4.8 Chemical Transport Model

4.8.1 Introduction

JMA started to provide Kosa information in January 2004. JMA also started to provide UV index information in May 2005. The products are provided via internet by JMA and the Japan Meteorological Business Support Center. The sample products are shown in Fig. 4.8.1 to Fig. 4.8.3. The Chemical Transport Models (CTM) are the basis of these products. In the CTM, the chemical modules are directly coupled with the MRI-JMA98 General Circulation Model (Shibata et al., 1999) and can make use of several GCM parameters without temporal or spatial interpolation. The schematic illustration of the structure of CTM is shown in Fig. 4.8.4 and 4.8.5. The resolutions of the GCM are T106L30 for Kosa prediction model and T42L68 for stratospheric ozone model, respectively. The forecast period of these models is 2 days. For UV index information, the radiative transfer model (Aoki et al., 2002) is also used to calculate UV index based on the total ozone amount predicted by the CTM.

4.8.2 General Circulation Model

(a) Basic framework

The GCM is based on a global spectral model, which was operationally used for weather forecasting at the JMA (GSM9603). The GCM was improved in some physical processes (Shibata et al., 1999). The radiation scheme was upgraded to the solar and terrestrial radiation scheme (Chiba et al., 1996) to yield sufficient accuracy in the middle atmosphere. The ground hydrology scheme



Fig. 4.8.1 Kosa information web page (http://www.jma.go.jp/jp/kosa/).



Fig. 4.8.2 Clear sky UV index forecast (http://www.jma.go.jp/en/uv/).



Fig. 4.8.3 UV index forecast (http://www.jma.go.jp/en/uv/).

was also updated. Soil layers for temperature were increased from two to three layers, similar to those for water, leading to a precise treatment of melting and freezing of water through the consistency between heat and water budgets.

(b) Relaxation to analyzed/forecasted field

In general, CTM needs more computational resources than GCM. Therefore a spatial resolution of CTM tends to be lower than an operational weather forecast model. To solve this problem, the GCM has a built-in, four-dimensional data assimilation system with a nudging scheme incorporating an assimilated and forecasted meteorological field as in equation 4.8.1, where x is a dynamical variable, x_{analysis} is an analyzed/forecasted variable, and T is the time scale of relaxation (currently set to 12 - 24 hours). This scheme

enables the CTM to realistically simulate a meteorological field during a forecast period.

$$\left(\frac{\partial x}{\partial t}\right)_{nudging} = -\frac{x - x_{analysis}}{T}$$
(4.8.1)

4.8.3 Chemical Module (Kosa prediction model)

(a) Basic framework

The Chemical Transport Model used for Kosa information is called MASINGAR (Model of Aerosol Species IN Global Atmosphere; Tanaka et al., 2003). The MASINGAR includes non sea salt sulfate, carbonaceous, mineral dust and sea—salt aerosols, and accounts for advective transport (3D semi-Lagrangian scheme), sub-grid scale eddy diffusive and convective transport, surface emission and dry/wet depositions as well as chemical reactions. To provide Kosa information, we focus on mineral dust aerosol. The vertical resolution of the chemical module is reduced to T106L20 from the GCM (T106L30) in order to decrease computational cost. The emission flux of mineral dust aerosol depends on meteorological, geographical and soil surface conditions, such as wind speed, land use, vegetation, soil moisture and soil types. The dust emission flux F is expressed as a function of wind speed at 10m (U_{10}) and the



Fig. 4.8.4 The schematic illustration of the structure of CTM (Kosa prediction model).



Fig. 4.8.5 The schematic illustration of the structure of CTM (stratospheric ozone model).

threshold wind velocity U_t as in equation 4.8.2.

$$F = CMA \frac{W_{gt} - W_g}{W_{gt}} (U_{10} - U_t) U_t^2 \quad for \quad U_{10} > U_t \quad and \quad W_{gt} > W_g$$
(4.8.2)

where *C* is a dimensional factor, *M* is the ratio of mass of dust in the size bin to total mass, *A* is the erodible fraction of the surface, W_g is the soil moisture, and W_{gt} is the threshold soil moisture (currently set to 0.3kg/m^2). The threshold wind velocity U_t is set to 6.5 m/s.

(b) Relaxation to analyzed/forecasted field

Due to the lack of real-time observational data of Kosa concentration, the chemical module in Kosa prediction model does not have Kosa assimilation system at this time. As the land surface conditions (soil water and snow) affects the amount of Kosa emission, the chemical module in Kosa prediction model has a data assimilation system which could assimilate snow depth analysis mentioned in section 3.11. This system can remove snow at the surface of GCM where there is no observational snow. The schematic table of data assimilation in Kosa prediction model is shown in table 4.8.1.

 Table 4.8.1. The schematic table of data assimilation in Kosa prediction model.

 From -24 hour to initial
 Initial to 48 hour forecast

	From -24 hour to initial	Initial to 48 hour forecast
Meteorological field	Global analysis	Global forecast
Snow depth	Snow depth analysis	-

(c) Verification

Currently, we do not have the Kosa quantitative observational data, therefore the forecast by Kosa prediction model is verified against the surface synoptic observation (present weather (ww)). We have calculated the model score using categorical verification similar to section 4.9 (shown in Table 4.8.2). The threshold value for Kosa forecast (currently set to 150µg/m³) is determined to maximize the Equitable Threat Score (ETS). The ETS of Kosa prediction model (24hr forecast, Japan area) are 0.26, 0.12 and 0.15 in 2004, 2005 and 2006 spring, respectively. In the spring of 2007, we have a plan to update Kosa prediction model. The first main change is to update surface vegetation data obtained by the satellite observation. The second change is to enhance the relaxation to analysis/forecast field.

Table 4.8.2 Verification indices for categorical forecast.

	Observed(ww=06-09, 30-35,98)	Not Observed (ww=00-05)		
Forecasted (Surface Kosa concentration is larger than $150\mu g/m^3$)	FO	FX		
Not Forecasted (Surface Kosa concentration is smaller than $150\mu g/m^3$)	ХО	XX		

4.8.4 Chemical Module (stratospheric ozone model)

(a) Basic framework

The chemical module in stratospheric ozone model was developed in Meteorological Research Institute (MRI) (Shibata et al., 2005). The chemical module is composed of chemical processes and a transport process. The chemical process is based on the family method and contains major stratospheric species, i.e., 34 long-lived species including 7 families and 15 short-lived species with 79 gas phase reactions and 34 photodissociations. The names of these species are shown in table 4.8.3. Two types (I and II) of polar stratospheric clouds (PSCs) and sulfate aerosols are included with six heterogeneous reactions on PSCs and three heterogeneous reactions on sulfate aerosols, respectively.

Long-lived						
01: N ₂ O	02: CH ₄	03: H ₂ O	04: NO_{y}	05: HNO ₃	06: N ₂ O ₅	
07: Cl_{y}	08: O _x	09: CO	10: OClO	11: CO ₂	12: Aerosols	
13: HCl	14: ClONO ₂	15: HOCl	16: Cl ₂	17: H ₂ O ₂	18: ClNO ₂	
19: HBr	20: BrONO ₂	21: NO _x	22: HO ₂ NO ₂	23: ClO _x	24: BrO _{<i>x</i>}	
25: Cl ₂ O ₂	26: HOBr	27: CCl ₄ (CFC-10)	28: CFCl ₃ (CFC-11)	29: CF ₂ Cl ₂ (CFC-12)	30: Br _v	
31: CH ₃ Cl	32: CH ₃ Br	33: CF ₂ ClBr(Halon1211)	34: CF ₃ Br(Halon1301)			
$O_x = O_3 + O(^{3}P) + O(^{1}D)$						
$ClO_x = Cl + ClO$ $Cl_y =$		$Cl_{y} = ClO_{x} + OClO + 2 Cl_{2}O_{2} + HCl + ClONO_{2} + HOCl + 2 Cl_{2} + ClNO_{2} + BrCl$				
$NO_x = NO + NO_2 + NO_3$ $NO_y = NO_x + N + HNO_3 + 2N_2O_5 + HO_2NO_2 + CIONO_2 + CINO_2 + BrONO_2$						
$BrO_x = Br +$	$BrO_x = Br + BrO + BrCl$ $Br_y = BrO_x + HBr + HOBr + BrONO_2$					
Short-lived						
$01: O(^{1}D)$	02: OH	03: Cl	$04: O(^{3}P)$	05: O ₃	06: HO ₂	
07: NO ₂	08: NO	09: Br	10: N	11: ClO	12: BrO	

Table 4.8.3 Names of species in the chemical module (ozone).

The transport scheme of chemical species is a "hybrid" semi-Lagrangian scheme, which is formulated to be compatible with the continuity equation, resulting in different forms for horizontal and vertical directions. The horizontal form is an ordinary semi-Lagrangian scheme. The vertical form is equivalent to a mass-conserving flux-form.

The operational global spectral model mentioned in section 4.2 makes use of the 3-dimensional monthly mean ozone climatology calculated by the stratospheric ozone model nudging with analyzed meteorological field and satellite data as a boundary condition.

(b) Relaxation to observational data

14: BrCl

15: H

13: NO₃

The chemical module in the stratospheric ozone model has an assimilation system similar to meteorological field (equation 4.8.1) which could assimilate total ozone obtained once a day by Ozone Monitoring Instrument (OMI) of the

Aura spacecraft (NASA). The weight of the model guess and OMI data are determined by the root mean square error against the surface observational data. We adopt the mixing ratio for nudging of CTM and OMI as 1:3. The schematic table of data assimilation in stratospheric ozone model is shown in table 4.8.4.

Table 4.0.4. The schematic table of data assimilation in stratospheric ozone model					
	From -24 hour to initial	Initial to 48 hour forecast			
Meteorological field	Global analysis	Global forecast			
Total ozone	OMI daily data	-			

Table 4.8.4. The schematic table of data assimilation in stratospheric ozone model

(c) Verification

The CTM's predictability on total ozone is investigated for up to 4 weeks from 1997 to 2000 (Sekiyama et al., 2005). Global root-mean-square errors (RMSEs) of a control run are approximately 10 DU (3% of total ozone) throughout the year; the control run results are used as initial values for hindcast experiments. RMSEs of the hindcast experiments globally range from 10 to 30 DU. The anomaly correlation between the 5-day forecasts and satellite measurements is approximately 0.6 throughout the year in the mid- and high latitudes of both the Northern and Southern Hemispheres. Thus, the model has potential for utilization on total ozone forecasts up to 5 days. In the northern mid- and high latitudes, the model produces better total ozone forecasts up to 2 weeks than the persistence.

4.8.5 Radiative transfer model (Look-Up Table method)

(a) Basic framework

UV index is calculated by the radiative transfer model (Aoki et al., 2002). Considering the computational cost, the Look-Up Table method (LUT) is adopted. The basic parameters of LUT are solar zenith angle and total ozone predicted by the CTM. The clearsky UV index is corrected by aerosol (climatology), the distance from the sun, altitude and surface albedo (climatology). The forecasted UV index is also corrected by categorized weather forecast mentioned in section 5.6.

(b) Verification

The clear sky UV index calculated by the LUT is verified



Fig. 4.8.6 Verification of UV index calculated by LUT against observation.

against the UV index observation. A verification result is shown in Fig. 4.8.6, where the 'x' shows the UV index considering measured aerosol optical depth and '+' shows the UV index without aerosol correction. The result shows the importance of the aerosol treatment in UV index calculation. The mean error of the calculated clear sky UV index is 0.0 and the RMSE is 0.5.

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