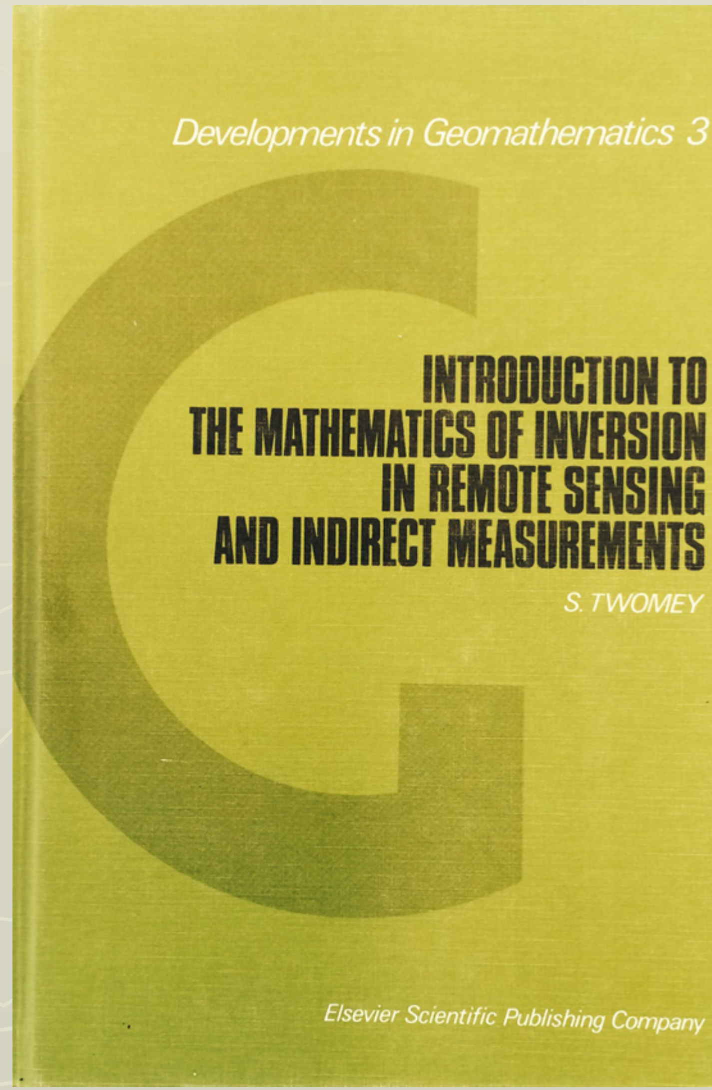
Motivation behind the Development of Inversion Methods in Geophysics: Sean Twomey and his Influence

Michael D. King
Laboratory for Atmospheric and Space Physics
University of Colorado Boulder

- Motivation behind inversion methods
  - Matrix inversion & instability
  - Solving one matrix inversion
- Applications
  - Aerosol size distribution
  - Satellite sounding of atmospheric temperature & ozone
- Influence on inversion of spectral aerosol optical thickness
  - Aerosol size distribution
  - Lagrange multiplier
- AERONET global observations
  - Aerosol size distribution
  - Single scattering albedo



Background
(ca. 1955, 1962)

- Solving a 'simple' electrical test network
  - A linear system with 6 unknowns
  - Spent more than a day solving this with a desk calculator
    - ✓ Results were disastrous, with negative resistances
  - Tried to hide results from boss because he felt he had wasted a day of time to obtain meaningless results
  - He was convinced that if he had greater accuracy he would have gotten the 'right' result
- Many years later, with the advent of computers, and having forgotten his earlier experience, he used the power of computers to invert a 20×20 system of linear equations
  - Nonsensical answers resulted, including negative values, for a known test case of hypothetical measurements, which he was able to reproduce to one part in 10^8
  - He had missed the essential point, the perils of instability and the practical equivalence of near-singularity and indeterminacy
- What was needed was a rephrasing of the question because it was the question, not the answer, that was wrong

Constrained Linear Inversion
(Phillips, 1962)

Many remote sensing problems can be formulated as a Fredholm integral equation of the first kind

$$\int_a^b K(y,x)f(y)dy = g(x) + \varepsilon(x)$$

- Examples
  - Vertical distribution of ozone from ultraviolet spectral measurements (Twomey 1961)
  - Inference of atmospheric temperature profile from thermal emission measurements
  - Inference of aerosol size distribution from optical transmission or scattering measurements
  - Path length distribution in radiative transfer
  - Aerosol size distributions from inversion of transmission through nuclepore filters
- When the kernel $K(y,x)$ is 'smooth', then large oscillations are possible in the 'solution' $f(y)$ that give satisfactory results for $g(x)$
  - Demonstrated by Phillips (1962)
    - ✓Solved for the same number of equations as unknowns by inverting 2 matrices
    - ✓Introduced smoothness constraint

Constrained Linear Inversion
(Twomey, 1963)

Expressing the Fredholm integral equation as a quadrature of the form

$$\mathbf{Af} = \mathbf{g} + \boldsymbol{\varepsilon}$$

- Twomey (1963) showed that the solution of this equation is an extension of least-squares fitting where one minimizes a performance function *Q* defined as

$$Q = Q_1 + \gamma Q_2$$

where

$$Q_1 = \boldsymbol{\varepsilon}^{\mathrm{T}}\boldsymbol{\varepsilon} = \sum_i \varepsilon_i^2$$

$$Q_2 = (\mathbf{Kf})^{\mathrm{T}}\mathbf{Kf} = \mathbf{f}^{\mathrm{T}}\mathbf{Hf}$$

and

H is a symmetric matrix of the form $\mathbf{K}^{\mathrm{T}}\mathbf{K}$

γ is an unspecified Lagrange multiplier to adjust the smoothing (constraint)

- Twomey's well-known solution involves a single matrix inversion and allows for more measurements than unknowns

$$\mathbf{f} = \left(\mathbf{A}^{\mathrm{T}}\mathbf{A} + \gamma\mathbf{H}\right)^{-1}\mathbf{A}^{\mathrm{T}}\mathbf{g}$$

Various Possibilities for Constraints

- Sum of the squares of second difference ($\sum(f_j - 2f_{j-1} + f_{j-2})^2$)
  - The data points to be inverted should be equally spaced (in radius, pressure, etc.) for easiest implementation
- Variance ($\sum(f_j - \bar{f})^2$)
- Deviation from a first guess (trial solution)
- Some of the squares of third differences

- Twomey himself never incorporated uncertainties into the measurements, nor uncertainties (error bars) into the solution

$$\mathbf{f} = \left(\mathbf{A}^T\mathbf{S}_e^{-1}\mathbf{A} + \gamma\mathbf{H}\right)^{-1}\mathbf{A}^T\mathbf{S}_e^{-1}\mathbf{g}$$

$$\mathbf{S} = \left(\mathbf{A}^T\mathbf{S}_e^{-1}\mathbf{A} + \gamma\mathbf{H}\right)^{-1}$$

where

$\mathbf{S}_e$ = uncertainty matrix of the measurements (often assumed diagonal with no correlation between measurements

$\mathbf{S}$ = uncertainty matrix of the solution (including non diagonal correlations)

Take Away Message

- The ambiguity in inversions is fundamental
  - Caused by the kernels, which describe the underlying physical connection between measured and sought functions
  - A successful algorithm can only succeed by making an acceptable selection from all the possibilities
- For real atmospheric physics problems, the kernel is fundamentally smooth
  - Smoothness implies a diminishing sensitivity of the measurements $g(x)$ to the high frequency components of $f(y)$
  - This has nothing to do with the inversion algorithm
- Twomey simulated data from known $f(y)$ and inverted these $g(x)$ 'measurements'
  - Constrained linear inversion
  - Backus-Gilbert method
  - Iterative (Chahine) method
  - Chahine-Twomey inversion (modification of the kernel)
- The nature of the constraints affects the final answer and too much constraint can lead to both good results and poor results, depending on *a priori* knowledge

Twomey (1977)

Aerosol Size Distribution by Multiple Filter Measurements

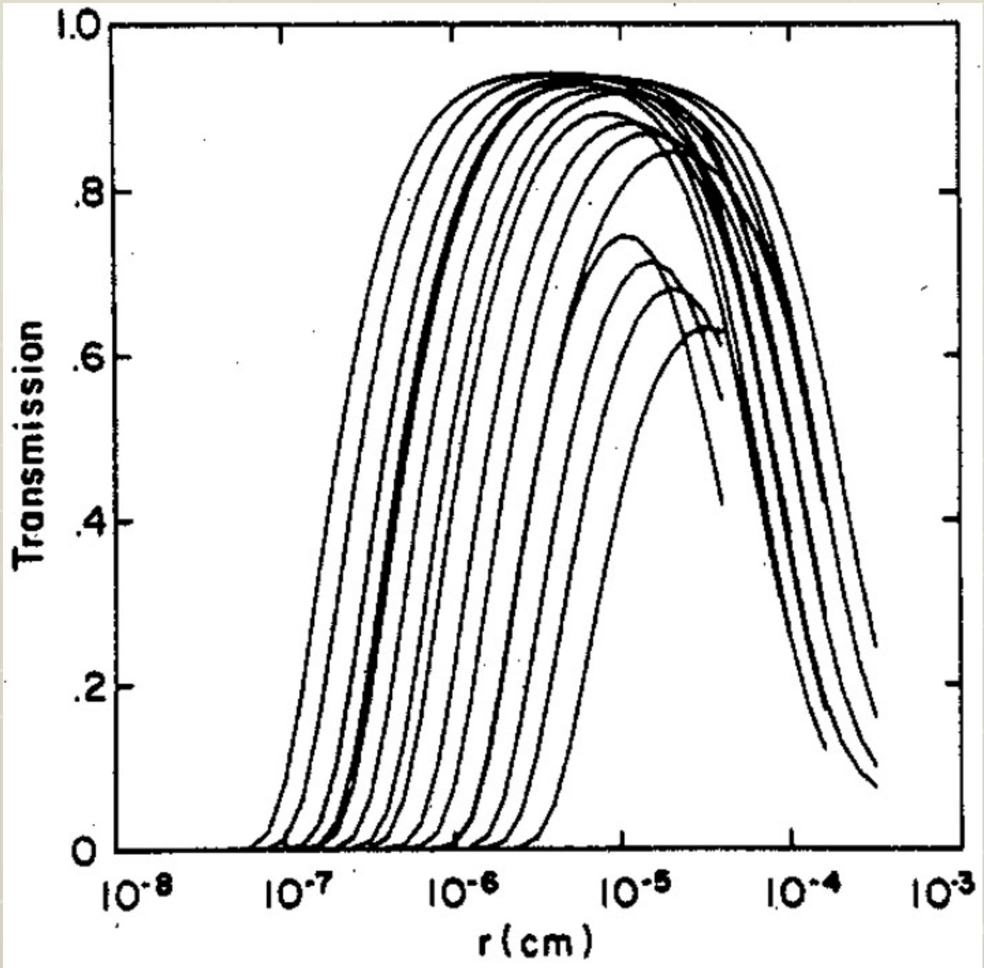
- Drew in large volume of air into an aluminized Mylar bag inside a rigid barrel
- Air is then pushed through a set of four nuclepore filters
  - Various hole diameters (0.95-4.5μm)
  - Pushed air through at four flow rates (24.2-171.6 $cm^3\ s^{-1}$)
- Measured the emerging particle concentrations with a Pollak photoelectric nucleus counter
  - He reproduced a Pollak counter based on Pollak's (1957) design
  - Problem with customs bringing Pollak counter into the United States from Australia
    - ✓Duty was collected for a 'heavy' device not found on any computer printout
- Inversion problem
  - Fredholm integral equation of the first kind
    - ✓Modified to account for decay of particle concentration with time while stored in the Mylar storage bag (diffusion loss)

$$g_i = \int K_i(x) e^{-\eta D(x) t_i} f(x)\, dx$$

Twomey (1976)

Kernel Functions for Nuclepore Filter Transmission

- A typical set of filter transmission curves



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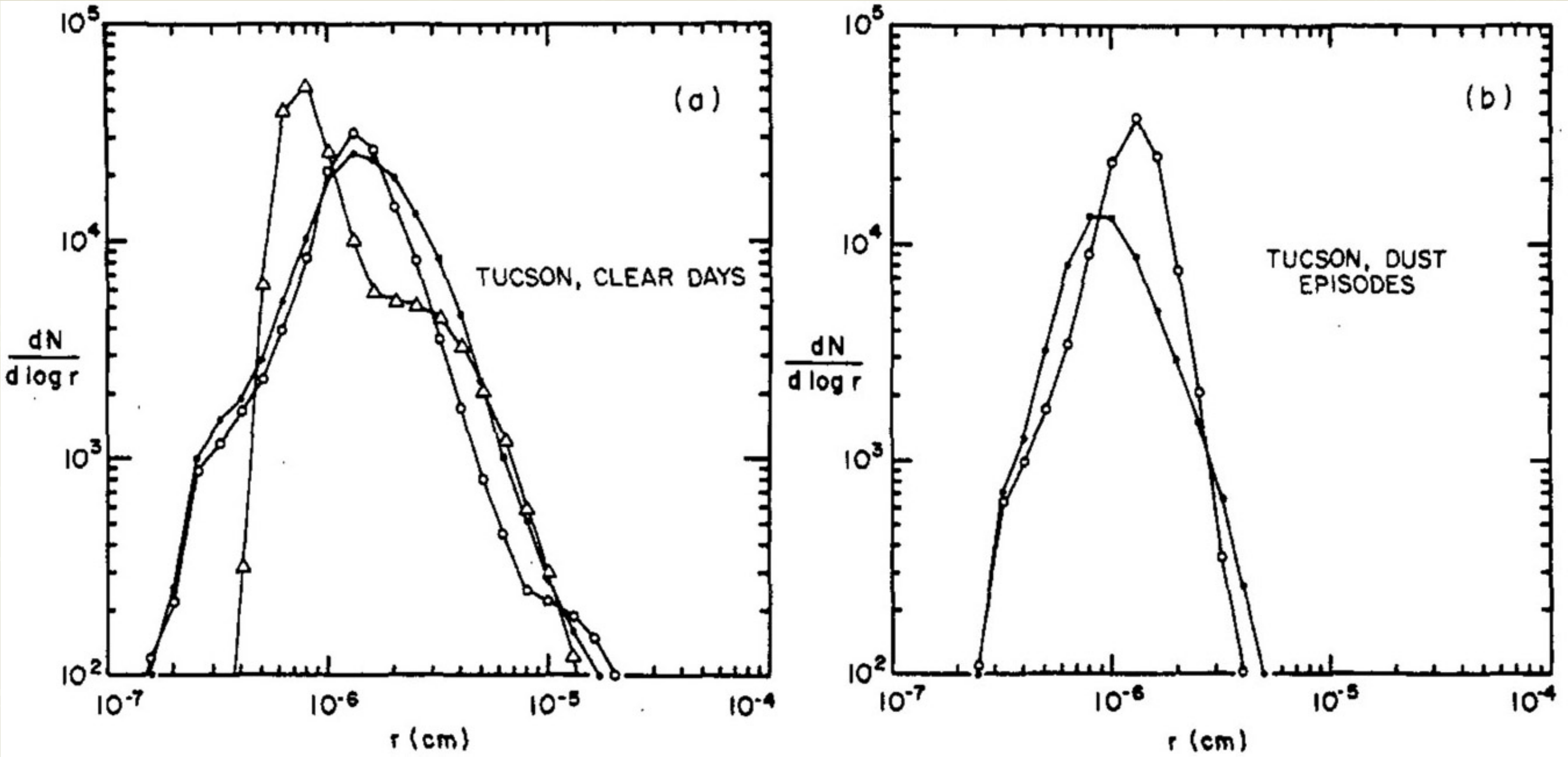
Twomey and Zalabsky (1981)

Size Distribution of Natural Aerosol in the Free Atmosphere

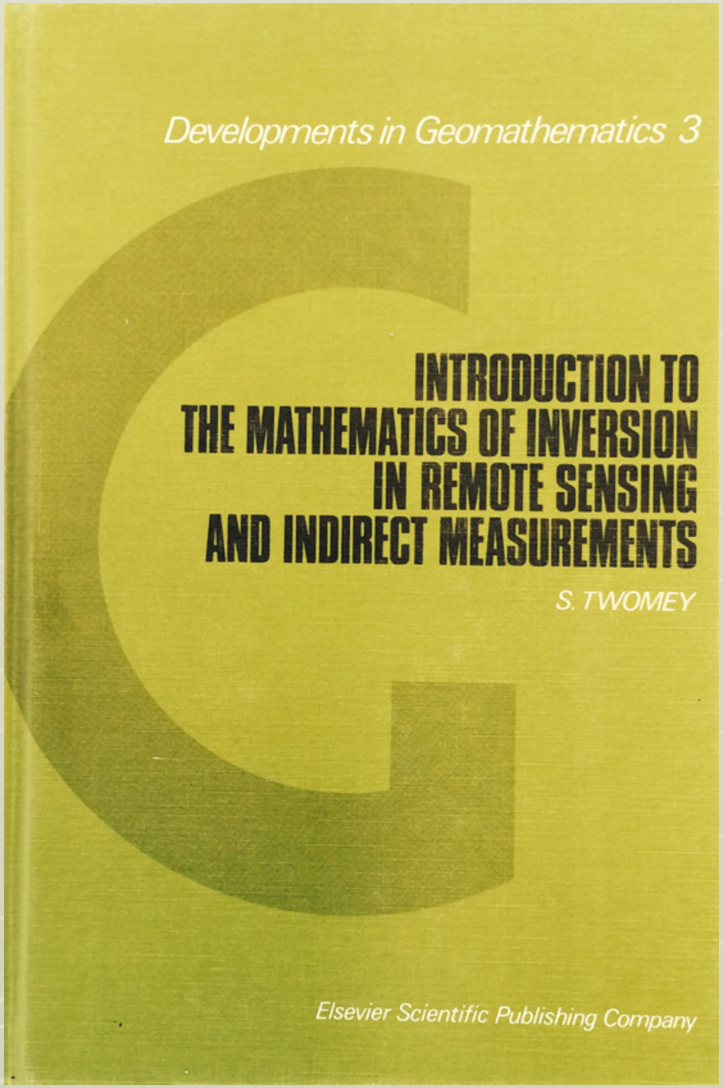
- Tucson (clear and dusty days)



Twomey and Zalabsky (1981)

Introduction to the Mathematics of Inversion in Remote Sensing and Indirect Measurements

- Introduction
  - Mathematical description
- Simple problems involving inversion
- Theory of large linear systems
- Physical and geometric aspects of vectors and matrices
- Linear Inversion methods
  - Least squares
  - Constrained linear inversion
- Further inversion techniques
- Information content of indirect sensing
- Appendix



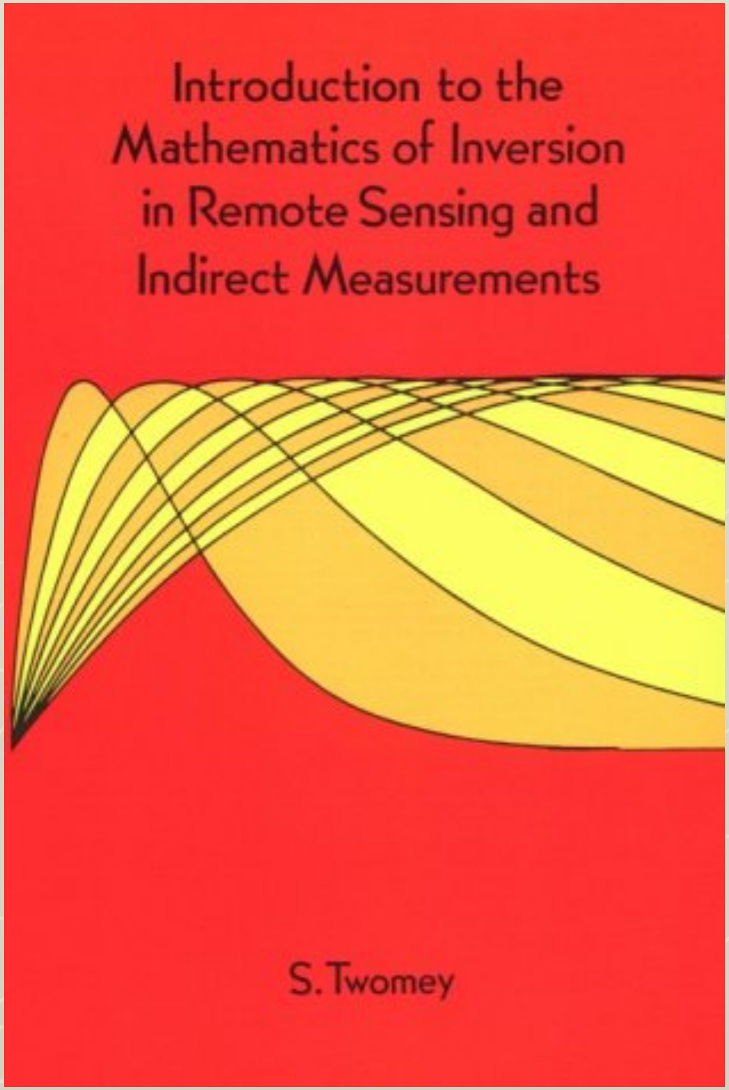
Twomey, S., 1977: Introduction to the Mathematics of Inversion in Remote Sensing and Indirect Measurements, Elsevier Scientific Publishing Company, 243 pp.

Introduction to the Mathematics of Inversion in Remote Sensing and Indirect Measurements

After being out of print, Dover picked up this publication and published it as a paperback (like they did with Chandrasekhar's radiative transfer text)

Twomey, S., 1996: Introduction to the Mathematics of Inversion in Remote Sensing and Indirect Measurements, Dover Publishing, 243 pp.

Twomey, S., 2014: Introduction to the Mathematics of Inversion in Remote Sensing and Indirect Measurements, Second Edition, Dover Publishing, 243 pp. [printed after Twomey passed away]



Aerosol Size Distribution from Spectral Optical Thickness

- Measure optical thickness as a function of wavelength
  - Subtract Rayleigh and molecular (ozone) optical thickness
- The aerosol optical thickness is related to the columnar aerosol size distribution as

$$\tau_{aer}(\lambda) = \int \frac{3}{4\pi r^3} \pi r^2 Q_{ext}(r, \lambda) v_c(\ln r) d\ln r$$

where

$v_c(\mathrm{r})$ = columnar volume aerosol size distribution

$K(\mathrm{r}, \lambda)$ = Kernel function = $\frac{3}{4\pi r^3} \pi \mathrm{r}^2 Q_{ext}(r, \lambda)$

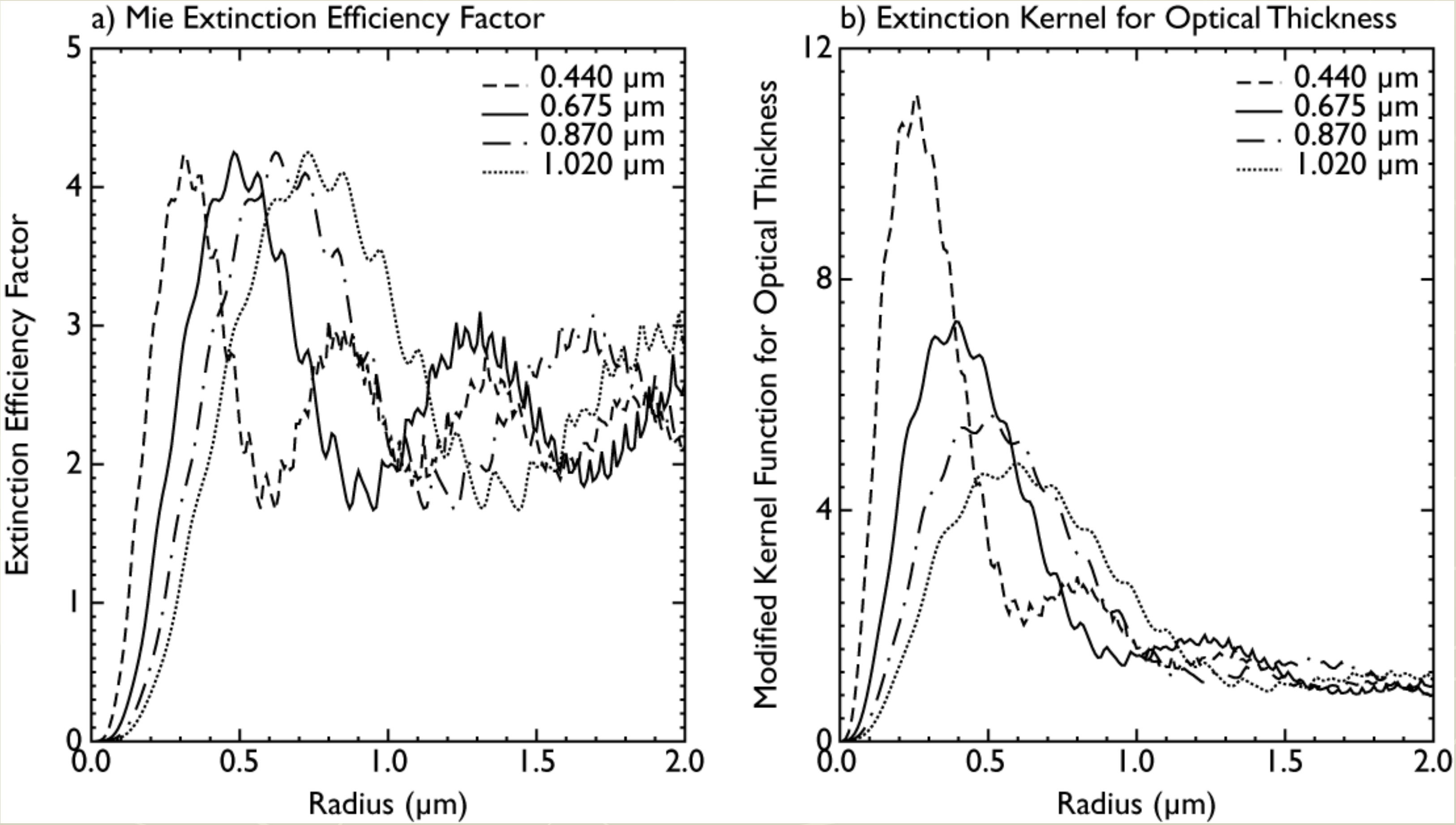
$Q_{ext}(\mathrm{r}, \lambda)$ = extinction efficiency factor

- Inversion problem
  - Fredholm integral equation of the first kind
  - Invert data after varying the Lagrange multiplier

King et al. (1978)
King and Dubovik (2013)

Extinction Kernel for Spectral Optical Thickness

- Aerosol efficiency factor and extinction kernel for volume size distribution inversion at 4 AERONET wavelengths



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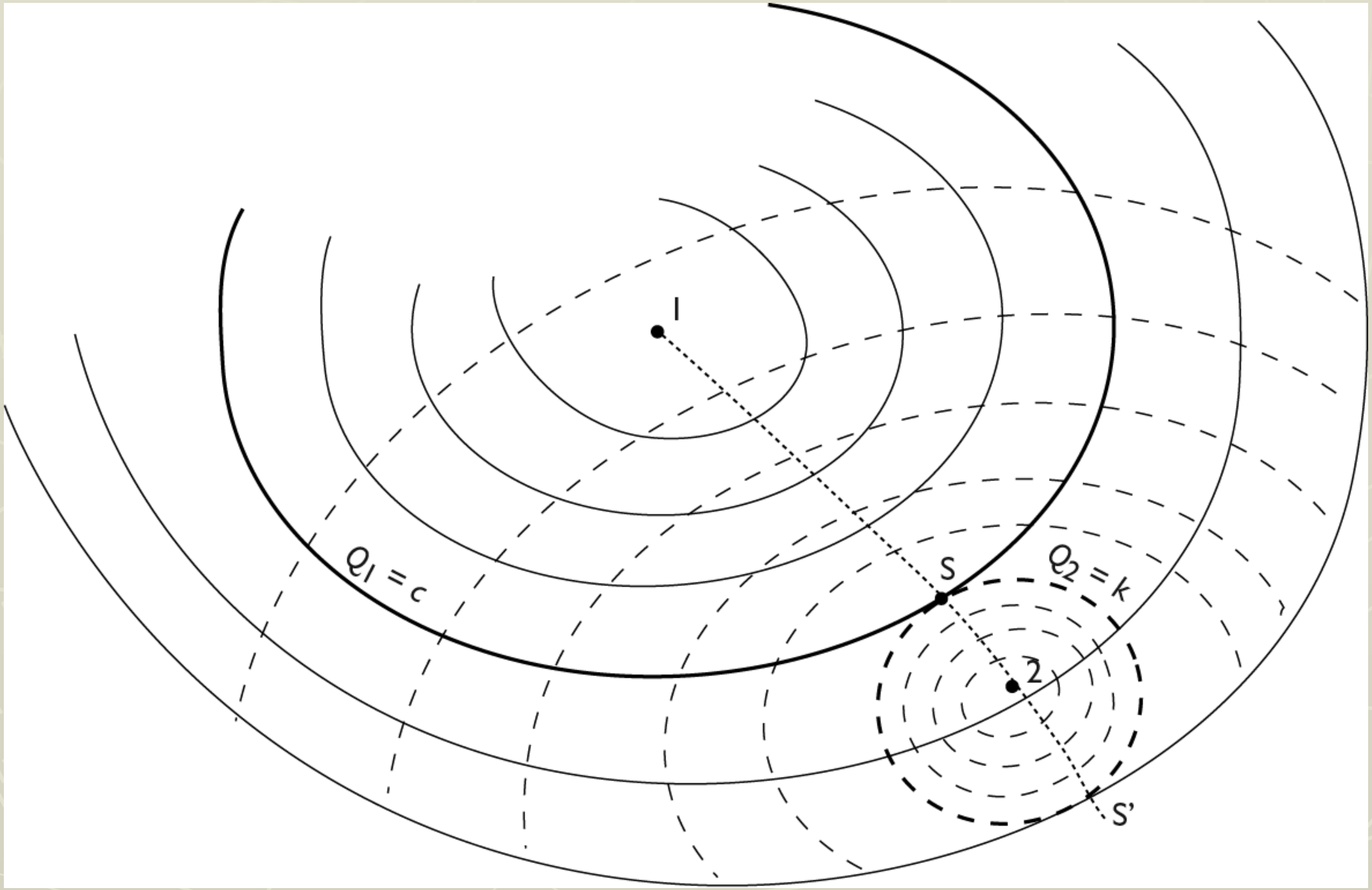
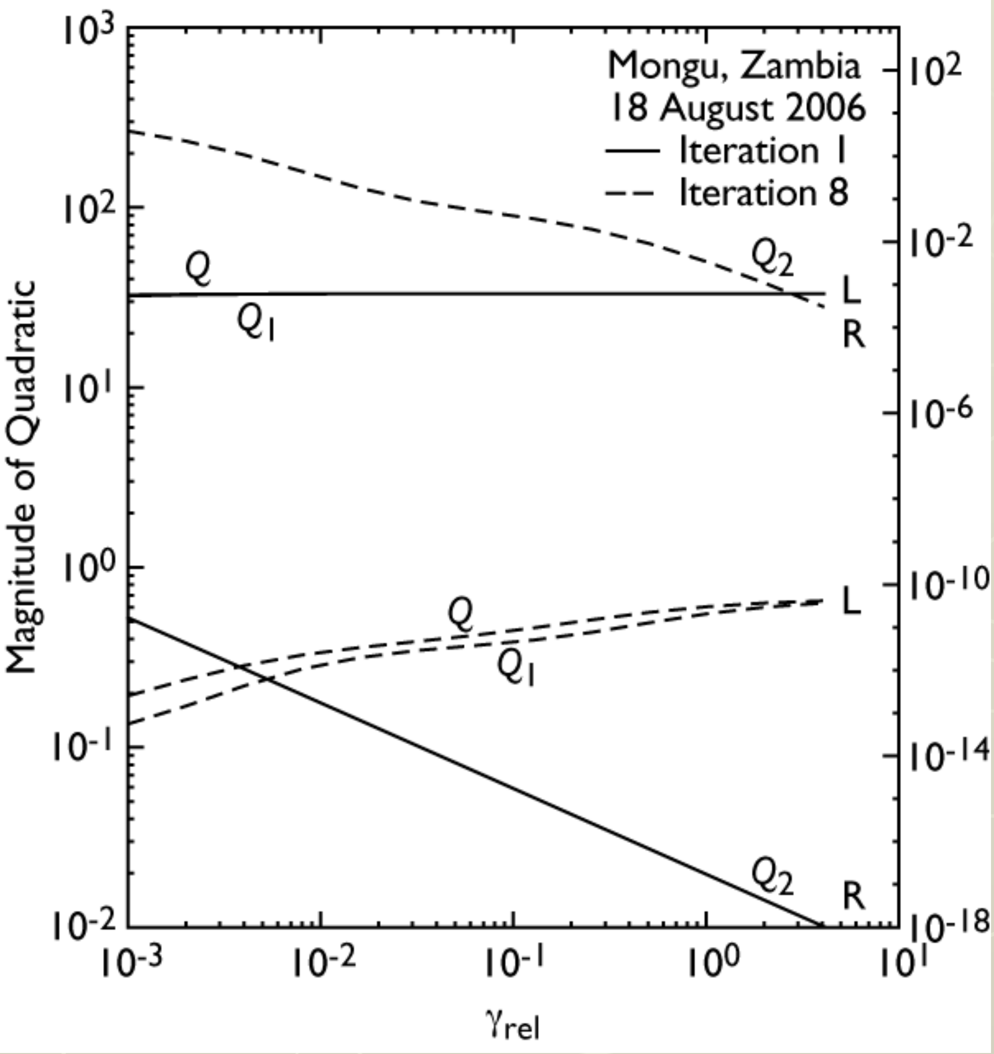
Selection of the Lagrange Multiplier

- Vary the Lagrange multiplier between 0 (Q_1 minimum with best match to measurements) and Q_2 minimum (very smooth but far from measurements)



Twomey (1977)

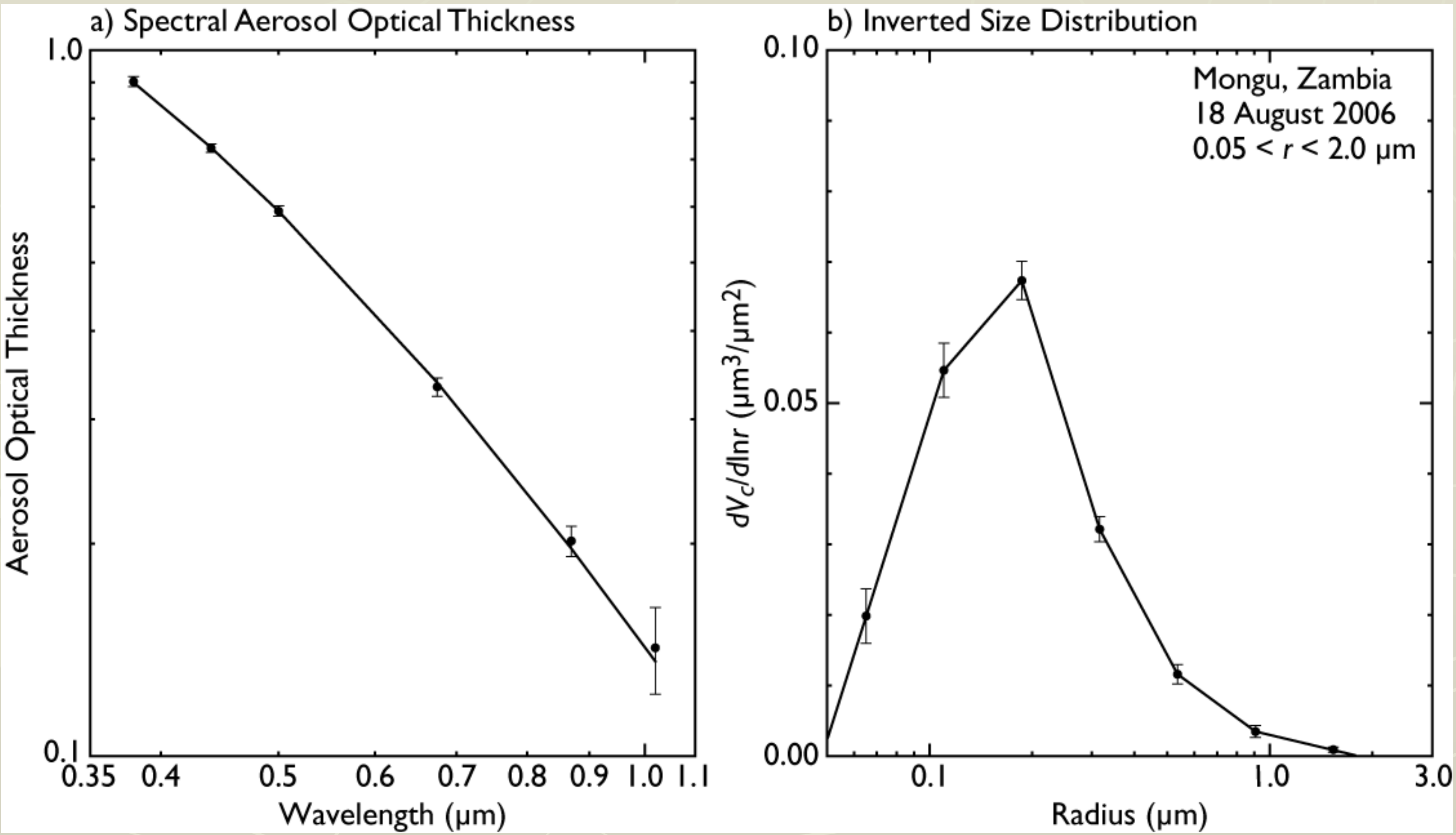
Magnitude of Quadratics Q_1, Q_2, and Q as a function of the Lagrange Multiplier



King (1982)
King and Dubovik (2013)

Inferring Aerosol Size Distribution from Spectral Aerosol Optical Thickness

- AERONET sunphotometer measurements from Zambia (18 August 2006)
- Derived volume size distribution (and error bars)



King and Dubovik (2013)

Surface Measurements of Sun/Sky Radiation

(B. N. Holben, T. F. Eck, I. Slutsker et al. – NASA GSFC)

AERONET

- Automatic recording and transmitting sun/sky photometers
- Data Base: Aerosol optical thickness, size distribution, phase function, optical properties, and precipitable water
- Collaborative: NASA – instruments/sites and centralized calibration & database
Non-NASA – instruments/sites

Holben et al. (1998)

Aerosol Size Distribution and Single Scattering Albedo from Spectral Optical Thickness & Sky Radiance

- Measure aerosol optical thickness as a function of wavelength
- Measure sky radiance as a function of azimuth angle in almucantar ($\theta = \theta_0$)
- The aerosol optical thickness is related to the aerosol size distribution as

$$\tau_{\mathrm{aer}}(\lambda) = \int \frac{3}{4\pi r^3} \pi r^2 Q_{\mathrm{ext}}(r, \lambda) v_c(\ln r) d\ln r$$

- The sky radiance is related to the aerosol scattering properties as

$$I(\Theta_0, \lambda) = \frac{F_0 \mu_0}{4\pi(\mu - \mu_0)} \left(e^{-\tau/\mu} - e^{-\tau/\mu_0}\right)\left(\varpi_0 p(\Theta, \lambda) + G(\ldots)\right)$$

where

ϖ_0 = single scattering albedo

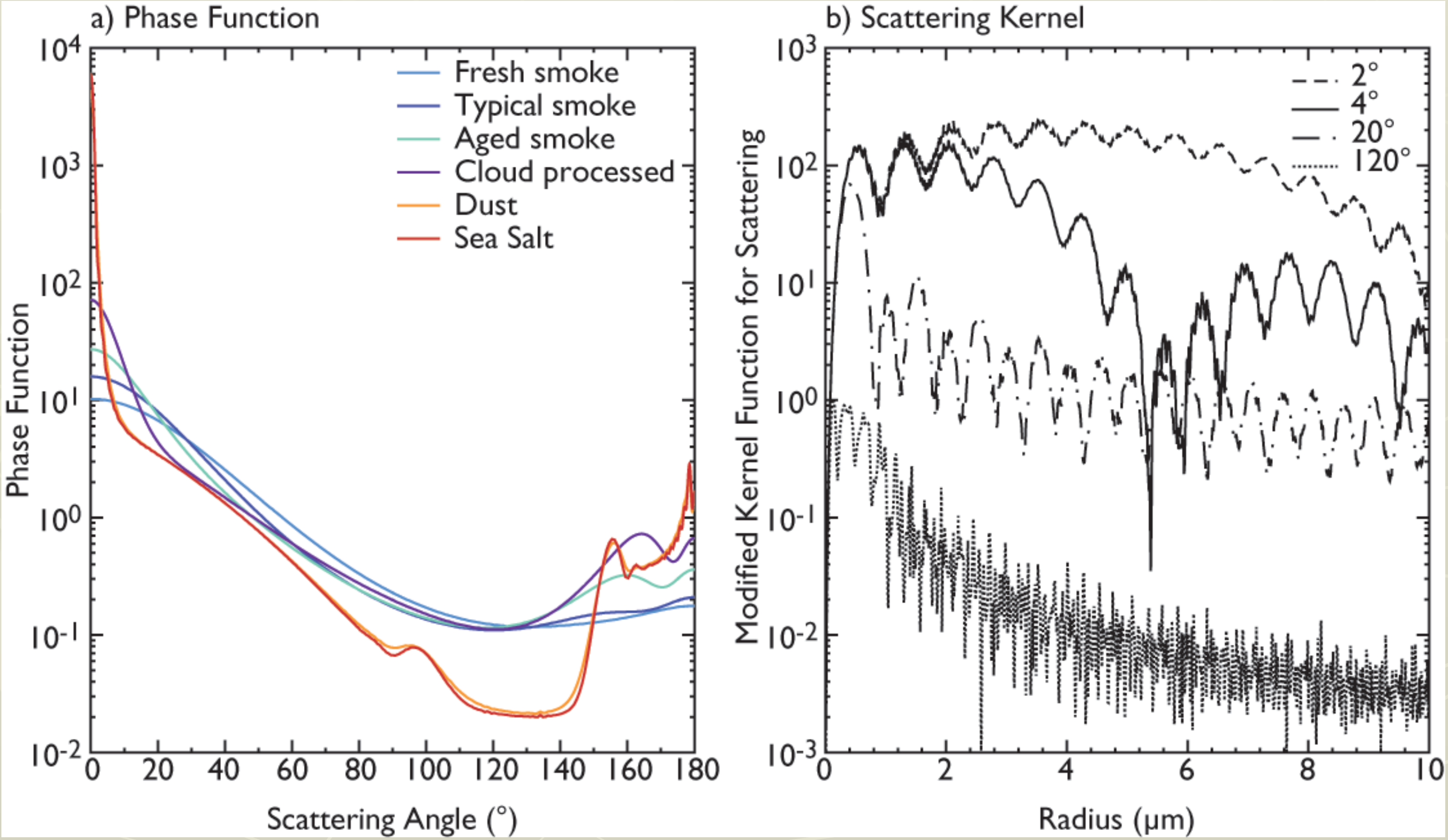
$p(\Theta,\lambda)$ = phase function

- Inversion problem
  - Fredholm integral equation of the first kind (multisource data)
  - Invert data after selecting the Lagrange multiplier

Dubovik and King (2000)
King and Dubovik (2013)

Scattering Kernel for Sky Radiance Measurements

- Aerosol phase function and scattering kernel for selected scattering angles used in inversion of AERONET sky radiance



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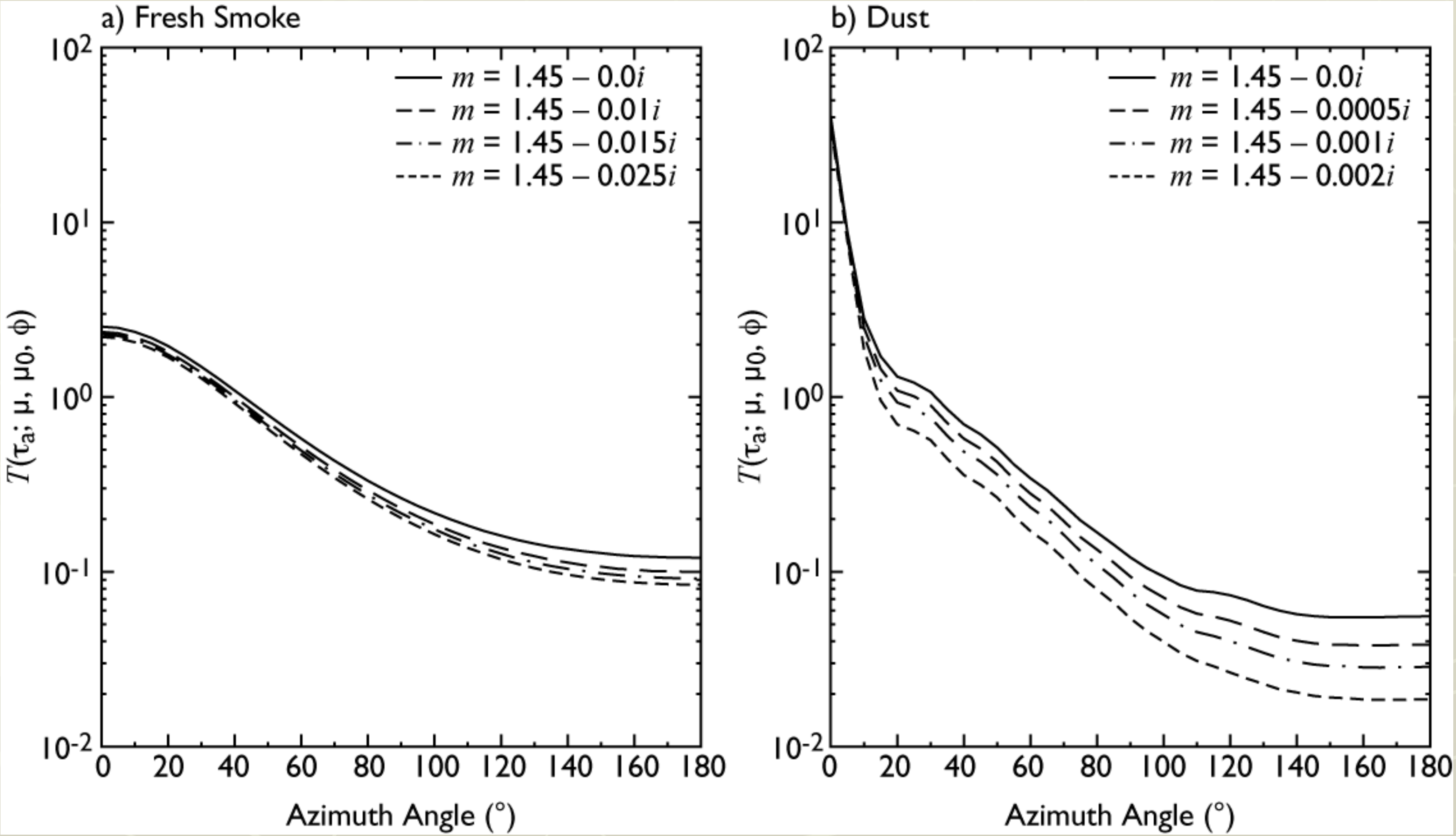
Sensitivity of Sky Radiance to Single Scattering Albedo

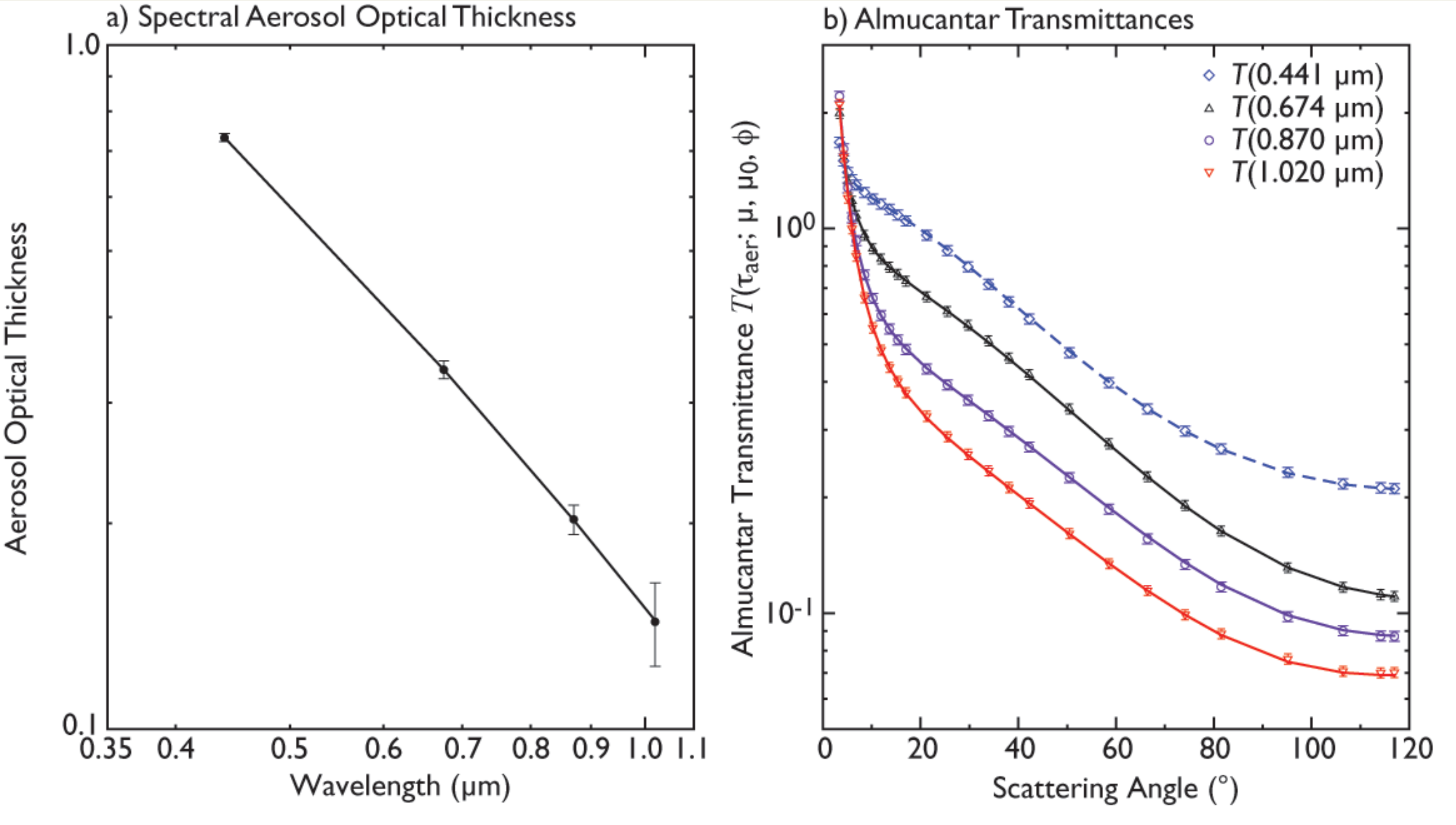
- Transmission function as a function of azimuth angle in the almucantar where $\theta = \theta_0$ for four values of the complex refractive index of aerosols



King and Dubovik (2013)

Spectral Aerosol Optical Thickness and Almucantar Transmittances

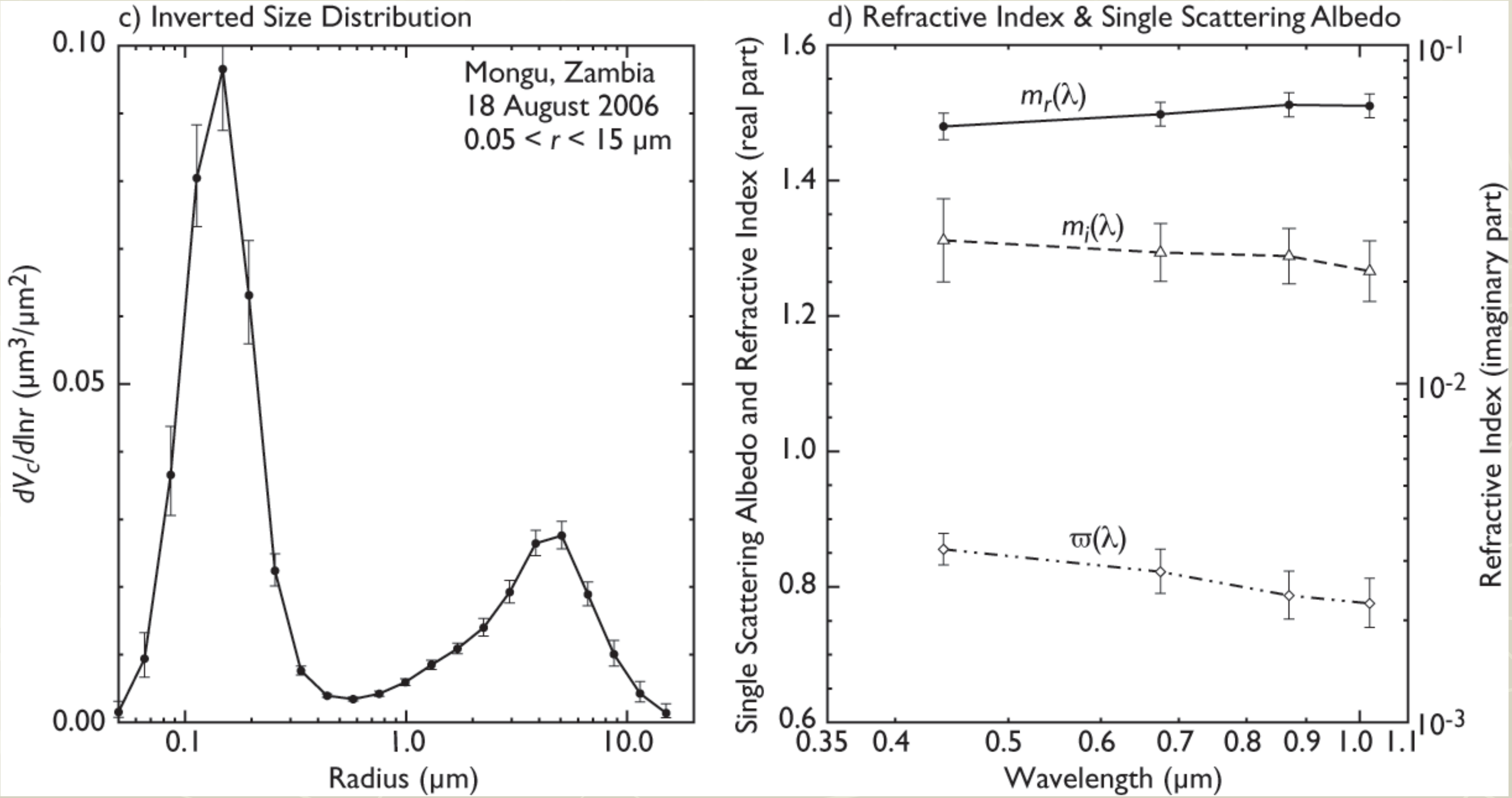
- AERONET sunphotometer measurements from Zambia (18 August 2006)
  - Optical thickness and almucantar measurements at 4 wavelengths



King and Dubovik (2013)

Inferring Aerosol Size Distribution from Spectral Aerosol Optical Thickness

- Derived volume size distribution (and error bars)
- Derived real and imaginary refractive index and single scattering albedo



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Summary and Conclusions

- Inversion problems received renewed attention in the early 1960s
  - Arrival of large computers
  - Launching of earth-orbiting satellites
    - ✓ Applications first generated unphysical answers with unwanted oscillations (negative temperatures) even though the forward problem could reproduce the measurements
  - Twomey realized that in the presence of measurement (and quadrature) errors, instability allowed many answers that were all possible to reproduce the measurements within experimental accuracy
    - ✓ Reframed the question and introduced smoothness constraints
    - ✓ He also explored the number of independent pieces of information whereby having more measurements (wavelengths, etc.) would not necessarily yield better results
- Pioneered constrained linear inversion method
  - Expanded David L. Phillips (1962) work, enabling one matrix inversion and unequal number of measurements and unknowns, and done in parallel with Andrey N. Tikhonov (1963)
    - ✓ Russian's used term 'regularization'
  - Published 12 papers on inversion techniques, its applications, and information content
  - Published 1 text book on the 'Introduction to the Mathematics of Inversion in Remote Sensing and Indirect Measurements'

Prof. Sean A. Twomey

Radiative transfer, aerosol and cloud microphysics, inversion theory, and mentor

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Photo by Glenn Shaw (1992)