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Global Lagrangian Atmospheric Dispersion Model

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Abstract—The Global Lagrangian Atmospheric Dispersion Model (GLADIM) is described. GLADIM is based on the global trajectory model, which had been developed earlier and uses fields of weather parameters from different atmospheric reanalysis centers for calculations of trajectories of air mass that include trace gases. GLADIM includes the parameterization of turbulent diffusion and allows the forward calculation of concentrations of atmospheric tracers at nodes of a global regular grid when a source is specified. Thus, GLADIM can be used for the forward simulation of pollutant propagation (volcanic ash, radionuclides, and so on). Working in the reverse direction, GLADIM allows the detection of remote sources that mainly contribute to the tracer concentration at an observation point. This property of Lagrangian models is widely used for data analysis and the reverse modeling of emission sources of a pollutant specified. In this work we describe the model and some results of its validation through a comparison with results of a similar model and observation data.

Keywords: Lagrangian model, air mass trajectory, turbulent diffusion, volcanic ash, carbon dioxide

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INTRODUCTION

Air-particle dispersion models are widely used in problems of the atmospheric transport of pollutants emitted during natural and technogenic catastrophes, such as volcanic eruptions and accidents at chemical plants and atomic power stations [1–4]. Such models were actively developed after the Chernobyl accident.

Dispersion models relate to the class of so-called Lagrangian models, where a change in the mixing ratio of any chemically active atmospheric pollutant is calculated along an air-particle trajectory, and the mixing ratio of a passive component along the trajectory remains constant. The absence of numerical diffusion, which is intrinsic to Eulerian (grid) models, originates due to the finite-difference representation of the continuity equation, and causes the artificial smoothing of tracer fields, is an advantage of Lagrangian models. In addition, it is difficult to specify a point source in grid models, e.g., an erupting volcano, since the initial ash concentration at the emission point instantly spreads over the grid cell. At the same time, Eulerian models have advantages in the long-term (over years) simulation of global propagation of atmospheric pollutants during a study of tropospheric-stratospheric exchange between hemispheres and climate changes, where Lagrangian models are not used due to significant computational efforts. Therefore, coupled Eulerian–Lagrangian models are currently being developed which combine the advantages of both approaches, e.g., [5].

Up-to-date dispersion models include such physical processes as advection, turbulent mixing, convection, gravity sedimentation, scavenging, etc. These models are used in the forward time direction, describing pollutant propagation from a source, and in the reverse direction, actually being conjugated models, which allows the detection of sources that affect the concentration at an observation point (receptor). The FLEXPART model [2] is an example of this class of model; its initial codes are freely accessible (http://transport.nilu.no/flexpart) and are widely used worldwide in view of validation in numerous international experiments. In this work, FLEXPART was used for calculating volcanic ash propagation to validate GLADIM.

Dispersion models are so-called off-line models, where prepared meteorological fields are used: reanalysis or prognostic data. To calculate trajectories, data from international weather analysis centers such as the National Centers for Environmental Prediction (NCEP), European Center for Medium-Range Weather Forecast (ECMWF), and Japan Meteorological Agency Climate Data Assimilation System (JCDAS) are used. These data are usually represented at nodes of a global regular grid at isobaric and model sigma-levels.

Existing and widely used Lagrangian dispersion models are mainly multitask and, hence, have a quite complicated structure, many components of which are not used when solving a specific task. In addition, there are problems the solution of which requires a modification of these models, which is often equivalent to the development of a new model. These circumstances inspire us to develop different versions of dispersion models specially intended for a more effective solution of a specific problem. A list of these problems and ways for their solution with the use of Lagrangian models are represented in [6] in sufficient detail.

In this work we describe GLADIM and the results of its testing and validation as applied to the propagation of volcanic ash and simulation of vertical profiles of carbon dioxide.

GLADIM DESRIPTION

The trajectory model of atmospheric pollutant transport TRACAO [7] is a key component of GLADIM. TRACAO was developed for the simulation of transport processes in the free atmosphere and for the analysis and planning of balloon and aircraft observations. The trajectory model and its version for accounting the turbulent mixing of air particles are briefly described below.

A fourth-order Runge–Kutta method with the linear spatial and temporal interpolation of wind data was used for the trajectory calculation. New horizontal coordinates of a moving air particle in spherical coordinates for a time step Δt can be found from the equations

$$\lambda(t + \Delta t) = \lambda(t) + \int_{t}^{t+\Delta t} \frac{u(\lambda, \varphi, t)}{R_e \cos\varphi} dt,$$

$$\varphi(t + \Delta t) = \varphi(t) + \frac{1}{R_e} \int_{t}^{t+\Delta t} v(\lambda, \varphi, t) dt,$$

where λ and φ are the longitude and latitude, respectively; u and v are the zonal and meridional wind speed and R_e is the Earth's radius.

The model uses data from international weather analysis centers specified on isobaric surfaces or at model sigma levels. The data can be represented on a Gaussian or regular grid with different spatial resolutions in a horizontal direction at each vertical level. The time resolution of meteorological fields is from 1 to 6 h. Three wind-speed components are key parameters for calculating 3D trajectories. To calculate isentropic trajectories, the horizontal components of wind and temperature are used. A vertical shift is calculated from the condition for potential temperature preservation; thus, an air particle moves along the same isentropic surface. Slow radiative heating/cooling is the main heat source in the stratosphere; therefore, adiabatic approximations are valid for trajectories of 10–15 days in duration. 3D trajectories are more reliable in the tropopause and troposphere, since adiabaticity is violated due to the latent heat of evaporation and condensation.

Thus, the trajectory model sets a bond between a source and a receptor in the form of the only trajectory. However, the turbulent mixing of air particles should be considered in real atmospheric conditions, especially near the Earth's surface. For example, the concentration of a pollutant from an emission source does not arrive unchanged to a certain point, but scatters in space in the form of cloud. The pollutant concentration measured at a certain point depends not on one emission source, but on their population. To consider the dispersion of air particles, the trajectory model was transformed into a multitrajectory model, which considers turbulent mixing of these particles. For this, a summand caused by turbulent mixing, which is considered a random process, is added to the advective shift of a particle at each time step. When simulating pollutant propagation with a short time step (about 1 s) near a source, a Langevin equation is solved to calculate the turbulent velocity in the boundary layer, where a correlation dependence between the velocities at neighbor time intervals should be considered. This algorithm requires significant computational efforts in the case of mesoscale and global simulation; therefore, longer time steps (15–20 min) are used in these cases, and the absence of a correlation dependence between velocities at neighbor time steps is assumed. In other words, the turbulent velocity at a time step is independent of the velocity at the previous step and particle coordinates are determined by a random value within limits specified by the diffusion coefficient. As was shown in [8], these models (the Monte Carlo model or random walk model) require significant less computational time without loss in quality when compared to more complicated models during mesoscale simulation. Since GLADIM was developed mainly for studying global atmospheric transport, this simplified algorithm was used in the model version presented.

An approach used in the SNAP model [9] was used in GLADIM for the parameterization of turbulent mixing. A horizontal shift induced by turbulent diffusion is written in spherical coordinates as

$$\Delta\lambda = \frac{rL}{R_e \cos(\varphi)}, \quad \Delta\varphi = \frac{rL}{R_e},$$

where $\Delta\lambda$ and $\Delta\varphi$ are the random walk path lengths in the zonal and meridional directions, λ and φ are the longitude and latitude, and r are random numbers with a homogeneous distribution in the range [–0.5, +0.5]. The random horizontal shift L is defined as [3]

$$L = aX^b$$

where $X = |V|\Delta t$, $|V| = \sqrt{u^2 + v^2}$, and $b = 0.875$ and $a = 0.5$ inside the boundary layer and 0.25 above it.

The particle coordinates inside the boundary layer in a vertical direction are determined based on the assumption of the homogeneous distribution in this region, i.e., complete mixing, which is valid for a

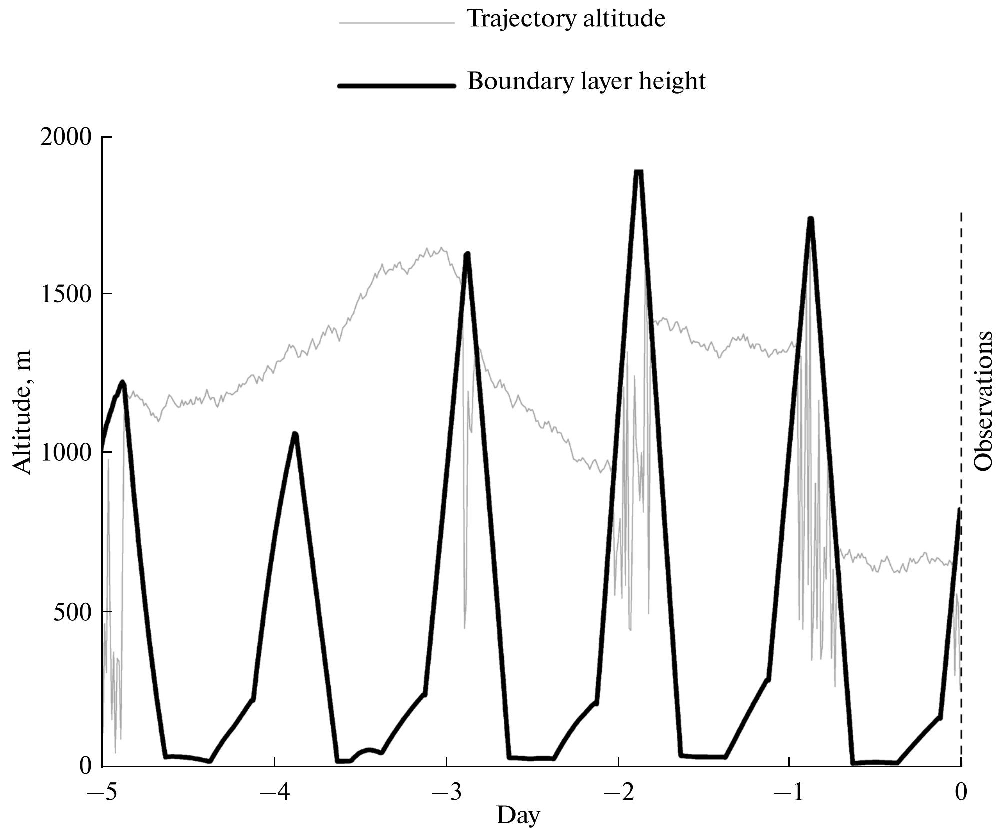

Fig. 1. Air-particle trajectory inside (gray curve) and outside (black curve) the boundary layer.

model time step of 15 min. Above the boundary layer, a vertical shift due to diffusion is defined as

$$\Delta p = g\rho r\sqrt{2\Delta t K_z},$$

where Δp is the random walk path length in the vertical direction (p is the pressure); g is the gravity acceleration; ρ is the air density; and K_z is the vertical diffusion coefficient, which is about 1 K_z in the free troposphere [10]. Figure 1 exemplifies variations in the air-particle altitude along a trajectory inside and outside the boundary layer. The parameterization described is applicable for simulating long-range atmospheric transport, including global transport. At the current stage, the model does not include convection parameterization, which is planned to be implemented in the following version of the model.

To calculated the mass concentration of a tracer (e.g., volcanic ash) in a 3D cell (i, j, k) of a regular grid at a source power specified, we used the equation

$$C^n_{i,j,k} = \frac{Mtn^n_{i,j,k}}{V_{i,j,k}N}10^6,$$

where $C^n_{i,j,k}$ is the concentration in the (i, j, k) cell at the time point t^n (mg/m^3), M is the source power (kg/s), t is the emission time (s), $n^n_{i,j,k}$ is the number of air particles in the (i, j, k) cell at the time point t^n, $V_{i,j,k}$ is the volume of the (i, j, k) cell (m^3), and N is the total number of air particles emitted. Thus, the propagation of a floating up cloud of particles is calculated during the forward simulation instead of a trajectory of an air particle; this allows the calculation of the concentration of these particles in cells of a global grid. During the reverse simulation, air-particle back trajectories are calculated from an observation point connecting a receptor with a potential source.

GLADIM VALIDATION

GLADIM operating in the forward time direction was validated with the use of FLEXPART calculation results of volcanic ash propagation after the Iceland volcanic eruption of April 14, 2010. The quality of FLEXPART calculations in that case was confirmed by lidar data from Troitsk for April 19, 2010 [11]. This GLADIM version does not consider particle sedimentation; therefore, calculations by both models were carried out for a passive tracer without accounting the sedimentation. Other input data for the models were taken from [11]. The GLADIM modification was mainly aimed at the model capability of calculating ash particle concentrations in cells of a regular grid at different altitude levels at certain time instants and the mean concentration in a specified air layer during a continuous 4-day emission.

Figure 2 shows the fields of the mean tracer concentrations in a 4–6-km layer calculated with FLEXPART

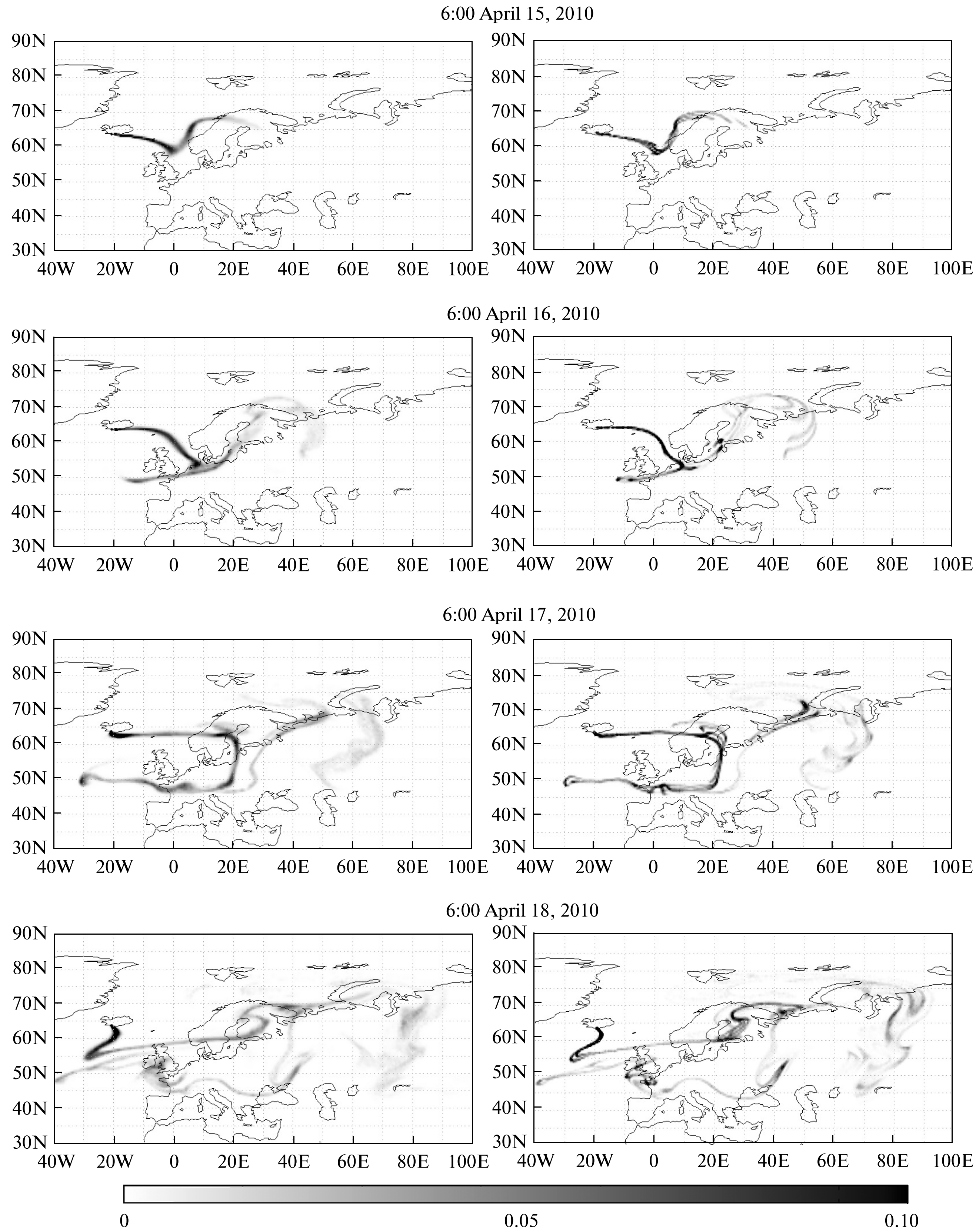

Fig. 2. Fields of the tracer concentration (mg/m^3) on the basis of FLEXPART (left) and GLADIM (right) model calculations.

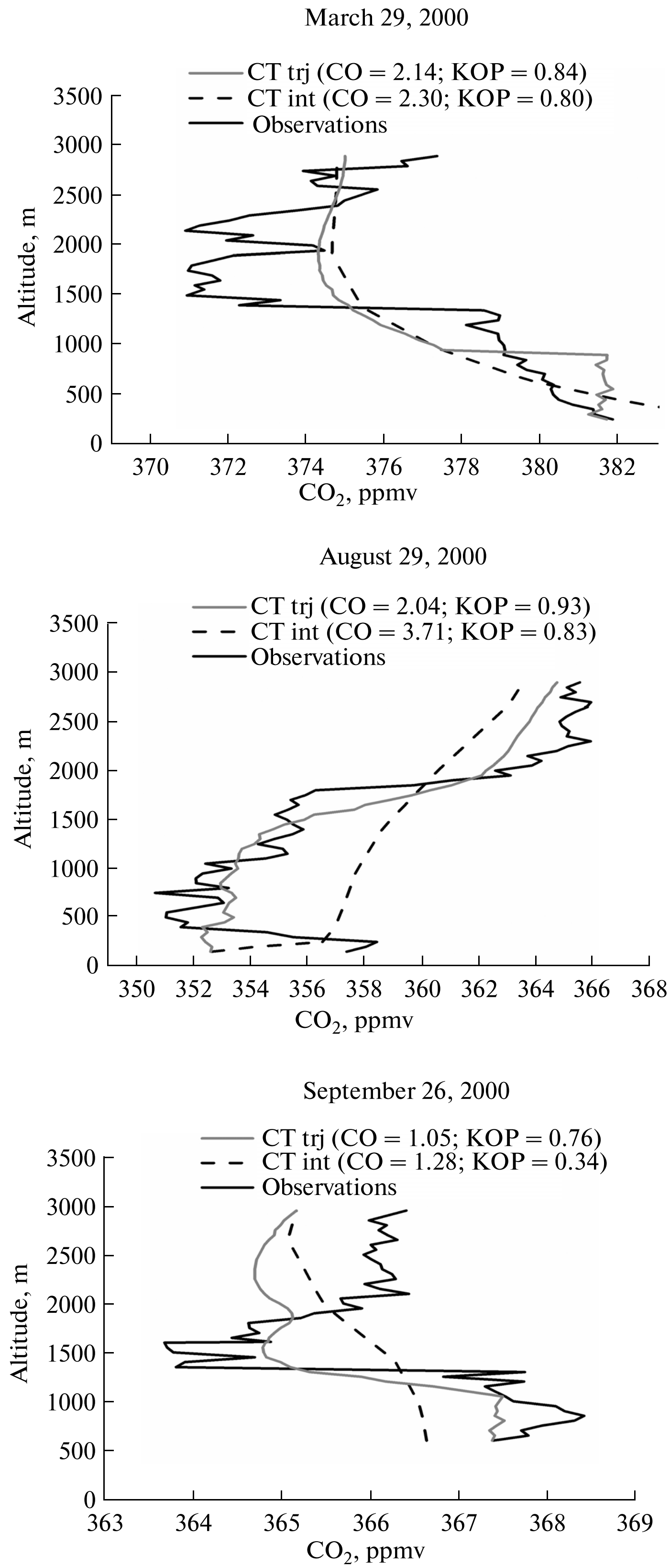

Fig. 3. Vertical CO_2 profiles: aircraft observations (solid black curve), interpolated CT data (dashed black curve), and GLADIM simulation results (gray curve).

(left) and GLADIM (right). ERA-Interim data on weather parameter [12] were used in the GLADIM calculations, and NCEP data [13] were used in the FLEXPART calculations. Though different models and different input data were used, the resulting concentration fields agree well. Thus, the results of the comparison show the efficiency of GLADIM.

To validate GLADIM operating in the reverse direction, the vertical profiles of carbon dioxide calculated with the model and measured with a high-resolution LICOR-6251 IR analyzer onboard an aircraft in a boundary layer from 0 to 3 km (st. Fedorovskoye (56° N, 33° E), 2000) were compared. The temperature and relative humidity were also measured. To simulate CO_2 vertical profiles with GLADIM, 100 air particles were initialized at each point of an aircraft profile, and 3-day back trajectories were calculated for each particle. CarbonTracker (CT) data [14], which are global 3D concentrations fields and 2D surface CO_2 fluxes, were used to calculate the CO_2 mixing ratios at the end points of back trajectories. Values of these initial concentrations were transferred invariably along the trajectories to an observation point in the free atmosphere. For trajectories inside the boundary layer, the depth of which was taken from the ERA-Interim database, concentrations were changed with accounting for contributions of surface CO_2 fluxes, also taken from CarbonTracker.

Figure 3 shows the comparison results for model and aircraft CO_2 profiles for March 29, August 29, and September 26, 2000. The aircraft profile is shown by the black curve; the (CT trj) model profile found from CT data trajectory attraction is shown by the solid gray curve and the (CT in) profile found from direct interpolation of CT data to an observation point from the nearest grid nodes is shown by the dashed curve. The standard deviation (SD) of the CT trj and CT int profiles from aircraft measurements and the corresponding correlation coefficients are also shown. It is evident from Fig. 3 that the model CO_2 profiles reproduce gradients at the boundary layer—free atmosphere interface better than the interpolated profiles. Thus, the results show that GLADIM can be used for the reconstruction of observation data on atmospheric component concentrations and, hence, for the reverse simulation of their surface sources.

CONCLUSIONS

The GLADIM global Lagrangian atmospheric dispersion model is described. It is based on a trajectory model that includes the parameterization of turbulent mixing of air particles. The parameterization supposes the stochastic character of diffusion and different values of mixing parameters in the boundary layer and free atmosphere.

To validate GLADIM, which operates in the forward time direction, the propagation of volcanic ash was calculated without accounting for sedimentation and the results were compared with similar calculations by the FLEXPART model. Fields of volcanic-ash concentrations found with the use of the two models show a good agreement.

GLADIM was also used to simulate vertical profiles of carbon dioxide. The comparison with aircraft observations has shown that the model profiles correlate with the observations better than profiles found from a simple interpolation of grid concentration values.

The model developed has been used for the planning and analysis of balloon and aircraft observations, as well as for the forward simulation of pollutant propagation and the reverse simulation of pollutant sources. In the future, we plan to include convection and dry and wet sedimentation processes in the model.

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