PROCEEDINGS OF THE 14TH ANNUAL REVIEW CONFERENCE ON ATMOSPHERIC TRANSMISSION MODELS, 11-12 JUNE 1991

EDITORS:
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F. X. KNEIZYS

26 FEBRUARY 1992

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PHILLIPS LABORATORY
AIR FORCE SYSTEMS COMMAND
HANSCOM AIR FORCE BASE, MASSACHUSETTS 01731-5000
"This technical report has been reviewed and is approved for publication"

William A. Blumberg, Chief
Simulation Branch
Optical Environment Division

ALAN D. BLACKBURN, Col, USAF, Director
Optical Environment Division

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L.W. Abreu and F.X. Kneizys

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- Atmospheric Transmittance
- Aerosols
- Atmospheric Propagation
- Clouds
- Radiative Transfer
- Optical Turbulence
- Molecular Absorption
- Ultraviolet
- Infrared
- Spectroscopy

Abstract:
Contains the viewgraphs and other materials for the 42 papers presented at the Fourteenth Annual Review Conference on Atmospheric Transmission Models held at the Geophysics Directorate, Phillips Laboratory (AFSC), Hanscom AFB, MA 11-12 June 1991
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INTRODUCTION

The Fourteenth DoD Tri-Service Review Conference on Atmospheric Transmission Models was held at the Geophysics Directorate, Hanscom AFB, Massachusetts on 11-12 June 1991. The purpose of the meeting was to review progress in the modeling of radiation propagating through the earth's atmosphere, identify deficiencies in these models, and make recommendations for improvements.

Approximately 140 scientists and engineers, representing DoD, other government agencies, industry, and the academic community were in attendance. The agenda consisted of forty two papers with sessions on aerosols and clouds, atmospheric propagation models, measurements and models and an extended Topical session on spectral line shapes hosted by Michael L. Hoke which included invited papers and contributed papers.

This proceedings volume summarizes the technical presentations at the conference. The main part of the report consists of the abstracts and copies of the viewgraphs or slides and other material as provided by the authors for the presentations. Preceding the viewgraphs for each session is a commentary prepared by the co-chairpersons on each presentation within that session. The Appendix includes the original call for papers and invitation to the meeting, a copy of the Agenda for the meeting, a list of the attendees, and an author index.

A special thanks is extended to Ronald G. Isaacs, Betty Stenhouse and Atmospheric and Environmental Research, Inc.

Francis X. Kneizys
Leonard W. Abreu
KEYNOTE:  Col. Grant Aufderhaar
USAF (OUSDA)
Pentagon
Washington, DC
DEFENSE CRITICAL TECHNOLOGIES PLAN
SUBMITTED ANNUALLY BY THE
DEPARTMENT OF DEFENSE
IN CONSULTATION WITH THE
DEPARTMENT OF ENERGY

TO THE

COMMITEES ON ARMED SERVICES
UNITED STATES CONGRESS

CRITICAL TECHNOLOGIES PLAN

HISTORICAL CONTEXT

• QUALITATIVE SUPERIORITY PROVIDES UNDERPINNING TO
  NATIONAL SECURITY

• U.S. SUCCESSFUL IN DOING SO FOR FORTY YEARS (B-52,
  MINUTEMAN, POLARIS, U-2, AIRCRAFT TURBINES, SENSORS,
  ACCURACY IN TARGETING, SATELLITES, ETC.)

RECENT TRENDS

• DECLINE IN FUNDING FOR TECHNOLOGY BASE SINCE 1965:
  — FEWER $ FOR BUDGET CATEGORIES 6.1, 6.2, 6.3A

CONSEQUENCES

• U.S. TECHNOLOGY BASE IS RUSTING
  — CONSISTS OF 80's RESEARCH AND EARLY 80's TECHNOLOGY

• RADICALLY NEW CONCEPTS ARE DIFFICULT TO IMPLEMENT
  — REGARDLESS OF MERIT
  — NOT ENOUGH $ TO DEMONSTRATE NEW TECHNOLOGIES

• EXPECTATIONS ARE UNSUSTAINABLE
CRITICAL TECHNOLOGIES PLAN

DEFENSE PLANNING GUIDANCE REQUIRES CONTINUED QUALITATIVE SUPERIORITY...

... AND CONTINUED QUALITATIVE SUPERIORITY REQUIRES ARRESTING EROSION OF THE TECHNOLOGY BASE THROUGH:

- CLEAR REALISTIC LONG-TERM GOALS
- A HEALTHY INFRASTRUCTURE
- ADEQUATE RESOURCES
  - TO DEVELOP NEW TECHNOLOGIES (6.1, 6.2)
  - TO DEMONSTRATE NEW SYSTEMS CAPABILITY USING NEW TECHNOLOGIES (6.3A)
- AN EFFICIENT MECHANISM FOR TURNING CONCEPTS INTO SYSTEMS
  - THAT ARE CAPABLE OF MEETING THE LONG-TERM GOALS

CONGRESSIONAL MANDATE

- PL 101-189

"THE SECRETARY OF DEFENSE ... SHALL SUBMIT ... AN ANNUAL PLAN FOR DEVELOPING THE TECHNOLOGIES CONSIDERED ... MOST CRITICAL TO INSURING THE LONG-TERM QUALITATIVE SUPERIORITY OF UNITED STATES WEAPON SYSTEMS."
CRITICAL TECHNOLOGIES PLAN

PRINCIPAL FEATURES OF THE PLAN

- LINKS CRITICAL TECHNOLOGIES TO DOD SCIENCE AND TECHNOLOGY STRATEGY
- SELECTS 20 CRITICAL TECHNOLOGIES
- PRIORITIZES THEM
- PROVIDES FUNDING ESTIMATES
- INDICATES MILESTONES TO 2005
- PROVIDES INTERNATIONAL COMPARISONS
- INCLUDES INDUSTRIAL BASE AND MANUFACTURING ISSUES

CRITICAL TECHNOLOGIES PLAN

ADDITIONAL CONSIDERATIONS FOR THE FY 1990 PLAN

- BROADER CONGRESSIONAL TASKING
- INCREASED DISCUSSION OF MANUFACTURING ISSUES
- NEW SELECTION CRITERIA
  - (INCLUDES: STRENGTHENING THE INDUSTRIAL BASE)
- FUNDING SHOWN OVER A DECADE (NOT JUST ONE YEAR)
- CRITICAL TECHNOLOGIES PRIORITIZED
- INTELLECTUAL CONSOLIDATION OF SOME CRITICAL TECHNOLOGIES
  - EMPHASIZING TECHNOLOGY RATHER THAN NEED
  - COMBINING CLOSELY RELATED TECHNOLOGIES

"SEC.801. ANNUAL DEFENSE CRITICAL TECHNOLOGIES PLAN

(A) INCREASED INFORMATION RELATING TO FUNDING ... 

(3) IDENTIFY EACH PROGRAM ELEMENT ...

FOR WHICH FUNDS ARE BUDGETED FOR THE SUPPORT OF THE DEVELOPMENT OF ANY CRITICAL TECHNOLOGY IDENTIFIED IN THE PLAN; AND

(4) FOR EACH SUCH ELEMENT --

(A) SPECIFY THE AMOUNT [IN FY92] INCLUDED FOR EACH CRITICAL TECHNOLOGY COVERED BY THE PROGRAM ELEMENT ... [AND COMPARE] ... WITH THE AMOUNT ... FOR THE [PRECEDING] FISCAL YEAR [FY91]..."
CRITICAL TECHNOLOGIES PLAN

THE PARTICIPANTS

STEERING COMMITTEE: SENIOR S&T MANAGERS FROM DOD, SERVICES, DOE

WORKING GROUP: OSD (CHAIRMANSHIP)
ARMY
NAVY
AIR FORCE
DARPA
DIA
DNA
SDIO
JCS

DOE HEADQUARTERS
DOE NATIONAL LABORATORIES:
LAWRENCE LIVERMORE
LOS ALAMOS
SANDIA

CRITICAL TECHNOLOGIES PLAN

SUBJECTS ADDRESSED IN THE REPORT

- DESCRIPTION OF THE TECHNOLOGY
- PAYOFF
- S&T PROGRAMS
- RELATED MANUFACTURING CAPABILITY
- R&D IN THE UNITED STATES
- INTERNATIONAL ASSESSMENT
LIST OF DEFENSE CRITICAL TECHNOLOGIES

- SEMICONDUCTOR MATERIALS AND MICROELECTRONIC CIRCUITS
- SOFTWARE PRODUCIBILITY
- PARALLEL COMPUTER ARCHITECTURES
- MACHINE INTELLIGENCE/ROBOTICS
- SIMULATION AND MODELING
- PHOTONICS
- SENSITIVE RADARS
- PASSIVE SENSORS
- SIGNAL PROCESSING
- SIGNATURE CONTROL
- WEAPON SYSTEM ENVIRONMENT
- DATA FUSION
- COMPUTATIONAL FLUID DYNAMICS
- AIR-BREATHING PROPULSION
- PULSED POWER
- HYPERVERSPEED PROJECTILES
- HIGH ENERGY DENSITY MATERIALS
- COMPOSITE MATERIALS
- SUPERCONDUCTIVITY
- BIOTECHNOLOGY MATERIALS AND PROCESSES
- FLEXIBLE MANUFACTURING

CRITICAL TECHNOLOGIES PLAN

TECHNOLOGY OBJECTIVES

- SEMICONDUCTOR MATERIALS AND MICROELECTRONIC CIRCUITS:
  — HIGH-SPEED COMPUTING AND SIGNAL PROCESSING, AUTOMATIC CONTROL, SENSITIVE RECEIVERS, MILLIMETER WAVE RADAR, PHOTONICS
- SOFTWARE PRODUCIBILITY:
  — AFFORDABLE, TRUSTED SOFTWARE, AUTOMATIC SOFTWARE GENERATION, REUSABLE SOFTWARE
- PARALLEL COMPUTER ARCHITECTURES:
  — ULTRA-HIGH-SPEED COMPUTING
- MACHINE INTELLIGENCE AND ROBOTICS:
  — BUILD HUMAN INTELLIGENCE INTO MECHANICAL DEVICES, MANUFACTURING, MAINTENANCE
- SIMULATION AND MODELING:
  — TESTING CONCEPTS AND DESIGNS WITHOUT EXPENSIVE REPLICA, TRAINING FOR COMPLEX MILITARY SCENARIOS
- PHOTONICS:
  — ULTRA-HIGH-DENSITY MEMORIES AND HIGH-VOLUME, HIGH-SPEED INFORMATION PROCESSING
- SENSITIVE RADARS:
  — NON-COOPERATIVE TARGET IDENTIFICATION, DETECTION OF LOW-OBSERVABLE TARGETS
CRITICAL TECHNOLOGIES PLAN

TECHNOLOGY OBJECTIVES (CONT.)

• PASSIVE SENSORS:
  — SILENT SENSING OF TARGETS OR ENVIRONMENT, MONITORING EQUIPMENT (CONDITION SENSING)

• SIGNAL PROCESSING:
  — PROCESSING SIGNALS FOR INFORMATION EXTRACTION, AUTOMATIC TARGET DETECTION/TRACKING/CLASSIFICATION/RECOGNITION

• SIGNATURE CONTROL:
  — CONTROLLING PLATFORM OR WEAPON SIGNATURES (RADAR, OPTICAL, ACOUSTIC, ETC.) TO ENHANCE THEIR SURVIVABILITY

• WEAPON SYSTEM ENVIRONMENT:
  — UNDERSTANDING OR PREDICTING THE BEHAVIOR OF THE ENVIRONMENT TO ENHANCE WEAPON EFFECTIVENESS

• DATA FUSION:
  — COMBINING AND INTERPRETING DATA FROM SEVERAL SOURCES AND PRESENTING IT IN A CONVENIENT FORM TO THE HUMAN OPERATOR

• COMPUTATIONAL FLUID DYNAMICS:
  — MODELING OF COMPLEX FLUID FLOW TO MAKE DEPENDABLE PREDICTIONS BY COMPUTING, THUS OBVIATING EXPENSIVE FACILITIES AND EXPERIMENTS

• AIR BREATHING PROPULSION:
  — LIGHT-WEIGHT, FUEL EFFICIENT ENGINES

• PULSED POWER:
  — COMPACT, LIGHT-WEIGHT, LOW-VOLUME DEVICES FOR HIGH-POWER MICROWAVES, HIGH-ENERGY LASERS, ELECTROTHERMAL GUNS, RADARS, ELECTROMAGNETIC LAUNCHERS, PARTICLE BEAMS

• HYPERVELOCITY PROJECTILES:
  — TO PENETRATE HARDENED TARGETS

• HIGH ENERGY DENSITY MATERIALS:
  — SAFE, TRANSPORTABLE, EFFICIENT ENERGETIC MATERIALS FOR EXPLOSIVES AND PROPELLANTS

• COMPOSITE MATERIALS:
  — HIGH-TEMPERATURE, HIGH-STRENGTH, LIGHT-WEIGHT COMPOSITE MATERIALS FOR AEROSPACE APPLICATIONS

• SUPERCONDUCTIVITY:
  — FABRICATION AND EXPLOITATION OF SUPERCONDUCTING MATERIALS

• BIOTECHNOLOGY:
  — SYSTEMATIC APPLICATION OF BIOLOGY IN MILITARY ENGINEERING OR MEDICINE
DEFENSE CRITICAL TECHNOLOGIES
PRIORITIZED IN THREE GROUPS
(FY92 FUNDING ESTIMATES FOR S&T PROGRAMS IN $M)

A
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- FLEXIBLE MANUFACTURING

NOTE: TECHNOLOGIES ARE LISTED IN ALPHABETICAL ORDER WITHIN EACH GROUP.
CRITICAL TECHNOLOGIES PLAN

CAVEATS

- CRITICAL TECHNOLOGIES ARE NOT THE ONLY IMPORTANT TECHNOLOGIES
  - THEY DO NOT EXIST IN ISOLATION
  - THERE ARE OTHER IMPORTANT TECHNOLOGIES
  - WHICH ARE DESCRIBED IN THE DOD S&T STRATEGY

- THEY ARE NOT TO BE CONFUSED WITH THE
  - "MILITARILY CRITICAL TECHNOLOGIES LIST" USED FOR EXPORT CONTROL PURPOSES

- FUNDING ESTIMATES ARE JUST THAT, NOT BUDGET NUMBERS

- PRIORITY GROUPINGS SHOULD NOT BE OVEREMPHASIZED

FOREIGN TECHNOLOGICAL CAPABILITIES

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<th>Critical Technologies</th>
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### FOREIGN TECHNOLOGICAL CAPABILITIES (CONT.)

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Session 1

Summary of the Session on Aerosols and Clouds

The session on Aerosols and Clouds included 7 papers. The first paper by Zardecki (Science & Technology Corp.) described the Boundary Layer Illumination Radiation Balance (BLIRB) model, which they are developing for the Army Atmospheric Sciences Laboratory (ASL), in support of the BTI/SWOE program. The model will calculate the direct and scattered sunlight reaching the ground through an atmosphere containing a 3-dimensional distribution of clouds and aerosols. The model, which is based on a modified version of LOWTRAN, includes some interactions between individual clouds, such as partial shadowing of the direct sunlight by an adjacent cloud.

There were two papers on cirrus clouds. The first of these by Cornette & Shanks (Photon Research Associates) reviewed the literature on modeling transmission through cirrus clouds. It provided a reasonable summary of the current research work. Kreiss & Vik (Horizon Technology Inc.) described the ICECLOUD cirrus transmittance model they are developing for AF Wright Labs as part of the IASPM (IR Atmospherics & Signature Prediction Model) project. This model is largely based on the Liou, Heymsfield et al. model in Applied Optics last May and presented at this meeting two years ago.

There were several papers on atmospheric aerosols and their effects on radiation. Volz (PL) showed that his observations of the brightness of the solar aureole are well correlated with the presence of large dust and pollen particles (5 to 50 μm) in the atmosphere. This aureole brightness has shown a steady decrease over the past twelve years, implying a corresponding decrease in the large aerosol particles in the atmosphere.

Rosen (LLNL) presented preliminary results on modeling the sensitivity of radiation in the atmosphere to different aerosol conditions using LOWTRAN. This work is being done in support of DOE's Atmospheric Radiation Measurements (ARM) program.

Hummel et al. (SPARTA, Inc.) described version 2 of the Lidar backscatter simulation computer code they developed for PL/OPA, named BACKSCAT. This code is written to run stand alone on a PC using the standard LOWTRAN aerosol and cirrus models, which are built in, and external molecular absorption profiles for the lidar wavelength (such as calculated by FASCODE). However, the scientific portion was written in FORTRAN, so it could be easily modified to be directly incorporated into FASCODE, or to run on other computers.

Gathman (NOSC) described the current status of the Navy Ocean Vertical Aerosol Model (NOVAM). This model describes the vertical structure of the optical IR properties of the atmospheric aerosols in the boundary layer above the ocean surface. It uses as input, the surface meteorological conditions and radiosonde profiles. The version of the Navy aerosol model which is currently implemented in LOWTRAN effectively applies the surface values of the NOVAM optical/IR properties to the entire boundary layer.
BOUNDARY LAYER ILLUMINATION RADIATION BALANCE MODEL: BLIRB

A. Zardecki
Science and Technology Corporation, 555 Telshor Blvd., Suite 200, Las Cruces, NM 88001

BLIRB provides direct and diffuse solar insolation at the earth's surface in the spectral range 0.4 to 12 \( \mu \text{m} \). The model is an extension of LOWTRAN 7 to 3-D cloud and aerosol distributions in the lower 5 km of the atmosphere. The propagation of radiation through clouds is formulated by a variant of the adding method, supplemented by a stochastic ray tracing algorithm to model the penumbra effect. With a spectral resolution of 20 cm\(^{-1}\), the spatial mesh can reach the size of 40X40X40 grid points in a physical volume whose extent is specified by the user. The full AFGL aerosol data base, including 40 boundary layer aerosol models, can be combined with six model atmospheres and five season-dependent visual range options. LOWTRAN 7 supplies the gaseous transmission to BLIRB, which offers four cloud options including cloud-free, horizontally homogeneous clouds, rectangular clouds, and a Cloud Scene Simulation prototype model developed by TASC.
Boundary Illumination Radiation Balance Model: BLIRB

A. Zardecki, R. Davis, B. Rappaport
Science & Technology Corporation
Las Cruces, New Mexico

A. Wetmore, J. Martin
Atmospheric Sciences Laboratory
White Sands Missile Range, NM

Annual Review Atmos. Transmission Models 1991

Boundary Illumination Radiation Balance Model: BLIRB

- Cloud Options
- Radiative transfer through 3-D clouds
- Atmospheric/aerosol data base
- Example of computation

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BLIRB: Cloud Options

- Cloud-free, aerosol loaded atmosphere
- Horizontally homogeneous clouds: cloudiness
- Rectangular clouds: composition
- Clouds Scene Simulation Model - TASC

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BLIRB: Radiative Transfer through 3-D Clouds

- Two-stream approximation: Coakley-Chylek 1975
- Doubling method for diffuse radiation
- IR radiation: average flux
- Stochastic ray tracing: penumbra effect

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Two-Stream Approximation

Reflection and transmission functions

\[ R(\mu) = \frac{(Q + 1)(Q - 1)[E - E^{-1}]}{(Q + 1)^2 E - (Q - 1)^2 E^{-1}} \]

\[ T(\mu) = \frac{4Q}{(Q + 1)^2 E - (Q - 1)^2 E^{-1}} \]

where

\[ E = \exp(\alpha \tau / \mu) \]

\[ Q = \frac{[1 - \omega_0 + 2 \omega_0 \beta(\mu)]^{1/2} [1 - \omega_0]^{1/2}}{[1 - \omega_0]^{1/2}} \]

\[ \alpha = [1 - \omega_0 + 2 \omega_0 \beta(\mu)]^{1/2} [1 - \omega_0]^{1/2} \]

Adding Method, Lacis & Hansen 1974

Let

\[ S = \frac{R_1 R_2}{1 - R_1 R_2} \]

then transmission & reflection between layers

\[ D = T_1 + ST_1 + S e^{-\tau_1 / \mu} \]

\[ U = R_2 D + R_2 e^{-\tau_1 / \mu} \]

Diffuse reflection and transmission

\[ R_{12} = R_1 + e^{-\tau_1 / \mu} U + T_1 U \]

\[ T_{12} = e^{-\tau_2 / \mu} D + T_2 e^{-\tau_1 / \mu} + T_2 D \]
Infrared Radiation

Monochromatic emissivity

\[ \epsilon(\nu) = 1 - \exp(-\sigma a z), \]

Flux transmissivity

\[ t_F(\nu) = \frac{\int_0^1 \exp(-\sigma a z/\mu) \mu \, d\mu}{\int_0^1 \mu \, d\mu} \]

\[ t_F(\nu) = e^{-\tau_a}(1 - \tau_a) + \tau_a^2 E_1(\tau_a) \]

where

\[ E_1(x) = \int_{x}^{\infty} s^{-1} \exp(-s) \, ds \]

Average IR flux, w/o scattering

\[ F \downarrow (\nu) = \int_{t_F}^1 B(\nu, T) \, dt_F \]

BLIRB: Stochastic Ray Tracing

- Random directions around the normal to earth’s surface
Angular Spread = 5 deg

Angular Spread = 15 deg
Angular Spread = 30 deg

Angular Spread = 45 deg
BLIRB: AFGL Data Base

- Four layers with different aerosol types
- Rural, urban, maritime, tropospheric aerosols
- RH between 0 and 99%
- Only first two (up to 5km) layers used by BLIRB

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BLIRB: Solar Radiation and Model Atmospheres

- Incident radiation: LOWTRAN 7/numerical fit
- Sky radiance - additional source
- Six temperature profiles
- Gaseous absorption from LOWTRAN 7

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BLIRB: Rectangular Clouds

- Regions: ID and bounding coordinates
- Fine mesh structure: MHX(l), XMS(l)
- Material: a mixture of up to 3 aerosols
- Assignment of materials to regions
- PFNDAT phase function data base

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BLIRB: Surface Albedo

- Areas: ID and bounding coordinates
- Albedo: ID and value from input file
- Albedo: tabulated, wavelength-independent
- Spectral albedo arrays pending realistic data

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BLIRB: Structure of the Code

![Diagram of the code structure]

BLIRB: Examples of Computation

- Physical region w. Water Cloud 2x2x1 km
  - Visible radiation
  - Stochastic ray tracing: 10 rays
  - Surface albedo: 0.2, 0.4

- Nonuniform mesh
  - Two rectangular clouds
  - Cloud region: 10 mesh points/km
  - Background region: 2 mesh points/km
BLURB: Input File

WAVL 0.55
VIS 1.0
BLIRB
MDL1  22.0000  6.0000  2.0000  0.0000  1.0000
MDL2  1.0000  292.0000 -1.0000  10.0000  0.0000
AREA  0.0000  5.0000  0.0000  4.0000  1.0000
AREA  3.0000  4.0000  2.0000  3.0000  2.0000
REGN  0.0000  5.0000  0.0000  4.0000  0.0000  5.0000  1.0000
REGN  1.0000  3.0000  1.0000  3.0000  3.0000  4.0000  2.0000
MEX  10.0000  5.0000
MESY  08.0000  4.0000
MESZ  10.0000  5.0000
ALBD  1.0000  0.2000
ALBD  2.0000  0.4000
MTRL  1.0000  0.1000  5.0000  0.1000  3.0000
MTTL -2.0000  3.0000  5.0000  0.1000
CLDS  2.0000  1.0000  1.0000
SUN  85.0000  000.0000  1.0000  1.0000
WAVN  18900.00  18940.00  20.0
RECL  1.0000
DONE
END
STOP
BLIRB: Conclusions

- Integrates clouds, aerosols, and gas absorption
- Direct and diffuse radiation 0.4 - 12 micro-m
- RT based on adding method and ray tracing
- Mesh 40x40x40 grid points
- AFGL data base for background aerosols
- Four cloud models implemented

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RELATIONS BETWEEN GIANT AEROSOLS NEAR THE SURFACE AND SOLAR AUREOLE BRIGHTNESS

F.E. Volz
Geophysics Directorate, Phillips Laboratory, Hanscom Air Force Base, MA 01731-5000

Observations of the sky brightness at the edge of the sun (aureole) to the west of Boston have shown a gradual decline since about 1979. The number of giant dust particles (with radii from 5 to 50 μm) suspended in the mixing layer at noontime appears to have decreased by more than a factor of ten. To correlate dust and pollen concentrations near the ground with simultaneous aureole data, those particles were collected by rotating impactor for over one year. Typical scattering functions for size distributions presented in the literature were calculated both for a point source and the sun; small-angle brightness of the latter is considerably lower.
BASIS OF METHOD:
SKY BRIGHTNESS AT SUN'S EDGE (SOLAR AUREOLE), which is governed by particles 3 to 100 microns in size.
AUREOLE BRIGHTNESS is measured by neutral-density filter needed to suppress glare.
OBSERVATIONS at AFGL and at home (Lexington).
Probably the only continuous data base existing.

AIRBORNE GIANT AEROSOLS - STRONG DECLINE

1988-89 TRENDS, GEOM. MEAN
THE COMPUTATION OF RADIATIVE TRANSFER THROUGH THE ATMOSPHERE INCORPORATING VARIOUS AEROSOL SCENARIOS*

L.C. Rosen
University of California, Lawrence Livermore National Laboratory, Atmospheric & Geophysical Sciences Division, Livermore, CA 94550

The Atmospheric and Geophysical Sciences Division at the Lawrence Livermore National Laboratory is participating in the Atmospheric Research Measurements (ARM) Program. In order to evaluate radiative measurements affected by aerosol environments, calculations are performed utilizing various aerosol scenarios. Mie calculations are done employing appropriate indices of refraction associated with aerosol constituents to yield aerosol extinction coefficients and asymmetry parameters. These results are integrated over aerosol size distributions and are used as data input to the LOWTRAN 7 code. The MIE calculations and integration technique are discussed. The radiative transfer results computed from the LOWTRAN 7 code are compared for the aerosol scenarios. The importance of differing aerosol contributions is discussed.

*Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under Contract No. W-7405-ENG-48.
The Computation of Radiative Transfer through the Atmosphere Incorporating Various Aerosol Scenarios

June 11, 1991

L. C. Rosen
Atmospheric & Geophysical Sciences Division
University of California
Lawrence Livermore National Laboratory

Goals

- Develop a capability within the Atmospheric & Geophysical Sciences Division, Lawrence Livermore National Laboratory

- Advise Atmospheric Radiation Measurement (ARM) Program as to the importance of aerosols to measurement plan
Computational Procedure

For a Given Aerosol Scenario

- Calculate extinction and scattering coefficients, asymmetry parameters from MIE code.

- Integrate extinction and scattering coefficients, asymmetry parameters over size distributions in quadrature code.

- Input averaged extinction, absorption coefficients asymmetry parameters into LOWTRAN7 code to yield radiances and atmospheric transmittances.

MIE Code

- Input indices of refraction

- Output of extinction and scattering coefficients, asymmetry parameters, extinction and scattering efficiency factors.

Quadrature Code

- Input aerosol size distributions, extinction and scattering coefficients, asymmetry parameters, scattering efficiency factors, frequency.

- Output of aerosol extinction and absorption coefficients, asymmetry parameters as a function of frequency.
The ICRCCM and other GCM intercomparison programs have highlighted an important area of scientific need associated with the understanding and prediction of global climate change. From the findings of those programs, the following scientific requirements emerge as the most critical:

- A quantitative description of the radiative energy balance profile under important physical circumstances must be developed. The descriptions must come from field measurements.
- The processes controlling the radiative balance must be identified and investigated. Validation must come from a direct, comprehensive comparison of field observations with detailed calculations of the radiation field and its cloud and aerosol interactions.
- The knowledge necessary to improve parameterizations of radiative properties of the atmosphere used in GCMs must be developed. This requires intensive measurements at a variety of temporal, spatial and spectral scales.
file 605: midlatitude summer
no aerosol
observer = 0.000
zenith angle =

Relative Humidity = \%.

MIDLATITUDE SUMMER

0.000
30.000

wavelength (microns)

file 605d: midlatitude summer
lowtran rural
vls = 5 km
observer = 0.000
zenith angle = 30.000

Relative Humidity = \%.

MIDLATITUDE SUMMER

wavelength (microns)
file 605b : midlatitude summer  
lowtran rural vis=23km
observer= 0.000 zenith angle= 30.000

file 605i : midlatitude summer  
no aerosol  humidity=50%
observer= 0.000 zenith angle= 30.000
file 605j: midlatitude summer
lowtran rural vis=23km
observer= 0.000
zenith angle= 30.000
humidity=50%

file 605k: midlatitude summer
lowtran rural vis=5km
observer= 0.000
zenith angle= 30.000
humidity=50%
file 60g: midlatitude summer
no aerosol
observer= 0.000 zenith angle= 30.000
humidity=20%

file 605g: midlatitude summer
lowtran rural vis=23km
observer= 0.000 zenith angle= 30.000
humidity=20%

wavelength (microns)

wavelength (microns)
file 605h: midlatitude summer
lowtran rural vis=5km humidity=20%
observer = 0.000 zenith angle = 30.000

file 529,20.6: midlatitude summer RH = 20%
o aerosol
observer = 0.000 zenith angle = 30.000
file 529b20.6:midlatitude $s$: $RH = 20\%$
lowtran rural vis=23km
observer= 0.000 zenith angle= 30.000

file 529d20.6:midlatitude summer $s$: $RH = 20\%$
lowtran rural vis=5km
observer= 0.000 zenith angle= 30.000
Future Work

- Rural aerosol scenarios
- Marine aerosol scenarios
- Clouds
- Comparison of radiances and atmospheric transmittances
Backscatter from atmospheric aerosols can produce significant returns in monostatic laser radar (lidar) systems. The Geophysics Directorate of Phillips Laboratory is developing lidar systems that will measure this backscatter. To aid in the design and use of such systems, SPARTA has developed a lidar simulation program, BACKSCAT, that calculates the backscatter return for various lidar systems, viewing aspects, and atmospheric conditions. This paper describes a new version of the simulation system, BACKSCAT Version 2.0. BACKSCAT Version 2.0 has been totally redesigned. Additional aerosol models and cirrus cloud models have been added. In addition, an all new user interface has been developed.
BACKSCAT, LIDAR BACKSCATTER SIMULATION
VERSION 2.0

By
John R. Hummel, David R. Longtin, Nanette L. Paul, & James R. Jones

11 June 1991
Annual Review Conference on Atmospheric Transmission Models
Hanscom AFB, Massachusetts

Contract F19628-88-C-0038

BRIEFING OUTLINE

• Background and Objectives of Work

• Overview of BACKSCAT

• New Features in BACKSCAT Version 2.0

• Summary and Recommendations for Future Work
BACKGROUND AND OBJECTIVES

BACKGROUND

- GL has Been Active in Developing and Fielding Atmospheric Backscatter Lidar Systems
- A Need Existed to Simulate the Aerosol Backscatter from Lidar Systems for Representative Atmospheric Conditions
- BACKSCAT Version 1.0 Was Developed to Meet That Need Using AFGL Atmospheric Models, circa LOWTRAN 6

OBJECTIVES

- Update BACKSCAT Aerosol Models to LOWTRAN 7 Levels
- Enhance BACKSCAT Based On User Feedback

OVERVIEW OF BACKSCAT

- BACKSCAT Simulates the Aerosol Backscatter from a Backscatter Lidar Operating Under User Defined Lidar, Atmospheric, and Viewing Conditions
- A Menu Driven “Front End” Simplifies Operation
- Code Implemented for the IBM PC Environment in “C” (Menu System) and FORTRAN 77 (Science Portion)
- Atmospheric Conditions are User-Defined Employing:
  - Built-in Aerosol and Atmospheric Models
  - User-Supplied Propagation Profile
OVERVIEW OF BACKSCAT
(Cont.)

BACKSCAT Version 2.0

NEW FEATURES IN BACKSCAT
VERSION 2.0

- Addition of Cirrus Clouds and Wind-Dependent Desert
  Aerosol Models

- Molecular Scattering Profiles Based On:
  - Built-in GL Model Atmospheres
  - User-Supplied Radiosonde Data

- Built-in "Quick View" Graphics Package

- All-New Menu Interface System
  - Easier to Use
  - Improved Error Checking
FEATURES OF BACKSCAT VERSION 2.0 (Cont.) - NEW MENU SYSTEM

BACKSCAT - LIDAR Backscatter Program

<table>
<thead>
<tr>
<th>Atmospheric Parameters File</th>
<th>Read in new File?</th>
<th>Seasonal Distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>NONE</td>
<td>N</td>
<td>FALL/WINTER</td>
</tr>
</tbody>
</table>

Boundary Layer -
- Height (km): 2.00000
- Type of Aerosols: RURAL
- Relative Humidity (%): 70.00
- Visibility at the Surface (km): 23.0000
- Wind Speed at 10m (m/s): 10.0000

Troposphere -
- Height (km): 2.00000
- Relative Humidity (%): 70.00

Stratosphere -
- Height (km): 29.0000
- Type of Aerosols: STRATOSPHERIC
- Aerosol Loading: BACKGROUND

Upper Atmosphere -
- Height (km): 100.000
- Type of Aerosols: METEORIC DUST
- Aerosol Loading: NORMAL

Cirrus Clouds -
- Cloud Type: NONE

Cirrus Cloud Types:
- NONE
- STANDARD CIRRUS
- SUBVISUAL CIRRUS

FEATURES OF BACKSCAT VERSION 2.0 (Cont.) - "QUICKVIEW OPTION"

Altitude (km) | BACKSCAT Results
---|---
0 | 100
10 | 90
20 | 80
30 | 70
40 | 60
50 | 50
60 | 40
70 | 30
80 | 20
90 | 10
100 | 0

Backscatter (1/(m*str))
FEATURES OF BACKSCAT VERSION 2.0
(Cont.) - RADIOSONDE DATA ENTRY

<table>
<thead>
<tr>
<th>ALTIMETRY</th>
<th>PRESSURE</th>
<th>TEMPERATURE</th>
<th>MOISTURE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Altitude (m)</td>
<td>Pressure (mb)</td>
<td>Temperature (°C)</td>
<td>Moisture (%)</td>
</tr>
<tr>
<td>1 79.00</td>
<td>1003.50</td>
<td>23.90</td>
<td>74.00</td>
</tr>
<tr>
<td>2 110.00</td>
<td>1000.00</td>
<td>23.60</td>
<td>74.00</td>
</tr>
<tr>
<td>3 555.00</td>
<td>950.00</td>
<td>18.60</td>
<td>87.00</td>
</tr>
<tr>
<td>4 585.00</td>
<td>946.84</td>
<td>18.30</td>
<td>88.00</td>
</tr>
<tr>
<td>5 1017.00</td>
<td>900.00</td>
<td>15.00</td>
<td>96.00</td>
</tr>
<tr>
<td>6 1091.00</td>
<td>892.55</td>
<td>14.50</td>
<td>97.00</td>
</tr>
<tr>
<td>7 1328.00</td>
<td>867.92</td>
<td>13.50</td>
<td>96.00</td>
</tr>
<tr>
<td>8 1498.00</td>
<td>850.68</td>
<td>11.60</td>
<td>74.00</td>
</tr>
<tr>
<td>9 1500.00</td>
<td>850.00</td>
<td>11.70</td>
<td>71.00</td>
</tr>
<tr>
<td>10 1582.00</td>
<td>842.17</td>
<td>12.60</td>
<td>37.00</td>
</tr>
<tr>
<td>11 1717.00</td>
<td>828.93</td>
<td>18.10</td>
<td>11.00</td>
</tr>
</tbody>
</table>

Ctrl-ENTER To ACCEPT DATA
ESC from MAIN Menu
ALTITUDE REFERENCE MSL
UNITS: Alt → m, P → mb, T → °C, M → RH(%)
CIRRUS CLOUD TRANSMISSION MODELLING*

W.M. Cornette, J.G. Shanks
Photon Research Associates, Inc., 9393 Towne Centre Drive, Suite 200,
San Diego, CA 92121

The modelling of transmission through a cirrus cloud is of significant concern to a
wide variety of users, including IRSTs and satellite systems. A model of cirrus
transmission involves a combination of characterizations of cirrus cloud properties and
radiative transfer. This presentation will summarize an assessment of current cirrus
transmission models, with recommendations for potential upgrades and additions to the
existing models. Also, several aspects for modelling transmission through cirrus clouds
are applicable to transmission through optically thick atmospheric layers by modelling
scattering in the forward direction as being no scattering at all, thereby producing a much
more reasonable result.

*This work was funded by the Air Force Geophysics Laboratory under Contract
No. F08606-87-C-0035; Dr. Donald Grantham, Technical Monitor.
CIRRUS CLOUD TRANSMISSION MODELING

JUNE 1991

Presented at the 14th Annual Review Conference on Atmospheric Transmission Models
11-12 June 1991, Geophysics Directorate, Phillips Laboratory, Hanscom AFB, MA

Work Funded In Part by the Air Force Geophysics Laboratory
Under Contract No. F08606-87-C-0035; Dr. D. Grantham, Technical Monitor

Presented By:
Dr. William M. Cornette
Dr. Joseph G. Shanks

Photon Research Associates, Inc.
9393 Towne Centre Drive, Suite 200
San Diego, CA 92121

OUTLINE

- Objective
- Cirrus Characterization
  - Mesoscale
  - Microscale
- Radiative Transfer
- Models
OBJECTIVE

To Assess the Current Capabilities in the Government, Contractor, and University Communities with Respect to the Present State of Technology in Cirrus Analysis and Attenuation Modeling.

- Cirrus (Ci)
- Cirrocumulus (Cc)
- Cirrostratus (Cs)
- Condensation Trails (Contrails)
- Nacreous (Stratospheric)
- Noctilucent (Mesospheric)

CIRRUS CLOUD ALTITUDES
CIRRUS THICKNESS

- Median Thickness = 1.0 km

![Graph showing cirrus thickness statistics]

Source: Hall et al. (1984)

OBSERVED SIZE DISTRIBUTIONS

- Lidar Measurements

![Graph showing observed size distributions]

Source: Sassen, Starr and Uttal, 1989
PARTICLE SIZE DISTRIBUTIONS

- Opaque Cirrus
- Thin, Translucent Cirrus
- Type 1 Subvisual Cirrus
- Types 1 & 2 Subvisual Cirrus
- Barnes (1982)

PHASE FUNCTIONS: OBSERVED

- Lyons and Schummers; 1984
- Platt and Dilley; 1984
1. Direct Line-of-Sight
2. Forward Scatter into Aperture
3. Scatter into Field of Regard

**CIRRUS CLOUD MODELS**

<table>
<thead>
<tr>
<th></th>
<th>RADIATIVE TRANSFER</th>
<th>PARTICLES</th>
<th>VERTICAL PROFILE</th>
<th>SIZE DISTRIBUTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>LOWTRAN</td>
<td>Beer's Law</td>
<td>Spherical</td>
<td>Uniform Layer</td>
<td>-</td>
</tr>
<tr>
<td>APART</td>
<td>Beer's Law and First Order Scattering</td>
<td>Spherical</td>
<td>Profile</td>
<td>-</td>
</tr>
<tr>
<td>SUBVIS</td>
<td>Beer's Law</td>
<td>Random Hexagonal</td>
<td>Uniform Layer</td>
<td>Temperature Dependent</td>
</tr>
<tr>
<td>Liou</td>
<td>Successive Order of Scattering</td>
<td>Random Hexagonal</td>
<td>Uniform Layer</td>
<td>Temperature Dependent</td>
</tr>
<tr>
<td>Rockwitz</td>
<td>Successive Order of Scattering</td>
<td>Oriented Hexagonal</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
MODELS

- "Comprehensive" Models
  - LOWTRAN 7
  - APART (Version 7.00)
  - SUBVIS and LOWTRAN
  - Liou

- "Element" Models
  - Pollack and Cuzzi
  - Liou, et al.
  - Rockwitz
  - Barnes
  - Hansen

LOWTRAN/APART CIRRUS MODEL

- Standard
- Subvisual
LOWTRAN/APART CIRRUS MODEL

- Standard
- Subvisual

![Graphs showing albedo vs. wavelength for Standard and Subvisual models.](image)

LOWTRAN/APART CIRRUS MODEL

![Graphs showing asymmetry factor vs. wavelength for Standard and Subvisual models.](image)
LOWTRAN/APART MODEL DEFICIENCIES

- LOWTRAN
  - Spherical Particles
  - Extinction Only
    - Multiple Scatter for Radiation Only, Not Transmittance
  - No Forward Scatter
  - Empirical Scaling Laws Not Based In Phenomenology

- APART
  - Same as LOWTRAN
    - EXCEPT
      - Forward Scattering Correction Included for Single Scatter into Field-of-Regard and Aperture

SUBVIS PARTICLE SIZE DISTRIBUTION
SUBVIS CIRRUS CLOUD

- 220, 230, 240, 250 K
- Geometrical Limit

SUBVIS MODEL DEFICIENCIES

- No Phase Functions
  \{ Input to LOWTRAN \}
- No Multiple Scattering
- Limited Spectral Region (2.2 - 6.2 \( \mu \text{m} \))
- Geometric Limit on Extinction
  - No Particles Less Than 20 \( \mu \text{m} \) Diameter
- Particles Randomly Oriented
CORRECTION FOR FORWARD SCATTER

• Replace

\[ \sigma_{\text{EXT}} = K_{\text{ABS}} + \sigma_{\text{SCAT}} \]

with

\[ \sigma_{\text{EXT}} = K_{\text{ABS}} + K \sigma_{\text{SCAT}} \]

Where \( g \) is Asymmetry Factor

• Sample Values of \( k \)
  - Hansen \((1 - g)\) \( \approx \) 0.49
  - Liou \( \approx \) 0.83
  - APART \( \approx \) 0.82 - 0.84

LIOU MODEL DEFICIENCIES

• Apparently Not Available

• Unknown Spectral Region

• Probable Geometric Limit
  - No Particles Less Than 20 \( \mu \text{m} \) Diameter

• Particles Randomly Oriented

• Unknown Term in Paper
SINGLE SCATTERING DIAGRAMS

- Upward Scattered Radiation

- Downward Scattered Radiation

DUAL/TRIPLE SCATTERING DIAGRAMS

- Dual Scattered
  - Upward 45°
  - Downward 45°

- Triple Scattered
RECOMMENDATIONS

- Incorporate Capabilities into APART/MODTRAN
  - SUBVIS Cirrus Model
  - Forward Scatter Correction (MODTRAN)
  - Different Size Distributions

- Upgrade Capabilities
  - Empirical Phase Function
  - Oriented Particles
  - Small Particle Sizes

- Perform Sensitivity Study

MULTIPLE SCATTERING (LIOU)

- Midlatitude Winter
- Sensor IFOV = 2°
- Cloud Top 8.5 km
- Cloud Thickness 0.5 km
ICE-CLOUD
A MODEL FOR IR TRANSMITTANCE THROUGH CIRRUS CLOUD

W.T. Kreiss, R. Vik
Horizons Technology, Inc., 3990 Ruffin Road, San Diego, CA  92123

ICECLOUD is a model for transmission of IR through cirrus clouds developed for the IASPM project. This task outlines the physical ideas on which the procedure is based. The model sets criteria for the occurrence of ice water and sets parameters defining the number, density and size distribution of the ice particles present. The ice particles are assumed to be hexagonal cylinders. Single particle optical scattering parameters appropriate to these particles (calculated using geometric optics) are used. The model represents transmission through dense cirrus clouds in a narrow region of the IR spectrum. The model can be improved, however, to broaden its applicability.
CIRRUS CLOUDS CAN HAVE SIGNIFICANT EFFECTS ON LONG-RANGE IR SENSOR PERFORMANCE

- IADM/IRSTS FLIGHT TESTS
  - ANOMALOUS DEGRADATION
  - SUBVISUAL CIRRUS POSSIBLE CAUSE

- LIDAR/RADIOMETER TEST PROGRAM
  - CHARACTERIZED CIRRUS AS AN IR ENVIRONMENT
  - POINTED TO USE OF LOWTRAN7 CIRRUS MODELS

- CONCLUSIONS
  - BACKGROUND RADIANCE IMPORTANT (AS WELL AS PATH TRANSMITTANCE)
  - LOWTRAN7 MODELS ARE USEFUL, BUT:
    - EMPLOY SPHERICAL PARTICLES
    - PROVIDE OPTICAL DEPTH FROM GEOMETRICAL THICKNESS

- REQUIREMENT FOR A BETTER CIRRUS MODEL FOR IASPM
REQUIREMENTS FOR A CIRRUS MODEL IN IASPM

- MUST INCLUDE SUBVISUAL CIRRUS
- MUST TREAT NON-SPHERICAL ICE PARTICLES
- OPTICAL DEPTHS MUST BE DETERMINED FROM OBSERVATIONAL DATA

EXISTING KNOWLEDGE

- OCCURANCE AND MICROPHYSICS OF CIRRUS CLOUDS (NCAR)
- HEXAGONAL ICE PARTICLE OPTICAL PROPERTIES (UTAH)

"ICECLOUD" MODEL

- GOOD FOR THE TIME
- WE KNOW HOW TO BUILD A BETTER MODEL NOW

PROGRAM ICECLOUD

REAL TREP, ICE
INTEGER ICL, IBOT, ITOP, ML, ICL, NCL
CHARACTER*64 INNAME, OUTNAM
CHARACTER*72 TITLE
PARAMETER (MAXP=1000, MAXL=34)
IONS = 0
OUTNAM = 'LOCARD'
INNAME = 'MOD1.INP'
OPEN(UNIT=1, FILE=INNAME, STATUS='OLD', IOSTAT=IOS)

CALL READSND
CLOSE(UNIT=1)
CALL PROFILE(ICL, IBASE, CBASE, ITOP, CTOP)
ML = 34

IF ( ICL .NE. 0 ) THEN
  PROFILE returns ICL = 1 if there is an ice cloud.
  CALL CLOUD(IBASE, IBOT, ITOP, TREP, ICE)
END IF

IF ( ICL .NE. 0 .AND. ICE.GT.1.E-06 ) THEN
  CALL LAYERS(ML, IBOT, ITOP, ICL, NCL)
  CALL BEBA(TREP)
ELSE
  CALL NOICE(ML)
ENDIF

CALL NEWCOM
CALL ARISPM(ML, ICE, OUTNAM)
STOP

1000 FORMAT (A64)

END
Figure 2. Cloud cloud ice water content plotted against temperature and parameterized in terms of relative humidity according to convective regions. (Inside symbol: synoptic type; Outside symbol: relative humidity).

Figure 3. Curves fitted to the average spectra for each temperature range.
The extinction cross-section, averaged over look angles is:

\[ C_0 = \frac{3}{2} (W/D)^2 \left( \sqrt{3} + 4D/W \right) \]

Figure 4. Definition of extinction cross-section.

\[ x = 2 m_1 x \]

\[ m_1 = \text{imaginary part of the refractive index} \]

\[ x = \text{size parameter}: \]
\[ x = \frac{2kW}{\lambda/2} \left( \frac{3\sqrt{3} - 4D/W}{3\sqrt{3} + 4D/W} \right) \]

Figure 5. Single scattering co-albedo.
\( X, \; \lambda = 20 \text{ micrometers} \)

**Figure 6.** Regions of validity of ICECLOUD.

"ICECLOUD" DEFICIENCIES

- DOES NOT APPLY TO SUBVISUAL CIRRUS
- APPLIES ONLY TO NARROW WAVELENGTH REGION
- SINGLE LAYER TRANSMITTANCE ONLY
- HIGH ALTITUDE WATER VAPOR MEASUREMENTS ARE DIFFICULT
ELECTRO-OPTICAL MODEL FOR AERIAL TARGETING (EMAT)  
(SUCCESSOR TO IASPM)

EMAT MODEL NEEDS

- BACKSCATTERING (BACKGROUND SCENES)
- PATH TRANSMITTANCE
- PATH RADIANCE
- MUST APPLY TO THIN AND SUBVISUAL CIRRUS
- CIRRUS CLIMATOLOGY/MORPHOLOGY
- A "PRESCRIBED" MODEL (STATISTICAL
- FULL WAVELENGTH COVERAGE
THE STATUS OF THE NAVY OCEANIC VERTICAL AEROSOL MODEL

S. Gathman
Ocean and Atmospheric Sciences Division, Naval Ocean Systems Center,
San Diego, CA 92152

The Navy has been working on the development of a vertical aerosol model called NOVAM for several years. This model uses the navy aerosol model as a kernel for estimation of optical / IR properties of the atmosphere near the ocean surface and provides vertical structure of these properties specifically matched to oceanic conditions. The model utilizes surface meteorological data and radiosonde data as input. The model has been tested off of the California coast during the FIRE experiment and in the tropics during the KEY 90 experiment. This paper shows some of the results of these tests where predicted extinction profiles are plotted along side of measured extinction profiles.
The Status of the Navy Oceanic Vertical Aerosol Model

Stuart G. Gathman
NOSC code 543
San Diego, CA

Naval Oceanic Vertical Aerosol Model
NOVAM

Type Selection

Well mixed
Weak convection
Stratus
Default
Future models

OPTICS

output

output

(for the future)

NRL code 4117
Testing of NOVAM

Difference Testing

Model Testing

Marine Atmosphere

NRL code 4117

NRL code 4117
NOVAM Testing

Testing Experiments
Field tests of NOVAM

- FIRE experiment at San Nicolas Island, CA. 1987
  Tethered Aerostat Balloon
  NOSC Navajo aircraft
  NPS on the ship, Point Sur

- KEY-90 experiment Marathon Florida, 1990
  Fishing boat for surface data
  NOSC Navajo aircraft
  NRL P-3A aircraft with LIDAR
  Shore base LIDAR

- East Coast Experiment - plans for 91/92
  Cooperation with IRAMMP, Summer 91
  Cooperation with ONR/NRL ATI, FALL 91/92

NRL code 4117
NOSC code 543
Aerostat Measurements SNI–87
(flight 1814)

NOVAM Grades

"A" = within data envelope 90% of time
"B" = within data envelope 50% of time
"C" = within 2X data envelope 90% of time
"D" = within 2X data envelope 50% of time

(SNI 1987)
KEY-90 - Verification of NOVAM in a "tropic like" environment

MEASURED EXTINCTION PROFILE

- Measured profile of Aerosol size distribution
  (Extinction calculated from Mie theory)
  NOSC aircraft with PMS probes
- Surface Aerosol size distribution
  Boat: UMIST PMS probe + TNO rotorod.
  (Extinction calculated from Mie theory)
- Surface extinction @ 3-5 and 8-12 bands
  Boat: PVM instrument.
- Downward looking lidar using aureole measurement.
  NRL P3 aircraft.
- TNO's lidar using the Kunz calibration.
  Shore based measurement.

NRL code 4117
KEY – 90

Experiment Days, July 1990

Extinction Profiles
(for NRL lidar)

Extinction (/km)

Height (m)

6.44:51
6.44:54
6.44:57
6.45:00
6.45:03
6.45:06

7/14/90; shots 725-730; 24°38'N, 80°56'W
Session 2

Summary of the Session on Atmospheric Propagation Models

The status of atmospheric propagation models is steadily improving. Problems that once appeared intractable are now being implemented on PCs. LOWTRAN has become a tri-service/industrial standard that is now commercially available. Other codes are also following suit. The increased resolution of new codes has allowed for examination of different problem areas. In particular, Non-LTE and other upper atmospheric problems are now being considered. This has brought attention to the altitude mismatch in results between various codes that work in the lower atmosphere and those which have been designed to operate in the upper atmosphere. This problem is being worked and should be resolved in the near future.

Comments on specific presentations:

MODTRAN/LOWTRAN: CURRENT STATUS, FUTURE PLANS
Presented by L. Abreu

MODTRAN compares well with SHARC. Favorable comparisons have also been done with LOWTRAN7 and FASCOD3. Improvements in MODTRAN will be in the area of radiative transfer (multiple scattering algorithms). World wide model atmospheres will be added, and the code will be made more modular. MODTRAN and APART will be integrated for work on spectral backgrounds.

FASCODE3: An Update
Presented by G. Anderson

The history of FASCODE development was presented. Currently FASCODE is trying to produce "exact" results in an optimized fashion (e.g. mathematical line shape, layer selection, etc.). Improvements underway currently consist of improving the portability, radiance algorithm, cross-sections, HITRAN capability, and dealing with non-local thermodynamic equilibrium (NLTE) and transitions from LTE to NLTE. Finally FASCODE3 has not been released because too many corrections/additions were needed.

EOSAEL 92
Presented by A. Wetmore

The 1992 version of the Electro-Optical Systems Atmospheric Effects Library (EOSAEL) will leave unchanged the following modules: NMMW, CLTRAN, COPTER, GRNADE, MPLUME, OVRCST, FCLOUD, ILUMA, FASCAT, LASS, GSCAT, NOVAE, and RADAR. The following modules will be upgraded: LOWTRN, IZTRAN, KWIK, XSCALE, TARGAC, COMBIC. The SABRE and MSCAT modules will be dropped. Four new modules will be added: BITS - to be used for broad-band integrated transmittance; FASCODE - GD's model; NBMSCAT - a radiative transfer approximation; and UVTRANS - a UV transmission, fluorescence, and lidar program. The various modules are also being made interactive.
HITRAN '91: The Contemporary Spectroscopic Molecular Database
Presented by L. Rothman

Major molecular parameter updates have been done for H2O, CO2, O3, methane, CO, NO, NO2, HNO3, and the hydrogen halides (HCl, HF, HI, HB). There have been minor changes in the trace gases (H2O2, C2H2, HCH6, SF6) and COF2 is being added. Provisions are also being made to convert HITRAN to run on a PC.

SHARC, An Atmospheric Radiation and Transmittance Code for Altitudes from 50 to 300 km
Presented by D. Robertson

SHARC was initially developed for SDIO for modeling radiance in the upper atmosphere. SHARC will handle Non-LTE conditions found in the upper atmosphere (50 - 300 km) in either ambient or auroral conditions. Current resolution is .5 inverse centimeters at wavelengths from 2 to 40 microns. A manual is currently being printed and will be available shortly.

Recent Development of the GENLN2 line-by-line model: studies in support of the UARS project
Presented by D. Edwards

GENLN2 is a line-by-line Non-LTE atmospheric transmittance and radiance code. It contains six GD model atmospheres, is modular, and will produce plots using NCAR graphics. Comparisons with ATMOS have been favorable, with reasonably good transmission over a variable spectral grid.

Present status of Transmittances and Radiances Modeling at L.M.D.
Presented by N. A. Scott

L.M.D. is investigating the impact of high resolution measurements for/on signatures. The fast-running, versatile codes compute transmittance and/or radiance for a variety of conditions.

AURIC (Atmospheric Ultraviolet Radiance Integrated Code): An Update
Presented by R. Huguenin

AURIC is being developed as an atmospheric UV spectral transmission and solar irradiance code. MODTRAN is the starting point; AURIC's structure will try to stay with MODTRAN's. The initial release will not include airglow, will have a resolution of 1 wavenumber with interpolation to .5 wavenumber. Optimum methods are being employed, particularly in the temperature dependent model, in order to have the code run faster.

ONTAR's PC Compatible LOWTRAN7 Package
Presented by J. Schroeder

ONTAR entered into a cooperative R & D agreement with GP in 1988. Since then, ONTAR has released various versions of GP's LOWTRAN code. The most recent version, release 3.8, has the full LOWTRAN7 implemented. Online help is available with this interactive version of LOWTRAN as are plotting routines which include overlays for different runs.
ONTAR's LOWTRAN7 has been certified by GP and runs in 640K on a PC with no memory extender required: however, a coprocessor is recommended.

Coupling Atmospheric and Background Effect
Presented by W. Cornette

The development of a computer model to determine thermal clutter in a scene with changing atmospheric conditions was described. The model is sensitive to solar radiation and includes numerous terrain materials for background effects. Terrain scenes and several cloud models at varying altitudes are included.

SENTRAN7: A Sensitivity Analysis Package for LOWTRAN7/MODTRAN
Presented by D. Longtin

SENTRAN7 was described as a user active analysis code designed to perturb various input parameters of LOWTRAN7 or MODTRAN. Graphical outputs are created in 2D and 3D formats. The code is currently designed to operate on VAX/VMS and SUN Unix systems. A complete description of the user input commands and the graphical requirements required was presented.

Atmospheric Models in the Strategic Scene Generation Model
Presented by W. Cornette

The Strategic Scene Generation Model was described in detail with special emphasis on the atmospheric propagation models currently implemented in the code. The background scene modules APART, GENESIS and CLDSIM were described with 2D simulations of terrain and cloud scenes. Simulations on varying resolution of transmittance, calculations were shown and some subtle differences between MODTRAN and APART were explained.

Review of the Chemical Kinetic Rate Constants Used in the SHARC Model
Presented by A. Pritt

As the title indicates, this was a comprehensive review of the chemical kinetic rate constants being used in the SHARC model. A basic explanation of SHARC and NLTE conditions was given, along with an explanation of the derivation of H2O and CO rate constants. The presenter showed numerous comparisons between SHARC and a large and impressive series of measurements.
MODTRAN/LOWTRAN: CURRENT STATUS, FUTURE PLANS

Geophysics Directorate, Simulation Branch (OPS),
Hanscom Air Force Base, MA 01731-5000

MODTRAN (public release: November 1990) is a 2 parameter (P&T) band model
code with moderate spectral resolution (2 cm\(^{-1}\) full width-half maximum). The
MODTRAN band model parameters were calculated by utilizing the HITRAN-86 data base.
The code is fully compatible with LOWTRAN 7 and the results can be degraded to between
2 and 50 wavenumber spectral resolution.

Future plans include an improved more accurate multiple scattering algorithm as
well as a realistic modelling of the atmosphere-to-background-to-atmosphere coupling
technique. A definitive set of worldwide model atmospheres is presently under
development.
MODTRAN/LOWTRAN: CURRENT STATUS, FUTURE PLANS

L.W. ABREU, F.X. KNEIZYS, G.P. ANDERSON
and J.H. CHETWYND

ANNUAL REVIEW CONFERENCE ON
ATMOSPHERIC TRANSMISSION MODELS

11-12 JUNE 1991
GEOPHYSICS DIRECTORATE
PHILLIPS LABORATORY

SOFTWARE DESCRIPTION FOR:
ATMOSPHERIC PROPAGATION MODELS AND DATA BASE:
FASCODE, MODTRAN, LOWTRAN, HITEMP

o Common Elements:
Transmittance and Radiance
Geometrical, thermal multiple scattering
Default atmospheric profiles
(Molecular, aerosol, particulates)
Spectral range: 0 to 50,000 cm⁻¹ (0.3μm to 200μm)
Interpolation, Scattering, and Fiber Functions

o FASCODE (FASCOD2-1986; FASCOD3-1990)
Resolution: Line-by-line (high)
Physics: Exact, Voigt
Altitude Range: 0 to space
Applications: High resolution simulations
Comments: Slow for large spectral range
Keeps external database (HITRAN)
Keeps NLDN specifications
Recognized International Standard

o MODTRAN (1990)
Resolution: 2 cm⁻¹ (moderate)
Physics: 2-parameter band model (P and T)
Altitude Range: 0 to 90 km
Applications: Moderate resolution simulations
Comments: Solar (direct and scattered)
Must use time consumption
Must use NLDN
Spectral database stored in 1 cm⁻¹ bins

o LOWTRAN (1989)
Resolution: 25 cm⁻¹ (low)
Physics: 1-parameter band model (P)
Altitude Range: 0 to 20 km (limited by band model)
Applications: Broad band spectral simulations
Comments: Solar (direct and scattered)
Limited to the same penalties
Loss of small scale spectral character
Recognized International Standard

o HITRAN (HITRAN86-1987; HITRAN90-1990)
Resolution: Infinite
Physics: Complete spectroscopic parameters for
over 30,000 species for
28 separate molecular species
Molecular cross sections for 9
additional species
Applications: Source data for high resolution line by
line synthesis of molecular
disruption properties
Emissivity data is HITRAN
Source of data is the HITRAN database
Recognized International Standard
THE LOWTRAN MODEL
-------------

ATMOSPHERIC TRANSMITTANCE.BACKGROUND RADIANCE
- 20 CM⁻¹ RESOLUTION

33 LAYER ATMOSPHERIC MODEL
- CHOICE OF MODEL ATMOSPHERES,
  AEROSOL MODELS
- USER DEFINED

GEOMETRY FOR ANY SLANT PATH
- LOOKING UP/DOWN
- TANGENT HEIGHTS
  - HORIZONTAL PATHS

PRODUCT TRANSMITTANCE DUE TO
- MOLECULAR ABSORPTION (BAND MODEL)
- MOLECULAR SCATTERING
- AEROSOL EXTINCTION
- CONTINUUM ABSORPTION

THERMAL EQUILIBRIUM IN EACH ATMOSPHERIC LAYER

LOWTRAN7

<table>
<thead>
<tr>
<th>ABSORBER</th>
<th>SPECTRAL RANGE (CM⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water Vapor (H₂O)</td>
<td>0-17860</td>
</tr>
<tr>
<td>Ozone (O₃)</td>
<td>0- 200, 515-1275, 1630-2295, 2670-3260, 13000-24200, 27500-50000</td>
</tr>
</tbody>
</table>

Uniformly Mixed Gases.

| Methane (CH₄)     | 1065- 1775, 2345- 3230, 4110- 4690, 5065- 6135 |
| Nitrous Oxide (N₂O) | 0- 120, 490- 775, 865- 995, 1065- 1385, 1545- 2040, 2090- 2655, 2705- 2865, 3245- 3925, 4260- 4470, 4540- 4785, 4910- 5165 |
| Oxygen (O₂)       | 0- 265, 7650- 8080, 9235- 9490, 12850-13220, 14300-14600, 15695-15955 |
| Carbon Monoxide (CO) | 0- 175, 1940- 2285, 4040- 4370 |
| Carbon Dioxide (CO₂) | 425- 1440, 1805- 2855, 3070- 4065, 4530- 5380, 5905- 7025, 7395- 7785, 8050- 8315, 9340- 9670 |

66
Trace Gases:

<table>
<thead>
<tr>
<th>Absorber</th>
<th>Spectral Range (cm⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitric Oxide (NO)</td>
<td>1700-2005</td>
</tr>
<tr>
<td>Nitrogen Dioxide (NO₂)</td>
<td>580-925, 1515-1695, 2800-2970</td>
</tr>
<tr>
<td>Ammonia (NH₃)</td>
<td>0-2150</td>
</tr>
<tr>
<td>Sulphur Dioxide (SO₂)</td>
<td>0-185, 400-650, 950-1460, 2415-2580</td>
</tr>
</tbody>
</table>

**LOWTRAN 7 BAND MODEL**

**TRANSMITTANCE FUNCTIONS**

\[
T = \exp(-C \cdot W) \\
W = \left(\frac{P}{P_0}\right)^n \times \left(\frac{T_o}{T}\right)^m \times U
\]

where:

\(a, n, m\) are BAND MODEL PARAMETERS

\(U = \text{ABSORBER AMOUNT}\)

\(C = \text{BAND MODEL ABSORPTION COEFFICIENT}\)
MODTRAN: Specific Attributes

* Moderate Spectral Resolution \(2 \text{ cm}^{-1}\) (FWHM)

* 2 Parameter Band Model \((P, T)\)

1 \(\text{ cm}^{-1}\) Bins Stored On Tape

Calculated From 1986 HI\(\text{FRAN}\) Data Base \((0 - 17900 \text{ cm}^{-1})\)

* Internal Triangular Slit Function

Degradable To Desired Spectral Resolution

* Atmospheric Molecules:

\[
\begin{align*}
&\text{H}_2\text{O} \quad \text{O}_3 \quad \text{CO}_2 \quad \text{CH}_4 \quad \text{N}_2\text{O} \quad \text{CO} \quad \text{N}_2 \\
&\text{O}_2 \quad \text{HNO}_3 \quad \text{NO} \quad \text{NO}_2 \quad \text{NH}_3 \quad \text{SO}_2
\end{align*}
\]

EXPANDED APPLICABILITY

* MODTRAN IS BETTER SUITED THAN LOWTRAN FOR ATMOSPHERIC PATHS ABOVE 30 KM

- Band Model Parameters Are Both Temperature and Pressure Dependent
- Transmittance Is Modeled With A Voigt Lineshape

* HOWEVER, MODTRAN STILL ASSUMES LOCAL THERMODYNAMIC EQUILIBRIUM
The diagram shows the comparison of transmittance between Modtran 10 to 20 and Lowtran. The x-axis represents the wavenumber in cm⁻¹, ranging from 1400 to 2600, and the y-axis represents the transmittance. The transmittance values range from 0.0 to 1.0. The diagram includes the text 'LOWTRAN' and 'FASCODE 3 10 to 20'.
### GL Atmospheric Propagation Models

<table>
<thead>
<tr>
<th>GENERAL PROPERTIES</th>
<th>FASCODE</th>
<th>MODTRAN</th>
<th>LOWTRAN</th>
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</thead>
<tbody>
<tr>
<td>SPECTRAL RESOLUTION</td>
<td></td>
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<tr>
<td>HIGH</td>
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<tr>
<td>MODERATE</td>
<td>X</td>
<td>X</td>
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<tr>
<td>LOW</td>
<td>X</td>
<td>X</td>
<td>X</td>
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<tr>
<td>CAPABILITIES</td>
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<tr>
<td>TRANSMITTANCE</td>
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<td>X</td>
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<td>BACKGROUND RADIANCE</td>
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<tr>
<td>THERMAL</td>
<td>X</td>
<td>X</td>
<td>X</td>
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<tr>
<td>SOLAR/LUNAR</td>
<td></td>
<td>X</td>
<td>X</td>
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<tr>
<td>NON-LTE</td>
<td></td>
<td></td>
<td>X</td>
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</tbody>
</table>

<table>
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<tr>
<th>SPECIFIC APPLICATIONS</th>
<th>FASCODE</th>
<th>MODTRAN</th>
<th>LOWTRAN</th>
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<tbody>
<tr>
<td>LASER PROPAGATION</td>
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<td></td>
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<tr>
<td>PLUME SIGNATURES</td>
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<tr>
<td>TARGET CONTRAST</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>REMOTE SENSING</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
</tbody>
</table>
FUTURE PLANS

* IMPROVED MULTIPLE SCATTERING ALGORITHM BASED ON THE DISCRETE-ORDINATE-METHOD
* WORLD-WIDE DATA BASE OF MODEL ATMOSPHERES
* MODULARIZATION OF CODES
* INTEGRATION OF MODTRAN AND APART
* SPECTRALLY DEPENDENT BACKGROUNDS
* IMPROVED GEOMETRY ROUTINES FOR 32 BIT MACHINES

DOD POINT OF CONTACT FOR LOWTRAN 7 AND MODTRAN IS:

LEONARD W. ABREU
GL/OPS(AFSC)
HANSCOM AFB, MA 01731
(617) 377-2337 Autovon 478

DOD POINT OF CONTACT FOR FASCOD3 IS:

GAIL P. ANDERSON
GL/OPS(AFSC)
HANSCOM AFB, MA 01731
(617) 377-2335 Autovon 478

NOTE: DOD Contractors, please have your contract monitor make the request.

The codes are publicly available through:

National Climatic Data Center, NOAA
Environmental Data Services
Federal Building
Asheville, NC 28801
FASCOD3: AN UPDATE

Geophysics Directorate, Hanscom Air Force Base, MA 01731-5000

S.A. Clough, R.D. Worsham
Atmospheric and Environmental Research, Inc., 840 Memorial Drive, Cambridge, MA 02139

E.P. Shettle
Naval Research Laboratory, Code 6522, Washington, DC 20375

FASCOD3, a line-by-line atmospheric radiance-transmittance code, is currently available in a beta-test version. As with FASCOD2, the program is applicable to spectral regions from the microwave to the middle ultraviolet, employing standard spectroscopic parameters supplied from external line atlases. New FASCOD3 capabilities include: multiple scattering of thermal radiation, CO2 and O2 temperature-dependent line coupling for selected bands, UV diffuse absorption (O2 and O3), improved weighting functions, enhanced non-local thermodynamic equilibrium (NLTE) calculations, and, perhaps most importantly, compatibility with the HITRAN91 database, including temperature-dependent cross sections. NLTE input requirements include LTE temperature and density profiles plus adequate descriptions of the NLTE population profiles for the specified excited vibrational states. Auxiliary NLTE line positions, halfwidths, strengths and vibrational-rotational assignments must also be provided.
FASCOD3: An Update

(Geophysics Lab (AFSC))

S.A. Clough, R.D. Worsham
(Atmospheric and Environmental Research, Inc.)

E.P. Shettle
(Naval Research Laboratory)

Presented at the:

Annual Review Conference on Atmospheric Transmission Models
11-12 June 1991

FASCODE: Fast Atmospheric Signature Code

Version 3 - \( \beta \)

AFGL: F.X. Kneizys
S.A. Clough
G.P. Anderson
J.H. Chetwynd
L.W. Abreu
W.O. Gallery
L.S. Rothman
M.L. Hoke
E.P. Shettle
R.D. Worsham

Primary
UV, Constituent Profiles
Programming, Validation
LOWTRAN7 Compatibility
Geometry
Line Atlas
Line Coupling
Aerosols/Hydromet.ors
X-sections, etc.

1 currently at Atmospheric and Environmental Research, Inc.
2 currently at Naval Research Laboratory
3 at Atmospheric and Environmental Research, Inc.
Some thoughts on FASCOD3 presentation: 1 June 1991

1. Authorship  2. History/Contractor Support
3. FASCOD2/FASCOD3 in 1990 - "The Way We Were"
4. Delays in FSC3 release - why?

FASCODE: Fast Atmospheric Signature Code
Version 2 and Version 3-β

Visidyne:  
H.J.P. Smith  - contributions to FASCOD1C (1978)
D.J. Dube
M.E. Gardner
T.C. Degges  - NLTE theory (1977, 1985)

Sonicraft:  
W.L. Ridgway  - contributions to FASCOD2 (1985)
R.A. Moose
A.C. Cogley

AER, Inc.:  
R.D. Worsham  - programming contributions to FASCOD3 & MS (1988-91)
S.A. Clough  - radiance algorithm, etc. (1990-1991)
FASCODE2/3: Fast Atmospheric Signature Code

Introduction: (or "Just what is so difficult anyway?" and "Why bother?")

- Line-by-Line Radiance/Transmittance Model which attempts:
  - to provide "exact" solution to radiative transfer problem -
    - Beer's Law \[ T = \exp(-a(i)*N(i)) \]
    - Planck Function \[ B = f(n(T)) \]
    - Radiance Eqn \[ R = B dT \]
  - to optimize mathematics for rapid solution
  - to account for realistic atmospheric lines-of-sight
    - (not including non-linear "seeing")
  - to maintain "state-of-the-art" spectroscopy
  - to unify physical description for all frequencies
  - to accommodate instrument design characteristics

- Limiting Considerations
  - Spectral sampling - governed by "true" line shape
  - Atmospheric layering - governed by Curtis-Godson approximation
  - Computer allocations - historic

- Solutions (?)
  - Optimize:
    - line shape per layer
    - layer selection
    - merging of adjacent layers
  - Provide "all" default options (realistic)
  - Maintain LOWTRAN compatibility for all non-molecular parameters
  - Support user-friendly I/O:
    - documentation, distribution, maintenance
    - user services
FASCODE2/3: Fast Atmospheric Signature Code

Basic Input/Output:

o INPUT

Mode

- optical depth
- transmittance
- radiance

Spectroscopic variables for line-by-line calculations

- external data bases (HITRAN86, NLTE, coupling coef.)
  [driven by LNFL routines for FASCOD3;
   BCDMRG routines for FASCOD2]
- internal block data (mm with coupling coef.)
- line shape including far wings and continua

Spectral range and sampling

- 500 cm⁻¹ limit
- "buffering" at boundaries
- monochromatic option (laser)
- "natural" frequency spacing
dv = 4 pts/halfwidth
- "instrumental" frequency spacing
  scanning and filter options

Line-of-sight/geometry

- horizontal
- H1 to H2 (-/ + 90°)
- tangent
- layering (boundaries and/or selection criteria)

Path characterization

- pressure, temperature
- constituent (trace) profiles
- hydrometeor profiles (clouds, rain, fog)
- particulate profiles (aerosols, dust, etc.)
Basic Input/Output:

- OUTPUT

Echo all input parameters

Path description

- layer selection
  - pressure, temperature
  - atmospheric constituent profiles*
  - aerosol/hydrometeor profiles
  - line shape, halfwidth

- geometry
  - path type
  - bending
  - integrated amounts (layer, total)
  - particulate absorption (layer, total)

Spectroscopic

- number of lines/species
- layer specific
  - \( v, v_2, dv \) (natural)
  - optical depth, transmittance, radiance
- total path
  - (same)
- scanned
  - \( dv \) (scan), type (triangular, rectangular, etc.)
- filtered
  - \( v, v_2 \) shape
- plotted (all of above)
- layer boundary info: \( T/p(l), T/p(l-1), \) etc.

FASCOD3: Fast Atmospheric Signature Code

Version 3

Generic Capabilities:

- Line-by-line molecular spectroscopy including line coupling
- Uniform physical definitions (0-50000cm\(^{-1}\))
- Full geometric path flexibility, 0-120 km,
  - all lines of sight with spherical refraction
- Access to arbitrary databases (HITRAN91/86, NLTE, etc.)
- Voigt line shape at all altitudes and/or pressures
- Mathematical optimization for layering and spectral sampling algorithms
- Default or user-supplied atmospheric profiles,
  - \( p, T \), and mixing ratios for 28 constituents
- Absorption x-section implementation from HITRAN86/90
- Additional default & user specifications for 10 green-house gases
- Default or user-supplied aerosol and hydrometeor profiles;
  - full LOWTRAN7 compatibility
- Laser (monochromatic) options
- Non-local thermodynamic equilibrium; NLTE populations must be provided
  - from outside source (i.e. Degges, SHARC, AARC, etc.)
- Weighting functions, merge options, ground reflection
- Thermal multiple scattering, layer fluxes
- Standard "user" options (plot, scan, filter, etc.)
4. Delays in FSC3 release - why?

90/91 SCIENCE:

i. improved radiance algorithms:
   \[ T_{\text{bar}}(l) \text{ replaced by weighted } (T(b) + T(b+1)) \]
   [non-compatible with m.s. algorithm??]
   Default "fine" layer at observer

ii. x-sections including:
   - p-broadening, T-dependence,
   - default profiles from M. Allen, 1990

iii. "linear" Planck function interpolation

iv. HITRAN91 compatibility:
   - Line coupling and cross sections

v. TIPS: Total Internal Partition Sum
   - from Gamache & Rothman, with FSC3 extrap.

vi. isotopic implementation

vii. revised NLTE coding,
    - including efficient 4th function

viii. dayside NLTE populations from SHARC (Sharma and Robertson), ARC (Wintersteiner & Picard), and HAIRM (Degges) (composite)

ix. nightside NLTE populations being explored

x. H2O continuum extrapolation altered in near IR
   - (based on measurements at 1.06 microns)

xi. new defaults:
   - simple CO2 mixing ratio modification:
     - 330ppmv can be replaced with single option
   - default alpha(0) adjust. for line coupling:
     - 0.04cm-1 instead of 0.08 at 1 atm STP
   - default line rejection values:
     - fraction of Optical Depth & Continuum

xi. possible inclusion of GL/NRL Constituent Climatologies (CIRA-based)

90/91 CODE ENHANCEMENTS:

i. scanning/interpolation upgrades:
   - SINC, SINC**, fixed sampling
   - FTS simulations/functions (Gallery)

ii. much improved "weighting function" options:
   - renamed "sequential" transmittance/radiance
   - reduced storage requirements, E/O systems compatibility

iii. improved efficient 4th function sampling

iv. corrected FASLOW compatibility (layering)

v. I/O improvements: ASCII/binary options

vi. portability!!
   - UNIX, IBM, CRAY(?), Workstation, Apollo, etc.
   - NCAR/IDL Graphics

90/91 OTHER:

i. future directions - ? (let's get there first!)
SPECIAL OPTIONS:

- Thermal multiple scattering - (Radiance ONLY)
  
  encouraged for long slant paths at moderate to high pressure (i.e. below 15km) in the presence of scatterers (aerosols and/or clouds)
  
  10-20% effect in IR
  
  activated by IMS = 1
  
  directionally dependent
  
  increases total radiance when looking down
  
  decreases " " " up
  
  strong function of viewing angle
  
  function of scattering opacity vs total opacity
  
  ** increases FASCOD3 runtime by at least a factor of 2-3
  
  modularized coding (if IMS = 0, normal FASCOD3 execution occurs)
  
  new input parameters - surface T and emissivity
  
  - min and max altitudes for calc.
  
- Non-local thermodynamic equilibrium (NLTE) - Radiance
  
  appropriate for spectral ranges and altitudes where "hot" bands occur
  
  potentially large effects, particularly for paths above 50km
  
  activated by HIRAC = 4
  
  new input parameters - vibrational ID's
  
  - vibrational Ts or populations
  
  - standard line parameters (S, v)
  
  modularized coding
  
  improved line shape for far wings
  
  increases runtime in proportion to no. of lines

80
FASCOD3: Fast Atmospheric Signature Code

SPECIAL OPTIONS (con’t #1):

o Line coupling - Optical depth, transmittance, and radiance

  important in vicinity of strong Q-branches and other
  "dense" band systems for which coupling coefficients
  are available (CO2 and O2 for now)
  moderate effects (contamination of remote sensing channels
  leading to T-determinations with errors > 5-10K)
  default option; activated whenever coef. are supplied
  new input parameters - coupling coef. as a fn(T)
  (recognized by LNFL routines)
  embedded coding
  modifies line shape and continua
  small effect on runtime

o Weighting Functions (Sequential Calculations)

  instrument design tool for ascertaining signature
  source regions as a fn(distance from observer)
  calculates cumulative transmittance from observer to
  points (layer boundaries) along the line-of-sight
  activated by IMRG = 3-8, 13-18, 23-28
  saves "layer-defined" monochromatic transmittances
    at dv(natural) for IMRG = 3-8; can consume large
    amnts of storage for moderate spectral range
  for IMRG = 13-18, will save only spectrally scanned
    cumulative transmittances while preserving proper
    line-by-line calculation
  for IMRG = 23-28, will save only filtered (spectrally
    integrated) cumulative transmittances, while
    preserving proper line-by-line calculation
  coding dependent on viewing geometry:
    line-by-line calc
    original pre-stored
    ground to space (IMRG = 4, 14, 24 6, 16, 26)
    space to ground (IMRG = 3, 13, 23 5, 15, 25)
    tangent (IMRG = 7, 17, 27 8, 18, 28)
  timing increases minimal to moderate
  does NOT work with IAERSL = 1,7 or IMS = 1
FASOOD3: Fast Atmospheric Signature Code

SPECIAL OPTIONS:

- Cross Section Capability - Radiance and Transmittance
  
  (activated by: IXSECT = 1)

  Currently reads HITRAN86 cross sections
  Will read HITRAN90 T-dependent cross sections
  Incorporates cross section into layer optical depths
    at the coarsest resolution possible:
      i.e. Function 1 (± 4α)
      Function 2 (± 16α)
      Function 3 (± 64α)
      Function 4 (± 25 cm⁻¹)

  ** Pressure broadened with Lorentzian convolution**

  Layer-dependent
  10 New default profiles for important greenhouse gases
    (based on M. Allen, 1990 photochemistry)

FASCODE2/3: Fast Atmospheric Signature Code

Recent Comparisons/Validation:

- Theoretical
  
    - compared with 6 line-by-line codes for
      limb, nadir, and microwave test cases
    - IR and mm wavelengths
    - line shape (including continua)
    - layering algorithm
    - transmittance, radiance, and weighting functions

  SHARC - Strategic High Altitude Radiance Code for
    NLTE comparisons (Sharma & Robertson)
  ARC/NLTE - Atm. Radiance Code (Picard & Wintersteiner)

- Laboratory (partial list; historic validation)
  
  Line coupling (Lafferty & Hoke, 1986-87)
  etc.
o Atmospheric Instruments

SCRIBE (Stratospheric Cryogenic Interferometric Balloon Experiment, AFGL) 1984-1988; multiple balloon flights with very high spectral resolution (0.06 cm\(^{-1}\)); limb and nadir radiance

HIS (High-Resolution Interferometer Sounder, Univ. of Wisconsin) 1985-1988; multiple airborne (balloon, aircraft, and shuttle) flights with high spectral resolution (0.5 cm\(^{-1}\)); limb and nadir radiance

ATMOS (Atmospheric Trace Molecule Spectroscopy instrument, JPL/NASA) 1985; spacelab (shuttle) flight with very high spectral resolution (0.01 cm\(^{-1}\)); solar occultation (transmittance)

IMORL (Infrared Mobile Optical Radiation Laboratory, NRL) 1976-1979; ground-based Fourier-transform spectrometer with very high resolution (0.06 cm\(^{-1}\)); transmittance

FASCOD3: Fast Atmospheric Signature Code

Version 3

Applications:

o Laser Propagation/
  Ground Based Laser

o Plume Signature/
  Infrared Search and Track

o Target Contrast/
  Tactical Decision Aids

o Remote Sensing/
  Improved Point Analysis Models

o Data Simulation/
  UV, Visible, IR, microwave
  NLTE, line coupling

o Instrument design & development/
  Information content, etc.

o Heating-Cooling Rate Calculations/
  Greenhouse gas absorption described by x-sections
FASCOD3: Fast Atmospheric Signature Code

DOCUMENTATION:

- "Instant" User Instructions (upon release)
  - Read tape
  - Unpack
  - Machine conversions
  - I/O "Parameter" definitions
  - Test cases
  - Sample output
  - Database access
    - (File management)

- User's Manual (release plus 5 months)
  - Expansion of "Instructions"
  - Scientific definitions
  - References
  - Description/justification of "default" choices
  - Subroutine descriptions and flow charts
  - Segment load file
  - File management

- Scientific Report (release plus 10 months)
  - All of the above AND:
    - Philosophy/history of FASCODE
    - Algorithm descriptions
      - Line-by-line functions *
      - Line shape *
      - Line coupling *
      - Continua *
      - Diffuse functions *
      - Geometry *
      - Layering selection *
      - Layer merging *
      - Weighting functions
        - Standard profiles (p, T, constituent) *
        - Aerosol/hydrometeor profiles (LOWTRA7)
        - NLTE
        - Multiple scattering
        - X-sections (greenhouse gases)
    - Test cases/templates
    - Validation
    - Comparisons
    - References
    - Hints/cautions
    - etc.
COMMON ELEMENTS: Model Atmospheres

Topics:

- Available "default" profiles for pressure, temperature, density, and molecular constituents: FASCODE, LOWTRAN, and MODTRAN all employ the same set; see AFGL Atmospheric Constituent Profiles (0-120km).

- User input options for these parameters: Again, the same type of options are employed by all three codes. However, the details of the input procedures differ, based primarily on the number of constituent variables (28 for FASCODE, 12+ for LOWTRAN and MODTRAN) and historic usage.

- New FASCOD3 "greenhouse" gas option: access to the molecular absorption cross sections available on the HITRAN86/90 databases has necessitated the addition of 10 new profiles.

- Natural climatological variability: Near-term availability of climatologically varying profiles and their statistical evaluation.

GREENHOUSE GAS PROFILES: New FASCOD3 Default Options


- FASCOD3 now includes "default" profiles for these gases, plus the capability to implement layer-by-layer optical depth/transmittance calculations.

- These profiles are based on a "one/two-dimensional photochemical model" with upgraded 1990 chemistry and/or measurements. (M. Allen, JPL)
The U.S. Army Atmospheric Science Laboratory (ASL) is planning to release the next version of the Electro-Optical Systems Atmospheric Effects Library (EOSAEL) during the first quarter of fiscal year 1992. This paper reports what the EOSAEL users have to look forward to. The climatology (CLIMAT) database has been expanded to include the continental United States and most of Canada. The aerosol phase function database (PFNDAT) database used by the EOSAEL has been expanded to include models of desert aerosols and lidar backscatter coefficients. A new Narrow Beam Multiple Scattering code will replace many of the previous scattering codes. An ultraviolet transmission and lidar code is being included. We are replacing LOWTRAN-6 with LOWTRAN-7 and including the capability of calculating contrast transmission. The target acquisition (TARGAC) and natural aerosol extinction (XSCALE) model have been improved and laser transmission (LZTRAN) should have several new wavelengths added. Several of the modules will sport an interactive interface.
The U.S. Army Atmospheric Sciences Laboratory (ASL) is planning to release the next version of the Electro-Optical Systems Atmospheric Effects Library (EOSAEL) during the first quarter of fiscal year 1992. There will be new models, upgrades to existing models, and obsolete models. Distribution will continue to be on magnetic tape and free to qualified recipients.
UNCHANGED MODELS

Many of the modules are unchanged in their physics. These are the near millimeter wave (NMMW), cloud transmission (CLTRAN), obscuration due to helicopter lofted snow and dust (COPTER), self-screening applications (GRNADE), missile smoke plume obscuration (MPLUME), contrast transmission (OVRCST) and contrast transmission (F CLOUD), natural illumination under realistic weather conditions (ILUMA), fast atmospheric scattering (FASCAT), large area screening systems applications (LASS), nonlinear aerosol vaporization and breakdown effects (NOVAE), and millimeter wave system performance (RADAR) modules.

UPGRADES TO EXISTING MODELS

• atmospheric transmittance and radiance (LOWTRN)
• laser transmission (LZTRAN)
• climatology (CLIMAT)
• munition expenditure module (KWIK)
• natural aerosol extinction (XSCALE)
• target acquisition (TARGAC)
• combined obscuration model for battlefield-induced contaminants (COMBIC)
ASL researchers are incorporating the Geophysics Laboratory’s (GL’s) latest upgrades to LOWTRAN 7, modifying the input routines to use the EOSAEL record order independent routines, and making some changes to improve portability.

The largest upgrades are the vertical structure algorithms. Bob Fiegel described this work last year.

We are writing *The Complete LOWTRAN Manual*.

Much of our time has been spent increasing the portability and putting reasonable limits and checks on many mathematical operations.

---

Several new laser wavelengths will be added.

It is not too late to request that your favorites be added.

Remember that LZTRAN is a near earth transmission code.
Data for Canada and the continental United States has been added.
An option to print out the summary data for all climate classes was added.
SOME PARTS OF NORTHERN CANADA NOT COVERED IN THIS STUDY

DISCUSSED IN US SECTION (SAME REGION NUMBERS)
• No new smoke munitions.
• Refinements to the calculation of extinction coefficients.
• The values of transmission reported by XSCALE are modified to better agree with experimental data.

XSCALE

• Increased speed in the calculations using the vertical structure models.
• The inversion–haze case has been compared with field data; good agreement was obtained.
• XSCALE now calculates transmission through thin cloud and haze layers. These paths may extend from above the layer, through the layer, to the ground below the layer.
• TARGAC has been upgraded to use the EOSAEL routine ILUMA. This replaces an independent routine that calculated illumination levels.

• A new thermal model (TCM2) for surfaces has been added. Turbulence and clutter calculations have been included in this model.

• An improved method of calculating the sky-to-ground ratio uses a delta Eddington model to account for path radiance and surface reflectance.

• COMBIC has had several modifications to fix minor bugs.

• A paper on using non-inventory smokes has been prepared.

• Instructions illustrating methodologies for adding "experimental" obscurants.
MODELS TO BE DROPPED

- The simulation of aerosol behavior in realistic environments (SABRE) and aerosol multiple scattering (MSCAT) modules will be dropped from the EOSAEL distribution.
- The SABRE model required too much customization to be used for different geographic sites.
- The MSCAT Monte Carlo code leaves far too many chances for misapplication. Most users who need a Monte Carlo code probably have their own. For those who were satisfied with MSCAT, the ASL will continue to supply it as a research code.

<table>
<thead>
<tr>
<th>NBMSCAT</th>
</tr>
</thead>
</table>

- NBMSCAT is a radiative scattering code developed by Luc Bissonnette of the Defence Research Establishment Valcartier, Canada.
- This code is an approximation to the radiative transfer equations suitable for narrow beams of light and observation points near the propagation axis.
- It handles arbitrary inhomogeneous obscurant clouds.
UVTRANS

- UVTRANS is an ultraviolet transmission, fluorescence, and lidar program developed for near earth applications.
- UVTRANS differs from LOWTRAN
  - flat earth and atmosphere approximations,
  - pressure parameterization valid for near earth only,
  - single aerosol model valid for visibilities less than 50 kilometers,
  - includes some different trace gasses.

USER INTERFACE IMPROVEMENTS

- We are developing an interactive user interface.
- There will be a demonstration available during the breaks. We would appreciate any comments on the work that is shown.
- We hope to have both a generic interface that can be used on any computer system and a more customized version for MS-DOS PC's.
- The interactive interface will also create a normal EOSAEL input file for later reuse or modification.
GRADE OF SOFTWARE

The ASL will be evaluating all of the modules to assign a grade. These grades are not the same as "validating" the codes.

| Research         | Describes phenomena based on a physical or meteorological theory.  
                   | Limited evaluations in the field or laboratory. |
|------------------|-------------------------------------------------|
| Developmental    | Tailored version of a research model.  
                   | Limits of applicability have been defined.  
                   | At least "several" evaluations have been made. |
| Fieldable        | Applicability has been defined.  
                   | Confidence has been established throughout the community.  
                   | "Many" evaluations have been "passed".  
                   | The model has been verified for its stated usage. |

AVAILABILITY

- EOSAEL92 is available to U.S. Department of Defense (DoD), specified allied organizations, and DoD authorized contractors at no cost. DoD agencies needing EOSAEL92 should send a letter of request, signed by a branch chief or division director, to the ASL. Contractors should have their DoD contract monitor send the letter of request. Allied organizations must request EOSAEL92 through their national representative.

- Please include, within security restrictions, your intended use(s). Also, indicate what type of nine-track tape your computer can read. We can make "ASCII" tapes, VAX VMS BACKUP tapes, and UNIX "tar" format tapes in either 1600 or 6250 bpi.

- (505) 678-5563 Commander/Director
  FAX (505) 678-2432 U.S. Army Atmospheric Sciences Laboratory
  DSN 258-5563 ATTN: SLCAS-AA-A (Dr. Wetmore)
  awetmore@wsmr-enh73.army.mil White Sands Missile Range, New Mexico 88002-5501
BATTLEFIELD ATMOSPHERICS CONFERENCE

Formerly the EOSAEL/TWI Conference
2-6 December 1991
Fort Bliss, Texas

Mailing Address:
Commander/Director
U.S. Army Atmospheric Sciences Laboratory
ATTN: Battlefield Atmospherics Conference
White Sands Missile Range, New Mexico 88002-5501
HITRAN'91:
THE CONTEMPORARY SPECTROSCOPIC MOLECULAR DATABASE

L.S. Rothman
Geophysics Directorate, Optical Environment Division, Simulation Branch (OPS),
Hanscom Air Force Base, MA 01731-5000

The spectroscopic molecular database, HITRAN, is the DOD and international standard compilation of absorption parameters that enable the calculation of atmospheric spectral simulations from the microwave through the visible. A new edition of HITRAN has been made available in the first quarter of 1991. The current edition contains over 65 megabytes of high resolution data of transitions for 30 species and their atmospherically significant isotopic variants. In addition, there is a file of new cross-sections for heavy molecular species, with bands at several representative temperatures that should facilitate some quantitative retrievals. This task will summarize some of the major updates, improvements, and modifications.
HITRAN'91:
The Contemporary Spectroscopic Molecular Database
Laurence S. Rothman
Geophysics Directorate
Optical Environment Division
Simulation Branch (OPS)
Hanscom AFB, MA 01731-5000 USA

Abstract

The spectroscopic molecular database, HITRAN, is the DOD and international standard compilation of absorption parameters that enable the calculation of atmospheric spectral simulations from the microwave through the visible. A new edition of HITRAN has been made available in the first quarter of 1991. This current edition contains over 65 Megabytes of high resolution data of transitions for 30 species and their atmospherically significant isotopic variants. In addition, there is a file of new cross-sections for heavy molecular species, with bands at several representative temperatures that should facilitate some quantitative retrievals. This talk will summarize some of the major updates, improvements, and modifications.

Major Molecular Parameter Updates

- H₂O
- CO₂
- O₃
- CH₄
- CO, HNO₃, HCl, HF, HI, HBr...
- Cross-sections (ClONO₂, CFC's, N₂O₅...
### Water Vapor (H₂O)

<table>
<thead>
<tr>
<th></th>
<th>V_{\text{min}}</th>
<th>V_{\text{max}}</th>
<th># bands</th>
<th># lines</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5904</td>
<td>7965</td>
<td>9</td>
<td>3112 *</td>
</tr>
<tr>
<td>2</td>
<td>8036</td>
<td>9482</td>
<td>9</td>
<td>1874</td>
</tr>
<tr>
<td>3</td>
<td>9603</td>
<td>11481</td>
<td>9</td>
<td>2484</td>
</tr>
<tr>
<td>4</td>
<td>11661</td>
<td>12741</td>
<td>5</td>
<td>714 *</td>
</tr>
<tr>
<td>5</td>
<td>13238</td>
<td>22657</td>
<td>41 (39,2)</td>
<td>4608</td>
</tr>
<tr>
<td>6</td>
<td>782</td>
<td>2745</td>
<td>2</td>
<td></td>
</tr>
</tbody>
</table>

All new regions have been taken at the Kitt Peak Solar Observatory using the FTS and long-path cell. These data replace older parameters that were observed using grating spectrometers and a path through the atmosphere. Most notable improvement in intensities of weak lines. In the case of data from Toth, a hybridization with '86 lines was used to supplement his data.

1. Toth, JPL
2. Flaud & Camy-Peyret (FCP), Paris
3. FCP
4. Toth
5. FCP | extends spectral range of compilation
6. Toth
Carbon Dioxide (CO$_2$)

1. **New Line Positions:** New fit of observed high resolution data by Hawkins & Rothman (including some DND points to supplement data). New data includes very high vibrational 4.3-μm observations of Bailly *et al.* (Orsay) and the 15-μm observations of Esplin *et al.* (GL).

2. **New Intensities:** New intensity observations of Dana *et al.* (Paris) and Johns (NRC). Calculations by Wattson & Rothman for unobserved bands, include Herman-Wallis coefficients.

3. **Revised Halfwidths:** Self- and Foreign-broadened halfwidths and temperature dependence now based on work at Ecole Centrale.

Ozone (O$_3$)

<table>
<thead>
<tr>
<th></th>
<th>$v_{\text{min}}$</th>
<th>$v_{\text{max}}$</th>
<th># bands</th>
<th># lines</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>557</td>
<td>900</td>
<td>2</td>
<td>12 085</td>
</tr>
<tr>
<td>2</td>
<td>919</td>
<td>1271</td>
<td>18</td>
<td>42 500</td>
</tr>
<tr>
<td>3</td>
<td>934</td>
<td>1178</td>
<td>4</td>
<td>13 590</td>
</tr>
<tr>
<td>4</td>
<td>1319</td>
<td>2322</td>
<td>19</td>
<td>44 926</td>
</tr>
</tbody>
</table>
Ozone (O₃)

1. New data for $v_2$ and $2v_2 - v_2$ from Pickett (JPL) et al.

2. Revamping of 10-μm region. This time includes many new bands and hot bands.

3. Isotopic bands of 10-μm region from FCP & Rinsland (NASA Langley)

4. Many new combination bands from Goldman (Denver)

Methane (CH₄)

<table>
<thead>
<tr>
<th>$v_{\text{min}}$</th>
<th>$v_{\text{max}}$</th>
<th># bands</th>
<th># lines</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>6185</td>
<td>31 (21,6,4)</td>
</tr>
<tr>
<td></td>
<td>37 207</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>2902</td>
<td>3147</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>309</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

1. Major improvement by Brown (JPL).

2. Updated mono-deuterated methane bands by Brown.
Other Molecular Species

- CO (carbon monoxide): Update, primarily for HITEMP (Tipping)
- NO (nitric oxide): Update of fundamental (Ballard)
- NO₂ (nitrogen dioxide): Update of ν₃ region (Perrin, FCP)
- HNO₃ (nitric acid): Addition of new bands (fundamentals and combinations, 410 to 1400 cm⁻¹) (Goldman, Maki, Perrin, et al.)
- HCl, HF, HI, HBr (hydrogen halides): Update, primarily for HITEMP (Tipping, et al.)

Other Molecular Species (continued)

- H₂O₂ (hydrogen peroxide): Update of ν₆ band, 138-1500 cm⁻¹ (Hillman)
- C₂H₂ (acetylene): Addition of ν₅ band, 1192-1470 cm⁻¹ (Rinsland et al.)
- C₂H₆ (ethane): Addition of ν₇ band, 2973-3000 cm⁻¹ (Goldman, Dang-Nhu, Bouanich)
- COF₂, SF₆: New species on compilation (Goldman, Rinsland, et al.)
- OCS, N₂ ...

Updates generally include all parameters of HITRAN format.
Cross-sections (Supplemental files)

CFC's now at six temperatures: 203, 213, 233, 253, 273, and 293K. N₂O₅ at 233, 253, 273, and 293K. ClONO₂ at 213 and 296K.

<table>
<thead>
<tr>
<th>Species</th>
<th>Vₘᵢₙ</th>
<th>Vₘₐₓ</th>
<th># lines</th>
</tr>
</thead>
<tbody>
<tr>
<td>CFC-11 (CCl₃F)</td>
<td>830</td>
<td>860</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1060</td>
<td>1107</td>
<td>31 146</td>
</tr>
<tr>
<td>CFC-12 (CCl₂F₂)</td>
<td>867</td>
<td>937</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1080</td>
<td>1177</td>
<td>67 542</td>
</tr>
<tr>
<td>CFC-13 (CCl₃F)</td>
<td>765</td>
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<td>1065</td>
<td>1140</td>
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<tr>
<td></td>
<td>1170</td>
<td>1235</td>
<td>72 804</td>
</tr>
<tr>
<td>CFC-113 (C₂Cl₃F₃)</td>
<td>780</td>
<td>995</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1005</td>
<td>1232</td>
<td>5304</td>
</tr>
</tbody>
</table>

Cross-sections (continued)

<table>
<thead>
<tr>
<th>Species</th>
<th>Vₘᵢₙ</th>
<th>Vₘₐₓ</th>
<th># lines</th>
</tr>
</thead>
<tbody>
<tr>
<td>CFC-114 (C₂Cl₂F₄)</td>
<td>815</td>
<td>860</td>
<td></td>
</tr>
<tr>
<td></td>
<td>870</td>
<td>960</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1030</td>
<td>1067</td>
<td></td>
</tr>
<tr>
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<tr>
<td></td>
<td>1680</td>
<td>1790</td>
<td>26 622</td>
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</tbody>
</table>

104
SELECT OPTIONS

Input:
1. \(v_1\) and \(v_2\) (Initial and final frequencies of selection)
2. Molecule
3. Isotope
4. \(v', v''\) (upper and lower "global" quanta)
5. \(S_{\text{crit}}\) (Intensity cutoff)

Output:
1. Batch file for input
2. Files for input to subsequent programs
   (direct image; '82 format; user defined)
3. Temperature Correction
4. Hard copy listing
   (codes converted to spectroscopic and chemical notations;
   80 or 132 columns printers)

MAJOR CONTRIBUTORS

D. C. Benner       J. W. C. Johns
L. R. Brown        A. G. Maki
V. Dana            S. T. Massie (NCAR)
V. Malathy Devi    C. P. Rinsland
J.-M. Flaud        L. Rosenmann
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A. Goldman         R. Tipping
J. M. Hartmann     R. A. Toth
R. L. Hawkins      R. B. Wattson
SUMMARY


★ Improvements notable for remote sensing, laser transmission, climate modeling, use of heavy species...

★ References and Error criteria now implemented.

★ SELECT faster and more flexible.

★ New media and structure for the database to materialize.

★ HITEMP to be available in '91.
The latest version of the Strategic High-Altitude Radiance Code (SHARC), SHARC-2, is now available. The new version contains significant upgrades, the most important being a fully integrated auroral model with time-dependent chemistry, extension down to 50 km altitude, and incorporation of the minor isotopes of CO$_2$. SHARC calculates atmospheric radiance and transmittance over the 2-40 $\mu$m spectral region and includes arbitrary paths within 50 and 300 km altitude. It models radiation due to NLTE (Non-Local Thermodynamic Equilibrium) molecular emission which are the dominant sources at these altitudes. It calculates molecular radiation on a line-by-line basis and has a spectral resolution of 0.1 cm$^{-1}$. SHARC uses an equivalent-width formalism to obtain the total transmittance for each line, thus alleviating the need for the usual numerical integration over the line shape.
SHARC
THE STRATEGIC HIGH-ALTITUDE RADIANCE CODE

BY
DAVID ROBERTSON, LARRY BERNSTEIN,
JAMES DUFF, JOHN GRUNINGER, ROBERT SUNDBERG,
SPECTRAL SCIENCES, INC.,
RAMESH SHARMA,
PHILLIPS LABORATORY/OPS
REBECCA HEALEY,
YAP ANALYTICS, INC.

11 JUNE 1991

OUTLINE

• SHARC-2 OVERVIEW

• MAJOR MODULES
  - RADIATIVE EXCITATION (NEMESIS)
  - AURORAL MODULE

• VALIDATION EXAMPLES

• ILLUSTRATIVE RUN TIMES

• CONCLUDING REMARKS
SHARC-2 OVERVIEW

- **SHARC calculates NLTE radiation from ambient and auroral atmospheres**

- **Basic Features:**
  - 50-300 km altitude regime
  - 2-40 μm with resolution of 0.5 cm⁻¹
  - Arbitrary viewing geometries
  - Interactive input module with error checking
  - Adjustable chemical kinetics mechanisms/rates
  - Automatically includes LTE & NLTE contributions
  - Ambient molecules include: \( \text{H}_2\text{O}, \text{O}_3, \text{CO}, \text{NO}, \text{OH}, \text{CO}_2 \), its important isotopes
  - Auroral module with: \( \text{NO}^+, \text{NO}, \text{CO}_2 \)
  - Multiple output options
  - FORTRAN source code provided

**ILLUSTRATIVE SHARC CALCULATION**

- Space viewing through a 50km limb path

![Illustrative SHARC Calculation Diagram](image)
SHARC-2 FLOW CHART

INPUT

SPECTRAL RADIANCE

OUTPUT


definition

radiances

layers

other environments

profile of excited-state populations

spectral radiances and transmittances

in-band radiant intensity

AMBIENT POPULATIONS MODULE

• SYMBOLIC DESCRIPTION OF CHEMICAL KINETICS MECHANISM
  - BASED ON WIDELY USED SANDIA CHEMKIN CODE
  - EXAMPLE:  \[ M + O + O_2 \rightarrow M + O_3(000) \]
  \[ M + O_3(001) \rightarrow M + O_3(000) \]
  \[ O_3(001) \rightarrow O_3(000) + h\nu \]

• RATE EQUATIONS SOLVED IN STEADY STATE
  - ASSUMES RATE EQUATIONS DEPEND LINEARLY ON VIBRATIONAL POPULATION

• MONTE CARLO CALCULATION FOR FIRST-ORDER RADIATIVE ENHANCEMENT
  - MULTIPLE APPLICATION YIELDS HIGHER ORDER ENHANCEMENTS
RADIATIVE EXCITATION MODULE
(NEMESIS)

- RADIATIVE EXCITATION SIGNIFICANTLY ENHANCES THE EXCITED-STATE POPULATIONS OF STRONG BANDS AND HENCE THE STRENGTH OF THEIR EMISSIONS

- BASIC MODEL ASSUMPTIONS
  - SEMI-INFINITE PLANE-PARALLEL HOMOGENEOUS LAYERS
  - VOIGT LINESHAPE
  - TRANSLATIONAL-ROTATIONAL EQUILIBRIUM
  - COMPLETE LINE FREQUENCY REDISTRIBUTION
  - COMPLETE ROTATIONAL LEVEL REDISTRIBUTION
  - NO LINE OVERLAP

ENHANCEMENT OF CO₂(ν₂)

- POPULATION ENHANCEMENT FACTOR DUE TO RADIATIVE EXCITATION

![Graph showing radiative enhancement over altitude with various enhancement orders]
RADIATIVE ENHANCEMENT FOR CO$_2$

- NO-NEMESIS CALCULATION SKIPS RADIATIVE EXCITATION

![Graph showing CO$_2$($v_2$) 15$\mu$m BAND]

SPECTRAL RADIANCE MODULE

- RADIATION TRANSPORT CALCULATION PERFORMED FOR EACH MOLECULAR LINE
  - USES GL ATMOSPHERIC ABSORPTION LINE DATABASE (HITRAN)

- RODGERS-WILLIAMS APPROXIMATION FOR THE EQUIVALENT WIDTH (W) OF A SINGLE LINE WITH A VOIGT LINESHAPE
  - NASA HANDBOOK APPROXIMATION FOR $W_D$ AND $W_L$

- LAYER-DEPENDENT LINE STRENGTHS
  - VIBRATIONAL AND ROTATIONAL TEMPERATURES

- CURTIS-GODSON APPROXIMATION
  - AVERAGING PROCEDURE FOR INHOMOGENEOUS PATHS

- LINE OVERLAP CORRECTION FOR DENSE REGIONS

- 50-70 TIMES FASTER THAN TRADITIONAL LBL APPROACH
SHARC AURORAL MODULE

- AURORAL PHENOMENOLOGY
  - STARTING POINT IS GL AARC CODE
  - ELECTRON DEPOSITION MODELS FOR DIFFERENT STRENGTH AURORAS: CLASS II, III, III+
  - SOLVES TIME/ENERGY DEPENDENT RATE EQUATIONS TO CALCULATE BOTH SECONDARY ELECTRON DISTRIBUTIONS AND THE KINETICS FOR IR RADIATORS
  - PRESENT IR MOLECULES ARE: NO, NO', CO₂

- SHARC AURORAL UPGRADE
  - GEAR'S STIFF ODE ALGORITHM USED AS REQUIRED
  - CAN ADD NEW RADIATORS VIA USER-DEFINED INPUT FILES
  - LOS CALCULATION COUPLED WITH AMBIENT REGION

- UPGRADED GEOMETRY MODEL INSURES THAT LOS TRAJECTORIES INTERSECT AURORA AS DESIRED

ILLUSTRATIVE AURORAL ENHANCEMENT

- RELATIVE STRENGTHS FOR PATH 90 km - SPACE

![Graph showing spectral radiance vs. frequency](image-url)
**COMPARISON TO AURORAL FIELD DATA**

- FWI DATA (FIELD WIDENED INTERFEROMETER)
- VERTICAL PATH TO SPACE FROM 90 KM
- CLASS II AURORA (~12 K RAYLEIGHS)
- SHARC CALCULATION FOR CLASS II (10 KR)
- MODEL CALCULATION USES A CONSTANT ELECTRON DOSE RATE BUT
- AURORA IS LIKELY STRONGLY PREDOSED

**LOCALIZED ATMOSPHERIC REGIONS**

- EXTENDED ATMOSPHERE PLUS LOCAL (AURORAL) REGIONS - POPULATIONS DEFINED IN EACH REGION
- LOS IS COMPOSED OF MULTIPLE HOMOGENEOUS SEGMENTS WITHIN EACH REGION
**SPIRE: DAYTIME CO$_2$ (4.3 µm)**

- STRONG SOLAR PUMPING VIA EXCITATION OF 2.7µm BAND

![Graph showing altitude vs. limb radianc](image)

**COMPARISON TO NO (5.3 µm) DATA**

- SIGNIFICANT VARIABILITY IN OBSERVED NO RADIANCES

![Graph showing altitude vs. limb radianc](image)
**COMPARISON TO O_3(9.6 \mu m) DATA**

- SPIRIT I AND SPIRE DATA FOR NIGHTTIME CONDITIONS

![Graph showing comparison between SPIRIT, SPIRE, and SHARC data for Limb Radiance (W/cm²/sr) versus Altitude (km).]

**RUN TIMES - CHEMISTRY**

- CHEMISTRY ONLY REPEATED FOR MODIFIED ATMOSPHERE

- AMBIENT POPULATIONS
  - 89 BANDS OF H_2O, CO_2, O_3, CO, NO, OH
  - 26 OF WHICH REQUIRE RADIATION TRAPPING TREATMENT
  - 66 ATMOSPHERIC LAYERS FROM 50 TO 300 KM

  DATA GENERAL AVION AV5100 (20 MIPS): 15.2 MIN
  DEC VAX 8800: 10.8 MIN
  DEC VAX 780: 80.1 MIN

- AURORAL POPULATIONS (ADDITIONAL TO AMBIENT)
  - 31 VIBRATIONAL STATES: NO(13), NO'(14), CO_2(4)
  - 37 RADIATING BANDS: NO(23), NO'(13), CO_2(1)
  - 36 LAYERS FROM 80 TO 150 KM

  DATA GENERAL AVION AV5100 (20 MIPS): 7-12 MIN
  DEC VAX 8800: 5-8.5 MIN
  DEC VAX 780: 37-64 MIN
RUN TIMES - LOS RADIANCE

- SPECTRAL RADIANCE - SINGLE BAND
  - 14-16 μm BAND OF CO₂ WITH 890 LINES
  - 131 LAYERS (50 KM LIMB)
    DATA GENERAL AViON AV5100 (20 MIPS): 5.2 SEC
    DEC VAX 8800: 3.7 * 
    DEC VAX 780: 27.6 *

- SPECTRAL RADIANCE - MULTIPLE BANDS
  - 1-40 μm BANDPASS: H₂O, CO₂, O₃, CO, NO, OH
    84,000 LINES
  - 131 LAYERS (50 KM LIMB)
    DATA GENERAL AViON AV5100 (20 MIPS): 6.3 MIN
    DEC VAX 8800: 4.5 *
    DEC VAX 780: 33.4 *

SUMMARY

- SHARC WAS DEVELOPED TO MEET SDIO REQUIREMENTS FOR A HIGH-ALTITUDE RADIANCE MODEL
  - AURORAL AND QUIESCENT ATMOSPHERES
  - MODULARIZED STRUCTURE
  - ARBITRARY PATHS ABOVE 50 km
  - FULLY INTEGRATED & LOCALIZED AURORAL REGION

- COMPATIBLE WITH SSGM STRUCTURE

- VALIDATED WITH GL FIELD DATA
**SHARC STATUS**

- **SHARC-2 WILL BE DISTRIBUTED IN JULY, 1991**
  - CODE IS READY
  - MANUAL IS BEING PRINTED

- **REQUEST (ON LETTERHEAD) FROM:**
  
  DR. RAMESH SHARMA  
  PHILLIPS LABORATORY (OL-AA)/GP/OPS  
  HANSCOM AFB, MA 01731-5000

- **ENCLOSE A 9-TRACK 1600-BPI TAPE**
RECENT DEVELOPMENTS OF THE GENLN2 LINE-BY-LINE MODEL:
STUDIES IN SUPPORT OF THE UARS PROJECT

D.P. Edwards
National Center for Atmospheric Research, Box 3000, Boulder, CO 80307

Recent developments of the general purpose line-by-line atmospheric transmittance and radiance model GENLN2 are described. Results will be presented of radiative transfer studies in support of algorithm development for the temperature sounding channels of infrared instruments aboard the Upper Atmosphere Research Satellite (UARS). The implications of spectral line shape modelling and line mixing have been considered for low altitude limb views and comparisons are made with spectra taken during the ATMOS experiment. The effect of high altitude non-LTE radiance in these channels has also been investigated.
GENLN2

Recent Developments and Studies in Support of the UARS Project

DAVID P. EDWARDS

Atmospheric Chemistry Division
National Center for Atmospheric Research
Boulder, CO

GENLN2 PROGRAMS

HITLIN
Purpose: Create fast access line data base.

- Binary, direct access line data base, allowing:
  - Fast search for first useful line
  - Pointer on each line to next line of same gas
  - Every 200 lines a record containing line number of next line of each gas
  - Ability to merge new lines into data base
  - Status number for each line indicating origin
  - Line strength scaling to avoid underflow of weak lines.
GENLN2 PROGRAMS

LAYERS
Purpose: Perform atmospheric layering.

- Model or user supplied atmospheric profile
- User specified viewing geometry
- Layer structure calculated according to max $\Delta T$ and $\Delta \alpha_{\text{Voigt}}$ across a layer or user supplied
- Ray tracing accounting for atmospheric refraction and variation of $g$.
- Curtis–Godson mean values for $T$, $p$ and gas amount.

GENLN2 PROGRAMS

GENLN2
Purpose: Line-by-line calculations.

- Spectral line shapes: Voigt (Humlicek, 1982), Doppler, Lorentz, Gross, Van-Vleck & Huber or user supplied
- CO$_2$ sub-Lorentzian line wings (Cousin et al., 1985)
- Line mixing (Edwards & Strou, 1991)
- Water vapour continuum (Clough et al., 1981)
- Heavy molecule absorption cross-sections (McDaniel et al., 1991)
- N$_2$ and O$_2$ pressure induced continua (Orlando et al., 1991)
- Temperature variation of line partition functions (Gamach et al., 1990)
- Non-LTE model based on vibrational temperature profile input (López-Puertas et al., 1986).
GENLN2 PROGRAMS

GENLN2

- Two stage line-by-line calculation: fine absorption grid close to line center, wider in the line wings
- Line cutoff at specified minimum intensity and at maximum value of $|\nu - \nu_0|$ 
- Vertical calculation: at any time the optical depth is known separately for each gas in every layer over a narrow wavenumber interval
- Parallel transmittance and radiance calculations
- Surface boundary options for radiance calculations
- Single gas emission studies for sensitivity calculations
- Gas-correlation, PMR and LMR calculation options.

GENGRP

Purpose: Graphics and spectra manipulation.

- Spectrum plotting based on NCAR graphics
- Spectra can be convolved with instrument function in the Fourier domain
- Boxcar, triangle, spectrometer (with apodizing functions) or user supplied instrument functions
- Spectrum convolution with broadband radiometer response
- Calculation of equivalent brightness temperatures.
Figure Captions

Fig. 1. A comparison of calculated transmittances and ATMOS spectra for a 22.4 km tangent height at the 617 cm\(^{-1}\) CO\(_2\) Q-branch. The upper panel shows calculated transmittance spectra (dashed line for simple Voigt model, solid line for line mixing model with sub-Lorentzian line wings). The lower panel shows the differences between the calculated transmittances and the ATMOS spectra (dashed line for the Voigt model, chain line for line mixing model with Lorentzian line wings and solid line for the line mixing model and sub-Lorentzian line wings).

Fig. 2. A comparison of calculated transmittances and ATMOS spectra for a 13.6 km tangent height at the 791 cm\(^{-1}\) CO\(_2\) Q-branch. The upper panel shows calculated transmittance spectra (dashed line for simple Voigt model, solid line for line mixing model with sub-Lorentzian line wings). The contribution of the CCl\(_4\) band is also shown (dotted line). The lower panel shows the differences between the calculated transmittances and the ATMOS spectra (dashed line for the Voigt model, chain line for line mixing model with Lorentzian line wings and solid line for the line mixing model and sub-Lorentzian line wings).

Fig. 3. ISAMS channel 7.1 radiometer signal at different tangent heights for the Voigt model (dashed line) and the line mixing model with sub-Lorentzian line wings (solid line). The wide-band signals are shown left and the PMR signals right.

Fig. 5. Calculated radiance spectra for a 13.6 km tangent height at the 791 cm\(^{-1}\) CO\(_2\) Q-branch. The upper panel shows calculated radiance spectra (dashed line for simple Voigt model, solid line for line mixing model with sub-Lorentzian line wings). The lower panel shows the CLAES blocker filter 8 etalon channel positions.

Fig. 6. CLAES blocker filter 8 etalon 3 channel radiance at different tangent heights for the Voigt model (dashed line) and the line mixing model with sub-Lorentzian line wings (solid line).
Vibrational Temperatures for CO$_2$ (11101)-(10002)
LTE 80km Limb Radiance: Subarc.Sum.#4.

NLTE 80km Day Limb Radiance: Subarc.Sum.#4, S&W.

Graph showing tangent height (km) on the y-axis and limb radiance (W/m².sr.cm⁻¹) on the x-axis. The graph includes various lines representing different conditions and equations, such as LTE, NLTE day, and NLTE night.
PRESENT STATUS OF TRANSMITTANCES AND RADIANCES MODELLING AT L.M.D.

N.A. Scott, A. Chédin, F. Chéruy, B. Tournier
(ARA/LMD) École Polytechnique, 91128 Palaiseau Cedex, France

The ARA/LMD group has years of experience in the modelling of transmittances and radiances: STRANSAC (1974), 4A (Automated Atmospheric Absorption Atlas, 1981) and 3R (Rapid Radiance Recognition, 1986) represent three generations of forward radiative transfer models characterized by their increasing efficiency regarding the computation time. They have already been and are involved in several international campaigns of intercomparisons (ITRA: Intercomparison of Transmittance and Radiance Algorithms, IRC/IAMAP). STRANSAC and 4A are presently used within the context of the modelling of high spectral resolution radiance measurements (AIRS experiment of the NASA EOS - Earth Observing System - Programme, and IASI experiment of the CNES-GLOBSAT Programme).

A description of these models as well as a report on the work in progress will be given at the time of the Conference.
"AURIC (ATMOSPHERIC ULTRAVIOLET RADIANCE INTEGRATED CODE): AN UPDATE"

R. Hugeunin, R. Hickey
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M. Minschwaner
Harvard University, Cambridge, MA 02138

G.P. Anderson, L.A. Hall, R.E. Huffman
Phillips Laboratory, Hanscom Air Force Base, MA 01731-5000

AURIC is an atmospheric ultraviolet spectral transmission and solar irradiance code that is being developed as a modification of MODTRAN. The modification provides an extension of atmospheric structure to allow more than 34 layers, including layers above 100 km. The modification also provides an extension of wavelength to 100 nm. Atmospheric specification will allow compatibility with layer specifications in SHARC. A new O2 Schumann Runge model is being developed for AURIC, but the initial release will not include airglow emissions.
AURIC
(ATMOSPHERIC ULTRAVIOLET RADIANCE INTEGRATED CODE)
AN UPDATE

ROBERT HUGUENIN AND ROBERT HICKEY (AERODYNE RESEARCH, INC.)
KEN MINSCHWANER (HARVARD UNIVERSITY)
GAIL ANDERSON, AL HALL AND ROBERT HUFFMAN
(PHILLIPS LABORATORY/GEOPHYSICS DIRECTORATE/AF SYSTEMS COMMAND)

PRESENTED AT
ANNUAL REVIEW CONFERENCE ON ATMOSPHERIC MODELS
PHILLIPS LABORATORY/GEOPHYSICS DIRECTORATE
AFSC, HANSCOM AFB, MA

11-12 JUNE 1991

AURIC DEVELOPMENT PROGRAM

GOAL: DEVELOP AN ATMOSPHERIC ULTRAVIOLET SPECTRAL TRANSMISSION
AND SOLAR IRRADIANCE CODE FOR DELIVERY TO SDIO BY
30 SEPTEMBER 1991
AURIC DEVELOPMENT PROGRAM

TECHNICAL APPROACH: MODIFY MODTRAN TO INCLUDE AN EXTENSION OF ATMOSPHERIC STRUCTURE AT ALTITUDES ABOVE 100 KM AND AN EXTENSION OF WAVELENGTH TO 100 NM. AIRGLOW EMISSIONS WILL NOT BE INCLUDED

SYSTEMS

HIGH ALTITUDE VERTICAL STRUCTURE EXTENSION

- MODTRAN/LOWTRAN7 CODE MODIFICATION TO REMOVE 33 LAYER LIMITATION
  - MODIFICATION OF EXISTING DIMENSION STATEMENTS
  - DEVELOPMENT OF NTH ORDER INTERPOLATION ROUTINE FOR CONSTITUENT PROFILES

- USER-DEFINED N-LAYER SPECIFICATION
  - LAYERS CAN BE ADDED ABOVE 100 KM
  - NUMBER OF LAYERS CAN BE INCREASED BELOW 100 KM
  - ALLOWS COMPATIBILITY WITH SHARC LAYER SPECIFICATIONS

- CONSTITUENT PROFILES WILL BE EXTENDED TO 1000 KM
  - BLOCK DATA STATEMENT EXTENSIONS
  - PROFILE SPECIFICATION IN PROGRESS
SYSTEMS

HIGH ALTITUDE VERTICAL STRUCTURE EXTENSION (CONT'D)

- STORAGE REQUIREMENTS (VIRTUAL MEMORY USED)
  - TESTS PERFORMED ON MICROVAX WITH MODTRAN CONSTITUENT PROFILES
    MODTRAN - APPROXIMATELY 533 KBYTES
    AURIC (50 LAYERS) - APPROXIMATELY 558 KBYTES
    AURIC (100 LAYERS) - APPROXIMATELY 670 KBYTES
    AURIC (200 LAYERS) - ESTIMATED, APPROX. 1 MBYTE

- ALL CURRENT FUNCTIONALITY OF MODTRAN/LOWTRAN7 HAS BEEN RETAINED

SYSTEMS

EXOATMOSPHERIC SOLAR IRRADIANCE EXTENSION

- INITIAL WAVELENGTH EXTENSION TO 1205Å
  - USE OF SUSIM (4000 - 1205Å) TABLES PLANNED
  - NOMINAL 1Å RESOLUTION DATA WITH INTERPOLATION

- SELECTION OF SOLAR ACTIVITY MODEL IN PROGRESS
**O2 SCHUMAN-RUNGE MODEL UPGRADE**

- Based on first principles model by K. Minschwaner and M. McElroy (Harvard University)

- Development of factorable temperature dependence model for compatibility with MODTRAN/LOWTRAN transmission formulation

**HARVARD SCHUMANN-RUNGE MODEL FEATURES**

- \(^3\Sigma_u^+\) and \(^3\Sigma_u^+\) energy levels from spectroscopic constants (Veseth and Lofthus, 1974; Cheung et al., 1986)

- Rotational dependence of predissociation widths (Cheung et al., 1990; Lewis et al., 1989)
HARVARD SCHUMANN-RUNGE MODEL FEATURES (CONT'D)

- Band oscillator strengths (Yoshino et al., 1983; Lewis et al., 1986); Hönl-London factors (Tatum and Watson, 1971); Full Boltzman calculation to determine individual line strengths

- Vibration: \( V' = 0, 1 \) and \( 2 \)
  \[ V'' = 0 \text{ to } 19 \]

- Rotation: \( N'' = 1 \) to 51
  \[ N' = 0 \text{ to } 50 \]

HARVARD SCHUMANN-RUNGE MODEL FEATURES (CONT'D)

- 2 principal branches \((\Delta N = \Delta J = \pm 1)\)
- 6 satellite branches \((\Delta N = \pm 1); \Delta J = 0, \pm 1; \Delta N \neq \Delta J)\)
- 2 forbidden lines \((\Delta N = \pm 3, \Delta J = \pm 1)\)
- Isotopic oxygen lines 16O 18O
- Underlying Herzburg-Schumann-Runge continua included
HARVARD SCHUMANN-RUNGE MODEL FEATURES (CONT'D)

- **INPUT**
  - O₂ SPECTROSCOPIC CONSTANTS
  - BAND OSCILLATOR STRENGTHS
  - LINE WIDTHS (FUNCTIONS OF UPPER STATE VIBRATIONAL /ROTATIONAL LEVELS)
  - TEMPERATURE

- **CALCULATION**
  - ENERGY LEVELS
  - POPULATION DISTRIBUTION
  - LINE POSITIONS
  - LINE STRENGTHS

- **SPECTRAL CALCULATION**
  \( a(\omega) = \sum \text{ALL LINES WITHIN 500 CM}^{-1}; \text{VOIGT LINE PROFILES} \)

- **VALIDATION AT 79°K AND 300°K FROM MEASUREMENTS BY HARVARD-SMITHSONIAN GROUP**

---

SCHUMANN-RUNGE TEMPERATURE DEPENDENCE MODEL

- **MODTRAN/LOWTRAN TRANSMISSION FORMULATION**

  \[
  t_v = \exp \left( -\sum \left( a_v + b_v T + c_v T^2 \right) n_j \right)
  \]

  \[
  = \exp \left( -a_v \sum n_k - b_v \frac{\sum T_k n_k}{T} - c_v \frac{\sum T^2 k n_k}{T^2} \right)
  \]

  STORED COLUMN AMOUNTS

- **TEMPERATURE DEPENDENCE MUST BE FACTORABLE, YIELDING \((a_v, b_v, c_v)\) VS. \(v\)**

  \( a_v(T) = a_v + b_v T + c_v T^2 \)

  OR \( a_v(T) = a_v + b_v T^2 + c_v T^4 \)
WORK IS PROCEEDING TO DETERMINE THE BEST SET OF BASIS FUNCTIONS AND OPTIMAL FITTING PROCEDURES TO COVER TEMPERATURE RANGE OF 100 - 500*K

- HOT AND COLD BANDS HAVE DIFFERENT TEMPERATURE DEPENDENCES
- ATTEMPTING TO FIT CROSS-SECTIONS WITH POLYNOMIALS IN TEMPERATURES
- DIFFERENT FITTING PROCEDURES REQUIRED ABOVE AND BELOW 275-300*K
- DOUBLE QUADRATIC FIT, PINNED TO 275*K DATA POINT YIELDS PROMISING RESULTS
Schumann–Runge Bands of $O_2$, $v''=0$
53250 to 53500 cm$^{-1}$
$T=300$ K

**Cross Section (cm$^2$)**

- Wavenumber (cm$^{-1}$):
  - 53250
  - 53300
  - 53350
  - 53400
  - 53450
  - 53500

**Absorption Cross Section (cm$^2$)**

- Wavenumber (cm$^{-1}$):
  - 53300
  - 53400
  - 53500
Atmospheric Transmission

--- Model Sigma       --- Exact Sigma (Harvard)

Optical Depth

52500  52550  52600  52650  52700  52750
Frequency - cm⁻¹

Transmission

52500  52550  52600  52650  52700  52750
Frequency - cm⁻¹
Atmospheric Transmission

--- Model Sigma --- Exact Sigma (Harvard)

Transmission

Frequency - cm⁻¹

Atmospheric Transmission

--- OD(m)/OD(e) --- TR(m)/TR(e)

Ratios

Frequency - cm⁻¹
SUMMARY

- AURIC IS AN EXTENSION OF MODTRAN
  - EXTENDED ATMOSPHERIC STRUCTURE
    - 33 LAYER LIMITATION REMOVED
    - LAYERS CAN BE ADDED ABOVE 100 KM
    - CONSTITUENT PROFILES EXTENDED TO 1000 KM
  - WAVELENGTH RANGE EXTENDED TO 1205 Å
    - EXTENSION OF EXOATMOSPHERIC SOLAR IRRADIANCE
    - ADDITION OF IMPROVED O\textsubscript{2} SCHUMANN-RUNGE MODEL
  - FULL MODTRAN FUNCTIONALITY RETAINED

- AURIC PROVIDES ATMOSPHERIC SPECTRAL TRANSMISSION AND SOLAR IRRADIANCE

- AURIC 1.0 WILL NOT INCLUDE AIRGLOW EMISSIONS

- DELIVERY TO SDIO BY 30 SEPTEMBER 1991
ONTAR'S PC COMPATIBLE LOWTRAN7 PACKAGE

P.V. Noah, J. Schroeder
Ontar Corporation, 129 University Road, Brookline, MA 02146

PCTRAN7 is an implementation of the Phillips Laboratory/Geophysics Directorate's LOWTRAN7 model and associated software for the IBM and compatible family of personal computers. The package contains software for input generation, help for LOWTRAN7 parameters, an ASCII text file viewer for output files, screen graphics capability, and hard copy graphics. The software has been validated by the PL/GP under a cooperative IR&D agreement with Ontar.

This paper will describe PCTRAN7, Version 2a, and demonstrate the capabilities of the package.
PCTRAN 7 [c]: An Implementation of the GP's

LOWTRAN 7 Model for the Personal Computer

USERS MODELING WORKSHOP
(LOWTRAN/MODTRAN/FASCODE-HITRAN)
PL/GP Hanscom AFB, MA

11 June 1991

Paul V. Noah and John Schroeder
Ontar Corporation
129 University Road
Brookline, MA 02146 - 4532
Tel: 617-739-6607  FAX: 617-277-2374

Cooperative R & D Agreement

With Geophysics Laboratory - Hanscom AFB, MA

September 1988

PC Implementation of a Software Package - LOWTRAN 7 - PCTRAN 7 [c]
LITERATURE AVAILABLE

SOFTWARE DEMONSTRATION

Ontar Corporation
129 University Road
Brookline, MA 02146 - 4532

PL/GP LOWTRAN 7 CODE

Computes Atmospheric Transmission and Radiance.

0 to 50,000 Cm\(^{-1}\) Spectral Coverage @ 5 to 20 Cm\(^{-1}\) Resolution.
All Viewing Geometries.
Default Atmospheric Profiles from Sea Level to 100 Km.
Capability for User Supplied Profiles.
Cloud, Rain and Aerosol Models.
Band Models for H\(_2\)O, O\(_3\), N\(_2\)O, CH\(_4\), CO, O\(_2\), CO\(_2\), NO, NO\(_2\),
NH\(_3\) and SO\(_2\). New UV parameters for O\(_2\) (Schumann-Runge bands and
Herzberg continuum) and updated O\(_3\) Hartley and Huggins bands.
PCTRAN 7 [c] * Version 2a

PC Version of the PL/GP LOWTRAN 7 Atmospheric Radiance & Transmission Code

Complete Implementation of the LOWTRAN 7 Code - Release 3.8.
Installation Program.
Interactive User Input Software.
Help Screens for All Input Variables.
Screen and Hard Copy Graphics Output.
Tabular Output in ASCII Format.
Batch Processing Input Software.
Plotting from Different LOWTRAN Calculations.
Expert Help.
CERTIFIED for ACCURACY by the GEOPHYSICS DIRECTORATE.

Hardware and Software Requirements

Personal Computer - XT, AT, 80386, 80486 (Compatible, Clone)

1.2 Mbyte Diskette Drive, Hard Disk

640 Kbytes of Memory

CGA, EGA, or VGA Graphics Board and Monitor - for Screen Plots

Printer - for Hard Copy

Numeric Co-processor Highly Recommended
Setup Program

Semi-automatic Installation Procedure.

Copies all files to target drive.

Sets up Printer Support.

Defines Graphics Adapter Type.

Capable of Printer ONLY Installation.

Checks Available Disk Space.

ONTAR Corporation, 129 University Road, Brookline, MA 02146, 617-739-6607

ONTAR's LOWTRAN Modules Program Suite -- Version 7.2a
LOWTRAN7/MODTRAN/SENTRAN

a. Input Shell
b. Execute Program
c. Data Plotting
d. Printer Plotting
e. View Data Output
f. View FILE7
g. View FILE8
h. Filter Input
i. Execute Filter Program
j. View Filter Output
k. Execute Scanning Program
l. Scanning Plotting
m. View FILE9
n. Multiple FILE7 Plots
o. Expert Help
x. Return to DOS

Input Function:
Initial Altitude (km) 1.500
Final Altitude/Tangent Height (km) 10.000
Initial Zenith Angle (degrees) .000
Path Length (km) .000
Earth Center Angle (degrees) .000
Radius of Earth (km) [.000 - default] .000
Type of Path Short

Initial Frequency 2000.000 cm⁻¹ Wavelength 4.000 m
Final Frequency 2500.000 cm⁻¹ Wavelength 5.000 m
Frequency Increment (wavenumber) 5.000

Run # 2 of 4 LOWTRAN7 Cards 3 & 4

PC-TRAN7 Batch Mode Manager.
ESC - Quit LOWIN (write LOWIN and LOWPLT.DAT)
F2 - Edit current run.
F3 - Edit next run.
F4 - Edit previous run.
F5 - Add new run (to end) and go to that run
F6 - Delete current run.
F7 - Go to run.

Database name MCASE3
Number of runs in this database 4 Current run 3

LOWTRAN7 Card 5
Plot Type
Type of X Axis
Type of Y Axis
Number of Decimal Digits for Y Axis
Length of X Axis (in inches)
Beginning Wavenumber/Wavelength
Ending Wavenumber/Wavelength
X Axis Annotation Interval
X - Number of Minor Ticks / Division
Length of Y Axis (in inches)
Autoscale Y Axis
Minimum Transmittance/Radiance
Maximum Transmittance/Radiance
Y Axis Annotation Interval
Y - Number of Minor Ticks / Division
Plot Grids (Graph Paper)

Transmittance in m
Linear
Linear
2
7.0000 m
4.0000 m
5.0000 m
.2000 m
5
2.00E-01
5
Coarse Grid

Run # 2 of 4 LOWPLT Scaling Plot # 1
Multiple Run Plotting Inputs

<table>
<thead>
<tr>
<th>Filename</th>
<th>Run</th>
<th>Plot Mode</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>CASE-A</td>
<td>1</td>
<td>Transmittance</td>
<td>1976 U S STANDARD</td>
</tr>
<tr>
<td>CASE-A</td>
<td>2</td>
<td>Transmittance</td>
<td>SUBARCTIC WINTER</td>
</tr>
<tr>
<td>CASE-A</td>
<td>3</td>
<td>Radiance /w Scattering</td>
<td>SUBARCTIC SUMMER</td>
</tr>
<tr>
<td>CASE-A</td>
<td>4</td>
<td>Radiance</td>
<td>MIDLATITUDE SUMMER</td>
</tr>
<tr>
<td>CASE-B</td>
<td>1</td>
<td>Transmittance</td>
<td>1976 U S STANDARD</td>
</tr>
<tr>
<td>CASE-B</td>
<td>2</td>
<td>Radiance</td>
<td>TROPICAL MODEL</td>
</tr>
<tr>
<td>CASE-B</td>
<td>3</td>
<td>Radiance /w Scattering</td>
<td>MIDLATITUDE SUMMER</td>
</tr>
<tr>
<td>CASE-B</td>
<td>4</td>
<td>Transmittance</td>
<td>SUBARCTIC SUMMER</td>
</tr>
<tr>
<td>CASE-C</td>
<td>1</td>
<td>Transmittance</td>
<td>1976 U S STANDARD</td>
</tr>
<tr>
<td>CASE-C</td>
<td>2</td>
<td>Radiance</td>
<td>TROPICAL MODEL</td>
</tr>
<tr>
<td>CASE-C</td>
<td>3</td>
<td>Radiance /w Scattering</td>
<td>New Model Atmosphere</td>
</tr>
<tr>
<td>CASE-C</td>
<td>4</td>
<td>Transmittance</td>
<td>Met Data (Hor Path)</td>
</tr>
</tbody>
</table>

LOWWMIP Select Runs
PCTRAN7 Expert Help

Online Expert Help.

Guides you through common user problems.

Draws on over 5 years of PCTRAN user support.

Aides in selecting Appropriate Model:

- LOWTRAN7
- MODTRAN
- SENTRAN
- FASCODE

Helps in model parameter selection/setup.
COUPLING ATMOSPHERE AND BACKGROUND EFFECTS*

W.M. Cornette
Photon Research Associates, Inc., 9393 Towne Centre Drive, Suite 200, San Diego, CA 92121

The available atmospheric transmission models typically represent the atmosphere in significant detail, but have traditionally modelled the background very simplistically, if at all. The impact that the atmosphere has on the background (e.g., convection, evaporation, condensation, evapotranspiration, radiative loading, cloud shadowing) has recently been modelled in some detail in a computer code developed for the U.S. Army Atmospheric Sciences Laboratory (ASL). This presentation will outline the model and will discuss some of the additional atmosphere-to-background and background-to-atmosphere coupling required (e.g., surface air heating by the background).

*This work was funded by the U.S. Army Atmospheric Sciences Laboratory under Contract No. DAAD07-90-C-0149; Dr. Patti Gillespie, Technical Monitor
COUPLING ATMOSPHERE AND BACKGROUND EFFECTS

JUNE 1991

Presented at the 14th Annual Review Conference on Atmospheric Transmission Models
11-12 June 1991, Geophysics Directorate, Phillips Laboratory, Hanscom AFB, MA

Work Funded In Part by the U.S. Army Atmospheric Sciences Laboratory
Under Contract No. DAAD07-90-C-0149; Dr. P. Gillespie, Technical Monitor

Presented By:
Dr. William M. Cornette

Photon Research Associates, Inc.
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San Diego, CA 92121

OBJECTIVE

Development of a Computer Model Which May be Used to
Characterize the Amount of Thermal Clutter in a Scene
Viewed by a Thermal Imager and How the Clutter Level
Changes with Changing Atmospheric Conditions
ATMOSPHERIC EFFECTS ON BACKGROUND

- Temperature
  - Convection
  - Evaporation/Condensation/Evapotranspiration

- Radiative Loading
  - Direct Solar Loading
  - Scattered Solar Loading
  - Thermal Loading
  - Scattered Thermal Loading

- Background Type
  - Polar Regions
  - Mid-Latitudes
  - Deserts
  - Tropics

ENERGY FLUX

- Radiation
  - Emitted
  - Absorbed Solar
  - Absorbed Thermal

- Sensible (Direct)
  - Free Convection
  - Forced Convection

- Latent (Indirect)
  - Evaporation
  - Condensation
  - Evapotranspiration

- Ground/Submedium
  - Conduction
  - Convection (Water)
TERRAIN MATERIALS

- Water
- Snow
- Ice
- Broadleaf Trees*
- Pine Trees
- Irrigated Low Vegetation
- Meadow Grass
- Tundra
- Scrub
- Sand
- Rock
- Packed Dirt
- Tilled Soil
- Urban Commercial
- Urban Residential
- Asphalt
- Concrete
- Metal Building Roof

* Summer and Winter Variations

PARAMETERS

- Atmosphere
  - Pressure Profile
  - Temperature Profile
  - $\text{H}_2\text{O}$, $\text{CO}_2$, $\text{O}_3$ Profiles
  - Wind Speed
  - Cloud Cover and Altitude

- Background
  - Solar Absorptivity \{ From Reflectivity
  - Thermal Emissivity
  - Thermal Conductivity
  - Submedium Temperature
  - Roughness
  - Density
  - Specific Heat

- General
  - Latitude
  - Time
  - Date
TERRAIN ALTITUDE MAP

- National Geophysical Data Center (NGDC) Global 10-Minute Terrain Data Base

- Resample with $1^\circ$ Latitude and Variable Longitude Resolution

GLOBAL TERRAIN SCENES (DETERMINISTIC)

- City/Harbor Land/Sea Interface
- Arctic Tundra Land/Sea Interface
- Forested Low Relief Terrain
- Subarctic Rocky Land/Sea Interface
- Forested Terrain/Agricultural Terrain
- Flat Agricultural
- Desert Pavement with Dunes
- Desert Land/Sea Interface
- Forested Mountains/Cultural
- Multi-Year Sea Ice
- Arctic Mountains with Scrub
- Arctic Tundra with Melt Lakes
- Open Ocean
- Mixed Farmlands/Orchards
- Southern California Land/Sea Interface

San Diego, CA
Point Barrow, AK
Wa Wa, Ontario, Canada
Trondheim, Norway
Fulda, Germany
Alberta, Canada
Imperial Valley, CA
Salton Sea, CA
Santa Cruz, CA
Beaufort Sea
Brooks Range, AK

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GLOBAL TERRAIN SCENES (MODIFIED)

- Tundra
- Pine Forest
- Mixed Forest/Farmland
- Grass Land - Savannah
- Scrub - Chaparral
- Scrub - Desert
- Urban
- Rural Land/Sea Interface
- Tropical Forest
- Tropical Savannah
- Tropical Desert
- Tropical Land/Sea Interface

SCENE TYPE MAP

Blue - Ocean
Light Blue - Sea Ice
White - Continental Ice
Green - Tropical Forest
Tan - Grassland
Brown - Scrub Desert
Grey - Mixed Forest/Farmland
Red - Forested Mountains
Pink - Arctic Mountains
Purple - Tropical Savannah
Black - Other
HEAT BALANCE OF THE EARTH

- Solar Radiation

- Terrestrial Radiation

HEAT TRANSFER

LAYERS

HIGH CLOUDS

MIDDLE CLOUDS

LOW CLOUDS

GROUND

- Short Wave ($\alpha_s$)
  (0.25 - 4.0 $\mu$m)
  - Direct Beam
  - Upward Diffuse
  - Downward Diffuse

- Long Wave ($\varepsilon_{th}$)
  (4.0 $\mu$m - 25 $\mu$m)
  - Upward Diffuse
  - Downward Diffuse

- Multiple Scattered
SURFACE TEMPERATURE MAPS

- NOAA Nimbus-7 C-Matrix Data Base
- Air Force Surface Temperature Analysis Base

CLOUD COVER MAPS
(NOAA NIMBUS-7 C-MATRIX DATA BASE)
TROPICAL ATMOSPHERE

- Thermal Loading by Atmosphere Dominates at Night
- Heavy Cloud Cover Prevents Cooling at Night
- No Day-Night Air Temperature Variations

SUBARCTIC SUMMER ATMOSPHERE

- Driven by Local Air Temperature
- Cooling Observed at Night Below Local Air Temperature
- Large Day-Night Air Temperature Variations
SUBARCTIC WINTER ATMOSPHERE

- Small Thermal and Solar Effects
- No Day-Night Air Temperature Variations
- Numerical "Noise" of Algorithm Seen in Temperature Curves

SANTA CRUZ, CALIFORNIA, SCENE

- Dawn Plus One Hour
- Noon
FULDA, GERMANY, SCENE

- Noon
- 3.7 - 4.1 μm

OPEN OCEAN SCENE

- 8 - 12 μm
SAN DIEGO, CALIFORNIA, SCENE

- Noon
- 3.7 - 4.1 \( \mu \)m

**Probability Density Function**

**Power Spectral Density**

---

**SKY NOISE**

- Thermal Sky Noise
  - Due to Temperature Fluctuations
  - Derived from \( C_n^2 \) Profiles
  - Based on Work of Kent and Korf at AMOS

- Scatter Sky Noise (Pending)
  - Variations in Aerosol Number Density
  - Variations in Aerosol Particles
  - Variations in Molecular Density
  - Variations in Index of Refraction
BACKGROUND EFFECTS ON ATMOSPHERE

- Altitude/Profile
- Atmospheric Heating
- Free Convection
- Wind Speed and Direction
- Relative Humidity
- Pollutants
- Aerosols
- Turbulence
- Cloud Cover/Type/Altitude

CURRENT STATUS

- CLUTTR Code Developed
  - Calculates PDF's and PSD's
  - Includes Atmospheric Thermal Sky Noise
  - Includes Sensor Effects, Including Human Factors

- Future Development
  - Add Atmospheric Scatter Sky Noise
  - Improve Interfaces
  - Validate Algorithms and Data Bases
  - Extend Data Bases

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SENTRAN7: A SENSITIVITY ANALYSIS PACKAGE FOR LOWTRAN 7 AND MODTRAN

D.R. Longtin, F.M. Pagliughi, N.L. Paul
SPARTA, Inc., 24 Hartwell Avenue, Lexington, MA 02173

The computer code SENTRAN, originally developed by researchers at The Pennsylvania State University, permits users to rapidly evaluate transmittances and radiances from LOWTRAN in response to perturbations of input atmospheric conditions. The code provides a friendly and efficient interface to create multiple LOWTRAN input decks as well as graphical representation of the output in both 2D and 3D formats.

In the current effort, SENTRAN has been upgraded for use with LOWTRAN 7 and MODTRAN. The new computer code is called SENTRAN7. As part of the upgrade, SENTRAN7 contains improved error checking on user inputs, an enhanced online help capability and smarter editing restrictions that reflect inputs from other LOWTRAN 7 or MODTRAN input cards. Additionally, users are able to graphically display results from the standard TAPE7 and TAPE8 files. New features of SENTRAN7 include the capability to run LOWTRAN 7 or MODTRAN internally, and screen display of available input files. Finally, the framework for a sensitivity package for FASCODE will be discussed.
SENTRAN7: A SENSITIVITY ANALYSIS PACKAGE FOR LOWTRAN7/MODTRAN

Presented at
The Annual Review Conference on Atmospheric Transmission Models
June 12, 1991

David R. Longtin, Nanette L. Paul and Frank M. Pagliughi
SPARTA, Inc.
24 Hartwell Avenue
Lexington, MA 02173

Contract F19628-88-C-0038

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• We Wish to Thank the Following Individuals

– Gail Anderson and Jim Chetwynd of The Geophysics Directorate
– Charles Randall of The Aerospace Corporation
– Charles Lo Presti of The Battelle Pacific Northwest Laboratory
– Ken Tomiyama and Michael Hogan of The Pennsylvania State University
Outline of Talk

- Introduction to SENTRAN7
  - Software and Hardware Requirements
- Capabilities of SENTRAN7
  - Examples of Menus
  - New Features
- Ongoing Efforts
  - Sensitivity Package for FASCODE, SENCODE

What Is SENTRAN7?

- User Interface System Designed to Evaluate the Sensitivity of LOWTRAN7/MODTRAN* Transmittances and Radiiances to Input Variations
  - Interactive Input Module to Perturb LOWTRAN7/MODTRAN Input Parameters
  - Automatic Generation of LOWTRAN7/MODTRAN Input Decks
  - Autonomous Post-Processing of TAPE7 and TAPE8 Outputs
  - Graphical Representation of Output in 2D and 3D Formats
- Based on Original SENTRAN for LOWTRAN6 By K. Tomiyama and M. Hogan

* MODTRAN: Moderate Resolution Model for LOWTRAN7 Developed By Spectral Sciences, Burlington, MA
Software and Hardware Details
For SENTRAN7

• Structural Design
  – SENTRAN7 Coded in Fortran-77
  – Graphics Consistent with Tektronix 4014 Standards
  – Terminal Control Follows ANSI Standards

• Hardware Requirements
  – Software Developed for VAX/VMS and SUN Unix Computer Systems
  – Interactive Viewing of SENTRAN7 Graphics Use VT240 Terminal or Emulator
  – Hard Copy Output Requires Tektronix 4014 Compatible Printer/Plotter or Device Able to Interpret Tektronix 4014 Files via Special Translating Programs

• SENTRAN7 Utilizes Standard Input and Output Formats from LOWTRAN7/MODTRAN Codes

Main Menu of SENTRAN7

WELCOME TO SENTRAN7
THE SENSITIVITY ANALYSIS PROGRAM FOR LOWTRAN7/MODTRAN

1 - LOAD/SAVE
2 - EDIT
3 - COMPILE
4 - SELECT LOWTRAN7/MODTRAN
5 - RUN LOWTRAN7
6 - GRAPH & ANALYZE
7 - HELP
8 - QUIT
Description of Main Modules

- LOAD/SAVE: Load or Save SENTRAN7 Methodology Files
  - Methodology Files Contain Images of LOWTRAN7 Input Cards and Directives for Their Perturbation

- EDIT: Interactive Editing Module for Specifying LOWTRAN7 Cards and Directives for Their Perturbation
  - Editor Emulates Logical Flow Through LOWTRAN7 Input Decks
  - Each LOWTRAN7 Input Described by a Nominal Value and an Optional Perturbation Directive

- COMPIL: Creates LOWTRAN7 Input Decks Based on Information in the EDIT Module
  - Provides List of Active Molecular Absorbers in the Spectral Interval of Interest

Description of Main Modules (cont.)

- SELECT LOWTRAN7/MODTRAN: Determines Code To Be Run

- RUN LOWTRAN7/MODTRAN: Executes Selected Code

- GRAPH AND ANALYZE: Generates Graphical Plots of Data
  - Screen or Files For Hard Copy Available
  - Additional Features Include Data Manipulation and Analysis

- HELP: Provides Information About and Examples For Most SENTRAN7 Commands

- QUIT: Exit SENTRAN7 Code
FOLLOWING PARAMS. USE A PERTURBATION VALUE

\begin{align*}
M1 & \ldots & 0.000 & \text{TO 20 STEP 2} \\
M2 & \ldots & 0.000 \\
\text{ANGLE} & & 0.000 \\
\text{RANGE} & & 1.000 & \text{TO 10} \\
\text{DETA} & & 0.000 \\
\text{BO} & \ldots & 0.000
\end{align*}

FOLLOWING PARAMS. USES A PERTURBATION LIST (* IMPLIES PERTURBATION RESTRICTIONS)

LEN * 0

ALL PARAMETERS FOR CARD 3 O.K. (Y/N) [Y]

---

**Graph and Analyze Module**

- **Main Capabilities**
  - Handles TAPE7 and TAPE8 Files from LOWTRAN7 Plus Raw X-Y-Z Data Files
  - Includes Tools for Data Analysis and Archiving
  - Generates Screen Plots of Data and Graphics Files for Hard-Copy Output

- **3-D Plotting Details**
  - Permits User-Defined Rotation Angles
  - $X$ and $Y$ Axes Can Represent Wavenumber, or the First or Second LOWTRAN7 Variables Perturbed
  - Conversion to Micrometers Are Available
  - Plots For Layer-By-Layer Calculations from TAPE8 Always Make $X$-Axis the Wavenumber and and $Y$-Axis the Layer Number
Available Plots in SENTRAN7

<table>
<thead>
<tr>
<th>PLOT CATEGORY</th>
<th>SPECIFIC PLOTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Raw-XYZ</td>
<td>Transmittance: total, log of total, uniform mixed gases, trace gases, molecular scattering, H₂O, H₂O continuum, O₃, N₂ continuum, aerosol and hydrometeor, CO₂, CO, CH₄, N₂O, O₂, NH₃, NO, NO₂, SO₂, HNO₃, Aerosol and Hydrometeor Absorption</td>
</tr>
<tr>
<td>Transmittance</td>
<td>Transmittance: total, log of total, uniform mixed gases, trace gases, molecular scattering, H₂O, H₂O continuum, O₃, N₂ continuum, aerosol and hydrometeor, CO₂, CO, CH₄, N₂O, O₂, NH₃, NO, NO₂, SO₂, HNO₃</td>
</tr>
<tr>
<td>Thermal Radiance</td>
<td>Transmittance: total, log of total, Atmospheric Radiance</td>
</tr>
<tr>
<td>Differential Transmittance and Black Body Function</td>
<td>Differential Transmittance (DTAU), DTAU/layer thickness</td>
</tr>
<tr>
<td>Fluxes/Irradiance</td>
<td>Fluxes: upward total, upward solar, downward total, downward solar</td>
</tr>
<tr>
<td>Solar/Lunar Radiance</td>
<td>Transmittance: total, log of total, Radiance: total, atmospheric, path scattered, single scattered, total ground reflected, direct reflected</td>
</tr>
<tr>
<td>Direct Solar Radiance</td>
<td>Transmittance: total, log of total, solar irradiance</td>
</tr>
</tbody>
</table>

Example 3-D Plot From SENTRAN7

Total Transmittance at 1300 cm⁻¹ Versus H1 and RANGE for a Horizontal Path
Other Features of SENTRAN7

- Original SENTRAN Code Upgraded for Use with LOWTRAN7
  - Smarter Editing Restrictions That Reflect Previous User Inputs
  - Improved Error Checking on User Inputs
  - Refined Identification of Major Molecular Absorbers

- New Features in SENTRAN7
  - Compatibility with the Moderate Resolution Code, MODTRAN
  - Ability to Access LOWTRAN7/MODTRAN Codes Internally
  - Screen Display of Available Methodology and Other Input Files
  - Safeguards to Prevent Existing Files From Being Overwritten
  - Increased Portability Across Hardware Platforms
  - Online Help Available Within Editing Module
  - Tick Marks on Plots
  - Graphical Display of User-Defined Trace Gas Profiles, Card 2C Series

Ongoing Work:
Sensitivity Package For FASCODE, SENCODE

- General Approach
  - Develop Parallel Package For FASCODE, But Retain SENTRAN7 Framework
  - Use Many of SENTRAN7’s Supporting Routines
  - Limit Those FASCODE Input Cards That Can Be Perturbed

- Future Obstacles
  - Method of Effectively Dealing With FASCODE Output Files
  - Output May Exceed SENTRAN7’s Plotting Capabilities
  - Some Sensitivity Studies May Grossly Interfere with FASCODE’s Atmospheric Layering Package
The Strategic Scene Generation Model (SSGM) produces scenes of interest to a strategic space-based sensor, including terrain, clouds, earth limb, aurora, zodiacal light, and stars as background; and missile plumes and fuselages, post-boost and reentry vehicles as targets. In support of the various components of the SSGM are several atmospheric codes, which provide basic information regarding transmission and emitted and scattered path radiance, plus additional information required by the various background and target models. An overview of the SSGM will be presented, with emphasis on how the various atmospheric models are utilized. Comparisons between the codes will be presented, together with recommendations for upgrades to insure consistency.

*This work is being funded by the Naval Research Laboratory under Contract No. N00014-89-C-2283; H. Heckathorn, Technical Monitor.
ATMOSPHERIC MODELS IN THE STRATEGIC SCENE GENERATION MODEL

JUNE 1991

Presented at the 14th Annual Review Conference on Atmospheric Transmission Models
11-12 June 1991, Geophysics Directorate, Phillips Laboratory, Hanscom AFB, MA

Work Funded in Part by Naval Research Laboratory Under Contract No. N00014-89-C-2283
H. Heckathorn, Technical Monitor

Presented By:
Dr. William M. Cornette
David C. Anding
Photon Research Associates, Inc.
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STRATEGIC SCENE GENERATION MODEL (SSGM)

**Definition**
- Computerized Methodology Founded on State-of-Science Knowledge, Empirical Data Bases, Phenomenological Models to Generate LOS Radiometrics, 2-D Radiance Maps, Time-Sequenced Scenes, and Observables Data Bases for SDI Applications

**Objectives:**
- Provide Focus for SDIO Scene Generation Requirements
- Serve as a Standard for Testing SDI Concepts and Designs Which is Traceable to a Consistent Set of Physical Assumptions, Conditions

**Requirements:**
- **Phenomenology** = Targets, Target Related Events, Natural and Nuclear Backgrounds
- **Scenarios** = All Vehicle Types (Launch, Midcourse, Re-Entry)
- **Dimensions** = Spatial, Temporal, Spectral Sampling Regimes
- **Geometry** = All Sensor/Scene/Target Locations and Time-History Sequences
- **Connectivity** = Event-Driven, Both Passive and Active (Illuminated) Signatures
SSGM FUNCTIONAL FLOW DIAGRAM DESIGN

SSGM ATMOSPHERIC MODELS

- Earthlimb
  - MODTRAN (<60 km)
  - SHARC (>60 km)

- Backgrounds
  - APART (Terrain)
  - APART (Clouds)

- Targets
  - APART (TARSIS)
  - SIRRM (Plumes)
  - Simple Extinctions (Plumes)
SSGM PHENOMENOLOGY

SSGM EARTH LIMB PROFILES

- **Day**
  - 2.000 μm
  - 4.235 μm
  - 12.104 μm

- **Night**
  

RADIANCE (W/cm² sr⁻¹)
EARTH LIMB MODELING

- U.S. Standard Day
- 2.5 - 2.9 μm

![Graph showing limb radiance vs. altitude with LTE (MODTRAN) and NLTE (SHARC) models.](image)

**Target Altitude (km)**

**Limb Radiance (W/cm² sr)**

**Limb Radiance (W/cm² sr)**

- SHARC
- MODTRAN
- APART

![Diagram of Earth limb with models](image)
BACKGROUND SCENE MODELS

- GENESIS (Generic Scene Simulation Software) and CLDSIM (Cloud Simulation) are Collections of Computer Codes Which Generate 2-D Images of Terrestrial and Cloud Scenes

- GENESIS Uses First-Principles Algorithms Which Include Those for:
  - Surface Temperature Heat Transfer
  - Solar-Viewer Shadowing and Scene Projection
  - Thermal Emission, Solar-Skyshine Reflection
  - Atmospheric Absorption, Scattering, Emission

  Using an Input Scene Data Base Consisting of:
  - Digital Elevation Map
  - Earth Surface Material Assignment

- CLDSIM Uses the Following Assumptions and Treatments:
  - Cloud Tops are Treated as Surfaces, Emitting and Reflecting According to a Bidirectional Reflectance Function (BRDF). BRDF Varies with Cloud Optical Properties, Altitude, and Wavelength.
  - Clouds Can be Optically Thin and Transmit Radiation from Below
  - Cloud Top Temperatures Set Equal to Ambient
  - Skyshine Reflection Neglects Radiation from Neighboring Clouds

  Using an Input Scene Data Base Consisting of:
  - Digital Cloud Top Altitude Map
  - Cloud Types
GENESIS SIMULATION OF SOUTHERN CALIFORNIA COASTLINE (NADIR VIEW)

1024 x 1024 Pixels, 400 Meter Resolution, 10 - 12 μm
GENESIS SIMULATION OF CAMARILLO, CALIFORNIA (NADIR VIEW)

512 x 512 Pixels, 30 Meter Resolution, 3.6 - 4.0 μm

CLDSIM CLOUD SCENE MODEL

Atmospheric Molecular Absorption, Scattering Emission

Viewer Shadowing

Solar Reflection

Cloud Shadowing

Attenuated Background

Cloud Top Altitudes Derived From Satellite Imagery and Surface Texturing

Cloud Attenuation

Cloud Temperatures Set Equal to Ambient

Earthshine
CLDSIM SIMULATION OF MULTIPLE CLOUD TYPE HORIZON SCENE

4000 x 4000 Pixels, Nominal 400 Meter Resolution, 2.6 - 2.6 μm

APART RADIATIVE ENVIRONMENT CODE

- Full LOWTRAN 7 Compatibility
- Observables-Driven Architecture
- Molecular Absorption
  - 5 cm⁻¹ Resolution
  - 0.2-50 μm
  - Five Parameter Voight Model
- Five-Flux Multiple Scattering
- Turbulence/Sky Noise
- Forward In-Scatter
- Backgrounds
  - Contrast
  - Structured
  - Global Data Base
  - Bidirectional Materials
- Global Atmosphere Data Base
- Hydrometeors
  - Clouds (Water/Ice)
  - Fog
  - Rain
  - Snow
ATMOSPHERE MODELS

- Latitude Dependent
  - Equatorial (Summer/Winter)
  - Tropical (Summer/Winter/Annual)
  - Subtropical (Summer/Winter)
  - Midlatitude (Summer/Winter/Spring-Fall)
  - Subarctic (Summer/Winter/Special)
  - Arctic (Summer/Winter)
  - Polar (Summer/Winter)

- Special
  - U.S. Standard (1976)
  - Israeli Standard (Day/Night)
  - User-Defined

NORTHERN HEMISPHERE MODEL ATMOSPHERES

<table>
<thead>
<tr>
<th>Type</th>
<th>Latitude</th>
<th>Seasons</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equatorial</td>
<td>0°</td>
<td>Summer Winter</td>
</tr>
<tr>
<td>Tropical</td>
<td>15°</td>
<td>Annual Summer Winter</td>
</tr>
<tr>
<td>Subtropical</td>
<td>30°</td>
<td>Summer Winter</td>
</tr>
<tr>
<td>Midlatitude</td>
<td>45°</td>
<td>Summer Winter Spring/Fall</td>
</tr>
<tr>
<td>Subarctic</td>
<td>60°</td>
<td>Summer Winter Winter (Cold) Winter (Warm)</td>
</tr>
<tr>
<td>Arctic</td>
<td>75°</td>
<td>Summer Winter Winter (Cold) Winter (Warm)</td>
</tr>
<tr>
<td>Polar</td>
<td>90°</td>
<td>Summer Winter</td>
</tr>
<tr>
<td>U.S. Standard</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Israeli Standard</td>
<td>-</td>
<td>Day/Night</td>
</tr>
</tbody>
</table>
AEROSOL TYPES AND HAZE PROFILES

APART

METEORIC DUST

STRATOPAUSE

STRATOSPHERIC AEROSOLS (TEMPERATURE DEPENDENT 180 - 200 K)

TROPOPAUSE

TROPOSPHERIC AEROSOL (RELATIVE HUMIDITY DEPENDENT)

2 Km AGL

BOUNDARY LAYER AEROSOL (RELATIVE HUMIDITY DEPENDENT)

GROUND LEVEL

ATTENUATION COEFFICIENT AT 0.65 μm (Km⁻¹)

M ARITIME, RURAL AND URBAN SURFACE VISIBILITIES 80, 22, 10, 5, 2Km

GROUND LEVEL

GROUND LEVEL

RADIATIVE TRANSFER

• Three Parameter Band Model
• Volght Line Shape
• Foreign-Broadened Line Wings
• Self-Broadened Line Wings
• Spectral Region 0.20 - 0.50 μm
• Band Parameters from 1986 AFGL Line Atlas
• User-Defined Resolution (5 - 200 cm⁻¹)
• Molecular Oxygen Model Added In UV
BAND CORRELATION

- A Passive Observable Consists of
  - Thermal Emission
  - Solar Reflections
  - Skyshine Reflections
  - Earthshine Reflections
- Each Component Transmits Differently Due to Band Averaging

- Options
  - 5 cm\(^{-1}\) Resolution
  - Multiples of 5 cm\(^{-1}\) Resolution
  - "Constant" Wavelength Resolution
ATMOSPHERIC TURBULENCE EFFECTS

- Turbulence Induced Irregularities Cause Spatial and Temporal Variations of Atmospheric Index of Refraction
  - Spatial and Temporal Variations of Wavefront Amplitude
  - Spatial and Temporal Variations of Wavefront Phase
  - Scintillation
  - Image Blur

- Turbulence Induced Irregularities Also Cause Atmospheric Radiance Variations
  - Sky Noise
  - Increased Path Radiance

- These Effects Can be Estimated Using Weighted Integrals of $C_n^2$, the Index of Refraction Structure Parameter, Over the Propagation Path

APART/MODTRAN DIFFERENCES

- BAND PARAMETERS
  - Spectral Resolution
  - Spectral Range
  - Variable Resolution
  - Wavelength Resolution

- REFRACTIVITY

- RAY TRACING

- FULL SOLAR GEOMETRY

- SOLAR AND LUNAR EPHEMERIS

- MOLECULAR SCATTERING

- RELATIVE HUMIDITY (GOFF-GRATCH)

- MODIFIED PHASE FUNCTION

- ADDITIONAL MODEL ATMOSPHERES

- MULTIPLE SCATTER
  - Four-Stream
  - Exponential Sum Fit
  - Coupling

- EQUATION OF TRANSFER

- TEMPERATURE DEPENDENT BACKGROUND STRATOSPHERIC AEROSOL (150 - 300 K)

- HAZE PROFILE AND AEROSOL TYPE
  - Boundary Layer
  - Tropopause
  - Stratosphere

- HYDROMETEORS
ADDITIONAL APART CAPABILITIES

- **TURBULENCE**
  - Thermal Sky Noise
  - Scatter Sky Noise
  - Scintillation

- **ATMOSPHERE**
  - Diurnal Variations
  - Geographic Variations

- **HEAT TRANSFER**
  - Cloud Cover
  - Surface Temperature
  - Background Temperatures

- **CORRECTION FOR LAYERING PROBLEM**

- **LINE CORRELATION**

- **INTEGRATION WITH OTHER CODES**
  - Target - Multiple Scatter
  - Plume - Heat Transfer
  - Terrain - Cloud

- **FORWARD SCATTER**

- **BACKGROUNDs**
  - Space (Zodiacal, Stars, Galactic)
  - Global Scene Types
  - Materials
    - Diffuse
    - Directional
    - Bidirectional
  - Terrain Blockage

- **USER-DEFINED**
  - Atmosphere
  - Aerosol (Layered Species)
  - Hydrometeors
  - Background Scenes and Materials

- **ULTRAVIOLET**
  - \( \text{O}_2 \) - \( \text{N}_2\text{O} \)
  - \( \text{O}_3 \) - \( \text{NO}_2 \)
  - \( \text{H}_2\text{O} \) - \( \text{N}_2\text{O}_2 \)
  - \( \text{SO}_2 \) - \( \text{D}_2\text{O}_2 \)

SIRRM ATMOSPHERIC MODEL

- SIRRM Uses Early (1981) Version of APART

- Can Easily Upgrade SIRRM for Latest Version of APART
## CONCLUSIONS

<table>
<thead>
<tr>
<th>PROBLEM</th>
<th>CURRENT SOLUTION</th>
<th>DESIRED SOLUTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>LTE/NLTE &quot;Discontinuity&quot;</td>
<td>Interpolate</td>
<td>Single Code</td>
</tr>
<tr>
<td>Earthlimb vs. Backgrounds</td>
<td>None</td>
<td>Compatible or Single Code</td>
</tr>
<tr>
<td>Plume vs. Background</td>
<td>None</td>
<td>Compatible or Single Code</td>
</tr>
</tbody>
</table>
REVIEW OF THE CHEMICAL KINETIC RATE CONSTANTS USED IN THE SHARC MODEL

V.I. Lang, A.T. Pritt, Jr.
The Aerospace Corporation, PO Box 92957, Los Angeles, CA 90009

The SHARC (Strategic High Altitude Radiance Code) predicts the infrared (1-40 μm) radiance background of the Earth's atmosphere from 50 - 300 km for a variety of viewing geometries. At these altitudes the molecular species are no longer in thermodynamic equilibrium, requiring that the state populations of each emitter be calculated based on a steady state solution to a set of first-order differential equations describing the kinetic development of each emitter. Presented here is a review of the rate constants used to calculate specific vibrational level populations for H₂O, CO₂, and O₃ which are important molecular species emitting in the infrared.
REVIEW OF THE CHEMICAL KINETIC RATE CONSTANTS USED IN THE SHARC MODEL

V. I. Lang and A. T. Pritt, Jr.
The Aerospace Corporation

prepared for the
Annual Review of Atmospheric Models
June 11 - June 12, 1991

work supported by the Geophysics Directorate, Phillips Laboratory
Dr. R. Sharma, Program Manager

STRATEGIC HIGH ALTITUDE RADIATION CODE
(SHARC)
Features: NLTE Code
1 - 40 μm
50 - 300 km
Quiescent and Auroral
Various Viewing Geometries
OUTLINE

WHAT IS SHARC?

WHY AN NLTE MODEL?

CO RATE CONSTANTS

H₂O RATE CONSTANTS

NEW WORK

Solar Radiation

\[
\begin{array}{c}
\text{Absorbers} \\
\text{CO₂} \\
\text{O₃} \\
\text{CO} \\
\text{H₂O} \\
\text{OH}
\end{array}
\quad \leftrightarrow \\
\begin{array}{c}
\text{Non-Emitters} \\
\text{N₂} \\
\text{O₂}
\end{array}
\]

More

\[
\begin{array}{c}
\text{NO} \\
\text{NO}^+
\end{array}
\]
EARTH'S ATMOSPHERE

\[ \text{CO(1) + N}_2(0) \rightarrow \text{CO(0) + N}_2(1) \]

No change in rate constants.
CO(1) + O₂(0) → CO(0) + O₂(1)

CO(1) + M → CO(0) + M
CO(1) + O → CO(0) + O

TABLE 1: Revisions to CO Kinetics

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Current SHARC Coefficients(a)</th>
<th>Revised Coefficients(a)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$A_i$</td>
<td>$C_i$</td>
</tr>
<tr>
<td>M + CO(1) - M + CO(0)</td>
<td>6.67e-08</td>
<td>208.3</td>
</tr>
<tr>
<td>M + CO(0) - M + CO(1)</td>
<td>6.67e-08</td>
<td>208.3</td>
</tr>
<tr>
<td>M + CO(2) - M + CO(1)</td>
<td>1.33e-07</td>
<td>208.3</td>
</tr>
<tr>
<td>M + CO(1) - M + CO(2)</td>
<td>1.33e-07</td>
<td>208.3</td>
</tr>
<tr>
<td>M + CO(2) - M + CO(0)</td>
<td>1.33e-07</td>
<td>208.3</td>
</tr>
<tr>
<td>M + CO(0) - M + CO(2)</td>
<td>1.33e-07</td>
<td>208.3</td>
</tr>
<tr>
<td>O + CO(1) - O + CO(0)</td>
<td>9.90e-08</td>
<td>118.1</td>
</tr>
<tr>
<td>O + CO(0) - O + CO(1)</td>
<td>9.90e-08</td>
<td>118.1</td>
</tr>
<tr>
<td>O + CO(2) - O + CO(1)</td>
<td>1.98e-07</td>
<td>118.1</td>
</tr>
<tr>
<td>O + CO(1) - O + CO(2)</td>
<td>1.98e-07</td>
<td>118.1</td>
</tr>
<tr>
<td>O + CO(2) - O + CO(0)</td>
<td>1.98e-07</td>
<td>118.1</td>
</tr>
<tr>
<td>O + CO(1) - O + CO(2)</td>
<td>1.98e-07</td>
<td>118.1</td>
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</table>
TABLE I (cont.): Revisions to CO Kinetics

<table>
<thead>
<tr>
<th>V-V Reactions(^{(d)})</th>
<th>Current SHARC Coefficients</th>
<th>Revised Coefficients</th>
<th>(A_i)</th>
<th>(C_i)</th>
<th>(D_i)</th>
<th>(A_i)</th>
<th>(C_i)</th>
<th>(D_i)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO((0) + N_2(1) \rightarrow CO(1) + N_2(0))</td>
<td>6.98e-13</td>
<td>25.6</td>
<td>0.0</td>
<td>2.20e-13</td>
<td>18.7</td>
<td>0.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CO((1) + N_2(0) \rightarrow CO(0) + N_2(1))</td>
<td>6.98e-13</td>
<td>25.6</td>
<td>268.5</td>
<td>2.20e-13</td>
<td>18.7</td>
<td>268.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CO((0) + O_2(1) \rightarrow CO(1) + O_2(0))</td>
<td>3.50e-10</td>
<td>124.0</td>
<td>844.4</td>
<td>1.68e-13</td>
<td>50.2</td>
<td>844.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CO((1) + O_2(0) \rightarrow CO(0) + O_2(1))</td>
<td>3.50e-10</td>
<td>124.0</td>
<td>0.0</td>
<td>1.68e-13</td>
<td>50.2</td>
<td>0.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(hv) Emission(^{(e)})</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CO((1) \rightarrow CO(0) + hv)</td>
<td>30.96</td>
<td>0.0</td>
<td>0.0</td>
<td>30.96</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td></td>
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<tr>
<td>CO((2) \rightarrow CO(1) + hv)</td>
<td>60.45</td>
<td>0.0</td>
<td>0.0</td>
<td>60.45</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CO((2) \rightarrow CO(0) + hv)</td>
<td>1.03</td>
<td>0.0</td>
<td>0.0</td>
<td>1.03</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- a) Landau-Teller function: \(k = A_i T^{B_i} \exp(-C_i T^{333} - D_i T^{-1})\); \(B_i = 0\) for all reactions included here.
- b) \(D_i = \Delta E (cm^{-1})^{1.44}\)
- c) efficiencies of collision partner are listed below each reaction
- d) rate units are \(cm^3\) molecules\(^{-1}\) s\(^{-1}\)
- e) rate units are s\(^{-1}\); rates for reverse processes are zero

Old SHARC CO Kin
Revised CO Kinetics
Atmosphere: Equator
Day 180, noon
Path: 200 km limb

FIG. 1: CO (1-0) and (2-1) BAND RADIANCE
FIG. 2: CO (2-0) BAND RADIANCE

\[ \text{H}_2\text{O} (010) + \text{M} \rightarrow \text{H}_2\text{O} (000) + \text{M} \]
### TABLE 1: Rate Coefficients for Relaxation of H₂O (kᵢ = Aᵢ Tᵢ exp[-ΔCᵢ / T] - Eᵢ / T)

<table>
<thead>
<tr>
<th>REACTIONS</th>
<th>REVISED RATE COEFFICIENTS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Aᵢ</td>
</tr>
<tr>
<td>M + H₂O(010) = M + H₂O(000)</td>
<td>5.37E-10</td>
</tr>
<tr>
<td>M + H₂O(000)</td>
<td>4.60E-13</td>
</tr>
<tr>
<td>M + H₂O(010)</td>
<td>5.37E-10</td>
</tr>
<tr>
<td>M + H₂O(010)</td>
<td>5.37E-10</td>
</tr>
<tr>
<td>M + H₂O(000)</td>
<td>4.60E-13</td>
</tr>
<tr>
<td>M + H₂O(000)</td>
<td>5.37E-10</td>
</tr>
<tr>
<td>M + H₂O(010)</td>
<td>5.37E-10</td>
</tr>
<tr>
<td>M + H₂O(010)</td>
<td>5.37E-10</td>
</tr>
<tr>
<td>M + H₂O(000)</td>
<td>5.37E-10</td>
</tr>
<tr>
<td>M + H₂O(010)</td>
<td>5.37E-10</td>
</tr>
<tr>
<td>M + H₂O(000)</td>
<td>5.37E-10</td>
</tr>
<tr>
<td>M + H₂O(010)</td>
<td>5.37E-10</td>
</tr>
<tr>
<td>M + H₂O(000)</td>
<td>5.37E-10</td>
</tr>
</tbody>
</table>

*Numbers in italics indicate that no change has been made from the original SHARC value.

** The Eᵢ terms (i.e., the energy differences between levels) are not listed here for the V-T processes because these are obtained from the H₂O QSTAT.DAT file in SHARC 2.0.
# Table 2: Band Radiance Comparison

<table>
<thead>
<tr>
<th>Transition</th>
<th>Frequency</th>
<th>Band Radiance (W/SR/cm²)</th>
<th>Radiance Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>(010)-(000)</td>
<td>1594.750</td>
<td>0.37277e-6</td>
<td>1.05</td>
</tr>
<tr>
<td>(020)-(000)</td>
<td>3151.630</td>
<td>0.11184e-8</td>
<td>5.22</td>
</tr>
<tr>
<td>(001)-(000)</td>
<td>3657.053</td>
<td>0.87024e-9</td>
<td>1.82</td>
</tr>
<tr>
<td>(001)-(000)</td>
<td>3755.930</td>
<td>0.35921e-7</td>
<td>0.994</td>
</tr>
<tr>
<td>(000)-(000)</td>
<td>4666.793</td>
<td>0.11070e-11</td>
<td>12.6</td>
</tr>
<tr>
<td>(000)-(000)</td>
<td>5234.977</td>
<td>0.63862e-11</td>
<td>2.56</td>
</tr>
<tr>
<td>(000)-(000)</td>
<td>5331.269</td>
<td>0.20763e-8</td>
<td>1.62</td>
</tr>
<tr>
<td>(001)-(010)</td>
<td>1556.880</td>
<td>0.39202e-7</td>
<td>5.22</td>
</tr>
<tr>
<td>(000)-(010)</td>
<td>2062.303</td>
<td>0.13254e-9</td>
<td>1.81</td>
</tr>
<tr>
<td>(000)-(010)</td>
<td>2161.180</td>
<td>0.16949e-8</td>
<td>1.00</td>
</tr>
<tr>
<td>(000)-(010)</td>
<td>3072.043</td>
<td>0.17710e-9</td>
<td>12.6</td>
</tr>
<tr>
<td>(000)-(010)</td>
<td>3640.227</td>
<td>0.39018e-10</td>
<td>2.55</td>
</tr>
<tr>
<td>(000)-(010)</td>
<td>3736.519</td>
<td>0.82490e-8</td>
<td>1.62</td>
</tr>
<tr>
<td>(000)-(010)</td>
<td>1515.163</td>
<td>0.32288e-8</td>
<td>12.6</td>
</tr>
<tr>
<td>Pure Rotational Lines</td>
<td></td>
<td>0.99151e-10</td>
<td>1.00</td>
</tr>
<tr>
<td>Total Overlap Corrected Band Pass Radiance</td>
<td>0.46488e-6</td>
<td>0.40686e-6</td>
<td>1.14</td>
</tr>
</tbody>
</table>

Model Atmosphere: DAYSUBAR.DAT  
Limb View, 64 km Tangent  
Lat. 0°, Long. 0°  
Solar Zenith Angle 0°

**Fig. 1:** Radiance Calculation Comparison  
(Including H₂O (020) Band; 3151.6 cm⁻¹)
Fig. 2: Radiance Calculation Comparison
(Including H₂O (030) Band; 4666.8 cm⁻¹)

Fig. 3: Radiance Calculation Comparison of H₂O Bands
NEW WORK

OZONE RATE CONSTANTS

NO RATE CONSTANTS

OH RATE CONSTANTS

LIMITATIONS OF KUYMER-JAMES MODEL

REVIEW ARTICLE
Session 3

Summary of the Session on Measurements and Models

This session addressed model applications, enhancements, validations, and potential new directions; the singular laboratory measurement paper described work on the UV Schumann-Runge bands. Because of the large number of separate issues covered, this synopsis is arbitrarily divided into two categories: "New Directions" and "Measurements and Validations".

NEW DIRECTIONS:

"Atmospheric Ultraviolet Radiance and its Variation": In the realm of new directions for PL/GP models, Computational Physics (CPI) outlined its approach to modeling UV/Visible airglow features and their variability. This modeling effort will eventually be merged with the lower atmosphere AURIC, MODTRAN, and SHARC (see previous papers, Huguenin et al.; Abreu et al.; Robertson et al.). Such syntheses will eventually produce a seamless code covering solar, thermal, and airglow features throughout the ultraviolet to far IR spectral ranges.

"Improved HNO$_3$ Band Model Parameters": Currently a full spectroscopic description for HNO$_3$ at 11.3 microns requires thousands of transitions. Implementing this system into a line-by-line algorithm consumes large amounts of time and storage; therefore, the authors propose an efficient temperature dependent band model, suitable for incorporation into LOWTRAN and MODTRAN.

"Line-by-Line Calculations of Atmospheric Fluxes and Heating Rates": Interest in Global Climate Change within the scientific community has driven the evolution of FASCOD3 into the arena of energy deposition within the atmosphere. AER has extended the code to produce heating and cooling rates for a variety of atmospheres, comparing those results to prior calculations (ICRCCM). The contour plots of line-by-line heating and cooling rates, as a function of both pressure and frequency, readily demonstrates the importance of correct detailed spectroscopy, particularly regarding "feature overlap" and the H$_2$O continuum, on potential global change predictions.

"A Comparison of Computational Approaches for the Voigt Function": F. Schreier of the Optoelectronics Institute, Germany, presents a comprehensive (and elegant) investigation of computational procedures for calculating the Voigt function. Coding implementation and subsequent timing runs were described.

"Spectral Smoothing in the Fourier Domain: A Software Package for Line-by-Line Calculations": With the growth of Fourier transform spectrometric techniques, used in both laboratory and field measurements (surface, airborne, balloon, shuttle, and satellite), the need for rapid FTS simulation capability became apparent. This new routine (developed at Optimetrics and Stewart Radiance Lab) provides a set of FTS scanning functions, including apodization, that can be used in conjunction with FASCOD3 output. The functions include sinc, sinc$^2$, Beer, Hamming, and Hanning.

MEASUREMENTS AND VALIDATIONS:

"Photoabsorption Cross Sections in the Transmission Window Regions of the Schumann-Runge Bands of Oxygen": This paper describes laboratory work done at Harvard-
Smithsonian to improve the measurements of the Schumann-Runge Band absorption in the window regions between stronger rotational lines, including the pressure dependence. These data are particularly important when calculating penetration of solar UV into the mesosphere and stratosphere. Eventually, full cross sections based upon the Harvard measurements will be incorporated into AURIC (see previous papers: Hugeunin et al., Link et al.).

"High-Resolution Spectral Measurements of Upwelling and Downwelling Atmospheric Infrared Emission with Michelson Interferometers": FASCOD3 validation is critically dependent upon good high-resolution radiance and transmittance measurements; the atmospheric data presented by the University of Wisconsin-Madison provide well calibrated IR radiance at both surface and aircraft altitudes (downwelling and upwelling). The data are of sufficient quality to infer necessary changes to CO2 and H2O spectral line parameters; independently those same parameters were updated for HITRAN91 based on laboratory data (see Rothman). The role of FTS in interpreting the atmosphere (temperature, constituent, and particular profiles) is strongly reinforced by this excellent program.

"Validation of HIS Spectral Measurements with the FASCODE Line-by-Line Model": This is a companion paper to the Wisconsin (Revercomb et al., above) instrument presentation, further describing inferences drawn from comparisons between HIS atmospheric measurements and FASCODE calculations. Cloud (sub-visual cirrus) and fluorocarbon signatures, in addition to ozone, water, and carbon dioxide, are readily apparent, supporting the development of high resolution measurements in more operational modes.

"Comparison of FASCOD2 and LOWTRAN7 Models with FIT Spectral Transmittance Measurements in the 3-12 micron Region": The Canadian research group has compared high resolution interferometric transmittance measurements (winter and summer, high and low humidity) with both FASCOD2 and LOWTRAN7 (after degrading the data to LOWTRAN resolution; agreement is, in general, very good (<18%)). However, their analyses point out some of the same problem areas in H2O lines (updated in HITRAN91), along with concerns about the self and foreign continua. This latter problem is being addressed; see Special Session discussion.

"LOWTRAN7 Comparisons with Field Measurements": As the title indicates, the Army Night Vision Laboratory conducted an extensive set of comparisons of LOWTRAN7 with transmissometer measurements at 1.54, 3-5, and 8-12 micron frequencies. Measurements were made in Virginia, Panama, Alaska, and Utah. The quality of agreement was, in most cases, as good as the supporting meteorological data (humidity, etc.). An initial comparison of MODTRAN and high resolution Fourier transform transmissometer measurements also showed excellent agreement, further supporting the development for the E/O community to convert from LOWTRAN to MODTRAN.

"Spectral Solar Radiation Modeling, Measurement, and Data Base Activities at the Solar Energy Resolution Institute (SERI)": SERI outlined their interest, motivation, and measurement program in the near UV through near IR spectral ranges. This program is driven by the need to assess performance of solar energy conversion devices. Both MODTRAN and LOWTRAN provide similar modeling capability, so the SERI development offers parallel validation of the DoD codes.

"Incorporation of LOWTRAN7 into the ACQUIRE Model": LOWTRAN7 has been modified for the Army to be compatible with EOSAEL 92; this has required changing the input to EOSAEL flexible formatting and adding target contrast calculations along with new aerosol and multiple scattering algorithms.

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ATMOSPHERIC ULTRAVIOLET RADIANCE AND ITS VARIATIONS

Computational Physics, Inc., P.O. Box 788, Annandale, VA 22003

CPI is developing numerical codes for the Atmospheric Ultraviolet Radiance Integrated Code (AURIC) development effort of the Phillips Laboratory Geophysics Directorate in the area of Ionospheric Impact on Air Force Systems - Ultraviolet Remote Sensing. The modules will calculate thermospheric emission spectra and radiances in the 1000 - 6500 Å wavelength region for dayglow, nightglow, twilight and electron aurora, and will account for solar, photoelectron, auroral electron, and chemical excitation processes, pure and self absorption, and multiple scattering effects. The modules will provide the capability to calculate emission spectra as a function of wavelength and look angle, or provide radiances integrated over specified wavelength intervals for user-selected viewing geometries. An orbit code will be provided for satellite viewing geometries. An interface to MODTRAN will be provided for calculating Rayleigh scattering contributions. The integrand codes will provide the analyst with a powerful tool for predicting UV optical backgrounds, analyzing optical data, and designing sensors.
PHOTOABSorption CROSS SECTIONS IN THE
TRANSMISSION WINDOW REGIONS OF THE SCHUMANN-RUNGE
BANDS
OF OXYGEN

Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138

A.S-C. Cheung
Chemistry Department, University of Hong Kong, Hong Kong

We have completed measurements of the absorption cross sections of the
Schumann-Runge bands in the window regions between the rotational lines in the
wavelength region 180-199 nm. The measurements have been done with many different
pressures of oxygen, 50-76 torr, so that the pressure dependent absorption can be
separated from the main cross sections. The measured cross section \( \sigma_p(\lambda) \) at the window
region is linearly dependent on the pressure \( P \) of \( O_2 \), 
\( \sigma_p(\lambda) + \alpha(\lambda)P \). \( \alpha(\lambda)P \) is the cross section of \( O_2 \) extrapolated to zero pressure and \( \alpha(\lambda)P \) is the cross section involving two molecules
of \( O_2 \). They are used to eliminate the pressure dependent part of the cross sections from
the measured cross sections in the transmission window regions. The absorption cross
sections at the window region have been obtained for (2,0) - (12,0) bands. The total cross
sections are obtained from the combination of the window cross sections here and the peak
cross sections previously obtained by Yoshino et al. (1983).
\[ \sigma_P(\lambda) = \sigma_0(\lambda) + \alpha(\lambda)P \]

\[ \sigma_0(\lambda) = \sigma_{SR}(\lambda) + \sigma_H(\lambda) + \sigma_R(\lambda) \]

- \( \sigma_{SR}(\lambda) \): Wing effects of the Schumann-Runge bands
  - Temperature dependent
- \( \sigma_H(\lambda) \): Herzberg continuum
- \( \sigma_R(\lambda) \): Rayleigh scattering

**Herzberg Continuum Cross Sections, \( \sigma_H \)**

![Graph showing Herzberg Continuum Cross Sections with data points and curves from different studies: Coquart et al. (1990), Cheung et al. (1984), and Yoshino et al. (1988).](image-url)
5.
4.
3.
2.
0.
Wavelength, nm

CROSS-SECTION

2-0 BAND
P15 R17
P13 R15
P11 R13
P9 R11
P7 R9
P5 R7
P3 R5
P1 R3
R1

5-1 BAND
P19 R21

3-0 BAND
P29

CONTINUUM $= 7.53 \times 10^{24}$ cm$^2$
(50500 cm$^{-1}$)

---
LABORATORY
---
CALCULATION

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Observed Cross Sections
Temperature: 293 K
Temperature: 293 K
Continuum: \( 9 \times 10^{-24} \text{ cm}^2 \)
8\( \times 10^{-24} \text{ cm}^2 \)
7\( \times 10^{-24} \text{ cm}^2 \)
6\( \times 10^{-24} \text{ cm}^2 \)
5\( \times 10^{-24} \text{ cm}^2 \)
4\( \times 10^{-24} \text{ cm}^2 \)

Temperature: 293 K
Continuum: \( 9 \times 10^{-24} \text{ cm}^2 \)
8\( \times 10^{-24} \text{ cm}^2 \)
7\( \times 10^{-24} \text{ cm}^2 \)
6\( \times 10^{-24} \text{ cm}^2 \)
5\( \times 10^{-24} \text{ cm}^2 \)
4\( \times 10^{-24} \text{ cm}^2 \)

Observed Cross Sections
Temperature: 293 K
Published Cross Sections
INCORPORATION OF LOWTRAN 7 INTO THE ACQUIRE MODEL

S.G. O'Brien
Las Cruces Scientific Consulting, 3373 Solarridge Street, Las Cruces, NM 88001

The Night Vision Laboratory ACQUIRE computer program is designed to calculate range performance predictions that are based upon results from the FLIR90 sensor performance model. ACQUIRE combines MRT data, target characteristics, and atmospheric conditions to predict the probability of accomplishing various acquisition tasks as a function of range. The addition of a modified version of LOWTRAN 7 to perform the atmospheric characterization task is described.
Incorporation of LOWTRAN 7 into the ACQUIRE Model

Sean G. O’Brien
Las Cruces Scientific Consulting

Incorporation of LOWTRAN 7 into ACQUIRE

Implementation

- Use ACQUIRE as the driver
- Input of negative transmission triggers LOWTRAN 7 execution
- Modified LOWTRAN 7 (EOSARL LOWTRAN) already performs target contrast computation
- Modify ACQUIRE range performance algorithms to include contrast results
Incorporation of LOWTRAN 7 into ACQUIRE

Goals

- Use modified LOWTRAN 7 to calculate observer-target and observer-background transmissions and radiances in ACQUIRE, and calculate target contrast

- Modify ACQUIRE to adjust target acquisition results using LOWTRAN 7 target contrast results

- Test and document the resulting code

NVL ACQUIRE Model Input/Output

- Input
  - target: height, length, delta T
  - environment: atmospheric transmittance, smoke mass extinction coefficient, smoke concentration length, max range
  - device: # of MRT data points, number of resolvable cycles on target corresponding to 50% probability of performing tasks #1 and #2 (#2 is used for search detection task), WFOV/NFOV ratio, search time

- Output
  - echo of input
  - NFOV P(#1), P(#2), and P(#2,t) as functions of range
  - NFOV R(#1), R(#2) as functions of probability
  - Corresponding WFOV results (if any)
NVL ACQUIRE Model

- Uses FLIR90 model output as input
- FLIR90 predicts device-dependent performance parameters measurable in the laboratory
  - NETD (noise equivalent temperature difference)
  - MTF (modulation transfer function)
  - MRTD (minimum resolvable temperature difference)
- ACQUIRE accepts MRTD data and predicts field performance
  - probability of detection and recognition of military targets as a function of range
  - 2-D range performance
  - optional 1-D range performance
- NVL search model is embedded in ACQUIRE
  - allows time-dependent probability of detection analysis, given search period criterion

Modifications to LOWTRAN 7

- Adapted to be driven by EOSAEL 92 control program
- Change of input format to EOSAEL card order-independent format
- Addition of target contrast calculation
- Comparison to UV transmission models and data
- Documentation of LOWTRAN 7
  - upgrade to include new features:
    - target contrast
    - new aerosol models (e.g., desert model)
    - multiple scattering of atmospheric radiance
The University of Wisconsin Space Science and Engineering Center has developed instruments for the measurement of accurately calibrated atmospheric emission both from the ground and from an aircraft platform (NASA ER-2). These instruments have been used in recent field experiments to obtain extensive data sets of combined radiances and in-situ atmospheric measurements. Some of the interesting results from these experiments that will be presented include: clear air spectroscopic differences with line-by-line code, ice and liquid water cloud radiative signatures, and atmospheric state parameter retrievals from the infrared measurements. Results of comparisons of observations with FASCOD2 and Beta-FASCOD3 will be presented as well as the impact of improvements in the CO₂ line parameters over those found in HITRAN86.
COMPARISON OF FASCODE SPECTRA WITH HIS OBSERVATIONS (II)

H.E. Revercomb, R.O. Knuteson, W.L. Smith, H.M. Woolf*, and H.B. Howell*

University of Wisconsin
Space Science and Engineering Center
1225 West Dayton Street
Madison, WI 53706
USA

* NOAA/NESDIS Systems Design and Applications Branch,
1225 West Dayton Street, Madison, WI 53706

for
Annual Review Conference on
Atmospheric Transmission Models
Geophysics Laboratory
Hanscom AFB, MA
11-12 June 1991

TOPICS

• HIS (High-resolution Interferometer Sounder) OBSERVATION HISTORY

• SUMMARY OF 1989 FASCODE2 / HIS COMPARISONS

• CO2 RESULTS FROM FASCODE3

• NEW 1991 OBSERVATIONS
6-YEAR HISTORY OF ATMOSPHERIC OBSERVATIONS

- NASA U2/ER2 AIRCRAFT (NADIR VIEWING)
  - KITT PEAK, APRIL 1986
  - COHMEX, JUNE / JULY 1986
  - FIRE, WISCONSIN, OCT / NOV 1986
  - NASA AMES, PACIFIC OCEAN, MAY 1991
  - CAPE, SERON, FIRE; 2ND HALF 1991

- NOAA P3 AIRCRAFT (NADIR VIEWING)
  - MIAMI, 1 TEST FLIGHT, NOV 1988

- GROUND BASED (ZENITH VIEWING)
  - MADISON, NOV 1986
  - GAPEX, DENVER, OCT / NOV 1988
  - MADISON / LIDAR, NOV / DEC 1989
  - WISP: COLORADO, FEB / MAR 1991
  - NSF SHIP, POINT SUR, MAY 1991
HIS GROUND-BASED OBSERVATIONS (Downwelling Compared to FASCODE)

University of Wisconsin
Space Science and Engineering Center

![Graphs showing downwelling compared to FASCODE.

DEMOnstration of ABSolute RADIOMETRY
(Intercomparison of 2 different interferometric systems)
H$_2$O CONTINUUM: 1989 Summary

- HIS AGREES REASONABLY WELL WITH FASCOD2 FROM 750 TO 1000 cm$^{-1}$ (10 TO 13 μm)
  (A 10% increase of the continuum strength would improve agreement)

- REDUCTION OF THE FOREIGN-BROADENING CONTINUUM BY 60% BETWEEN 1300 AND 1400 cm$^{-1}$ (8 TO 9 μm)
  WOULD ACCOUNT FOR THE DISCREPANCY BETWEEN HIS AND FASCOD2 FOR DRY ATMOSPHERES.
TRACE GASES: 1989 Summary

- CFC 11 AND CFC 12 ARE IDENTIFIABLE IN THE REGION FROM 1050 TO 1200 cm\(^{-1}\), IN ADDITION TO THE REGION PREVIOUSLY IDENTIFIED FROM 840 TO 940 cm\(^{-1}\)

- CCl\(_4\) IS IDENTIFIABLE CENTERED AT ABOUT 800 cm\(^{-1}\)
LINE STRENGTH ADJUSTMENTS:
1989 Summary

- H₂O LINE STRENGTHS FROM 1090 TO 1200 cm⁻¹ NEED ABOUT 30% INCREASE

- CO₂ LINE STRENGTHS FROM ABOUT 700 TO 760 cm⁻¹ NEED TO BE INCREASED

FASCOD2 - HIS 1 NOV. 11Z GAPEX UPLOOKING

SUGGESTS CO₂ LINE STRENGTHS NEED TO BE INCREASED

SUGGESTS H₂O LINE STRENGTHS NEED TO BE INCREASED

WAVENUMBER (CM⁻¹)
CO₂ RESULTS FOR FASCOD3

- AUGUST 1990 BETA TEST VERSION OF FASCOD3
- 1990 WATTSON / ROTHMAN CO₂ LINES
- RINSLAND H₂O LINES AUGMENTING HITRAN '86

RADIANCE DIFFERENCES HIS - FASCOD3

[Graph showing radiance differences for various conditions and locations]
HIS
Downlooking: April 15, 1986
Resolution = 0.7 cm⁻¹ (apodized)
HIS & FASCOD2
Downlooking: April 15, 1986

FASCOD2 = dashed

-FASCODE+ HIS
Downlooking: April 15, 1986

FASCOD2, 1986 CO2

FASCODE3, 1990 CO2
NEW 1991 OBSERVATIONS


- **Pacific Ocean, off Monterey: Uplooking from ship "Pt Sur" & downlooking from NASA ER2, Very moist, 7-9 May 1991**

- **Cape Canaveral (CAPE) & Southeast US (Seron): Downlooking from NASA ER2, July-August 1991**

- **Coffeyville, Kansas (Fire & Spectre): Downlooking from NASA ER2 & uplooking, Nov-Dec 1991**

![Graph showing radiance vs. wavenumber for WISP, Platteville, CO on 28 Feb 1991, 3:25 Z]
Pts Sur

May 7, 1991 2:45pm

NASA ER-2 at 20km

May 7, 1991 2:45pm
Monterey May 7, 1991

ER2 @ 20km
SUMMARY

- FASCOD3 with line mixing and the new Wattson/Rothman CO2 lines substantially improves agreement with HIS observations in the 15 µm region.

- New HIS observations for different atmospheric conditions have been acquired during 1991 and more are expected.
VALIDATION OF HIS SPECTRAL MEASUREMENTS
WITH THE FASCODE LINE-BY-LINE MODEL

S.A. Clough, R.D Worsham
Atmospheric and Environmental Research, Inc., 840 Memorial Drive, Cambridge, MA 02139

G.P. Anderson, M.L. Hoke, F.X. Kneizys
Geophysics Laboratory (OP), Hanscom AFB, MA 01731

M. Wagner, R.M. Goody
Harvard University, Department of Applied Sciences, Pierce Hall, Cambridge, MA 02138

An extended version of FASCODE (Clough et al., 1986) has been utilized in conjunction with the GL HITRAN database (Rothman et al., 1987) and carbon dioxide line coupling coefficients (Hoke et al., 1988), to perform spectral radiance comparisons with data from the High-Resolution Interferometer Sounder (HIS; Revercomb et al., 1987). Validations have been performed with down viewing spectra from 19.6 km and up viewing spectra from the surface for the 600-1100 cm⁻¹ spectral region. Effects that are observed include improvements relating to the 1991 HITRAN line parameters for water vapor and carbon dioxide, line coupling effects in carbon dioxide and absorption by anthropogenic molecules including CCl₄, CFC11, and CFC12. Of particular interest is the apparent effect of attenuation by sub-visual cirrus clouds and the correlation of the spectral residuals with carbon dioxide quantum number.
Validation of HIS Spectral Measurements with the FASCODE Line-by-Line Model

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution/Department</th>
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<tr>
<td>S.A. Clough</td>
<td>Atmospheric and Environmental Research, Inc.</td>
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<td>M.V. Wagner</td>
<td>Harvard University</td>
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<td>R.M. Goody</td>
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<td>Platform</td>
<td>U2</td>
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<tr>
<td>Altitude</td>
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Radiance spectrum in equivalent brightness temperature for the long wave spectral region from 600 to 1100 cm\(^{-1}\). The data were taken with the U. of Wisconsin High-Resolution Interferometer Sounder (HIS), Smith et al. (1983).

**WAVELENGTH (MICROMETER)**

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<td>600</td>
<td>720</td>
<td>840</td>
<td>960</td>
<td>1080</td>
<td>1200</td>
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</table>

**RADIANCE WATTS / (CM\(^2\) STERADIAN)\(^{-1}\)**

**HIS/FASCODE Comparison**

**Data:**
- unappodized
- field of view correction in time domain
- FFT to spectral domain

**Calculation:**
- line by line (FASCODE)
- sinc scanning function
- radiances at same spectral values as data
HIS - Calculated
HITRAN 86 Line Parameters

WAVELENGTH (MICROMETER)

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WAVENUMBER (CM$^{-1}$)

-4.0 -2.0 0.0 2.0 4.0 6.0 8.0 10.0 12.0 14.0 16.0

Temperature Difference

600 700 800 900 1000 1100

x - line mixing: CO2 Q branches

Parameters for FASCODE Calculation

Spectral parameters

Temperature profile

Water vapor profile

Ozone profile

Surface temperature

1986 HITRAN database

radiosonde

radiosonde

U.S. Standard profile

obtained from window radiance
The effects of line coupling including its temperature dependence have been accounted for using the line coupling coefficients of Hok et al. (1988) multiplied by a factor of 1.3 based on this and related spectra. Essential to these results are improved interim carbon dioxide line parameters provided by L.S. Rothman (1990). The improvements in the carbon dioxide line intensities are qualitatively consistent with those developed for ATMOS, Brown et al. (1987). The residuals for ozone have been reduced through the application of a retrieval algorithm to obtain an improved ozone profile. The remaining residual associated with the main Q-branch of carbon dioxide at 667 cm⁻¹ is due to warmer gas close to the instrument.

The same as the previous figure except that the effects of the absorption by the heavy molecules have now been included. This has been accomplished by using the cross sections of Massie et al. (1985) and the mixing ratios from the AER/NASA community model. The broad spectral features associated with CCl₄, CFC11 and CFC12 are well accounted for.
The same as the previous figures except that the effects of extinction due to a thin cirrus cloud at 13 km have been included. The cloud has an optical thickness of 0.05 at 0.55 microns. For computational expediency conservative scattering has been invoked. The cloud model used for this example is one developed for LOWTRAN7 by Eric Sattle; spherical particles are assumed with a mode radius of four microns. The spectral characteristics of this cloud type provide a marked improvement in the spectral residuals. The idea of looking at this issue had its origins with the paper by Prabhakara et al. (1988).

The effect on the spectral residuals of performing a temperature retrieval based on the spectral interval from 680-780 cm⁻¹. It may be noted that the mean error is improved from Fig. 5, but that the rms error about the mean is not greatly improved. Most of the irregular spaced residuals are due to incorrect intensities of pure rotational water lines.
Radiance spectrum in equivalent brightness temperature for the long wave spectral region from 680 to 780 cm\(^{-1}\). The data were taken with the U. of Wisconsin High-Resolution Interferometer Sounder (HIS), Smith et al. (1983).

The difference spectrum in equivalent brightness temperature between the HIS spectrum and a calculated spectrum using an advanced version of FASCODES.
Residual Correlations

1) residuals vs. brightness temp. 680-780
   a) all points
   b) peaks
   c) valleys

2) residuals vs. brightness temp. for reduced spectral regions

3) residuals vs. quantum number by band
   a) 667 2-1
   b) 720 5-2
   - residuals at the peak
   - doubly sampled data from U. of Wisconsin
     - 4 point Interpolation
   - doubled the sampling frequency for calibration
     - 4 point Interpolation
Band 2-1, R lines.

Band 5-2, R lines.
Summary

Conclusions:
- data are extremely good
- '91 line parameters significantly better than '86
- line coupling (some remaining issues)
- cross sections
- effects of thin cloud (Prabhakara et al.)

Remaining Issues:
- residuals ~1-2 K in CO2 region
  - not calibration
  - not temperature profile
  - CO2 line parameters: widths, strengths?
  - additional intervening cloud?
- residuals associated with water vapor lines
  - pure rotation: strengths and widths
IMPROVED HNO$_3$ BAND MODEL PARAMETERS

N. Jones, A. Goldman, D. Murcray, F. Murcray, W. Williams
Department of Physics, University of Denver, Denver, CO 80206

Band model temperature dependent parameters for HNO$_3$ have been recalculated for the 11.3 µm bands using the best available molecular parameters and integrated band strengths. Parameters are calculated with a 1 cm$^{-1}$ resolution and for several temperatures appropriate to the lower stratosphere. The new parameters should be suitable for both MODTRAN and LOWTRAN. A brief presentation of the calculations as well as sample results will be included.
IMPROVED HNO$_3$ BAND MODEL PARAMETERS
FOR THE 11.3$\mu$ REGION

Nicholas Jones
Aaron Goldman
David Murcray
Frank Murcray and
Walter Williams

University of Denver
Department of Physics
Denver, CO 80208

Annual Review Conference
on
Atmospheric Transmission Models
Hanscom AFB

11-12 June, 1991

ABSTRACT

- HISTORY
- METHODS
- PRELIMINARY RESULTS
- COMPARISONS
- FUTURE WORK
HISTORY OF HNO₃ MODELS

<table>
<thead>
<tr>
<th>Date</th>
<th>Group</th>
<th>Data Base</th>
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HNO₃ BAND MODEL PARAMETERS

Method of calculation

- Calculate Band Model Coefficients for several temperatures using
  HNO₃ line parameters and Goodys' Statistical method

\[
x/L = \frac{S^0}{2\pi\gamma^0} - \frac{1}{8}\left(\sum_{i=1}^{N} S_i^0\right)^2, \quad \beta = \frac{2\pi\gamma^0}{d} - \frac{8}{\Delta v} \left(\sum_{i=1}^{N} (S_i^0 \gamma_i^0)^{1/2}\right)^2 \sum_{i=1}^{N} S_i^0
\]

\[
S^0/d - \left(\frac{2\pi\gamma^0}{d}\right)(x/L) = \frac{1}{\Delta v} \sum_{i=1}^{N} S_i^0
\]

- Approximate Band Model Coefficients with Linear Coefficient
  \[ K = S^0/d \]

- Derive Temperature Dependent Linear Coefficients
  \[ K(T) = K_0(T_0)(T_0/T)^\nu \]
HNO₃ calculated average cross-section

Temperature coefficient for $S^0/d$

$0.4 \text{cm}^{-1}$ filter
Average Cross-section 1.2 cm\(^{-1}\) filter

solid calculated points Giver (1986)
Calculated at 260K
SIGNIFICANCE OF TEMPERATURE DEPENDENCE

T-Dep Results
- Many Spectral Regions have \( \leq 5\% \) T-Dep
- Some Spectral Regions have \( \geq 20\% \) T-Dep
- Strongest T-Dep In Wings
- Incomplete "Hot Bands" Analysis

Applications
- Select Optimum Spectral Regions for HNO$_3$ Measurements:
  Regions w/wo Interference (F11, F12, H$_2$O)
  Regions w/wo T-Dep
- Verify T-Profile used for Analysis of Emission Data

REMAINING TASKS

- Extend Coefficients into the Wings
- Further Compare Line Parameters and Band Model Parameters with High Resolution and Low Resolution Lab Data
- Publish Results
- Make Data Base Available
LINE-BY-LINE CALCULATIONS OF ATMOSPHERIC FLUXES AND HEATING RATES

S.A. Clough, M.J. Iacono, J.-L. Moncet
Atmospheric and Environmental Research, Inc., 840 Memorial Drive, Cambridge, MA 02139

A rapid and accurate radiance algorithm has been developed to provide enhanced capability for the line-by-line calculation of fluxes and heating rates using FASCODE for thermally inhomogeneous non-scattering atmospheres. First moment quadrature is utilized to obtain fluxes from the radiances, providing accuracies of 1% for two angles and 0.2% for three angles. Optical depths are calculated for a single zenith angle, generally the nadir. Extensive calculations have been performed for water vapor using the mid-latitude summer atmosphere in the context of the ICRCCM campaign. Comparisons with other line-by-line models have been conducted. Effects of line cutoff procedures have been studied in detail and will be discussed. The role of the water vapor continuum (Clough et al., 1989) will be described in detail. The heating rate and flux calculations are presented spectrally to provide insight into the correlation of the radiative effects between spectral domain and altitude. The importance of the 300-600 cm\(^{-1}\) region for the upper tropopause will be discussed. Calculations have also been performed for the tropical and subarctic winter atmospheres with important implications related to the water vapor continuum.
Line-by-line Calculations of Atmospheric Fluxes and Heating Rates: Application to Water Vapor

S. A. Clough
M. J. Iacono
J.-L. Moncet
Atmospheric and Environmental Research, Inc.

12 June 1991

ICRCCM: InterComparisons of Radiation Codes for Climate Models

LBL: W.L. Ridgway - Goddard Laboratory for Atmospheres (GLA)

Model Atmospheres:
- Mid-Latitude Summer
- Tropical
- Sub Arctic Winter
- 66 layers

Line-by-Line Calculation
Advanced version of FASCODE.
G.P. Anderson & F.X. Kneizys Radiance Algorithm
Topics

Calculation:

heating rate: flux divergence
flux: first moment quadrature
radiance: inhomogeneous atmosphere
spectral integration: box car

Application:

spectral sampling error at high altitudes (GLA)
# of quadrature points
spectral extent of line contributions
water vapor continuum
model atmospheres
spectral mapping of cooling rate vs. altitude

Heating Rate:

\[
\left( \frac{\partial T}{\partial t} \right)_{IR} = -\frac{1}{c_{P}P} \frac{\Delta F}{\Delta Z}
\]

\(F\): net flux
\(F_{i} = F_{i+} - F_{i-}\)
\(\Delta F = F_{1} - F_{-1}\)

Flux:

\[
F_{o}^{\pm} = \int_{0}^{\frac{\pi}{2}} \int_{0}^{\pi} I_{o}(\theta, \phi) \cos \theta \, s \rho \, \theta \, d\theta d\phi
\]

\(I_{o}\): monochromatic radiance

\[
= 2\pi \int_{0}^{1} I_{o}(\mu) \mu d\mu
\]

\(\mu\): direction cosine

\[
= 2\pi \sum_{j=1}^{N} w_{j,N} I_{o}(\mu_{j})
\]

\(w_{j,N}\): first moment quadrature
Radiance Algorithm:

\[ I_v = \hat{B}_v (1 - T_v) \]

- Isothermal (old FASCODE)

\[ I_v^i = \hat{B}_v (1 - T_v) \]

- Linear in \( \tau \)

\[ I_v^l = B_v^U (1 - T_v) - (B_v^L - B_v^U) T_v + \frac{B_v^L - B_v^U}{\tau_v} (1 - T_v) \]

- New algorithm (new FASCODE)

\[ I_v^n = \left\{ (\hat{B}_v + a \tau_v B_v^U) / (1 + a \tau_v) \right\} (1 - T_v) \]

- Limits:

<table>
<thead>
<tr>
<th></th>
<th>Isothermal</th>
<th>Linear in ( \tau )</th>
<th>New</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thin (( \tau \to 0 ))</td>
<td>( \hat{B}_v \tau_v )</td>
<td>( \frac{B_v^U + B_v^L}{2} \cdot \tau_v )</td>
<td>( \hat{B}_v \tau_v )</td>
</tr>
<tr>
<td>Thick (( \tau \to \infty ))</td>
<td>( \hat{B}_v )</td>
<td>( B_v^U )</td>
<td>( B_v^U )</td>
</tr>
</tbody>
</table>

Spectral Radiance

![Spectral Radiance Graph](image)
Approx. - 'Correct'

**new algorithm**

**isothermal**

Approx: 1 layer
2.5 km thick
5.2 K differential

'Correct': 5 layers
each layer 0.5 km thick
uses new algorithm for radiance

**MLS, H_2O lines only, LS=10**

325-400 cm\(^{-1}\)

PRESURE (mb)

COOLING RATE (x10^4 K/day)

320-325 cm\(^{-1}\)

PRESURE (mb)

COOLING RATE (x10^4 K/day)
Flux Errors (%): Quadrature vs. 25 pt. trapezoidal

<table>
<thead>
<tr>
<th># angles</th>
<th>quadrature</th>
<th>first moment quadrature</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>up</td>
<td>down</td>
</tr>
<tr>
<td>1</td>
<td>-2.3</td>
<td>8.5</td>
</tr>
<tr>
<td>2</td>
<td>-0.13</td>
<td>0.99</td>
</tr>
<tr>
<td>3</td>
<td>0.006</td>
<td>0.16</td>
</tr>
<tr>
<td>4</td>
<td>-0.009</td>
<td>0.04</td>
</tr>
</tbody>
</table>

Mid-lat summer, H₂O lines only

10-500 cm⁻¹

---

PRESSURE (mb) vs. TOTAL FLUX (W/m²)
ICRCCM Temperature Profile

- Tropical
- Mid-lat summer
- Subarctic winter

Mid-latitude summer, H₂O 10-3000 cm⁻¹

- H₂O lines only
- H₂O lines & continuum
LBL COOLING RATE

MLS, H$_2$O lines only

Contours: $x \times 10^3$ K/(day cm$^{-1}$)

Wavenumber (cm$^{-1}$)

Pressure (mb)

LBL COOLING RATE

TRP, H$_2$O + Continuum

Contours: $x \times 10^3$ K/(day cm$^{-1}$)

Wavenumber (cm$^{-1}$)

Pressure (mb)
COMPARISON OF FASCOD2 AND LOWTRAN7 MODELS WITH FIT SPECTRAL TRANSMITTANCE MEASUREMENTS IN THE 3-12 μm REGION

J.M. Thériault
DREV-Defense Research Establishment Valcartier,
P.O. Box 8800, Courcelette, Québec, Canada, GOA-1RO

A comparison is made between FASCOD2 and LOWTRAN7 predictions with experimental measurements carried out at DREV over a 5.7 km transmission path under a wide range of ambient temperature (-9° to 30° C) and humidity conditions (1.1 to 14.2 g/m³). Following a brief review of the FIT instrumentation\(^1\), low and high resolution measurements (20 and 1 cm\(^{-1}\)) of atmospheric transmittance in the 3-12 μm region are reported. The most significant differences have been recorded in winter and spring conditions. The analysis of the results suggests that the water vapor continuum modeling in the 7-12 μm region has some limitations at low ambient temperature in both models. Furthermore, the comparison of LOWTRAN7 with measurements has revealed an unexpected difference of 12%, independent of temperature and humidity conditions in the important transmission window near 3.6 μm. This difference is attributed to the modeling of the 3020 cm\(^{-1}\) absorption band of methane.

COMPARISON OF FASCOD2 AND LOWTRAN7 MODELS WITH FIT SPECTRAL TRANSMITTANCE MEASUREMENTS IN THE 3-12 μm REGION

J.-M. Thériault

DREV-Defence Research Establishment Valcartier
P.O. Box 8800, Courcelette, Quebec, Canada, GOA-1RO

also with
(Mar. 91- Feb. 92)

CIMSS-Cooperative Institute for Meteorological Satellites Studies
University of Wisconsin
Space Science and Engineering Center
1225 West Dayton Street
Madison, WI 53706

Presented at the
1991 Annual Review Conference on Atmospheric Transmission Models, AFGL
11-12 June 1991

High Resolution Atmospheric Transmission Measurement

- 5.7-km transmission range
- FIT-Fourier Interferometric Transmissometer
- Quebec city area: Wide range of ambient temperature and humidity conditions

Current work:

- Transmissometer calibration techniques
- Water vapor and temperature effects
- Comparison with FASCOD2 and LOWTRAN7 predictions
FIT-Receiver:
1 - Parabolic Newtonian 17-in diameter F/4.6 telescope
2 - BOMEM DA2.02 field Interferometer:
   - Resolution from 0.04 cm\(^{-1}\) to 64 cm\(^{-1}\)
   - Clear optical beam cross section – 14 cm\(^2\)
   - Bandpass: 2.8-12 \(\mu\)m MCT det. and BaF\(_2\) beamsplitter
3 - System field of view: 0.5 mrad

FIT-Calibration:
\[
T_{\text{atm}}(\nu) = \frac{1}{K(\nu)} \frac{P_{d}(\nu)}{P_{loc}(\nu)}
\]
- Calibration factor:
\[
K(\nu) = \frac{A_{m}}{\Delta^{2}} \frac{f_{1}^{2}}{f_{2}^{2}} \cdot (RQ)
\]
- In the Mid-IR: Verification of results with a wideband transmissometer (3.4-4.1 \(\mu\)m).
- In the Far-IR: Correction Factor \(F_{c}(\mu) = R^{2}(\mu)\cdot Q\)

Comparison of Measurements with FASCOD2:

1 - Resolution of 1 cm\(^{-1}\)
2 - Spectral region: 850-3500 cm\(^{-1}\)
3 - Temperature Range: -8.55 to 29.4 C
4 - Humidity Range: 1.16 to 14.2 g/m\(^3\)
5 - HITRAN Database: 1986 Edition
6 - Contributions of other active molecules namely O\(_3\), N\(_2\)O, CH\(_4\), CO, O\(_2\), and N\(_2\): AFGL Mid-summer or Mid-winter conditions except for the CO\(_2\) (350 ppm)
7 - Aerosol model: Rural Type
8 - Visibility evaluation: Matching FASCOD2 spectra with measurements at 2684 cm\(^{-1}\)
Visibility Evaluation

![Graph showing visibility evaluation with different wavelengths and transmittance values.]

VALIDATION OF TRANSMITTANCE MEASUREMENTS

![Graph showing transmittance measurements with different wavelengths and transmittance values.]

- Problem with Al-mirror
- FIT
- 17" Collimator
Typical Measurements (winter / summer)

27 MARCH 1990
T=0.22°C
H=1.55 g/m³
V_m=42 km

26 JULY 1990
T=28.0°C
H=13.26 g/m³
V_m=15.2 km

Comparison winter/summer for the 7.4-11.8 μm region

27 MARCH 1990
T=0.22°C
H=1.55 g/m³
V_m=42 km

25 JULY 1990
T=24.2°C
H=14.07 g/m³
V_m=20.0 km
Comparison winter/summer in the 4.5-5.5 μm region

27 MARCH 1990
T=0.22°C
H=1.55 g/m³
Vₚ=42 km

26 JULY 1990
T=28.0°C
H=13.3 g/m³
Vₚ=15.9 km

Comparison winter/summer in the 3.3-4.3 μm region

27 MARCH 1990
T=0.22°C
H=1.55 g/m³
Vₚ=42 km

26 JULY 1990
T=28.0°C
H=13.3 g/m³
Vₚ=15.9 km
H$_2$O-continuum evaluation (cold conditions)

$$T^C_{\text{EXP}} = \frac{T_{\text{EXP}}}{(T^L_{\text{FAS2}} \cdot T^A_{\text{FAS2}})}$$

Winter Condition (4.5-5.5 μm)

18 APRIL 1990

T = 0.22 C
H = 1.55 g/m³

Transmission of the H$_2$O-Continuum
H₂O-continuum evaluation (cold conditions)

\[ T_{\text{MEAS}}^C = \frac{T_{\text{MEAS}}^L}{T_{\text{FAS2}}^{L} \cdot T_{\text{FAS2}}^{AE}} \]

- H₂O-Foreign Broadening Coeff.
- Transmission H₂O-cont (EXPE)
- Transmission H₂O-cont (FAS2)

Edges of the 6.3 μm Band

18 APRIL 1990
T = 0.22 C
H = 1.55 g/m³

WAVENUMBER (cm⁻¹)

TRANSMTANCE
Comparison of Measurements with LOWTRAN7:

1 - Resolution degraded to 20 cm\(^{-1}\)
2 - Spectral region: 850-3500 cm\(^{-1}\)
3 - Temperature Range: -8.55 to 29.4 C
4 - Humidity Range: 1.16 to 14.2 g/m\(^3\)
5 - Contributions of other active molecules namely O\(_3\), N\(_2\)O, CH\(_4\), CO, O\(_2\), and N\(_2\): AFGL Mid-summer or Mid-winter conditions except for the CO\(_2\) (350 ppm)
6 - Aerosol model: Rural Type
7 - Visibility evaluation: Matching FASCOD2 spectra with measurements at 2684 cm\(^{-1}\)

Comparison winter/summer for the 3-12 \(\mu\)m region:

- 27 MARCH 1990
  - T = 0.22 C
  - H = 1.55 g/m\(^3\)
  - \(V_{\text{fit}}\) = 42 km

- 25 JULY 1990
  - T = 24.2 C
  - H = 14.0 g/m\(^3\)
  - \(V_{\text{fit}}\) = 20.0 km
LOWTRAN7 - MEASURE (year)

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Humidity (g/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>T=25.2 C</td>
<td>H=14.2 g/m³</td>
</tr>
<tr>
<td>T=19.6 C</td>
<td>H=9.49 g/m³</td>
</tr>
<tr>
<td>T=9.41 C</td>
<td>H=3.79 g/m³</td>
</tr>
<tr>
<td>T=4.15 C</td>
<td>H=2.08 g/m³</td>
</tr>
<tr>
<td>T=0.22 C</td>
<td>H=1.55 g/m³</td>
</tr>
<tr>
<td>T=8.55 C</td>
<td>H=1.16 g/m³</td>
</tr>
</tbody>
</table>

Comparison of Models with Measurements

19 April 1990
SUMMARY(FASCOD2)

1 - Overall agreement with measurements is very good. The average difference over the 3-12 μm region is generally smaller than 15% (ΔT/T). The remaining differences have been attributed to the water vapor and to the ozone.

2 - The analysis of results suggest that for

H₂O - The self broadening continuum absorption should be increased by approximately 10-15% in the 850-1000 cm⁻¹.

- The Foreign broadening continuum absorption should be reduced by approximately 50% at the edges of the 6.3 μm absorption band (5.3 μm and 7.5 μm): Assuming that the lines parameters are perfect.

- The absorption of several lines in the 1100-1250 cm⁻¹ region should be increased by approximately 20-50%.

O₃ - Generally for temperatures smaller than 10 C, the FASCOD2 transmittance of the ozone band at 9.6 μm is higher than the experimental one by approximately 10% on the average. Both the concentration and the absorption parameters may be the cause of this.

SUMMARY(LOWTRAN7)

1 - The average difference is generally smaller than 18%.

2 - The analysis of results suggest that for

H₂O - Continuum: (same remarks as for FASCOD2)

CH₄ - In the transmission window near 3.6 μm, LOWTRAN7 is always smaller than the measured one by approximately 12%, independently of the temperature and humidity conditions. It is attributed to the modeling of the 3020 cm⁻¹ absorption band of methane.
SPECTRAL SOLAR RADIATION MODELING, MEASUREMENT, AND
DATA BASE ACTIVITIES AT THE SOLAR ENERGY RESEARCH
INSTITUTE

C.J. Riordan, R.L. Hulstrom
Solar Energy Research Institute, 1617 Cole Boulevard, Golden, CO 80401

The Solar Energy Research Institute uses atmospheric transmission codes and data
to characterize spectral solar radiation (0.3-3.0 μm) at the earth's surface for designing and
predicting the performance of spectrally selective solar energy conversion devices, such as
solar electric cells (photovoltaics). We use a simple model called SPCTRAL2 that was
developed at SERI using comparisons with more complex codes, such as LOWTRAN, and
comparisons with limited measured data. We also maintain a data base with 3000
measured spectra, 0.3-1.1 μm at a 2-nm resolution. Our current activities include
participation in a new International Energy Agency, Solar Heating and Cooling Program,
Task 17 on Measuring and Modeling Spectral Radiation Affecting Solar Systems and
Buildings. We will present an overview of all of our spectral solar radiation modeling,
measurement, and data base activities at SERI.
Spectral Solar Radiation Modeling, Measurement, and Data Base Activities at the Solar Energy Research Institute

Carol Riordan and Roland Hulstrom

Solar Energy Research Institute
Golden, Colorado
303-231-1344  303-231-1220

June 1991

Objective

Briefly describe SERI's interests and activities in spectral solar radiation, and identify conference participants with similar interests.
Interests

Spectral solar radiation at the earth's surface from 280 to 3000 nm at about 1-nm resolution for designing and predicting the performance of spectrally selective solar energy conversion devices (e.g., photovoltaics).
Modeling - Measurements

International Energy Agency
Solar Heating and Cooling Programme Annex 17
Measuring and modeling spectral
radiation affecting solar systems and buildings

A. Narrow-band spectral and broad-band infrared
radiometry
B. Broad-band visible radiometry
C. Narrow-band spectral radiation data acquisition and
analysis
D. Narrow-band spectral radiation modeling-SERI
E. Broad-band visible radiation data acquisition and analysis
F. Broad-band infrared radiation data acquisition and analysis
Measurements

Spectroradiometers

Geophysical Environmental Research  300-3000 nm
LI-COR LI-1800  300-1100 nm
Optronic Laboratories - 752D  200-800 nm
Instruments S.A. DH10  200-800 nm

Direct Normal UV Spectral Irradiance
SERI/Solar Radiation Research & Metrology
Branch (SRR&M)
ISA/DH10 Spectroradiometer Jan 05 1990

280
Measurements

Department of Energy
Atmospheric Radiation Measurement (ARM) Program

Characterizing, evaluating, and calibrating instruments for measuring atmospheric properties and radiation at the Clouds and Radiation Testbed (CART) Sites
This paper presents comparisons between LOWTRAN 7 and field measurements taken during a number of field tests conducted by the US ARMY Center for Night Vision and Electro-Optics. The data was taken by the TECOM Ft. Belvoir Meteorological Team. Transmission data in the .4 to .7 micron, 3 to 5 micron, and 8-12 micron bands were taken at Ft. A.P. Hill, VA in March and April 1991. Data at 1.54 micron was taken at Ft. Greely, AK in February and at Ft. Clayton, Panama during March and April 1991. A description of the equipment is provided along with the input values used for the LOWTRAN calculations.
LOWTRAN 7 COMPARISONS WITH FIELD MEASUREMENTS

R.W. SMITH, T. CORBIN, N. MCNABB, K. HAMMERDORFER
TECOM FT BELVOIR METEOROLOGICAL TEAM

This paper presents comparisons between LOWTRAN 7 and field measurements taken during a number of field tests conducted by the US ARMY Center for Night Vision and Electro-Optics at several different locations. The data was collected by the TECOM Ft Belvoir Meteorological Team. Data includes transmission at 1.54 microns, 3-5 microns, and 8-12 microns. A brief description of the equipment and meteorological parameters are presented along with the measured transmission and calculations using LOWTRAN 7 and in one example, MODTRAN.

INTRODUCTION

One of the most important measurements made by this team in support of test operations is that of atmospheric transmission. It is essential to evaluate the performance of the many different articles our customers test ranging from R&D to operational evaluation. Transmission models are also of great importance to us. We use them in studies and we use them in field support. In field support, we often use LOWTRAN calculations whenever it is not possible or practical to use our measurement equipment due to size of the test or other considerations. For example, it is generally not practical to provide support which takes four days to set up to support a one day test. At times, we must support one test with LOWTRAN while our equipment is in use on another test. We also use LOWTRAN to monitor the behavior of our equipment and compare it with the behavior of our technicians compare to the measured data. In this manner, we can detect problems quickly and take corrective action. This is built into our automated run stream and serves as a good quality control mechanism. It is obvious that we must have confidence in the transmission model in use and have a feel for how it performs under various conditions.

A few comments may be appropriate before we launch into the data. First is that this data was collected as part of testing programs with specific objectives and unfortunately collecting nice clean data for these comparisons were not among them. So we have to live with real world problems of power, equipment changes, unwanted vehicle traffic, etc. These will be pointed out whenever possible. The second comment concerns the meteorological data. In some tests, we have to use locally collected data which is not designed to support E-O testing. Some problems with this will be pointed out. During large tests where we are collecting all data ourselves, we feel much more comfortable in its quality and representativeness.

The discussion will be organized with a brief description of our equipment at the beginning, then we will look at data collected at Ft AP Hill, Va in the 3 to 5 micron band and the 8-12 micron band. Visible data could not be obtained during this test because of a broken beam combiner at the transmssometer source. Next we will look at data taken for the Miniature Eyesafe Laser Infrared Observation System at 1.54 microns. This data was taken in Alaska, Panama, and Utah. Finally, and example involving MODTRAN will be presented. In all the comparisons, I must give credit to MajOWz) Bob Hughes of the Wright-Patterson AFB Staff in for supplying the computer version of LOWTRAN. I should point out that lowtran was run using 1.54 microns +/- 10 wave numbers.

1. INSTRUMENTATION

The transmssometer system used for all the data except the section on modtran was a Barnes 4.5 inch research radiometer system with a 1000 C blackbody source for the 3-5 and 8-12 bands, and an InSb detector for 3-5 microns and MCT for the 8-12 band. Both detectors are LEM cooled. For the 1.54 transmission, a Germanium detector was used with a high intensity quartz halogen light source. Precision optics are used for even distribution of the energy and the beam is highly collimated. The system was calibrated by abutting the source and receiver to eliminate atmospheric and system effects. Then appropriate corrections for range and optics were applied. The result is a measurement of absolute transmission. Discussion of the equipment used for the higher resolution data is described in that section.

2. Ft A.P. Hill, Va Data

The following data was taken as part of the Multisensor Automated Targeting field test. This data was taken over a two week period with extensive meteorological measurements taken at both ends and optical turbulence measurements taken at the first kilometer of the path. Temperature and humidity measurements were done with Vaisala humicaps, visibility using a NBS visibility meter, rate of rain with a NFR optical rainimage instrument, pressure by an AIR digital barometer and with a Vaisala Laser Cislometer. Many other parameters were measured, such as soil temperature, solar radiation, and wind and are available on floppy disk. Meteorological data are collected on an automated system and represent 15 minute averages. Two days of data are presented, the data is presented in charts at the end of the text, hopefully in the correct order.

a. 20 Mar 81: This was a partly cloudy day with no clouds below 12000 ft. Optical turbulence was in the light range so that data is not presented. Looking for good data was quite exciting except for three spikes. These are periods were equipment was being changed or repaired causing a period of bad data (eliminated in the official test data base). Only one site data is included because site two data is identical.

The first comparison shows 3-5 microns. We had significant power stability problems due to cool weather with its use of heaters and due to the number of test participants. During the period before 1400 our data was well below lowtran. We did not have a select amplifier in use on the 3-5 system so holding a good signal was difficult. We did achieve stable power by 1400 and the comparison to lowtran now becomes quite good. One minute data
shows the problems clearly, especially the two periods when the
lock-in amplifiers were turned off to reset the system.

The 8-12 system had a select amplifier so we actually
obtained good data sooner. The one minute data indicates that
while the data stabilizes easier, twitching the system takes
longer. I should point out that the spike at about 0900 coincident
with the met equipment problem is just that coincidence.

b. 22 Mar 91: This day brings change with higher humidity
and a period of rain. Site one data only for temperature and
pressure are shown because they are identical. Both sites are
shown for RH and visibility because differences are indicated.
Note that differences in visibility increase with increasing
visibility. That is common with the H85 instrument. But below 10
km the differences are real. Cloud height is shown as is a
comparison of the rain rates (sites 344 are further down range).
The difference between site one and two were verified by our
observations. In this case we show our data compared to lowtran
using data from both met sites. You are invited to make your own
comparisons. I will say that these comparisons are consistent
with what we usually observe.

3. Panama

Next we will travel south to Panama and look at the 1.84
micron region. Again we had a two kilometer path length but this
time looking down some 300 meters and crossing the panama canal
as shown on the map. Met data comes from the receiver site so its
representativeness is in question. Two days are presented.

a. 30 Mar 91: The only comment to be made about the met data
is that the visibility was estimated by a human and is not
representative of the path. Many fires from burning crops were in
the area and especially dense during one afternoon period. The
break in the measured data was caused by lunch. Note the very
good agreement during the last hour.

b. 1 Apr 91: This day had no fires to contend with and the
comparison is straight forward. Some of the difference is probably
due to our detector band width.

4. Alaska

This was done with the cold weather testing of the MELIOS
at the Cold Regions Test Center, Ft. Greely, Alaska. Part of this
test involved smoke. Again, met data was taken at the receiver
site. The comparison chart shows mainly why we were still in
business. Between generator smoke and the obscuring smoke,
comparisons are not really possible. For this paper, we will not
discuss the type of obscuring used

5. Utah

The final stop on our support of MELIOS was the Dugway
Proving Ground in Utah. Met data is again at the receiver site by
a human, the path is two kilometers and very flat, but now the
altitude is near 4000 ft. In this case three days are shown.

6. May 91: The met data is included for reference. This
was a clear warm day and had very strong optical turbulence, I
would estimate in the 10E-12 range. The first comparison shows
our hour averaged data with measured being somewhat lower than
lowtran. Near the end of the day, dust from vehicles came over
our path dropping the transmission but the observer could still
see the top of the mountain 90 miles away. The fact that we could
not see the base 10 miles away was not recorded. The effect of
the turbulence can be seen on the one minute data.

b. 22 May 91: This day was cloudy and cooler and the observed
turbulence was slight. Now we have excellent agreement between
measured and calculated. The one minute data captures a vehicle
which kept crossing our line of sight, a problem we were able to
resolve with our powers of persuasion.

c. 23 May 91: This day was partly cloudy with moderate
turbulence. Lack of turbulence measurements is a bother. But again
in this case, with a uniform path and moderate turbulence, we
found very good agreement with lowtran 7.

6. Summary

The above data gives us considerable confidence in using
LOWTRAN as a tool of great usefulness. When one has good met
measurements which describe the path, good comparisons can be
obtained by scintillation, it most certainly is a factor in
obtaining field measurements, but that is another topic which we
intend to address in another paper.

7. Bonus

We would like to present some data we took in Germany in
1988 using our Nicolet FTIR transmissometer. This instrument has
a HCTA detector with a ZnSe beamsplitter and can produce a two
wavenumber resolution. The data were taken over a path of about
700 meters. The first chart shows the data obtained. The DF
refers to distance and optics corrections. The second chart is a
lowtran run using met data at both ends of the path including
measured visibility. Incidentally, that was also our data. The third
chart shows a MODTRAN run of the same time. The agreement is very
good, in fact remarkable considering our field conditions with
the very sensitive FTIR.

We are currently working a PC version of MODTRAN and feel
that it will eventually replace LOWTRAN in some of our support
activities. Our manning and workload has interfered with our
work with the FTIR but we think that that will soon change.

FINAl SUMMARY

To provide support to our customers in the E-O world, we
must have the capability for both measuring and calculating
atmospheric transmission. We in fact use LOWTRAN as a quality
control tool. Accordingly our confidence must be high that it is
an accurate product. We feel that it is, at least to the
accuracies we need and in our near the ground application. Our
data shows that if the input data is accurate, so is the result.
LOWTRAN7/TRANSMISSION

22 MAR 1991 8–12m

LOWTRAN7/TRANSMISSION

22 MAR 1991 8–12m
RELATIVE HUMIDITY
PANAMA MAR 30 1991

PRESSURE
PANAMA 30 MAR 91
LOWTRAN7/TRANSMISSION
DUGWAY MAY 23 1991 1.54m

TRANSMISSION

TIME

DUGWAY TRANSMISSION
MAY 23 1991

TIME
SPECTRAL SMOOTHING IN THE FOURIER DOMAIN:
A SOFTWARE PACKAGE FOR LINE-BY-LINE CALCULATIONS

W. Gallery
Atmospheric and Environmental Research, Inc., 840 Memorial Drive,
Cambridge, MA 02139

M. Esplin
Stewart Radiance Laboratory, 139 Great Road, Bedford, MA 01730

We have developed a software package which will convolve a spectrum with a
spectral scanning function using Fourier transforms. This technique mimics the operation
of Fourier transform spectroscopy and preserves the full extent of the scanning function,
which is particularly important for functions like sinc. This package has the following
features:

1. It gives the user a choice of 5 scanning functions commonly used in Fourier
transform spectroscopy, including sinc, sinc^2, Hamming, Hanning, and Beer, plus triangle
and Gauss, and may be easily modified to include other functions.

2. There is no limitation on the size of the spectrum (a disk-based Fourier
transform method is used for spectra exceeding the available memory).

3. If possible, it optimizes the calculation by prescanning the spectrum with a
rectangle narrow compared to the scanning function, resulting in significant time and size
savings.

4. It has been adapted to read and write FASCODE binary files.

Sample calculations will be shown comparing measured spectra with calculated
spectra smoothed using this technique.

William O. Gallery
OptiMetrics, Inc.

Mark Esplin
Stewart Radiance Lab, Bedford, MA

*Now with Atmospheric and Environmental Research, Inc., Cambridge, MA

Introduction

- Line-by-Line Calculation are Often Compared to FTS Measurements
  - e.g., Scribe, CIRRUS, HIS, ATMOS, Lab Measurements
- Scanning Function Is Determined by the Apodization Function Applied to the Interferogram
- The Calculation Should Accurately Match the Scanning Function
  - Extent (Especially Important for Sinc, Sinc²)
  - Shape
Program FFTSCAN

- A Software Package for Convolving a Spectrum with a Spectral Scanning Function Using Fourier Transforms
- Mimics the Operation of a Fourier Transform Spectrometer
  - Transforms the Calculated Spectrum Into an "Interferogram"
  - Apodized the Interferogram
  - Transforms Back to the Spectral Domain
- Choice of 5 Common FTS Scanning Functions
  - Sinc, Sinc\(^2\), Hamming, Hanning, Beer
  - Also Triangle, Gauss, and Box

Scanning Functions and Associated Apodization Functions

The Five Scanning Functions and Their Associated Apodization Functions. The functions shown here model the HIS interferometer, with a maximum optical path difference of 1.8 cm.
Program Details

- Program Reads and Writes Fascode Files
- Can Handle Arbitrarily Large Spectra By Using A Disk-Based FFT
- Input Spectrum Can be Pre-Scanned with a Boxcar and Deconvolved
- Apodization Function Can Be Calculated Either Analytically or As the Fourier Transform of the Scanning Function

Disk Based FFT

- Disk Based FFT Courtesy of Mark Esplin, Steward Radiance Lab
- If the Number of Points Exceeds the Available Memory, A Disk-Based FFT is Used
  - Input Data Points Are Sorted Into Blocks and Written To Disk as Direct Access Files
  - Only 2 Blocks Reside in Memory
  - A Standard FFT is Applied to Each Block
  - Data From the Various Blocks is Combined to Obtain the FFT of the Entire Dataset
  - Sorting of Data and Combining of the Blocks is Analogous to the Method of a Standard FFT
- Time Penalty For a Disk-Based FFT Compared to an In-Memory FFT is 35 % on a Sun 360 Workstation for the Same Total Number of Points
- Caution With Virtual Memory
- VAX: Direct Access Blocks Blocks Limited to 2048 Points
Prescanning

- Prescan Input Spectrum With a Boxcar (Rectangle) If Input $\delta \nu < \alpha / M$
- $\delta \nu =$ input frequency spacing, $\alpha =$ scanfunction halfwidth at halfmaximum, $M = 5$
- $M$ Points From Input Spectrum Are Averaged To Obtain One Output Point
- Prescanning Results in Significant Time and Memory Savings
- Smoothing Effect of the Boxcar Can Be (Partially) Reversed By Deconvolving Resampled Spectrum

Example of Prescanned and Deconvolved Line

Lorenz Line, $\text{HWHM} = 0.04 \text{ cm}^{-1}$, $\text{du} = 0.01 \text{ cm}^{-1}$, Scanned with a Beer Scanning Function, $\text{HWHM} = 0.2645 \text{ cm}^{-1}$ (HIS Resolution), Prescanned With $M = 5$, Output $\text{du} = 0.05 \text{ cm}^{-1}$
• **Resolution:**
  - Half Width at Half Maximum of the Scanning Function, or
  - Maximum Optical Path Difference of an Equivalent Interferometer

• **Frequency Range**
  - Adjusted to Fit Input Spectrum
  - User Must Allow For Edge Effects, Which Can be Quite Extensive For the Sinc Function

• **Transmittance or Radiance**
  - Program Recognizes Different Fascode File Types

• **Scanning Function**

• **Selectable Options:**
  - Prescanning
  - Deconvolution
  - Apodization Function Calculated as the FFT of the Scanning Function
A COMPARISON OF COMPUTATIONAL APPROACHES FOR THE VOIGT FUNCTION

F. Schreier
DLR - Deutsche Forschungsanstalt für Luft- und Raumfahrt, Institute of Optoelectronics
D-8031 Oberpfaffenhofen (Fed. Rep. Germany)

Several computational procedures for the Voigt function are discussed and compared for accuracy and speed. Vectorization of the codes was applied where possible. This resulted in a variation of computational speed over two orders of magnitude. However, even without vectorization restructuring of the programs can yield a significant acceleration. For applications with least-squares-fitting the evaluation of the complex error function provides an efficient way to calculate both the Voigt function and its partial derivatives.
A Comparison of Computational Approaches for the Voigt Function

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ABSTRACT

Several computational procedures for the Voigt function are discussed and compared for accuracy and speed. Vectorization of the codes was applied where possible. This resulted in a variation of computational speed over two orders of magnitude. However, even without vectorization restructuring of the programs can yield a significant acceleration. For applications with least-squares-fitting the evaluation of the complex error function provides an efficient way to calculate both the Voigt function and its partial derivatives.

The Voigt Function — Definitions

\[ g_V = g_L \otimes g_D = \frac{2\ln 2/\pi}{\gamma_D} K(x, y) \]

\[ K(x, y) = \frac{y}{\pi} \int_{-\infty}^{+\infty} \frac{e^{-t^2}}{(x-t)^2 + y^2} \, dt \]

where

\[ x = \sqrt{\ln 2} \frac{\tilde{\nu} - \tilde{\nu}_0}{\gamma_D} \]

\[ y = \sqrt{\ln 2} \frac{\gamma_L}{\gamma_D} \]

and \( \tilde{\nu}_0 \) line center

\( \gamma_L, \gamma_D \) Lorentzian and Gaussian half width

representation in complex plane \( (z = x + iy) \):

\[ W(z) = K(x, y) + iL(x, y) = \frac{i}{\pi} \int_{-\infty}^{+\infty} \frac{e^{-t^2}}{z-t} \, dt \]

Complex error function:

\[ w(z) = e^{-z^2} \left( 1 + \frac{2i}{\sqrt{\pi}} \int_0^z e^{t^2} \, dt \right) \]

\[ = e^{-z^2} \text{erfc}(-iz) \]

\( W(z) \) and \( w(z) \) are identical for positive \( y \):

\[ w(z) = \begin{cases} W'(z) & \text{for } y > 0 \\ W'(z) + 2e^{-z^2} & \text{for } y < 0 \end{cases} \]
Voigt function: Armstrong's algorithm

imaginary part of complex error function: Hui’s algorithm

<table>
<thead>
<tr>
<th>author(s)</th>
<th>region(s)</th>
<th>method</th>
<th>total accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Armstrong</td>
<td>$y &lt; 1.0, x &lt; 4$ or $y &lt; \frac{4}{x}, x &gt; 4$</td>
<td>Hummer-Faddeeva/Terent’ev power series 20-term Gauss-Hermite integration</td>
<td>1-2 digits in 6th significant figure</td>
</tr>
<tr>
<td>Drayson</td>
<td>$y &gt; 1.0, x &lt; 2$ or $0.5y$</td>
<td>Taylor expansion, Chebyshev expansion continued fraction 4-term or 2-term Gauss-Hermite integration</td>
<td>one part in $10^4$</td>
</tr>
<tr>
<td>Gautschi</td>
<td>all $r, p$</td>
<td>truncated Taylor expansion</td>
<td>10 decimal places after decimal point</td>
</tr>
<tr>
<td>Hui et al.</td>
<td>all $r, p$</td>
<td>rational approximation</td>
<td>rel. error $&lt; 10^{-8}$</td>
</tr>
<tr>
<td>Humícak</td>
<td>$y &gt; 0.85$ or $</td>
<td>x</td>
<td>&lt; 18.1y + 1.8y$</td>
</tr>
</tbody>
</table>
| Humícak       | $16 + 1.15 \leq |y| < 16.3|y| \leq 16$ 
|               | $|x| + y < 0.8$ and $y \geq 0.148(y - 0.17y)$ | rational approximations                                             | $10^{-4}$ relative error |
| Karp          | all $r, p$       | Fourier transform                                                       | $10^{-4}$ relative to peak value |
| Kyslopof      | all $r, p$       | weighted sum of Lorentz and Gauss function                             | $10^{-4}$ relative to peak value |
| Pierluissi et al. | $0 \leq x < 1, 0 \leq y < 1$ | series expansion                                                        | peak deviation $\leq 1.4 \cdot 10^{-3}$, RMS deviation $\leq 3.1 \cdot 10^{-3}$ |
|               | $0 \leq x < 1, 1.6 \leq y < 4$ | 6-point Gauss-Hermite integration                                      |                              |
|               | $x \leq 2, y \geq 2$ | 6-point Gauss-Hermite integration                                      |                              |
| Whiting       | all $r, p$       | weighted sum of Lorentz and Gauss function                             | 1% at worst                   |

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Humlicek vs IMSL-ZERFE
1979

Humlicek 1982
vs Armstrong (Re) vs IMSL-ZERFE (Im)

\[ K(x,y) \sim \{1 - \eta(y)\}G(x) + \eta(y)L(x) + \text{correction} \]

Kielkopf vs Armstrong

Whiting vs Armstrong
Comparison: Computational times

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Function</th>
<th>CRAY Y-MP2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0 &lt; y &lt; 1</td>
<td>1 &lt; y &lt; 10</td>
</tr>
<tr>
<td></td>
<td>0 &lt; y &lt; 1</td>
<td>1 &lt; y &lt; 10</td>
</tr>
<tr>
<td>Armstrong</td>
<td>1.36</td>
<td>1.04</td>
</tr>
<tr>
<td>Drymon</td>
<td>0.35</td>
<td>0.21</td>
</tr>
<tr>
<td>Hui et al.</td>
<td>0.48</td>
<td>0.48</td>
</tr>
<tr>
<td>Hamelin 70</td>
<td>0.87</td>
<td>0.76</td>
</tr>
<tr>
<td>Hamelin 82</td>
<td>0.45</td>
<td>0.29</td>
</tr>
<tr>
<td>IMSL CERF</td>
<td>5.97</td>
<td>3.18</td>
</tr>
<tr>
<td>Pieni ni et al.</td>
<td>0.51</td>
<td>0.24</td>
</tr>
</tbody>
</table>

SUBROUTINE

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Function</th>
<th>CRAY Y-MP2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0 &lt; y &lt; 1</td>
<td>1 &lt; y &lt; 10</td>
</tr>
<tr>
<td></td>
<td>0 &lt; y &lt; 1</td>
<td>1 &lt; y &lt; 10</td>
</tr>
<tr>
<td>Hui (vector)</td>
<td>0.093</td>
<td>0.093</td>
</tr>
<tr>
<td>Kiehlhof (vector)</td>
<td>0.051</td>
<td>0.051</td>
</tr>
<tr>
<td>Kiehlhof (vector)</td>
<td>0.17</td>
<td>0.17</td>
</tr>
<tr>
<td>Whiting (vector)</td>
<td>0.15</td>
<td>0.15</td>
</tr>
<tr>
<td>Whiting (vector)</td>
<td>0.36</td>
<td>0.36</td>
</tr>
</tbody>
</table>

The CPU time used by each function or subroutine has been determined by the IMSL routine CTIME. Jobs were run on a IBM 3080-305 V1.0 under MV5/IXA operating system and with VS FORTRAN Version 6 Release 4.8 Compiler. The CRAY Y-MP2/16 runs under UNICOS operating system with a CFT77 compiler. Highest optimization level has been used on both systems.

Implementations of Hui's algorithm

Vectorization of Hui's algorithm

rational approximation (Hui et al., 1978):

\[ w(z) = \sum_{m=0}^{6} a_m (y - iz)^m \]

\[ b_7 = 1 \]

\[ \sum_{n=0}^{7} b_n (y - iz)^n \]

\[ \Rightarrow \text{computational effort (for each line and grid point )}: \]

12 complex multiplications and one complex division, equivalent to 54 real multiplications and one real division

optimization:

complex polynomial in \( \hat{z} = y - iz \) with real coefficients \( c_m \)

\[ P(\hat{z}) = \sum_{m=0}^{M} c_m (y - iz)^m \]

polynomial in \( z \) with complex coefficients \( d_m(y) \)

\[ M \]

\[ = \sum_{m=0}^{M} d_m(y) z^m \]

\[ = \sum_{m, even} d_m z^m + i \sum_{m, odd} d_m z^m \]

where

\[ d_k = (-i)^k \sum_{l=0}^{M-k} \binom{l + k}{k} c_{l + k} y^l \]

\[ \Rightarrow 21 \text{ real multiplications and one real division} \]
Computing times: Hui's algorithm

<table>
<thead>
<tr>
<th></th>
<th>IBM 3090</th>
<th>CRAY Y-MP2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0 &lt; y &lt; 1</td>
<td>1 &lt; y &lt; 10</td>
</tr>
<tr>
<td>function</td>
<td>0.48</td>
<td>0.49</td>
</tr>
<tr>
<td>subroutine (vector)</td>
<td>0.053</td>
<td>0.083</td>
</tr>
<tr>
<td>optimized subroutine (vector)</td>
<td>0.037</td>
<td>0.037</td>
</tr>
<tr>
<td>opt. subroutine, no vector</td>
<td>0.14</td>
<td>0.14</td>
</tr>
<tr>
<td>opt. sub., Karp's mod., vector</td>
<td>0.046</td>
<td>0.037</td>
</tr>
<tr>
<td>opt. sub., Karp, no vector</td>
<td>0.14</td>
<td>0.14</td>
</tr>
</tbody>
</table>

(Karp’s modification is used only for y ≤ 0.1)

Computing times: Humlicek’s algorithm (1979)

<table>
<thead>
<tr>
<th></th>
<th>IBM 3090</th>
<th>CRAY Y-MP2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0 &lt; y &lt; 1</td>
<td>1 &lt; y &lt; 10</td>
</tr>
<tr>
<td>function, region I and II, real*4</td>
<td>0.87</td>
<td>0.76</td>
</tr>
<tr>
<td>function, region I and II</td>
<td>1.29</td>
<td>0.95</td>
</tr>
<tr>
<td>subroutine, only region I</td>
<td>0.18</td>
<td>0.18</td>
</tr>
<tr>
<td>subroutine, region I and II</td>
<td>0.43</td>
<td>0.18</td>
</tr>
<tr>
<td>subroutine, I and II, no vector</td>
<td>0.05</td>
<td>0.83</td>
</tr>
</tbody>
</table>

(Except for the first row double precision arithmetic has been used in the CRAY version)

---

Voigt and complex error function: computational approaches

**Fourier Transform Methods**

- **advantage:** simple Fourier representation of Voigt function
  \[ K(x, y) = \frac{1}{\sqrt{\pi}} \int_{0}^{\infty} e^{-y^2/4-y^2} \cos qx dq \]

- **Karp:**
  - direct methods: \( n \times n \) evaluations
  - FT methods:
    - only sines, cosines and exponentials for each line
    - and two FFT's for entire frequency range

- **but:** FT method also requires \( n \times n \) evaluations in the Fourier domain plus two FFT's

- **???:** comparable computational effort

- **for direct and FT methods**

- **problems:** restriction for the number of grid points to powers of 2
  error sources like aliasing

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Karp's Fourier Transform Algorithm

total absorption coefficient for \( n_I \) lines

\[
k(\tilde{\nu}) = \sum_{l=1}^{n_I} \frac{S_l}{\eta_i} \frac{\sqrt{\eta_i^2/2}}{P} K(x_l, y_l)
\]

insert Fourier representation for \( K(x, y) \)

use \( \delta_l \equiv \frac{\eta_i^2}{\sqrt{\eta_i^2}} \) and \( \lambda_l \equiv \eta_i \),

change of variables \( qx_l = \tilde{\nu} - \nu_l \)

\[
k(\tilde{\nu}) = \frac{1}{\pi} \int_0^\infty dp \cos \tilde{\nu} \left[ \sum_l S_l e^{-\lambda_l^2/4} \delta_l \cos \nu_l \right] + \frac{1}{\pi} \int_0^\infty dp \sin \tilde{\nu} \left[ \sum_l S_l e^{-\lambda_l^2/4} \delta_l \sin \nu_l \right]
\]

estimate of computing time

\[
t_{\text{Karp}} \approx n_I n_\nu \left( t_{\text{exp}} + 2t_{\text{sin}} + 6t_{\text{mult}} + 3t_{\text{add}} \right)
\]

equidistant grid points \( p_j = j \Delta p \):

recursive relations for exponential and trigonometric functions

\[
t_{\text{Karp}} \approx n_I n_\nu \left( 12t_{\text{mult}} + 4t_{\text{add}} \right)
\]

\[
+ n_I \left( 2t_{\text{exp}} + 2t_{\text{sin}} + 6t_{\text{mult}} \right) + 2n_\nu \log_2 n_\nu T_{FFT}
\]

Absorption coefficient: Hui's rational approximation

total absorption coefficient for \( n_I \) lines

\[
k(\tilde{\nu}) = \sum_{l=1}^{n_I} \frac{S_l}{\eta_i} \frac{\delta}{\delta_l} \sum_{m,n=0}^6 \frac{a_m(\eta_l - i\tilde{\nu})^m}{\sum_{n=0}^n b_n(y_l - i\tilde{\nu})^n}
\]

requires \( n_I n_\nu \) evaluations of \( z_l(\tilde{\nu}_l) \) and of fraction of polynomials

define new coefficients for all lines

\[
\alpha_{ml} \equiv \frac{S_l a_m}{\delta^{m+1}}
\]

\[
\beta_{ml} \equiv \frac{S_l b_m}{\delta^{m+1}}
\]

\[
= \bullet \quad \text{absorption coefficient}
\]

\[
k(\tilde{\nu}) = \sum_{l=1}^{n_I} \frac{\delta}{\delta_l} \sum_{m,n=0}^6 \frac{\alpha_{ml}(\lambda_l - i(\tilde{\nu} - \nu_l))^m}{\sum_{n=0}^n \beta_{ml}(\lambda_l - i(\tilde{\nu} - \nu_l))^n}
\]

with rearrangement of the complex polynomials

\[
t_{\text{Hui}} \approx n_I n_\nu \left( 16t_{\text{mult}} + t_{\text{div}} + 13t_{\text{add}} \right)
\]

\[
+ n_I \left( 10t_{\text{mult}} + t_{\text{div}} + t_{\text{add}} \right)
\]
Derivatives of the Voigt function

Differential equation \((z = x + iy)\)

\[ w'(z) = \frac{2i}{\sqrt{\pi}} - 2z w(z) \]

use Cauchy-Riemann conditions or
direct differentiation of \(K(x, y)\) and partial integration

\[
\frac{\partial K(x, y)}{\partial x} = -2 \Re\left(z w(z)\right)
\]

\[
\frac{\partial K(x, y)}{\partial y} = +2 \Im\left(z w(z)\right) - \frac{2}{\sqrt{\pi}}
\]

Voigt function and derivatives calculated simultaneously !!!

numerics:
subtracting two numbers of approximately equal magnitude

Conclusions and Remarks

Accuracy:
sufficient accuracy of most algorithms, but
for applications further aspects are important, too:

- other error sources:
  - limited accuracy of molecular line parameters
  - uncertainties from exact temperature dependence of \(\gamma_L\)
  - deviations from pure Lorentzian line shape
- least-squares-fits in molecular spectroscopy:
  higher accuracy for computation of derivatives

Computational Speed:
- "black boxes": quick implementation for single applications
  but possibly time consuming otherwise
- vectorization: significant acceleration (factor 140 for Hui)
- restructuring: subroutine instead of functions
  invariant code
- usefulness of imaginary part of \(w(z)\)
Session 4

Summary of the Topical Session on Spectral Line Shapes

The inclusion of the Topical Session on Spectral Line Shape, as part of the Annual Review Conference on Atmospheric Transmission Models, was an effort to introduce the workshop attendees to some of the basic physics of spectral line shape, to some of the recent research results in this field of study, to the ways those results are manifest in radiative transfer computer codes and to the effects the new results have on the problems of radiative transfer and remote sensing. A particular feature of the topical session was that special consideration was given to providing a tutorial overview of the subject with some emphasis on historical developments.

Within the constraint of time, there were two particular objectives. First, that there should be some presentation in outline tutorial form of the basic physics of spectral line shape. The intention was to stress the physics and not the mathematical theory. The second objective was that there should be detailed consideration of recent research results concerning (1) the shape of far wings of water vapor spectral lines and their aggregate affect on the water vapor continuum, especially in the "window" spectral regions, and (2) the shape of overlapped spectral lines, in particular in the microwave spectrum of oxygen and in the spectrum of carbon dioxide Q branches in the fifteen micron spectral region. The question of the shape of the far wings of water vapor spectral lines is a long standing and much studied theoretical and experimental problem. The questions concerned with the shape of overlapping spectral lines were first addressed almost thirty-five years ago, both theoretically and experimentally in the study of the microwave spectrum of oxygen. However, the discovery, within the last ten years, of line coupling effects in laboratory and atmospheric spectra of many other molecules has brought this effect considerable new attention. Both problems are important to studies related to radiative transfer and remote sensing.

Five invited and five contributed papers composed the topical session. Both invited and contributed papers included original research results. In addition, however, the authors of the invited papers were asked to include tutorial and historical material, related to the general topic of their respective papers. The inclusion of historical material was considered appropriate and was specifically encouraged to address the lack of background knowledge of some of the conference attendees concerning the physics of spectral line shape. In compensation for the added requirement the invited presentations were allotted slightly more time than the contributed papers.

Copies of the transparencies of all of the presentations, both invited and contributed are collected together on the following pages. The authors of the invited papers were asked to prepare and submit summaries of their papers, including references, in particular because these papers contained interesting tutorial and historical materials. Some authors were not able to honor the request, and in part for that reason a very brief description of each paper, along with a few references, is given below.

The first paper, 4a1, "Basis of the Water Vapor Continuum Coefficients in the GL Models" was presented by S.A. Clough (Atmospheric and Environmental Research, Inc. and formerly of the Air Force Geophysics Laboratory). The results of the studies of S.A. Clough, F.X. Kneizys and their co-workers (1), are incorporated in the Geophysics...
Directorate's computer code FASCODE. This paper covered some of the general dynamical and statistical considerations for spectral line shape. In particular as they apply to the shape of the far wings of water vapor spectral lines, the frequency dependence of the self and nitrogen broadened Chi-factors and continua. Some of their research is based on the studies of Huber and Van Vleck (2).

The second paper, 4a2, "Water Vapor Continuum Absorption Measurements with Line Shape Interpretations", was presented by M. Thomas (Johns Hopkins University Applied Physics Laboratory). This paper was concerned with the application of a line shape model developed by George Birnbaum (3). Birnbaum's stated objective was to develop a line shape which is applicable from resonance to the far wings. To achieve this he focused his attention on the dipole autocorrelation function, seeking to bridge the gap between the known long and short time behavior of the correlation function with a well chosen empirical interpolation function.

The third paper, 4a3, "Line Coupling for Microwave Oxygen Lines", was presented by P.W. Rosenkranz (Massachusetts Institute of Technology). This paper was concerned with the effect of line mixing in the microwave spectrum of oxygen. The line coupling effect was first observed in the microwave spectrum of oxygen and Rosenkranz was among the first to model the effect (5), employing a perturbation approximation to the line shape matrix. Rosenkranz's presentation included an historical overview of the study of the line coupling effect and recent results for the microwave oxygen band obtained in collaboration with H.J. Liebe (see contributed paper 4b2). Rosenkranz's data analysis technique is unique and differs from that of most other researchers in that the first order perturbation theory line coupling coefficients are inferred directly from the spectral data. Rosenkranz's presentation did not cover the technique but focused on the results of the analysis. However, a discussion of the technique has been presented by Rosenkranz in the literature (6).

The fourth paper, 4a4, "Laboratory Measurements of Line Coupling in CO2 and N2O" was presented by L.L. Strow (Univ. of Maryland). This paper considered laboratory measurements and analyses of spectra of carbon dioxide and nitrous oxide which Strow and his co-workers have made. The presentation also included a discussion of the technique most often used to model the line coupling effect in spectral data. Most often rate matrix parameters, and from them line coupling coefficients, are inferred from the spectral line widths, using "gap" laws, for example exponential gap or exponential-power gap laws, to model off diagonal elements of the rate matrix (7,8,9, see also contributed paper 4b3). First or second order perturbation theory is applied to the line shape operator (10) to yield the description in terms of the line coupling parameters ($y_i$).

The fifth paper, 4a5, "Line Mixing: A Near Wing and Far Wing Problem", was presented by J.M. Hartmann (Ecole Centrale, Paris). This paper, the last of the invited papers, was designed to iterate and tie together some of the basic physical ideas which were presented in the preceding four papers. Hartmann's presentation also illustrates those ideas with some of his and his co-worker's results (11,12) from studies of spectra of water vapor and carbon dioxide.

The sixth paper, 4b1, "Far Wing Line Shape Contribution to the Water Continuum in the Millimeter and Infrared Regions", was presented by R.H. Tipping (Univ. of Alabama). In this paper Tipping presented a theoretical collision broadened line shape, developed in collaboration with Q. Ma (Goddard Instituted for Space Studies) (13). The
theory assumes only the known values of (a) the permanent dipole moment, (b) the rotational constants and (c) the Lennard-Jones potential parameters. Their theory predicts, in particular, the experimentally observed negative temperature dependence of the molecular absorption by water vapor. Their theory partially follows the theoretical studies of Rosenkranz (14).

The seventh paper, 4b2, "Laboratory Measurements of the 60 GHz O2 Spectrum in Air", was presented by Hans J. Liebe (Institute for Telecommunication Sciences). In this paper Liebe discussed his experimental apparatus which he used to make new measurements of the spectrum of O2. Liebe also presented some of the experimentally recorded data and some data analyses. Liebe's data were the basis of analyses presented by Rosenkranz (see paper 4a3).

The eighth paper, 4b3, "Line Mixing in Polar and Nonpolar Molecules", was presented by A.S. Pine (National Institute of Standards and Technology; NITS). In this paper Pine presented data of HCN and HCCH which he collected and analyzed in collaboration with J.P. Looney (NITS). Pine reported new measurements and analysis of HCN; their studies of HCCH have been reported previously (15). Pines' presentation compared and contrasted results of data analyses employing various semi-empirical gap laws; an exercise which no one else has to date performed.

The ninth paper, 4b4, "Study of CO2 Blue Wing in the 4.1 Micron Region", was presented by C.T. Delaye (Applied Physics Laboratory, the Johns Hopkins Univ.) and covered research performed in collaboration with M.E. Thomas (also of the Applied Physics Laboratory); see paper 4a2. Delaye presented interferometric data collected at the Applied Physics Laboratory of carbon dioxide in the 4.3 micron region. Delaye also presented an analysis of this data performed using the same Birnbaum line shape (3) which had been discussed by M. Thomas in paper 4a2. An important result of this study was the applicability of the line shape from the band head region into the far wing of the band and from this the implication that the Birnbaum line shape offered a convenient and accurate expression which would be useful in radiative transfer calculations.

The tenth paper, 4b5, "Theoretical Approach to the Line Wing Problem", was presented by L. Sinitsa (Institute of Atmospheric Optics, Tomsk, USSR). The presentation covered theoretical studies of spectral line shape and approximations with applications to a variety of experimental data from the infrared to the microwave region.

References:


BASIS OF THE WATER VAPOR CONTINUUM COEFFICIENTS IN THE GL MODELS

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A formulation is developed in which the contribution of the far wings of collisionally broadened spectral lines to the water vapor continuum absorption is established. The effects of deviations from the impact (Lorentz) line shape due to duration of collision effects are treated semi-empirically to provide agreement with experimental results for the continuum absorption and its temperature-dependence. The continua due to both water-water molecular broadening (self-broadening) and water-air molecular broadening (foreign broadening) are discussed. Several atmospheric validations of the present approach are presented.
Line Shape and the Water Vapor Continuum

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ABSTRACT


A formulation is developed in which the contribution of the far wings of collisionally broadened spectral lines to the water vapor continuum absorption is established. The effects of deviations from the impact (Lorentz) line shape due to duration of collision effects are treated semi-empirically to provide agreement with experimental results for the continuum absorption and its temperature-dependence. The continuum due to both water-water molecular broadening (self-broadening) and water-air molecular broadening (foreign broadening) are discussed. Several atmospheric validations of the present approach are presented.

RESUME

On développe une formule dans laquelle on établit la contribution des raies élargies par collision au continuum d'absorption de la vapeur d'eau. Les effets des déviations de la forme de raie d'impact (Lorentz) sont traités de façon semi-empirique pour fournir un accord avec les résultats expérimentaux concernant le continuum d'absorption et sa dépendance en température. Les contributions dues à l'élargissement moléculaire eau-eau (self-broadening) et air-eau (foreign broadening) sont discutées. Plusieurs validations atmosphériques de cette approche sont présentées.

INTRODUCTION

The continuum absorption due to water vapor has posed a complex problem for researchers concerned with atmospheric radiative problems. In fact, a universally accepted definition of continuum absorption has not been established making more difficult the discussion of the effect. The regions of the atmospheric spectrum in the microwave and the infrared with the greatest transparency, the windows, are strongly dependent on the water vapor continuum. These spectral regions are at 0 cm$^{-1}$, 800-1200 cm$^{-1}$ and 2000-3000 cm$^{-1}$. Laboratory measurements of the water vapor continuum are made difficult by the long path lengths required with conventional spectroscopic techniques or by the complexities encountered with methods of high sensitivity such as spectrophotometer detection. Atmospheric measurements are adversely affected by the difficulty in adequately characterizing the path, aerosol attenuation, turbulence, scintillation and instrument calibration. From a theoretical point of view, the continuum has posed a comparably complex problem and still lacks a completely satisfactory explanation. The issue of whether the absorption represents an excess or deficiency is fundamentally dependent on the line shape formulation chosen as reference as well as on the frequency regime of interest. A theoretical understanding of this problem entails a satisfactory description of the line shape and its temperature-dependence from line center to the far line wing requiring a proper treatment of the physical processes occurring in the time associated with the duration of collision. Further, an adequate model must also address the issue of collision-induced spectra as well as the possibility of dimer absorption.

LINE SHAPE FORMULATION

In our consideration of the continuum, we start with a line shape formulation for the absorption coefficient $k(\nu)$ (cm$^2$/molec.), that is applicable from the microwave to the infrared (Clough et al., 1983):

$$k(\nu) = R(\nu) \left( \phi(\nu) + \phi(-\nu) \right)$$  \hspace{1cm} (1)

with:

$$R(\nu) = \frac{1 - e^{-\beta\nu}}{1 + e^{-\beta\nu}}$$  \hspace{1cm} (2)

$$\nu \approx \tanh(\beta\nu/2)$$  \hspace{1cm} (3)

where $\nu$ is the wavenumber value, $R(\nu)$ (cm$^{-1}$) is a radiation field term at temperature $T$ with $\beta = h\nu/kT$ (cm), and $\phi(\nu) + \phi(-\nu)$ is the symmetrized power spectral density function (Van Vleck and Huber, 1977). The term $R(\nu)$ includes the effect of stimulated emission. This formulation has a number of attractive properties: its appropriateness to all spectral domains and the fact that the symmetrized power spectral density function satisfies an important intensity sum rule, the Nyquist theorem. For the application of this formalism to the computation of spectra in terms of line transition data, we obtain:
\[ k(\nu) = \nu \tanh(\beta \nu / 2) \]

\[ \times \sum \frac{\hat{S}(\nu)}{R_0} \frac{\alpha_i}{(\nu - \nu_i)^2 + \alpha_i^2} \chi(\nu_i - \nu + \nu_i) \]

where \( \hat{S} \) (cm\(^2\)/molec.) is the intensity of the transition at wavenumber value \( \nu \) (cm\(^{-1}\)) and halfwidth \( \alpha_i \) (cm\(^{-1}\)). The Lorentz function, \( f(\nu - \nu_i) \) (cm):

\[ f(\nu - \nu_i) = \frac{\alpha_i}{\pi (\nu - \nu_i)^2 + \alpha_i^2} \]

is the line shape function appropriate to the impact approximation for which the collision time is assumed to be instantaneous. The \( \chi \) function is a semi-empirical function applied to the impact result to correct for duration of collision effects and to attain agreement between calculated and measured spectra. With \( \chi = 1 \), this line shape reduces to the Lorentz shape in the infrared, since \( R(\nu - \nu_i) \) for \( |\nu - \nu_i| \ll \alpha_i \), and to the Van Vleck-Weisskopf shape in the microwave, since \( R(\nu) \approx \beta \nu^2 / 2 \). We adopt a notation in which a tilde over a quantity indicates that the radiation term, \( R(\nu) \), has been excluded from that quantity.

At this stage we define a continuum absorption by excluding from the power spectral density function fast spectral components associated with the line center. The continuum, \( \check{C}(\nu) \), is given by:

\[ \check{C}(\nu) = \sum \hat{S}(\nu) \chi(\nu_i - \nu) \]

where \( f_i \) is a line shape with the strong central component excluded (Clough et al., 1980). We systematically define \( f_i(\nu \mp \nu_i) \) in the following way:

\[ f_i(\nu \mp \nu_i) = \frac{1}{\pi} \frac{\alpha_i}{(\nu \mp \nu_i)^2 + \alpha_i^2} \]

\[ |\nu - \nu_i| \leq 25 \text{ cm}^{-1} \]

\[ |\nu - \nu_i| > 25 \text{ cm}^{-1} \]

The function \( f_i \) is indicated schematically in Fig. 1 by the solid curve. Another function that has been used by Burch in some of his work is indicated by the dashed line in Fig. 1. The lack of agreement among researchers on the line shape formulation and on the definition of the function \( f_i \) has inhibited the intercomparison and validation of continuum. It must be emphasized that the continuum and the details of the line-by-line calculation are intrinsically related. The present formulation for the continuum is consistent with the FASCODE line-by-line model (Clough et al., 1986). Similarly, it is important to recognize that band models developed to describe molecular absorption, must also be derived in the context of a consistent treatment of the continuum. To

![Fig. 1. The line shape function, \( f_1(\nu) \), used to develop the continuum (solid curve). The dashed curve represents the function used by Burch.](image)
satisfactorily described through an empirical exponent, \( m \), determined from measurements for \( \alpha \), where:

\[
\alpha \rho T = \alpha_0 (T/T_0)^m (\rho/\rho_0)
\]

For the line shape factor \( \chi \) the situation is more complicated. Near line center, \( |\nu - \nu_c| < 5 \text{ cm}^{-1} \), \( \chi \) is essentially unity for all temperatures. However far from line center the temperature dependence for \( \chi \) must be inferred from the temperature of the absorption resulting from many overlapping lines.

**WATER VAPOR**

We are now in a position to apply the formulation we have developed to water vapor absorption. Performing a line-by-line calculation using the entire set of water vapor lines from 0 cm\(^{-1}\) to 10,000 cm\(^{-1}\), we obtain the power spectral density function for self-broadened water vapor shown in Fig. 2. The dotted curve is obtained by utilizing the continuum line shape function, \( f_0 \), thus excluding from the power spectral density function the contribution of the line centers, and providing a spectrum of low spectral content designated as the continuum. The well known water vapor bands associated with pure rotation (0 cm\(^{-1}\)), \( \nu_2 \) (1600 cm\(^{-1}\)), \( \nu_3 \) of HDO (2720 cm\(^{-1}\)), 2\( \nu_3 \) (3100 cm\(^{-1}\)), \( \nu_4 \) (3660 cm\(^{-1}\)) and \( \nu_5 \) (3760 cm\(^{-1}\)) are evident in Fig. 2. In Fig. 3 we indicate two continua, one obtained using the impact line shape (\( \chi = 1 \)), and the other with a function obtained by adjusting the parameters in an empirical \( \chi \) function to attain agreement with the indicated spectral results (Burch, 1981; Burch and Alt, 1984; Burch, 1985).

Note that in Fig. 3 the continuum coefficient for self-broadened water vapor, \( \tilde{C}_0 \), exhibits an excess absorption with respect to the reference impact continuum (\( \chi = 1 \)) in the center of the bands at 0–500 cm\(^{-1}\) and 1400–1800 cm\(^{-1}\) and a deficiency between central band absorption regions, 800–1200 cm\(^{-1}\) and 1800–3300 cm\(^{-1}\). This result is consistent with theoretical requirements and is a direct consequence of the formulation. The \( \chi \) function associated with the line shape for self-broadened water vapor, designated \( \chi_0 \), is shown by the solid curve in Fig. 4. The functional form of \( \chi \) is given by:

\[
\chi = 1 - (1 - \chi') \frac{(\nu + \nu_0)^2}{25^2} \quad |\nu + \nu_0| \leq 25 \text{ cm}^{-1}
\]

\[
\chi' = \left\{ \begin{array}{ll}
0.83 \exp(-z_1^2) & |\nu + \nu_0| > 25 \text{ cm}^{-1}
\end{array} \right.
\]

where for self-broadening \( \chi_0 \) is obtained by setting \( \chi' = \chi' \) with:

\[
\chi'_0 = 8.03 \exp(-z_1^2) + (0.83z_1 + 0.33z_1^2) \exp(-|z_1|)
\]
where \( x_1 = (v + \nu) / 400 \) and \( x_2 = (v + \nu) / 250 \) at 296 K. From eq. 12 and Fig. 4 we note that \( x \) is continuous at 25 cm\(^{-1}\), but that the first derivative is discontinuous. This is a direct consequence of the choice of \( f \) (eq. 8) but causes no particular problems in the formulation.

The self-continuum of water vapor demonstrates a rather strong temperature-dependence, particularly in the 1000 cm\(^{-1}\) window. It is an important shortcoming of the current state of line shape theory for molecular collisions, that the temperature-dependence of the far wings, or alternatively of the continuum in the window regions, is not explained. Rosenkrantz (1985, 1987), in two particularly interesting papers, has proposed an alternative formulation to eqs. 1 and 3, which leads to a strong temperature-dependence consistent with observations in the far-wing regions. This proposed formulation warrants additional scrutiny. The dimer has often been postulated as a source of the continuum absorption primarily as a consequence of its simple and attractive temperature-dependence. However, the absence of spectral structure, difficulties in explaining spectral pressure-dependence and the fact that the absorption in the windows as developed in this paper represents an excess with respect to the impact line shape are in direct contradiction with the dimer theory. On the other hand, dimers should be formed under atmospheric conditions so that the central issue becomes the question of dimer lifetime (Suck et al., 1979).

For pragmatic purposes the temperature-dependence of the continuum has been treated as follows: the parameters in an analytical \( x \) function are obtained by least-squares fitting the calculated continuum to the data of Burch at 296 K and 338 K. These parameters for 296 K and 338 K are then extrapolated to 260 K and a continuum for that temperature is calculated. This is potentially a source of error; however, validations for atmospheric measurements have provided remarkably good results. Continua for 338 K, 296 K and 260 K are shown in Fig. 5.

An analogous treatment is performed for air-broadening of water vapor, referred to as foreign broadening. Fig. 6 shows the empirical continuum, \( \chi_f \), fit to the data of Burch as well as the continuum for the impact approximation. For the foreign-broadened case, the line wings decay much more rapidly as a function of wave number difference from line center than for the self-broadened case. This is reflected in the foreign chi-function, \( \chi_f \), shown by the dashed curve in Fig. 4. For the foreign continuum \( \chi_f \) is obtained by setting \( x' = x_f \) in eq. 12 with:

\[
\chi_f = 6.65 \exp(-x_f^2)
\]

where \( x_f = (v + \nu) / 75 \). For the window regions of the foreign continuum, 1000 cm\(^{-1}\) and 2500 cm\(^{-1}\) in Fig. 6, an absorption coefficient has been added to the continuum resulting from the present formalism in order to attain agreement with atmospheric measurements (Roberts et al., 1975). The contribution of the foreign continuum is very small in these spectral regions making the measurements particularly difficult. The observed effect may be due to collision
induced spectra or humidity-dependent aerosols. No significant temperature-
dependence has been observed for the foreign continuum.

The total absorption coefficient due to self- and foreign-water-vapor continuum, $k_t(ν)$, is given by the relation:

$$k_t(ν) = ν \tanh (βν/2) \left[ \hat{C}_v(ρ_v/ρ_0) + \hat{C}_f(ρ_f/ρ_0) \right]$$

(15)

It is an important point that for atmospheric conditions, the foreign continuum is dominant for in-band absorption and the self continuum is dominant for the out-of-band absorption, the window regions of water vapor spectrum.

**ATMOSPHERIC VALIDATION**

The most important element in the development of an atmospheric transmittance/irradiance model is validation with atmospheric data. Since the atmospheric window at 1000 cm$^{-1}$ (10 μm) is of such importance, we consider that spectral region in more detail. The continuum currently being used in FASCODE2 has been adjusted to fit the more recent measurements at 1000 cm$^{-1}$ of Burch and Alt, 1984 (Fig. 7). In Fig. 8 we show a plot of the optical depth for a 1-km path at 990 cm$^{-1}$ as a function of water vapor density from LOWTRAN7 (Kneizys et al., 1988) which incorporates this continuum de-

Fig. 6. The continuum for foreign-broadened water vapor. The solid curve is the calculated continuum with the z function adjusted to fit the experimental data of Burch, 1981. The broadening pressure is 1013 mb.

Fig. 7. Details of the self-broadened continuum at 1000 cm$^{-1}$. The solid line is the calculated continuum at 296 K. The data for 284 K and 296 K are from Burch and Alt (1984); the other data are from Burch (1981).

development. We consider two sets of atmospheric measurements: one from the Air Force Wright Aeronautical Laboratories (AFWAL) taken over an 8-km path and for a range of visibilities (Kneizys et al., 1984) and the other from the Technion Institute in Israel over an 8.6-km path (Oppenheim and Lipson, 1986). Both of these sets of measurements were taken with circular variable filter (CVF) spectrometers. Since the atmospheric measurements include extinction due to aerosol effects, the calculated optical depths, which do not include aerosol contributions, are less than those for the atmospheric measurements. The calculations do take into effect the contribution from other molecules (intercept) and from the local water vapor lines. Spectral validation of the continuum model with the Technion measurements for the 8–12 micron window is shown in Fig. 9 and for the 3–5 micron window in Fig. 10. Of particular note is the excellent agreement between calculation and observation obtained at 4.75 μm and 3.2 μm. These two regions demonstrate the predictive capability of the current formulation since there has been no adjustment with data in these spectral regions. With respect to the continuum beyond 5000 cm$^{-1}$, it should be emphasized that the calculations are essentially qualitative and unvalidated. This is particularly the case for the self-broadened continuum, important between the bands.
Fig. 8. The optical depth for a 1-km path at 990 cm⁻¹ as a function of water vapor density. The calculations are from LOWTRAN with the self-continuum of Fig. 7. The solid curve is for 298 K and the dashed curve is for 284 K. The data are from Kinetza et al., 1984. The X-symbols are for cases with visibilities > 15 km.

Fig. 9. Spectral comparison between a CVF measurement in the 8-12 micron window over a 5.637-km path by Tinsley (Oppenheim and Lipson, 1985) and a LOWTRAN calculation with the FASCOD2 continuum (dotted curve). The measurement conditions: T = 297.5 K, P = 1008 mb, RH = 85%, and visibility = 15 km.

Fig. 10. Spectral comparison between a CVF measurement in the 3-5 micron window over a 10.37-km path by Tinsley (Oppenheim and Lipson, 1985) and a LOWTRAN calculation (dotted curve). The measurement conditions: T = 297 K, P = 890 mb, RH = 65% and visibility = 41 km.

SUMMARY

The present discussion is not intended as a comprehensive review of the water vapor continuum problem. It is rather a description of a specific approach that is consistent with the physics of the problem and that has been constrained to provide results consistent with experimental measurements. The choice of measurements used for this discussion has been highly selective. This is related to a need for internal consistency of the observations, our estimation of the accuracy of the measurements and a treatment of the data that is in the context of the current development. The present status should be regarded as useful if not definitive. In order to meet current objectives in atmospheric remote sensing and related phenomena, more observations of high accuracy both in the laboratory and in the atmosphere are required, and significant advances in the theoretical treatment of the effects of collision on molecular line shape need to be achieved. A floppy disk containing a program to calculate continuum absorption coefficients as described here and consistent with FASCOD2 and LOWTRAN is available from the authors.

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calculations leading to the current results. We would also like to thank our many colleagues, experimentalists and theoreticians, for the discussions that have clarified our understanding of a very difficult problem. The discussion and experimental results due to Darrel Burch have been invaluable in reaching the present state of understanding. To our other colleagues not mentioned here, we hope to do greater justice in a more extensive paper in preparation.

REFERENCES


WATER VAPOR CONTINUUM ABSORPTION MEASUREMENTS WITH A LINE SHAPE INTERPRETATION

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A review of water vapor continuum experimental data is presented as a function of frequency, partial pressures, and temperature for atmospheric windows from the millimeter wave to 1 \( \mu \)m. The millimeter wave and 10 \( \mu \)m regions are the most extensively characterized. The behavior of the continuum can be represented in the form of simple well behaved functions, yet a physical interpretation has been elusive. For the millimeter wave window, the continuum frequency dependence is frequency squared. For infrared windows, the continuum frequency dependence is exponential always decreasing away from strongly absorbing bands for both self and foreign broadening. These observations have lead to line shape interpretations of the water vapor continuum.

A particular line shape of interest has been developed by G. Birnbaum in the late 1970's. It has a closed form solution, has a continuous representation from line center to the far wing and thus is normalizable, has an exponential far wing and is consistent with many line shapes at line center. In short, it is a versatile and practical line shape. Line-by-line calculations based on this line shape are compared to the experimental data base with interesting results. The agreement with experimental data is best when the continuum is at a minimum, but deviates below observation towards the bordering absorption band. However, this formalism does not include line mixing (or coupling) and this is certainly important. Far wings must play some role in continuum absorption, but a definitive model will require a complete theory.
WATER VAPOR CONTINUUM ABSORPTION MEASUREMENTS WITH LINE SHAPE INTERPRETATIONS

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Absorption by molecules defines the atmospheric windows and is an important mechanism of tropospheric attenuation at millimeter and infrared wavelengths, especially in the marine environment. Therefore, the understanding and accurate modeling of absorption by atmospheric molecules are important to atmospheric remote sensing, infrared imaging systems, long-path laser propagation, electro-optical systems, radar, and atmospheric meteorology. Figure 1a shows low-resolution infrared transmittance of the atmosphere and demonstrates the importance of water vapor over other atmospheric constituents\(^{(1)}\). The \(H_2O\) absorption bands, along with those of \(CO_2\), define the atmospheric window regions in the infrared. At millimeter and microwave wavelengths, \(O_2\) and \(H_2O\) determine the window regions.

The main rotational and vibrational bands have been extensively characterized by many investigators\(^{(2,3,4)}\). This work has resulted in a compendium of absorption-line parameters, maintained by the Air Force Geophysics Laboratory \(^{(5,6)}\) (AFGL), which represents a significant contribution to absorption calculations. The database also contains parameters for weak absorption lines in the window regions. However, this information is, in general, not as accurate as that of the main bands.

The comparatively weak absorption that does occur in the window regions can be described as arising from two distinct sources, local line and continuum absorption, as illustrated in the high-resolution computed spectrum of Fig. 1b for the 10 \(\mu\)m window region. Weak absorption bands of \(CO_2\) and \(H_2O\), along with other \(H_2O\) absorption lines in the window regions, compose the local line contribution. The continuum contributes an additional, gradually varying, frequency-dependent background to the total absorption. A general empirical form for the continuum absorption coefficient used to represent the data\(^{(7)}\) is

\[
\beta_{\text{cont}}(\nu,T,P_f,\ldots,P_k) = \frac{P}{R} \sum_i [C_i(\nu,T)P_i + C_i(\nu,T)P_k]
\]

where \(C_i\) is the self-broadening coefficient of the absorbing gas, \(C_f\) is the foreign broadening coefficient due to the \(i^{th}\) type foreign gas, and \(R\) is the ideal-gas constant. The equation can be conveniently rewritten for \(i = 2\) to obtain

\[
\beta_{\text{cont}}(\nu,T,P_f) = \frac{P}{R} \sum_i [C_i(\nu,T)P_i + C_i(\nu,T)P_k]
\]

Figure 1. (a) Low-resolution solar spectrum compared with laboratory spectra of atmospheric gases. (b) Local line structure plus continuum in the 10-\(\mu\)m region.
\[ \beta_{\text{abs}}(\nu, T) = \frac{C_1(v, T)P_T}{R_T} P_T + F(\nu, T)P_T + B(\nu, T)P_T \]

where \( F = C_4/C_3 \) and \( B = C_6/C_3 \) are the dimensionless broadening coefficients. Near line center, \( B \) has the value of 5 for water vapor relative to nitrogen. In the real atmosphere, the effects of oxygen broadening must also be included. The dimensionless broadening coefficient \( B \) accounts for oxygen. However, many laboratory experiments ignore the effects of oxygen and use only nitrogen as the broadening gas along with the absorbing gas.

Water vapor absorption

As previously mentioned, molecular absorption in the window regions manifests itself as local line and continuum type absorption. Narrow band systems can avoid local line effects but not continuum absorption. Broad band systems must account for both.

Local lines

Local line structure of the 10- and 6 \( \mu \)m water vapor window regions has been experimentally characterized by Thomas\(^{(39)} \) and Long and Dason\(^{(40)} \). The 1 to 1.1 \( \mu \)m local line structure based on experimental data has been reported by Gallery et al.\(^{(41)} \). The data demonstrate the importance of local line structure in the case of water vapor. The NITRAN database also represents local line structure based on experimental data and/or theoretical calculations.

Continuum

In 1942, Slesinger\(^{(1)} \) recognized a continuum in the 13- to 8 \( \mu \)m window region, which he attributed to the far wings of the \( \nu_1 \) and \( \nu_2 \) rotational and vibrational bands of H\( \text{O} \). Further verification of this nonlocal line absorption feature was provided by Yates and Taylor\(^{(8)} \), who studied total-attenuation along horizontal paths at sea level. Solar spectra studies also indicated continuum absorption in the 13- to 8 \( \mu \)m window\(^{(9,11)} \). The nature of the continuum, if by those measurements, was uncertain. It could be due to far wings (far from the band center) of strong absorption bands or to scattering and absorption by particulates.

In an effort to determine the cause of continuum absorption in the 13- to 8 \( \mu \)m window, Bignell\(^{(12)} \) in 1963 examined solar spectra while monitoring the atmosphere for aerosol concentrations and studying CO\( \text{O} \) far-wing contributions. He concluded that the amount of continuum absorption observed could not be explained by aerosol attenuation or far-wing absorption by CO\( \text{O} \). An attempt was then made to model the continuum by far wings of the bordering \( \nu_1 \) bands. The important contribution from this initial work was the realization of major water vapor contributions to the continuum. A second paper by Bignell\(^{(13)} \) in 1970 described a careful examination of water vapor absorption in the window regions and of use of a multiple-transversal absorption cell and grating spectrometer. Two important characteristics of the 13- to 8 \( \mu \)m window were noted: (a) a large ratio of water vapor self-to-foreign-gas broadening ability (see Eq. 2) and (b) a strong negative temperature dependence. Neither of these findings was anticipated on the basis of the far-wing approaches of Bignell’s 1963 paper\(^{(12)} \). Also reported by Bignell\(^{(13)} \) was a similar, but much weaker, continuum absorption in the 4 \( \mu \)m region. (The 4 \( \mu \)m region also features a collision-induced absorption band of nitrogen\(^{(14,15)} \). The band is of comparable strength to the water vapor continuum in the earth’s atmosphere. It is a smooth absorption band showing no structure; thus, it is often referred to as the nitrogen continuum. Also, a far-wing continuum of CO\( \text{O} \) beyond the \( \nu_2 \) band head is observed between 4.1 and 4.0 \( \mu \)m\(^{(38)} \).)

Since these initial experimental efforts to characterize water vapor continuum absorption, many measurements have been made. They fall into three categories: (a) measurements within the earth’s atmosphere or field measurements, (b) laboratory measurements using a long-path cell and a spectrometer, and (c) laboratory measurements using a long-path cell or a photoacoustic cell and a laser. Although continuum absorption was first observed through long-path field measurements, its precise characterization requires control and knowledge of the propagation path. The effects of turbulence, particulate scattering, temperature variations, and partial-pressure variations are difficult to determine in a field measurement. Thus, laboratory measurements are needed to characterize the pressure and temperature dependence of each atmospheric constituent. Spectrometer measurements determine the frequency dependence of the window regions, i.e., local lines and continuum absorption. Laser measurements are limited to discrete frequencies, but because of the laser’s higher power and stability, greater accuracy can be obtained; this is particularly true for photoacoustic techniques. Laboratory transmittance measurements require very long path lengths (\(~1 \text{ km} \)) and thus are difficult to obtain. The photoacoustic cell, on the other hand, is compact (about 30 cm) but still maintains considerable sensitivity. Of course, field measurements will have the final say in the validation of atmospheric propagation computer codes.

As a result of these experiments, a good characterizalation of the commonly used window regions exists today. An excellent review of the field is given by the recent work of Hinderling et al.\(^{(42)} \). They emphasize the 8- to 14- \( \mu \)m window region, which, along with the millimeter-wave window, is the most extensively measured. A review of the current experimental data for all the window regions is given in the next section, followed by a brief review of the theoretical and empirical models used to explain the experimental data.

Millimeter-wave window

Figure 1.3.10\(^{(14-22)} \) shows continuum absorption from 10 to 1000 GHz (total absorption minus local lines). The solid line represents an empirical formula given by Gaut and Raffenetti:\(^{(14)} \)

\[ \kappa_{\text{continuum}} = (1.08 \times 10^{-6}) P_w \left( \frac{300}{T} \right)^{3/2} \left( \frac{P_T}{101} \right)^{1/2} \quad (\text{km}^{-1}), \]

where \( P_w \) is the water vapor density (g/m\(^3 \)), \( P_T \) is the total pressure (kPa), and \( f \) is the frequency (GHz). The plotted points indicate experimental data. The formula correctly demonstrates the frequency dependence of the continuum but not

3
the temperature and pressure dependence. Note recent work by Liebe\(^{33}\) uses a
continuum formula, fitted to experimental data at 138 GHz, of the form

\[
\beta_{\text{continuum}} = (6.73 \times 10^{-4}) \frac{\rho_0}{T} \left( \frac{300}{T} \right)^{3.5} \left( \frac{P_o}{P_p} \right)^{1.1} \left( \frac{P_p}{P_o} \right)^{0.3} \quad \text{(cm}^{-1}\text{)},
\]

(4)

where \(f\) is gigahertz, \(T\) is in kelvins, and \(P_o\) and \(P_p\) (\(P_f = P_T - P_o\)) are in
kilopascals. A strong dependence on the water vapor partial pressure is shown
\((\beta \gg 5)\). The continuum calculated using Eq. 4 is smaller than that calculated
using Eq. 3 because of improved local line modeling. On the basis of the work
by Liebe and Layton\(^{24}\), the parameter \(\beta\) grows as the frequency decreases from 833
to 110 GHz (see Table 1). This dependence is expected based on the far-wing
model of Birnbaum\(^{37}\) and leads to the following empirical model (for \(f < 1000 \text{ GHz}\)
and in units of \text{cm}^{-1}\))\(^{24}\)

\[
\beta_{\text{continuum}}(f) = (6.73 \times 10^{-4}) f^6 \rho_o [\rho_p + 40.9 \times 0.001 (f_0 - \rho_o)]
\]

(5)

where \(\theta = (300/T)\) and the other variables have the same units as above.

<table>
<thead>
<tr>
<th>(f) (GHz)</th>
<th>(\omega) (cm(^{-1}))</th>
<th>(\theta) ((\omega, 300))</th>
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<tr>
<td>833</td>
<td>27.8</td>
<td>7.4</td>
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Table 1. Experimental frequency dependence of \(\beta\) (\(\omega, 300\))

As Eq. 4 indicates, \(\beta\) is not only a function of frequency but a strong
function of temperature as well. Although Liebe\(^{33}\) chooses to represent his data
in a power law form, a comprehensive study at 213 GHz by Llewellyn-Jones\(^{35}\)
shows the data fits an Arrhenius plot with the functional form

\[
\beta(v, T) = e^{bT},
\]

(6)

\(b = 5 \times 10^4\) K. Again, a strong negative temperature dependence is observed at
this frequency as well. Figure 3 illustrates the experimental results of
Llewellyn-Jones\(^{35}\).

In summary, the millimeter-wave water vapor continuum falls off as
frequency squared, has an enhanced self-broadening contribution that grows with
decreasing frequency, and has a strong negative temperature dependence.
Based on the data presented and Birnbaum's line shape formula, a simple formula for the nitrogen broadened water vapor continuous absorption coefficient from 700 to 1100 cm\(^{-1}\) and for typical atmospheric temperatures is given by \(\text{Eq. 3}\):

\[
\beta_{\text{continuum}} = 6.41 \times 10^3 \exp(-0.00835v) \\
x + (T_0/T)^{1/2} P_0 = 16.80 \left(1/T - 1/T_0\right) P_0 \left(1 - \frac{P_0}{P_0}\right) \quad \text{[km}^{-1}\text{]} \tag{8}
\]

where \(P_0\) is atmospheres, \(v\) is wave numbers and \(T_0 = 296\) K.

An excellent review of experimental measurements in the 10-\(\mu\)m region by Grant \(\text{Eq. 3}\) makes the following additional points:

1. Oxygen does not broaden as effectively as nitrogen and must be included in a realistic model of the earth's atmosphere. A broadening coefficient of \(F/0.75 \pm 0.1\) for oxygen relative to nitrogen was measured by Nordstrom et al. \(\text{Eq. 3}\) using Eq. 3, this means air has an effective broadening of 0.95.

2. Understanding the local line structure is critical in determining the true continuum. Line positions are known reasonably well; however, line strengths and half-width are not known with enough accuracy.

Long-path field measurements by Devir et al. \(\text{Eq. 3}\) are in excellent agreement with the laboratory measurements of Burch and Alc \(\text{Eq. 3}\) and Peterson et al. \(\text{Eq. 3}\) in this window region concerning the water vapor continuum. The measured spectral range of Devir extends the range covered by Burch and Alc \(\text{Eq. 3}\) and shows the water vapor continuum increasing with increasing frequency. The minimum occurs at 9.0 \(\mu\m (1111 \text{ cm}^{-1})\). The nature of 8-12 \(\mu\m\) continuum absorption appears to be understood on the basis of the agreement between laboratory and field measurements.
Figure 5. Nitrogen broadening coefficient as a function of wave number from 700 to 1000 cm⁻¹ at 296 K.

Figure 6. Water vapor partial pressure dependence in the 10 μm region.

Figure 7. Temperature dependence of self-broadening coefficient in the 10 μm region.

The 3- to 5-μm window

The 3- to 5-μm continuum region has a different frequency dependence compared with the millimeter and 8- to 12-μm regions. Figure 1.3.16b displays a nearly parabolic dependence with a minimum at a wavenumber of 2600 cm⁻¹. As shown by the spectrometer measurements of Burch and Alt (27) (Fig. 8a), the self-broadening coefficient has an exponential falloff at wavenumbers up to 2550 cm⁻¹, then the falloff rate decreases as the frequency increases. Figure 8b shows long-path white cell DF laser measurements (27) taken under atmospheric conditions, which indicate continuum absorption levels roughly 50% higher than those indicated by Burch and Alt (27). The level of absorption in the 6-μm region is roughly an order of magnitude less than that in the 10-μm region. Long-path CO, DF, and HF laser measurements near room temperature again indicate large values for CO in the continuum region, ranging from 10 to 20 at 3 μm (28) to approximately 50 to 60 at 4 μm (29) and back down to 10 at 3 μm (29).

A strong negative temperature dependence is again observed for the self-broadening coefficient. Figure 9 shows the results of laboratory long-path spectrometer measurements by Burch and Alt (27). The temperature dependence at 2600 cm⁻¹ exhibits exponential falloff similar to that in the 10-μm and millimeter regions. However, the curves at 2500 and 2600 cm⁻¹ show double exponential trends. The nature of the water vapor continuum in this window region is more complicated than the other windows previously discussed.
More experimental data is needed to generate a meaningful empirical model of the continuum absorption coefficient. An attempt at representing the existing data is given by the following formula for the nitrogen broadened water vapor continuum absorption coefficient valid from 2400 to 2800 cm\(^{-1}\) [33a].

\[
A_{\text{continuum}} = 7.34 \times 10^{24} \left[ \frac{1}{P_{\text{H}_2} + 2293} \right] C_{\nu} (\nu, T) P_{\text{H}_2} + C_{\nu} (\nu, T) P_{\text{H}_2} \]  

(9)

where

\[
C_{\nu} (\nu, T) = 1.77 \times 10^{-20} \exp \left( \frac{-3.32 \times 10^{13}}{\nu} \right) \exp \left( \frac{1236}{T - 273} \right) + 3.91 \times 10^{-25} \exp \left( \frac{3.66 \times 10^{-13}}{\nu} \right) \exp \left( \frac{2625}{T - 273} \right)
\]

and

\[
C_{\nu} (\nu, T) = \left( \frac{1}{296/73} \right) 7.16 \times 10^{10} \exp \left( -6.45 \times 10^{-14} \nu \right) + 2.73 \times 10^{-25} \exp \left( 6.45 \times 10^{-14} \nu \right)
\]

Again, long-path field measurements by Devitt et al. [38] are in good agreement with Burch and Ali [27] in this window region concerning the water vapor continuum. The results of Devitt et al. [38] also point out the importance of the water vapor continuum between 4.5 and 5.0 \(\mu\)m. In this region, local line contributions can be significant as well, thus masking to some extent water vapor continuum absorption. CO laser transmission measurements as a function of water vapor partial pressure show an increase in the dimensionless self-broadening coefficient \(B\), over the near line center value [39]. As observed in the previous window regions, this observation is indicative of continuum absorption.

Field measurements between 4.1 and 3.8 \(\mu\)m reveal that other continuum sources exist. The far blue wing beyond the band head of the fundamental \(v_3\) band of CO [41] and the collision-induced absorption band of nitrogen [42] also contribute to continuum-type absorption in this window region and will be discussed later.

The 2.0- to 2.5-\(\mu\)m window

This window region has not received the same attention as the longer-wavelength windows; as a result, no experimental continuum absorption has been previously reported. Recent measurements [43], however, indirectly suggest that continuum absorption does exist. Transmission measurements on hot (7 - 685 K) high-pressure (up to 4.8 kPa) water vapor show the continuum absorption in the 2.1- and 4- \(\mu\)m regions (Fig. 10). Absorption levels at 4 \(\mu\)m are consistent with the extrapolated values from the curves in Fig. 9. The point to be made is that a similar continuum absorption process occurs in the 2.1- \(\mu\)m region, as shown in Fig. 10. If we assume that an extrapolation to lower temperature follows the same trend as at 4 \(\mu\)m, then a continuum exists in the 2.0- to 2.5- \(\mu\)m window that is very similar to the 3- to 5- \(\mu\)m window under normal atmospheric conditions.

1.7 to 1.5 \(\mu\)m window and beyond

Figure 10 shows the beginning of the continuum centered at 1.6 \(\mu\)m. Again, this suggests a water vapor continuum in this window region at a weaker level than at 4 and 2 \(\mu\)m. Based on this observation, it is expected that every window in the infrared has a water vapor continuum at some absorption level. This level should become weaker as the frequency increases.
of past line-shape theories is in their failure to predict the observed strong negative temperature dependence characteristic of all the window regions, except for the recent line shape model of Ha and Tipping at the millimeter wave window. But this weakness is the very strength of an alternative hypothesis to explain the water vapor continuum: the water dimer. The formation of water vapor dimers has a strong negative-temperature dependence that closely matches the temperature dependence of the continuum absorption in the 10-μm region. However, this near match does not occur in the microwave window or in the 4-μm window. This approach also requires dimer absorption bands to account for the continuum. However, the hypothesis would require a dimer absorption band in every water vapor window, a condition that has not been experimentally found or theoretically shown. Furthermore, measurements on supercooled water vapor indicate that dimer absorption is an order of magnitude too small to account for the water vapor continuum at 10 μm. In spite of these shortcomings, the dimer hypothesis demonstrates the importance of understanding water-vapor water-vapor interaction to explain the continuum absorption temperature dependence.

A semi-empirical line shape model developed by Birnbaum with validity from line center to the far wing (when line mixing can be ignored) predicts an exponential wing as observed experimentally and can be properly normalized. This model has been successfully applied to the CO₂ blue wing of the 4.3 μm band. Application of this line shape to line-by-line calculations indicate that this model is not complete enough to represent the water vapor continuum throughout the entire infrared region. The experimental data previously described are reasonably represented by these models. The strength of this approach is accounting for spontaneous emission and the fluctuation dissipation theorem in enforcing detailed balance across the entire line shape. This results in a physically meaningful far wing and a more versatile line shape overall.

Although no definitive interpretation of the water vapor continuum exists, the experimental and theoretical evidence indicates that far wing absorption contributions by the bordering strong water vapor bands play a dominant role. The evidence is based largely on the frequency dependence of the continuum in the first four spectral windows reviewed (i.e., the shape of the continuum as a function of frequency and growth of the dimensionless broadening coefficient, ε, away from a band as a function of frequency). The shortcoming of the far wing approach is predicting the temperature dependence, but the character of a far wing must be driven by close binary interactions much like the creation of a dimer, which does exhibit the observed temperature dependence in the 10-μm window region. This point has been verified by the recent work of Ha and Tipping.

REFERENCES


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Prepared for: Annual Review Conference on Atmospheric Transmission Models
Topical Session on Spectral Line Shapes
June 12, 1991
Geophysics Directorate, Phillips Laboratory
Hanscom Air Force Base
BIRNBAUM’S LINE SHAPE

Ignoring line mixing, the absorption coefficient is:

\[ \beta(\nu) = \sum_j S_j \frac{\nu}{\nu_j} \frac{\tanh \frac{hc\nu}{2kT}}{\tanh \frac{hc\nu_j}{2kT}} j(\nu, \nu_j) \]

WHERE \( S_j \) IS THE LINE STRENGTH OF THE JTH LINE,

\( \nu \) IS THE FREQUENCY IN WAVE NUMBERS.

\( j(\nu, \nu_j) \) IS THE FOURIER TRANSFORM OF THE DEPENDENT AUTOCORRELATION FUNCTION \( C(r) \):

\[ j(\nu, \nu_j) = \frac{1}{N} \frac{1}{\pi} \int_0^{\infty} \text{d}r \cos 2\pi c \nu r \left( e^{j2\pi c \nu_j r} C(r) + e^{-j2\pi c \nu_j r} C^*(r) \right) \]

\( N \) IS THE NORMALIZATION FACTOR OF THE LINE PROFILE. AT INFRARED FREQUENCIES \( N = 1 \).
Birnbaum uses the following semi-empirical expression for $C(r)$:

$$ C(r) = \exp\left[\frac{r_{12}^2 - (r_{12}^2 + r^2 - 21r_{12}r^2)^{1/2}}{r_{12}}\right] $$

and $C(r) = C_a(r) + C_b(r) + \ldots + C_m(r)$

where the subscripts designate the different molecules in the system.

$t_{A1}$ and $t_{S1}$ represent the long time and short time behavior of the autocorrelation function respectively.

$t_0$ is a thermal time defined by:

$$ t_0 = \frac{\hbar}{4\pi k_T} $$

In the case of pure gases, $J(\omega, \omega_0)$ is written (with $\omega = 2\pi c$):

$$ J(\omega, \omega_0) = \frac{1}{N} \frac{r_1}{\pi} e^{r_1^2/2} \left\{ e^{\text{ih}_{\omega_0} \omega_0} \frac{Z_K(Z)}{1 + ((\omega - \omega_0) t_1)^2} + e^{\text{ih}_{\omega_0} \omega_0} \frac{Z_K(Z)}{1 + ((\omega + \omega_0) t_1)^2} \right\} $$

where $Z_2 = (r_1^2 + \omega_2^2) + (r_0^2 + \omega_1^2)$ and

$\omega_2 = \omega \pm \omega_0$

$K_1(Z)$ is the modified Bessel function of the second kind. $r_1$ is written as

$$ r_1 = \frac{1}{2\pi c t_1} $$

where $t_1$ is the self broadened coefficient for each absorber molecule $i$. We assume that $r_2$ is constant for each molecule and for each studied frequency range.
Far Wing line shape.

\[ \text{SN} = \frac{\tanh(hc_{i}/2k_{i}T)}{\tanh(hc_{j}/2k_{j}T)} \cdot j_{N}(v) \]

and

\[ j_{N}(v) = (\frac{\text{SN}}{2\pi})^{1/2} \frac{1}{v_{i}} \frac{\exp(-2\pi c_{i} v_{i}v)}{\sqrt{2\pi c_{i}}} \exp(2\pi c_{i} v_{i}v) \]

The exponential wing is consistent with experimental observation \([13,16]\). The general far wing result for a binary mixture can be obtained by solving a convolution integral of the individual line shape functions \((j, \text{and } j_{b})\) in the far wing limit. Thus, given

\[ j_{b}(v) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \ e^{2\pi c_{i}v} C_{b}(v), \]

\[ j_{l}(v) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \ e^{2\pi c_{i}v} C_{l}(v), \]

and

\[ j(v) = \int_{-\infty}^{\infty} j_{b}(v)j_{l}(v - v_{l} - x)dx. \]

Then using contour integration and in the far wing limit

\[ j_{N}(v) = (\frac{\text{SN}}{2\pi})^{1/2} \frac{1}{v_{i}} \frac{\exp(-2\pi c_{i} v_{i}v)}{\sqrt{2\pi c_{i}}} \exp(2\pi c_{i} v_{i}v) \]

\[ \ast (\frac{\text{SN}}{2\pi})^{1/2} \frac{1}{v_{i}} \frac{\exp(-2\pi c_{i} v_{i}v)}{\sqrt{2\pi c_{i}}} \exp(2\pi c_{i} v_{i}v). \]

Note:

\[ \int_{F_{W}}(v) \xrightarrow{v \to 0} 2^{y} \]

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A general empirical form for the continuum absorption coefficient used to represent the data (5) is

$$\beta_{\text{cont}}(v, T, P_i; ... P_n, P_k) = \frac{P_i}{RT} \sum_i \left[ C_i(v, T) P_i + C_f(v, T) P_k \right]$$

where $C_i$ is the self-broadening coefficient of the absorbing gas, $C_f$ is the foreign broadening coefficient due to the ith type foreign gas, and $R$ is the ideal-gas constant. The equation can be conveniently rewritten for $i = 2$ to obtain

$$\beta_{\text{cont}}(v, T) = \frac{C_2(v, T) P_2}{RT} \left[ P_2 + C(v, T) P_2 + B(v, T) P_2 \right]$$

where $P = C_2 / C_1$ and $B = C_1 / C_1$ are the dimensionless broadening coefficients. Near line center, $B$ has the value of 5 for water vapor relative to nitrogen. In the real atmosphere, the effects of oxygen broadening must also be included. The dimensionless broadening coefficient $P$ accounts for oxygen. However, many laboratory experiments ignore the effects of oxygen and use only nitrogen as the broadening gas along with the absorbing gas.

**EXPERIMENTAL WATER VAPOR CONTINUUM DATA**

![Graph showing water vapor continuum absorption coefficient as a function of frequency.](Image)

**Figure 1.3.10** Water vapor continuum absorption coefficient as a function of frequency. The solid line is an empirical fit to the experimental data points as given by Eq. 1.3.92. The plotted points are (+) [20], (-) [21], and (x) [22] for $T = 300 \text{ K}$, $P_2 = 101 \text{ kPa}$ and $\rho_a = 10^{-3} \text{ kg/m}^3$. 

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Figure 1.3.11 Temperature dependence of millimeter wave water vapor continuum. Solid curve represents empirical fit to data as given by Eq.

<table>
<thead>
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Figure 1.3.12 Self-broadening coefficient as a function of wave number from 700 to 1100 cm\(^{-1}\) at 296 K[27].

Figure 1.3.13 Nitrogen broadening coefficient as a function of wave number from 700 to 1000 cm\(^{-1}\) at 296 K[27].

Figure 1.3.14 Water vapor partial pressure dependence in the 10 \(\mu\)m region.

Figure 1.3.15 Temperature dependence of self-broadening coefficient in the 10 \(\mu\)m region.
4-μm continuum of H₂O

Figure 1.3.16 4 μm water vapor continuum region at T= 296K. (a) C₄ vs wave number [27] and (b) absorption coefficient vs wavelength [37,38].

Temperature (K)

Figure 1.3.17 Plots of the water vapor self-broadening coefficients at 2400, 2500 and 2600 cm⁻¹ vs reciprocal temperature [27]. The symbols †, ■, and ▲ represent the experimental data points.
Pure water vapor absorption coefficient at \( T = 685 \text{K} \) and three different pressures.

* The 1 \( \mu \text{m} \) window water vapor continuum has been measured by a novel interferometric calorimeter technique.

A pulsed Nd-glass laser is used to heat a nitrogen buffered water vapor sample placed in the arm of He–Ne Mach–Zehnder interferometer. Variations in the index of refraction due to the heating cause measurable fringe shifts proportional to the absorption coefficient.

* The resulting continuum absorption coefficient measured at 9466 \( \text{cm}^{-1} \) is \( 6 \times 10^{10} \text{ cm}^{-1} \) for a water vapor partial pressure of 16.5 Torr buffered by nitrogen to a total pressure of 1 atmosphere at 30°C.

Thus, the water vapor continuum is roughly two orders of magnitude weaker near 1 \( \mu \text{m} \) than at 4 or 2 \( \mu \text{m} \).

* Further measurements to determine the water vapor partial pressure dependence and temperature dependence are needed.
The tragedy of experimental water vapor continuum characterization is that unlike nitrogen and CO₂ experiments, it presently cannot be done at high pressure. High-pressure water vapor measurements also require high-temperature and thus a theoretical understanding of the continuum absorption temperature dependence to extrapolate back to atmospheric temperatures.

LINE-BY-LINE CALCULATIONS

HITRAN DATABASE AND BIRNBAUM'S LINE SHAPE

Pure H₂O
Continuum
Band = 1500 cm⁻¹
Local = 25 cm⁻¹

![Graph showing line-by-line calculations with experimental data and model predictions.](image-url)
OVERVIEW OF LINE COUPLING IN THE 5 mm BAND OF OXYGEN

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Nearly forty years ago, measurements of microwave absorption in oxygen indicated that pressure broadening became less effective, by approximately a factor of two, at pressures approaching one atmosphere than at lower pressures where the individual lines in the band were resolved. The explanation of this behavior of oxygen by means of overlapping line theory eventually led to methods of calculating absorption by oxygen that could be based on parameters determinable from careful laboratory measurements. Only recently, however, have such measurements explored an extensive range of frequency, pressure and temperature. These measurements (made by H.J. Liebe) are interpreted to determine the variation with temperature of the parameters that characterize line coupling. Possible revisions in transmittances for weather satellite frequencies are discussed.
Overview of Line Coupling in the 5 mm Band of Oxygen

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Abstract: Nearly forty years ago, measurements of microwave absorption in oxygen indicated that pressure broadening became less effective, by approximately a factor of two, at pressures approaching one atmosphere than at lower pressures where the individual lines in the band were resolved. The explanation of this behavior of oxygen by means of overlapping line theory eventually led to methods of calculating absorption by oxygen that could be based on parameters determinable from careful laboratory measurements. Only recently, however, have such measurements explored an extensive range of frequency, pressure and temperature. These measurements (made by H. J. Liebe) are interpreted to determine the variation with temperature of the parameters that characterize line coupling. Possible revisions in transmittances for weather satellite frequencies are discussed.

When microwave absorption in oxygen began to be measured, it was recognized very early (e.g., Crawford and Hogg, 1956 - Fig. 1) that at pressures near 1 atmosphere where the lines overlapped into a band, pressure broadening seemed to be less effective, by approximately a factor of two, than at much lower pressures where the individual lines were resolved. Meeks and Lilley (1963) proposed the use of the oxygen band for remote measurements of atmospheric temperature from satellites. They also devised a scheme for calculating absorption by assuming that the ratio of linewidth to pressure varied with altitude (Fig. 2). Similar absorption models were devised by Carter, Mitchell and Reber (1968) and Reber (1972). By and large, these models represented atmospheric opacity on the far wings of the oxygen band reasonably well. However, when the Nimbus 5 Microwave Spectrometer was launched into space in 1972, some systematic discrepancies from calculated brightness temperatures were observed, in particular near 58.8 GHz (Waters et al., 1975 - Fig. 3).

Gordon (1967) had already explained the relative narrowness of the oxygen band at high pressures by means of the theory of overlapping lines. This theoretical framework had been originated by Baranger (1958) and Kolb and Gnem (1958) and had been further developed by Fano (1963) and Ben-Reuven (1966). In the impact approximation, the pressure-proportional width parameter that applies to an isolated line is replaced, for a band of lines, by a pressure-proportional matrix \( \mathbf{w} \) whose diagonal elements are width parameters for each line, and whose off-diagonal elements represent the coupling of each pair of lines by collisions. Calculation of the band shape involved the inversion of a complex matrix (Fig. 4); however, a first-order perturbation expansion (Rosenkrantz, 1975 - Fig. 5) made it feasible to use the theory for atmospheric radiative-transfer calculations.

In the first-order approximation, the influence of the off-diagonal matrix elements occurs through the addition of dispersion-shaped functions to the usual resonant line shapes that describe isolated lines. Because of the way in which the signs of the coefficients associated with the former terms depend on rotational quantum number, the effect is an increase in absorption near the band center, and a decrease on the wings (Fig. 6).

Initially these coefficients (of the dispersion-shaped terms) were obtained from a method that estimated the largest of the off-diagonal elements of \( \mathbf{w} \). A later refinement (Rosenkrantz, 1988) allowed their determination directly from laboratory measurements. Direct calculation of the \( \mathbf{w} \) matrix has been carried out by Lam (1977) (whose results were revised by Smith, 1981 - Fig. 7), and by Minglegrin et al. (1972, 1979 - Fig. 8). These calculations obtained agreement with measurements at normal laboratory temperature and at pressures up to at least seven atmospheres (although the exact matrix inversion is required above one atmosphere).

Despite the success of overlapping line theory in accounting for laboratory measurements of absorption and dispersion as well as atmospheric opacity on the far wings of the band, it has not eliminated all discrepancies between calculations and measurements for satellite-based radiometers. Grody (1983) discusses some of these systematic offsets in data from the Microwave Sounding Unit on NOAA satellites (Fig. 9). They reach 1 to 2% in the channels at 55 and 58 GHz, which measure thermal emission from the upper troposphere and lower stratosphere. These brightness temperature differences could be explained by an increase in absorption of approximately 10%.

The association of these offsets with the colder parts of the atmosphere suggested that the temperature dependence of the line coupling might be different from that which had been assumed. A recently completed series of measurements by Liebe et al. (1991) on dry air at 279, 303 and 327 K provide the opportunity to test this hypothesis (Fig. 10). Coefficients for the line interference effect have been extracted from these measurements by the method described by Rosenkrantz (1988). For the lower rotational quantum levels (1, 3, 5, 7) their temperature dependence is \( T^{-0.8} \) (Fig. 11), similar to the line widths. The higher levels have some further variation with temperature, to which a linear function of the reciprocal temperature variable \( \theta = 300/T \) was fitted.

Atmospheric absorption can be calculated by extrapolating this fitted temperature dependence, and the new coefficients produce slightly less absorption than previously calculated at 53.7 and 55 GHz. The calculated brightness temperatures at these frequencies
have changed by less than 0.4 K. At 58 GHz there is essentially no change from the older calculation. Possibly, one could choose different functions to represent the variation with temperature that might fit the data equally well over the measured temperature range, yet extrapolate differently to colder temperatures. On the basis of the present laboratory measurements, however, the discrepancies observed by the MSU do not find an explanation.

An aircraft-based radiometer experiment is planned for the summer of 1991. It is hoped that these measurements, in the zenith-observing mode, will provide the lower-temperature test points that could validate (or not validate) the new oxygen-band line parameters.

References


Viewgraphs:

1. Absorption in air at sea level, from Crawford and Hogg (1956).
3. Calculated minus measured NEMS brightness temperatures at 58.8 GHz, from Waters et al. (1975).
4. Complex index of refraction.
5. Absorption at 58.8 GHz, from Rosenkranz (1975).
6. The effect of off-diagonal elements of w.
8. $O_2$ spectrum, from Mingelgrin et al. (1972).
10. New laboratory measurements on dry air by Liebe et al. (1991). Interference coefficients were fitted to the 101 kPa data.
11. Derived interference coefficients at three temperatures. The plotted coefficients are adjusted to 100 kPa pressure and normalized by the factor $\theta^{0.8}$.

Note: Figs. 10 and 11 were revised after the conference.
Fig. 8—Calculated and measured absorption by air at sea level. The dots represent the experimental data; the vertical lines indicate the spread in the measured values. Curves A and B are calculated curves of oxygen absorption using line-breadth constants of 600 and 1200 mc, respectively, and a temperature of 293° K. (Courtesy of T. F. Rogers, Air Force Cambridge Research Center.)
Complex index of refraction:

\[ m(\nu) - m(0) = -\frac{8\pi \mu_0 N_0}{3} \int \frac{\Delta \nu}{T} (\nu - \nu_0 - i \nu)^{-1} J_\nu d\nu \]
Fig. 3. Absorption in dry air at 58.82 GHz and 295 K, computed for three models. Measurements are by Poon [30].
Pressure in kPa

FIG. 8. Dispersion\textsuperscript{21} at 59.591 GHz as a function of pressure at a temperature of 300 K. Experimental points, solid and open circles, obtained from two independent unpublished measurements.\textsuperscript{4}

MINGELGRIN, GORDON, FRENKEL, AND SULLIVAN

Fig. 7. Calculated vs experimental line shape of pure O\textsubscript{2}.
LABORATORY MEASUREMENTS OF LINE COUPLING IN CO₂ AND N₂O

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Laboratory studies of line coupling in a number of CO₂ and N₂O Q-branches will be presented. Coupling calculations based on very simple scaling laws for rotational relaxation give good agreement with observation for self-broadened spectra over a wide temperature range (200 to 350K). N₂-broadened CO₂ Q-branches, however, exhibit more line coupling than calculated unless one forces the f→f collision rate in the Π state to be larger than the f→e collision rate. These two collision rates are approximately equal for self-broadened line coupling. Similar, but more extreme differences in these collision rates have been observed in CO₂ Q-branches broadened by He. Laboratory measurements of line coupling in the Q-branch at the Π–Δ band of CO₂ will also be presented. All previous measurements of Q-branch line coupling in CO₂ have involved Π–Σ bands. Examples of line coupling in N₂O Q-branches will also be presented.
Laboratory Measurements of Line Coupling in CO$_2$ and N$_2$O

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- Line Mixing – also known as
  - Line Coupling
  - Rotational Collisional Narrowing
  - Q-branch Collapse

- Previous Work
  - Raman – CO$_2$, NO, N$_2$, O$_2$, CO
    - 1932, 2070 cm$^{-1}$ CO$_2$ Q branches, self- and N$_2$-broadened; 597 cm$^{-1}$ Q-branches, H$_2$-broadened.
    - 720 cm$^{-1}$ CO$_2$ Q branch, self-broadened
    - N$_2$O Q branches, self-broadened (1880, 2800 cm$^{-1}$), N$_2$-broadened (2800 cm$^{-1}$)
    - C$_2$H$_2$, HCN, etc. Q branches, self-broadened
    - $\nu_3$ R-branch bandhead of CO$_2$

- Atmospheric Implications
  - Temperature Sounding: UARS (CLAES, ISAMS), EOS (AIRS, TES), ATMOS, HIS

Line Coupling Theory

- $\Pi - \Sigma$ band, $l=1$ in $\Pi$ state
- Line mixing absorption coefficient given by
  \[ k(\nu) = \frac{N}{\pi} \text{IM} \left\{ \sum_{i,k} d_i(\langle j|[(\nu - \nu_e) - iPW]^{-1}|k\rangle) \rho_k \right\}, \]

- Determine $W$ matrix ($\Pi - \Sigma$ bands) from
  \[ W_{jj} = -\frac{1}{2} \left( \sum_{j'\neq j} K_{j'j}^{(e-o)} - \frac{1}{2} \left( \sum_{j'\neq j} \beta K_{j'j}^{(e-e)} + \sum_{j'\neq j} (1 - \beta) K_{j'j}^{(o-o)} \right) \right), \]
  where $W_{jj}$ is the linewidth, and $K_{j'j}$ is modeled with the hybrid power-exponential-gap (PEG) law
  \[ K_{j'j} = a_2(T_o/T)^{0.5} \frac{\left[ \frac{\Delta E_{j'j}}{B_0} \right]^{-\alpha}}{\exp \left( \frac{-a_3 \Delta E_{j'j}}{kT} \right)}, \]
  for $j' > j$. Detailed balance gives $K_{j'j}$ for $j' < j$. $\Delta E_{j'j} = E_{j'} - E_j$ is the rotational energy gap. For CO$_2$-CO$_2$, N$_2$O-N$_2$O collisions $\beta \approx 0.50$. For CO$_2$-N$_2$ collision $\beta \approx 0.625$, for CO$_2$-He collisions $\beta \approx 0.75$. $W$ is obtained by letting
  \[ W_{jj} = -\beta K_{j'j}^{(e-e)} \]
- Only $\beta$ must be determined from spectra exhibiting mixing
Calculational Details

\[ k(\nu) = \frac{N}{\pi} \text{IM} \left\{ \sum_{j,k} d_j \langle j | \left[ (\nu - \nu_o) - iPW \right]^{-1} | k \rangle d_k \rho_k \right\}, \]

can be rewritten as

\[ k(\nu) = \frac{N}{\pi} \text{IM} \{ d \cdot G(\nu)^{-1} \cdot \rho \cdot d \}, \]

where

\[ G = \nu - H, \quad H = \nu_o + iPW. \]

Diagonalizing \( H \) with \( L \)

\[ A^{-1} \cdot H \cdot A = L \]

allows \( k(\nu) \) to be rewritten

\[ k(\nu) = \frac{N}{\pi} \text{IM} \left\{ \sum_i \frac{(d \cdot A)_i (A^{-1} \cdot \rho \cdot d)_i \nu - l_i}{\nu - l_i} \right\} \]

which is an algebraic sum.

1% CO2 in 50, 100, 360, 720 Torr N2
Data - Ishus
Calc. - Helle et al.
20 meter path
0.1% CO₂ in Ne
552 Torr Ne

Fig. 14a. The CO₂ 1500 band absorption spectra at 3920. Two solid curves are the experimental data taken using the gas cell. The long dashed curve is the Voigt calculation. The short dashed curve is the Lorentzian.

Fig. 14b. The CO₂ 1500 band absorption spectra at 251 K. The solid curve is the experimental data taken using the gas cell. The long dashed curve is the Voigt calculation. The short dashed curve is the Lorentzian.

Fig. 14c. The CO₂ 1500 band absorption spectra at 292 K. The solid curve is the experimental data taken using the gas cell. The long dashed curve is the Voigt calculation. The short dashed curve is the Lorentzian.

Fig. 14d. The CO₂ 1500 band absorption spectra at 351 K. The solid curve is the experimental data taken using the gas cell. The long dashed curve is the Voigt calculation. The short dashed curve is the Lorentzian.

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720 Torr CO₂

Transmission

791.2 791.4 791.6 791.8
Frequency (cm⁻¹)

360 Torr CO₂

Transmission

791.2 791.4 791.6 791.8
Frequency (cm⁻¹)

Error

Obs-Calc

791.2 791.4 791.6 791.8
Frequency (cm⁻¹)

360 Torr CO₂, Equal f→f, f→e

Transmission

791.2 791.4 791.6 791.8
Frequency (cm⁻¹)

360 Torr CO₂, no f→e (δ=1)

Transmission

791.2 791.4 791.6 791.8
Frequency (cm⁻¹)

Obs-Calc

791.2 791.4 791.6 791.8
Frequency (cm⁻¹)
1% CO₂ in 720 Torr N₂

1% CO₂ in 360 Torr N₂

CO₂ Q Branch -- 1% CO₂ in 740 Torr N₂
ATMOS Spectrum

--- VOIGT
--- LINE MIXING

RESIDUAL (%)

SS07
14.8 KM

SIGNAL

WAVENUMBER (cm⁻¹)

1.0
0.8
0.6
0.4
0.2
0.0

NO
H₂O

0.2 0.4 0.6 0.8 1.0

1931 1932 1933

CALCULATED TRANSMITTANCES

Mixed Lorentz
Mixing (with x-function)

0.2 0.4 0.6 0.8 1.0

616 617 618 619

WAVENUMBER (cm⁻¹)

0.00 0.05 0.10 0.15 0.20 0.25 0.30

ATMOS-Lorentz
ATMOS-Mixing (no x-function)
ATMOS-Mixing (with x-function)

378
$\beta = 0.5$

$\beta = 0.75$

Experimental Spectra: Diff-Freq Laser

\[ P = 20,200,400,740 \text{ Torr}; \ L = 5.8 \text{ cm} \]

---

**Results of least-squares fit to \( \nu D \) \( \Delta \)-branch**

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**Observed Spectrum**

**No Mixing**

**Mixing**

---

Wavenumber
Experimental Spectra; Diode Laser

P = 2, 100, 380, 740 Torr; L = 1.12, 417 cm

Transmission

Frequency (cm⁻¹)
See previous figure for definitions of (a) - (d). Sign of error reversed here.
12.17 meters, 296.7K

401 torr, 1.00% CO₂

![Graph of transmission vs. frequency](image)

- Data
- All lines mixed
- No mixing
- Quasi mixing

![Graph of transmission vs. frequency](image)

- Data
- Lorentz
- Mixing

![Graph of deviation vs. frequency](image)

- Lorentz deviation
- Mixing deviation

---

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Line Coupling in the \( \nu_3 \) Bandhead of \( \text{CO}_2 \) at 4.3 \( \mu \text{m} \)

- Line coupling accounts for much of the sub-Lorentz absorption in the bandhead region which is used for temperature sounding.
- Duration-of-collision effects may also be important inside the bandhead.
- Trade-offs between high-J behavior of rotational relaxation (is the scaling law any good at high J?) and the duration-of-collision parameter give good results for room-temperature spectra of pure \( \text{CO}_2 \).

We use a semi-empirical lineshape in this region:

\[
k(\nu)_{\text{empirical}} = k_{\text{mixing}}(\nu) \cdot \chi(\Delta \nu), \quad \Delta \nu_i = \nu - \nu_i.
\]

\[
\chi_i = z_i K_1(z_i) \exp(\tau_2 \alpha_{L_i} + \tau_0 \Delta \nu_i),
\]

where

\[
z_i = \sqrt{(\alpha_{L_i}^2 + \Delta \nu_i^2)(\tau_0^2 + \tau_2^2)}, \quad \tau_0 = \frac{0.72}{T}, \quad \tau_2 \sim 0.0275.
\]
Line Coupling in R-branch Bandhead of CO\textsubscript{2} at 4.3 μm
(Data from Grier, pre CO\textsubscript{2} at ~32 m)

Wavenumber (cm\textsuperscript{-1})

Ratio of Measured k(G) to Lorentz k(G) for Δ\textsuperscript{4}-branch CO\textsubscript{2}
(Expt. Data from Coisin et al.)

Lines denote centers of A1E3 Channels

Wavenumber (cm\textsuperscript{-1})
Conclusions

- CO₂–N₂ calculations predict less coupling than observed indicating some propensity to conserve vibrational angular momentum, this propensity is more pronounced for CO₂–He collisions
- CO₂ self-broadening models also very accurate over a wide temperature range
- Line coupling models sufficiently accurate for Q-branches important for CLAES, AIRS, HIS retrievals
- Atmospheric measurements (ATMOS, HIS) indicate that temperature dependence of line coupling is in relatively good shape for air-broadening
- More parameters needed to model Π-Δ Q-branches at 740 and 97 cm⁻¹
- One N₂-broadened N₂O study shows good agreement using self-broadened collision model (β = 0.50), some further work warranted on other bands, and with O₂-broadening
- Good progress made with R-branch coupling at 4.3 μm. Further work with N₂-broadening, low temperature, high-resolution spectra required for AIRS temperature sounder which operates inside the R-branch
LINE-MIXING: A NEAR AND FAR LINE WING PROBLEM

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Line mixing is a problem of crucial importance for modeling of gas absorption spectra. For this reason, much experimental and theoretical studies have been made in the infrared and Raman domains. In particular, absorption in Q-branches and troughs between lines of P and R-branches, which are affected by line-interferences at moderate densities have been widely investigated. Various models have been proposed for the modeling of such phenomenon, which are generally based on the impact approximation. Studies of absorption at elevated density and in the very far wings of lines have demonstrated that these models can be very inaccurate. Other approaches, which account for the finite collision duration, have been proposed quite recently which lead to satisfactory results.

The author will try to present a comprehensive révue of experimental and theoretical results connected with the influence of line-mixing on absorption spectra. The advantages and limits of approaches based on the impact approximation will be discussed. The state of the art and perspectives for measurements and calculations of high density spectra and continuum absorption will be discussed.
LINE - MIXING: NEAR AND FAR
LINE - WING PROBLEMS

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1. WHAT HAPPENS?
2. IMPACT APPROXIMATION
   - MODELLING
   - REMAINING PROBLEMS
3. FAR WING
The Hamiltonian of the isolated molecule is perturbed during each collision. The energy levels of the molecule are then modified and functions of time.

All the more important that the interaction potential is large and spread (long range), and that the collision duration is long (low T).
LINE MIXING: WHAT HAPPENS?

- NEAR LINE CENTER

\[ \Delta E = h(v_1 - v_0) \]
\[ \Rightarrow \text{efficient if } |v_0 - v_1| \ll \gamma \]

- Dominant process:
\[ p_0 \sigma_{0 \rightarrow 1} = p_1 \sigma_{1 \rightarrow 0} \]
\[ \Rightarrow \text{if } (p_0 > p_1, \ i.e. \ S_0 > S_1) \sigma_{1 \rightarrow 0} \text{ more efficient} \]
\[ \Rightarrow \text{molecules which are on } \sigma \text{ above at } v_1 \]
\[ \Rightarrow \text{intensity taken from weak lines given to strong lines} \]

Conclusion: from line center to line center
- only if \( \gamma \gg |v_0 - v_1| \) (large potential)
- only if \( \neq \) populations at the levels (low T)
- from weak to strong lines
- Energy: $|\Delta E| = |h(V_0 - V_i + \Delta V)|$

- Efficiency: when $|V_0 - V_i| \ll \Delta V$
  the jump is $\Delta V$ \text{ as efficient as the broadening up to } \Delta V

\text{\text{\text{\begin{itemize}}}
  \item Take intensity in the wings to give to line centers
  \item Oscillator will go to zero in far wing
\end{itemize}}
Similar results in N₂O, CO₂
Hartmann et al. 1988
Straw et al. Noguchi et al.
1: experimental
—: Lorentzian calculation
—: EGL fitting law line mixing calculation.

Trough Between $R_{66} - R_{68}$ CO$_2$ lines  CO$_2$ - N$_2$
Similar results for CO, N₂O...
\[
\alpha(\omega) = \frac{8 \pi^3 \sigma}{3 h \pi c} N_a \sum_{i \neq f} \left[ \rho_i - \rho_f \right] d_{i f} \frac{\sinh \left( \frac{\hbar \sigma_{1/2} \omega}{2kT} \right)}{\sinh \left( \frac{\hbar \sigma_{1/2} \omega}{kT} \right)}
\]

\[
\times \left\{ \sum_{i \neq f} d_{i f} \text{Im} \left[ \langle \phi_i | \tilde{\sigma}_\omega \tilde{\sigma}_{\omega_i} - i N_a \tilde{W}(\omega) \rangle^{-1} \langle \phi_i | \tilde{\sigma}_\omega \tilde{\sigma}_{\omega_i} - i N_a \tilde{W}(\omega) \rangle \right] \right\}
\]

\[\tilde{W}:\text{relaxation operator - All the influence of collisions.}\]

\[2\pi c |\sigma - \sigma_{ib}| \ll c \implies \tilde{W} \text{ independent on } \sigma\]

\[\text{ (Impact approximation)}\]

\[\langle \phi_i | \tilde{\sigma}_\omega \tilde{\sigma}_{\omega_i} - i N_a \tilde{W}(\omega) \rangle^{-1} \langle \phi_i | \tilde{\sigma}_\omega \tilde{\sigma}_{\omega_i} - i N_a \tilde{W}(\omega) \rangle \approx \delta_{i f} - i \Delta i f\]

\[\tilde{W} \text{ diagonal \Rightarrow Lorentz shape}\]

\[\langle \phi_i | \tilde{\sigma}_\omega \tilde{\sigma}_{\omega_i} \rangle^{-1} \langle \phi_i | \tilde{\sigma}_\omega \tilde{\sigma}_{\omega_i} \rangle \approx \delta_{i f} - i \Delta i f\]

\[\text{In Raman (isotropic)}\]

\[\sum_{i', f'} \langle \phi_i | \tilde{\sigma}_\omega \tilde{\sigma}_{\omega_i} \rangle^{-1} \langle \phi_i | \tilde{\sigma}_\omega \tilde{\sigma}_{\omega_i} \rangle = - \langle \phi_i | \tilde{\sigma}_\omega \tilde{\sigma}_{\omega_i} \rangle^{-1} \langle \phi_i | \tilde{\sigma}_\omega \tilde{\sigma}_{\omega_i} \rangle\]

\[\text{In infrared (within 10SA)}\]

\[\sum_{i', f'} \frac{d_{i' f'}}{d_{i f}} \langle \phi_i | \tilde{\sigma}_\omega \tilde{\sigma}_{\omega_i} \rangle^{-1} \langle \phi_i | \tilde{\sigma}_\omega \tilde{\sigma}_{\omega_i} \rangle = \langle \phi_i | \tilde{\sigma}_\omega \tilde{\sigma}_{\omega_i} \rangle^{-1} \langle \phi_i | \tilde{\sigma}_\omega \tilde{\sigma}_{\omega_i} \rangle\]
LINE MIXING MODELS
W( = )

Statistically based FITTING LAWS

\[ \langle i f \mid W(0) \mid i' f' \rangle \neq \langle i f \rangle = F(i, i') \]

Exponential Gap Law

\[ \rho_i = \exp[-\beta (E_i - E_t)] \]

Polynomial Energy Gap Law

\[ \rho_i = (\Sigma_k - |E_i - E_t|)^{-k} \]

Isotropic Raman Sum Rule

\[ \sum_{i' f' \neq i f} \langle i f \mid W(0) \mid i' f' \rangle = -\langle i f \mid W(0) \mid i f \rangle \]

Widely used in Raman (Greenhalgh, Hall, Rosasco, Robert, Bonamy, ...)
in IR (Stron, Gentry, Lacombe, Boulet, Harothon, Nacloux, ...)

Dynamically based SCALING LAWS (De Fristo, Rabitz, 1979)
(10S, ECS)

\[ \langle i f \mid W(0) \mid i' f' \rangle \propto \sum_{L} \bar{F}(i, i', b, b', L) \to L \]

Angular momenta
Energy Corrections
Detailed Balance

Direct calculation (10S, CS, CC) (Green, Boulet, 1989)
Inversion from broadening (De Fristo, Rabitz, Bonamy, Robert, 1989)

More accurate than fitting laws. Correct J dependence (interbranch mixing)
MODELS within the IMPACT APPROX

Absorption coefficients

$$K_{\nu}^{\text{LC}}(T,P) = \text{Im} \left\{ P \left( \frac{8\pi^2 \nu}{3hc} \right) \left[ 1 - \exp(-h\nu/kT) \right] \sum_{IF} \rho_I(T) \; d_{IF} \right\}$$

$$W(T) : \text{relaxation operator. Contains all the influence of collisions. Relation with line-broadening:}$$

$$\langle IF|W(T)|IF\rangle = \gamma_{IF}(T) - i\Delta_{IF}(T)$$

No line-mixings --> W diagonal --> lorentzian shape.

$$K_{\nu}^{\text{LR}}(T,P) = \sum_{IF} \left\{ \rho_{IF}(T) \sum_{IF} \langle IF|W(T)|IF\rangle \right\}$$

Problem: Model the off-diagonal elements of W

Fitting laws

$$\langle IF|W(T)|I'F'\rangle = f(a_1, a_2, \ldots, a_n, I, I') \quad (I \neq I')$$

Exponential Gap Law: $$\gamma_I \cdot \exp(-b|E_I-E_{I'}|)$$

parameters deduced from isotropic Raman sum rule:

$$\sum \langle IF|W(T)|I'F'\rangle = -\langle IF|W(T)|IF\rangle$$

Scaling relations (Energy Corrected Sudden Approximation).

$$\langle ji'jf'|WECS|jijf\rangle = -(Nv/2\pi c) \; A(ji, ji') \; A(jf, jf')$$

$$\exp[(E_{ji} - E_{ji'})/kT] \sum_{L\ell_0} F_1(ji'jf'|lijjf|L00) \; A(L,0) - 2 (2\ell + 1) \sigma_{OL}$$

$$F_1(ji'jf'|lijjf|L00) = (-1)^{n+jf+jf'+L(2ji'+1)+v((2jf+1)(2jf'+1))}$$

$$\left\{ \begin{array}{ccc} ji & jf & n \\ ji' & L & ji' \\ jf' & L & ji \\ 0 & 0 & 0 \end{array} \right\}$$

$$A(j, j') = [1 + \Omega(j, j') \ell_c/v]^2/24]^{-1} \quad (\ell_c \text{ scaling length})$$

calculation or analytical law for $$\sigma_{OL}$$ (example: $$A(L(L+1))^{-\alpha}$$

parameters (including $$\ell_c$$) deduced from line-broadening:

$$\langle ji'jf'|WECS|jijf\rangle = \gamma_{ji'jf} = (Nv/2\pi c) \; A(ji, ji) A(jf, jf)$$

$$\left\{ \sum_{L\ell_0} F_n(ji'jf'|lijjf|L00) \; A(L,0) - 2 (2\ell + 1) \sigma_{OL} \right\}$$
$10^{-3} \text{ cm}^{-1} \text{ atm}^{-1}$

P lines - $R_2$

$R_2$ - R lines

(a)

$J_i$

40 20 0 20 40

(b)

$R_{18}$ - P lines

$R_{18}$ - R lines

---

- ECS
- MEGL only intra-branch
- MEGL intra + inter branch

Pure CO$_2$ 296 K: $<E||W(O)||E'>$
Pure CO₂ V band Raman Q branch

$T = 295 \text{ K}$

$\rho = 25.8$ amagat

---

PEGGL line mixing

lorentzian

Hillot et al. 1987

---

N₂ ECS MODEL

$P = 9.54$ Amagat $T = 506.0$ K

pure N₂ Raman

---

Boñamy et al., Berger et al. 1989
PurE CO₂ IR Q-Branch 296 K, 30 atm

Very similar results:
- Strrow et al.
- Haugan et al.

Still problems in IR Q-Branch (Ω-P, Ω-R mixing)
Statistical quasistatic approach
- Danes et al.
- From first principles
FREQUENCY $\omega$ (cm$^{-1}$)

$\alpha(\omega) \times 10^{22}$ (cm$^2$ molecule$^{-1}$ atm$^{-1}$)

+ 'CHP (Burch)
O, A Cole. (Tipping et al. Similar to Ramskog
pure H$_2$O 296 K

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CONCLUSION

Impact Models

- Quite accurate by using empirical factors for inter/intra branch or e/\phi levels
- Still problems: why intra branch mixing has to be lowered in the IR (OK in IR even with models (105, ECS) which should account correctly for coupling between levels of \phi symmetry
- Efforts on \phi-branched \textit{CO}_2-He? Close coupling?

FAR WING

- Very difficult problem
- Results are very sensitive to the interaction potential (particularly in far wing \textarrow{\rightarrow} short range interactions)
- Theory only for very far wing (quasistatic)
  \textarrow{\Rightarrow} How to connect with impact
- Still quite untractable for molecule-molecule with many levels and multi-component interaction
Theoretical calculations of the contributions from the far wings of allowed transitions to the continuous absorption by water vapor have been carried out for both the millimeter and infrared spectral regions. The theory is based on the quasistatic approximation and assumes as input only the known rotational constants and dipole moment matrix elements, and two Lennard-Jones potential parameters describing the isotropic interaction between two molecules. Results will be compared to recent laboratory data, and the implications for atmospheric applications discussed.
INTRODUCTION

1.1) IMPORTANCE OF MILLIMETER AND INFRARED RADIATION IN ATMOSPHERES

(1) Controls the energy balance and affects the climate of the Earth.

(2) Widely used in remote sensing, atmospheric communications, etc.

(3) To determine characteristics of planetary atmospheres from experiment data.
1.2) ATMOSPHERIC WINDOWS AND CONTINUUM ABSORPTION

Opaque regions and windows:
The opaque regions are mainly determined by H$_2$O lines, along with O$_2$ and CO$_2$ lines. Between them there are "WINDOWS".

The weak absorption in windows:
(1) Some weak local lines of H$_2$O, O$_2$ and CO$_2$.
(2) A gradually varying background, i.e. continuum absorption.

---

Fig. 57: Microwave absorption due to atmospheric gases: (a) average absorption coefficient $\kappa_f/\kappa_s$ at sea level and (b) trace species, both at the surface conditions $P_s = 1013$ mbar, $T_s = 293$ K, and $n_0 = 7.5$ g cm$^{-2}$. Solid curves are calculated according to theory, and dots are measured.
1. "CONTINUUM" - ABSORPTION NOT ASSOCIATED WITH NEARBY LINES. THIS DOES NOT IMPLY THAT IT IS ASSOCIATED WITH UNBOUND STATES.

2. EXCESS ABSORPTION OR DEFICIENT ABSORPTION?

1.3) BASIC CHARACTERISTICS OF CONTINUA

There are two kinds of water continua:
(1) \( \text{H}_2\text{O} - \text{H}_2\text{O} \) (self) continuum
(2) \( \text{H}_2\text{O} - \text{N}_2, \text{O}_2 \) (foreign) continuum

Usually, the self-continuum is dominant.

CHARACTERISTICS OF THE SELF-CONTINUUM:
(1) Varies smoothly with frequency.
(2) Proportional to \( n^2 \).
(3) Very strong negative temperature dependence.
1.4) MAIN THEORIES OF WATER CONTINUUM

THREE MECHANISMS FOR SELF-CONTINUUM:

(1) Collision broadened far-wings of allowed water vapor lines.
(2) Collision-induced absorption.
(3) Water dimers.

All three mechanisms vary as $n^2$, but there are large differences in the temperature dependencies and in the magnitudes of the absorption.
BRIEF HISTORY OF COLLISION-BROADENING MECHANISM FOR THE WATER CONTINUUM:

(1) In 1938, Elsasser first proposed that the water continuum was due to far-wings of allowed lines.

(2) Anderson-type theories with the impact approximation.

(3) Clough et al. considered the finite duration of collisions.

(4) Boulet and Robert, Birnbaum, etc. obtained exponential-like far wings.

(5) Rosenkranz's quasistatic method based on two approximations:
   (a) the far wing limit: \( \omega \gg \omega_{fi} \)
   (b) the narrow band approximation:
       \( \omega \gg \omega_{fi} \).

RESULTS:
In the IR, the temperature dependence and the magnitude of \( \alpha(\omega) \) were in reasonable agreement with experiment but there are significant differences in some regions, and this method is NOT APPLICABLE IN THE MILLIMETER REGION.
THEORY MILLIMETER REGION

\[ \alpha(\omega) = \frac{4\pi^2}{3hc} \omega \tanh(\beta\omega/2) \left[ F(\omega) + F(-\omega) \right] \]

\[ = \frac{4\pi^2}{3hc} \omega \left( e^{\beta\omega} - 1 \right) F(\omega) \]

\[ F(\omega) = (2\pi)^{-1} \int_{-\infty}^{+\infty} e^{i\omega t} <\hat{\mu}(0) \cdot \hat{\mu}(t)> dt \]

\[ <\hat{\mu}(0) \cdot \hat{\mu}(t)> = \sum_i \rho_i <i|\hat{\mu}(0) \cdot \hat{\mu}(t)|i> \]

\[ F(\omega) = -(n)^{-1} \text{Im} \text{Tr} \left( \hat{\mu}(0) \frac{1}{\omega - \hat{\sigma}} \rho \hat{\mu}(0) \right) \]

APPROXIMATIONS

1. BINARY COLLISIONS
2. PAIR POTENTIAL
   \[ V = V_{\text{ISO}} + V_{d-d} \]
3. QUASISTATIC

INPUT DATA

A, B, C, \mu

\[ S_{\mu}, \epsilon, \sigma^- \]

415
FIG. (1) FREQUENCY \(\omega (\text{cm}^{-1})\)

---

416
FIG. (4) FREQUENCY $\omega$ (cm$^{-1}$)

FIG. (6) FREQUENCY $\omega$ (cm$^{-1}$)

$T = 430K$

$T = 296K$
LABORATORY MEASUREMENTS OF THE 60-GHz O2 SPECTRUM IN AIR

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The O2-spectrum of dry air was studied with a resonance spectrometer under controlled laboratory conditions. Key parts of the instrumentation were an automatic network analyzer and a one-port Fabry-Pérot resonator affording an effective path length of 240 m. Measurements were made at frequencies between 49.3 and 67.2 GHz in 0.1 GHz increments for eleven pressure steps (1-100 kPa) and three different temperatures (7-30-53°C). More than $5 \times 10^6$ data points ($S_{11}$ parameters) have been recorded and reduced to about 5,000 absorption values $\alpha$ (dB/km). Measurement uncertainties were estimated to be typically the worse of ±0.05 dB/km or 2 percent. The collective spectral behavior of 38 pressure-broadened O2 lines is described by the model MPM (NTIA Report 91-272, March 1991). A comparison of the absorption results with MPM predictions reveals systematic differences which correlate with O2 line width and overlap parameters. An interpretation of the extensive data set with Rosenkranz's overlap theory [JQSRT 39(4), 287-297, 1988] is underway.
LABORATORY MEASUREMENTS
OF THE 60-GHz O$_2$ SPECTRUM IN AIR

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Microwave Line Spectrum of Dry Air

Line-by-line summation of 40 Q transitions ($n^2 = 1$ to 39) to yield the complex refractivity ($4 \times 40 = 200$-parameter problem),

$$\mathcal{N} = \sum_{i} S_i \mathcal{P}_i \quad \text{ppm}$$

where the line strength is

$$S_i = S_i \mathcal{P}_i \exp\left(a_i(1 - b_i)\right) \quad \text{Km}$$

and $S_i$ is a complex shape function in KHz$^{-1}$. The Van Vleck-Weisskopf shape function of a pressure-broadened line was modified by Rosenkrantz (1968) to account for overlap interferences,

$$\mathcal{P}(f) = \frac{1 + f_b}{f_b} \left[ \frac{1 - f_b}{f_b - f + f_b} - \frac{1 - f_b}{f_b + f - 2f_b} \right]$$

which rationalizes to absorption ($\delta'$) and dispersion ($\delta'$) profiles

$$\delta'(f) = \frac{A}{X + Y} - \frac{B}{(1 - B)X + (1 + B)Y}$$

and

$$\delta'(f) = \frac{A}{(1 - B)X + (1 + B)Y} + \frac{B}{2A(X - Y)}$$

with the abbreviations

$$A = \frac{\gamma_i}{\gamma_b}, \quad B = \frac{f}{\gamma_b}, \quad X = f/((\gamma_b - f)^2 + \gamma_b^2), \quad Y = f/((\gamma_b + f)^2 + \gamma_b^2).$$

Width and interference parameters are for Q$_2$ lines in air.

$$\gamma_b = 2g_2\left(n - n_2\right) \quad \text{GHz} \quad k \cdot f$$

and

$$S_i = (a_i + a_i f)g_2^{n-1} \quad k \cdot f$$
O2-Spectrum in Dry Air

- 300 K
- Strength
- Width
- Overlap

Relative Units

Frequency $f$, GHz

50 55 60 65 70
-101.3 kPa, 30°C

DRY AIR (h = 12 km)
P = 19.49 kPa
\[ h = 9 \text{ km} \]

**EXP - MPM91**

Frequency \( f \), GHz

Residual Attenuation \( \delta \alpha \), dB/km

\[ h = 18 \text{ km} \]

**EXP - MPM91**

Frequency \( f \), GHz
LINE MIXING IN POLAR AND NONPOLAR MOLECULES

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Line mixing has been observed for three infrared Q branches of HCN and HCCH, self-broadened at subatmospheric pressures, using a difference-frequency laser spectrometer. Broadening coefficients and line-coupling effects are independent of vibration in these species. The broadening coefficients monotonically decrease with J for HCCH whereas they peak near the Boltzmann population maximum for HCN. Empirical energy-gap rate laws adequately describe the broadening and line mixing in HCCH provided that a decoupling factor, representing collisional cross relaxation between the q and f levels of the II bending vibrations, be included. These rate laws do not fit the line mixing in HCN whereas an energy-corrected-sudden (ECS) scaling law does. Here the cross relaxation decoupling is smaller than for HCCH, indicating a slight propensity for preserving vibrational angular momentum in polar molecule collisions.
LINE MIXING IN POLAR AND NONPOLAR MOLECULES

(HCN)     (HCCH)

A. S. Pine and J. P. Looney

Molecular Physics and Thermophysics Divisions
National Institute of Standards and Technology
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EMPIRICAL COLLISION RATE FITTING LAWS

R-T Hybrid Power-Exponential-Gap (PEG) Law

\[ R_{J\rightarrow K} = a_1 (E_{KJ}/B)^{-a_2} \exp(-a_3 E_{KJ}/kT) \]

where \( E_{KJ} = E_K - E_J \) and \( k = k_B/h_c \)

R-T Modified-Exponential-Gap (MEG) Law

\[ R_{J\rightarrow K} = a_1 \frac{[1+1.5(E_J/a_2 kT)]}{[1+1.5(E_J/kT)]} \exp(-a_3 E_{KJ}/kT) \]

R-R Resonant-Exponential-Gap (REG) Law

\[ R_{J\rightarrow K} = a_1 \rho_K \sum_{LM} \rho_{LM} \exp(-a_3 |E_{KJ}+E_{ML}|/kT) \]

where \( \rho_J = \rho_J(2J+1)\exp(-E_J/kT)/2R \)

for upward collisional transitions, \( K \geq J \).

Downward transitions related by detailed balance, \( R_{K\rightarrow J} = R_{J\rightarrow K} \rho_J/\rho_K \).
ENERGY-CORRECTED-SUDDEN (ECS) SCALING LAWS

R-T Inelastic Collision Rates

\[ R_{J+K} - (2K+1) \exp\left(-E_{KJ}/kT\right) \sum_{L}(2L+1) \left(\begin{array}{c} J \\ K \end{array}\right) \left(\begin{array}{c} L \\ 0 \end{array}\right) \left(\begin{array}{c} I \\ 0 \end{array}\right)^2 \]
\[ \times \left[1+\left(a_4E_{L_0}\right)^2/BkT\right]^2/\left[1+\left(a_4E_{L_0}\right)^2/BkT\right] \]

where \( E_{KJ} = E_K - E_J \) and \( k = k_B/hc \).

\( E_K - E_K - I \) for \( I = 1 \) (dipole)
or \( I = 2 \) (quadrupole),

\[ R_{L+0} - a_1 \left(E_L/B\right)^{a_2} \exp\left(-a_3E_L/kT\right) \] (PEG)

R-R Inelastic Collision Rates

\[ R_{J+K} - a_1(2K+1) \sum_{L} \rho_L \exp\left(-\Delta E/kT\right) \left(\begin{array}{c} J \\ K \end{array}\right) \left(\begin{array}{c} L \\ 0 \end{array}\right) \left(\begin{array}{c} I \\ 0 \end{array}\right)^2 \]
\[ \times \left(2M+1)(2I+1)/\left[1+(a_4(E_{KJ}+E_{ML}))^2/BkT\right] \right]^2 \]

where \( \rho_L = g_L(2L+1)\exp\left(-E_L/kT\right)/Z_R \),

\( K = J+I, \ M = L-I, \) for \( I = 1 \) or 2,
\( \Delta E = E_{KJ}+E_{ML} \) if \( > 0 \) or \( -0 \) if \( \leq 0 \)

for upward collisional transitions, \( K > J \).

Downward transitions related by
detailed balance, \( R_K\rightarrow J - R_{J\rightarrow K} \rho_J/\rho_K \).
**HCN Self Broadening: ECS Scaling**

**LINE COUPLING or LINE MIXING**

Absorption Coefficient (impact approximation)

\[ \kappa(\nu) = \frac{(N/\pi)}{\text{Im}(\sum_{j} (d_{j} - k_{j})/(\nu - \omega_{j}))} \]

where

- \( d_{j} = \frac{\mu_{j}}{[1 + \alpha_{ij}(J+j)]^{4}} \)
- \( \mu_{j} = \delta_{j} \exp(-\frac{\hbar c E(J)}{k_{B} T}) \)
- \( \omega_{j} \) are complex eigenvalues of complex matrix
- \( H = \nu_{o} + \mu_{j} \)

whose eigenvectors are columns of matrix \( \Lambda \)

\( \Lambda^{-1} \cdot H \cdot \Lambda = \Omega \) where \( \nu_{ij} = \delta_{ij}, \omega_{j} \)

\( \nu_{o} \) is a diagonal matrix of transition frequencies, \( \nu_{j} \)

\( \Omega \) is relaxation matrix whose diagonal elements are broadening coefficients and off-diagonal elements are line-coupling coefficients.
RELAXATION MATRIX

Diagonal Elements (Broadening)

\[ \Sigma_{JK} = h \sum_{K} \left( R_{J\rightarrow K}(\Sigma, e\rightarrow e) + R_{J\rightarrow K}(\Pi, f\rightarrow f) + R_{J\rightarrow K}(\Pi, f\rightarrow e) \right) \]

Off-Diagonal Elements (Coupling)

\[ \Sigma_{JK} = -F R_{J\rightarrow K}(\Pi, f\rightarrow f) \]

\( F \) is an empirical coupling factor.

HCN \( \nu_1 + \nu_2 \) 100 Torr

Absorbance

Points

435
HCN $\nu_1 - \nu_2$ 100 Torr

Obs - Calc

Points

HCCH

P=1.04 Torr

Observed

Calculated

O branch

$\nu_3 + \nu_2$

Observed

Calculated

O branch

$\nu_3 + 2\nu_2 + \nu_1$

Observed

Calculated

O branch

Wave number (cm$^{-1}$)
STUDY OF THE CO$_2$ BLUE WING IN THE 4.1 $\mu$m REGION

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In the 4.1 $\mu$m region, continuum type absorption by CO$_2$ is the blue wing of the $\nu_3$ fundamental band. Correct modeling of absorption in the wings of CO$_2$ vibrational bands is required to calculate the shape of atmospheric windows.

Birnbaum's line shape is used to calculate absorption coefficients beyond 2380 cm$^{-1}$. This line shape allows a continuous representation from local calculations near resonance to continuum calculations in the far wings. It is incorporated in a line by line calculation, where it can be used with up to date spectroscopic databases. The calculation duplicates the shape of the wing, but not the magnitude. Line mixing effects are not taken into account in this model and an empirical scaling factor is required to match the model with the experimental data. This scaling factor remains constant below 1 atmosphere and increases, as expected, with increasing density. However, it is not possible to deduce a relation between this coefficient and the pressure. At high pressure, collision induced absorption (CIA) bands appear, which are forbidden, in the infrared. These bands are centered at 2669 cm$^{-1}$ and at 3015 cm$^{-1}$, and they modify the shape of the far wing. Beyond 2380 cm$^{-1}$, no strong temperature dependence has been observed. Experimental data have been obtained with a 10 meter long White cell and with a 30 cm long high pressure high temperature cell. Comparisons with calculations are presented.
STUDY OF CO₂ BLUE WING IN THE 4.1 μm REGION

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STUDY OF CONTINUUM ABSORPTION

- RADAR
- ELECTRO-OPTICAL SYSTEMS
- ATMOSPHERIC REMOTE SENSING
- INFRARED IMAGING SYSTEMS
- ATMOSPHERIC METEOROLOGY ...

CO₂

CO₂ - N₂

4.1 μm REGION [2380 - 2600] cm⁻¹

BIRNBAUM'S MODEL

EFFECTS OF LINE MIXING — EMPIRICAL SCALE FACTOR
In the far wing:

\[ g_{\text{FW}}(\omega) = \frac{1}{\pi} \left\{ \sum_{i} \frac{\rho_i d_i^2}{\Delta_i^2} B_{\mu}(\Delta_i) + \sum_{i \neq j} \frac{\rho_i d_i d_j}{\Delta_i \Delta_j} B_{\mu}(\Delta_j) \right\} \]

\( \Delta_j = \omega_j - \omega \)

\( \rho_i \) POPULATION OF THE ACTIVE MOLECULE

\( d_i \) REDUCED DIPOLE MATRIX ELEMENT

\( B_{\mu}(\Delta) \) FREQUENCY DEPENDENT LINE WIDTH

\( B_{\nu}(\Delta) \) FREQUENCY DEPENDENT CROSS-RELAXATION FUNCTION WHICH PRODUCES LINE INTERFERENCE

BIRNBAUM'S MODEL:

\[ B_{\mu}(\Delta_j) = \gamma_{\mu} b_{\mu}(\Delta_j) \]

\[ B_{\nu}(\Delta_j) = \gamma_{\nu} b_{\nu}(\Delta_j) \]

\[ b_{\mu}(\Delta_j) = \frac{H_{\mu}(\Delta_j)}{H_{\mu}(0)} \]

\[ H_{\mu}(\Delta_j) = \frac{1}{2} \frac{x^{n-1}}{(n-2)!} e^{-\frac{2x^2}{n}} \cdot \frac{\tau_{\mu} K_{\mu}(x)}{1 + (r_{\mu}/r_{\nu})^2} \]

\[ x = |\Delta_j| \left[ \frac{\tau_{\mu}}{\tau_{\nu}} + \frac{\tau_{\nu}}{\tau_{\mu}} \right]^{n/2} \]

approximations → \( b_{\mu}(\Delta_j) \approx b_{\mu}(\Delta_j) \)

→ \( r_{\mu} = \frac{1}{n} \)

→ \( \Delta_{\mu} = \omega_j + \Delta \omega \)

sum rule → \( \sum_{i \neq j} \rho_i d_i d_j \gamma_{\mu} = \rho_j d_j \gamma_{\mu} \)

\[ g_{\text{FW}}(\omega) = \frac{1}{\pi} \left\{ \sum_{i} \frac{\rho_i d_i^2 \gamma_{\mu}}{\Delta_i^2} b_{\mu}(\Delta_i) \left[ 1 - \left(1 - \frac{\Delta \omega}{\Delta_i} \right) \right] \right\} \]

scale factor

\[ a = \frac{\Delta \omega}{\Delta_i} \]

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MIXTURE CO₂ - N₂

\[ r_{1}(\text{CO}_2 - \text{CO}_2) = r_{1}(\text{CO}_2 - \text{N}_2) \]

\[ \gamma_{\text{g}} = \gamma_{\mu \text{co}_2 - \text{co}_2} \cdot \gamma_{\mu \text{co}_2 - \text{N}_2} \]

\[ -\varepsilon_{\text{m}}(\omega) = \frac{1}{\pi} \left\{ \sum_{i} \frac{\rho_{i}d_{i}^{2}y_{i}}{a_{i}^{2}} b_{i}(\lambda_{i}) \right\} \cdot \alpha \]

- ABSORPTION CELL

10 M WHITE CELL
(40 TRAVERSALS)

P < 1 ATM

ROOM TEMPERATURE

![Diagram](image)

- HIGH PRESSURE - HIGH TEMPERATURE CELL

L = 30 CM

P' = 1 ATM - 35 ATM

T = 296K - 370K
$\text{CO}_2$ absorption coefficient in m$^{-1}$ at $T=329K$ and $p=28.9$atm.

$\text{CO}_2$ absorption coefficient in m$^{-1}$ at $T=295K$ and $p=35.5$atm and at $T=367K$ and $p=29.9$atm.
CO₂ absorption coefficient in \((cm^{-1}(mole.cm^3)^2)\) at 295K.

\[\text{Absorption coefficient (cm}^{-1}(\text{mole.cm}^3)^2)\]

Wave numbers [cm⁻¹]

CO₂-N₂ absorption coefficient in \((cm^{-1}(mole.cm^3)^2)\) at 295K.
Relative difference in percent between experimental and calculated data.

\[
\begin{align*}
\text{CO}_2 & \\
T &= 296K \quad 329K \quad 367K \quad 534K \quad 627K \\
\alpha &= 0.35 \quad 0.25 \quad 0.19 \quad 0.22 \quad 0.14
\end{align*}
\]

\[
\begin{align*}
\text{CO}_2 \cdot \text{N}_2 & \\
T &= 296K \quad 550K \quad 643K \\
\alpha &= 0.125 \quad 0.08 \quad 0.25
\end{align*}
\]

Scale factor \( \alpha \) for \( \text{CO}_2 \) and \( \text{CO}_2 \cdot \text{N}_2 \) at different temperatures.

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CONCLUSIONS

BIRNBAUM'S LINESHAPE

VERSATILE LINE SHAPE (H\textsubscript{2}O, CH\textsubscript{4},...)

EASILY UTILIZED IN A LINE-BY-LINE CALCULATION

AGREEMENT WITH EXPERIMENTAL DATA AT ROOM TEMPERATURE FOR CO\textsubscript{2} AND CO\textsubscript{2}N\textsubscript{2}

UNDERSTANDING OF TEMPERATURE DEPENDENCE OF THE CONTINUUM ABSORPTION
(TEMPERATURE DEPENDENCE OF THE SCALE FACTOR)
THEORETICAL APPROACH TO THE LINE WING PROBLEM

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Theoretical approach to the line wing problem

\[ H = H_0 + H_{\text{or}} = \left(H_1 + H_2 + H_3 + U\right) + H_{\text{or}} \]  

- \( H_1 \): absorbing molecule
- \( H_2 \): surrounding molecule
- \( H_3 \): kinetic energy of mass centers
- \( U \): intermolecular interaction

Dynamic subsystem \( \Phi_1 \)

Dissipative subsystem \( \Phi_2 \)

Interaction between subsystems \( \Phi_3 \)

First order perturbation theory in \( H_{\text{or}} \)

\[ \alpha \sim \text{Re} \text{e}^{i\omega t} \int_{-\infty}^{\infty} F(t) e^{-i\omega t} dt \]  

Long-wave approximation

\[ \alpha \sim \text{Re} \text{e}^{i\omega t} F(t) dt \]

Kinetic equation, semiclassical description

\[ F = \text{Sp}_p M(t) = \text{Sp}_p \text{Me}^{-\frac{i}{\hbar} \int_{\text{Sp}} R(t) S(t) - F(t) S(t) Me^\frac{i}{\hbar} \int_{\text{Sp}} R(t) dt} \]  

\[ \rho = \text{Pr}_{P, P} \text{v} = \text{Sp}_p P(t) \text{v} \]  

\[ i(\omega - \omega_{\text{nn}}) \rho_{\text{nn}} + (\rho \rho_{\text{nn}})^{\text{int}} = \rho_{\text{nn}}^{\text{int}} \rho_{\text{nn}} + \rho_{\text{nn}} \]
Theoretical approach to the line wing problem

\[
H = H_0 + H_{OR} = (H_1 + H_2 + H_3 + U) + H_{OR} \tag{1}
\]

- \(H_1\)-absorbing molecule
- \(H_2\)-surrounding molecules
- \(H_3\)-kinetic energy of mass centers
- \(U\)-intermolecular interaction

First order perturbation theory in \(H_{OR}\)

\[
\chi \sim \text{Re} \int dt e^{i\omega t} \text{Sp} F(t) \equiv \int d\delta(S - F) S(t) \text{Me}^{i\omega t} \tag{2}
\]

- \(M\)-dipole moment of absorbing molecule
- \(i\hbar \frac{\partial S}{\partial t} = H_{OR} S\), \(S(0) = 1\), \(\rho = \frac{1}{Z} e^{-\mu}/kT\)

Long-wave approximation

\[
\chi \sim \text{Re} \int_0^\infty F(t) dt \tag{3}
\]

Kinetic equation, semiclassical description

\[
F = \text{Sp}_{p} p M(t) = \text{Sp}_{p} M(t) + S^{-1} M S, Q = \text{Sp}_{p} p M(t) \tag{4}
\]

- classical \(U\)
- \(U\)-intermolecular potential

\[
i(\omega - \omega_m) Q_{mn} + (M_{p1})_{mn} = (\omega - \omega_m) I_{mn} + I_{mn} \tag{5}
\]

Asymptotic cases

\[
\begin{array}{c|c}
\text{Small } \omega & \text{Large } \omega \\
\hline
\xi = \frac{\omega_{mn}}{\omega_{mn}^2} I_{mn} & \xi = \text{D}_{1}^{-1} S^{-1} w F(R(\omega), T) \tag{6} \\
\end{array}
\]

\[
\phi(V) \equiv F(R(\omega), T) = \int_{V_u} R \, dV \, \exp \left( -\frac{w F(R(\omega), T)}{2} \right) \tag{7}
\]

- \(R_1 = C\sqrt{\omega} \\frac{\omega}{U} \tag{8}
\]

- \(R_1\)-the root of the Equation

\[
\delta E_{mn} = h\omega \tag{9}
\]

\[
\delta E_{mn} \sim \frac{C\sqrt{\omega}}{R} \tag{10}
\]

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\[ i(\omega - \omega_{mn})q_{mn} + (\mathcal{M}_i)_{mn} = (\omega - \omega_{mn})I_{mn} + \mathcal{I}_{mn} \] 

\[ \Phi(V) \, U \]

**Asymptotic cases**

<table>
<thead>
<tr>
<th>Small ( \omega )</th>
<th>Large ( \omega )</th>
<th>Line wing theory</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \omega \approx \omega_{mn} )</td>
<td>( \omega \approx \infty )</td>
<td>( \Phi(V) , U )</td>
</tr>
</tbody>
</table>

\[ \omega \approx \frac{\gamma}{\frac{y}{y+1} \omega^2} \]

\[ \omega = D_a \sum \omega^{2-3/2} F(R(\omega), T) \]

\[ \Phi(V) \, U \]

\[ F(R(\omega), T) = \frac{1}{R_i} \int_{R_i}^\infty dR e^{-\lambda R} k R(R_i - R)^{3/2} \]

\[ R_i - \text{the root of the Equation} \]

\[ \Delta E_{mn} = \hbar \omega \]

\[ \Delta E_{mn} \sim \frac{Ca}{R^2} \]

---

**Fundamental CO Band**

- **Experiment:** • Buotia et al. (1984)
- **Calculation:** — Line wing theory (1988)
- **Calculations using four nearest lines with Lorentz profile**

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![Graphs](image_url)
Fundamental CO Band

experiment: • - Buntin et al. (1984)
calculation: —— line wing theory (1989)
- - - - calculations using four nearest lines with Lorentz profile

experiment between the $R_{00}$ and $R_{01}$ lines:  

calculation —— line mixing theory  
- - - - line wing theory (1989)
$T = 298 \text{ K}$

$T = 370 \text{ K}$

experiment between the $R_{gg}$ and $R_{gs}$ lines:

- calculation
- line mixing theory
- line wing theory (1989)

$4.3 \mu m, \text{CO}_2 - \text{CO}_2$

experiment:
- Le Doucen et al (1985)
- Bulanin et al (1976)

calculation, line wing theory (1987)
\[ x_2(T, \omega) \text{ cm}^{-1} \text{Angstrom}^{-1} \]

Experiment:
- Le Doucen et al. (1985)
- Gattsev et al. (1984)
- Bulanin et al. (1976)

Calculation: Line wing theory (1987)

\[ \chi = \frac{x_2(T, \omega)}{\sum x_2^{\infty}(\omega)} \]

\[ x_2(T, \omega, \text{cm}^{-1}) \]

Experiment:
- 193 K Cousin et al. (1986)
- 296 K Cousin et al. (1986)
- Calculation: 193 K Cousins (1986)
\[ x = \frac{x(\omega,T)}{\Sigma x_2(\omega)} \]

Experiment: 193K Cousin et al. (1986)

Calculation: 296K Cousin et al. (1986)

- 296K
- 193K (Brilliard et al. 1986)
DISTRIBUTION

1. The extended DoD Plan for Atmospheric Transmission Research and Development tasks the Air Force to conduct an annual review conference to provide for tri-service discussion of model deficiencies and recommend corrective action.

2. The 14th Annual Review Conference will be held at the Geophysics Laboratory (now designated the Geophysics Directorate, Phillips Laboratory), Hanscom Air Force Base, Bedford, Massachusetts during the second week in June (11-12 June 1991). The objectives of the meeting are to review the current status of transmittance/radiance models and in hearing your recommendation regarding how we can overcome any identified deficiencies.

3. Areas of interest include molecular and aerosol effects on atmospheric radiative transfer, lidar, turbulence, remote sensing, the impact of trace atmospheric constituents on climate, and the general topic of spectral line shapes including both continua and line coupling effects.

4. This letter is intended to solicit contributions to this conference. If you would like to present a paper, please provide an unclassified abstract which should be double-spaced and no more than 12 lines. Please send abstracts to L.W. Abreu, GL/OPS (AFSC), HANSCOM AFB, MA 01731-5000 by 19 April 1991 (Telephone 617-377-2337).

5. Note all sessions will be open, and it is anticipated that foreign nationals will be permitted to attend. Allow sufficient time to obtain the necessary clearances for your papers. Immediately following this meeting, on 13-14 June the workshop on the HITRAN database will be held. For those interested in also attending this workshop, contact L.S. Rothman, GL/OPS, Hanscom AFB, MA 01731 (Telephone 617-377-2336).

6. If you plan to participate in the conference, but not make a presentation, please notify us in writing, by 19 April 1991 (non-US citizens should allow at least 6 weeks for visit approval). Send your letter to L.W. Abreu, GL/OPS (AFSC), Hanscom AFB, MA 01731-5000. (Telephone 617-377-2337). If you have any questions contact us at the numbers listed. AUTOVON prefix for Hanscom AFB is 478.

FRANCIS X. KNEIZYS
Simulation Branch
Optical Environment Division

LEGNARD W. ABREU
Simulation Branch
Optical Environment Division
REPLY TO
ATTN OF

SUBJECT
Annual Review Conference on Atmospheric Models
(11-12 June 91) (OPS Ltr, 28 Jan 91, same subj::)

TO
DISTRIBUTION

1. On the basis of responses to our January 28th letter announcing the Annual Review Conference on Atmospheric Transmission Models, we have constructed the enclosed tentative agenda for a two-day meeting on 11-12 June 1991. In general, we have reduced some initial time requests slightly to allow for adequate discussion. Speakers should plan on a maximum total presentation time of 15 minutes. Viewgraphs are preferable as visual aids in the talks. The meeting will be unclassified.

2. We ask that all conference speakers provide us with hard copies of viewgraphs used in your presentation at the meeting. You can either mail them to L.W. Abreu GL/CPS, Hanscom AFB, MA 01731-5000, or bring a copy to the meeting.

3. We will meet on 11-12 June (starting at 0845 on the 11th and 0830 on the 12th in the GL Science Center, Bldg 1106, Hanscom AFB. (See attached map). Please plan to arrive by 0830 on the eleventh to allow time for registration on the first day.

4. We do not intend to make motel reservations for any participants, but we have enclosed a list of motels which are reasonably close to Hanscom AFB (although you will need a car for transportation). On-base government quarters are limited, so if you require VOQ accommodations, please make your reservations early by calling 617-377-2112. The AUTOVON prefix for Hanscom AFB is 478.

FRANCIS X. KNEIZYS
Simulation Branch
Optical Environment Division

LEONARD W. ABREU
Simulation Branch
Optical Environment Division

3 Atchs
1. Agenda
2. Map
3. List of Motels
ANNUAL REVIEW CONFERENCE ON ATMOSPHERIC TRANSMISSION MODELS

11-12 June 1991

Geophysics Directorate, Phillips Laboratory
Hanscom Air Force Base
Science Center, Building 1106

PROGRAM

Tuesday, 11 June 1991
(0845 - 1200)

WELCOME - R.E. Good, OP/Geophysics Directorate

KEYNOTE - Col. G. Aufderhaar, USAF (OUSDA)

SESSION 1 - AEROSOLS AND CLOUDS
(Co-Chairpersons: E.P. Shettle (NRL) and J.R. Hummel (SPARTA))

"Boundary Layer Illumination Radiation Balance Model: BLIRB"
A. Zardecki (Science and Technology Corporation)

"Relations Between Giant Aerosols Near the Surface and Solar Aureole Brightness"
F.E. Volz (Geophysics Directorate)

COFFEE BREAK (1000 - 1015)

"The Computation of Radiative Transfer Through the Atmosphere Incorporating Various Aerosol Scenarios"
L.C. Rosen (University of California, Lawrence Livermore National Laboratory)

"BACKSCAT Lidar Backscatter Simulation: Version 2.0"
J.R. Hummel, D.R. Longtin, N.L. Paul, J.R. Jones (SPARTA, Inc.)

"Cirrus Cloud Transmission Modelling"
W.M. Cornette, J.G. Shanks (Photon Research Associates, Inc.)

"ICE-CLOUD - A Model for IR Transmittance Through Cirrus Cloud"
W.T. Kreiss, R. Vik (Horizons Technology, Inc.)

"The Status of the Navy Oceanic Vertical Aerosol Model"
S. Gathman (Naval Ocean Systems Center)

LUNCH (1130 - 1330)
Tuesday, 11 June 1991
(1330 - 1700)

SESSION 2 - ATMOSPHERIC PROPAGATION MODELS
Co-Chairpersons: L.W. Abreu (PL), R. Shirkey (ASL) and J.E.A. Selby (Grumman)

"MODTRAN/LOWTRAN: Current Status, Future Plans"

"FASCODE3: An Update"
S.A. Clough, R.D. Worsham (Atmospheric and Environmental Research, Inc.), E.P. Shettle (Naval
Research Laboratory)

"EOSAEL92"
A.E. Wetmore (U.S. Army Atmospheric Sciences Laboratory)

"HITRAN'91: The Contemporary Spectroscopic Molecular Database"
L.S. Rothman (Geophysics Directorate)

"SHARC, An Atmospheric Radiation and Transmittance Code for Altitudes from 50
to 300 km"
D. Robertson, L. Bernstein, J. Duff, J. Gruninger, R. Sundberg (Spectral Sciences, Inc.),
R. Sharma (Geophysics Directorate), R. Healey (Yap Analytics, Inc.)

"Recent Developments of the GENLN2 Line-by-Line Model: Studies in Support of
the UARS Project"
D.P. Edwards (National Center for Atmospheric Research)

COFFEE BREAK (1500 - 1515)

"Present Status of Transmittances and Radiances Modelling at L.M.D."
N.A. Scott, A. Chédin, F. Chéruy, B. Tournier (ARA/LMD - Ecole Polytechnique)

"AURIC (Atmospheric Ultraviolet Radiance Integrated Code): an Update"
R. Huguenin, R. Hickey, K. Minschwaner (Aerodyne Research, Inc.), G.P. Anderson, L.A. Hall,
R.E Huffman (Phillips Laboratory)

"Ontar's PC Compatible LOWTRAN Package"
J. Schroeder, P. Noah (Ontar Corporation)

"Coupling Atmosphere and Background Effects"
W.M. Cornette (Photon Research Associates, Inc.)
Tuesday, 11 June 1991  
(1330 - 1700)

SESSION 2 - ATMOSPHERIC PROPAGATION MODELS (continued)  
Co-Chairpersons: L.W. Abreu (PL), R. Shirkey (ASL) and J.E.A. Selby (Grumman)

"SENTRAN7: A Sensitivity Analysis Package for LOWTRAN7 and MODTRAN"  
D.R. Longtin, F.M. Pagliughi, N.L. Paul (SPARTA, Inc.)

"Atmospheric Models in the Strategic Scene Generation Model"  
W.M. Cornette, D.C. Anding (Photon Research Associates, Inc.)

"Review of the Chemical Kinetic Rate Constants Used in the SHARC Model"  
V.I. Lang, A.T. Pritt, Jr., (The Aerospace Corporation)

SOCIAL HOUR/DINNER
SESSION 3 - MEASUREMENTS AND MODELS
Co-Chairpersons: G.P. Anderson (PL), R. Smith (TECOM) and H. Revercomb (Univ. of Wisconsin)

"Atmospheric Ultraviolet Radiance and its Variations"
R. Link, D.J. Strickland and D.E. Anderson Jr. (Computational Physics, Inc.)

"Photoabsorption Cross Sections in the Transmission Window Regions of the Schumann-Runge Bands of Oxygen"
K. Yoshino, J.R. Esmond, D.E. Freeman, W.H. Parkinson (Harvard-Smithsonian Center for Astrophysics), A.S-C. Cheung (Chemistry Department - University of Hong Kong)

"Incorporation of LOWTRAN7 into the ACQUIRE Model"
S.G. O'Brien (Las Cruces Scientific Consulting)

"High-resolution Spectral Measurements of Upwelling and Downwelling Atmospheric Infrared Emission with Michelson Interferometers"
H.E. Revercomb (University of Wisconsin - SSEC)

"Validation of HIS Spectral Measurements with the FASCODE Line-by-Line Model"

"Improved HNO3 Band Model Parameters"
N. Jones, A. Goldman, D. Murcray, F. Murcray, W. Williams (University of Denver, Department of Physics)

COFFEE BREAK (1000 - 1015)

"Line-by-line Calculations of Atmospheric Fluxes and Heating Rates"
S.A. Clough, M.J. Iacono, J.-L. Moncet (Atmospheric and Environmental Research, Inc.)

"Comparison of FASCOD2 and LOWTRAN7 Models with FIT Spectral Transmittance Measurements in the 3-12\,\mu m Region"
J.M. Thériault (DREV-Defense Research Establishment Valcartier)

"Spectral Solar Radiation Modeling, Measurement, and Data Base Activities at the Solar Energy Research Institute"
C.J. Riordan, R.L. Hulstrom (Solar Energy Research Institute)
Wednesday, 12 June 1991
(0830 - 1200)

SESSION 3 - MEASUREMENTS AND MODELS (continued)
Co-Chairpersons: G.P. Anderson (PL), R. Smith (TECOM) and H. Revercomb (Univ. of Wisconsin)

"LOWTRAN 7 Comparisons with Field Measurements"
R. Smith, N. McNabb, K. Hammerdorfer, T. Corbin (TECOM Fort Belvoir Met Team)

W. Gallery (Atmospheric and Environmental Research, Inc.), M. Esplin (Stewart Radiance Lab)

"A Comparison of Computational Approaches for the Voigt Function"
F. Schreier (Deutsche Forschungsanstalt fur Luft- und Raumfahrt, Institute of Optoelectronics)

LUNCH (1200 - 1330)
SESSION 4 - TOPICAL SESSION ON SPECTRAL LINE SHAPES
Chairperson: M.L. Hoke (PL)

SESSION 4a - INVITED PAPERS

"Basis of the Water Vapor Continuum Coefficients in the GL Models"
S.A. Clough (Atmospheric and Environmental Research, Inc.)

"Water Vapor Continuum Absorption Measurements with Line Shape Interpretations"
M. Thomas (Johns Hopkins University)

"Line Coupling for Microwave Oxygen Lines"
P.W. Rosenkranz (Massachusetts Institute of Technology)

"Laboratory Measurements of Line Coupling in CO₂ and N₂O"
L.L. Strow (University of Maryland)

COFFEE BREAK (1500 - 1515)

"Line Mixing: A Near Wing and Far Wing Problem"
J.-M. Hartmann (Ecole Centrale Paris)

SESSION 4b - CONTRIBUTED PAPERS

"Far-wing Lineshape Contribution to the Water Continuum in the Millimeter and Infrared Regions"
R.H. Tipping (University of Alabama), Q. Ma (Goddard Space Flight Center)

"Laboratory Measurements of the 60-GHz O₂ Spectrum in Air"
H.J. Liebe (U.S. Department of Commerce)

"Line Coupling in Polar and Nonpolar Molecules"
A.S. Pine and J.P. Looney (NITS)

"Study of CO₂ Blue Wing in the 4.1 μm Region"
C. Delaye, M. Thomas (Johns Hopkins University)
### Attendance List

<table>
<thead>
<tr>
<th>Name</th>
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### Appendix

**Annual Review Conference on Atmospheric Transmission Models**

**11-12 June 1991**

**Attendance List**

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<tr>
<th>Name</th>
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<td>Photon Research Associates, Inc. 9393 Town Center Drive San Diego, CA 92121</td>
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### Annual Review Conference on Atmospheric Transmission Models

**11-12 June 1991**

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## Annual Review Conference on Atmospheric Transmission Models
### 11-12 June 1991
### Attendance List

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<td>Harvard University</td>
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<td>Livermore, CA 94550</td>
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<th>Name</th>
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<tr>
<td>Dr. L. A. Hall</td>
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### Annual Review Conference on Atmospheric Transmission Models

**11-12 June 1991**

#### Attendance List

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| Mr. Edward R. Niple | Aerodyne Research, Inc.  
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<td>Dr. Anthony Ratkowski</td>
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