Modeling Titan’s Upper Atmosphere

By

Jared M. Bell

09-19-2012

Overview

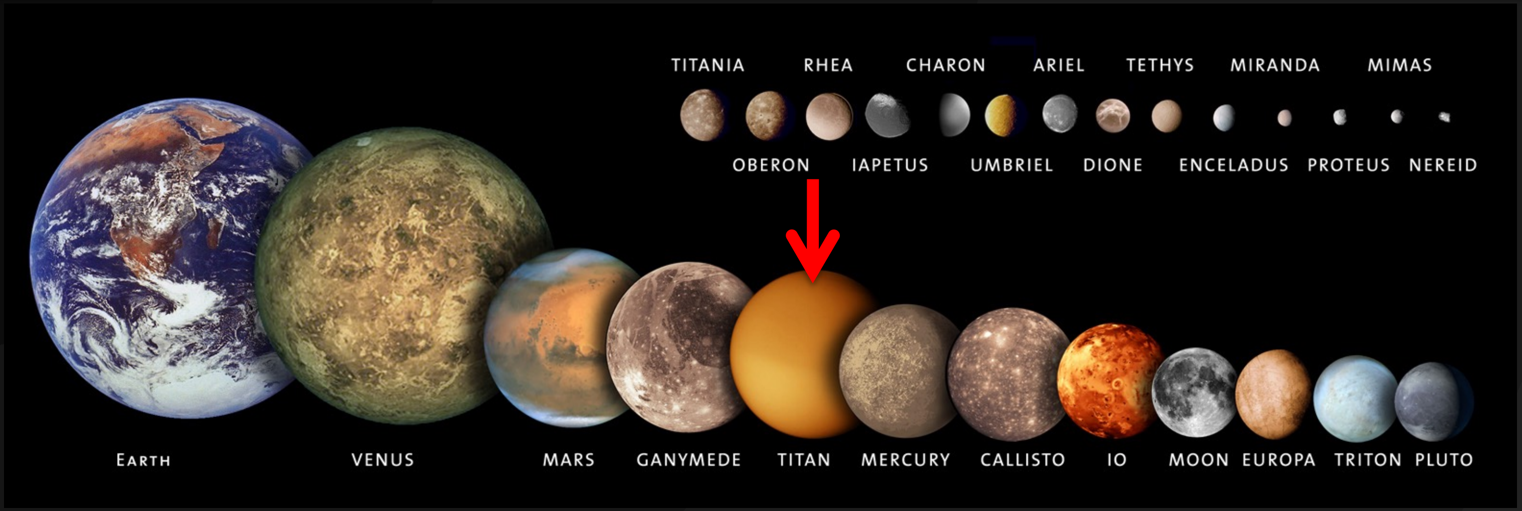
1. Introducing Titan‘s upper atmosphere.

2. Observations of the upper atmosphere.
    1. Neutral thermosphere
    2. Ionosphere

3. Modeling the coupled thermosphere-ionosphere.
    A. Overview of the Titan GITM.
    B. Modeling the Thermosphere.
        - Atmospheric escape
        - Magnetospheric heating of the atmosphere
    C. Modeling the Ionosphere.

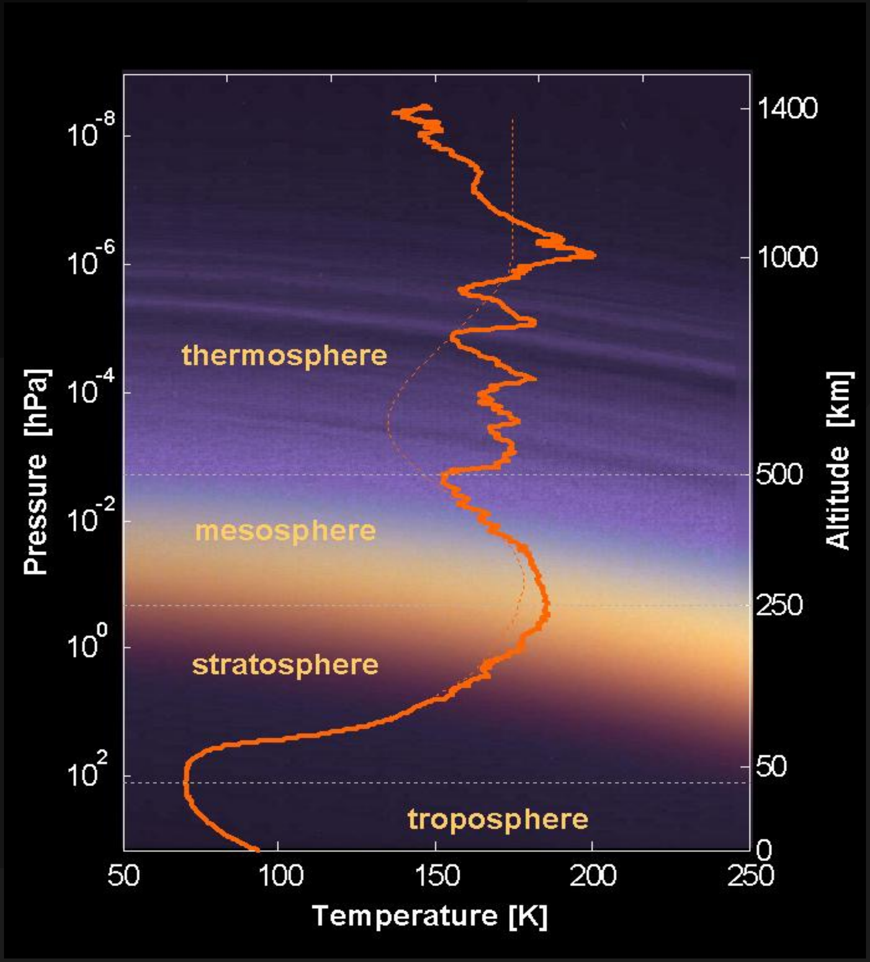
4. Summary and Discussion.

Introducing Titan



- Titan is 2nd largest moon (2575 km radius).
  - Largest of Saturn's moons.
- Significant N_2 atmosphere (1.5 bar)
- Non Magnetic
  - Venus-like Magnetosphere-Ionosphere coupling.

A Very Extended Atmosphere

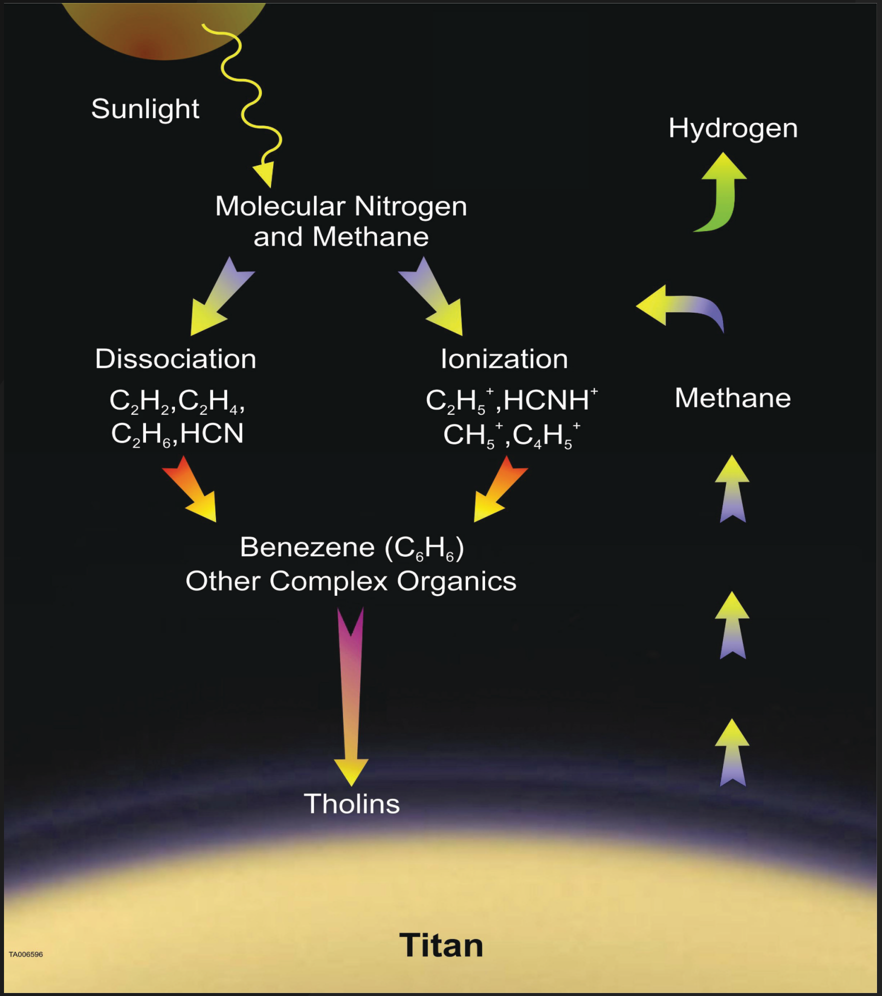


Huygens Temperature Profile
Fulchignoni et al. [2005]

- The exobase is almost 0.6 Titan radii above the surface.
- Due to the low gravity.
- Some have suggested high atmospheric escape.
  - *Strobel* [2008,2009, 2010]
  - *Yelle et al*. [2008]
  - *Bell et al*. [2010a, 2010b].

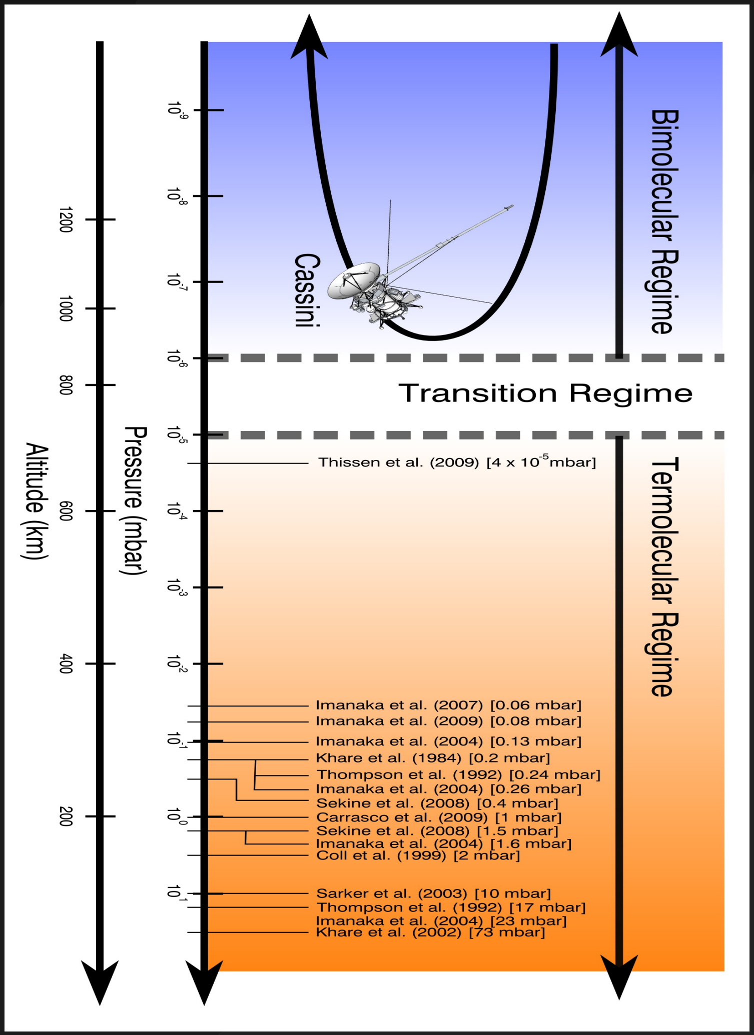
An Organic Chemistry Lab at 9.5 AU

- Unanticipated large molecules in the thermosphere (>100 amu).
- Negative ion clusters, ionized aerosol embryos, hazes...
- Could be a pre-biotic earth!

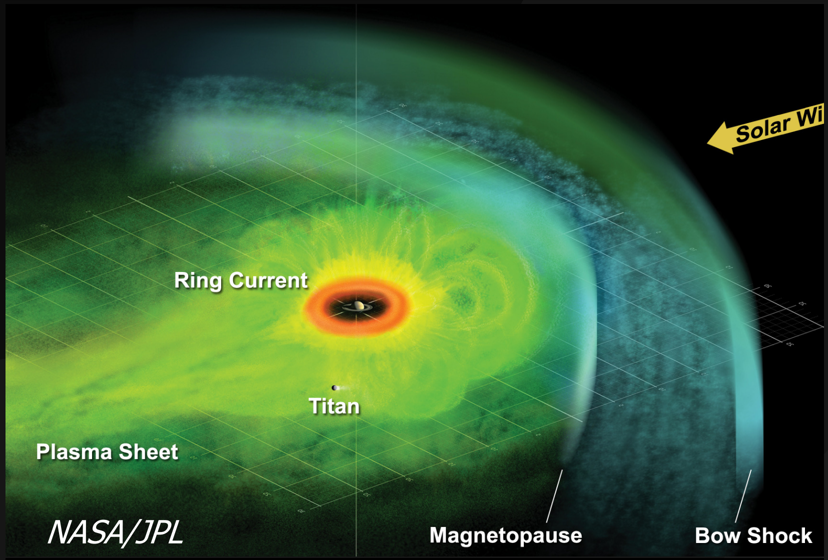


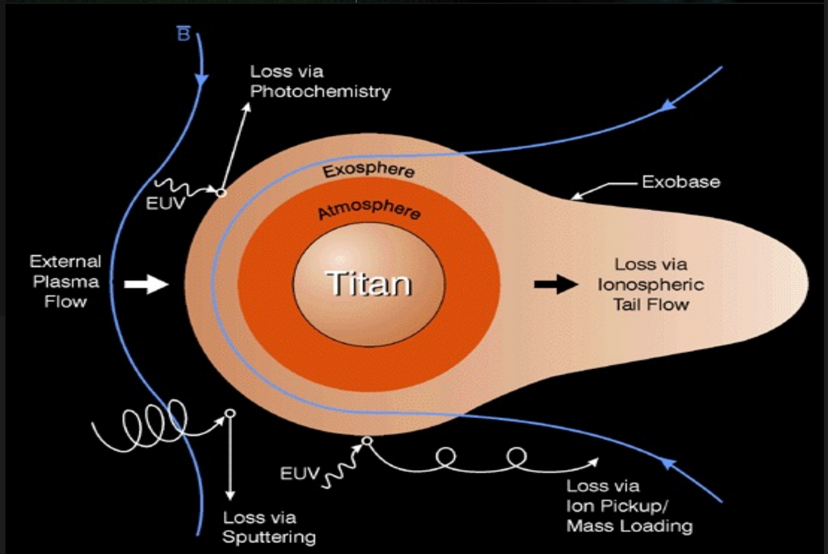
Poorly Constrained Chemistry

- Chemical reaction rates are poorly understood in the altitude regime of interest.
- So we have complex chemistry and very little certainty in the rates!



Titan’s Plasma Environment





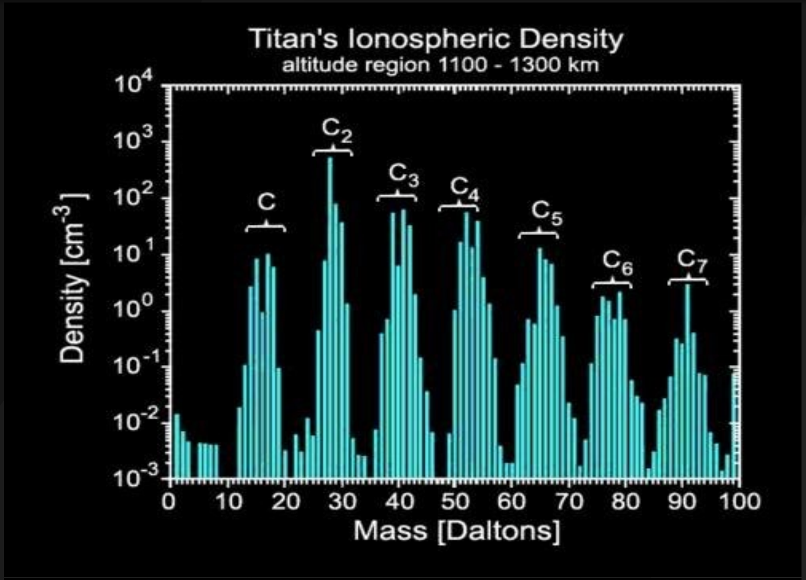
- Titan immersed in Saturn’s magnetosphere.
- In the magnetosphere most of the time (*Bertucci et al*. [2009]).
- Variations in local plasma seem to impact Titan’s upper atmosphere.
  - neutral and ionosphere
- Complex interaction.

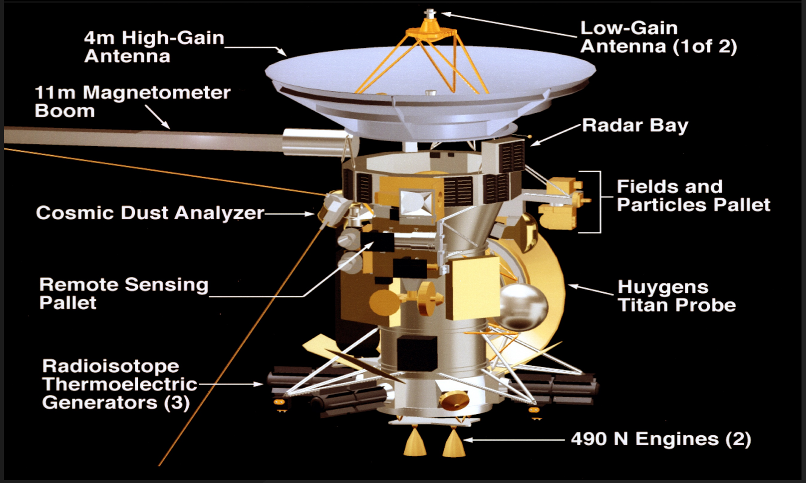
MEASURING THE UPPER ATMOSPHERE:

THE CASSINI ION-NEUTRAL MASS SPECTROMETER

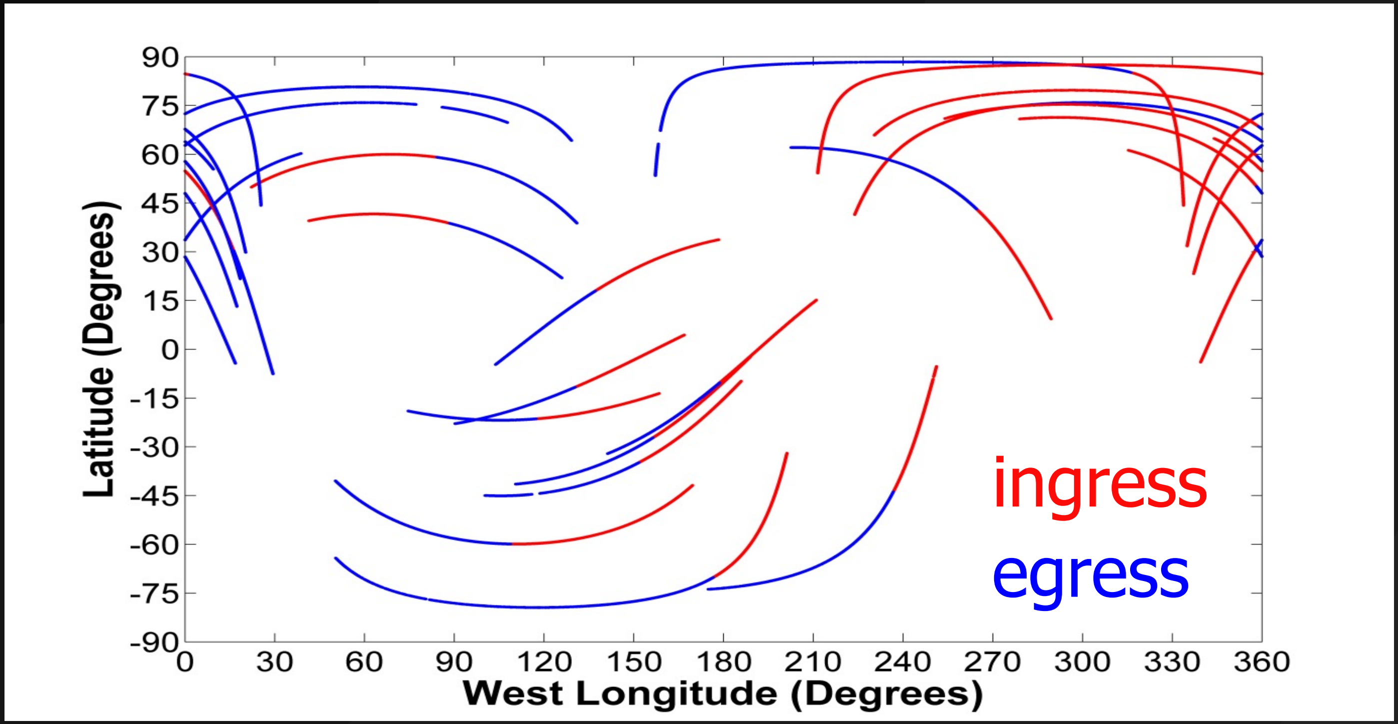
The Cassini INMS

- The Ion-Neutral Mass Spectrometer.
- Takes *in-situ* measurements above 900 km.
  - both neutral and ion densities.
- Sampling the upper atmosphere since 2004.
  - SOI: Saturn Orbit Insertion
- Due to mission constraints, this sampling is sporadic in space and time.





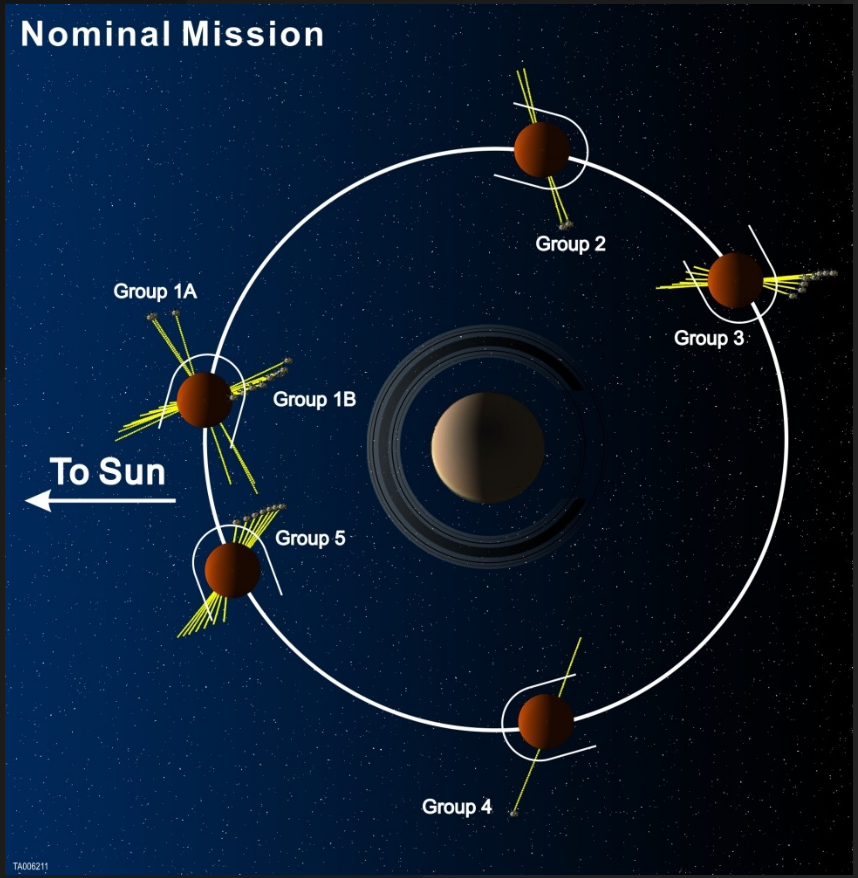
Some Sampling by INMS



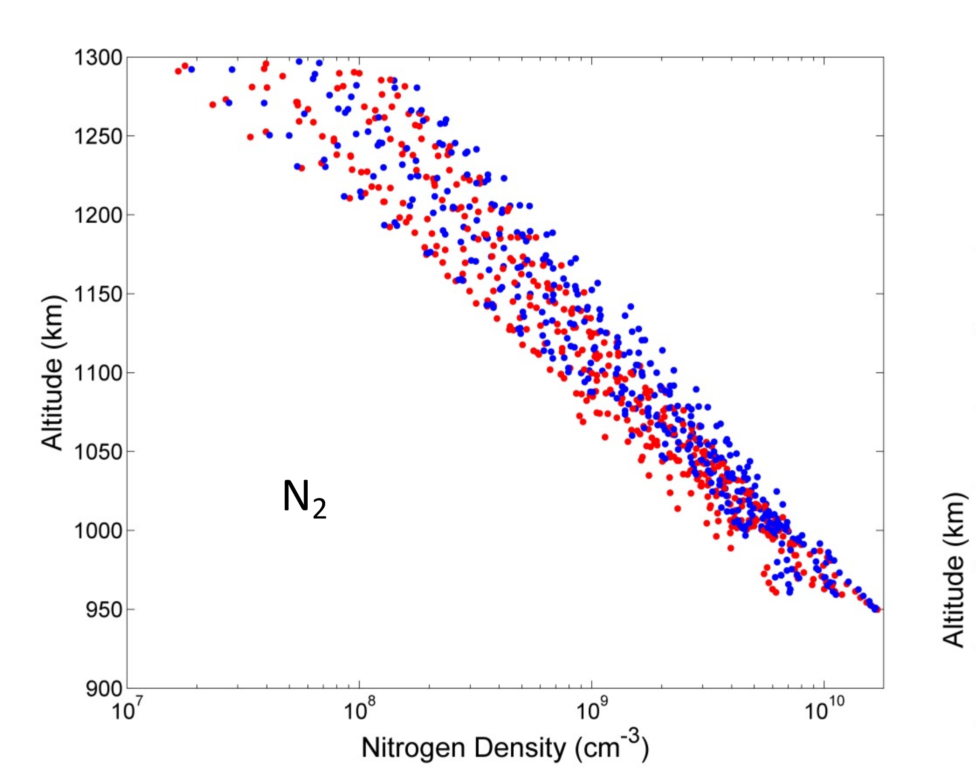
- Sporadic spatial sampling.
- Difficult to extract spatial vs. temporal variations from the data.

Saturn Orbit Sampling

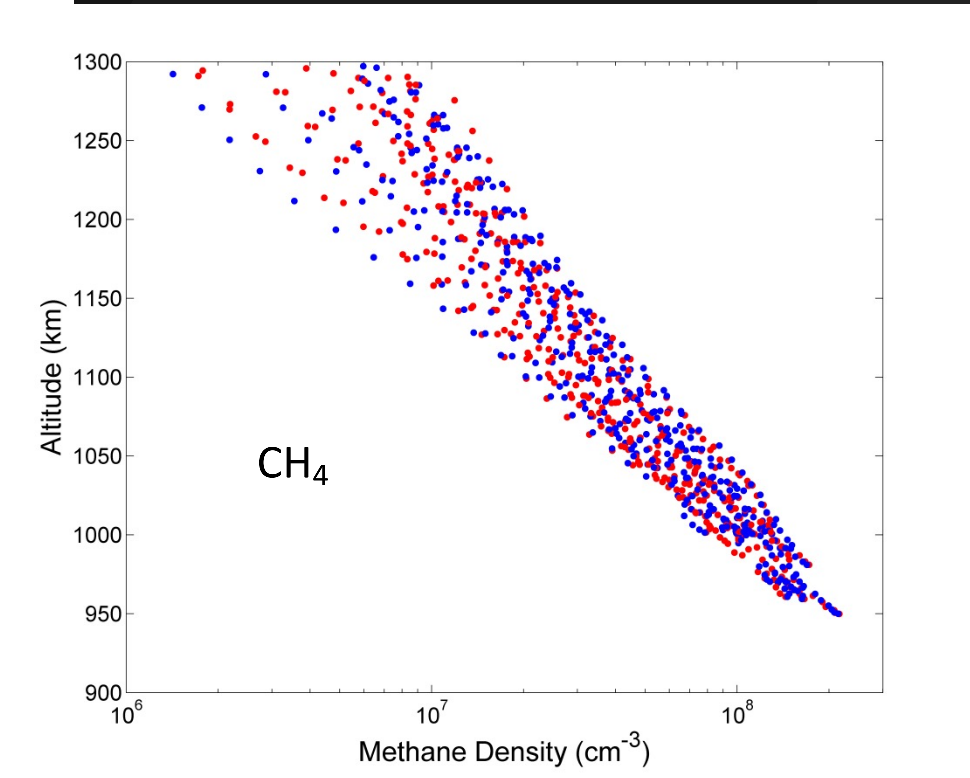
- INMS samples Titan's atmosphere at only discrete points in Saturn's magnetosphere.



Example Neutral Data



- INMS samples number (mass) density.

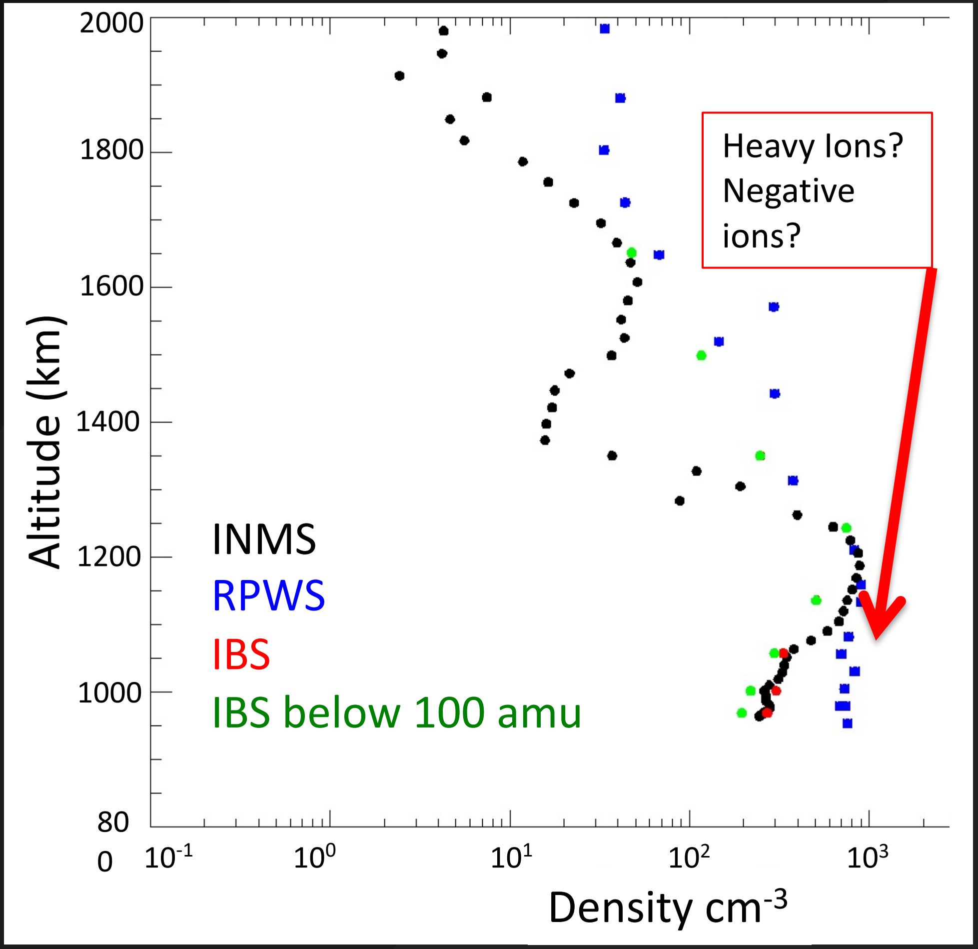


- On-going calibration efforts to reconcile with other instruments.

Sample Ion Data

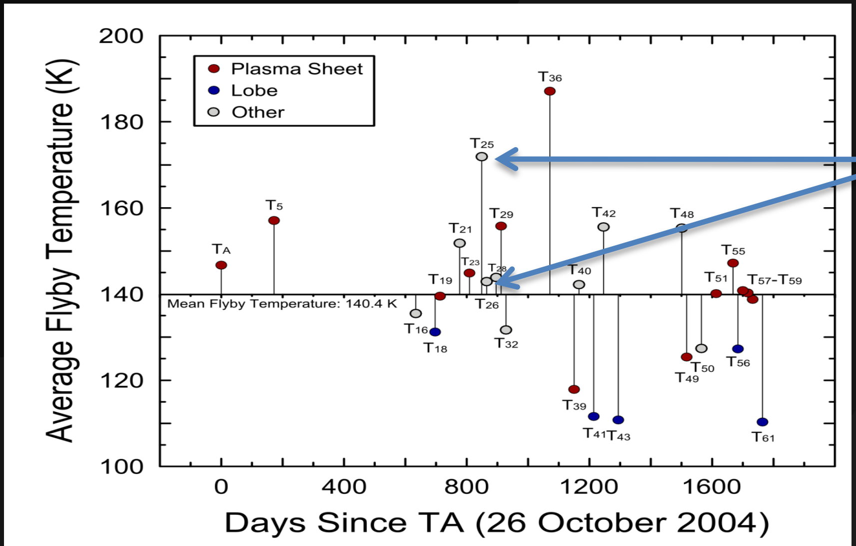
- Measured directly by INMS.
  - Peak ions near ~1100 km.
  - On-going extensive calibrations for both Neutral and Ion data.
    - *Mandt et al.*, *Waite et al.*, and *Gell et al.*

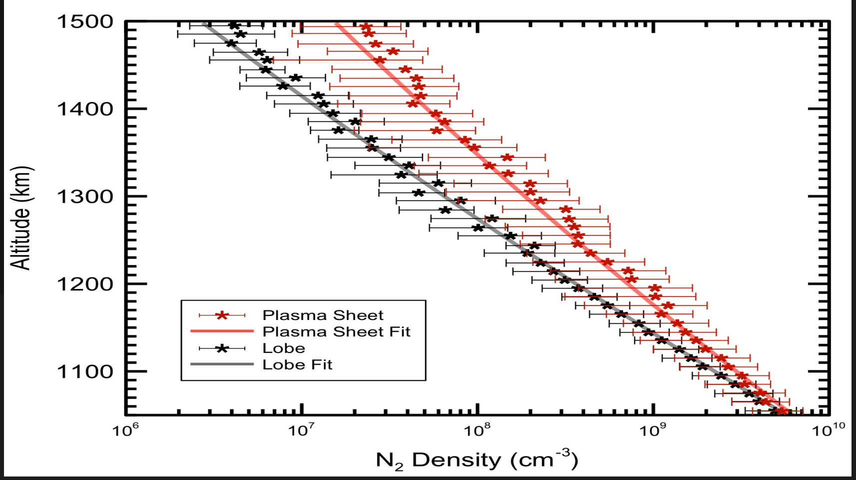
- Cross-calibrated with the
  - Radio and Plasma Wave Science (RPWS)
  - CAPS Ion Beam Spectrometer (IBS)



Mandt et al. [2011] (in prep)

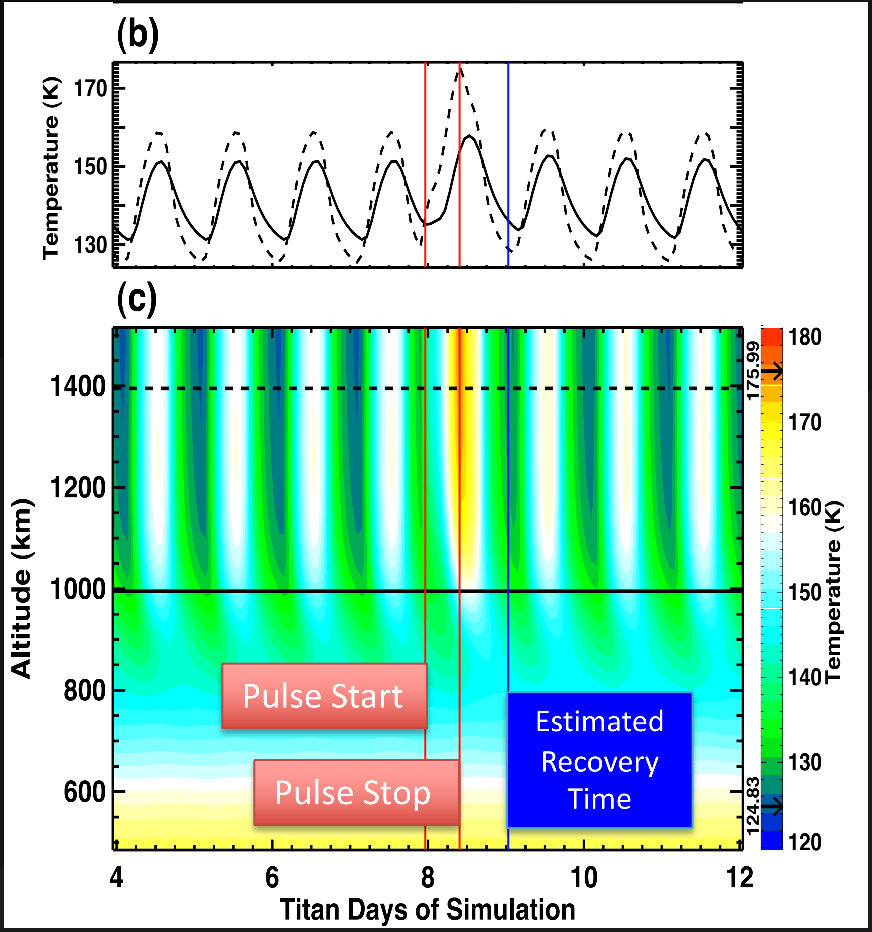
Puzzling Variations





- Cassini INMS detects large, relatively rapid temperature variations.
  - 25 K changes in 1 orbit.
  - Thermosphere temperature ~150 K on average.
- INMS N_2 densities appear to be correlated with intensity of surrounding plasma.
  - *Westlake et al*. [2011] posited a magnetospheric driver.
- Can we validate this hypothesis?
  - Yes! With modeling

A Potential Solution with T-GITM



Bell et al. [2011a]

- We modeled these temperature/density variations using T-GITM.
- Titan Global Ionosphere-Thermosphere Model.
  - Part of University of Michigan's Space Weather Modeling Framework (SWMF).
  - Based upon Earth GITM (*Ridley et al.* [2006])
- Include momentum, energy, and chemistry into a unified model.
  - Include Solar EUV/UV Heating
  - HCN Rotational Cooling
  - No Photoelectrons (important later).

Why Data and Models are needed

- Cassini INMS is measuring Titan sporadically in space and in time.

- There are large, unexpected variations in the upper atmospheric densities closely correlated with Saturn’s plasma environment.

- Given the constraints on further data collection, the best way to maximize the utility of both the INMS neutral and ion data is to use time-dependent global models to help guide our scientific understanding.

MODELING TITAN’S COUPLED IONOSPHERE-THERMOSPHERE SYSTEM: T-GITM.

Global Ionosphere-Thermosphere Model (GITM)

- 3-D, non-hydrostatic, altitude-based atmospheric model
  - Developed at the University of Michigan.
  - Can run in 1-D and 3-D.

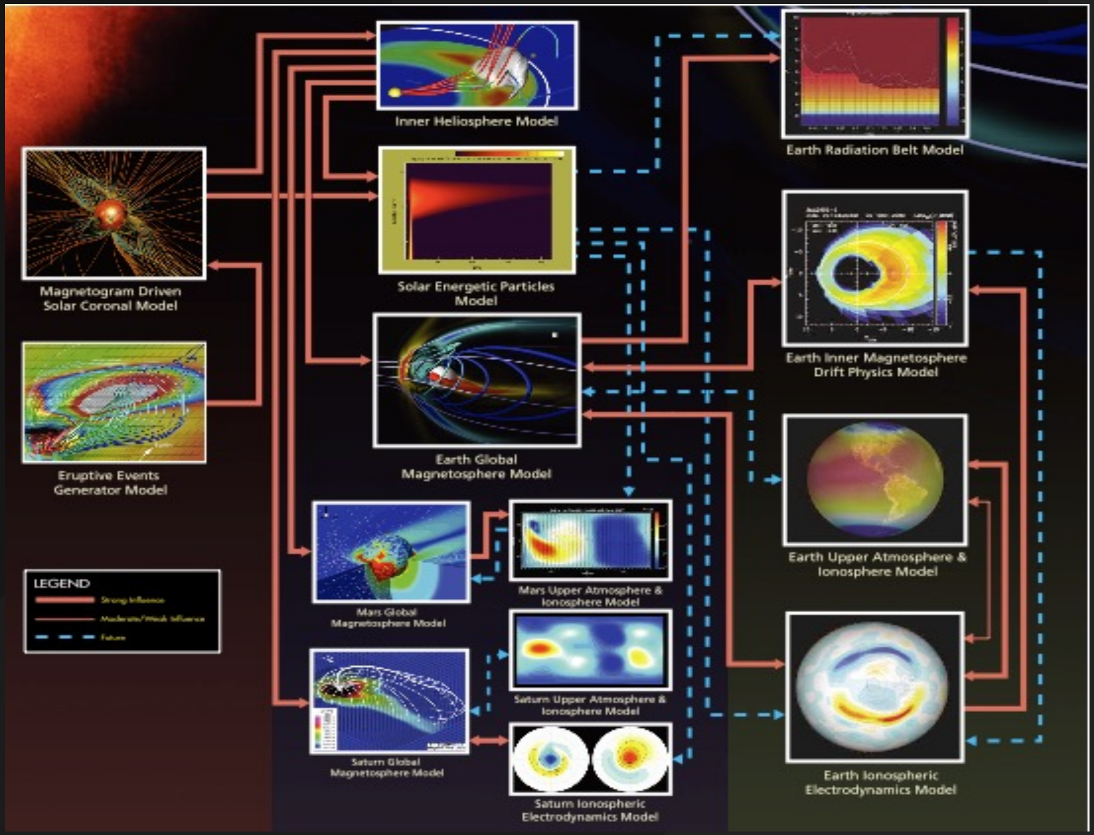
- Applied to Earth, Mars, Titan (and now Jupiter and Saturn).

- It solves the time-dependent Navier-Stokes equations.
  - 2nd order Total Variation Diminishing (TVD) MUSCL Scheme.
  - Block-based Massively Parallel Framework
  - Updating with 4th order Runge-Kutta Time-stepping.

- Part of the Space Weather Modeling Framework (SWMF).
  - Readily couples with MHD models.
  - Radiation belt models.

The Larger Family of models

- GITM fits within a larger family of models.
- Coupling is relatively straight-forward.
- Allows system-wide studies.



3-D Titan GITM

- We model from 500 km altitude (roughly the top of the stratosphere) up to 1500 km (the exobase).

- We use a uniform 10 km radial resolution.
  - 0.25 scale heights near 500 km.
  - 0.10 scale heights near 1500 km.

- We use uniform 2.5 degrees latitude and 5 degrees longitude resolution.

- Typically run for ~20 Titan days (~1 Earth Year).
  - Runs on ~500 processors and takes 1 week of simulation.
  - Use NASA High End Computing (HEC) Pleiades cluster.

1-D T-GITM

- GITM can run in a 1-D mode and 3-D mode.
- For a 1-D mode, we ignore horizontal transport.
- User dials in a preferred latitude and longitude.
- GITM then simulates a 1-D, “spherical” column rotating with the planet.
- Simulates what you would see on Titan if you were at a fixed point on the planet and looked up.

We Constrain T-GITM with Data

Table 3. T-GITM lower boundary settings and associated Cassini-Huygens constraints.

T-GITM Lower Boundary Field	Cassini-Huygens Range
$\chi_{CH_4} = 1.44\%$	1.48 ± 0.9 % (GCMS[a]) and $1.6 \pm 0.5\%$ (CIRS[b])
$\chi_{H_2} = 2.00 \times 10^{-3}$	$1.0 \pm 0.5 \times 10^{-3}$ (CIRS[c]) and $1.01 \pm 0.16 \times 10^{-3}$ (GCMS[a])
$\chi_{Ar^{40}} = 3.30 \times 10^{-5}$	$3.39 \pm 0.12 \times 10^{-5}$ (GCMS[a])
$\chi_{HCN} = 4.00 \times 10^{-6}$	$2.0 \times 10^{-7} - 2.0 \times 10^{-5}$ (CIRS[d])
$^{14}N/^{15}N = 167.7$	167.7 ± 0.6 (GCMS[a])
T = 175.0 K	160.0 – 190.0 (CIRS[e])
$n = 9.6 \times 10^{19}$ (m^{-3})	$\sim 8.2 \times 10^{19}$ (m^{-3}) (HASI[f])

[a]*Niemann et al.* [2010], [b]*Flasar et al.* [2005], [c]*Jennings et al.* [2009], [d]*Teanby et al.* [2007],

[e]*Achterberg et al.* [2008], [f]*Fulchignoni et al.* [2005]

Titan-specific Physics

- Solar EUV/UV heating (of N_2, CH_4, and H_2).
- We account for the chemistry of Titan.
  - Based upon a simplified ion-neutral chemical scheme of *De La Haye et al*. [2008].
  - Focus on the formation of HCN (main radiative coolant).
- Thermal molecular conduction.
- We can specify magnetospheric heating rates due to plasma precipitation.
  - DSMC simulations, Hybrid simulations, and MHD calculations.
  - Constrained by Cassini-mission data for energy inputs.

Radiative Cooling

- HCN is the major radiative cooling mechanism.
  - *Yelle* [1991].
- A Linear, asymmetric molecule, allows for efficient radiative cooling from the rotational lines (LTE).
  - Treated with a line-by-line code, developed by myself.
  - Based upon work by *Yelle* [1991] and *Mueller-Wodarg et al.* [2000]
- We couple the chemistry leading to the formation of HCN to its dynamical transport and its radiative effects.
  - Allows T-GITM to capture the non-linear feedback between chemistry, momentum, and energy balance.

Science Topics Addressed by T-GITM

1. Estimated atmospheric escape of key constituents: N_2, CH_4, and H_2
   - Important for understanding atmospheric evolution.
   - *Bell et al*. [2010a, 2010b, 2011b].

2. The role of magnetospheric heating on the neutral atmosphere.
   - *Bell et al*. [2011a], *Westlake et al*. [2011a]

3. Simulated the 3-D ionosphere and made observations about likely missing ion-neutral chemical processes.
   - *Westlake et al*. [2011b], *Bell et al*. [2012] (in prep.)

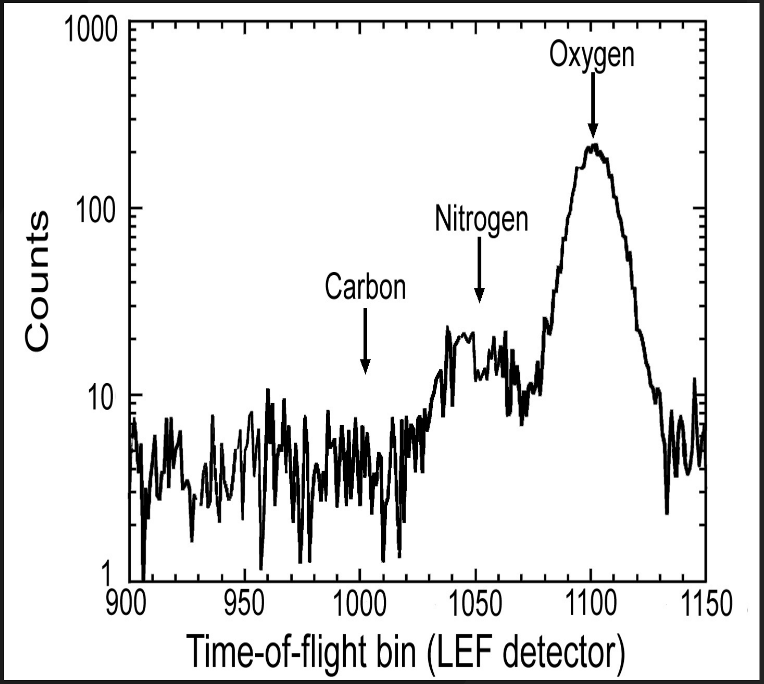
Atmospheric Escape

- *Strobel* [2008, 2009, 2010] and *Yelle et al*. [2008] suggested high escape rates of CH_4 are required to reproduce INMS data with models.
  – Based upon INMS composition and lower atmosphere composition.
  – Suggested 40 – 60 kg/s escaping (Enceladus estimated at 200 kg/s).
  – Called this *slow hydrodynamic escape*.

- The only problem is that there is no evidence (directly or indirectly for this).

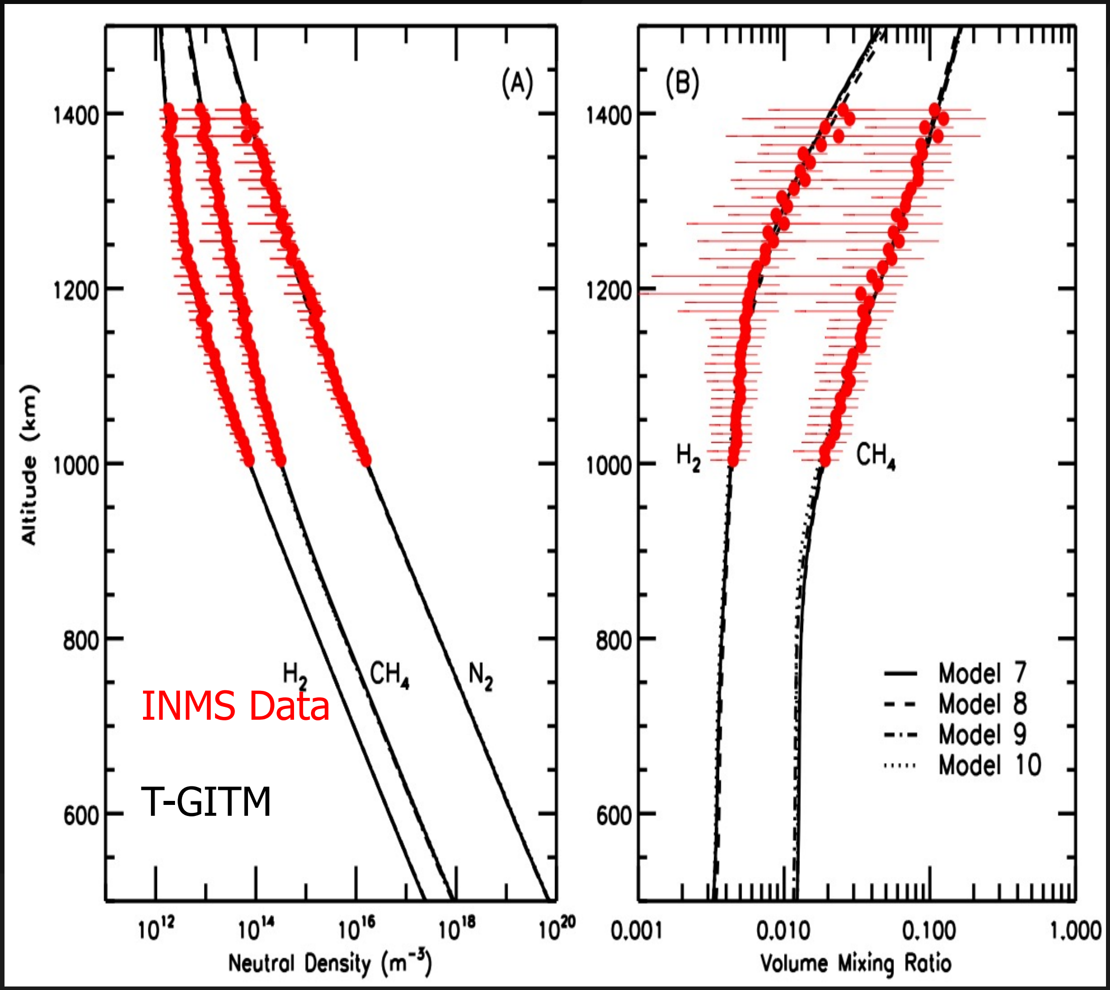
No Carbon Ions!

- Cassini Plasma Spectrometer (CAPS) reveals no Carbon ions near Titan.
- Co-added spectrum of ions over 6 years of data near Titan's orbit.
  - remove Titan's ionosphere
- Possible that all the methane just slips away undetected...
  - However we see Titan producing H_2^+ ions (*Tseng et al*. [2011])



Courtesy: Frank Crary (unpublished)

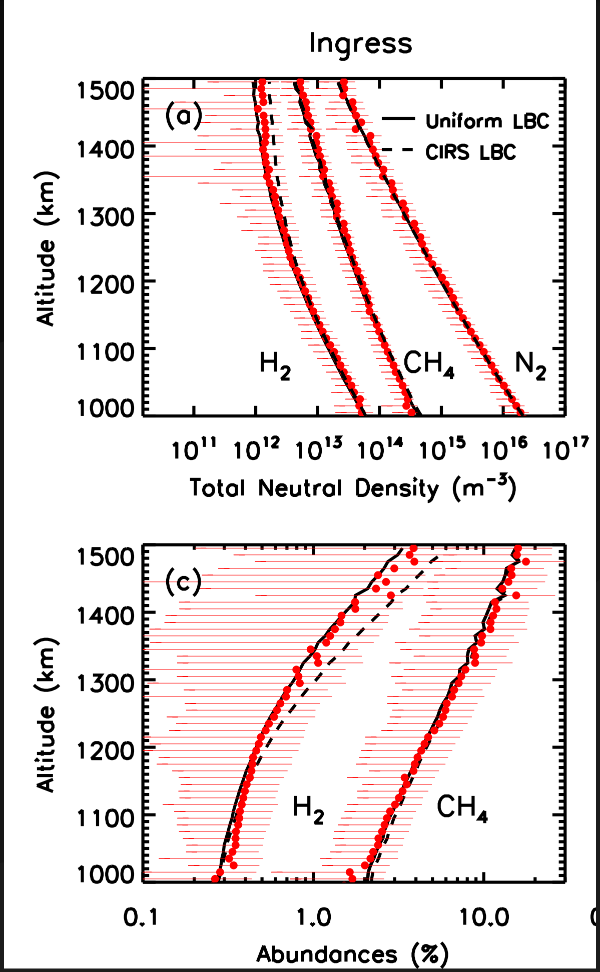
Sample 1-D T-GITM Results



Bell et al. [2010b]

- We used Titan-GITM to explore the possibility that no CH_4 escapes.
- Results shown to the left have only 0.01 kg/s escape rates
  - Consistent with CAPS data.
- Used a higher homopause and included CH_4 chemical losses.
- Combined effect is to limit CH_4 escape in the model.

3-D Atmospheric Escape



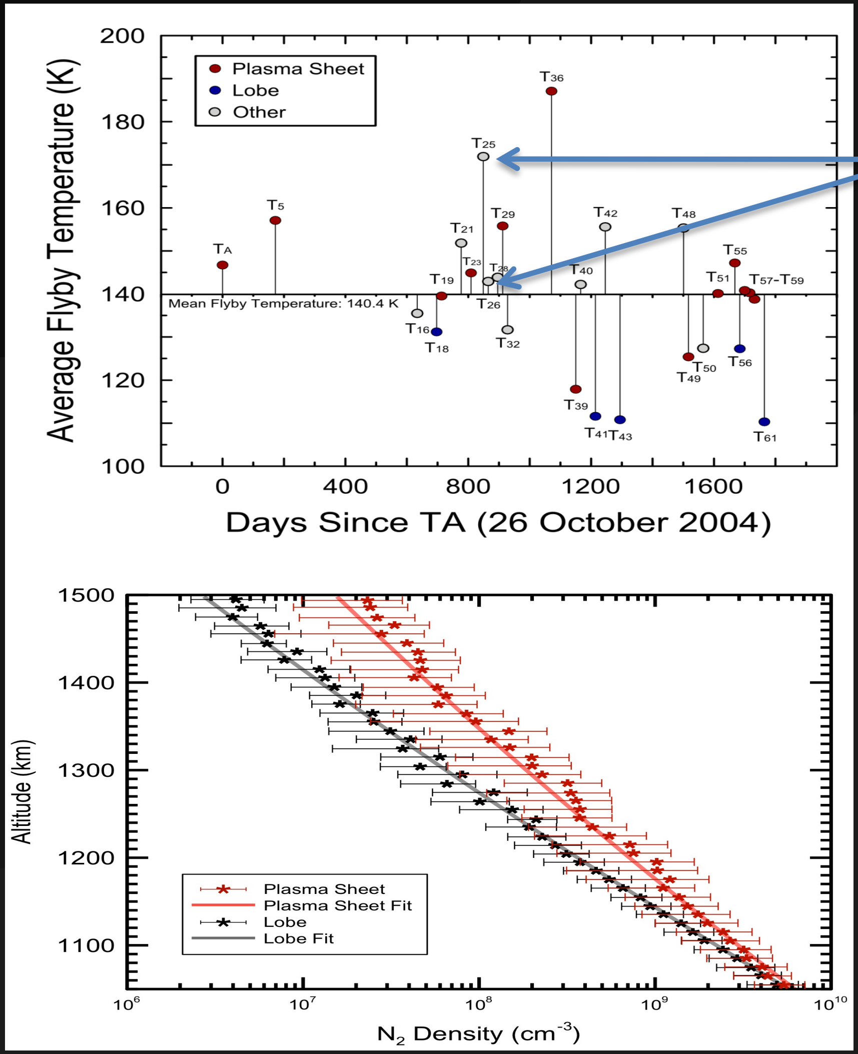
Bell et al. [2012a, b], in prep.

- 3-D T-GITM also reproduces INMS composition (solid black line) along TA-T40 flybys.
  - Using a uniform (flat LBC) or a CIRS-driven latitude-varying Lower boundary.
- I sampled the model along all INMS flybys between TA and T40 (in full 3-D space).
- Created a synthetic "T-GITM dataset" and them compared that to the actual INMS.
- Little to no CH_4 escape was required to reproduce INMS.

Atmospheric Escape Summary

- Based upon our simulations, INMS data is a weak constraint on atmospheric escape estimates.
  - even when constrained to match lower atmosphere data (i.e. HASI, GCMS, CIRS, UVIS).
- High homopause, low escape rate scenario is consistent with INMS and other instrument datasets.
  - Also consistent with CAPS magnetosphere observations (i.e. no Carbon ions).
- No need to impose high escape rates of methane, as suggested to *Strobel* [2008, 2009, 2010] and *Yelle et al*. [2008].
  - Emphasize that T-GITM corroborates their findings under very specific parameter values.
  - This does not “refute” hydrodynamic escape scenarios, it only offers and alternative.

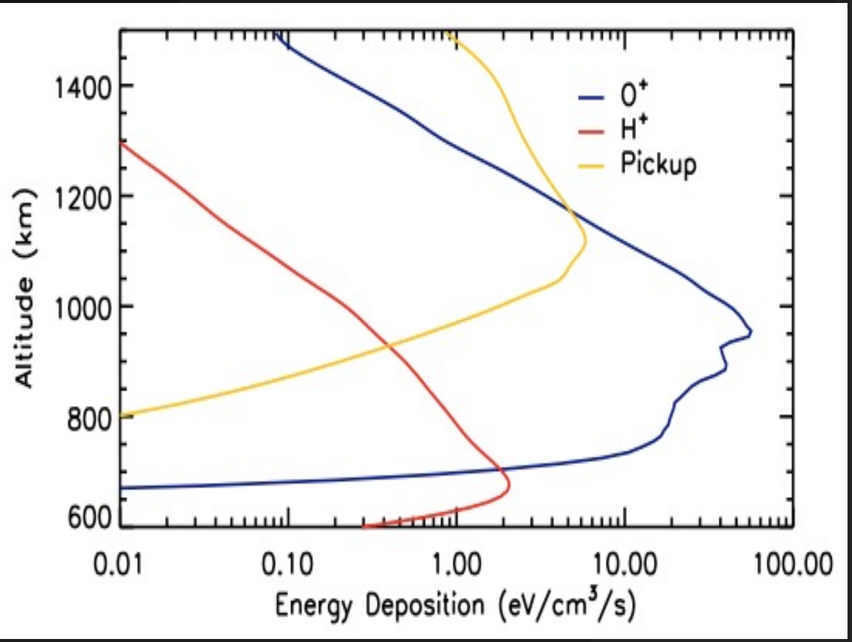
Potential Magnetospheric Heating?



- "Rapid" variations in inferred temperatures suggest a mechanism operating within a Titan orbit.
- Solar activity has been very constant and low.
- Variations are strongly correlated with plasma environment.
- Suggests a magnetospheric driver.

Simple 1-D Heating Rates

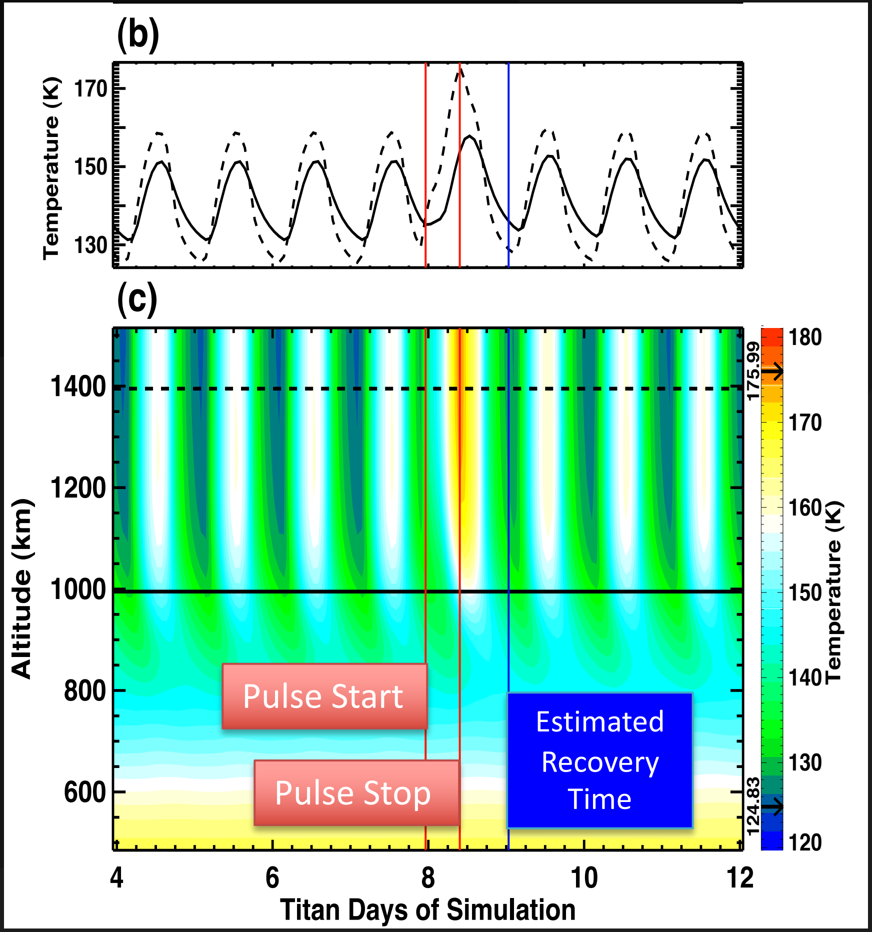
- We take heating rates from ion precipitation.
  - *Shah et al*. [2011], *Smith et al.* [2009], *Michael and Johnson* [2005].
  - e^- precipitation is complicated by **B**-field (*Gronoff et al*. [2009a,b]).
  - Joule heating also dependent upon **B**-field.



- From *Bell et al.* [2011a]

- "Hit" T-GITM with a pulse of magnetospheric energy:
  - Would it heat?
  - Would it cool back down within a Titan orbit?

1-D T-GITM Simulation

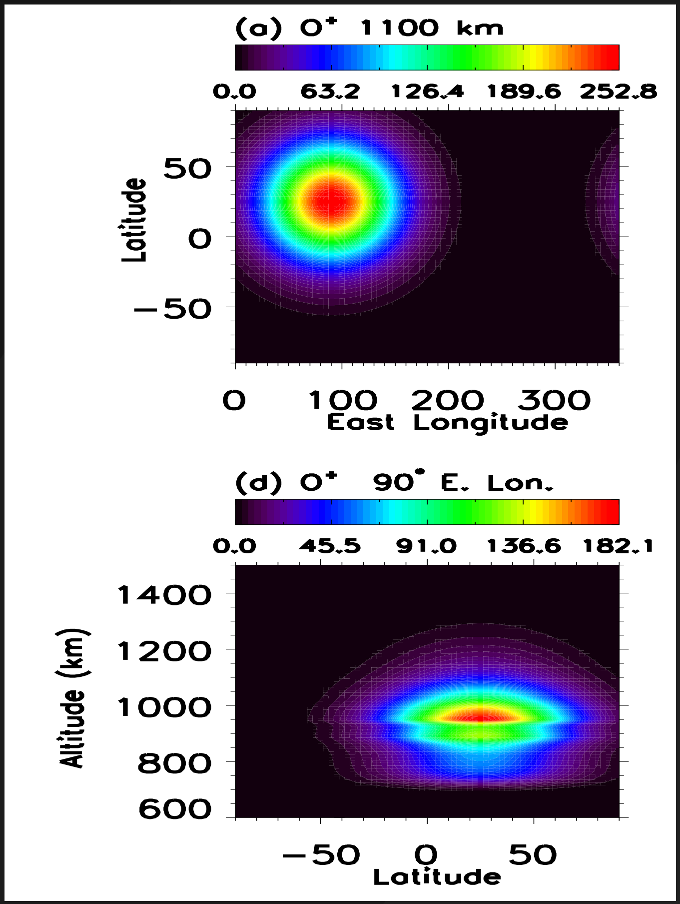


Bell et al. [2011a]

- Began with a solar-only simulation.
- Initiated a magnetospheric pulse at Titan day 8
  - lasted for 8 Earth days (0.5 Titan days).
- Ended on Titan day 8.5.
- Titan temperatures recovered within 10 Earth days
  - less than a Titan orbit.
- Most variation seen above 1100 km
  - Where INMS observes it.

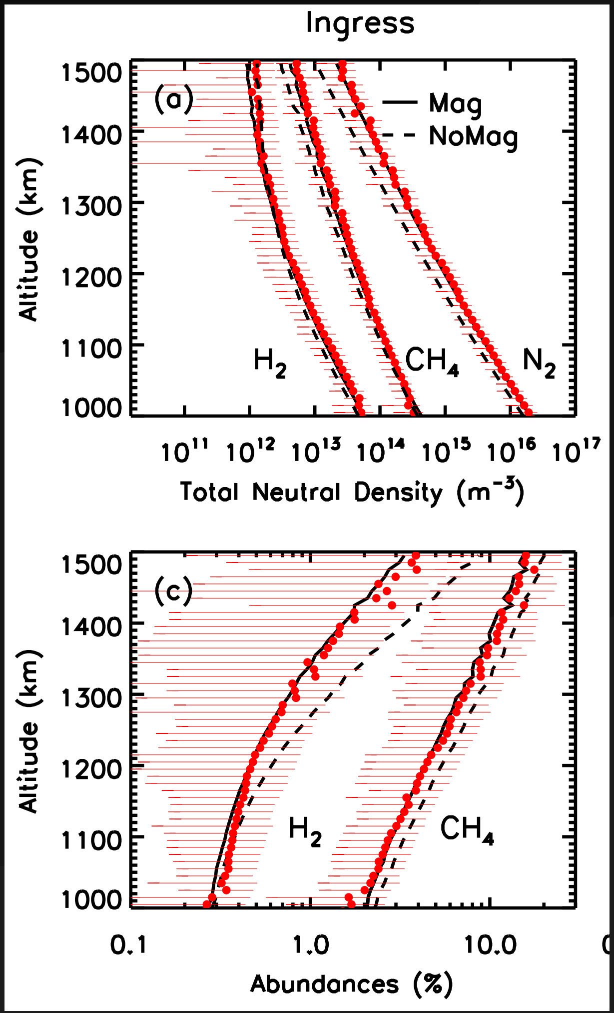
3-D Magnetospheric Heating

- Need Multi-dimensional heating functions from hybrid models.
- Major heating from O^+ and pickup ions.
- Maps taken from *Sillanpaa et al*. [2007] for O^+ and H^+.
- Pickup ions from *Tseng et al*. [2008].



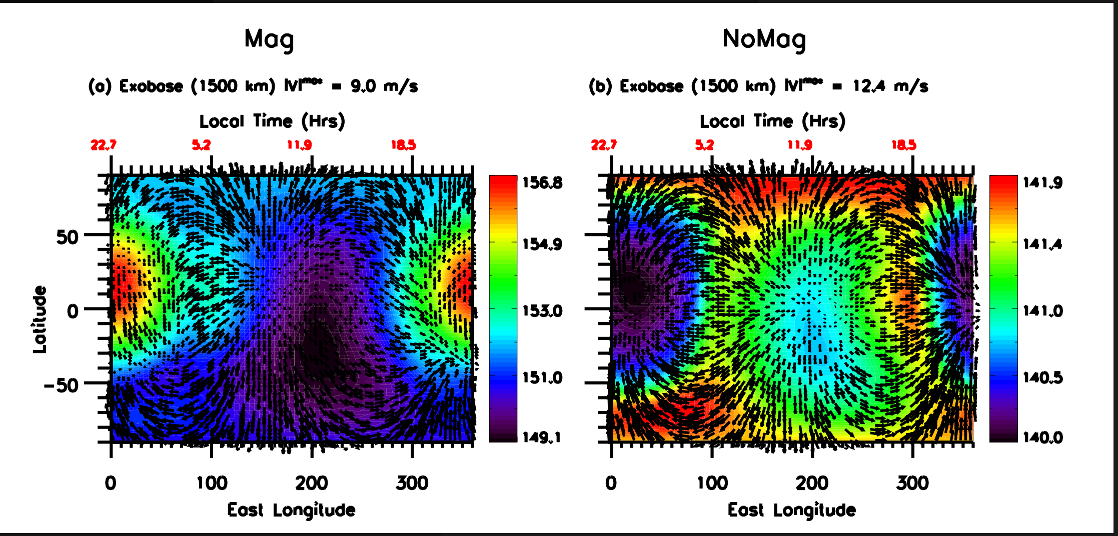
Bell et al. [2012a, b] (in prep.)

Neutral Atmosphere 3-D Modeling



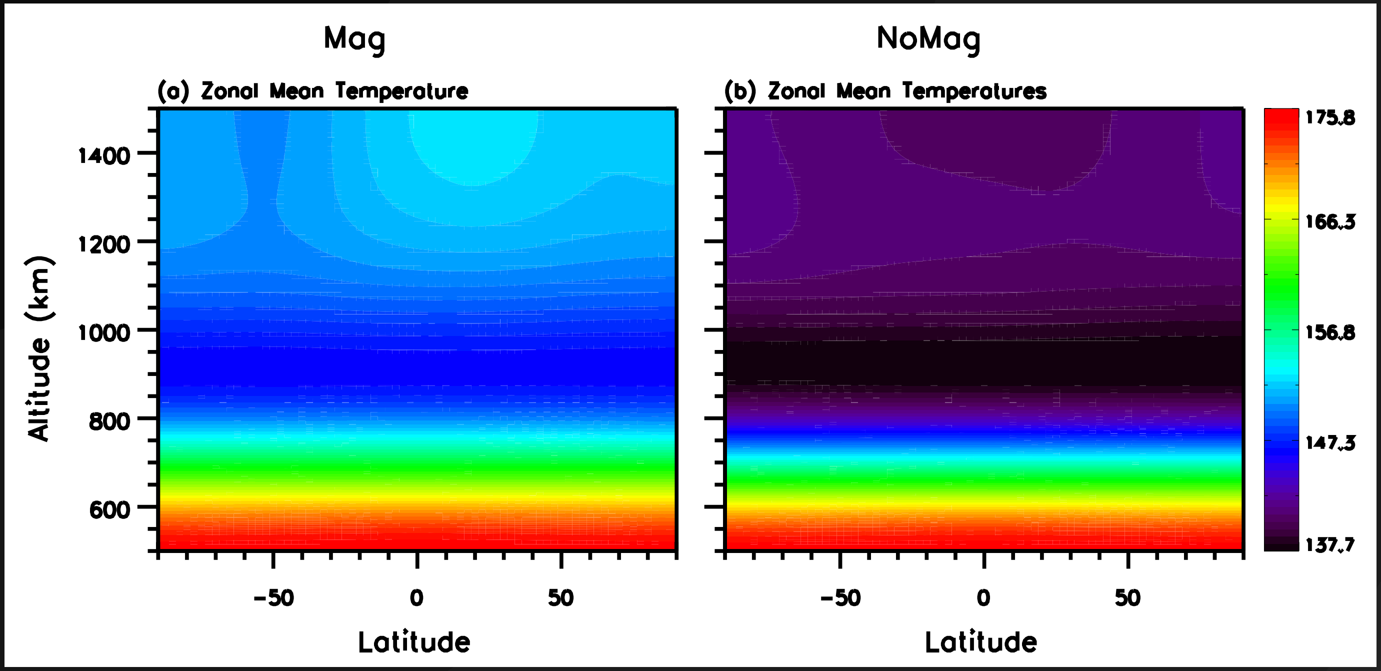
- 3-D T-GITM (black lines) compared with INMS data (red circles and error bars).
- "Fly" through the model along all trajectories between TA-T40 and extract fields.
  - Average them together.
- Upshot: Magnetospheric Heating required to reproduce INMS.
  - During the TA-T40 timeframe.
  - More high energy plasma environment Titan encounters.
  - Paper(s) being submitted to JGR-Planets.
- Other time-frames might reveal different results.

Exobase Temperatures



- Sample exobase temperatures and winds from T-GITM.
- Two observations:
  1. Diurnal variations are muted.
  2. Magnetospheric heating differences are much larger.
- This is consistent with INMS observations (*Westlake et al*. [2011]).

Zonal Mean Temperatures

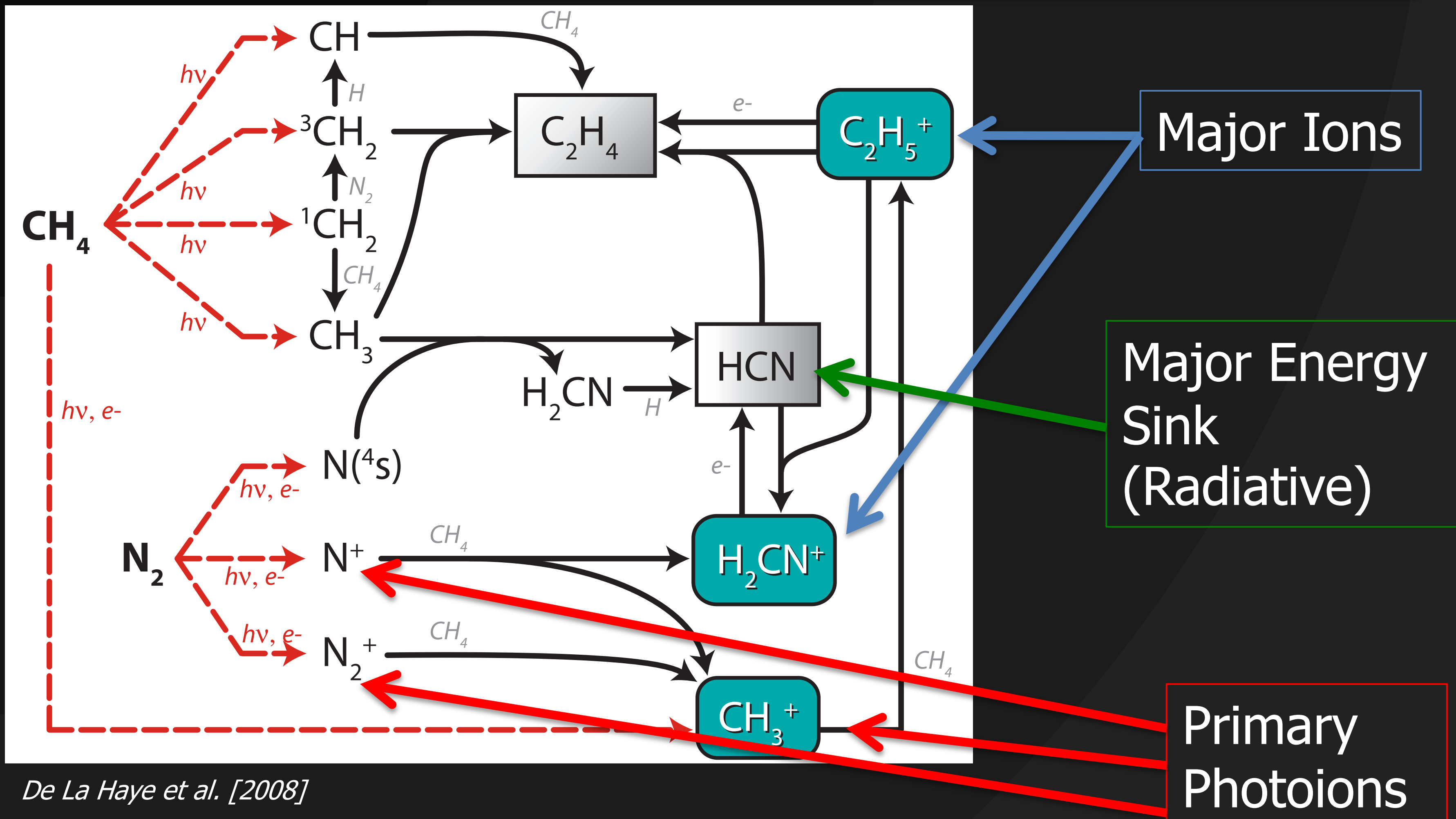


- Zonal average (longitude-averaged) temperatures.
- Lefthand plot has magnetospheric heating and solar EUV/UV.
- Right plot is solar EUV/UV heating only.

Thermosphere and Ionosphere

- The results just presented all hinge upon properly simulating HCN.
  - Has a huge radiative cooling impact on the thermosphere.
- HCN is directly tied into ion-neutral chemistry.
  - Characterizing the ionosphere is very important.
  - Ion chemistry is very complex and potentially tied to dynamics and electron precipitation.
    - *Cravens et al*. [2010], or *Gronoff et al*. [2009a, 2009b]

T-GITM Ion-Neutral Chemistry

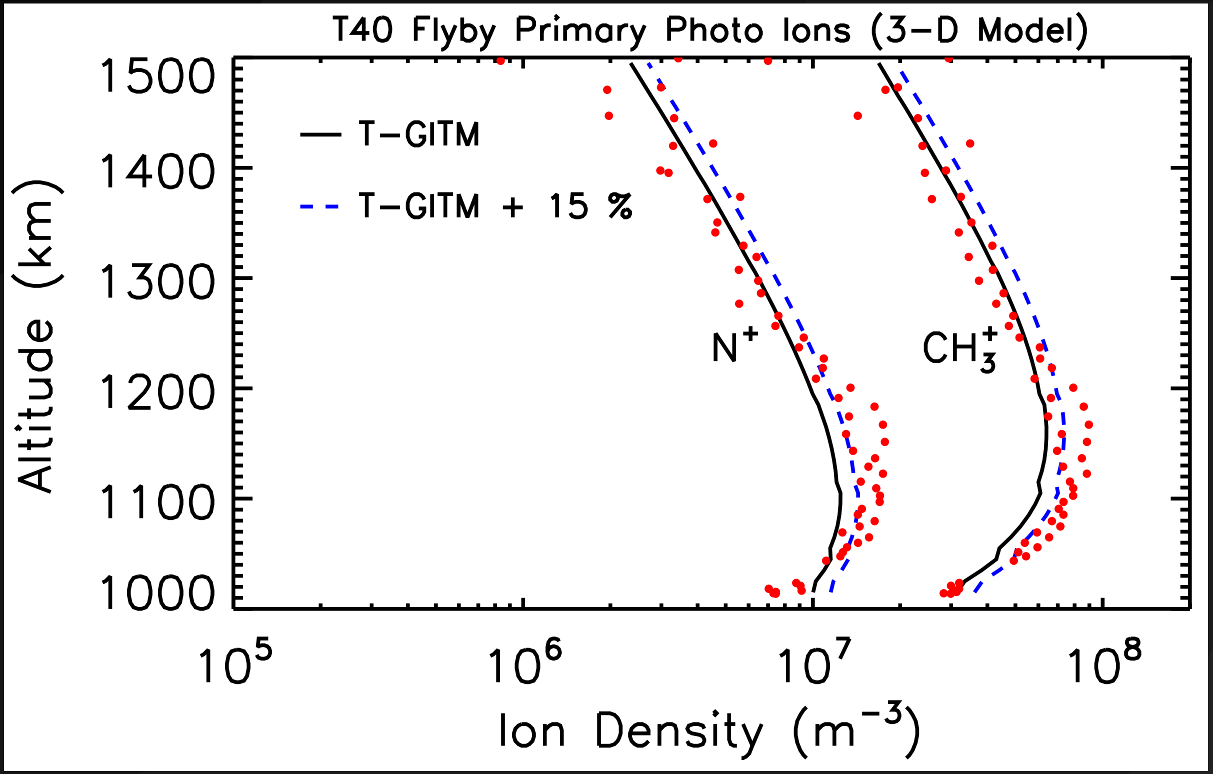


De La Haye et al. [2008]

Approach to the Ionosphere

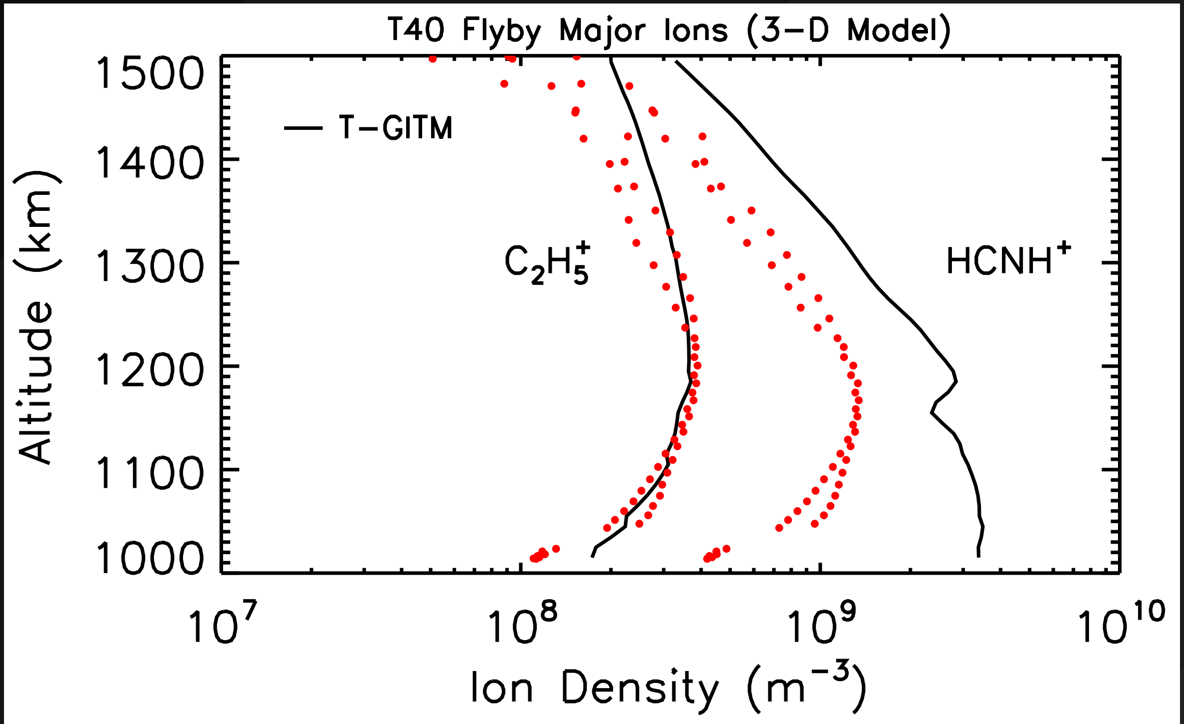
- We need to benchmark the Ionosphere
- Focus on the principle photoion fragments of N_2 and CH_4.
- Then, examine the major ions, which are molecular ions.
  - $C_2H_5^+$ and $HCNH^+$
  - We currently do not carry CH_4^+ or CH_5^+.
- We will consider only solar photons (not e^-).
- Examine a day-side flyby, since we ignore e^- precipitation on the nightside.

Simulated Primary Photoions



- Red circles are INMS T40 (dayside) data.
- Model Fields extracted along T40 flyby latitudes, altitudes and local times (capture SZA effects).

Major Molecular Ions



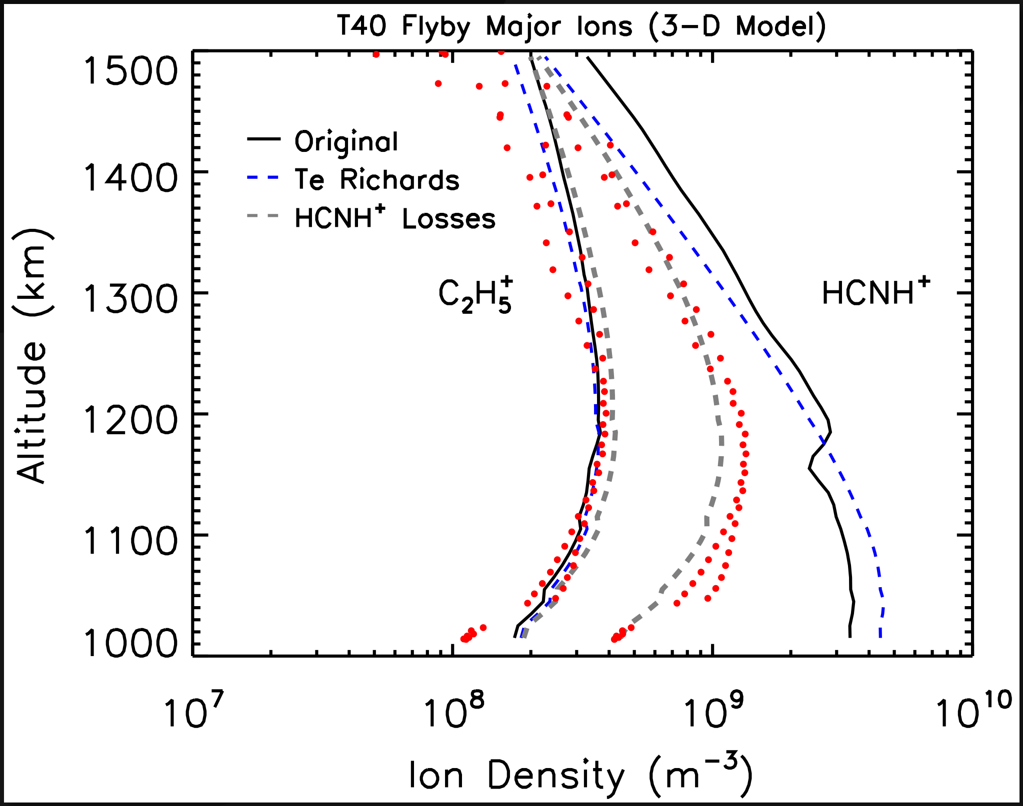
- Reasonable match to $C_2H_5^+$
- Model is too high for $HCNH^+$
  - Total ions are thus too high!
  - Important implications for HCN (major coolant).

Possible Remedies

- Examined in detail by *Westlake et al*. [2011b] (JGR-Planets)

- Suggested the following tests:
  1. Changing T_e from RPWS to one similar to *Richard et al.* [2011] (model).
  2. Adding Additional reactions, such as
     1. $HCNH^+ + C_2H_4 \rightarrow$ Not $HCNH^+$ ($k = 5.0 \times 10^{-10}$ cm^3/s)
  3. Examining Dynamics (Ion flows).

HCNH$^+$ Needs Additional Chemical Losses



Bell et al. [2012c] (in prep.)

- Two tests shown here.
- Blue dashed line is a change in electron temperature
  - enhanced electron recombination rate.
- Grey dashed lines is added chemical losses
  - C_2H_4 + HCNH$^+$ -> not HCNH$^+$
- Our results indicate chemical losses most likely candidate for improving HCNH$^+$ comparisons.
- Ion dynamics do not matter so much.

Ions Discussion

- The 3-D T-GTIM does a reasonable job with primary photo ions
  - N^+, CH_3^+, (N_2^+ swamped by $HCNH^+$)
  - Similar to *Richard et al*. [2011] and *Cravens et al*. [2009]

- Major Ion $C_2H_5^+$ is modeled reasonably well
  - Similar to *Westlake et al*. [2011].

- Some issues with $HCNH^+$
  - Additional chemical losses for $HCNH^+$ missing.
  - Including these chemical losses does reduce the need for magnetospheric heating to reproduce INMS (by ~10%).

Conclusions

- We are capable of modeling the mean state of Titan's Neutral and Ionized Upper Atmosphere from first principles.
- 3-D Titan GITM simulations compare well with INMS observations.
- We find that the magnetosphere is playing a major role in determining the thermal structure above 1000 km.
- There is no apparent need for large escape fluxes of N_2 or CH_4 from Titan's upper atmosphere.

Going Forward

- Next step is to approach Titan as a system.
  - Couple with MHD and Hybrid codes from above (beyond 1500 km).
- Improve radiative transfer in hydrocarbons
  - Need improved chemical calculations of these heavy hydrocarbons.
- Need to include kinetic treatments near the exobase
  - DSMC models of the atmospheric escape.

THANK YOU!