SABER ALGORITHM UPDATE

SABER Software Critical Design Review

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&

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Outline

Review SABER data products

Discuss the challenge of generating these data

Algorithm status

Algorithm roadmap from here to launch and beyond

Summary

SABER MEASUREMENT REQUIREMENTS

The overarching goals of the TIMED mission are

- *Quantify the thermal structure of the 60-180 km region*

- *Understand the energy balance of this region*

These two goals are tightly coupled because it is the energetics which determines the thermal structure

The TIMED region is also unique in that chemistry and the transport of chemical energy plays a crucial role in the energy/thermal balance

The SABER measurements are chosen to:

- *Provide global thermal structure, day and night*

- *Provide key photochemically active species abundances*

- *Provide direct measures of energy gain and loss*

SABER MEASUREMENTS

SABER Measurements	Geophysical Information
CO_2 (15 μm)	Temperature, Radiative Cooling
O_3(9.6 μm)	Ozone, Solar Heating, Radiative Cooling
H_2O (6.7 μm)	Water vapor, Radiative Cooling, Chemistry
NO (5.3 μm)	Radiative Cooling
CO_2(4.3 μm)	Dynamical tracer
OH(1.6 μm)	Chemical heating, chemistry, airglow loss
OH(2.0 μm)	Chemical heating, chemistry, airglow loss
O_2(1.27 μm)	Ozone, solar heating, airglow loss

These measurements enable a virtually complete description of solar heating, radiative cooling, chemical heating, and airglow losses in addition to the thermal structure

SABER DATA PRODUCTS

There are numerous data products that will be derived from the SABER measurements.

Two classes of data products, Routine and Analysis

Routine: Regularly produced

Analysis: Requires additional processing/work/modeling

SABER "Routine" Data Products

- KINETIC TEMPERATURE (T_K)
- OZONE (O_3)
- WATER VAPOR (H_2O)
- EXCITED STATE ABUNDANCES/Volume Emission Rates
  - NO(υ)
  - OH(υ = 7, 8, 9)
  - OH(υ = 3, 4, 5)

- $O_2(^1\Delta)$

SABER DATA PRODUCTS

SABER Analysis Products

- Constituent Abundances:
  - CO_2 (100-160 km)
  - O (80-100 km)
  - H (80-100 km)

- Cooling Rates
  - CO_2(15 μm)
  - NO (5.3 μm)
  - O_3 (9.6 μm)
  - H_2O (6.7 μm and far-infrared)

- Solar Heating Rates
  - O_3 (Hartley, Huggins, Chappuis, and other UV)
  - O_2 (Schumann-Runge, Ly-α, Herzberg, Atmospheric Bands)

CO_2 (near-ir)

SABER DATA PRODUCTS

SABER Analysis Products (continued)

- Chemical Heating Rates

  $H + O_3 \rightarrow OH + O_2$

  $O + O + M \rightarrow O_2 + M$

  $O + O_2 + M \rightarrow O_3 + M$

  $O + OH \rightarrow H + O_2$

  $H + O_2 + M \rightarrow HO_2 + M$

  $O + O_3 \rightarrow O2 + O_2$

  $OH + O_2 \rightarrow HO_2 + O$

- Airglow/Chemiluminescent Emission/Heating Efficiencies

  $O_2(^1\Delta)$ (Hartley band solar heating)

  $OH(\upsilon = 7,8,9)$

  $OH(\upsilon = 3, 4, 5)$

SABER DATA - The Challenge

Ultimately, SABER measures radiation emitted by the atmosphere in 10 narrow spectral intervals as a function of altitude

The challenge is to interpret these measurements in terms of temperature, minor species, and rates of heating and cooling

This interpretation requires an understanding of the physics and chemistry which result in the generation of radiation by infrared active species

All of the SABER measurements in the TIMED core region (60-180 km) are of non-LTE radiative emission

The pertinent radiative transfer equation for SABER limb viewing is

$$R = \int_{\nu_1}^{\nu_2} \int_{x} J_\nu(x) \, \partial\tau_\nu(x) \, d\nu$$

Where J is the source function and $\partial\tau$ is the transmittance gradient

SABER DATA - The Challenge

There are 2 challenges to the interpretation of SABER data:

1. *Understanding the physical, radiative, and chemical processes which result in the non-LTE energy level populations in the SABER-observed emissions and accurately modeling these processes*

These “non-LTE models” are non-trivial to develop and implement

Members of the SABER science team possess comprehensive, *peer-reviewed* “non-LTE” models for each SABER-observed molecule

Challenge is to develop techniques to extract the geophysical information from the radiances using these models

2. *Be able to calculate rapidly and accurately the limb radiance for a specified non-LTE condition*

The RTE above is evaluated numerous times for each single profile of measured radiance

Fast techniques, applicable to non-LTE, have been developed and published

SABER Non-LTE MODEL STATUS

SABER Channel	Geophysical Data	Model
CO_2 (15 μm)	T_K, cooling rate	Lopez-Puertas et al., QJRMS, 1992
Ozone (9.6 μm)	O_3, solar heating, ir cool	Mlynczak and Drayson, JGR, 1990
H_2O (6.7 μm)	H_2O, cooling rate	Lopez-Puertas et al., JGR, 1995
NO(5.3 μm)	NO(υ), cooling rate	Picard et al. (numerous JGR)
CO_2 (4.3 μm)	CO_2 abundance	Lopez-Puertas et al., JGR, 1989
OH (1.6 μm)	H, chemical heating	Mlynczak and Solomon, JGR 1993, 1991
OH (2.0 μm)	H, chemical heating	Mlynczak and Solomon, JGR, 1993, 1991
$O_2(^1\Delta)$ (1.27 μm)	O_3, O, energy loss	Mlynczak et al. , JGR, 1991, 1993

Radiative Transfer Modules (LINEPAK, BANDPAK; Gordley et al; Marshall et al; JQSRT 1994)

JGR: Journal of Geophysical Research
JQSRT: Journal of Quantitative Spectroscopy and Radiative Transfer
QJRMS: Quarterly Journal of the Royal Meteorological Society

SABER ALGORITHMS -- ADDITIONAL NEEDS

Non-LTE models require a priori specification of numerous parameters

- Einstein A coefficients for spontaneous emission
- Einstein B coefficients for absorption
- Collisional quenching rates
- Collisional excitation rates
- Photochemical rates and quantum yields

Virtually all of these rate “constants” are measured in controlled laboratory experiments

Accuracy of SABER data products is directly dependent on accuracy to which the numerous rates are known

Many rates are not well-known and significant improvement is required

We are systematically examining the improvements in kinetics and spectroscopy for each SABER data product and publishing (*GRL*) our requirements

SABER ALGORITHM ADDITIONAL NEEDS

Kinetics and Spectroscopy

- Within the last year, defined kinetics and spectroscopy needs:
  - Ozone (9.6 μm retrieval)
  - Chemical Heating (H + O_3)
  - Water Vapor

These requirements published in Geophysical Research Letters (3 papers in 1998)

Numerous proposals submitted to NSF and NASA to make necessary measurements

Thus, the “plan” is working --

State our needs through formal publication in refereed literature

Tie them to an upcoming spaceflight program

Lab community recognizes funding opportunity and proposes

SABER ALGORITHM STATUS

Routine Products:

Product	Conceptual Approach	Prototype Software	Operational Software	Kinetics Needs/ Error Analysis
T_K	yes	underway	no	underway soon
O_3 (9.6 μm)	yes	yes[a]	underway	yes (*GRL*)
O_3(1.27 μm)	yes	yes	underway	yes (*GRL*)
H_2O	yes	yes	underway	yes (6/98)
Vol. Em. Rates				
NO	yes	yes	no	yes (Laboratory)
OH(1.6 μm)	yes	yes	no	yes (*GRL*)
OH(2.0 μm)	yes	yes	no	yes (*GRL*)
$O_2(^1\Delta)$	yes	yes	no	yes (*GRL*)

Notes:

a) Prototype software for weak-line radiative transfer regime, z > 70 km only

(*GRL*) means publication in Geophysical Research Letters of requirements

(Laboratory) implies new laboratory measurements recently reported

SABER ALGORITHM STATUS

Analysis Products:

Product	Conceptual Approach	Prototype Software	Operational Software	Kinetics Needs/ Error Analysis
Minor species				
CO_2	yes	yes	no	underway
O	yes	no	no	no
H	yes	yes	no	yes
Cooling rates				
CO_2 (15 µm)	yes	yes	no	underway
O_3(9.6 µm)	yes	yes	no	underway
NO (5.3 µm)	yes	no	no	(Laboratory)
H_2O(6.7, far-ir)	yes	yes	no	underway
Solar Heating				
O_3	yes	yes	no	yes
O_2	yes	yes	no	yes
CO_2	yes	yes	no	yes

SABER ALGORITHM STATUS

Analysis Products:

Product	Conceptual Approach	Prototype Software	Operational Software	Kinetics Needs/ Error Analysis
Chemical Heating				
$H + O_3$	yes	yes	no	yes
O + O + M	yes	no	no	no
$O + O_2 + M$	yes	no	no	yes
O + OH	yes	no	no	yes
$H + O_2$	yes	no	no	N.A.
$O + O_3$	yes	no	no	N.A.
$OH + O_2$	yes	no	no	N.A.

Note:

Prototype software for some chemical heating reactions is only a few lines of code once the reactants are known -- e.g., once [H] is derived then heating due to reaction of H and O_2 is very simple to calculate.

SABER ALGORITHMS: Roadmap

Roadmap from now to launch:

- Implement temperature retrieval algorithm -- focus of team effort
- Implement water vapor, ozone, and V.E.R. retrievals in operational software
- Implement Analysis products in operational software as possible (e.g., solar heating, chemical heating, and radiative cooling)
- Prepare for analysis products which require iteration/interaction with numerical models (e.g., Nitric Oxide cooling)

Goal:

Have publications submitted to refereed journals detailing algorithm approaches for *all routine products* before launch

SABER ALGORITHMS: Summary

SABER measurements and data products are sufficient to meet TIMED goals of thermal structure and energy balance

Radiative transfer calculation approaches/techniques for non-LTE are developed

Non-LTE/Statistical Equilibrium Models exist for all SABER channels

All transfer calculation approaches (Non-LTE EGA, and Line-by-Line) and Non-LTE models have been published in the peer-reviewed literature

We have essentially completed error analysis and specification of kinetics needs

Major science team effort now to implement concepts in operational software

The SABER algorithm development is a team effort drawing on the unique, diverse skills of many individuals

Recent SABER-Related Bibliography (since 1994)

Gordley, L.L., B. T. Marshall, and D. A. Chu, LINEPAK: Algorithms for modeling spectral transmittance and radiance, J. Quant. Spectrosc. Radiat. Transfer, 52, 563-580, 1994.

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