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• **News & Views** •

A Newly Established Air Pollution Data Center in China※

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ABSTRACT

Air pollution in China covers a large area with complex sources and formation mechanisms, making it a unique place to conduct air pollution and atmospheric chemistry research. The National Natural Science Foundation of China's Major Research Plan entitled "Fundamental Researches on the Formation and Response Mechanism of the Air Pollution Complex in China" (or the Plan) has funded 76 research projects to explore the causes of air pollution in China, and the key processes of air pollution in atmospheric physics and atmospheric chemistry. In order to summarize the abundant data from the Plan and exhibit the long-term impacts domestically and internationally, an integration project is responsible for collecting the various types of data generated by the 76 projects of the Plan. This project has classified and integrated these data, forming eight categories containing 258 datasets and 15 technical reports in total. The integration project has led to the successful establishment of the China Air Pollution Data Center (CAPDC) platform, providing storage, retrieval, and download services for the eight categories. This platform has distinct features including data visualization, related project information querying, and bilingual services in both English and Chinese, which allows for rapid searching and downloading of data and provides a solid foundation of data and support for future related research. Air pollution control in China, especially in the past decade, is undeniably a global exemplar, and this data center is the first in China to focus on research into the country's air pollution complex.

Key words: air pollution, data center, platform, multi-source data, China

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1. Introduction

The Major Research Plans funded by the National Natural Science Foundation of China (NSFC) usually focus on themes of fundamental research that have an urgent need for research to be conducted towards understanding the mechanisms underpinning challenging scientific questions. The Major Research Plan entitled "Fundamental Researches on the Formation and Response Mechanism of the Air Pollution Complex in China" (hereafter referred to as the Plan) is one of these Plans, which was funded in 2015 and has supported 76 research projects towards understanding the formation mechanisms and physical and chemical processes of haze, including the coupling between them (Zhu, 2017).

The Plan was initiated at a time when China, especially the North China Plain region, was experiencing severe haze cov-

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erage (An et al., 2019), seriously impacting visibility and human health (Parrish and Zhu, 2009). Based on numerous studies, the Chinese government believed that $PM_{2.5}$, or fine particulate matter, was the major cause of the haze problem, and therefore a new National Air Quality Standard was established for $PM_{2.5}$ in 2012 (Ministry of Environmental Protection of the People's Republic of China and General Administration of Quality Supervision, Inspection and Quarantine of the People's Republic of China, 2016). To reduce the concentration of $PM_{2.5}$ and achieve a blue sky, the NSFC funded a joint program entitled "Formation Mechanisms, Health Effects and Mitigation Strategies of the Air Pollution Complex in China" in 2015 in order to provide scientific support for formulating policies and cleaning the air. This joint program included two Major Research Plans. The Plan was one of them, focusing on air pollution formation mechanisms, while the other concentrated on human health impacts.

In 2020, five years later, the 76 projects supported by the Plan have provided valuable insights into the haze problem in China. Zhu et al. (2023) summarized the main research findings of the projects supported by the Plan and major advancements in atmospheric chemistry research in China, covering sources and emission inventories, atmospheric chemical processes, interactions of air pollution with meteorology, weather and climate, interactions between different interfaces, and data assimilation. More importantly, as most projects are data-type projects, a huge amount of valuable data has emerged. Although in recent years a significant amount of data has been acquired from many research projects related to air pollution in China, a unique and high-quality database of air quality from China is still not available due to, for example, the lack of data compilation, quality control, sharing mechanisms, and effective data platforms.

Therefore, a data integration project entitled "Developing a Comprehensive Data Sharing Platform for the Air Pollution Complex in China" was funded by the Plan to collect these data from the Plan and include all data on a public data platform, which would be open to both domestic and international scientists. Based on the data from 76 individual projects supported by the Plan, this project aimed to collect and classify all raw data, establish expert groups for quality control, set up data sharing mechanisms, and finally form a representative and sustainable large database of air pollution in China, including the following data categories: emission inventory, chemical reanalysis, field measurements, and physical and chemical parameters from laboratory experiments. These different categories of data are described in detail below.

2. The China Air Pollution Data Center

An online data platform, named the China Air Pollution Data Center (CAPDC), with its own website (www.capdatabase.cn) and DOI (doi.org/10.12423/capdb_PKU.20200101), has been successfully established. The platform was built by 3Clear Science & Technology Co., Ltd., with their staff responsible for all technical issues of the website. The CAPDC is available in both Chinese and English versions. The configuration of the website consists of seven major functions at the top and eight major categories of project outputs on the left side. The seven functions include Home, the Major Research Plan, Download Data, Data Visualization, About, Open Statistics, and Personal Center. The research outputs from the Plan

Fig. 1. The eight categories of the China Air Pollution Data Center and the number of datasets in each category.

are classified into eight categories—six data-type categories and two non-data-type categories (Fig. 1). The data-type categories are Emission Inventory, Chemical Reanalysis, Field Observation, Satellite Observation, Laboratory Measurement, and Source Profile, while the non-data-type results are classified into two categories named New Technology and Online Source Apportionment Technology. In addition to the DOI of the CAPDC website, each category has its own DOI (see Table 1).

3. Description of data categories

3.1. *Emission Inventory*

This category is organized and integrated by the research group of Prof. Qiang ZHANG from Tsinghua University, and includes nine datasets from nine projects and one dataset linked with the Multi-resolution Emission Inventory model for Climate and air pollution research (MEIC) database (Li et al., 2017; Zheng et al., 2018). The nine datasets are: (1) The High-resolution Integrated Emission Inventory of Air Pollutants for China in 2017; (2) Gridded Emission Inventory of Semi-volatile and Intermediate Volatile Organic Compounds (VOCs) in China (Wu et al., 2021); (3) Anthropogenic Chlorine Emission Inventory for China (ACEIC) (Hong et al., 2020); (4) Yangtze River Delta (YRD) Air Pollutant Emission Inventory (An et al., 2021); (5) Ship Emission Inventory in East Asia (Liu et al., 2019); (6) Vehicle Emission Inventory for the Beijing–Tianjin–Hebei (BTH) Region (Yang et al., 2019); (7) Open Biomass Burning Emission Inventory established by Beijing University of Technology (BJUT-OBB) (Zhou et al., 2021); (8) Anthropogenic Emission Inventory of VOCs for the BTH Region in 2013 (Li et al., 2019); and (9) High-resolution Biogenic Emissions Inventory from Urban Green Spaces in China established by the Ocean University of China (OUC-BUGS) (Wu et al., 2022). Both anthropogenic sources (industrial, electricity, etc.) and natural sources are included in these inventories with a variety of temporal (year/month/day/hour) and spatial (Asia/mainland China/regional/city) resolutions.

Among these inventories, the High-resolution Integrated Emission Inventory of Air Pollutants for China is a national-scale emission inventory for 2017, jointly developed by the MEIC team from Tsinghua University and several research groups. After comprehensive comparison, uncertainty analysis, and evaluation of multi-source data, several multi-scale high-resolution emission inventories have been integrated into the MEIC model to improve the data accuracy for specific regions, sources and species. The inventories integrated with MEIC include the YRD Air Pollutant Emission Inventory (An et al., 2021), the Greater Bay Area-Emission Inventory (GBA-EI) in the Pearl River Delta developed by Prof. Junyu Zheng from Jinan University (Huang et al., 2021), the PKU-NH_3 (Kang et al., 2016) and the Open Biomass Burning Emission Inventory (Huang et al., 2012) developed by Prof. Yu Song from Peking University, and the Shipping Emission Inventory in East Asia (Liu et al., 2019). The missing sources in MEIC (e.g., open biomass burning and ship emissions) are supplemented, the data accuracy for specific regions (YRD, GBA, etc.) and species (e.g., VOCs, ammonia) is improved, and monthly emissions at 0.1° (~10 km) of nine major air pollutants in China are provided in the inventory for 2017 on the website. The nine major pollutants include sulfur dioxide (SO_2), nitrogen oxides (NO_x), carbon monoxide (CO), non-methane VOCs (NMVOCs), NH_3, inhalable particulate matter (PM_{10}), fine particulate matter ($PM_{2.5}$), black carbon (BC), and organic carbon (OC).

3.2. *Chemical Reanalysis*

This category is led by the research group of Prof. Jiang ZHU from the Institute of Atmospheric Physics (IAP), Chinese Academy of Sciences. Three main datasets are provided in this category from two projects and one linked to EAC4 (ECMWF Atmospheric Composition Reanalysis 4). One major dataset, a high-resolution air quality reanalysis dataset over China (CAQRA), is produced by IAP in collaboration with the China National Environmental Monitoring Centre (CNEMC) and other research institutes, with part of the support from the Plan. CAQRA has assimilated data from over

Table 1. DOIs for the China Air Pollution Data Center and its eight categories.

Category	DOI
China Air Pollution Data Center	doi.org/10.12423/capdb_PKU.20200101
Emission Inventory	doi.org/10.12423/capdb_PKU.2023.EI
Chemical Reanalysis	doi.org/10.12423/capdb_PKU.2023.DA
Field Observation	doi.org/10.12423/capdb_PKU.2023.OB
Satellite Observation	doi.org/10.12423/capdb_PKU.2023.SAT
Laboratory Measurement	doi.org/10.12423/capdb_PKU.2023.LAB
Source Profile	doi.org/10.12423/capdb_PKU.2023.SOURCE
New Technology	doi.org/10.12423/capdb_PKU.2023.TECH
Online Source Apportionment Technology	doi.org/10.12423/capdb_PKU.2023.SA

1000 surface air quality monitoring sites of the CNEMC based on the ensemble Kalman filter (EnKF) algorithm and the Nested Air Quality Prediction Modeling System (NAQPMS). Its method has overcome challenges of instability, insufficient adjustment, and negative assimilation effects in atmospheric chemistry data assimilation, and has developed multi-air pollutant collaborative assimilation methods, including monitoring data automatic quality control methods, adaptive model error estimation, and other advanced algorithms. Data of six conventional air pollutants ($PM_{2.5}$, PM_{10}, SO_2, NO_2, CO and O_3) and the simulated surface wind speed, pressure, relative humidity, and temperature from 2013 to 2022 are provided with a spatial and temporal resolution of 15 km and 1 h, respectively. The 2013–18 data have been published in Science Data Bank, where the dataset is described and validated in detail (Kong et al., 2021).

Another important dataset in this category is the high-resolution simulation dataset of $PM_{2.5}$ composition (including BC, OC, sulfate, nitrate, ammonium, etc.) over China (CAQRA-aerosol), using the methods of emission inversion and high-resolution numerical simulation. First, the $PM_{2.5}$ composition simulation module was improved in NAQPMS to reduce the simulation errors of $PM_{2.5}$ compositions. Furthermore, data from over 1000 surface air quality monitoring sites from the CNEMC have been assimilated by the Chemical Data Assimilation System (ChemDAS) developed by the IAP to constrain the emission inventory of $PM_{2.5}$ and its precursors. This method has overcome the problems of underestimation of background model errors and large biases in the a priori emission inventory, and thus it has improved the model performance in simulating compositions of $PM_{2.5}$. After that, the high-resolution simulation dataset of $PM_{2.5}$ composition over China has been produced based on the numerical simulation by NAQPMS with the inversed emission inventory, providing aerosol component data from 2013 to 2022 with resolutions of 15 km and 1 h. In the future, the above CAQRA and CAQRA-aerosol datasets will be continuously updated on this platform.

3.3. *Field Observation*

This category has involved the collection of data from a total of 27 projects funded by the Plan, spanning from 2011 to 2021 and comprising 41 sites. This compilation has ultimately resulted in 221 datasets, including various critical parameters of the atmospheric measurements. The data variables mainly cover the following categories (Table 2): (1) cloud parameters, including 5 datasets related to the microphysical properties of clouds; (2) atmospheric parameters, including 8 datasets for boundary layer properties, 95 datasets for near-surface properties, and 16 datasets for upper-atmospheric properties; (3) aerosol parameters, including 11 datasets for aerosol optical and radiative properties, 77 datasets for aerosol physical and chemical properties, and 8 datasets for other aerosol properties. Each dataset is accompanied by a comprehensive data description file, which contains information such as data provider, data variable, sampling site, instrument, and measurement period. These detailed descriptions serve as invaluable resources, helping users to gain a better understanding of the data and related information.

3.4. *Satellite Observation*

This category includes satellite data from one project funded by the Plan and nine ChinaHighAirPollutants (CHAP) datasets. The retrieved NO_2 column concentration dataset from the TROPOspheric Monitoring Instrument (TROPOMI) in China is provided in the first dataset. Based on the spectral data of the European Space Agency's S5P satellite (effective spatial resolution: 3.5 × 5.5 km), an NO_2 inversion algorithm that includes spectral inversion, tropospheric separation, and radiation transfer calculation has been developed independently (Zhang et al., 2020). Data of the tropospheric NO_2 column concentration and whole-layer NO_2 column concentration from 2019 to 2020 at a 0.01° and daily resolution are available through the platform. In the nine CHAP datasets, a variety of high-resolution and high-precision atmospheric parametric satellite remote sensing products (including PM_{10}, $PM_{2.5}$, PM_1, O_3, NO_2, SO_2, and CO) are produced through multi-source satellite sensors with

Table 2. Parameter categories of field observation data from 27 projects in the Plan.

Parameter category	Subcategory	Parameters	Number of datasets
Cloud parameters	Microphysical properties	Cloud base height, cloud boundary, vertical structure, etc.	5
Atmospheric parameters	Boundary layer properties	Boundary layer height, turbulence parameter, etc.	8
	Near-surface properties	Basic meteorological variables, atmospheric NO, NO_2, NO_x, CO, SO_2, O_3 concentrations, profiles and flux, etc.	95
	Upper-atmospheric properties	Profiles of basic meteorological variables, etc.	16
Aerosol parameters	Optical and radiative properties	Aerosol extinction, backscattering and absorption coefficient, optical depth, etc.	11
	Physical and chemical properties	Aerosol chemical components, particle number size distribution, aerosol hygroscopicity, etc.	77
	Other aerosol properties	Cloud condensation nuclei number concentration, aerosol activation characteristics, $PM_{2.5}$ carbon isotopic characterization, etc.	8

a variety of temporal (year/month/day/hour) and spatial (10 km/5 km/1 km) resolutions (Wei et al., 2021). The CHAP data are also available on the CHAP platform (https://zenodo.org/communities/chap/).

3.5. *Laboratory Measurement*

This category comprises six datasets covering more than 400 entries of parameters from 12 projects funded by the Plan. The data in this category originate from 140 peer-reviewed papers. The platform categorizes laboratory parameter datasets into two main classes: physicochemical property parameters and chemical reaction parameters. They are further subdivided into six datasets, covering deliquescence point and efflorescence relative humidity, hygroscopicity, secondary organic aerosol yield, heterogeneous reaction uptake coefficient, gas-phase reaction rate constant, and liquid-phase reaction rate constant. Based on the characteristics of laboratory parameters, the datasets are classified into two levels, with Level 1 from published laboratory data from the 140 peer-reviewed papers, and Level 2 from comprehensive reviews of literature data and recommended values by invited experts. Among the six datasets, deliquescence and efflorescence relative humidity are Level 2 data.

Each dataset allows for data querying and downloading. Users can retrieve relevant data based on species, reaction conditions, reaction parameters, or other information, enabling efficient parameter searches. For datasets at Level 1, each entry contains details on the measurement conditions and measurement method, and a link to the source paper, which is convenient for users with different levels of expertise to assess the applicability of the corresponding parameters and to trace the literature. For datasets at Level 2, not only are recommended values presented, but literature summaries of the specific parameters are also provided as separate pdf files.

3.6. *Source Profile*

This category has five datasets from five projects supported by the Plan. The sources encompass industrial combustion sources (power plants, boilers, etc.), industrial process sources, other industrial sources (industrial rubbers and plastics, synthetic fiber, etc.), road mobile sources (gasoline, diesel, etc.), non-road mobile sources (e.g., ship emissions), residential combustion sources (wood, straw, bituminous coal, anthracite, etc.), and biomass burning sources (wood, straw). Apart from traditional species including OC, EC, water-soluble ions and metals, species covering VOCs, intermediate/oxygenated VOCs, organic amines, and primary and secondary organic tracers are also provided. Additionally, the platform provides links to two other existing comprehensive source profile databases: Source Profiles of Air Pollution (SPAP) developed by Nankai University, and Main Emission Source Profile Database of $PM_{2.5}$ in China developed by the Chinese Academy of Sciences. Users can navigate to the respective database webpages through the links.

3.7. *New Technology*

With the support of the Plan, significant progress has been made in novel applications of measurement principles in spectroscopy, mass spectrometry and integrated technologies through seven projects. In this project, new technologies are introduced with detailed information in each report to enhance understanding of the essential advancements in technology development in the Plan. This category provides 11 reports on new technologies, including seven spectroscopy technical reports, two mass spectrometry technical reports, and two integration technical reports (Table 3). Each report consists of several sections including scientific background, principles of instrument, quality assurance and control, instrument application, commercial promotion plan, etc.

3.8. *Online Source Apportionment Technology*

Regional air pollution has occurred in many regions of China, and concentrations of pollutants such as $PM_{2.5}$ could experience explosive increases with large amplitudes during very short periods. Therefore, rapid and accurate source apportionment is the foundation of effective air quality management, calling for high time-resolved online monitoring and source apportionment techniques to help to understand the causes of heavy pollution. Four online source apportionment technology reports based on four projects funded by the Plan are available in this category (Table 3) to provide reliable references for future research, which are based on different instruments and principles.

The four technologies are:

(1) Online measurements by multiple instruments, including the Aerodyne Aerosol Chemical Speciation Monitor (ACSM), seven-wavelength aethalometer (AE-31), Ambient Continuous Multi-Metals Monitor (Xact-625i), and Synchronized Hybrid Ambient Real-time Particulate Monitor (SHARP-5030i), are combined to achieve 1-h measurements of mass concentrations of $PM_{2.5}$ and its components. Local source profiles are derived from source apportionment results of historical data through the Positive Matrix Factorization (PMF) model, and an online source apportionment platform based on the Chemical Mass Balance (CMB) model has been established.

(2) An online measurement system of air pollutants with a 5–10-min resolution based on Time of Flight-Aerosol Chemical Speciation Monitoring (TOF-ACSM) has been established. Based on the PMF model, a new online organic aerosol source apportionment method has been developed and optimized using constraints such as inorganic components.

Table 3. New technology and online source apportionment technology reports.

Category	Subcategory	Technology
New Technology	Spectroscopy technique	(1) A portable cavity ring down spectroscopy instrument for simultaneous and in situ measurement of NO_3 radicals and N_2O_5
		(2) Measurement of HO_x radicals by fluorescence assay by gas expansion technology
		(3) Laser-induced fluorescence method for measuring HO_x radicals in the atmospheric environment
		(4) Amplitude modulated cavity-enhanced nitrogen dioxide analyzer
		(5) Broadband cavity enhanced absorption spectroscopy based on an iterative algorithm to measure HONO and NO_2
		(6) Total OH reactivity measurement instrument
		(7) Atmospheric total peroxy radicals analyzer
	Mass spectrometry technique	(8) A vacuum ultraviolet photoionization aerosol mass spectrometer
		(9) Detection of RO_2 by microwave discharge flow tube photoionization mass spectrometry
	Integration technique	(10) Online analysis of the dynamic process of atmospheric ultrafine particle condensation growth
		(11) A twin open-top chambers method to measure soil HONO emission
Online Source Apportionment Technology*	–	(1) $PM_{2.5}$ source apportionment combining integrated instruments**, using source profiles from PMF and online source apportionment platform based on CMB
		(2) Organic aerosol source apportionment based on TOF-ACSM measurement and optimized PMF
		(3) $PM_{2.5}$ source apportionment based on multiple instrument measurement*** and models including PMF and NAQPMS
		(4) $PM_{2.5}$ source apportionment by traditional PMF model as well as novel technology based on SPAMS

* The full names of all methods and instruments are provided in section 3.8.
** Instruments include ACSM, AE-31, Xact-625i, and SHARP-5030i.
*** Instruments include Sunset OCEC, IGAC, Xact-625i, TAG, etc.

(3) Hourly monitoring data of organic and inorganic components of $PM_{2.5}$ are provided by instruments including the Sunset Semi-Continuous Organic Carbon/Elemental Carbon (Sunset OCEC) aerosol analyzer, In-situ Gas and Aerosol Composition (IGAC), Xact-625i, and Thermal desorption Aerosol Gas chromatography (TAG). Both PMF and NAQPMS are used to quantify the sources of $PM_{2.5}$.

(4) Single Particle Aerosol Mass Spectrometry (SPAMS) is used to resolve sources of $PM_{2.5}$. Meanwhile, traditional $PM_{2.5}$ source apportionment using PMF is conducted with online hourly measurements from IGAC, Sunset OCEC, and Xact-625i. Source apportionment results from the two methods are compared in the report.

4. Features of the China Air Pollution Data Center

4.1. *Data visualization*

In order to preview and visualize the required data, the platform is equipped with a rapid data visualization feature based on key-word querying or webpage options. Three categories of data, including Emission Inventory, Chemical Reanalysis, and Satellite Observation, can be visualized before download. Users can filter data based on target parameters, time range, temporal resolution, etc., for further investigation. Static visualization of data is available, allowing users to view the spatial distribution of parameters at a specific time point. Additionally, dynamic visualization is feasible through a slideshow, enabling users to observe the trend of parameter changes over a certain period of time. The platform supports the download of high-quality visual products in both static and dynamic formats for presentation or report purposes.

4.2. *Multiple data download options*

Currently, over one terabyte of data have been successfully uploaded to the platform, and most of the data are provided freely for download after registration. Information including name, affiliation, email address, etc., needs to be provided for registration. An account will be issued after evaluation and signing the agreement. To make data downloads more accurate, simple, and efficient, the platform has designed flexible retrieval and download solutions based on the nature of different datasets. For example, for chemical reanalysis datasets, three distinct data filtering options have been developed, allowing users to directly download raw files, filtered based on requirements (including time period, region, temporal resolution, parameters, etc.) or by manually selecting a map area to download specific data. For field observation datasets, users can filter the dataset based on target parameters and observation sites, or by manually selecting the target area. For only a few datasets, users are encouraged to contact data providers before downloading data, as required by the data providers (e.g., the retrieved NO_2 column concentration dataset from TROPOMI in China in the Satellite Observation category, and the deliquescence and efflorescence point dataset in the Laboratory Measurement category).

4.3. *Data provider information*

In order to aid users to gain related information of the data quickly, the platform has set several avenues for finding information about projects: (1) The platform features a display page showing projects supported by the Plan. This page offers functions such as project querying, data upload status inquiries, and viewing detailed introductions. The introduction page of each project also provides links to relative data. (2) The download interface of the desired data provides detailed information and links to relative projects. (3) The data visualization interface also offers detailed information and links to the source projects.

In addition, to safeguard the interests of data providers, the platform has formulated a comprehensive data agreement for users, specifying detailed instructions regarding data use. Users are also reminded to acknowledge and cite relevant projects and publications through pop-up notifications when downloading data.

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