Data Rescue of Temperature-Dependent Optical Constants of Water for the Thermal Infrared

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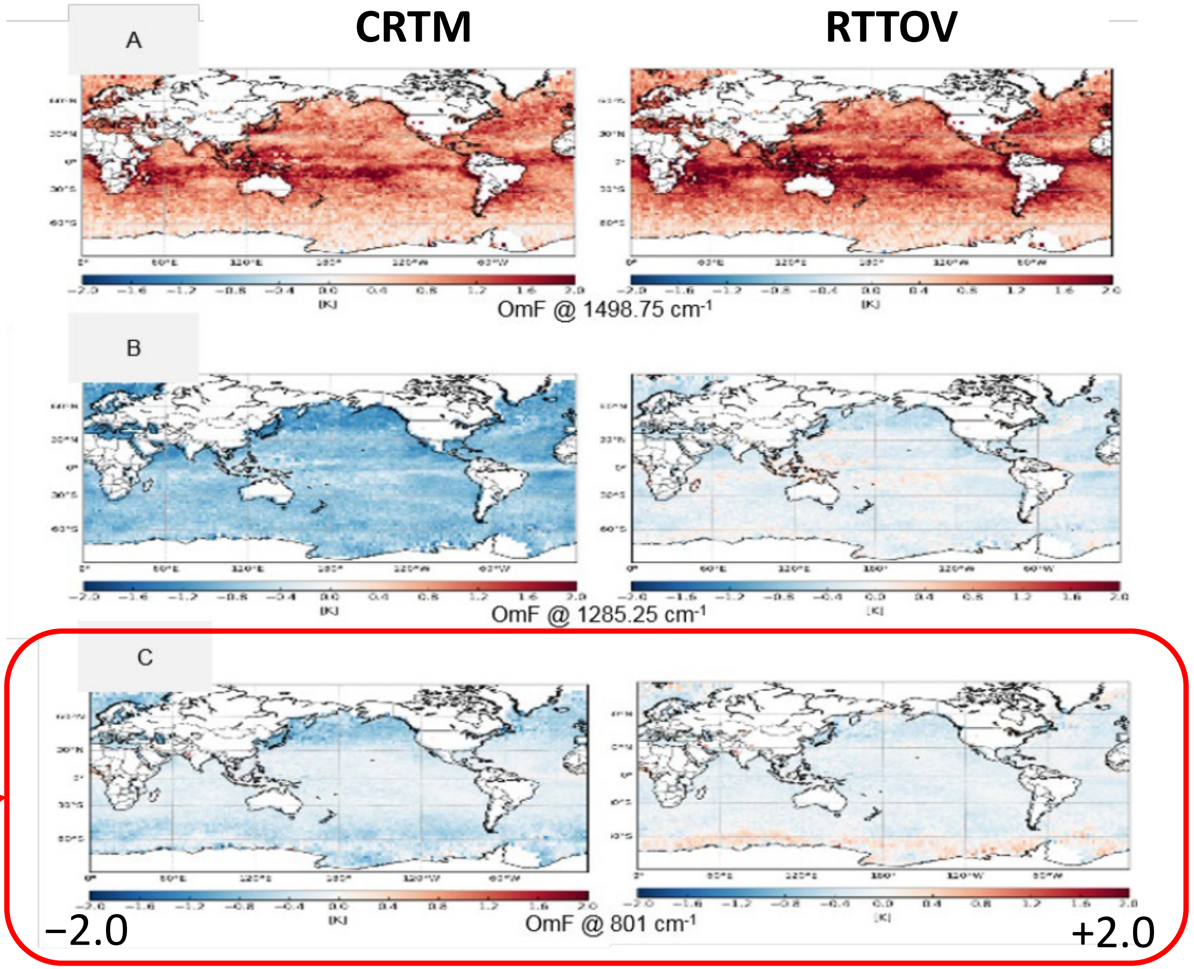
- *The scientific results and conclusions, as well as any views or opinions expressed herein, are those of the author(s) and do not necessarily reflect those of NOAA or the Department of Commerce.*

Introduction

- For satellite thermal IR remote sensing applications, the **surface emissivity** must be specified with a high degree of absolute accuracy
  - **0.5%** uncertainty ⇒ ≈**0.3–0.4 K systematic error** in LWIR window channels
- The **Community Radiative Transfer Model (CRTM) IR sea surface emissivity (IRSSE) model** was derived based on field observations to account for the BRDF in a manner practical for operational assimilation and retrievals
- However, recent findings (*Liu et al.* 2019) have revealed **significant systematic latitudinal biases** (0.5 K) on a **global scale**

***From Liu et al.* (2019)**



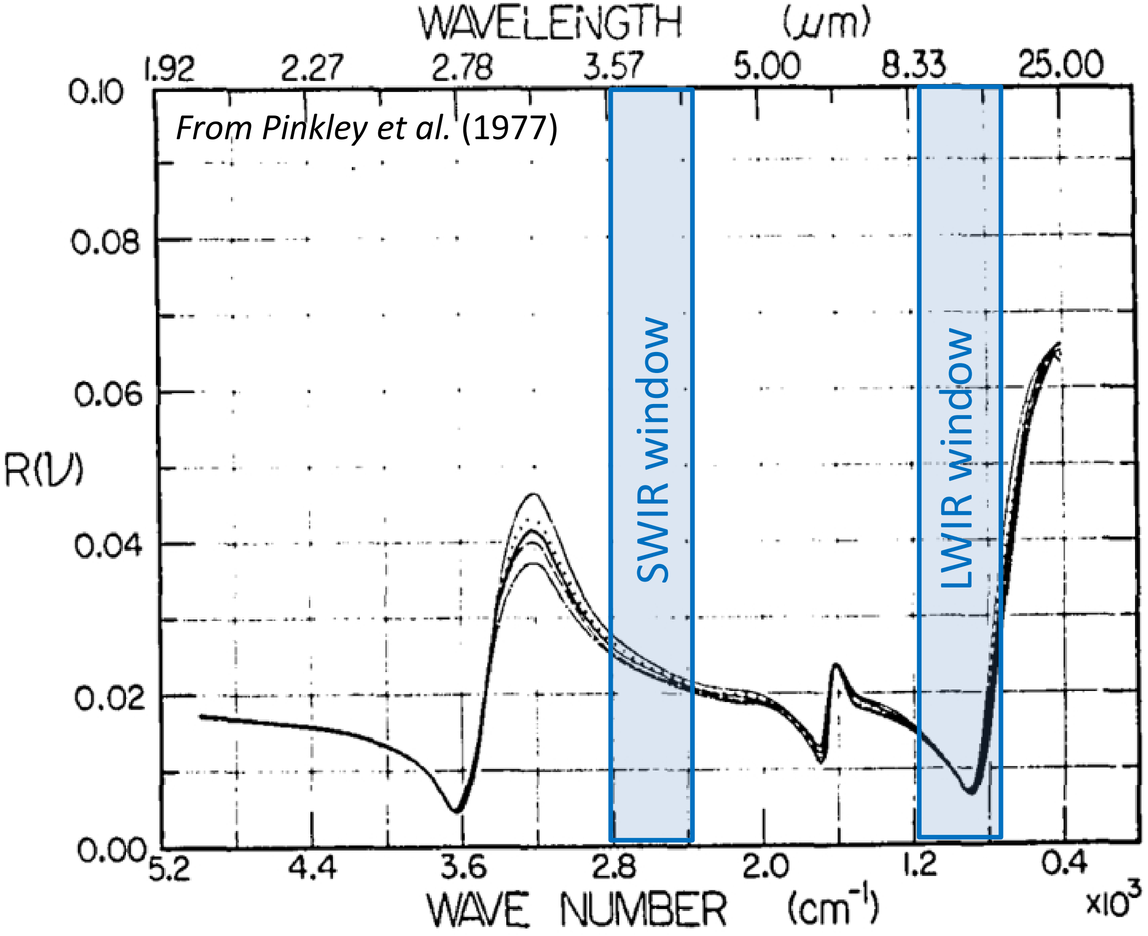
Temperature-Dependent IR Optical Constants

- The **temperature dependence** stems from the dependence of the **complex IR refractive index, N_ν**, on the water density
- Thus, we have sought to upgrade the IRSSE model to account for *T*-dependence
- To our knowledge, ***Pinkley et al.* (1977)** are the only complete set of laboratory derived ***T*-dependent IR optical constants** of **water** at surface temps
  - *Rowe et al.* (2020) are for supercooled water (cloud droplet applications)
  - *Newman et al.* (2005) are field-derived and do not span full IR spectrum
- However, their data is of **limited practical use as published**
  - Includes only **a small spectral subset**
  - **Severely truncated to 3 significant digits**
- To address this problem, we sought to perform a **data archeology and rescue** of their temperature-dependent optical constants via digitization of their figures
  - This effort was responsive to ITSC-22 RTSP-WG Action RTSP-5: *Identify up-to-date and develop new laboratory measurements across spectral ranges*
  - However, we eventually found that naïve digitation of their derived optical constants was *ad hoc* at best

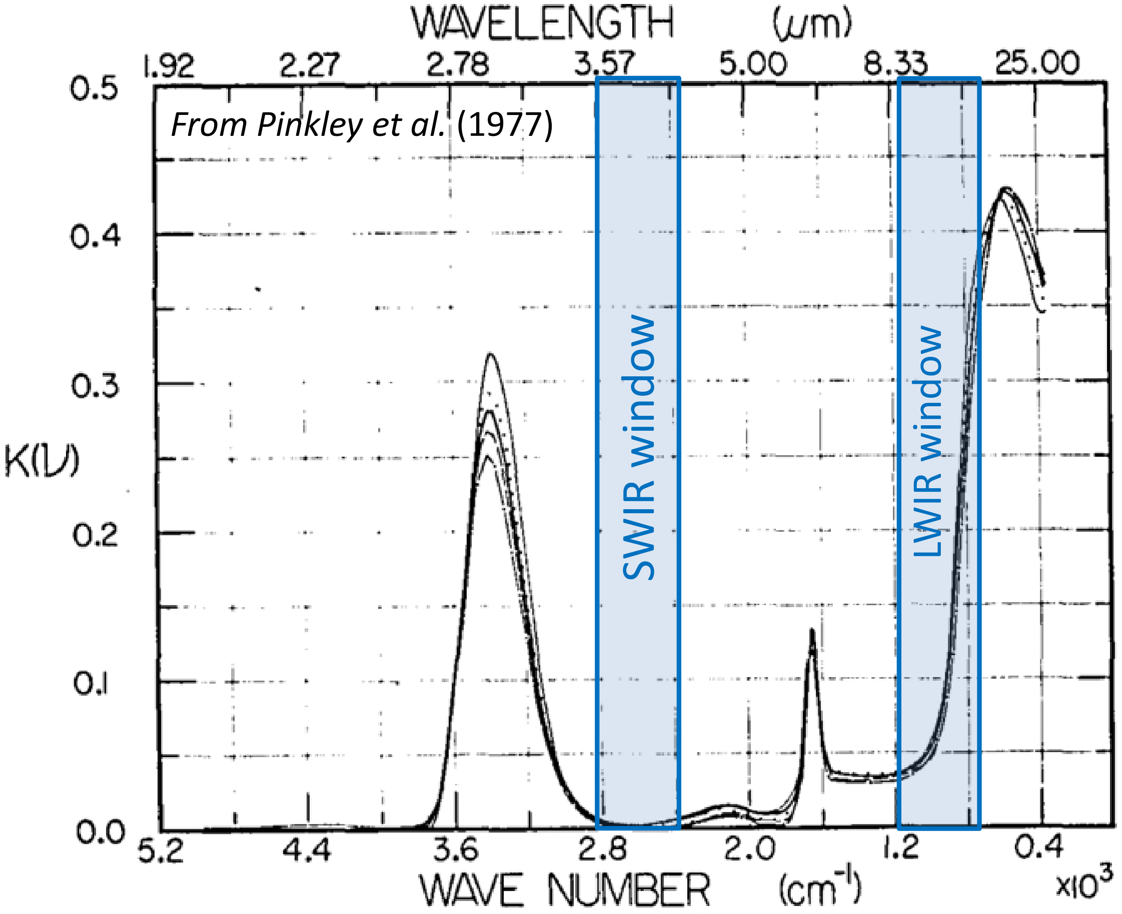
Electronic Reprints of *Pinkley et al.* Optical Constants

Temperatures = 1, 16, 39, 50°C

Real Part, $\Re(N_\nu)$ (Figure 3 *op. cit.*)



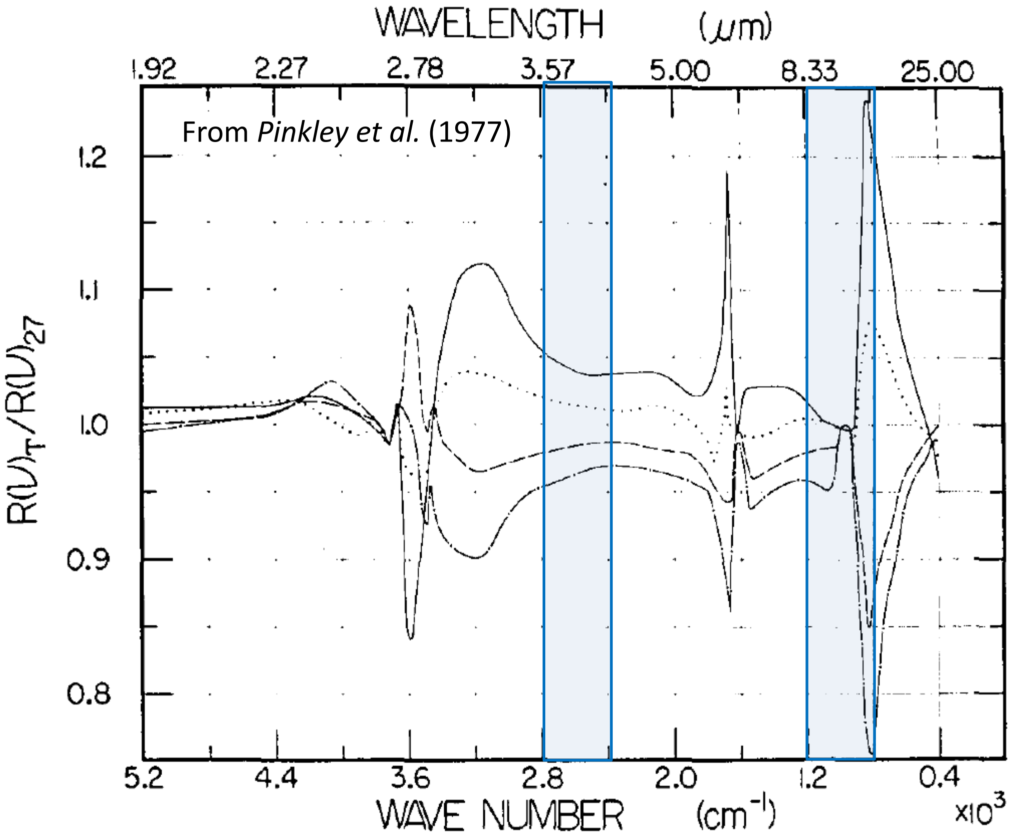
Imaginary Part, $\Im(N_\nu)$ (Figure 4 *op. cit.*)



Digitization of Laboratory Measured Reflectance-Ratios

- To get around this problem, we decided to perform a rigorous data rescue based on **Pinkley's original laboratory-measured reflectances**, along with **Kramers-Kronig (KK) analysis** to extract temperature-dependent optical constants from existing laboratory datasets
- The first step was to digitize their Figure 1, which showed **ratios of laboratory measured spectral reflectances** taken at 4 different temperatures (1, 16, 39, 50°C) with those measured previously at 27°C
  - This figure shows **significant *T*-dependence** not resolved in their figure showing the derived optical constants

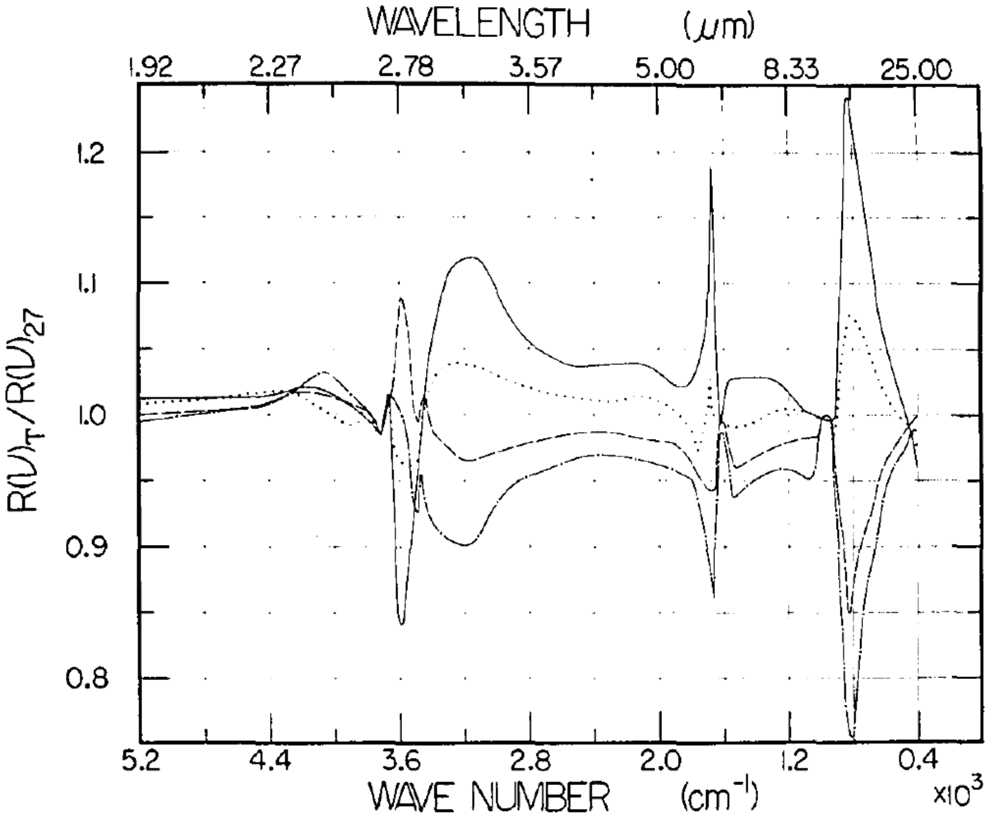
Reflectance Ratios (Figure 1 *op. cit.*)



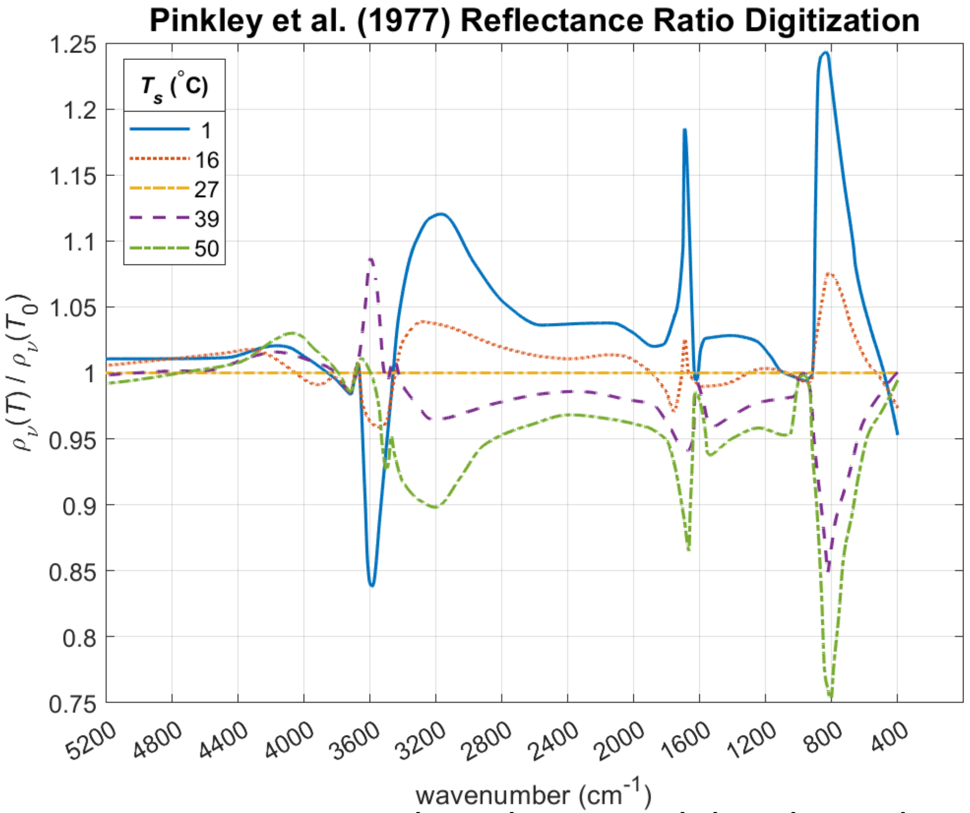
Note that **significant temperature-dependence** is clearly evident in **measured reflectance** space.

Digitization of Laboratory Measured Reflectance-Ratios

Original Figure from *Pinkley et al.* (1977)



Digitization



The digitization is accurate, but the *T*-peak has been broadened in the 900 cm^{-1} range based on NCEP GSI Assimilation Feedback.

KK Methodology for Deriving the Optical Constants

- We can derive the refractive index, n_ν, and extinction coefficient, k_ν, from the **Fresnel relations at normal-incidence**:

$$n_\nu(T) = \frac{1-\rho_\nu(T)}{\rho_\nu(T) - 2\sqrt{\rho_\nu(T)}\cos[\phi_\nu(T)] + 1},$$

$$k_\nu(T) = \frac{2\sqrt{\rho_\nu(T)}\sin[\phi_\nu(T)]}{\rho_\nu(T) - 2\sqrt{\rho_\nu(T)}\cos[\phi_\nu(T)] + 1}.$$

- The **phase shift** ϕ_ν can be obtained as a function of temperature from measured nadir reflectances and **KK analysis** (after *Pinkley et al.*)

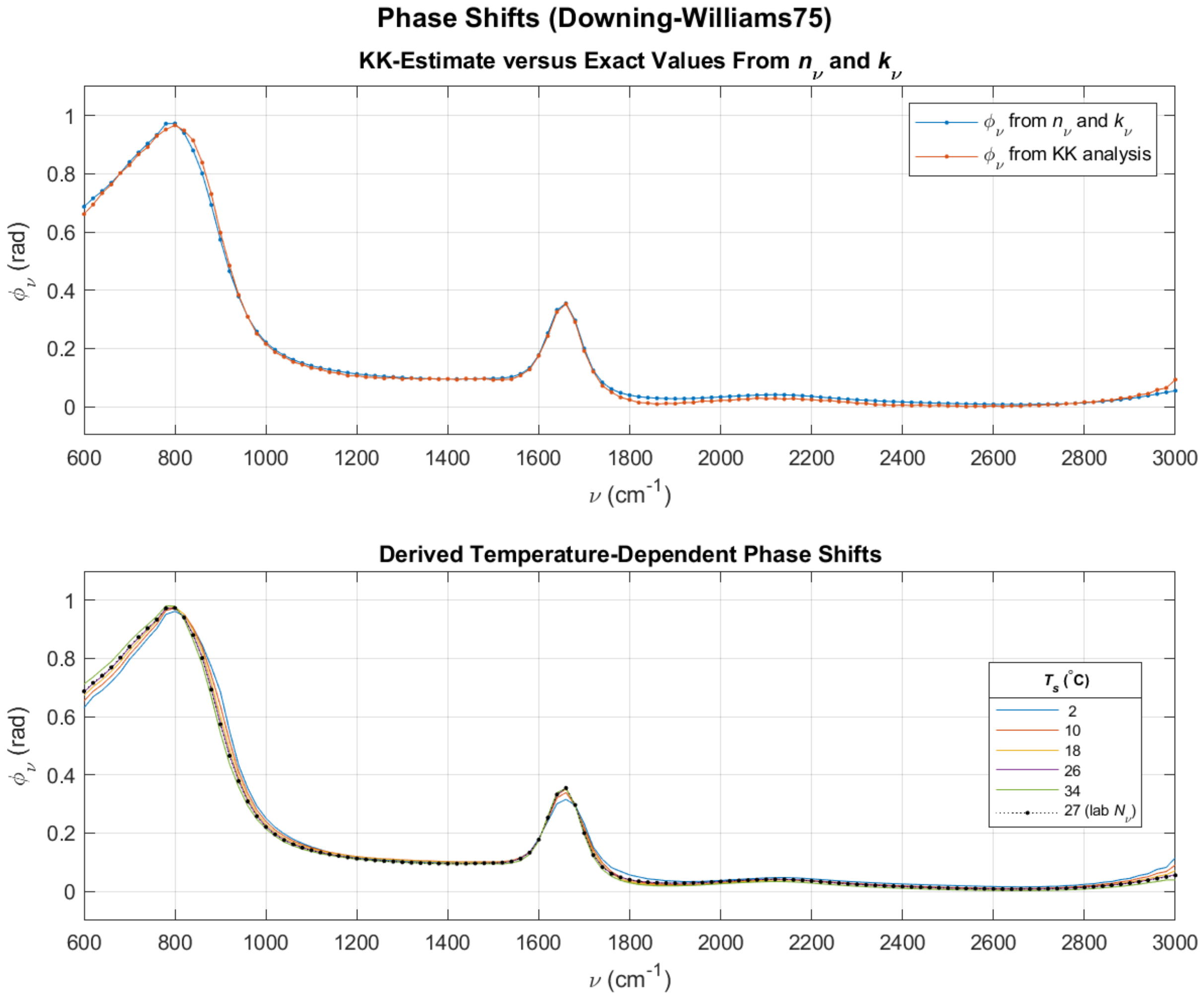
$$\widehat{\phi}_\nu(T) = \frac{2\nu}{\pi} P \int_0^\infty \frac{\ln\sqrt{\rho_{\nu'}(T)}}{\nu^2 - \nu'^2}\, d\nu',$$

$$\Delta\phi_\nu(T) = \widehat{\phi}_\nu(T) - \widehat{\phi}_\nu(T_0)$$

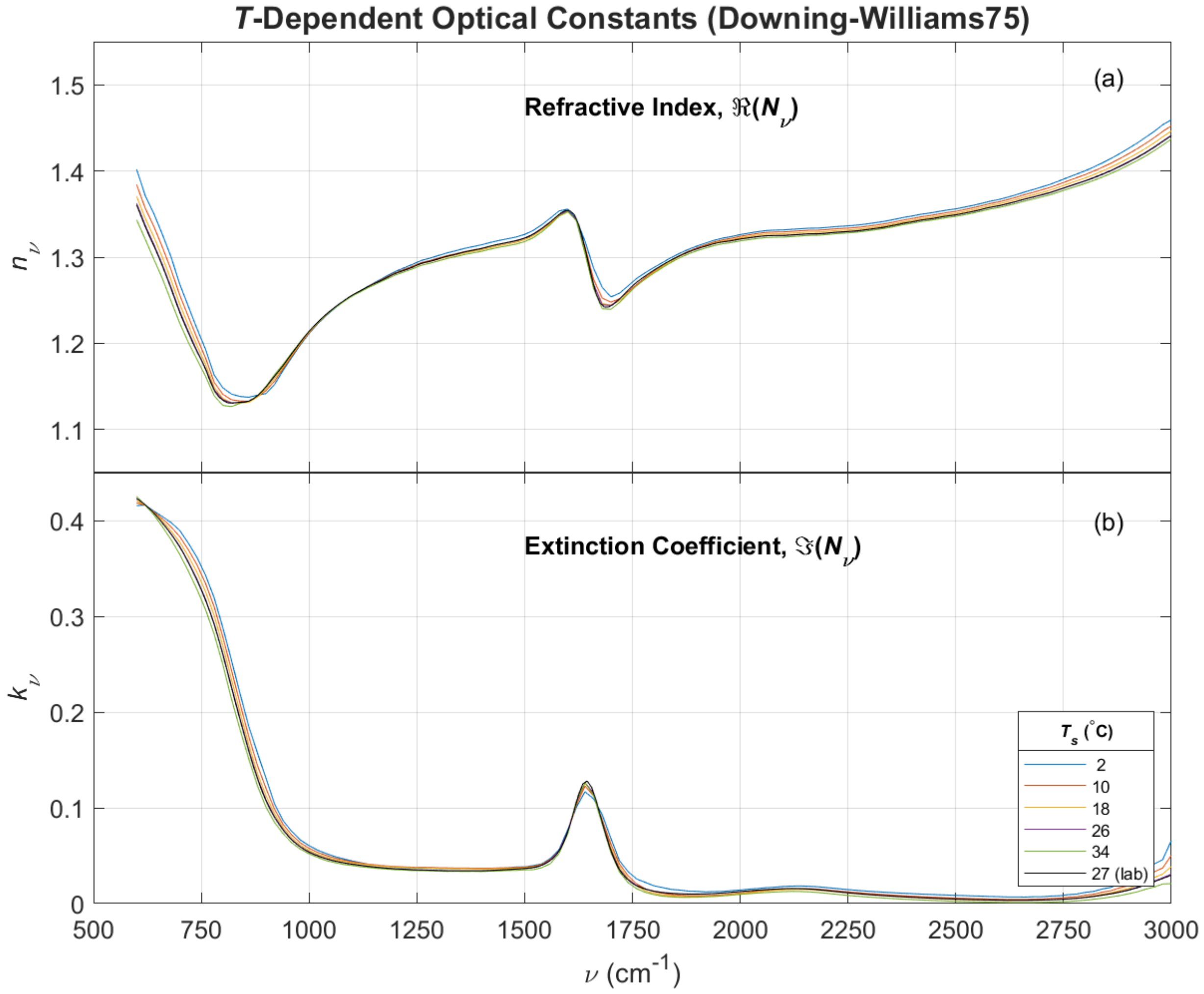
$$\phi_\nu(T) = \phi_\nu(T_0) + \Delta\phi_\nu(T)$$

Results: Temperature-Dependent Optical Constants
(based on *Downing and Williams*, 1973)

KK-Estimated and Exact Phase Shifts



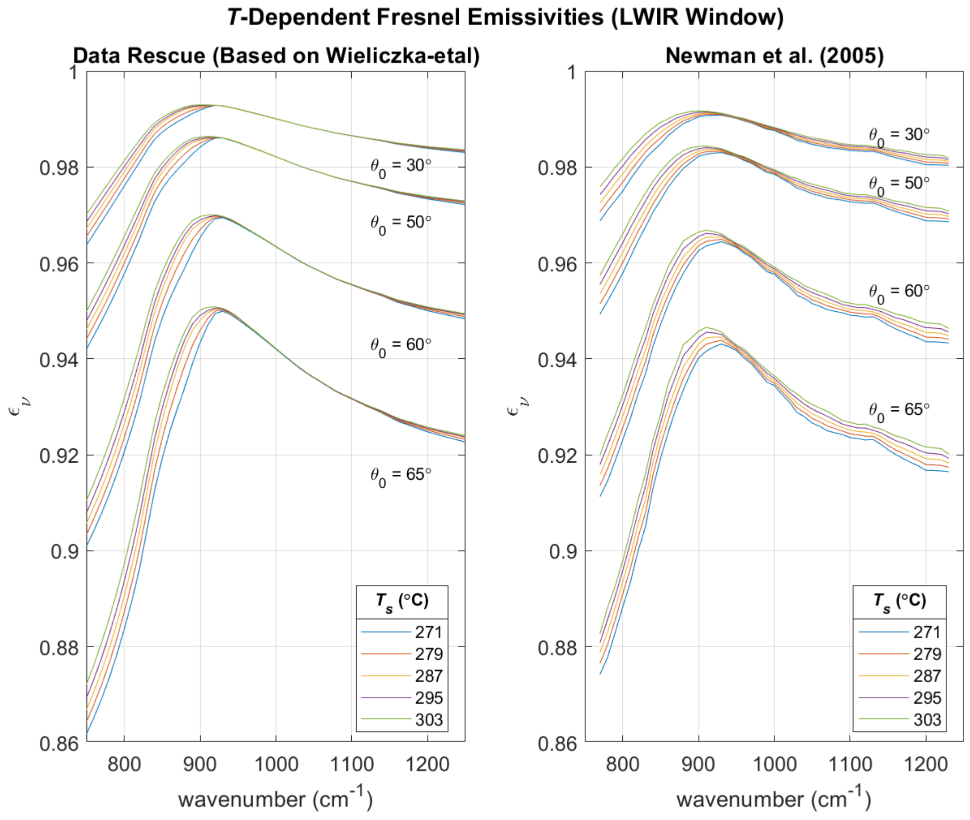
Optical Constants



Results: LWIR and Far-IR Fresnel Emissivities

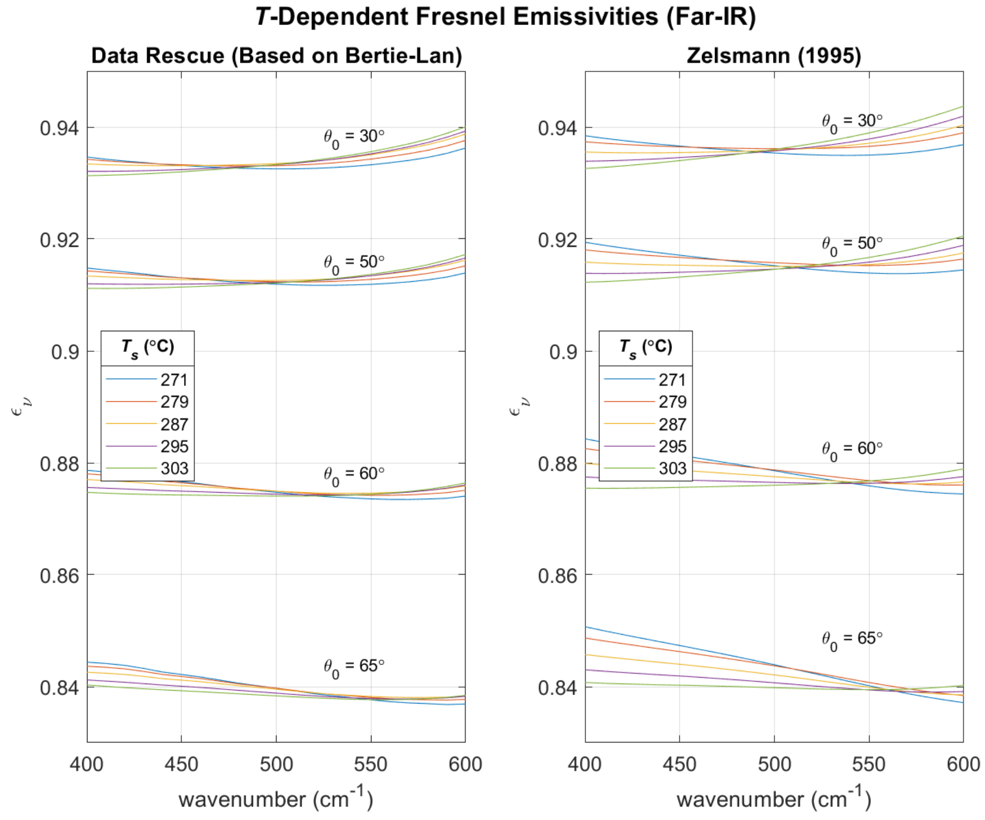
LWIR Window Region vs *Newman et al.* (2005)

(based on *Wieliczka et al.* 1989)



Far-IR Region vs *Zelsmann* (1995)

(based on *Bertie and Lan* 1996)



Summary

- Using the methodology described herein, we have successfully rescued the Pinkley data and have derived **temperature-dependent IR optical constants of water** based on the following standard datasets
  - *Hale & Querry* (1973) @ 298 K
  - *Bertie & Lan* (1996) @ 298 K
  - *Downing & Williams* (1975) @ 300 K
  - *Pontier & Dechambenoy* (1966) @ 300 K
  - *Segelstein* (1981) @ 303 K
  - *Wieliczka et al.* (1989) @ 303 K
- These data are currently being used for the upgraded **CRTM IRSSE v2.2**
  - The data are available as convenient lookup tables (LUTs), in both NetCDF and MATLAB formats, to radiative transfer modeling (RTM) teams upon request

Future Work

- Results using the rescued temperature-dependent optical constants within the new **CRTM IRSSE v2.2** will be subject of a forthcoming paper
- A manuscript detailing the results of the current work has been submitted for publication in *Optics Continuum*

- The IRSSE v2.2 is also being implemented within other radiative transfer models (e.g., PCRTM, kCARTA)
- We are currently looking into funded work (with UW/SSEC) to obtain an **updated laboratory set** of normal-incidence IR reflectance-ratios for deriving updated temperature-dependent optical constants

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Satellite Data Application, Validation, and Calibration for Atmospheric Observation II

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Deadline for manuscript submissions: 30 April 2022

Special Issue Information

Well-calibrated, remotely sensed spectral observations acquired from the growing constellation of environmental satellites flown in low-Earth orbit (LEO) and geosynchronous orbit (GEO) provide the vast majority of data for the purpose of observing the global atmosphere and oceans over varying space and timescales. While environmental satellite data have been critical in the improvement of numerical weather forecasts via data assimilation in recent years, a large complement of derived geophysical products and state parameters (e.g., environmental data records, climate data records) retrieved from sensor data records (i.e., spectral radiances) are used for Earth system observation at microscale, mesoscale, synoptic, and global climate scales. Because multiple independent passive and active sensors are sensitive to different portions of the EM spectrum and deployed onboard different satellite platforms, high absolute calibration accuracy is crucial for synergistic observations and data continuity, as well as for specifying reliable uncertainty estimates. Climate change detection, in particular, requires the capability to resolve small global signals over decadal timescales ($\Delta T \approx 0.1$ K per decade), which fundamentally requires stable sensor data records (SDRs) with high calibration accuracy. Routine monitoring of sensor calibration stability is facilitated via the validation of retrieved geophysical state parameters (i.e., SDRs, environmental (EDRs) and climate data records (CDRs)), which includes assessments of both absolute accuracy and precision with respect to independent reference measurements.

Special Issue

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THANK YOU! QUESTIONS?