GOME Total Ozone Column Retrieval Development

GOTOCORD

Project in Response to ESA ITT AO4235

PI: Mark Weber

Co-Is:

M. Coldewey, R. De Beek, M. Buchwitz, V. Rozanov,

and J.P. Burrows

Project Period: 2002/10/10-2003/10/10

Topics

- Background
- Proposal: GOTOCORD project
- Current Status
- Work Package Breakdown
- Contractual Issues
- Study Team
- „Company“ Profile: IUP University of Bremen
- First Phase Actions (M. Coldewey et al.)
  - WF DOAS
  - Iterative Scheme
  - Selection of Input Parameters
  - Ghost vertical column
  - Temperature and Albedo weighting function
  - Scan Simulation
  - Look-up tables
  - Ring effect
  - Model studies
  - Preliminary validation
  - First Phase Plan

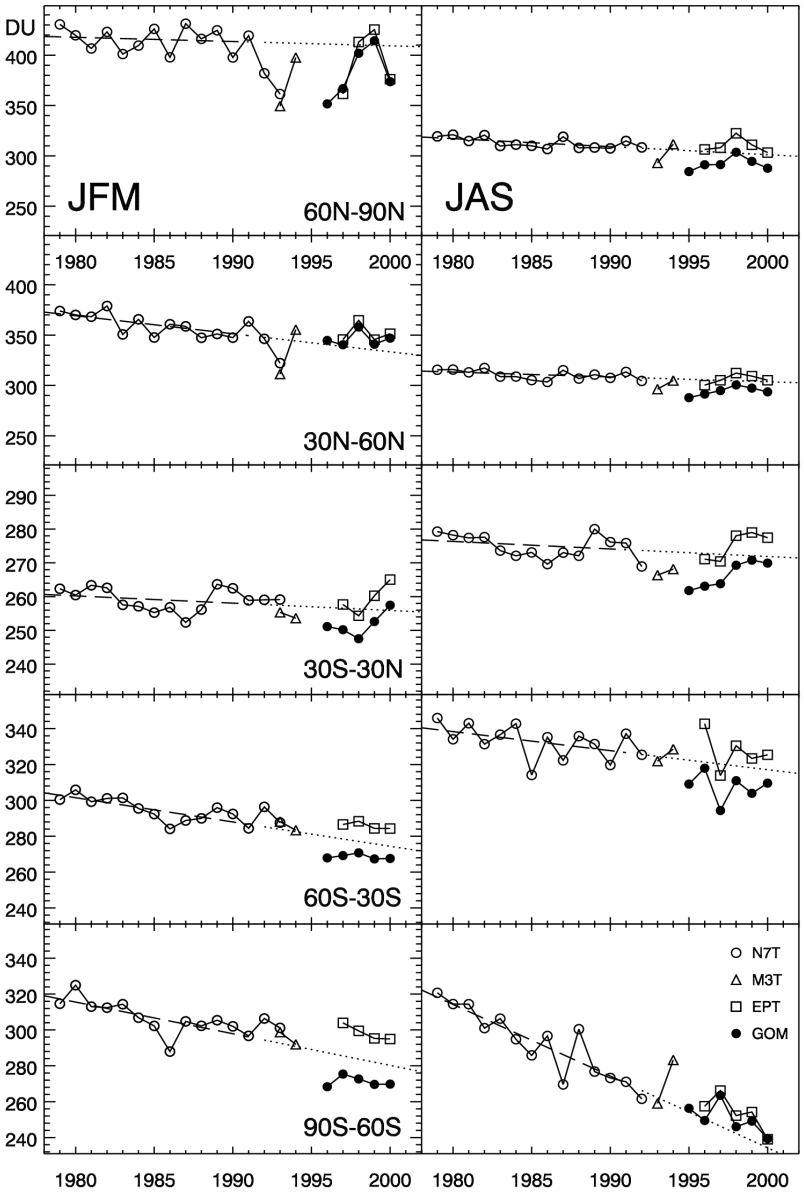
Background

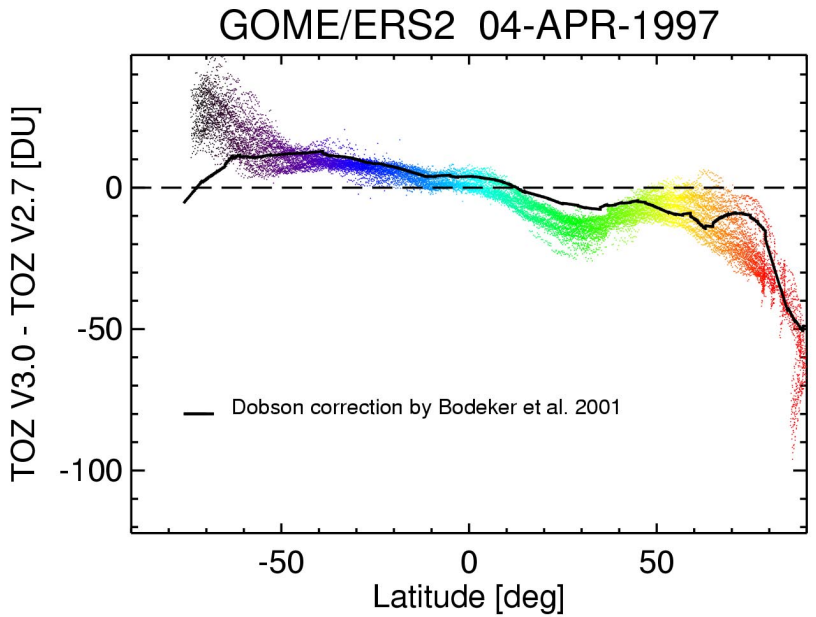
- Uncertainties exist about continuation of longterm global ozone trends and about possible first signs of recovery as a consequence of measures according to Montreal Protocol and its amendments
  - ➔ Maximum in chlorine loading in the stratosphere reached at the turn of the century
  - ➔ Moving away from linear trend in anthropogenic caused ozone changes
  - ➔ stratospheric cooling due to climate change

- Inconsistencies between TOMS, GOME, and groundbased Dobson data after mid-nineties (WMO Report 1998)
  - ➔ Data gap between 1994-1996 in the TOMS data series
  - ➔ Hemispheric bias in TOMS data
  - ➔ GOME seasonal variation with respect to groundbased data in V2.7 data and to a lesser extent in V3.0

- Requirement of internal consistency in longterm trends on the order of 1% (WMO, SPARC)

Background





Changes in GDP V3.0 data
(from Bramstedt et al. 2002)

- Seasonal variation reduced in V3
- Further improvements needed (Tiger team validation)

EU Report 2002
GOME V2.7 data

Proposal

- Development of a novel retrieval algorithm
  - ❍ Weighting Function DOAS (WF DOAS, Buchwitz et al. 2001)
    - ➔ Linearisation (Taylor series) of DOAS equation
    - ➔ Direct Fitting of vertical columns
    - ➔ RTM quantities in Look-Up Tables
    - ➔ Improved treatment of the Ring effect
- Prototype development of a quasi-operational processor
  - ➔ Retrieval software development
  - ➔ Generation of LUTs and optimisation (speed, interface)
  - ➔ Pre-Processing of data (cloud, Lambertian reflecitivities)
  - ➔ Definition of output (incl. Auxiliary information)
- Validation of new data products
  - ➔ Reference orbits (Tiger Team Validation Strategy)
  - ➔ WOUDC Dobson Brewer/Dobson (Bramstedt et al. 2002)

Current Status

- WF DOAS algorithm is ready, needs some optimisation for quasi-operational retrieval
  - Fortran 77/90 code
  - Input: GDP extracted Level-1 data
  - Interface to LUT
- Current computing facilities available (no cost basis)
  - alpha dec cluster
  - Sun Ultra cluster
  - Cray J90 with 16 processors
- Sensitivity studies are needed for final improvements
  - Selection of fitting parameters & spectral range
  - Ring effect
  - Cross-section
- Final Design of LUT to be found during this study
  - Parameter Space definition
  - Optimum coding of database with quick interface to retrieval algorithm

Work Package Breakdown

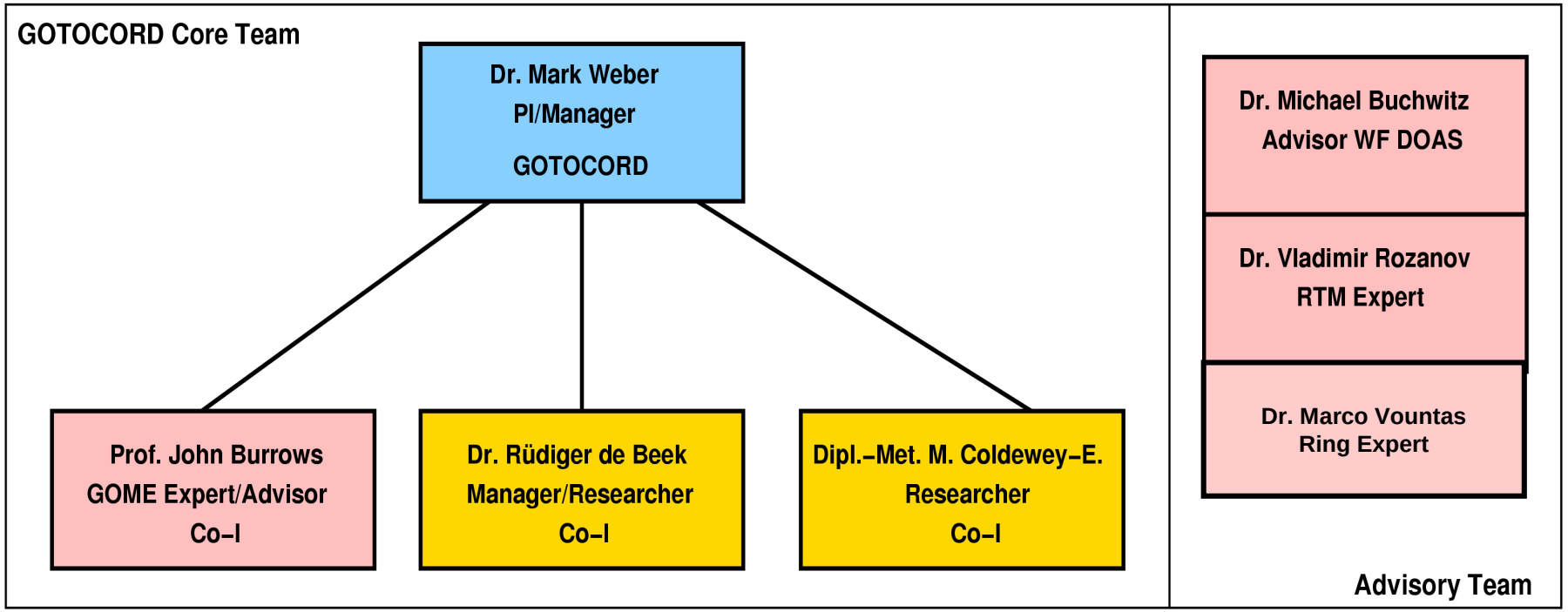
- WP 300 Phase 1: Sensitivity Study and Optimization (R. De Beek)
  - ➔ Duration: 4months
- WP 400 Phase 2: Algorithm Implementation (M. Coldewey)
  - ➔ Duration: 6 Months
- WP 500 Phase 3: Validation (M. Weber)
  - ➔ Duration: 2 months

Deliverables (Milestones):
ATBD, Software Requirements Document, Validation Report,
Software User Document, WF-DOAS Software CDs

Contractual Issues/ Requests

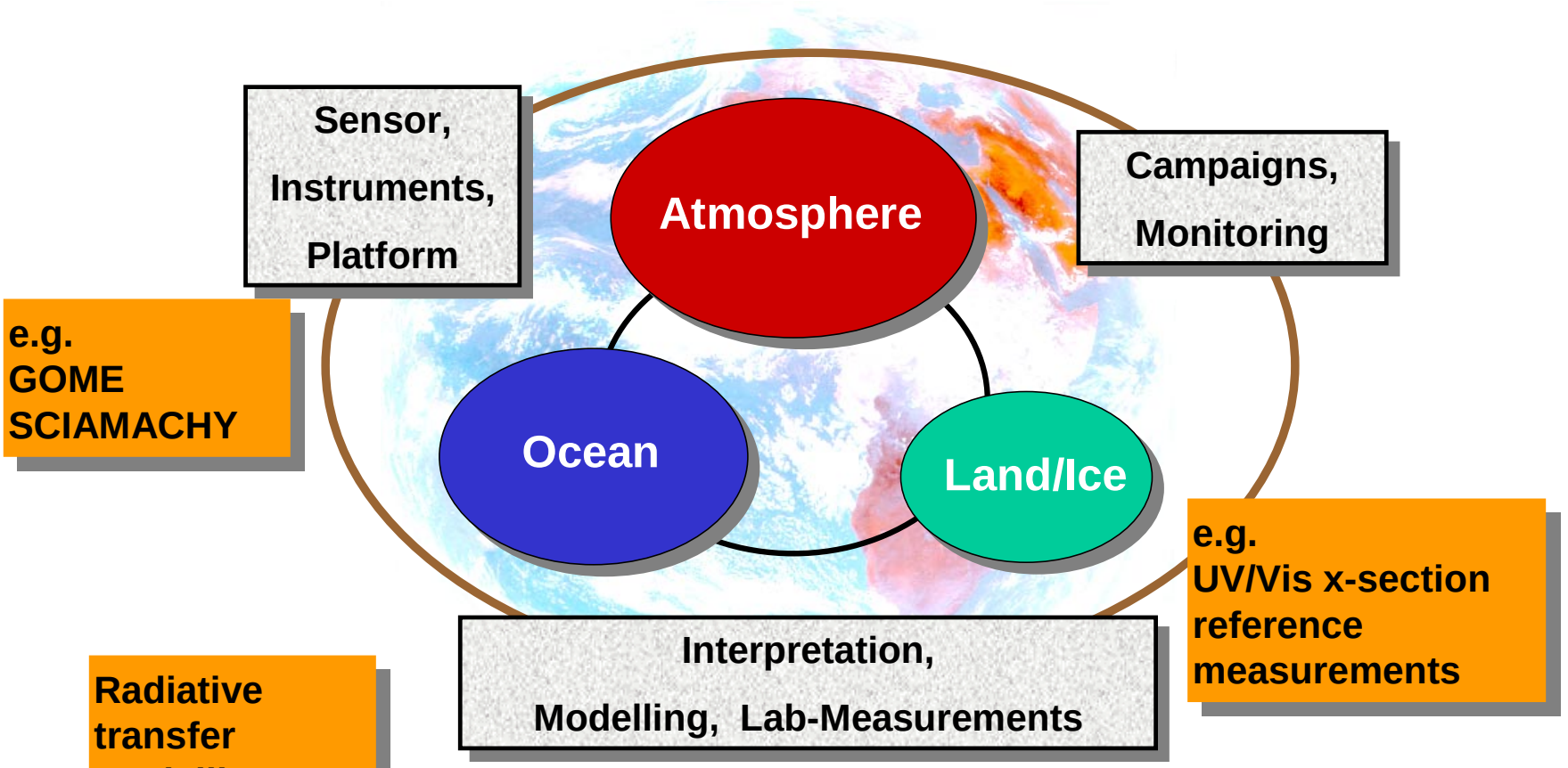
- Different time schedules for project due to different approach as stated in SOW
  - Proposed Modification in time schedule
    - ➔ Extention of first phase (Sensitivity Study and Optimisation) to 4 months
    - ➔ Second phase (Algorithm implementation) set to 6 months
- Request for reference orbits (level 1 data) collected on tape
- Access to GDP database
  - topography
  - ISCCP climatology (ICFA)

GOTOCORD Study Team



„Company“ Profile: IUP University of Bremen

Research at the Institute of Environmental Physics (IUP)



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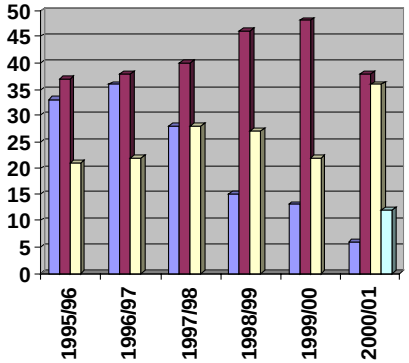
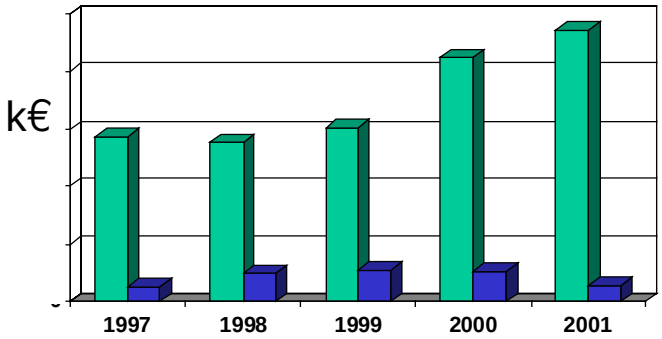
Some statistical information



Personnel (October 2001):

Total:	**105**
Scientists:	38%
PhD Candidates and Students:	48%
Technical:	14%



Finances:

Total amount in k€ excluding contributions from the University

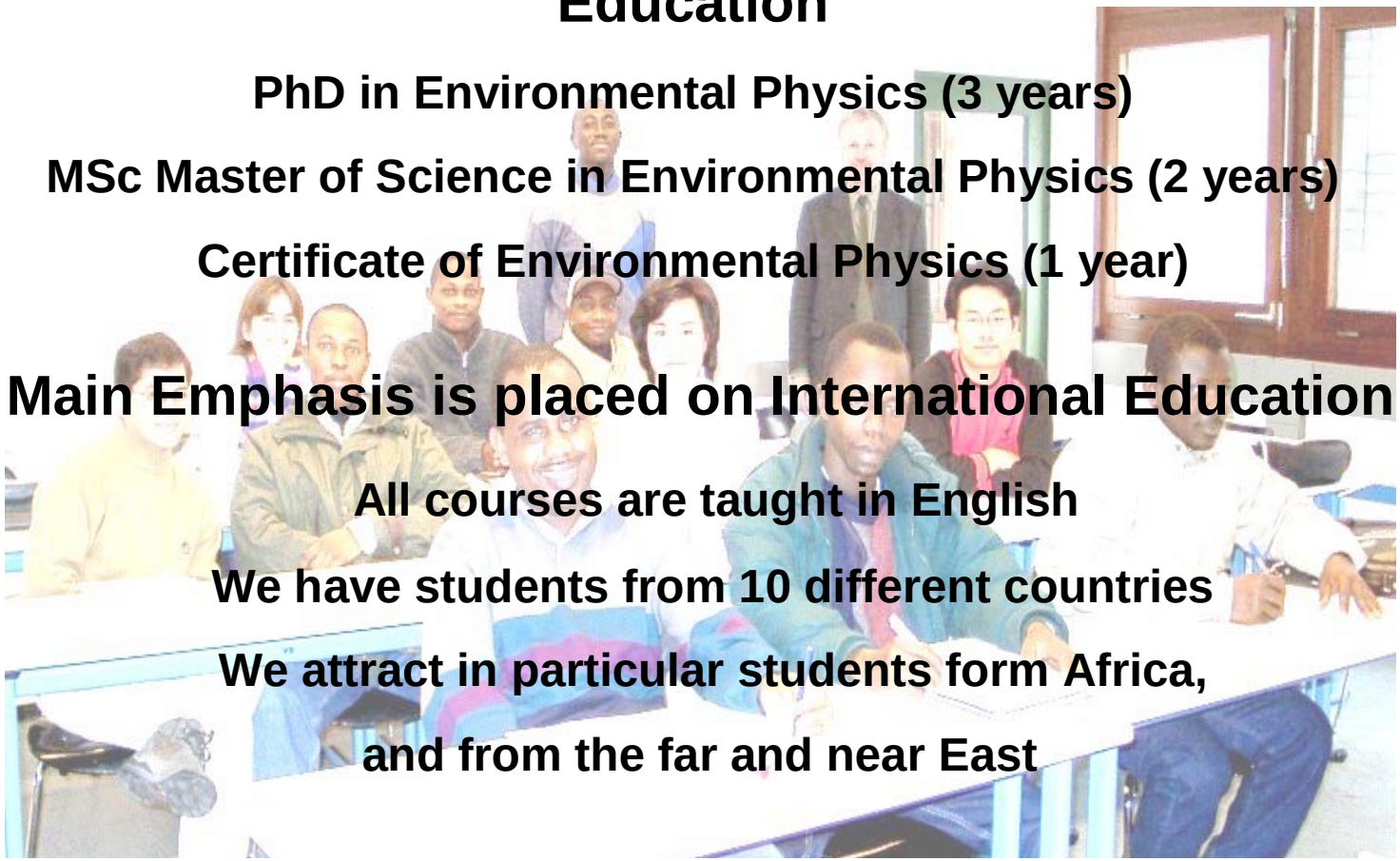
„Company“ Profile: IUP University of Bremen

Education

PhD in Environmental Physics (3 years)

MSc Master of Science in Environmental Physics (2 years)

Certificate of Environmental Physics (1 year)



Main Emphasis is placed on International Education

All courses are taught in English

We have students from 10 different countries

We attract in particular students form Africa,

and from the far and near East

Phase 1: Sensitivity Study and Optimisation

M. Coldewey, M. Weber, R. De Beek, and M. Buchwitz
Universität Bremen FB1
Institute of Environmental Physics

Table of Content

- WF DOAS
- Iterative Scheme
- Selection of Input Parameters
- Ghost vertical column
- Temperature and Albedo weighting function
- Scan Simulation
- Look-up tables
- Ring effect
- Model studies
- Preliminary validation (Antarctica & Mid-latitude)
- First Phase Plan

Weighting Function Modified DOAS — WFM-DOAS

$$\ln I_i^{mea}\left(V^t, \vec{b}^t\right) \approx \ln I_i^{mod}\left(V_0, \vec{b}_0\right)$$

$$+\frac{\partial \ln I_i^{mod}}{\partial V}|_{V_0} \times (\hat{V} - V_0)$$

$$+\sum_{j=1}^{F} \frac{\partial \ln I_i^{mod}}{\partial b_j}|_{b_{0,j}} \times (\hat{b_j} - b_{0,j})$$

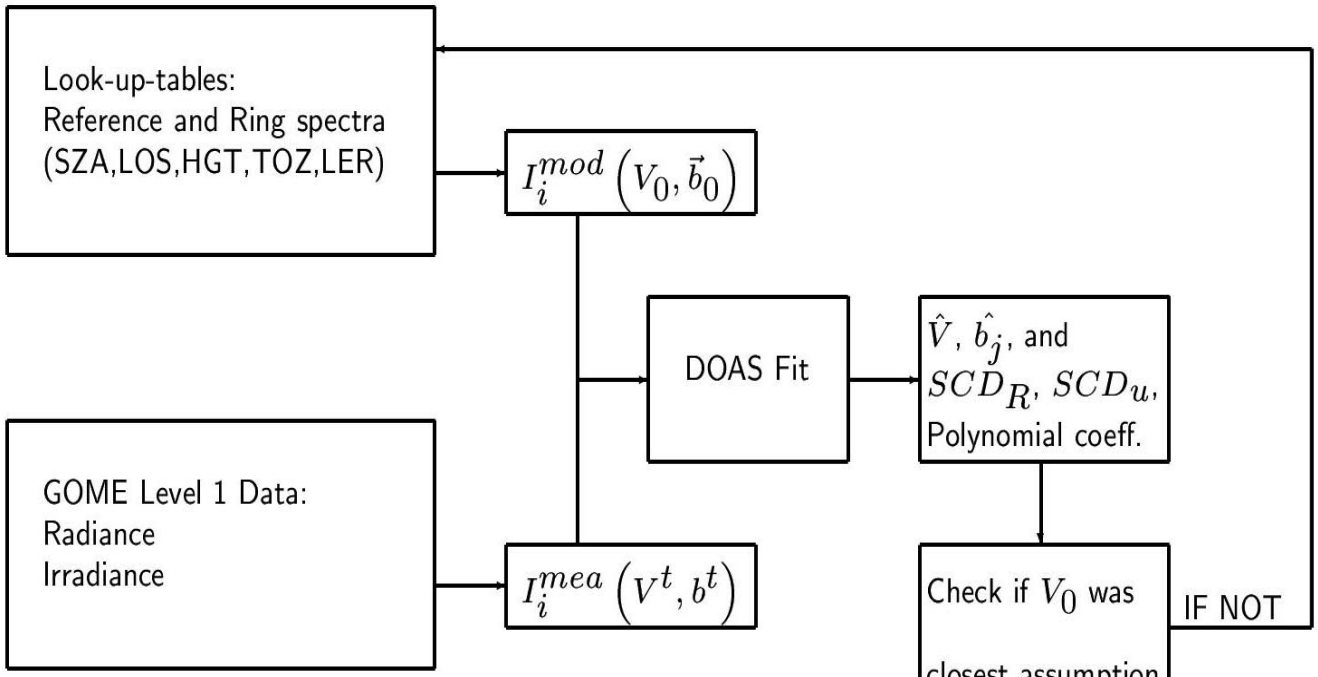
$$+SCD_{Ring} \cdot \sigma_{i,Ring}$$

$$+SCD_{usamp} \cdot \sigma_{i,usamp}$$

$$+P_i$$

- I_i Sun-normalized spectral radiance
- P_i Low-order polynomial
- V^t True vertical column
- $\vec{b}^t$ True atmosphere (pressure,temperature,...)
- V_0 Assumed model vertical column
- $\vec{b}_0$ Assumed model atmosphere
- $\hat{V}$ Vertical column fit parameter
- $\hat{\vec{b}}$ Atmospherical fit parameters
- σ_{Ring} Ring-Spectrum
- σ_{usamp} Undersampling-Spectrum
- i Wavelength index

WFM DOAS Iterative Scheme

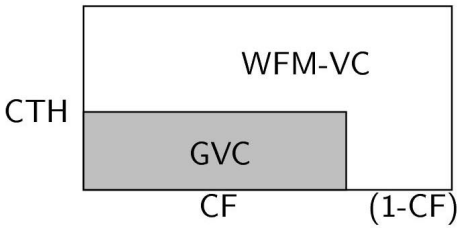


SZA : Solar zenith angle
LOS : Line-of-sight
HGT : Ground altitude
TOZ : Total ozone
LER : Lambertian equivalent reflectivity

Selection of relevant Input-Parameters

Parameter	Input
Total Ozone	WF
NO_2	WF or cross-section / SC Fit
BrO	WF or cross-section / SC Fit
Temperature	WF (?)
Pressure	WF (?)
Albedo	WF (?)
Ring-Effect	SC Fit
Undersampling	SC Fit

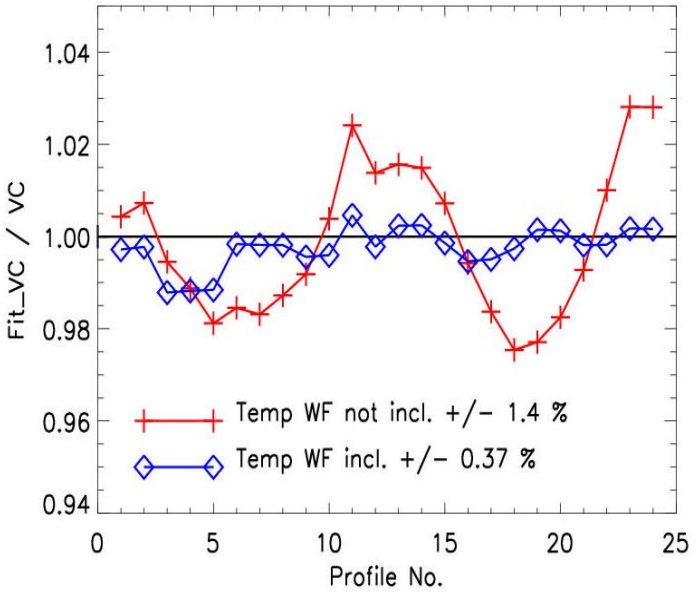
Ghost Vertical Column

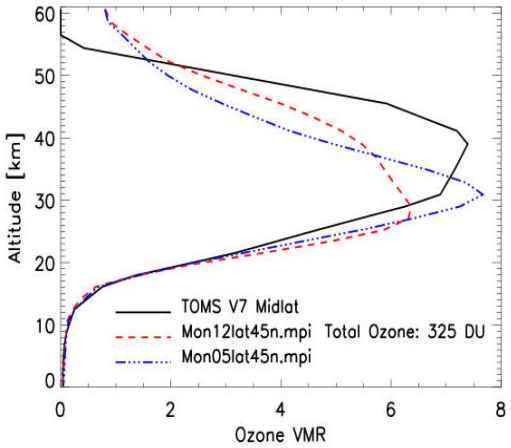


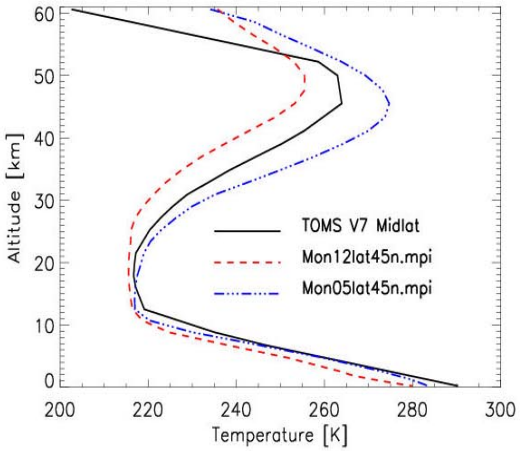
- ▷ FRESCO
- ▷ ICFA / ISCCP

Influence of temperature and ozone profile

- ▷ 24 simulated spectra using different MPI profiles (Mid latitudes)
- ▷ WF DOAS reference spectra calculated using one TOMS V7 profile (Mid latitudes)



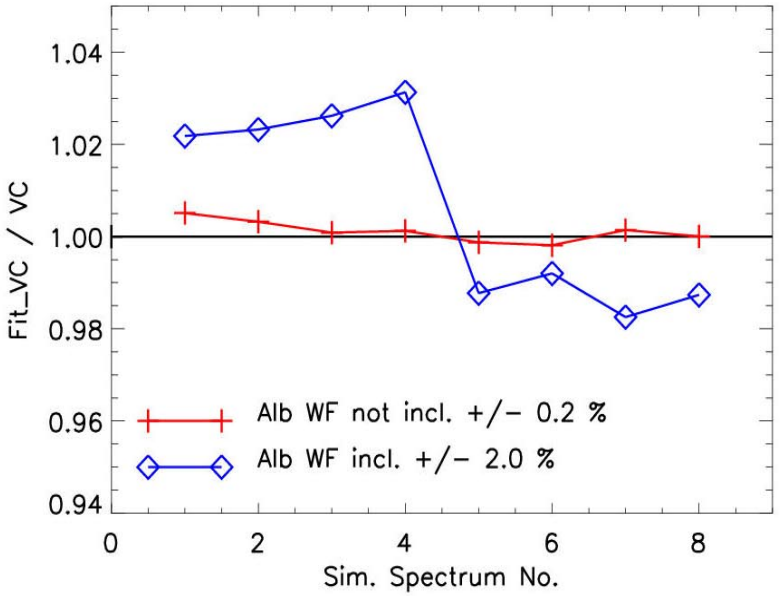




⇒ Include temperature weighting function !

Albedo weighting function

- ▷ 8 simulated spectra with surface albedo different from albedo in reference spectra
- ▷ Strong correlation between albedo WF and ozone WF



⇒ Albedo weighting function must not be included !

- ▷ LUT albedo spacing : 0.05, 0.2, 0.4, 0.6, 0.8, 0.98
- ▷ Linear interpolation of reference spectra

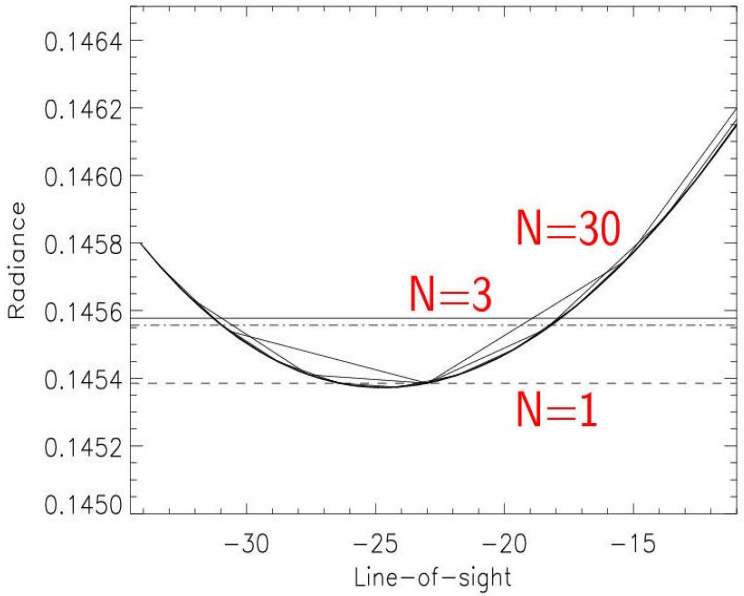
Scan Simulation

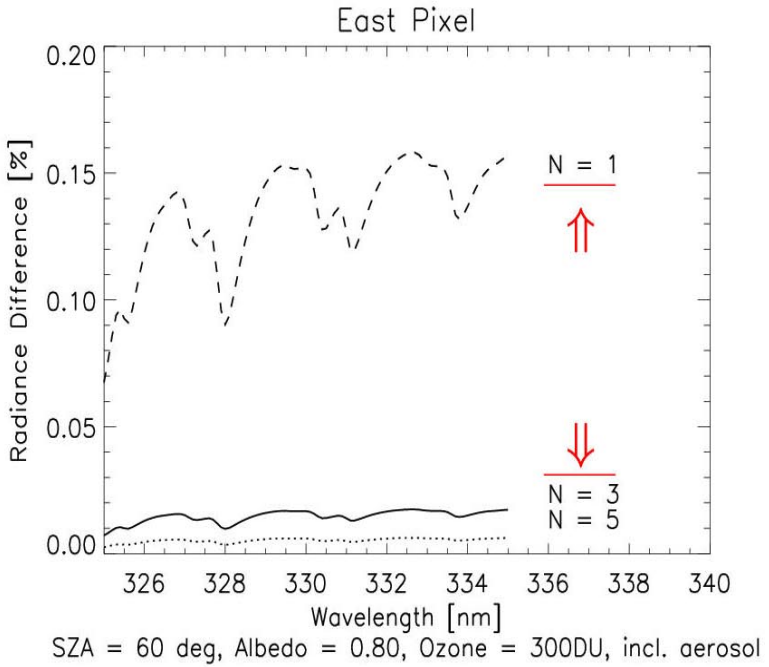
▷ Scan Simulation (east pixel / LOS $= 34.5^\circ - 11.5^\circ$) :

30 Spectra / $\Delta = 0.7\bar{6}^\circ$

3 Spectra / $\Delta = 7.\bar{6}^\circ$

1 Spectrum / LOS $= 23^\circ$





First Setup of Look-Up-Table

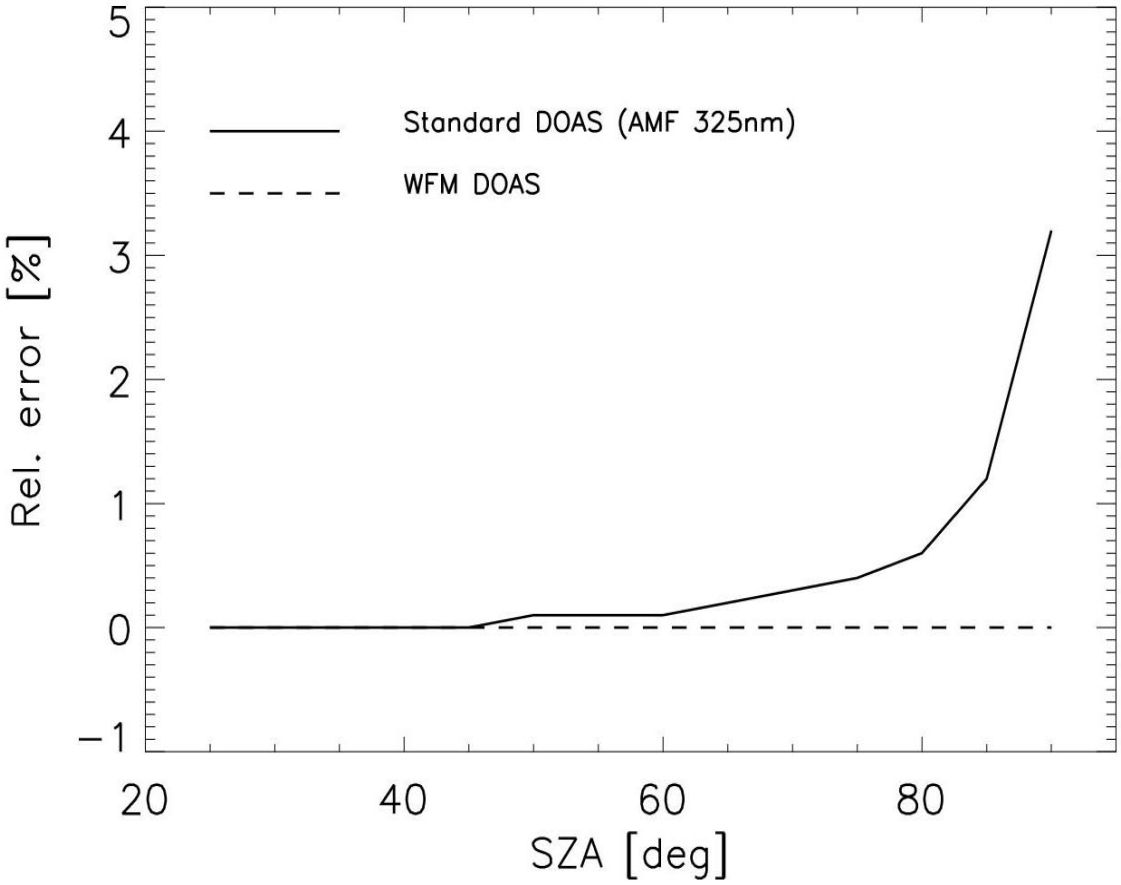
Optimum spacing has to be defined !

Atmospheric Parameter	Min	Max	Δ	N
Total Ozone (high latitudes)	125 DU	575 DU	50 DU	10
Total Ozone (mid latitudes)	125 DU	575 DU	50 DU	10
Total Ozone (low latitudes)	225 DU	475 DU	50 DU	6
Solar Zenith Angle	15°	90°	5° if SZA $\leq$ 70° 1° if SZA $>$ 70°	30
Line-Of-Sight	-34.5°	34.5°	11.5°	7
Surface Albedo	0.05	0.98	$\sim$0.2	6
Ground Altitude	0 km	6 km	2 km	4

Ring Effect Studies

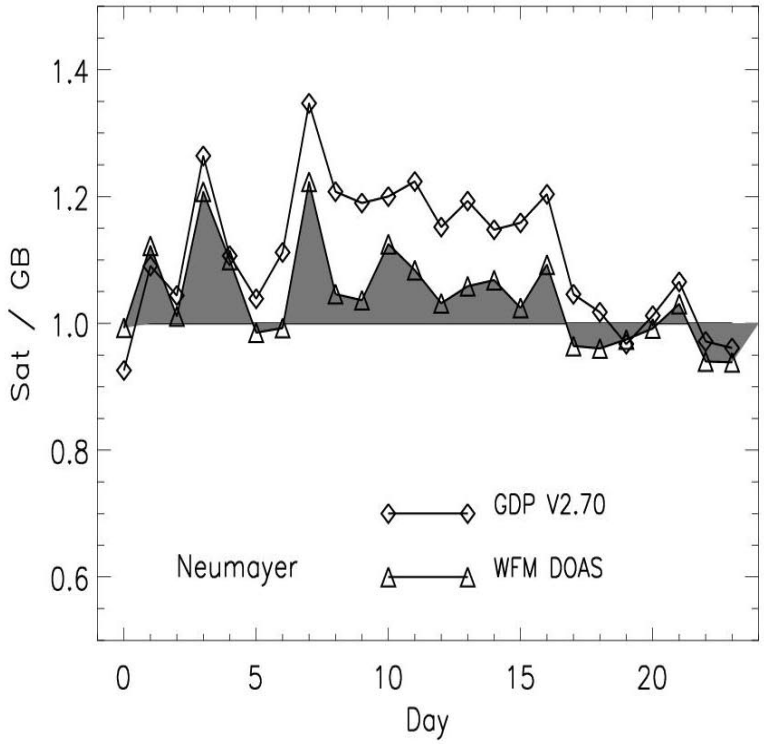
- Fraunhofer filling-in and molecular filling-in contribute to the Ring spectral signature
- Error in ozone retrieval $> 3\%$ for SZA $\geq 60^\circ$ when neglecting the ozone profile shape dependence
- Optimal extent of a Ring data base which includes the atmospheric parameter dependence (SZA, ozone profile shape, albedo, clouds, ...) has to be investigated
- In preparation: Ring spectra for representative trace gas scenarios (SLIMCAT), seasons (Jan, Apr, Jul, Oct), latitudes (5°, 55°, 75°), albedo (0.05, 0.8), and different line-of-sight (-32°, 0°, 32°)

Model Studies: WF DOAS vs. Standard DOAS



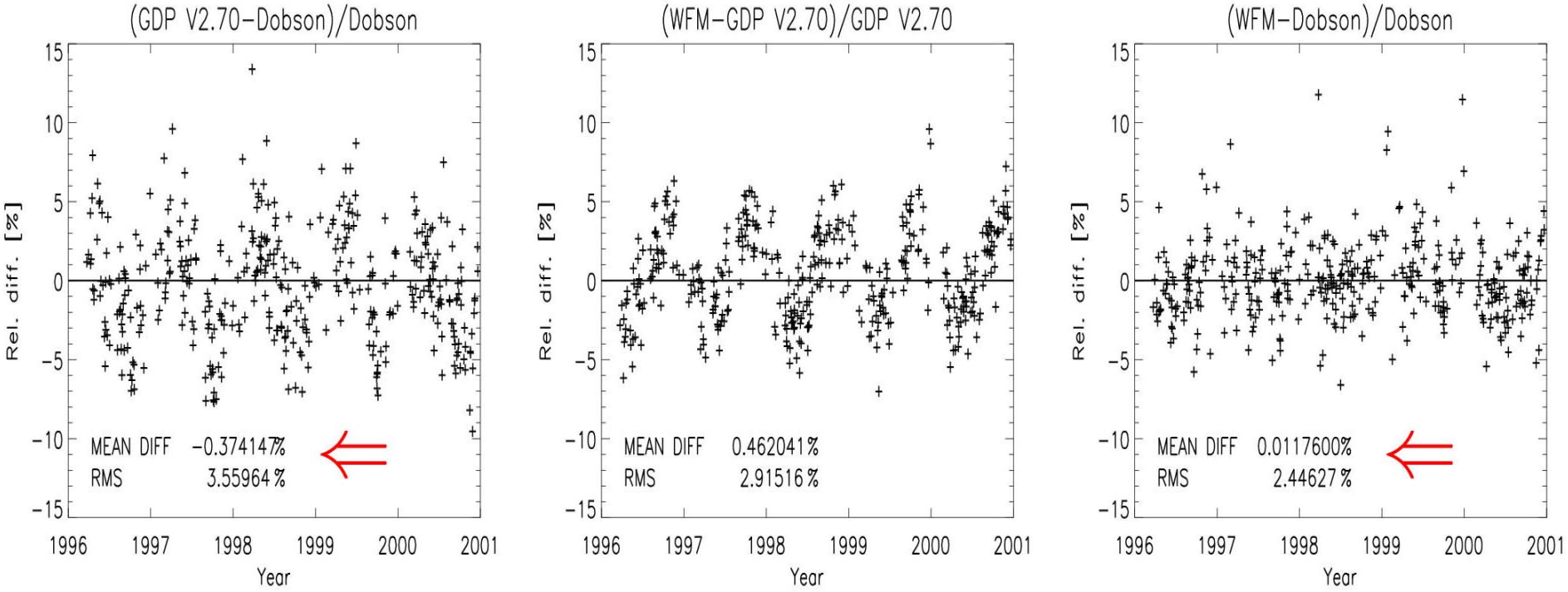
Comparison with Sonde Data from Neumayer (Ozone Hole)

- ▷ Neumayer-Station (70 S, 8 W)
- ▷ GOME overpasses from September to December 1997



Comparison with Ground-Based Ozone Data

- ▷ Hradec Kralove, Czech Republic (50 N, 15 E), Daily means
- ▷ GOME overpasses from 1996 to 2000



Data from K. Vanicek

First Phase Plan

- Selection of optimum spectral range and number of spectral points for WF DOAS fitting
- Selection of RTM, SCIATRAN or spherical CDI
- Definition of optimum parameter space for LUT (reference spectra and WF)
- Selection of optimum number of fitting parameters included in the fitting procedure
- Definition of an optimum Ring data base
- Investigate necessity of shift-and-squeeze and fixed-shift approach
- Decision of default ghost vertical column calculation (ICFA or FRESCO) and climatology data base (Gordon & Labow or TOMS V7)
- Selection of viewing geometry (ground or TOA)
- Selection of x–sections (GOME-FM98 or Bass-Paur)