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ARM data-oriented metrics and diagnostics package for climate model evaluation version 3 (ARM-DIAGS-V3)

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ARM data-oriented metrics and diagnostics package for climate model evaluation (ARM- DIAGS) version 3

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1. Introduction

A Python-based metrics and diagnostics package is currently being developed by the ARM Infrastructure Team at Lawrence Livermore National Laboratory to facilitate the use of long-term high frequency measurements from the ARM program in evaluating the regional climate simulation of clouds, radiation, precipitation, and aerosols. This metrics and diagnostics package computes climatological means of targeted climate model simulation and generates tables and plots for comparing the model simulation with ARM observational data. The CMIP model data sets are also included in the package to enable model inter-comparison as demonstrated in Zhang et al. (2018) and Zhang et al. (2020). The mean of the CMIP model can be served as a reference for individual models.

Basic performance metrics are computed to measure the accuracy of mean state and variability of climate models. The evaluated physical quantities include cloud fraction, temperature, relative humidity, cloud liquid water path, total column water vapor, precipitation, sensible and latent heat fluxes, aerosol optical depth, and radiative fluxes, with plan to extend to more fields, such as the evaluation of model simulated aerosol physicochemical properties and cloud microphysics properties. Process-oriented diagnostics focusing on aerosol, cloud, and precipitation-related phenomena are also being developed for the evaluation and development of specific model physical parameterizations. In addition to the Southern Great Plains (SGP), North Slope of Alaska (NSA) and Tropical Western Pacific (TWP) atmospheric observatories in the ARM-DIAGS version 2.0, the version 3.0 package have extended to the data collected at the ARM Eastern North Atlantic (ENA) atmospheric observatory and the Observation and Modeling of the Green Ocean Amazon (GOAMAZON) field campaign.

The metrics and diagnostics package are currently built upon standard Python libraries and additional Python packages developed by DOE (CDAT). The ARM metrics and diagnostic package is available publicly with the hope that it can serve as an easy entry point for climate modelers to compare their models with ARM data.

In this report, we first provide an overview of major metrics in section 2. The input data, which constitutes the core content of the metrics and diagnostics package, is summarized in section 3. A user's guide documenting the workflow/structure of the version 3.0 codes and including step-by-step instruction for running the package is described in section 4.

2. Overview of metrics in ARM-DIAGS

The standard metrics and diagnostics included in the ARM-DIAGS version 2.0 are summarized in Zhang et al. (2020), which covers basic climate variability, diurnal and seasonal cycle, as well as statistics that enables process level studies. Particularly, the convection onset statistics, which quantifies robust relationships between precipitation, column water vapor (CWV) and temperature, has been added to the ARM-DIAGS as the first suit of process-oriented diagnostics. This module allows users to compare diagnostics for the behavior of deep convection from ARM observations to model outputs.

One of the most important enhancements in the ARM-DIAGS version 3.0 is the implementation of metrics and diagnostics on the aerosol-cloud interactions (ACI). Statistical metrics, such as the annual cycle of aerosol optical depth (AOD), aerosol and cloud condensation nuclei (CCN) number concentrations, and aerosol chemicals (organic, sulfate, nitrate, etc.) are developed and currently available in the ARM-DIAGS version 3.0. Moreover, the aerosol-CCN activation metrics, which is process-oriented, are also created. Through quantifying the statistical relationship between the aerosol and CCN number concentration at certain supersaturation levels, this module provides a feasible tool for quick assessment of the aerosol activation parametrization in models as well as a solid entrance point for the further assessment on the simulated aerosol indirect effects.

A full list of metrics and diagnostics are as follows, with detailed information summarized in Table 1:

- a set of basic metrics tables: mean, mean bias, correlation and root mean square error based on the annual cycle of each variable.
- line plots and Taylor Diagrams (Taylor, 2001) for annual cycle variability of each variable.
- contour and vertical profiles of annual cycle and diurnal cycle of cloud fraction.
- line and harmonic dial plots (Covey et al. 2016) of diurnal cycle of precipitation.
- probability density function (PDF) plots of precipitation (Pendergrass & Hartmann, 2014).
- convection onset metrics showing the statistical relationship between precipitation rate and column water vapor (Schiro et al. 2016).
- aerosol-CCN activation metrics describing the percentage distributions of how many aerosols can be activated as CCN under certain supersaturation levels (Zheng et al., 2020).

Table 1. A list of metrics and diagnostics available in the ARM-DIAGS version 3.0

Basic Diagnostics Sets	Input Variables	Available Sites
Statistical summary of mean state (annual cycle, Taylor diagram)	<p><i>Aerosol properties:</i> CCN number concentration at 0.2% & 0.5% supersaturations*; Aerosol number concentration*; Aerosol chemical component mass concentrations*.</p> <p><i>Column properties:</i> Cloud fraction; Cloud optical depth*; Column precipitable water vapor; Aerosol optical depth.</p> <p><i>Surface properties:</i> Latent & sensible heat fluxes; Relative humidity; Temperature; Precipitation; Downwelling shortwave & longwave fluxes; Upwelling shortwave & longwave fluxes; Soil Moisture**.</p>	SGP C1; NSA C1; ENA C1; TWP C1, C2, C3; MAO M1

Vertical variabilities	Cloud Fraction	SGP C1; NSA C1; ENA C1; TWP C1, C2, C3; MAO M1
Diurnal and seasonal variabilities	Precipitation	SGP C1; ENA C1; TWP C1, C2, C3; MAO M1
Process-oriented Diagnostics Sets	Input Variables	Available Sites
Convection onset	Column precipitable water vapor & Surface precipitation (hourly)	SGP C1; ENA C1; TWP C1, C2, C3; MAO M1
Aerosol-CCN activation	Aerosol & CCN number concentrations (5-min)	SGP C1; ENA C1;

*Variables available at SGP C1 & ENA C1 only.

** Variables available at SGP C1 only.

3. Observations and Model Data Description

3.1 Observation Data Sets

The observations used to assess model performance primarily rely on the ARM Best Estimate (ARM-BE) data products (Xie et al. 2010) and other ARM value-added products (VAPs) (<https://www.arm.gov/capabilities/vaps>), which are available for all the ARM permanent research sites and some ARM mobile facilities. These data often rely on measurements at the ARM Central Facility (CF) locations (i.e., single point measurements). To improve model-observation comparison, the ARM long-term continuous forcing data derived based on a constrained variational analysis (VARANAL, Xie et al. 2004; Tang et al., 2019), which represents an average over a Global Climate Model (GCM) grid box, is also used when it is available. To derive the ACI metrics and diagnostics, here, we carefully processed, and quality controlled the data collected from the condensation particle counter (CPC), cloud condensation nuclei particle counter (CCN), aerosol chemical speciation monitor (ACSM), and multifilter rotating shadowband radiometer (MFRSR) at the SGP and ENA sites.

The detailed information about ARM data used in the ARM-DIAGS package is listed in Tables 2a and 2b. The observational data product consists of hourly averaged, diurnal cycle, monthly means or climatological summaries of the measured quantities, with variable names, units and vertical dimensions remapped to CMIP convention. They are currently available for the SGP, NSA, ENA, GO AMAZON Manacapuru site (MAO), and the TWP Manus, Nauru, and Darwin sites. Other than the ARM observations, ARM-DIAGS also includes simulation data from models participating CMIP5 and CMIP6 project, which will

allow climate-modeling groups to compare a new candidate version of their model to existing CMIP models.

Table 2a. Observational references using the ARM long-term continuous forcing dataset (VARANAL) at ARM SGP.

Quantities	ARM Data Products	Data Source/ Instruments	Time resolution	Spatial info
Surface Screen-Level Temperature/ Humidity	VARANAL	Surface Meteorological Observation System (SMOS), Oklahoma and Kansas mesonet stations (OKM and KAM) [Xie et al. 2004]	mon, day, hr	domain averaged
Temperature/Humidity profile/wind speed/large scale tendencies	VARANAL	NOAA/ NCEP Rapid Update Cycle (RUC) analysis data [Xie et al. 2004]	mon, day, hr	domain averaged
Surface Precipitation	VARANAL	Arkansas-Red Basin River Forecast Center (ABRFC) Nexrad radar precipitation estimates w/ rain gauge	mon, day, hr	domain averaged
Precipitable Water	VARANAL	Microwave Radiometer (MWR) water liquid & vapor along line of sight (LOS) path (MWRLOS)	mon, day, hr	domain averaged
Surface All Sky Radiative Fluxes	VARANAL	Data Quality Assessment for ARM Radiation Data (QCRAD) [Long and Shi, 2006, 2008]	mon, day, hr	domain averaged
Surface Latent/Sensible Heat	VARANAL	Best-Estimate Fluxes from EBBR Measurements and Bulk Aerodynamics Calculations (BAEBBR) [Cook and Sullivan, 2019] & Quality Controlled Eddy Correlation Flux Measurement [Cook and Sullivan, 2020]	mon, day, hr	domain averaged

*Time ranges for the ARM SGP C1 site is 2004-2015. All related data have been processed and quality controlled at 1-hour temporal resolution.

Table 2b. Observational references using the ARMBE and other VAP data at multiple ARM sites.

Quantities	ARM Data Products	Data Source/ Instruments	Time resolu	Spatial info
Cloud Fraction*	ARSCL	Active Remote Sensing of Clouds [Clothiaux et al, 2001]	mon, day, hr	SGP C1; NSA C1; ENA C1; TWP C1, C2, C3; MAO M1
Aerosol Optical Depth 550nm*	MFRSRAOD 1MICH	Multifilter Rotating Shadowband Radiometer (MFRSR) [Knootz et al.,2013]	mon	SGP C1 & E13 average; NSA C1; ENA C1; TWP C1, C2, C3; MAO M1
Surface Screen-Level Temperature/ Humidity*	ARMBEAT M	ARM-standard meteorological instrumentation at the surface [Xie et al. 2010]	mon	NSA C1; ENA C1; TWP C1, C2, C3; MAO M1

Surface Precipitation*	ARMBEAT M	Same as above	mon, hr	ENA C1; TWP C1, C2, C3; MAO M1
Precipitable Water*	ARMBEAT M	Microwave Radiometers Retrievals (MWRRET) [Xie et al. 2010]	mon, hr	NSA C1; ENA C1; TWP C1, C2, C3; MAO M1
Surface Radiative Fluxes*	ARMBECLD	Data Quality Assessment for ARM Radiation Data (QCRAD) [Long and Shi, 2006, 2008]	mon	NSA C1; ENA C1; TWP C1, C2, C3; MAO M1
Surface Latent/Sensible Heat*	QCECOR	Quality Controlled Eddy Correlation Flux Measurement [Cook and Sullivan, 2020]	mon	NSA C1; ENA C1; TWP C1, C2, C3; MAO M1
Surface Soil Moisture Content (10 cm)*	SWATS	Soil Water and Temperature System (SWATS) [Cook, 2018]	mon	SGP domain averaged
Cloud Optical Depth*	MFRSRCLD OD1MIN	Multifilter Rotating Shadowband Radiometer (MFRSR) [Knootz et al., 2013]	mon	SGP C1; ENA C1
Cloud Condensation Nuclei**	CCN1COL	Cloud Condensation Nuclei Counter (CCNC) [Uin, 2016]	mon, 5-min	SGP C1; ENA C1
Aerosol Number Concentration**	CPC	Condensation Particle Counter (CPC) [Kuang, 2016]	mon, 5-min	SGP C1; ENA C1
Aerosol Chemical Component**	ACSM	Aerosol Chemical Speciation Monitor (ACSM) [Watson, 2017]	mon, 5-min	SGP C1; ENA C1

*Time ranges for the ARM sites are: SGP C1 (2004-2015); NSA C1 (2001-2016); ENA C1 (2016-2019); TWP C1 (1998-2009), C2 (1999-2010), C3 (2003-2010); MAO M1 (2014-2015). All related data have been processed and quality controlled at 1-hour temporal resolution.

**Aerosols, CCN and COD data at SGPC1 ranged from 2011-2016, while at ENAC1 ranged from 2016-2019; CMIP simulation counterparts are not yet available. All related data have been processed and quality controlled at 5-min temporal resolution.

3.2 CMIP5 and CMIP6 AMIP Simulations

Simulations of 23 models contributing to the CMIP5 [Taylor et al., 2012] and the CMIP6 [Eyring et al., 2016] multi-model experiments have been used (see Table 3 for details). We evaluate these models from the CMIP atmospheric only (AMIP) experiments from year 1979 to 2008. The nearest model grid points to the ARM central facilities are selected. The CMIP6 simulations are set as default in the ARM-DIAGS version 3.0.

Table 3. CMIP5 and CMIP6 Models used in the evaluation

Modeling groups	CMIP5 Model Name	CMIP6 Model Name
Commonwealth Scientific and Industrial Research Organization; Bureau of Meteorology (BOM), Australia	ACCESS-1-0 ACCESS-3-0	ACCESS-ESM1-5
Beijing Climate Center, China Meteorological	BCC-CSM-1-1	BCC-CSM2-MR

Administration, China	BCC-CSM-1-1(m)	
College of Global Change and Earth System Science, Beijing Normal University, China	BNU-ESM	
Chinese Academy of Meteorological Sciences, China		CAMS-CSM1-0
Canadian Centre for Climate Modelling and Analysis, Canada	CanAM4	CanESM5
National Center for Atmospheric Research, USA	CCSM4	
Community Earth System Model Contributors	CESM1-CAM5	CESM2 CESM2-WACCM
Centro Euro-Mediterranean Centre on Climate Change, Italy	CMCC-CM	CMCC-CM2-SR5
Centre National de Recherches Météorologiques, France	CNRM-CM5	CNRM-CM6-1-HR
Commonwealth Scientific and Industrial Research Organization; Queensland Climate Change Centre of Excellence, Australia	CSIRO-Mk3-6-0	
Energy Exascale Earth System Model Contributors		E3SM-1-0
European Centre for Medium-Range Weather Forecasts	EC-Earth	EC-Earth3-AerChem
State Key Laboratory of Numerical Modeling for Atmospheric Sciences and Geophysical Fluid Dynamics, Institute of Atmospheric Physics, Chinese Academy of Sciences; Center for Earth System Science, Tsinghua University, China	FGOALS-g2 FGOALS-s2	FGOALS-f3-L
NOAA Geophysical Fluid Dynamics Laboratory, USA	GFDL-HIRAM-C360 GFDL-HIRAM-C180	GFDL-CM4
NASA Goddard Institute for Space Studies, USA	GISS-E2-R	GISS-E2-1-G
Met Office Hadley Centre, UK	HadGEM2-A	HadGEM3-GC31-L
Institute Pierre-Simon Laplace, France	IPSL-CM5A-LR IPSL-CM5B-LR IPSL-CM5A-MR	IPSL-CM6A-LR
Centre for Climate Change Research, Indian Institute of Tropical Meteorology, India		IITM-ESM
Institute for Numerical Mathematics, Russia	INM-CM4	INM-CM5-0
National Institute of Meteorological Sciences; Korea Meteorological Administration, Korea		KACE-1-0-G
Atmosphere and Ocean Research Institute; National Institute for Environmental Studies; and Japan Agency for Marine-Earth Science and Technology, Japan	MIROC5	MIROC6
Max Planck Institute for Meteorology, Germany	MPI-ESM-LR MPI-ESM-MR	MPI-ESM1-2-HAM MPI-ESM1-2-HR
Meteorological Research Institute, Japan	MRI-AGCM-3-2 MRI-CGCM-3	MRI-ESM-2-0
Earth System Modeling Center, Nanjing University of Information Science and Technology, China		NESM3
Norwegian Climate Centre, Norway	NorESM1-M	NorESM2-LM
Research Center for Environmental Changes, Academia Sinica, Taiwan, China		TaiESM1

*Note that for certain quantities, especially for sub-monthly output variables; only subsets of models are available for analysis.

3.3 Data Limitation/Uncertainty

The ARM data used in the package have been gone through stringent data quality control and are representing the "best" estimate of the selected quantities. Fully addressing data uncertainty is a challenging task and ARM is making efforts to address this issue. More information will be provided once the uncertainty of these selected fields is better quantified. We recommend the user to read the references on the observational data products and contact PIs of each data product for additional data quality information.

4. User's Guide

4.1 Package Overview / Workflow

Figure 1 illustrates the flowchart of creating the diagnostic results by applying the diagnostics tool. The steps are straightforward. the step-by-step procedure to set-up a working prototype is presented in section 3.

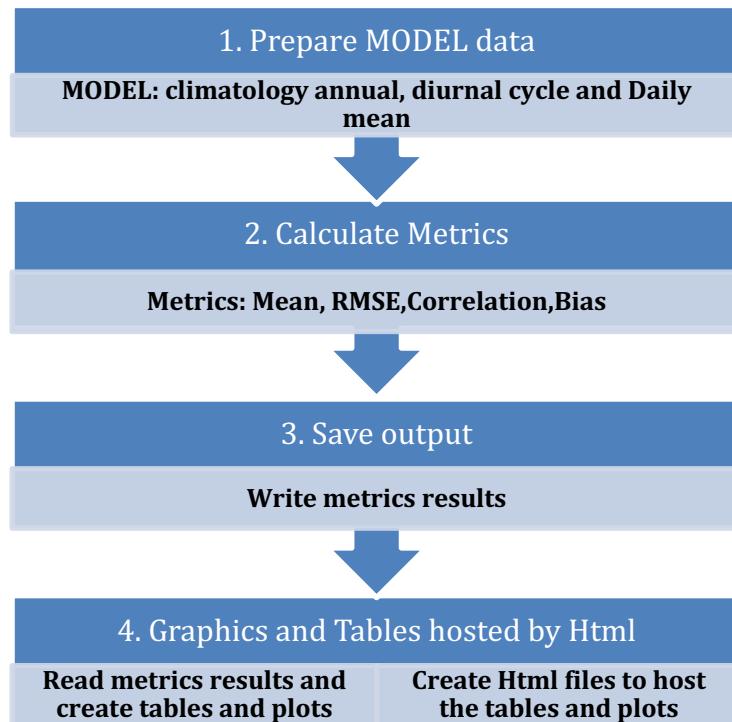


Figure 1. Work flow of the diagnostics package

The project has the following structure:

```

a |____ arm_diags
| |____.DS_Store
| |____ init__.py
| |____ arm_driver.py
| |____ arm_parameter.py
| |____ arm_parser.py
| |____ basicparameter.py
| |____ diags_all_multisites_for_cmip5.json
| |____ diags_all_multisites_for_cmip6.json
| |____ examples
| | |____ [example json files for different running tasks]
| |____ misc
| | |____ ARM_DIAGS_logo.png
| | |____ ARM_logo.png
| | |____ [multiple figures for webpage illustrations]
| |____ src
| | |____ init__.py
| | |____ aerosol_activation.py
| | |____ annual_cycle.py
| | |____ annual_cycle_aci.py
| | |____ annual_cycle_zt.py
| | |____ convection_onset_driver.py
| | |____ convection_onset_statistics.py
| | |____ create_htmls.py
| | |____ diurnal_cycle.py
| | |____ pdf_daily.py
| | |____ seasonal_mean.py
| | |____ taylor_diagram.py
| | |____ utils.py
| | |____ varid_dict.py
| | |____ convection_onset_driver.py
| | |____ convection_onset_statistics.py
| |____ ARM_DIAGS_TechReport_v3.docx

```

4.2 Obtain ARM-DIAGS

ARM-DIAGS version 3.0 with basic sets of diagnostics is now publicly available. The data files including observation, and CMIP5 and CMIP6 model data are available through ARM archive. The analytical codes to calculate and visualize the diagnostics results are placed via repository (arm-gcm-diagnostics) at <https://github.com/ARM-DOE/arm-gcm-diagnostics>

For downloading data:

- Click www.arm.gov/data/data-sources/adcme-123
- Following the **Data Directory** link on that page, it will lead to the area that the data files are placed. A short registration is required if you do not already have an ARM account.
- DOI for the citation of the data is 10.5439/1646838

For obtaining codes:

```
$ git clone https://github.com/ARM-DOE/arm-gcm-diagnostics/
```

4.3 Set-up a test case

The software environment is managed through conda. Either Anaconda or Miniconda needs to be installed for setting up the environment of the package

1. First to create a conda environment and then activate it:

```
$ conda create -n arm_diags_env_py3 cdp cdutil cdms2 libcdms matplotlib scipy
python=3 -c conda-forge
$source activate arm_diags_env_py3
```

2. To install the package, cd <Your directory>/, type following:

```
$python setup.py install
```

3. A working test case has been set up for the users to run the package out-of-the-box. In this case, all the observation, CMIP data, test data should be downloaded placed under directoris:

```
<Your directory>/arm_diags/observation
<Your directory>/arm_diags/cmip6
<Your directory>/arm_diags/testmodel, respectively.
```

4. To configure basic parameter file: basicparameter.py and edit parameters such as, input and output paths, model name (used to search the file), and case name (to create a new folder for the case).

5. To run the package, simply type in the terminal the following:

```
$ python arm_driver.py -p basicparameter.py
```

6. To view the diagnostics results:

For Mac OS:

```
$ open <User defined output directory>/html/ARM_diag.html
```

For Linux:

```
$xdg-open <User defined output directory>/html/ARM_diag.html
```

For setting up customized runs and creating new cases, check details at:

<https://github.com/ARM-DOE/arm-gcm-diagnostics/>

4.4 Diagnostics examples

Below shows the main html page hosting the results:

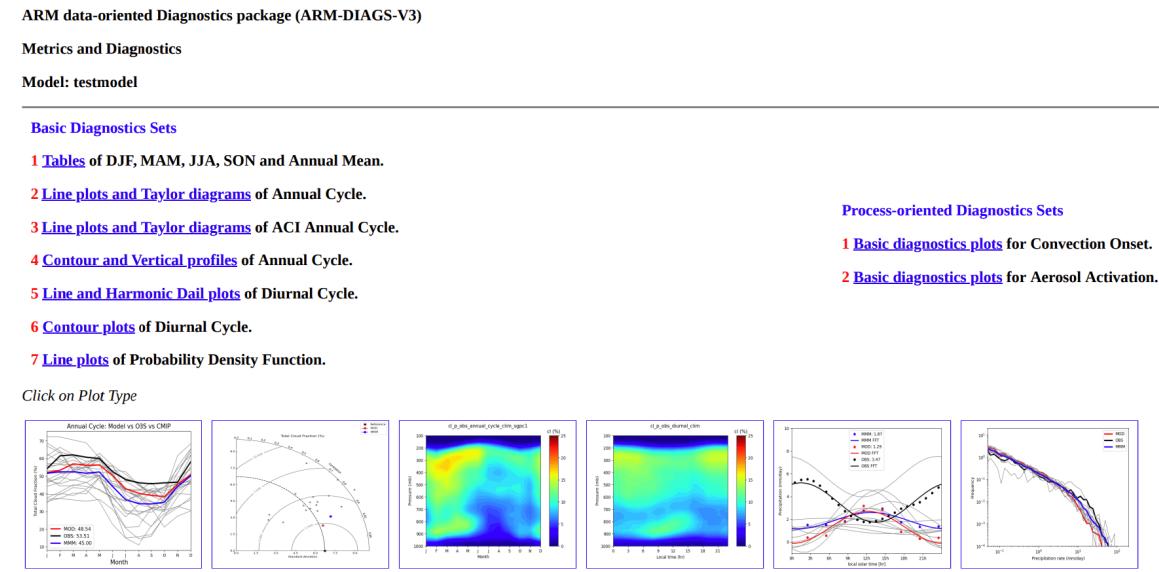


Figure 2. Main html page generated to host the diagnostic results

testmodel: ANN. Mean

Variables	Model	Obs	Model-Obs	CMIP6
Surface Temperature (C)	14.222	14.689	-0.467	17.108
Precipitation (mm/day)	2.058	2.346	-0.289	1.775
Total Cloud Fraction (%)	48.509	53.472	-4.964	44.96
Rel. Humidity (%)	63.02	66.094	-3.074	55.03
Sensible Heat Flux (W/m ²)	27.561	42.234	-14.673	39.345
Latent Heat Flux(W/m ²)	56.931	55.828	1.104	48.462
Upwelling LW (W/m ²)	390.813	394.03	-3.216	410.385
Downwelling LW (W/m ²)	319.408	332.95	-13.542	331.225
Upwelling SW (W/m ²)	42.498	41.675	0.824	38.412
Downwelling SW (W/m ²)	199.418	193.407	6.012	206.332
Surface Pressure (Pa)	96421.993	97111.059	-689.066	97228.305
Precipitable Water (mm)	18.86	22.05	-3.19	20.754
top 10 cm soil moisture content (mm)	21.645	28.924	-7.279	19.335
Aerosol Optical Depth	0.175	0.097	0.077	0.141

Figure 3. Tables summarizing annual mean climatology

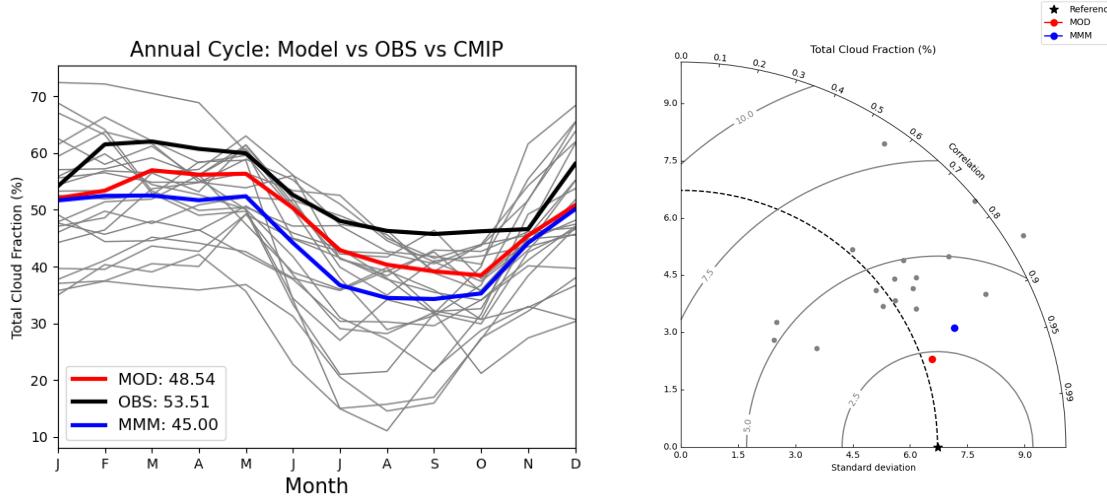


Figure 4. Line plots and Taylor diagrams for diagnosing annual cycle of cloud fraction. Black denotes observation, red denotes test model, blue denotes CMIP6 ensemble mean, and gray denotes CMIP6 individual model members.

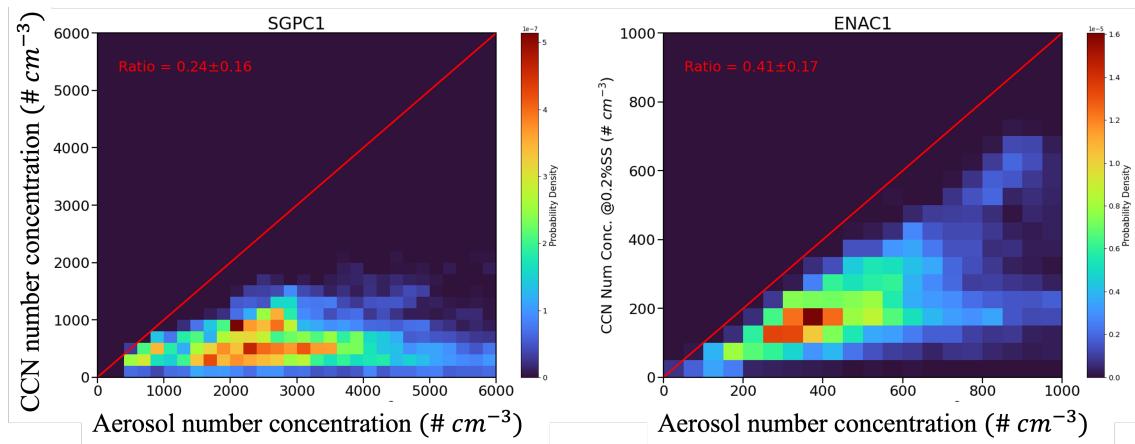


Figure 5. Probability density plots for aerosol number concentration (x-axis) versus CCN number concentration (y-axis) at 0.2% supersaturation level at the ARM SGP (left) and ENA site (right).

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