ESM Aerosol-Cloud Diagnostics Package (ESMAC Diags)

Version 1.0

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Abstract

This document describes the **version 1.0** of Earth System Model (ESM) aerosol-cloud diagnostics package (**ESMAC Diags**) that facilitate routine evaluation of aerosols, clouds and aerosol-cloud interactions simulated by the Department of Energy's (DOE) Energy Exascale Earth System Model (E3SM). The first version focuses on comparing simulated aerosol properties with in-situ aircraft, ship and surface measurements. Various types of diagnostics and metrics are performed for aerosol number, size distribution, chemical composition, and CCN concentration to assess how well E3SM represents observed aerosol properties and aerosol-cloud interactions across spatial scales. Metrics for various meteorological and aerosol precursor quantities from the same field campaigns are also included. As a technical documentation, this document will describe the structure of the diagnostics package, included field campaign measurements as well as the instruction of how to run or modify this package. The diagnostics package is coded and organized in a way that can be easily extended to other field campaign datasets and adapted to higher-resolution model simulations for user need.

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Field campaigns and observations

The diagnostics package initially focuses on four geographical regions: Eastern North Atlantic (ENA), Northeastern Pacific (NEP), Central U.S. (CUS, where the ARM Southern Great Plains, SGP, site is located in), and Southern Ocean (SO), where liquid clouds occur frequently and extensive measurements are available from ARM and other agencies. Aerosol properties also vary among these regions. Among the four testbeds, ENA, NEP and CUS are regions typically have high effective radiative forcing (ERF) associated with aerosol-cloud-radiation interactions, while SO is a remote region with more pristine conditions characterized by low ERF, which serves a good contrast to the other three testbeds. Six field campaigns from these four testbeds are selected in the initial phase of ESMAC Diags (Table 1). HI-SCALE and ACE-ENA are based on long-term ARM ground sites with aircraft field campaign sampling within a few hundred kilometers around the sites. Aircraft sampling during HI-SCALE and ACE-ENA occurred below, within, and above shallow clouds forming at the top of the convective and marine boundary layers, respectively. CSET and MAGIC are field campaigns with aircraft and ship platforms, respectively, that sample transects between California and Hawaii characterized by transitions between stratocumulus to cumulus dominated regions. SOCRATES and MARCUS are field campaigns with aircraft and ship platforms, respectively, based out of Hobart, Australia. Aircraft transects during SOCRATES extended south to around 60°S, while ship transects during MARCUS extended southwest from Hobart to Antarctica. The aircraft (black) and ship (red) tracks for these field campaigns are shown in Figure 1.

The instruments and measurements used in ESMAC Diags version 1 are listed in Tables 2 to 7. Each table corresponds to each field campaigns. Note that some instruments are only available for certain periods, so that model evaluation is limited by the availability of collected data. Currently the data are available through each individual DOI or link. In the future we will bundle them into one single DOI for easier download.

ESMAC Diags Structure

The diagnostics package is designed to be flexible so that additional field campaign measurements and functionality can be included in the future. The workflow of ESMAC Diags, illustrated in Figure 2, consists of four major components. The “scripts” directory contains executable scripts and user-specified settings. The “python” directory contains all source code including code used to preprocess model output, read files, merge aerosol size distributions, compute observed versus simulated statistical relationships, and plot results. All observational and model data are in the “data” directory and are organized by field campaign. The diagnostic

plots and statistics are put in the “figures” directory, also organized by field campaign. It is relatively straight-forward to add other field campaign datasets using this structure.

How to run ESMAC Diags.

1. **Get the code and download observation data**

The code of ESMAC Diags are available at GitHub: https://github.com/tangshuaiqi/ESMAC_Diags. Currently the directory “data” and “figures” are hyperlinks to keep the git code small. Users need to create their own “data” and “figures” location and update the links in the main directory. Users should also download the field campaign data and put into the “data” directory organized as shown in Figure 2 (e.g., SMPS data for HI-SCALE put in data/HI-SCALE/observed/surface/smps/). In the future we will bundle all observational data together for easier download.

2. **Get E3SM output**

Run E3SM and get output within field campaign regions in 1hr resolution. It should also include all aerosol-related variables for evaluation. A example of namelist in `user_nl_cam` in the E3SM running script is given below:

```
nhtfrq      = 0,-24,-3,-1
mfilt       = 1,1,8,24
               …     …       …
fincl4      = 'PS',       !! dynamical fields
              'U',        !! ..
              'V',        !! ..
              'T',        !! ..
              'Q',        !! vapor (kg/kg)
              'CLDLIQ',   !! cloud hydrometeors (kg/kg)
              'CLDICE',   !! ..
              'NUMLIQ',   !! ..
              'NUMICE',   !! ..
              'RAINQM',   !! ..
              'SNOWQM',   !! ..
              'NUMRAI',   !! ..
              'NUMSNO',   !! ..
              'PBLH',     !! PBL height
              'LHFLX',    !! energy fluxes
              'SHFLX',    !! ..
```

```
          'FLNT',     !! ..
          'FSNT',     !! ..
          'FLNS',     !! ..
          'FSNS',     !! ..
          'TREFHT',    !! ..
          'Z3',       !! geopotential height
          'RELHUM',    !! relative humidity (RH)
          'RHW',      !! RH with respect to water
          'RHI',      !! RH with respect to ice
          'RHICE',    !! RH before nucleation
          'RHCFMIP',   !! RH with respect to water above 273 K, ice below 273 K
          'CLOUD',    !! cloud fraction
          'AWNI',     !! in-cloud values
          'AWNC',     !! Average cloud water number conc (1/m3)
          'AQRAIN',    !! Average rain mixing ratio (kg/kg)
          'AQSNOW',    !! Average snow mixing ratio (kg/kg)
          'CCN1',     !! CCN concentration at S=0.1% (#/cm3)
          'CCN3',     !! CCN concentration at S=0.3% (#/cm3)
          'CCN5',     !! CCN concentration at S=0.5% (#/cm3)
          'AREI',     !! ..
          'AREL',     !! ..
          'FREQL',    !! frequency of cloud appearance
          'FREQI',    !! ..
          'FREQS',    !! ..
          'FREQR',    !! ..
          'PRECT',    !! precipitation
          'PRECC',    !! ..
          'PRECL',    !! ..
          'CDNUMC',    !! vertically-integrated droplet concentration (m-2)
          'CMELIQ',    !! rate of cond-evap of liq within the cloud (kg/kg/s)
          'DCQ',      !! Q tendency due to moist processes (kg/kg/s)
          'FICE',     !! ice mass fraction
          'IWC',      !! grid box average ice water content (kg/m3)
          'LWC',      !! grid box average liquid water content (kg/m3)
          'ICLDIWP',   !! in-cloud ice water path
          'ICLDTWP',   !! in-cloud total water path
          'TGCLDLWP',  !! liquid water path (including convective clouds)
          'TGCLDIWP',  !! ice water path (including convective clouds)
          'ICWNC',    !! prognostic in-cloud water number conc (m-3)
          'ICINC',    !! prognostic in-cloud ice number conc (m-3)
          'ICWMRST',   !! Prognostic in-stratus water mixing ratio (kg/kg)
          'ICIMRST',   !! Prognostic in-stratus ice mixing ratio (kg/kg)
          'AODVIS',    !! AOD
          'WP2_CLUBB', !! Vertical Velocity Variance (m2/s2)
```

```
          'DMS',      !!
          'SO2',      !!
          'H2SO4',    !!
          'bc_a1',    !! aerosols mass (kg/kg)
          'bc_a3',    !!
          'bc_a4',    !!
          'dst_a1',   !!
          'dst_a3',   !!
          'mom_a1',   !!
          'mom_a2',   !!
          'mom_a3',   !!
          'mom_a4',   !!
          'ncl_a1',   !!
          'ncl_a2',   !!
          'ncl_a3',   !!
          'pom_a1',   !!
          'pom_a3',   !!
          'pom_a4',   !!
          'so4_a1',   !!
          'so4_a2',   !!
          'so4_a3',   !!
          'soa_a1',   !!
          'soa_a2',   !!
          'soa_a3',   !!
          'num_a1',   !! aerosols number (#/kg)
          'num_a2',   !!
          'num_a3',   !!
          'num_a4',   !!
          'num_c1',   !! aerosols number (#/kg)
          'num_c2',   !!
          'num_c3',   !!
          'num_c4',   !!
          'dgnd_a01',  !! dry aerosol size
          'dgnd_a02',  !! ..
          'dgnd_a03',  !! ..
          'dgnd_a04',  !! ..
          'dgnw_a01',  !! wet aerosol size
          'dgnw_a02',  !! ..
          'dgnw_a03',  !! ..
          'dgnw_a04',  !! ..
          'EXTINCT',   !! Aerosol extinction (1/m)
          'AODABS',    !! Aerosol absorption optical depth 550 nm
          'ABSORB',    !! Aerosol absorption (1/m)
fincl4lonlat = '260e:265e_34n:39n',  ! SGP (~5x5 degs)
```

```
        '330e:335e_37n:42n',  ! ENA
        '202e:240e_19n:40n',  ! CSET
        '202e:243e_20n:35n',  ! MAGIC
        '60e:160e_42s:70s',   ! MARCUS
        '133e:164e_42s:63s',  ! SOCRATES
```

In a successful run, E3SM output files *.cam.h3.yyyy-mm-dd-00000.nc will contain hourly variables for each field campaign domain (e.g., “PS_ 260e_to_265e_34n_to_39n” for PS at SGP region).

3. Preprocessing:

Because of large size of hourly model output, we preprocess model output to extract the model variables at the surface site, along the flight tracks or along the ship tracks depending on what measurements are available for each field campaign. We also calculate aerosol size distribution from 1nm to 3000nm with 1nm increment in E3SM.

For some field campaigns (HI-SCALE and ACE-ENA), there are several instruments (e.g., FIMS, PCASP, OPC for aircraft, SMPS and nanoSMPS for ground) measuring aerosol size distribution over different size ranges. It is useful to merge these datasets to create a broader size distribution information. The aerosol concentrations in the “overlapping” bins measured by multiple instruments are weighted by the reliability of each instrument based on the knowledge of the instrument mentors. This is included in the preprocessing step.

To run the preprocessing code:

a. Enter scripts/ directory
b. Edit settings.py to setup the data paths. Campaign names, model labels and IOPs do not need to change since they will be overwritten by the .csh file
c. Edit scripts_preprocess.csh to choose the campaign names, model labels, IOPs and the types of preprocesses you want to perform.
d. Run scripts_preprocess.csh
e. Check data/*campaign*/model/ and data/*campaign*/obs/aircraft/merged_bin/ for the output data

an alternative way to run the preprocessing code is to run individual python code:

a. Enter python/preprocessing
b. Edit settings.py
c. Run the preprocessing code you want:

```
>> python prep_*.py
```

Plotting:

Currently, ESMAC Diags produces the following diagnostics and metrics:

For aircraft measurements:

- aircraft track maps.
- Timeseries of aerosol variables (total aerosol number concentration, size distribution of aerosol number, total composition, CCN number concentration) for each flight.
- mean aerosol size distribution for each field campaign or IOP.
- Percentiles of aerosol variables by height for each field campaign or IOP.
- Percentiles of aerosol variables by latitude for each field campaign or IOP.
- Vertical profile of cloud fraction, LWC and cloud droplet number concentration composite of aircraft measurements for each field campaign or IOP.
- Mean value, bias, RMSE and correlation of aerosol number concentration output as txt file

for surface measurements:

- Timeseries of aerosol variables (total aerosol number concentration, size distribution of aerosol number, total composition, CCN number concentration) for each field campaign or IOP.
- timeseries of aerosol size distribution for each field campaign or IOP.
- diurnal cycle of these surface measurements for each field campaign or IOP.
- mean aerosol size distribution for each field campaign or IOP.

- Pie/bar charts of observed and predicted aerosol composition averaged over each field campaign or IOP.
- Mean value, bias, RMSE and correlation of aerosol number concentration output as txt file.
- Timeseries of basic meteorological fields, time-height profile of cloud fraction.

For ship measurements:

- Ship track maps.
- Timeseries of basic meteorological fields, time-height profile of cloud fraction.
- Timeseries of aerosol variables (total aerosol number concentration, size distribution of aerosol number, total composition, CCN number concentration) for each ship trip
- timeseries of aerosol size distribution for each ship trip
- mean aerosol size distribution
- Percentiles of aerosol variables by latitude for each field campaign or IOP.
- Mean value, bias, RMSE and correlation of aerosol number concentration output as txt file.

To run the plotting code:

a. Enter scripts/ directory
b. Edit settings.py to setup the data paths. Campaign names, model labels and IOPs do not need to change since they will be overwritten by the .csh file
c. Edit scripts_plotting_jobsubmit.csh to choose the campaign names, model labels, IOPs and the types of figures you want to plot
d. Submit job:

```
>> sbatch scripts_plotting_jobsubmit.csh
```

e. Check figures/*campaign*/ for the figures

an alternative way to make plots is to run individual python code:

a. Enter python/plotting
b. Edit settings.py
c. Run the plotting code you want:

```
>> python xxx.py
```

Note: sometimes on certain servers there could be memory errors ("Bus error") for one or two .py files. This can be solved by running the code interactively (>>./scripts_***.csh or use the alternative way above). You can also download the package and run it in local machine. The observational data plus preprocessed model data from one simulation is less than 200GB for all six field campaigns.

The webpage of webpage/index.html provides an interface to look at the diagnostics plots. Users may also go to the subdirectories under figures/ to browse the plots and metrics.

Contact:

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Table 1. information of the field campaigns

Campaign name	Period	Measuring platform	Cloud/Aerosol properties	Reference
HI-SCALE	IOP1: 24 Apr – 21 May 2016 IOP2: 28 Aug – 24 Sep 2016	Ground, aircraft	Continental shallow cumulus clouds	(Fast et al. 2019)
ACE-ENA	IOP1: 21 Jun – 20 Jul 2017 IOP2: 15 Jan – 18 Feb 2018	Ground, aircraft	Marine PBL clouds	(Wang et al. 2021)
MAGIC	Oct 2012 – Sep 2013	Ship	Stratocumulus to cumulus transition	(Lewis and Teixeira 2015; Zhou et al. 2015)
CSET	1 Jul – 15 Aug 2015	Aircraft	Same as above	(Albrecht et al. 2019)
MARCUS	Oct 2017 – Apr 2018	Ship	Pristine region with low aerosol loading	(McFarquhar et al. 2021)
SOCRATES	15 Jan – 24 Feb, 2018	Aircraft	Same as above	(McFarquhar et al. 2021)

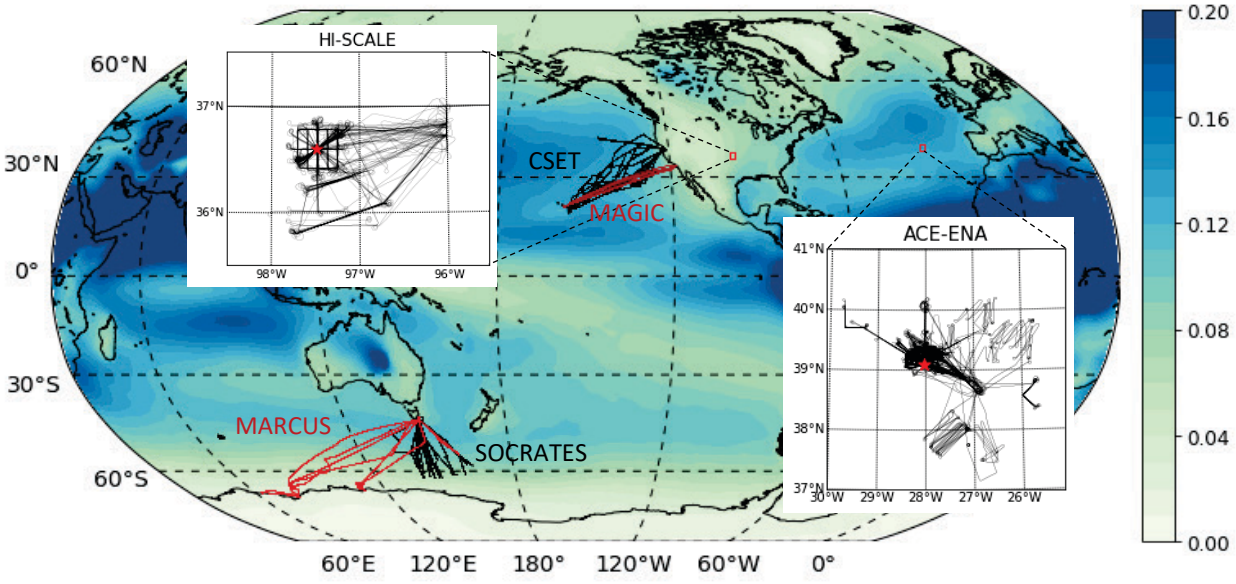

Figure 1. aircraft (black) or ship (red) tracks for the six field campaigns. Overlaid is aerosol optical depth at 550nm averaged from 2014 to 2018 simulated in EAMv1.

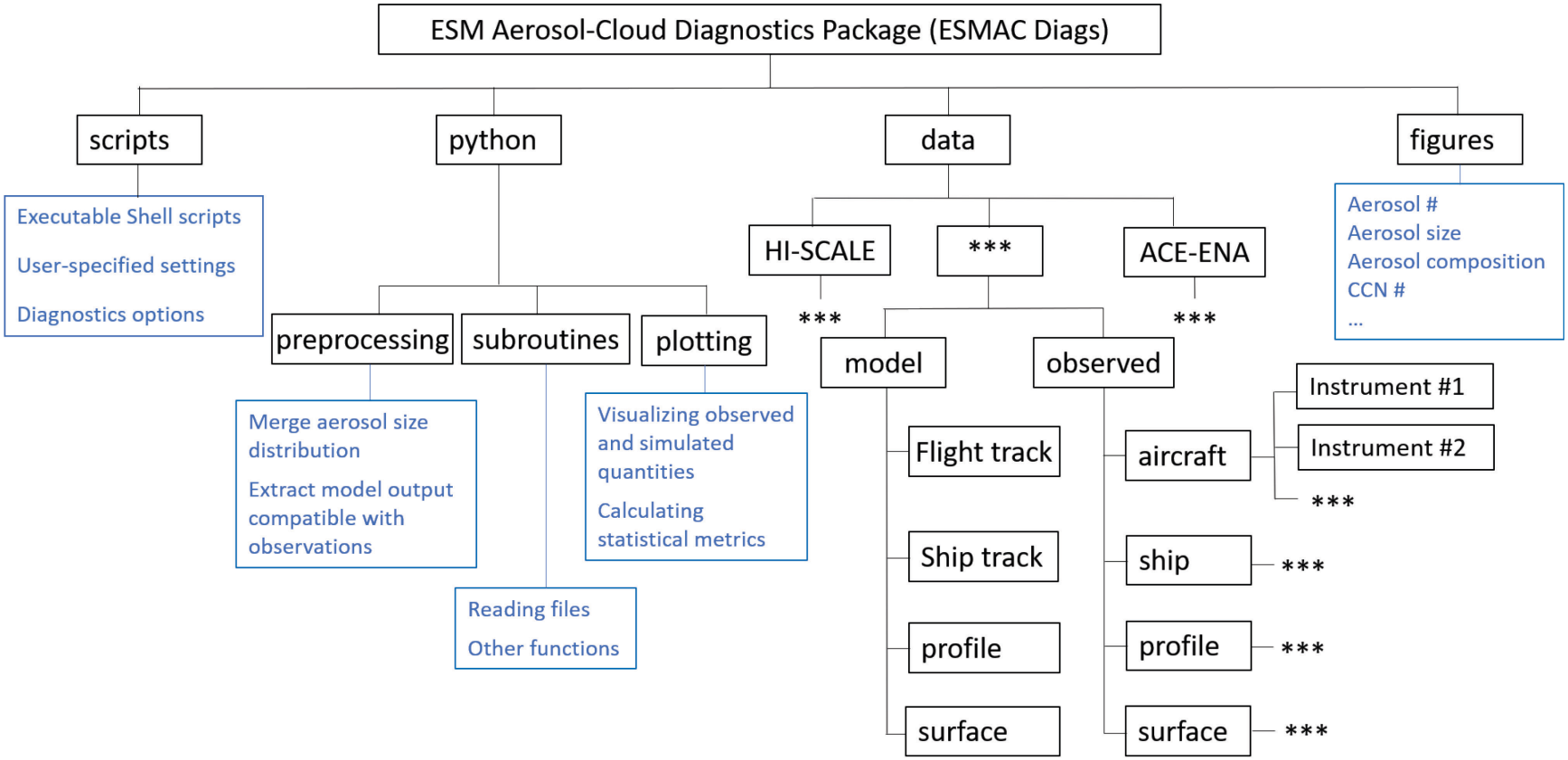

Figure 2: workflow of ESMAC Diags. Boxes in blue describe the functions or examples of the directory.

Table 2: Instruments for HI-SCALE

Platform	Instrument	Full name	Measurements	Particle diameter range	Datastream name	DOI or link
Ground	MET	Surface meteorology systems	Temperature, relative humidity, wind, pressure		sgpmetE13.b1	DOI: 10.5439/1786358
	SMPS	scanning mobility particle sizer	Aerosol size distribution	20-700 nm	sgpaossmpsS01.a1	DOI: 10.5439/1476898
	nanoSMPS	Nano scanning mobility particle sizer	Aerosol size distribution	2-150 nm	sgpaosnanosmpsS01.a1	DOI: 10.5439/1242975
	UHSAS	Ultra High Sensitivity Aerosol Spectrometer	Aerosol size distribution, number concentration	60 – 1000 nm	sgpaosuhsasS01.a1	DOI: 10.5439/1333828
	CPC	condensation particle counter	Aerosol number concentration	> 10 nm	sgpaoscpcC1.b1	DOI: 10.5439/1025152
	CPCU	condensation particle counter - ultrafine	Aerosol number concentration	> 3 nm	sgpaoscpcuS01.b1	DOI: 10.5439/1046186
	CCN	cloud condensation nuclei (CCN) counter	CCN number concentration		Two *.dat files from J. Fast	Not sure the public source
	ACSM	Aerosol Chemical Speciation Monitor	Aerosol composition		sgpaosacsmC1.b1	DOI: 10.5439/1762267
Aircraft	UHSAS	Ultra High Sensitivity Aerosol Spectrometer	Aerosol size distribution, number concentration	60 – 1000 nm	tomlinson-uhsas	https://iop.archive.arm.gov/arm-iop/2016/sgp/hiscale/tomlinson-uhsas
	CPC	condensation particle counter	Aerosol number concentration	> 10 nm	mei-cpc	https://iop.archive.arm.gov/arm-iop/2016/sgp/hiscale/mei-cpc

	CPCU	condensation particle counter - ultrafine	Aerosol number concentration	> 3 nm	mei-cpc	https://iop.archive.arm.gov/arm-iop/2016/sgp/hiscale/mei-cpc
	CCN	cloud condensation nuclei (CCN) counter	CCN number concentration		mei-ccn	https://iop.archive.arm.gov/arm-iop/2016/sgp/hiscale/mei-ccn
	IWG	Interagency Working Group for Airborne Data and Telemetry Systems	navigation information and basic atmospheric state parameters		mei-iwg1	https://iop.archive.arm.gov/arm-iop/2016/sgp/hiscale/mei-iwg1
	FIMS	Fast integrated mobility spectrometer	Aerosol size distribution	10 – 425 nm	wang-fims	https://iop.archive.arm.gov/arm-iop/2016/sgp/hiscale/wang-fims
	PCASP	passive cavity aerosol spectrometer	Aerosol size distribution	120 – 3000 nm	tomlinson-pcasp	https://iop.archive.arm.gov/arm-iop/2016/sgp/hiscale/tomlinson-pcasp
	AMS	Aerosol mass spectrometer	Aerosol composition		shilling-ams	https://iop.archive.arm.gov/arm-iop/2016/sgp/hiscale/shilling-ams
	WCM	water content measuring system	Cloud liquid and total water content		matthews-wcm	https://iop.archive.arm.gov/arm-iop/2016/sgp/hiscale/matthews-wcm

Table 3: Instruments for ACE-ENA

Platform	Instrument	Full name	Measurements	Particle diameter range	Datastream name	DOI or link
Ground	MET	Surface meteorology systems	Temperature, relative humidity, wind, pressure		enametC1.b1	DOI: 10.5439/1786358
	UHSAS	Ultra High Sensitivity Aerosol Spectrometer	Aerosol size distribution, number concentration	60 – 1000 nm	enaaosuhsasC1.a1	DOI: 10.5439/1409033
	HTDMA	humidified tandem differential mobility analyzer	Aerosol size distribution	20 – 2500 nm	enaaoshtdmaC1.a1	DOI: 10.5439/1095581
	CPC	condensation particle counter	Aerosol number concentration	> 10 nm	enaaoscpcfC1.b1	DOI: 10.5439/1046184
	CCN	cloud condensation nuclei (CCN) counter	CCN number concentration		enaaosccn1colavgC1.b1	DOI: 10.5439/1342133
	ACSM	Aerosol Chemical Speciation Monitor	Aerosol composition		enaaosacsmC1.b2	DOI: 10.5439/1762267
Aircraft	CPC	condensation particle counter	Aerosol number concentration	> 10 nm	mei-cpc	DOI: 10.5439/1440985
	CPCU	condensation particle counter - ultrafine	Aerosol number concentration	> 3 nm	mei-cpc	DOI: 10.5439/1440985
	CCN	cloud condensation nuclei (CCN) counter	CCN number concentration		enaaafccn2colaF1.b1, enaaafccn2colbF1.b1	No DOI
	IWG	Interagency Working Group for	navigation information and		mei-iwg1	https://iop.archive.arm.gov/arm-iop/2017/ena/aceena/mei-iwg1

		Airborne Data and Telemetry Systems	basic atmospheric state parameters			
	FIMS	Fast integrated mobility spectrometer	Aerosol size distribution	10 – 425 nm	wang-fims	https://iop.archive.arm.gov/arm-iop/2017/ena/aceena/wang-fims
	PCASP	passive cavity aerosol spectrometer	Aerosol size distribution	120 – 3000 nm	tomlinson-pcas	https://iop.archive.arm.gov/arm-iop/2017/ena/aceena/tomlinson-pcas
	OPC	Optical particle counter	Aerosol size distribution	390 – 15960 nm	pekour-opc_iso	https://iop.archive.arm.gov/arm-iop/2017/ena/aceena/pekour-opc_iso
	AMS	Aerosol mass spectrometer	Aerosol composition		shilling-hrfams	Doi: 10.5439/1468474
	WCM	water content measuring system	Cloud liquid and total water content		matthews-wcm	Doi: 10.5439/1465759

Table 4: Instruments for MAGIC

Platform	Instrument	Full name	Measurements	Particle diameter range	Datastream name	DOI or link
Ship	MET	Surface meteorology systems	Temperature, relative humidity, wind, pressure		raynolds-marmet	https://iop.archive.arm.gov/arm-iop/2012/mag/magic/reynolds-marmet/
	MWR	Microwave radiometer	Liquid water path, precipitable water vapor		magmwrret1liljclouM1.s2	DOI: 10.5439/1027369
	UHSAS	Ultra High Sensitivity Aerosol Spectrometer	Aerosol size distribution, number concentration	60 – 1000 nm	magaosuhsasM1.a1	DOI: 10.5439/1333828
	HTDMA	humidified tandem differential mobility analyzer	Aerosol size distribution	20 – 2500 nm	magaoshtdmaM1.a1	DOI: 10.5439/1095581
	CPC	condensation particle counter	Aerosol number concentration	> 10 nm	magaoscpcfM1.a1	DOI: 10.5439/1046184
	CCN	cloud condensation nuclei (CCN) counter	CCN number concentration		magaosccn100M1.a1	DOI: 10.5439/1227964

Table 5: Instruments for MARCUS

Platform	Instrument	Full name	Measurements	Particle diameter range	Datastream name	DOI or link
Ship	MET	Surface meteorology systems	Temperature, relative humidity, wind, pressure		maraadmetX1.b1	NO DOI
	MWR	Microwave radiometer	Liquid water path, precipitable water vapor		marmwrret1liljclouM1.s2	DOI: 10.5439/1027369
	UHSAS	Ultra High Sensitivity Aerosol Spectrometer	Aerosol size distribution, number concentration	60 – 1000 nm	maraosuhsasM1.a1	DOI: 10.5439/1333828
	HTDMA	humidified tandem differential mobility analyzer	Aerosol size distribution	20 – 2500 nm	maraoshtdmaM1.a1	DOI: 10.5439/1095581
	CPC	condensation particle counter	Aerosol number concentration	> 10 nm	maraoscpcf1mM1.b1	DOI: 10.5439/1418260
	CCN	cloud condensation nuclei (CCN) counter	CCN number concentration		maraosccn1colavgM1.b1	DOI: 10.5439/1342133

Table 6: Instruments for CSET

Platform	Instrument	Full name	Measurements	Particle diameter range	Datastream name	DOI or link
aircraft	UHSAS	Ultra High Sensitivity Aerosol Spectrometer	Aerosol size distribution, number concentration	60 – 1000 nm	Low Rate (LRT - 1 sps) Navigation, State Parameter, and Microphysics Flight-Level Data. Version 1.3	DOI: 10.5065/D65Q4T96
	CNC	condensation nuclei counter	Aerosol number concentration	12 – 70341 nm	Same as above	DOI: 10.5065/D65Q4T96
	PCASP	passive cavity aerosol spectrometer	Aerosol size distribution	120 – 3000 nm	Same as above	DOI: 10.5065/D65Q4T96

Table 7: Instruments for SOCRATES

Platform	Instrument	Full name	Measurements	Particle diameter range	Datastream name	DOI or link
aircraft	UHSAS	Ultra High Sensitivity Aerosol Spectrometer	Aerosol size distribution, number concentration	60 – 1000 nm	Low Rate (LRT - 1 sps) Navigation, State Parameter, and Microphysics Flight-Level Data. Version 1.3	DOI: 10.5065/D6M32TM9
	CNC	condensation nuclei counter	Aerosol number concentration	192 – 78846 nm	Same as above	DOI: 10.5065/D6M32TM9
	CCN	cloud condensation nuclei (CCN) counter	CCN number concentration		SOCRATES CCN measurements. Version 1.1	DOI: 10.5065/D6Z036XB