of Numerical Models

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Overview

- Discussion of what to expect from this tutorial.
- Select a tutorial example.
- Empirical Modeling.
- Physics Based Modeling.
- Numerical Schemes, or not!
- What can we infer from this example?
- An approach for inferring limitations of numerical models.

Discussion of what to expect from this tutorial.

- Have you used a numerical model?

  - Have you used a numerical model? (Someone else's.)

- Did you have concerns about the models limitations?

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  - Did you have concerns about the limitations?

- What did you do about addressing these burning concerns?

Discussion of what to expect from this tutorial.

- Have you used a numerical model? (Someone else's.)
- Did you have concerns about the limitations?
- What did you do about addressing these burning concerns?

ASSUMED IT DID NOT SUCK TOO MUCH!

Asked someone.

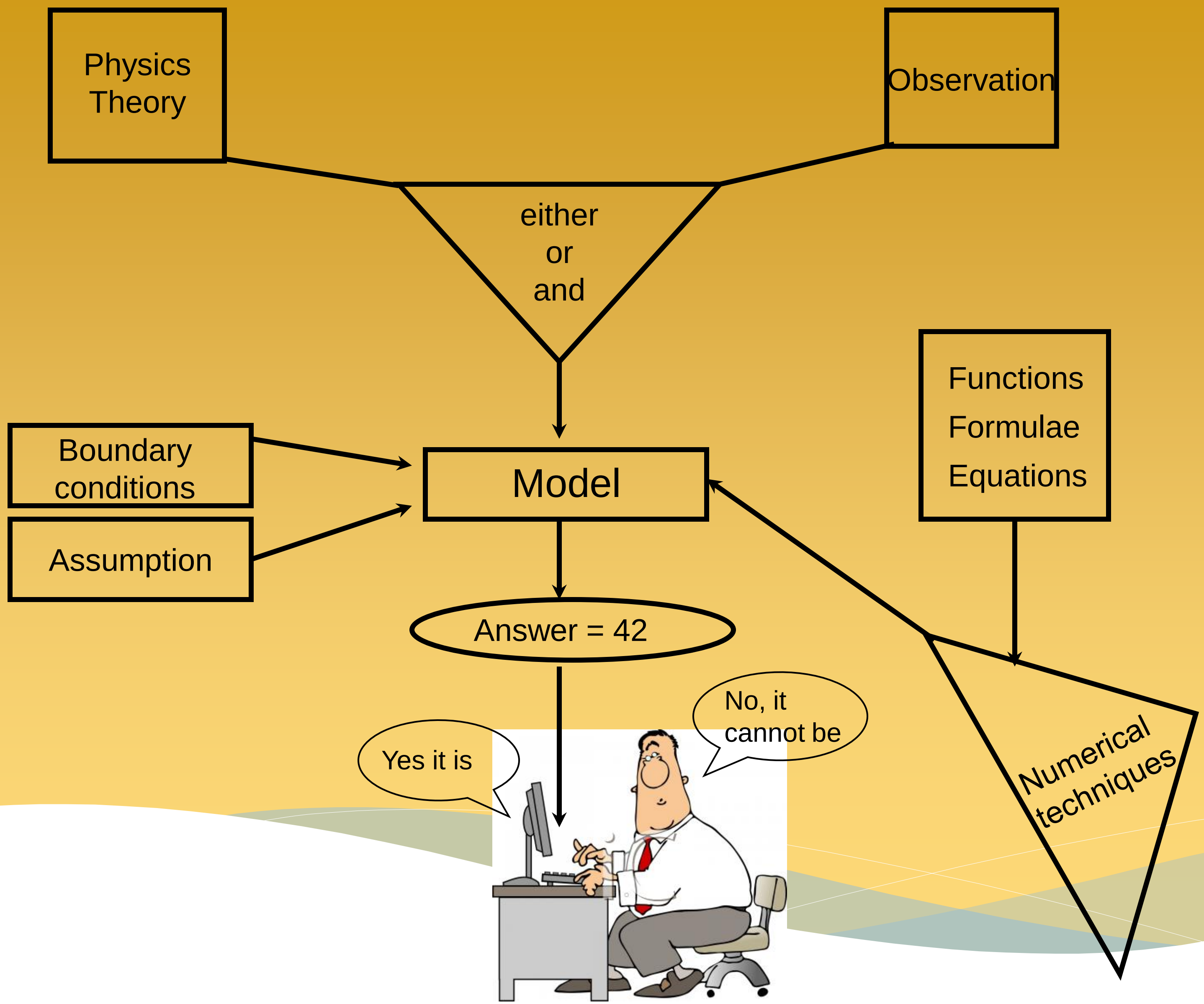
Asked the model developer.

Read the model paper.

Read the model paper's bibliography papers.

Think about the physical processes.

The Problem: A Canonical Black Box Model



Select a Tutorial Example

Assumptions

Every new model development of a particular phenomena was developed for 1 of 2 reasons.

1. To add more physics or observations with the honest intent of improving the description and prediction of the phenomena.
2. To duplicate or even strip down an existing model for a specific application.

We will discuss development 1 only.

The model you are about to use is expected to be an improvement over earlier models and hence what is this improvement?

Or put another way, what was missing in this and previous models?

- How many of you know the limitations of E-region numerical models?

Solomon, Bailey, and Woods [2001]

Titheridge (series of studies [1990 - 1997])

Buonsanto, Solomon and Tobiska [1992]

Rasmussen, Schunk, and Wickwar [1988]

Lilensten, Kofman, Wisemberg, Oran, and Devore [1988]

Muggleton [1972]

Empirical Modeling of the E-region

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L. M. Muggleton

University of Edinburgh, Scotland

Papers between 1969 and 1975

“A Method of Predicting f_oE at any Time and Place”

f_o ordinary mode of radio propagation.

Critical frequency of the E-layer peak.

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APPLETON E. V.	1953	*J. Atmosph. Terr. Phys.* **3**, 282.
CHAPMAN S.	1931	*Proc. Phys. Soc.* **43**, 483.
MUGGLETON L. M.	1970	*Electron. Lett.* **6** (24), 768.
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What were Muggleston's Model Limitations?

Numerical Model:

$$(f_oE)_\chi^{2} = (f_oE)_{\chi=0}^{2}\,\mathrm{Ch}^{-n}(x,\chi) \qquad (3)$$

Where n is the constant factor to be determined by least-squares analysis of ionosonde observations.

Chapman
Function

Least squares fit to 4 separate seasons, n = 0.35, 0.60, 0.30, 0.52. A higher correlation coefficient was obtained if he introduced a more sluggish ionospheric response to the solar radiation; following a 1952 suggestion of Appleton.

Regression analysis fit to 4 separate seasons, n = 0.61, 0.63, 0.60, 0.60.

- Time constant in E-region?
- Measurements where typically hourly values?

- A final reflection on the work of Muggleton and his colleagues is worth mentioning.
- While he was working in Edinburgh the other team developing these numerical models was “here” in Boulder.
- These studies/numerical models became the basis for the CCIR data sets which in turn were the basis for IRI [Rawer,Bilitza].

From Muggleton 1975

Table 1

r.m.s. values of the differences between solar-cycle averages of monthly-medians of the measured foE at each hour in each month, and corresponding values predicted by the Edinburgh method and the Boulder method.

Observatory	Geographic latitude (degrees)	Root mean square of deviation (MHz)		Number of comparisons (each method)
		Edinburgh method	Boulder method	
Oslo	59.97	0.09	0.14	133
Slough	+51.52	0.06	0.11	134
Washington	+38.73	0.10	0.17	142
Maui	:20.80	0.12	0.14	147
Singapore	+1.32	0.06	0.09	1530
Johannesburg	–26.20	0.06	0.13	153
Canberra	–35.32	0.06	0.10	152
Port Stanley	51.70	0.05	0.11	139

- Physics is limited other than Chapman Profile Concept: production/loss etc.

Physics Based Modeling of the E-region

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Lilensten, Kofman, Wisemberg, Oran, and Devore [1988]

- Decided that photoelectrons were more important than others were assuming.

Quote: *"However, in many ionospheric modeling efforts, no such detailed photoelectron transport equations are solved and the secondary ionization is then often assumed to be 30% of the primary [Roble et al., 1987]."*

Since late 1970's global models of the ionosphere and thermosphere were being developed! Even coupling them. Roble et al., Schunk & Sojka, Rees & Fuller-Rowell et al.

- This concern is still present today! The standard secondary electron transport-ionization codes are a serious CPU problem.

- They realized that penetration to E-region altitudes only occurred for certain wavelength mainly the XUV and this was not well represented.

- However their transport code had a boundary at 100 km and hence the E peak at 108 km was being affected by boundary condition numerics. (Numerical problem, Boundary problem.)

- They generate scaling factor profiles for secondary ionization as a function of the photoelectron energy and altitude. (Method still used today.)

Rasmussen, Schunk and Wickwar [1988]

- Why is the E-region important?

  i) Provides all of the Hall Conductivity.
  ii) 50% of the Pedersen Conductivity.
  iii) Magnetosphere models - need conductivities for M-I.
  iv) Thermosphere models - need conductivities for dynamo.
  v) Magnetogram inversion schemes.

- Model deals with secondary electron ionization by generating ion/electron pairs for every 35 eV of the photoelectrons energy.

- Is this a good method?
  How does it compare with a full transport model?

Photochemical Equilibrium Model

Continuity Equation

$$\frac{\partial n_s}{\partial t} + \nabla \cdot (n_s \mathbf{u}_s) = P_s - L_s n_s$$

becomes

$$P_s = L_s n_s$$

production equals loss

Momentum Equation

$$n_s m_s \frac{D_s \mathbf{u}_s}{Dt} + \nabla p_s + \nabla \cdot \tau_s - n_s m_s \mathbf{G} - n_s e_s \left[\mathbf{E} + \frac{1}{c}\mathbf{u}_s \times \mathbf{B}\right]$$
$$= -\sum_t n_s m_s \nu_{st} (\mathbf{u}_s - \mathbf{u}_t)$$
$$+ \sum_t \nu_{st} \frac{z_{st}\mu_{st}}{kT_{st}} \left[\mathbf{q}_s - \frac{\rho_s}{\rho_t}\mathbf{q}_t\right]$$

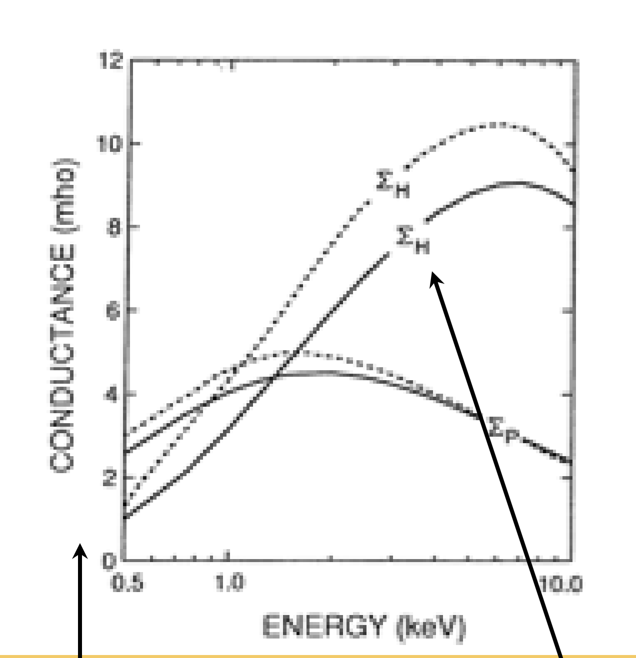
TABLE 1. Ion Chemistry

Reaction			
R1	$N_2 + h\nu$	$\rightarrow$	$N_2^+ + e$
R2	$O_2 + h\nu$	$\rightarrow$	$O_2^+ + e$
R3	$O + h\nu$	$\rightarrow$	$O^+ + e$
R4	$N_2^+ + e$	$\rightarrow$	$N + N$
R5	$O_2^+ + e$	$\rightarrow$	$O + O$
R6	$NO^+ + e$	$\rightarrow$	$N + O$
R7	$N_2^+ + O_2$	$\rightarrow$	$O_2^+ + N_2$
R8	$N_2^+ + O$	$\rightarrow$	$NO^+ + N$
R9	$N_2^+ + O$	$\rightarrow$	$O^+ + N_2$
R10	$N_2^+ + NO$	$\rightarrow$	$NO^+ + N_2$
R11	$O_2^+ + N_2$	$\rightarrow$	$NO^+ + NO$
R12	$O_2^+ + NO$	$\rightarrow$	$NO^+ + O_2$
R13	$O_2^+ + N$	$\rightarrow$	$NO^+ + O$
R14	$O^+ + N_2$	$\rightarrow$	$NO^+ + N$
R15	$O^+ + O_2$	$\rightarrow$	$O_2^+ + O$
R16	$O^+ + NO$	$\rightarrow$	$NO^+ + O$

• Take Away Message about the E-region and Conductivities

Figure 7

From Vickrey et al. [1981]



Photoelectrons
Pedersen > Hall

Auroral energetic electrons
Hall > Pedersen

• But this model is primitive in EUV - XUV, atmosphere and photoelectrons.

Buonsanto, Solomon, and Tobiska [1992]

Revised 1990 model used Lilensten's photoelectron scheme + updated chemistry.

Bank & Nagy 1970 photoelectron 2-stream model revised chemistry.

Supplied solar irradiance model XUV and EUV to both E-regions.

Buonsanto, Solomon, and Tobiska [1992]

<u>Chemistry differences</u>

Buonsanto scheme 13 reactions

Solomon scheme 22 reactions

- ? The more the better?
- Adding more cannot do any harm!

But how would you know?

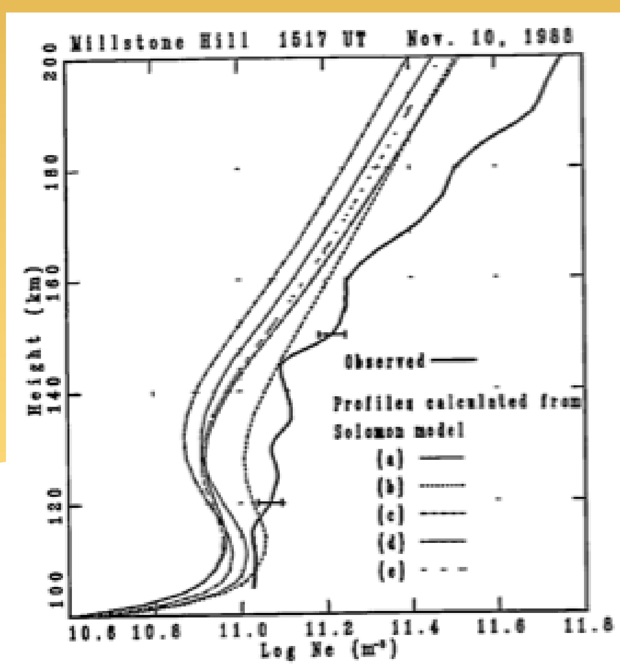
Revised Buonsanto Model

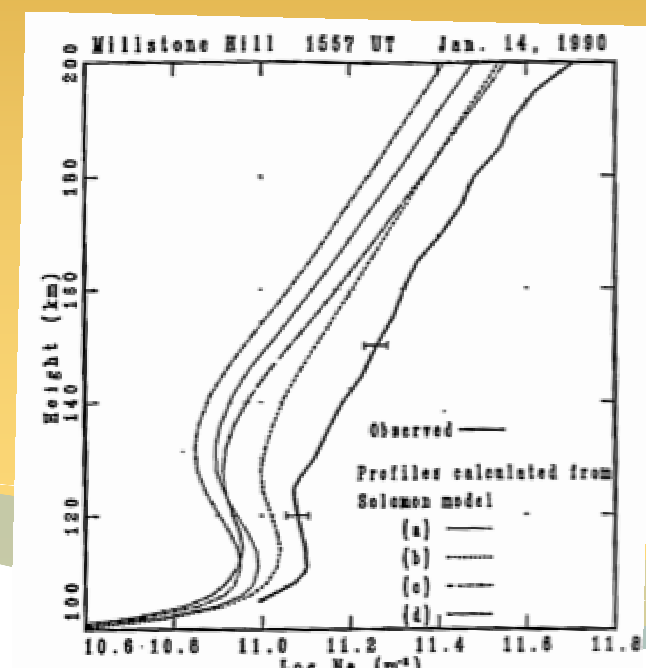
$O^+(^4S) + N_2 \rightarrow NO^+ + N$	$k_1 = 1.533\times10^{-18} - 5.92\times10^{-19}(T_f/300) + 8.6\times10^{-20}(T_f/300)^2$
$O^+(^4S) + O_2 \rightarrow O + O_2^+$	$k_2 = 1.25\times10^{-23}T_f^2 - 3.7\times10^{-20}T_f + 3.1\times10^{-17}$

Solomon Model

$O^+(^4S) + N_2 \rightarrow NO^+ + N$	$k_1 = 1.533\times10^{-18} - 5.92\times10^{-19}(T_f/300) + 8.6\times10^{-20}(T_f/300)^2$ $(T_f < 1700\ K)$ $k_1 = 2.73\times10^{-18} - 1.155\times10^{-18}(T_f/300) + 1.483\times10^{-19}(T_f/300)^2$ $(T_f > 1700\ K)$
$O^+(^4S) + O_2 \rightarrow O + O_2^+$	$k_2 = 2.82\times10^{-17} - 7.74\times10^{-18}(T_f/300) + 1.073\times10^{-18}(T_f/300)^2 - 5.17\times10^{-20}(T_f/300)^3 + 9.65\times10^{-22}(T_f/300)^4$

- More complicated: photoelectrons
  - : chemistry
  - : [NO], MSIS
  - : solar irradiance
- Compared with Millstone Hill ISR profiles
- E-region observations greater than all model runs.





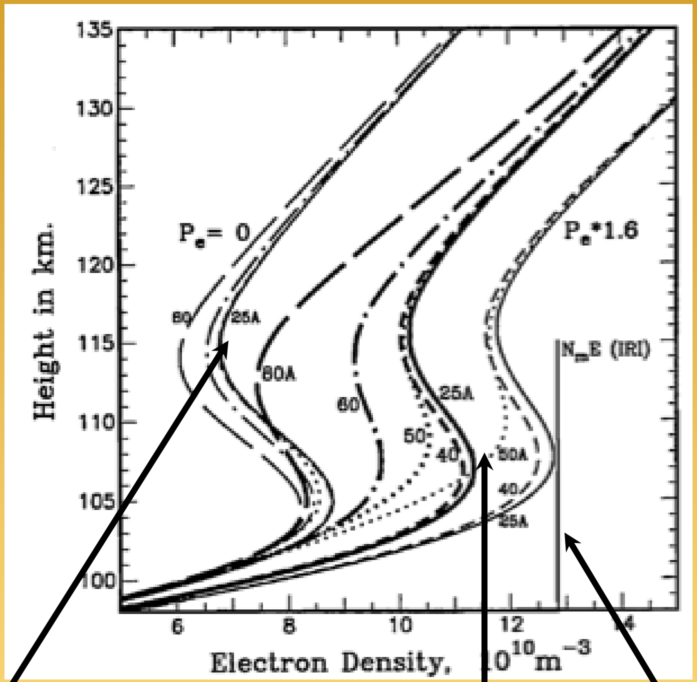
Note: Earlier paper by Buonsanto [1990] argued that scaling MSIS-86 and increasing XUV irradiance provides agreement with these Millstone Hill ISR observations.

- Is MSIS-86 reliable?
- XUV irradiance what did we know?

Titheridge papers

Titheridge (Series of studies 1990 – 1997)

- Revisited secondary production in the E and F1 regions.



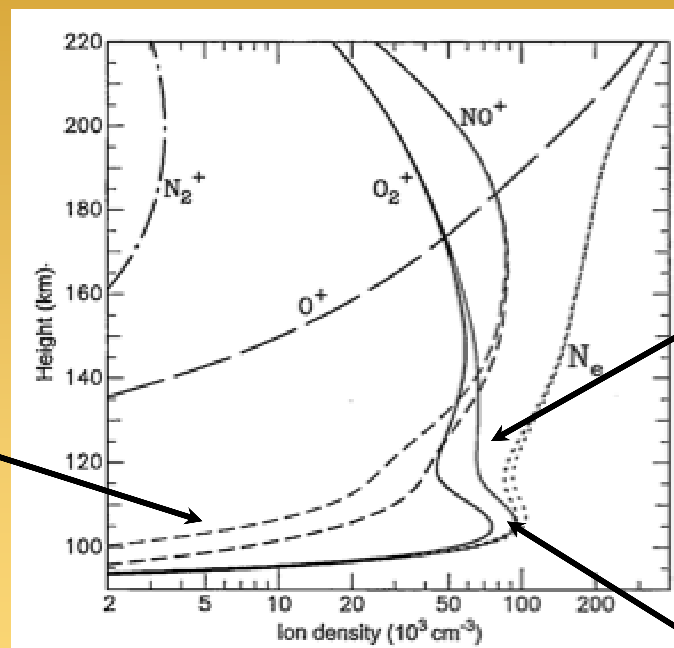
Height depends on Wavelength 2.5 to 8 nm

No secondary ionization 50% lower Ne than IRI

Increase secondary ionization by 60%

IRI is this ground truth

- The [NO] Problem
  - Direct production of NO^+ from [NO] is very small.
  - NO^+ produced indirectly.
  - But [NO] plays a role in conversion of O_2^+ to NO^+.



Valley region sensitive to [NO]

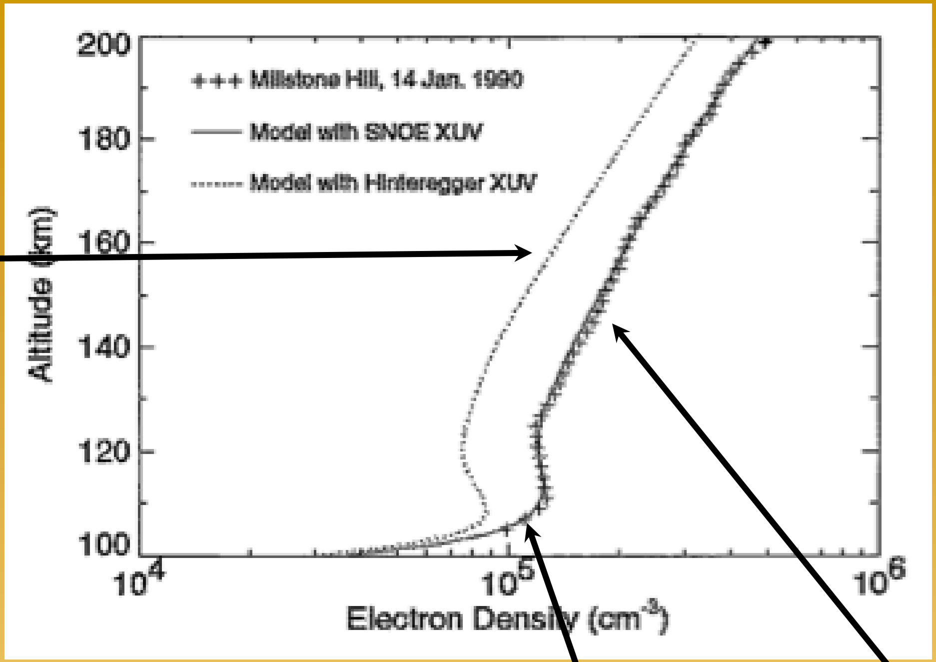
Remove [NO] Decreases NO^+

Remove [NO] Increases O_2^+ at E peak

- Still no good [NO] available!

Solomon, Bailey, and Woods [1996 – 2001]

- Addressing the XUV irradiance question.
- Why GOES x-ray is not sufficient.
- Student Nitric Oxide Explorer (SNOE)
- XUV, 2-7 nm
6-19 nm
17-20 nm
- Discovered that existing models needed to increase their XUV irradiance by factors of 2 to 6.



Unmodified XUV

Solomon et al. 2001

Millstone Hill ISR observations
14 January 1990

XUV modified by a factor of 4

- Does 100% agreement of 1 profile suggest there are no limitations for this model.
- Used MSIS-86.
- No [NO] mentioned.
- SNOE observations in late 1990s used to scale spectrum used for a 14 January 1990 ISR observation.

Numerical Schemes, or not!

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Inferring Limitation of E-region Models

- Solar Irradiance needs spectrally resolved XUV!
- Photoelectron ionization cascade!
- [NO]!
- Neutral atmosphere!
- Dawn & dusk, perhaps time-dependent numerics are needed!
- Did we mention night time?

Observations of Ground Truth Essential

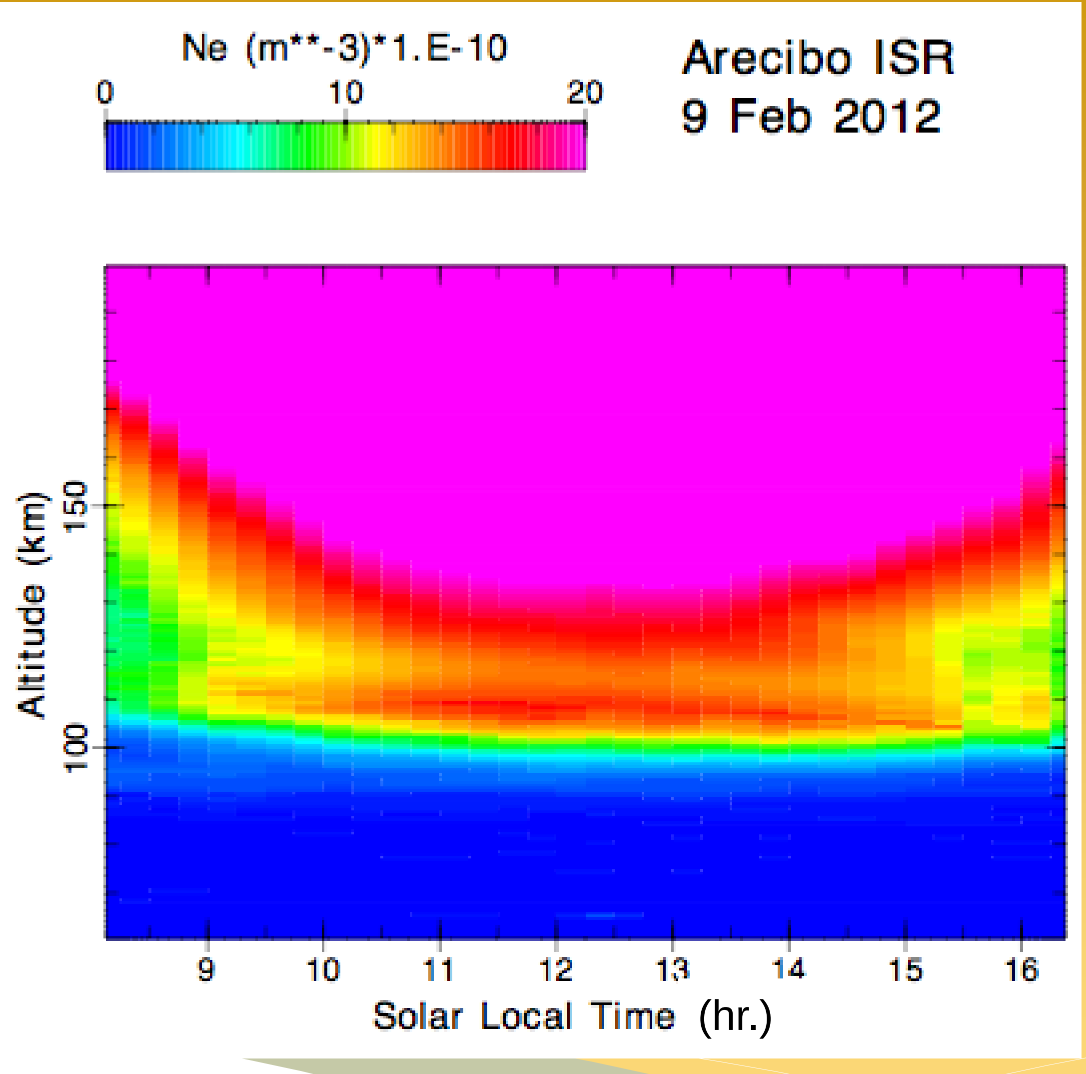
- Ionosonde
- Millstone Hill ISR (decades)
- Arecibo, EISCAT, ALTAIR

Need: better than 1 km altitude resolution (seasonal trend, profile.)

: need all local times (diurnal variation.)

: need many latitudes (NO, atmospheric dependencies, solar zenith angle.)

- ISR chain & SDO EVE simultaneous observations.


Ne (m**-3)*1.E-10
0
10
20
Arecibo ISR
9 Feb 2012
Altitude (km)
150
100
9
10
11
12
13
14
15
16
Solar Local Time (hr.)

An Approach for Inferring Limitations of Numerical Model X

- Focused literature search on MODEL X

  Goggle $\longrightarrow$ 2 days

  Library $\longrightarrow$ week

- List the science processes and solution schemes.
- Construct questions, specific concerns, about MODEL X.
- Politely E-mail these to the model developer(s).

  (Direct questioning of modeler possible afterwards.)

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