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Near real-time simulation data of atmospheric components and meteorology in the Arctic region using the WRF-Chem model from August to September 2016

Masayuki TAKIGAWA[1, 2]*, Masahiro YAMAGUCHI[1], Fumikazu TAKETANI[2, 1], Yugo KANAYA[2, 1] and Yutaka KONDO[3]

[1] Institute of Arctic Climate and Environmental Change Research, Japan Agency for Marine-Earth Science and Technology, 3173-25 Showa-machi, Kanazawa-ku, Yokohama, Kanagawa 236-0001.

[2] Reseach and Development Center for Global Change, Japan Agency for Marine-Earth Science and Technology, 3173-25 Showa-machi, Kanazawa-ku, Yokohama, Kanagawa 236-0001.

[3] Arctic Environment Research Center, National Institute of Polar Research, 10-3, Midori-cho, Tachikawa-shi, Tokyo 190-8518.

*Corresponding author. Masayuki TAKIGAWA (takigawa@jamstec.go.jp)

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Abstract: This study aims to develop a near real-time simulation system to assist in the preparation of the observational plan and the first analysis during the observational campaigns such as a cruise of the Research Vessel (R/V) *Mirai*. This system covers most of the Northern Hemisphere for the precise treatment of the intrusions of airmasses from the mid-latitudes to the Arctic. Day-to-day variations in the emissions are also taken into account, especially for emissions from biomass burning. The calculation is conducted using forecasted meteorological data for the target period, and the model data is finally overwritten by the output executed using the operational reanalysis data. The system has been applied to cruises of the R/V *Mirai* for MR1606 in 2016. Operationally, a 48-hour forecast calculation is conducted once a day and the result is shared with the researchers conducting the observations. Here, we present a dataset for the meteorological and atmospheric constituents, such as ozone and black carbon near the surface, during the MR1606 cruise of the R/V *Mirai* in 2016. This dataset can be used for the analysis of transport and transformation processes of chemical constituents that are observed during the cruise, and also the meteorological data can be used for the source analysis using trajectory models such as WRF-FLEXPART.

1. Background & Summary

Black carbon (BC), which is known to be a component of PM2.5, can change the Earth's albedo by changing the color of ice and snow via deposition onto the surface, and the impact of BC on the climate change appears to be larger at high-latitude regions in comparison with the other parts of the world[1]. The amount of local anthropogenic sources in high-latitude regions is relatively small, and the precise assessment of 1) impact of local sources, such as biomass burning, ship emissions, and gas flares, 2) amount of transport from mid-latitude regions such as China and Japan, and 3) the removal process during long-range transport is quite important for the estimation of climate change in Arctic region.

Chemical transport models have been used to estimate the burden and origin of BC and other pollutants in the Arctic region[2]. Global models have an advantage in their precise treatment of long-range transport; however, the horizontal resolution of these models is generally not sufficient to reproduce frontal activity[3,4], which is important for the eventual transport of polluted airmasses. High-resolution model calculations also reveal that more realistic representation of convection, clouds, and aerosol–cloud interaction processes is required for the precise estimation of wet deposition processes[5].

In this study, we have developed a model system which can take into account the impact of local and remote sources on the concentration or the budget of BC in the Arctic region using a regional model with several special treatments to improve the short-range variations. We have used a chemical transport model, which is mutually coupled with the meteorological process, to apply more precise vertical mixing within the planetary boundary layers. High-resolution biomass burning emissions are also applied as a local source in the Arctic region taking into consideration the release height corresponding to the activity of the burning. Here, we present a dataset of meteorology and chemical constituents that can be used to estimate the transport pathways of airmasses in the Arctic region.

2. Model Domain

The domain of the model is designed to cover the entire Arctic region and the most of the northern mid-latitude region, which is thought to be an important source of the pollutants in the Arctic (Figure 1). A polar-stereographic projection has been applied, and the center point and the true latitude are set to the North Pole and 70° N, respectively. The grid interval is set to 40 km near the true latitude and is slightly different near the pole and the equatorial regions due to the map projection effect. The number of horizontal grids is 399 × 399 for temperature, surface pressure, and tracers, such as the chemical constituents, water vapor, and clouds (water, ice, and graupel). Since the Arakawa C-grid[6] is used in the model, staggered grids are applied for the horizontal wind fields. The model has 32 vertical layers up to 50 hPa. Approximately seven layers are set to be within 1 km above the surface, and the height of the lowest level is about 20 m above the surface. Three-dimensional (3D) data are available upon request for a detailed analysis of the source–receptor relationships, and the data at the lowermost level (approximately 10 m above the ground level) are uploaded to the data server to reduce the disk space on the server.

3. Methods

We conducted model simulations over the target region using the regional chemical transport model WRF (Weather Research and Forecasting)/Chem[7] version 3.8.1 (cf. http://www2.mmm.ucar.edu/wrf/users/) following to our chemical weather forecasting system adopted for Tokyo[8]. The initial and lateral boundary conditions for the meteorology were taken from the National Centers for Environmental Prediction (NCEP) Global Forecast System (GFS)[9] (cf. http://www.nco.ncep.noaa.gov/pmb/products/gfs/). Since it is difficult to obtain near real-time model data for the chemical constituents, a global model output from MOZART[10] (Model for OZone and Related chemical Tracers) version 4 was applied only for the initial condition of the chemical constituents (cf. https://www.acom.ucar.edu/wrf-chem/mozart.shtml). Fixed vertical profiles were applied as the lateral boundary conditions of the chemical constituents; however, the effect of the lateral boundary is not significant for the BC concentration because the most part of the source region is located within the model domain.

Since the WRF/Chem model is an online model, the meteorological field is calculated at every time step and simple assimilation by nudging is applied to the calculated meteorology (horizontal wind, temperature, and humidity) using NCEP-GFS forecasted data to improve the forecast skill of the meteorological field. The timestep was originally set to 6 minutes and was diagnosed based on the computational stability; the Courant number was kept at 1.0 or lower for the horizontal and vertical dimensions during the calculation. The Mellor–Yamada–Nakanishi–Niino[11,12,13,14] level 2 scheme was used for the planetary boundary scheme. Morrison two-moment microphysics scheme[15] and the G3 convection scheme[16] were used for the calculation of the grid-scale and subgrid-scale clouds and precipitation, respectively.

RACM[17] (Regional Atmospheric Chemistry Mechanism) and GOCART[18,19] (Goddard Chemistry Aerosol Radiation and Transport) modules were used for the gaseous and aerosol chemistries, with a slight modification to include the OH dependency for the conversion from hydrophobic to hydrophilic BC and the wet deposition process of particles[20]. Vertical fluxes of the rainwater and snow calculated in the grid- and subgrid-scale cloud processes in the model were used to estimate the wet deposition of particles. Anthropogenic emissions were based on the annual mean of EDGAR[21] (Emissions Database for Global Atmospheric Research) version 4.2 for 2010, and the biomass burning was based on the near real-time version of FINN[22] (Fire

Inventory from NCAR) for each day (cf. http://www.acom.ucar.edu/acresp/MODELING/finn_emis_txt). A dataset of version 1.5 was used for the target period. A pyro-convection process was also considered to estimate the release height of the biomass burning emissions[23] using the stability calculated by the meteorological variables in the model for every hour. Biogenic emissions of VOCs (Volatile Organic Carbons) were estimated using MEGAN[24,25] (Model of Emissions of Gases and Aerosols from Nature) version 2.1, which is included in the model and uses the meteorology and radiation calculated in the model for each time step (typically 3 minutes, but it can be changed to keep the computational stability in the model).

The operational calculation is driven using near real-time meteorological data and biomass burning emissions. NCEP conducts operational forecasts four times in a day at 00, 06, 12, and 18Z. The maximum length of a forecast is 192 hours in NCEP-GFS. A 48-hour forecast from 12Z is conducted every day to provide an operational forecast to the researchers at the observational site. The temporal variation in the biomass burning is much larger than that of anthropogenic emissions, especially in the boreal forests, and the latest FINN emission is used for the calculations. Near real-time emissions are used for the analysis calculation as the spin-up, which is resumed from the restart file of the previous day's calculation. It is assumed that the biomass burning emission is maintained for two days for the forecast calculation. The calculation was executed on the supercomputer operated by JAMSTEC (SGI UV1000 until January 2018 and HP Apollo 6000 since February 2018). The original model data is automatically transported to the local file server.

4. Data Records

The original format of the output files was NetCDF (cf. https://www.unidata.ucar.edu/software/netcdf/). The output files contain 182 two-dimensional (2D) variables and 113 3D variables for the meteorology and chemistry, and the file size exceeds 2.5 GB for a 1-hour snapshot. The data at the lowest level is extracted from the model output for every 1-hour for selected variables (e.g., BC, ozone, and near-surface winds) to reduce the disk usage on the server, and the data files are archived at the National Institute of Polar Research (for details concerning the data reference, see Data Citations 1). The data size is 636,804 (4 × 399 × 399) bytes for a 1-hour snapshot for one variable. The order of the binary is big endian in the extracted data, and each variable is written as a 2-D array (x, y) of 4-byte real numbers in the direct access format. The data files are listed in Table 1, and the variables in each data files are listed in Table 2. Users can analyze or visualize the data using GrADS (cf. http://cola.gmu.edu/grads/) or other software. The horizontal distribution of the BC concentration at 00Z on 15 August is shown in Figure 2. The original output files are available upon request.

5. Technical Validation

The meteorological field calculated by the model is essentially important for the transport and removal processes of pollutants and is evaluated using the observational data along the ship track of the Research Vessel (R/V) *Mirai* during the MR1606 cruise. The period of comparison is from 22 August to 4 October 2016. The observational data are available from the JAMSTEC data site (http://www.godac.jamstec.go.jp/jmedia/portal/j/index.html). Instantaneous values at each one hour are compared for wind direction, wind speed, and relative humidity (Fig. 3). One-hour accumulated values are compared for the precipitation. The model generally succeeded in reproducing the temporal variations in the meteorological fields, except precipitation, which is not assimilated with the analysis or forecasted meteorological field of NCEP-GFS.

The concentrations of atmospheric constituents are evaluated using the observational data at Fukue Island in western Japan (32.75° N, 128.68° E). Long-term continuous measurements of BC and other chemical species have been conducted at Fukue. The BC mass concentrations were measured using a continuous soot monitoring system (COSMOS), which is a filter-based absorption photometer with a heated inlet[26,27,28]. The accuracy of COSMOS has been assessed to be about 10% in East Asia[27] and the Arctic region[28]. Fukue is located sufficiently far from the source region to allow for the state conversion of BC from hydrophobic to hydrophilic[29,30]. The model captured the temporal variations in the ozone concentration well (Fig. 4a). For BC, the model qualitatively captured the temporal variations but tended to underestimate the concentration (Fig. 4b). For ozone, the correlation coefficient (r) and root mean square error (RMSE) are 0.85 and 9.15 ppbv, respectively, and, for BC, the values are 0.82 and 0.22 μg/m^3, respectively.

6. Competing interests

The authors declare no competing financial interests.

7. Figures

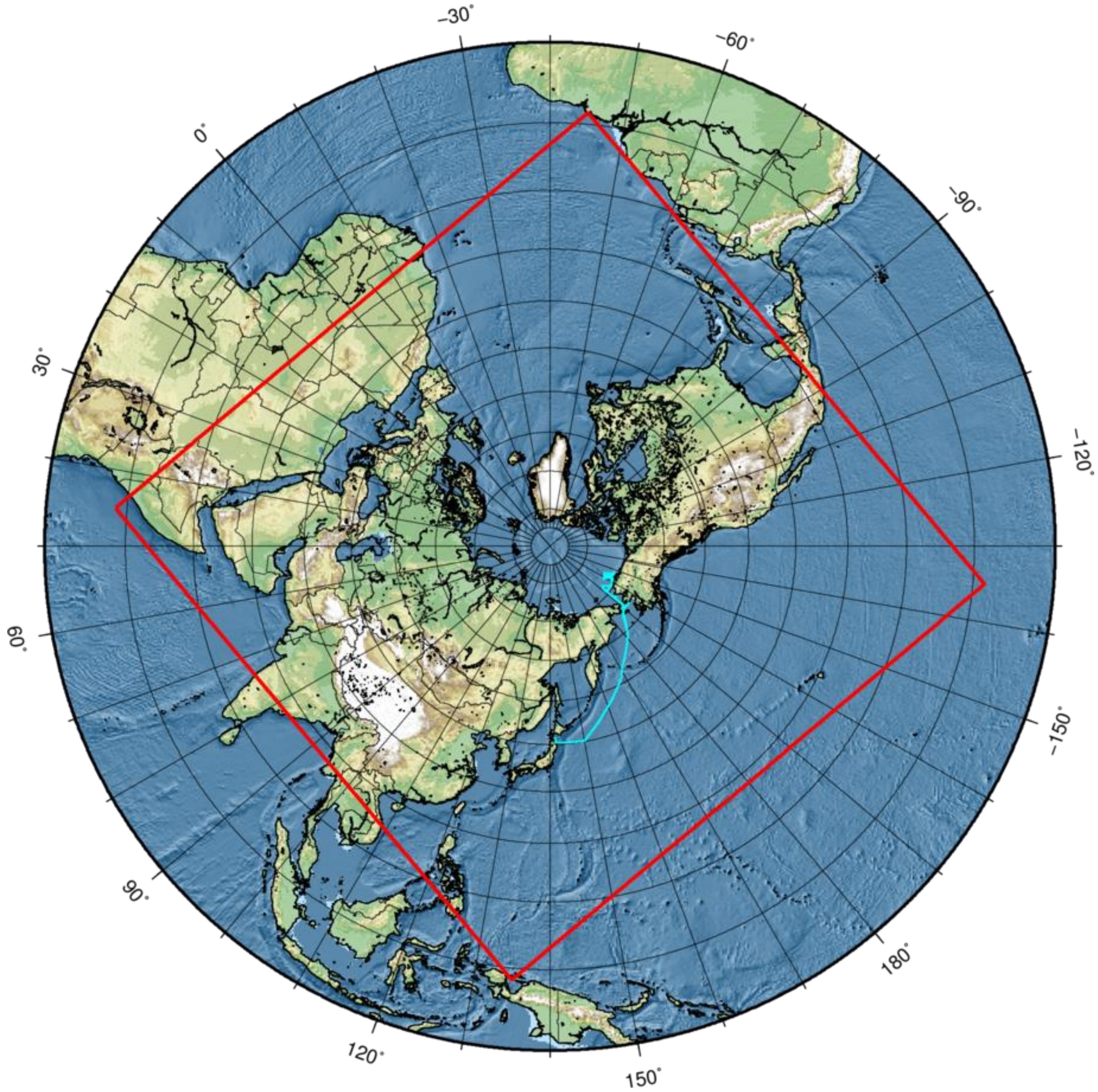

Figure 1. Map of the model domain. The red box indicates the area of the model. Light blue line denotes the ship track during the MR1606 cruise of the R/V *Mirai*.

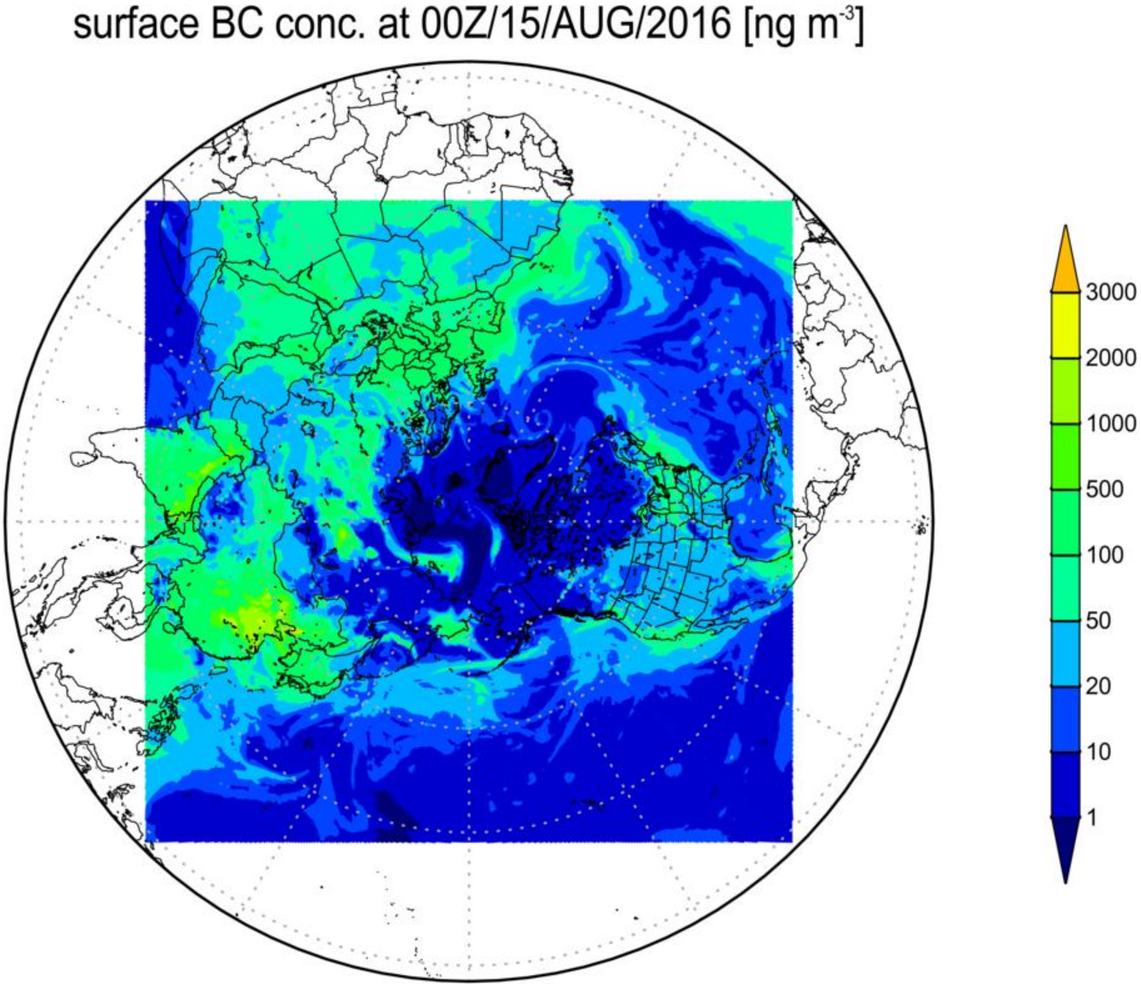

Figure 2. A sample of the output data. BC concentration (ng/m^3) near the surface at 00Z on 15 Aug 2016 calculated using the WRF/Chem model.

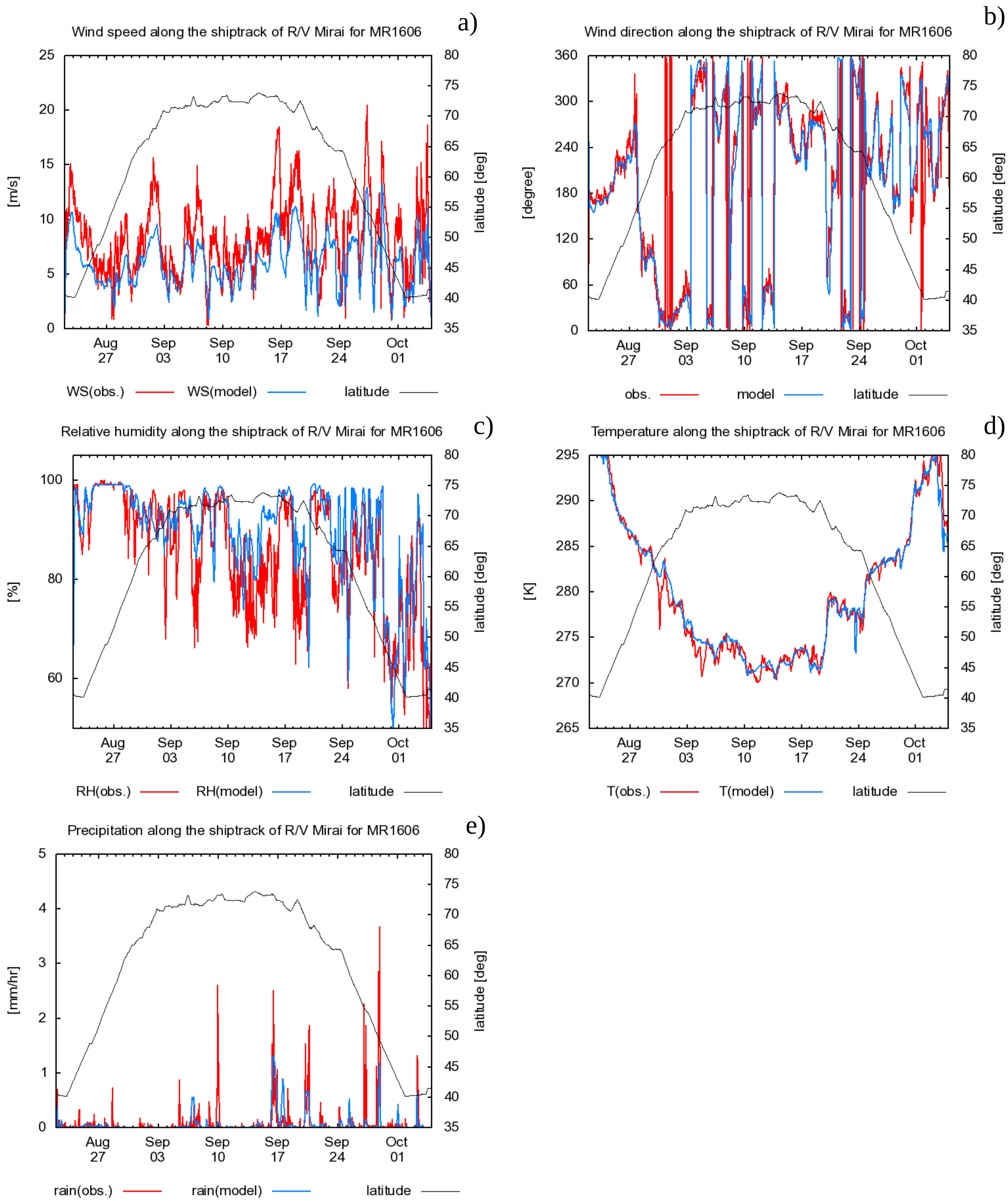

Figure 3. Meteorological data along the ship track during the MR1606 cruise of the R/V *Mirai*. Temporal variations in (a) wind speed, (b) wind direction, (c) relative humidity, (d) temperature, and (e) precipitation are shown. Red and blue lines denote the observations and model output extracted along the shiptrack, respectively. The latitude is also shown as a black line.

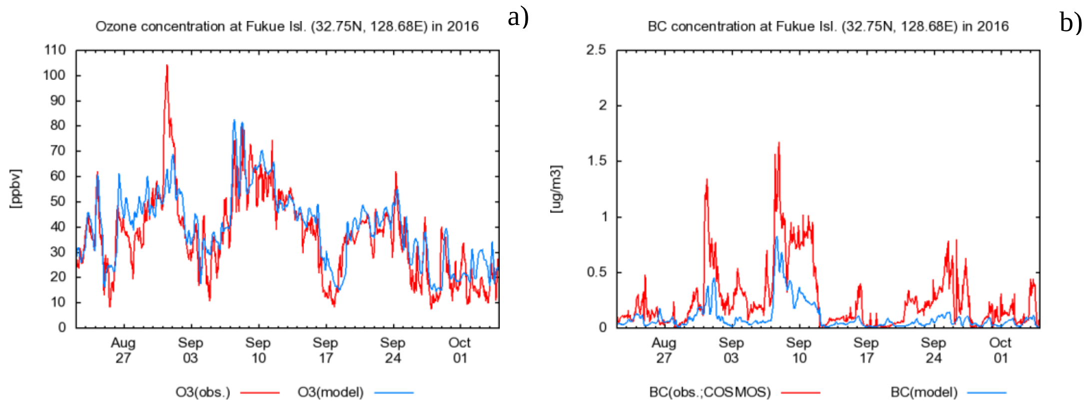

Figure 4. Concentrations of (a) ozone and (b) BC near the surface at Fukue from August to October 2016 in units of ppbv and μg/m^3, respectively. The red and blue lines denote the observations and the model, respectively.

8. Tables

Table 1. List of data files and sample files extracted from the original output files of the WRF/Chem model and sample control file for the analysis.

File names	Short description	notice
outYYYYMMDDHH.dat	Data files.	HH is in UTC.
extractCDF.tar	Sample program for the conversion from the WRF/Chem history file	Requires the NetCDF library and the Fortran90 compiler.
sample.ctl	Sample control file for GrADS	
full_list.txt	List of all variables in WRF/Chem	

Table 2. List of variables written in the data files.

Variable name	Units	Short description	Size
U10	m/s	Zonal wind at 10 m above the surface.	4 bytes × (399 × 399) grids
V10	m/s	Meridional wind at 10 m above the surface.	4 bytes × (399 × 399) grids
BC	ng/m^3	BC concentration near the surface.	4 bytes × (399 × 399) grids
Ozone	ppbv	Ozone concentration near the surface.	4 bytes × (399 × 399) grids

Author contributions

M. Takigawa designed the study and the model system. M. Yamaguchi performed the post-processing of the model data. Y. Kanaya and F. Taketani managed the field measurements for the validation of the model system. Y. Kondo developed COSMOS for BC measurements, assessed its accuracy, and deployed it at Fukue.

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Data Citation

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