

# ***SABER* ALGORITHM UPDATE**

## **SABER Software Critical Design Review**

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# Outline

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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

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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

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## SABER Measurements

CO<sub>2</sub> (15 μm)

O<sub>3</sub>(9.6 μm)

H<sub>2</sub>O (6.7 μm)

NO (5.3 μm)

CO<sub>2</sub>(4.3 μm)

OH(1.6 μm)

OH(2.0 μm)

O<sub>2</sub>(1.27 μm)

## Geophysical Information

Temperature, Radiative Cooling

Ozone, Solar Heating, Radiative Cooling

Water vapor, Radiative Cooling, Chemistry

Radiative Cooling

Dynamical tracer

Chemical heating, chemistry, airglow loss

Chemical heating, chemistry, airglow loss

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

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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

- $NO(v)$

- $OH(v = 7, 8, 9)$

- $OH(v = 3, 4, 5)$

- O<sub>2</sub>(<sup>1</sup>Δ)

# SABER DATA PRODUCTS

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## SABER Analysis Products

- Constituent Abundances:

  - CO<sub>2</sub> (100-160 km)

  - O (80-100 km)

  - H (80-100 km)

- Cooling Rates

  - CO<sub>2</sub>(15 μm)

  - NO (5.3 μm)

  - O<sub>3</sub> (9.6 μm)

  - H<sub>2</sub>O (6.7 μm and far-infrared)

- Solar Heating Rates

  - O<sub>3</sub> (Hartley, Huggins, Chappuis, and other UV)

  - O<sub>2</sub> (Schumann-Runge, Ly-α, Herzberg, Atmospheric Bands)

CO<sub>2</sub> (near-ir)

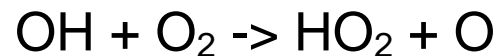
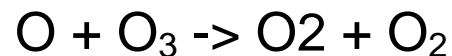
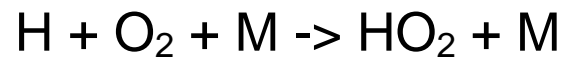
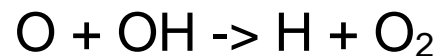
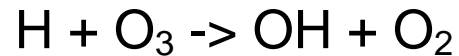


# SABER DATA PRODUCTS

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## SABER Analysis Products (continued)

### - Chemical Heating Rates



### - Airglow/Chemiluminescent Emission/Heating Efficiencies

$\text{O}_2(^1\Delta)$  (Hartley band solar heating)

$\text{OH}(\nu = 7, 8, 9)$

$\text{OH}(\nu = 3, 4, 5)$

## SABER DATA - The Challenge

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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

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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**

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<u>SABER Channel</u>	<u>Geophysical Data</u>	<u>Model</u>
CO <sub>2</sub> (15 μm)	T <sub>K</sub> , cooling rate	Lopez-Puertas et al., QJRMS, 1992
Ozone (9.6 μm)	O <sub>3</sub> , solar heating, ir cool	Mlynczak and Drayson, JGR, 1990
H <sub>2</sub> O (6.7 μm)	H <sub>2</sub> O, cooling rate	Lopez-Puertas et al., JGR, 1995
NO(5.3 μm)	NO( <i>v</i> ), cooling rate	Picard et al. (numerous JGR)
CO <sub>2</sub> (4.3 μm)	CO <sub>2</sub> 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 <sub>2</sub> ( <sup>1</sup> Δ) (1.27 μm)	O <sub>3</sub> , 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

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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

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## *Kinetics and Spectroscopy*

- Within the last year, defined kinetics and spectroscopy needs:
  - Ozone (9.6  $\mu\text{m}$  retrieval)
  - Chemical Heating (H + O<sub>3</sub>)
  - 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

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Routine Products:

<u>Product</u>	<u>Conceptual Approach</u>	<u>Prototype Software</u>	<u>Operational Software</u>	<u>Kinetics Needs/ Error Analysis</u>
T <sub>K</sub>	yes	underway	no	underway soon
O <sub>3</sub> (9.6 μm)	yes	yes <sup>a</sup>	underway	yes ( <i>GRL</i> )
O <sub>3</sub> (1.27 μm)	yes	yes	underway	yes ( <i>GRL</i> )
H <sub>2</sub> O	yes	yes	underway	yes (6/98)
Vol. Em. Rates				
NO	yes	yes	no	yes (Laboratory)
OH(1.6 μm)	yes	yes	no	yes ( <i>GRL</i> )
OH(2.0 μm)	yes	yes	no	yes ( <i>GRL</i> )
O <sub>2</sub> ( <sup>1</sup> Δ)	yes	yes	no	yes ( <i>GRL</i> )

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

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Analysis Products:

<u>Product</u>	<u>Conceptual Approach</u>	<u>Prototype Software</u>	<u>Operational Software</u>	<u>Kinetics Needs/ Error Analysis</u>
Minor species				
CO <sub>2</sub>	yes	yes	no	underway
O	yes	no	no	no
H	yes	yes	no	yes
Cooling rates				
CO <sub>2</sub> (15 μm)	yes	yes	no	underway
O <sub>3</sub> (9.6 μm)	yes	yes	no	underway
NO (5.3 μm)	yes	no	no	(Laboratory)
H <sub>2</sub> O(6.7, far-ir)	yes	yes	no	underway
Solar Heating				
O <sub>3</sub>	yes	yes	no	yes
O <sub>2</sub>	yes	yes	no	yes
CO <sub>2</sub>	yes	yes	no	yes

# SABER ALGORITHM STATUS

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Analysis Products:

<u>Product</u>	<u>Conceptual Approach</u>	<u>Prototype Software</u>	<u>Operational Software</u>	<u>Kinetics Needs/ Error Analysis</u>
Chemical Heating				
H + O <sub>3</sub>	yes	yes	no	yes
O + O + M	yes	no	no	no
O + O <sub>2</sub> + M	yes	no	no	yes
O + OH	yes	no	no	yes
H + O <sub>2</sub>	yes	no	no	N.A.
O + O <sub>3</sub>	yes	no	no	N.A.
OH + O <sub>2</sub>	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<sub>2</sub> is very simple to calculate.

# SABER ALGORITHMS: Roadmap

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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**

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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)

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- 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.
- Lopez-Puertas et al., Evidence for non-LTE in the 15- $\mu\text{m}$  bands of  $\text{CO}_2$  from ISAMS data, *Geophys. Res. Lett.*, 1997
- Lopez-Puertas, M., G. Zaragoza, B. J. Kerridge, and F. W. Taylor, Non-local thermodynamic equilibrium model for  $\text{H}_2\text{O}$  6.3 and 2.7-mm bands in the middle atmosphere, *J. Geophys. Res.*, 100, 9,131-9,147, 1995.
- Marshall, B. T., L. L. Gordley, and D. A. Chu, BANDPAK: Algorithms for modeling broadband transmission and radiance, *J. Quant. Spectrosc. Radiat. Transfer*, 52, 581-599, 1994.
- Mertens, C. J., M. G. Mlynczak, R. R. Garcia, and R. Portmann, A detailed evaluation of the stratospheric heat budget. Part I. Radiative transfer, *J. Geophys. Res.*, submitted, 1998.
- Mlynczak, M. G., D. S. Zaras, and M. Lopez-Puertas, Rapid computation of spectrally integrated non-LTE limb emission, *J. Geophys. Res.*, 99, 25761-25772, 1994.
- Mlynczak, M. G., Energetics of the Middle Atmosphere: Theory and Observation Requirements, *Adv. Space Res.*, 17, 117-126, 1995.
- Mlynczak, M. G., and J. M. Russell III, An overview of the SABER experiment for the TIMED mission, *Optical Remote Sensing of the Atmosphere*, 2, OSA Technical Digest Series, Washington, DC, 5-7, 1995.

## Recent SABER-Related Bibliography (since 1994)

---

- Mlynczak, M. G., and D. S. Olander, On the utility of the molecular oxygen dayglow as proxies for middle atmospheric ozone, *Geophys. Res. Lett.*, 22, 1377-1380, 1995.
- Mlynczak, M. G., and D. J. Nesbitt, The Einstein coefficient for spontaneous emission of the O<sub>2</sub>(a<sup>1</sup>D<sub>g</sub>) state, *Geophys. Res. Lett.*, 22, 1381-1384, 1995.
- Mlynczak, M. G., and B. T. Marshall, A reexamination of the role of the A, B, and g bands in the middle atmosphere heat budget, *Geophys. Res. Lett.*, 23, 657-660, 1996.
- Mlynczak, M.G., Energetics of the mesosphere and lower thermosphere and the SABER Experiment, *Adv. Space. Res.*, 20, 1177-1183, 1997.
- Mlynczak, M. G., and D.K. Zhou, Kinetic and spectroscopic requirements for the measurement of ozone at 9.6 mm under non-LTE conditions, *Geophys. Res. Lett.*, 25, 639-642, 1998.
- Mlynczak, M.G., D.K. Zhou, and S.M. Adler-Golden, Kinetic and spectroscopic requirements for the inference of chemical heating rates and atomic hydrogen densities from OH Meinel band measurements, *Geophys. Res. Lett.*, 25, 647-650, 1998.
- Mlynczak, M. G., C. Mertens, R. R. Garcia, and R. Portmann, A detailed evaluation of the stratospheric heat budget. Part II. Global radiation balance and diabatic circulations, *J. Geophys. Res.*, submitted, 1998.
- Mlynczak, M. G., D. K. Zhou, M. Lopez-Puertas, and G. Zaragoza, Kinetic requirements for the measurement of water vapor at 6.8 mm under non-LTE conditions, *Geophys. Res. Lett.*, submitted, 1998.

## Recent SABER-Related Bibliography (since 1994)

---

Russell, J. M., M. G. Mlynczak, and L.L. Gordley, Overview of the Sounding of the Atmosphere using Broadband Emission Radiometry (SABER) Experiment for the TIMED Mission, in *Optical Spectroscopic Techniques and Instrumentation for Atmospheric and Space Research*, Jinxue Wang, P.B. Hays, Editors, Proc. SPIE 2266, 406-415, 1994.

Zaragoza, G., M. Lopez-Puertas, A. Lambert, J. J. Remedios, and F. W. Taylor, Non-local thermodynamic equilibrium in the H<sub>2</sub>O 6.9 mm emission as measured by the Improved Stratospheric and Mesospheric Sounder, *J. Geophys. Res.*, submitted, 1998.

Zhou, D.K., M. G. Mlynczak, M. Lopez-Puertas, and G. Zaragoza, Evidence for non-LTE in mesospheric water vapor as determined from spectrally-resolved emissions measured by CIRRIS-1A, *Geophys. Res. Lett.*, submitted, 1998.

Zhou, D. K., M. G. Mlynczak, G.E. Bingham, J. O. Wise, and R. M. Nadile, CIRRIS-1A limb spectral measurements of mesospheric 9.6 mm airglow and ozone, *Geophys. Res. Lett.*, 25, 643-646, 1998.