Title – NOAA PSL Thermodynamic profiles from infrared spectrometers retrieved with TROPoe

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1.0 Data Set Description

This dataset contains daily files with thermodynamic profiles retrieved with the optimal estimation physical retrieval TROPoe (TROPoe, Turner and Löhnert 2014; Turner and Blumberg 2019; Turner and Löhnert 2021). The profiles are retrieved every 10 min from instantaneous radiances observed with an infrared spectrometer (IRS). The IRS are Atmospheric Sounder Spectrometer by Infrared Spectral Technology (ASSIST, Rochette et al. 2009) and manufactured by LRTech. They were deployed during the Propagation, Evolution and Rotation in Linear Storms (PERiLS) experiment in Columbia, LA, and Courtland, AL. The IRS are operated continuously between the middle of February 2022 and the middle of May 2023.

The spectral bands used in the retrieval are in the wavenumber range from 612 - 905.4 cm-1 and are specified in Turner and Löhnert (2021). Additional input data in TROPoe are cloud base height from a collocated ceilometer, temperature, water vapor mixing ratio, and pressure from collocated near-surface measurements, from hourly virtual temperature profiles measured by collocated Radio Acoustic Sounding System (RASS), and from hourly analysis profiles from the operational Rapid Refresh (RAP, Benjamin et al. 2021) weather prediction model at the closest grid point. The latter are used only outside the atmospheric boundary layer (ABL) above 4 km above ground level (AGL) and provide information in the middle and upper troposphere where little to no information content is available from the infrared radiances. The RASS were associated with a 915 MHz radar wind profiler. In Courtland, a second RASS was associated with a 449 MHz radar wind profiler. The inclusion of RASS and RAP were both shown to improve the retrieval accuracy (Djalalova et al. 2022, Bianco et al. 2024).

In addition to these temporally resolved input data, TROPoe requires an a priori dataset (prior) which provides mean climatological estimates of thermodynamic profiles and specifies how temperature and humidity covary with height as an input (for details see e.g. Djalalova et al. 2022). The prior is a key component of the retrieval and provides a constraint on the ill-posed inversion problem. For this study, we computed the prior from operational radiosondes launched at Shreveport, LA, for the retrievals at Columbia and at Birmingham, AL, for the retrievals at Courtland.

- Data status: Final
- Time period:

Columbia, LA: 9 February 2022 – 20 May 2023
Courtland, AL: 11 February 2022 – 18 May 2023

- Physical location:
  Columbia, LA: 32.124322 N, 92.055569 W, 20 m above mean sea level
  Courtland, AL: 34.66 N, 87.35 W, 187 m above mean sea level
- Data Frequency: continuous every 10 min
- Data set restrictions: none

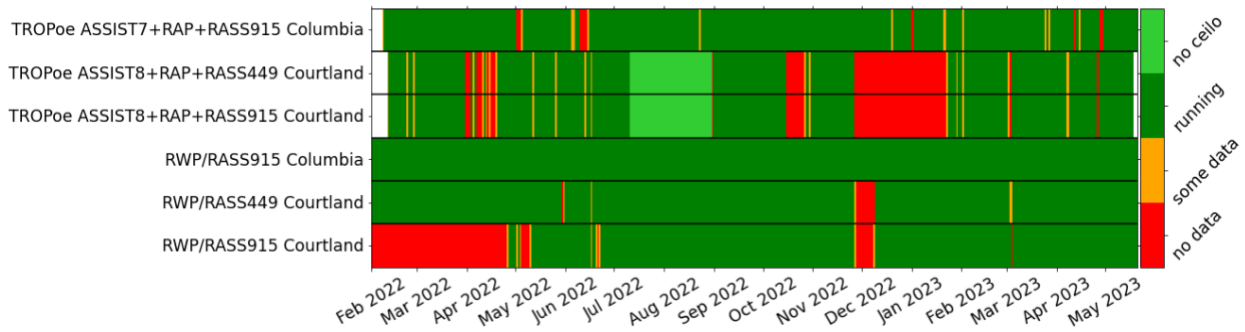
2.0 Instrument Description

The IRSs are passive spectrometers that receive downwelling infrared radiation between the wavelengths of 3.3 and 19 μm (520-3000 cm^{-1}) at a spectral resolution of about 0.5 wavenumber (Knuteson et al. 2004a,b). The instruments have a hatch that closes during precipitation events to protect the fore optics, which inhibits measurements during rain or snow.

3.0 Data Collection and Processing

Data are collected continuously. The infrared radiances were noise filtered using a principal component analysis before being used as input to TROPoe (Turner and Blumberg, 2019) using the software package IRS-Noise-Filter (https://github.com/OAR-atmospheric-observations/IRS-Noise-Filter). In TROPoe, we applied a spectral calibration factor determined from a clear-sky radiosonde launch in February 2022 (Knuteson et al. 2004b).
We used the TROPoe version 0.13 (available from DockerHub as davidturner53/tropoe/v0.13). This version includes recent improvements that helps with increasing valid solution availability (Adler et al. 2024) in very humid environments such as the south-eastern United States.

The following schematic displays availability of TROPoe retrievals at Courtland and Columbia. Dark green means that TROPoe retrievals were available during at least 50 % of the day. Data gaps are related to power failures and AC and instrument issues or to periods when the hatch was closed. Red means that no data were available at all and yellow means that less than 50 % of data were available on a specific day. At Courtland, a weed vine was partially blocking the ceilometer window reducing the backscatter signal, between July 10 and August 30 2022 (light green). Because of this, the automatic cloud base height detection in CL-view hardly detected any cloud bases during this period. This means that the default cloud base height was used in the TROPoe retrievals and cloudy profiles are not recommended for use without careful inspection during this period. Suggestions for filtering are given below to assure the use of high-quality data only.
RASS data were included in the TROPoe retrieval when available. The availability of RASS data (RASS915 and RASS449 at Courtland and RASS915 at Columbia) is given in the last three rows of the schematic. For example, the RASS915 at Courtland was not operational until the end of April 2022. For the advanced user, information on data which are used in the observation vector as input to the retrieval are included in the variables obs_flag, obs_dimension, obs_vector, and obs_vector_uncertainty in the TROPoe netcdf output files.



4.0 Data Format

The daily files are in netcdf format and the file naming conventions for the files are as follows:
clbtropoeASSIST7_RAP_RASS915.final_v2.yyyymmdd.HHMMSS.cdf
ctdtropoeASSIST8_RAP_RASS915.final_v2.yyyymmdd.HHMMSS.cdf
ctdtropoeASSIST8_RAP_RASS449.final_v2.yyyymmdd.HHMMSS.cdf

with
yyyy: Year
mm: Month
dd: Day
HH: Hour
MM: Minute
SS: Second

The time stamp of all data is in UTC and HHMMSS indicate the time of the first retrieved profile of the day. The netcdf file contain a larger number of diagnostic variables that can be used by the experienced TROPoe user to assess details of the retrieved profiles. For most users the following variables are sufficient:

Name	Dimension	Unit
base_time	Single value	Seconds (since 00 UTC 1 Jan 1970)
time_offset	Time	Second (since base_time)
hour	Time	Hours since 00UTC this day
height	Height	km AGL
temperature	Time, Height	C, temperature
waterVapor	Time, Height	g/kg, water vapor mixing ratio
theta	Time, Height	K, potential temperature
lwp	Time	g/m^2, Liquid water path
pressure	Time, Height	hPa, pressure
rh	Time, Height	%, relative humidity
dewpt	Time, Height	C, dew point temperature
thetae	Time, Height	K, equivalent potential temperature
sigma_temperature	Time, Height	C, 1-sigma uncertainty temperature
sigma_waterVapor	Time, Height	g/kg, 1-sigma uncertainty water vapor
cdfs_temperature	Time, Height	cumulative degrees of freedom for temperature

cdfs_waterVapor	Time, Height	Cumulative degrees of freedom for water vapor
gamma	Time	Gamma parameter
rmsa	Time	Root mean square error between observation vector and the forward calculation

Bold variables are the main retrieved meteorological variables, from which the other variables are derived.

Note that the vertical resolution of the retrieved profiles decreases with height, because of the broadening of the weighting function as a function of height. Thus, there are relatively few independent pieces of information in the profiles, this is reflected in the cumulative degree of freedom variables. The majority of the information from the IRS is in the lowest 2-3 km, above that most information comes from the RAP model.

To assure that only high-quality thermodynamic profiles are used, the following quality control steps are recommended. The thresholds given here are rather strict and it might be desirable for some case study to relax the thresholds for higher data availability, e.g. not all cloudy profiles with higher LWP are suspicious and data below cloud base may still be good.

1. RMSA filter: Large RMSA values indicate a large discrepancy between the solution and the observations, even though the retrieval found a solution. We suggest to only use profiles with rmsa < 3.
2. Gamma filter: The scalar γ is used to stabilize the retrieval when iteration number is small. It is a function of iteration number and cycles through a fixed sequence of integer values ranging from 1000 to 1. It decreases to unity for larger n and is used to change the relative weight between the prior information and the observation, where $\gamma > 1$ corresponds to less information from the observations relative to the prior (more details are provided in Turner and Löhnert, 2014). We suggest to use profiles with gamma =1.
3. LWP filter: Because of strong emission in the infrared from clouds, clouds strongly impact the ability to retrieve profiles from the IRS. For a statistical analysis, we suggest to only use profiles with LWP < 8 g/m2. For the analysis of individual days, thresholds of 50 g/m2 or even more may be acceptable (more details in Turner 2007).

5.0 Data Remarks

None

6.0 References

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7.0 Appendix

GCMD keywords

EARTH SCIENCE	SPECTRAL/ENGINEERING	INFRARED WAVELENGTHS	INFRARED RADIANCE			69f475b6-42af-4822-ae57-6c8fd8ebad4a