DMS model Calibration Using Genetic Algorithm

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Abstract— Recent researchers suggested Dimethyl sulphide (DMS) flux emission in Arctic Ocean plays an important role for the global warming. A Genetic Algorithm (GA) method was developed and used in calibrating the DMS model parameters in Barents Sea in Arctic Ocean (70-80N, 30-35E). Two-step GA calibrations were performed. First step was to calibrate the most sensitive parameters based on Chlorophyll_a (CHL) satellite SeaWIFS 8-day data. DMS model was then calibrated for another 5 most sensitive parameters. The best fitness was as good as -0.76 for CHL calibration in 1998-2002. The GA proved an efficient tool in the multiple-parameter calibration task. Model simulations indicate significant inter-annual variation in the CHL amount leading to significant inter-annual variability in the observed and modeled production of DMS and DMS flux in the study region in Arctic Ocean.

Keywords—Genetic Algorithm; Arctic; Calibration; Dimethyl sulphide flux; Chlorophyll_a

I. INTRODUCTION

Dimethyl sulphide (DMS) is the main sulphur released during the decay of ocean biota [1]. Aerosols formed from the conversion of DMS to sulphate and methanesulphonic acid (MSA) can exert a climate cooling effect directly by scattering and absorbing solar radiation, and indirectly by promoting the formation of cloud condensation nucleii (CCN) and hence increase the albedo of clouds, reflecting more solar radiation back to space, thus cool the climate [2]. DMS has been estimated to contribute 60% of the natural emissions of sulphur to the atmosphere [3].

As the 80% Arctic Ocean is covered by ice, the steady decreasing rate of ice cover would give rise to a stratified and nutrient-rich euphotic zone, which supports pronounced spring bloom in the marginal ice zone (MLZ)[4]. Ice melting phenomenon also affects the sea levels and ocean circulations, hence it has significant impact on global climate. The Barents Sea has been indicated as a major productivity site that transports the productivity signal to all water masses in the Eurasian Basin (Olli et al., 2002). Gabric et al. (1999) [5] calculated DMS production and cycling in the central Barents Sea based on data sampled in May 1993 in the four stations [6]. where dynamics of vernal bloom and their contribution to DMS (DMSP) were discussed early by in Matrai and Vernet [6]. This paper will investigate the impact of simulated climate change on the DMS in the year 1998 to 2002 based on the calibrated satellite data (CHL) in the same study region.

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A noval Genetic Algorithm was developed to calibrate the most sensitive parameters in DMS model. DMS and DMS flux concentration in the study region were produced and compared.

II. THE MODEL AND METHOD

A. The updated DMS model

The DMS model was firstly introduced by Gabric, et al., (1993)[7] which was adapted the ecological structure of the nitrogen-based plankton community model of (Moloney et al., 1986). The model was a depth averaged model and was developed and used for sub-Antarctic southern ocean modeling [8]. The DMS model parameters are as Table 1.

TABLE I. DMS MODEL COMPARTMENT

Compartments	Description
XI = P	Phytoplankton
X5=Z	Zooplankton
X6=N	Nitrogen (as nitrate)
X7=DMSP	Dimethyl sulfoniopropionate
X8=DMS	Dimethyl sulfide

The basic equations for DMS model is listed below:

$$\frac{dP}{dt} = k_{23} \left(\frac{N}{N + k_{24}} \right) P - k_4 P Z \tag{1}$$

$$\frac{dZ}{dt} = k_4 (1 - k_{20}) P Z - k_{19} Z \tag{2}$$

$$\frac{dN}{dt} = k_{19}Z + k_4k_{20}PZ - k_{23}\left(\frac{N}{N+k_{24}}\right)P$$
(3)

$$\frac{\partial DMSP}{\partial t} = k_5 P + k_{21} Z - k_{27} DMSP - k_{31} DMSP$$
(4)

$$\frac{\partial DMS}{\partial t} = k_6 P + k_{27} DMSP - k_{28} DMS - k_{29} DMS - k_{30} DMS$$
(5)

where parameter k_i (1<*i*<31) are listed in Table 2.

TABLE II. PARAMETER VALUES QUATED FOR THE DMS MODEL

PAR	PROCESS		
k4	Z grazing rate on P		
k5	Release rate of DMSP by P		
k6	Release rate of DMS by P		
k19	Z soecufuc N excretion rate		
k20	Prop of N uptake excreted by Z		
k21	DMSP excretion rate by Z		
k23	Maximum rate of N uptake by P		
k24	Half-sat const for P uptake of N		
k27	DMSP-DMS conversion rate		
k28	DMS consumption rate by B		
k29	Maximum DMS photo-oxidation rate		
k30	DMS ventilation rate to atmosphere		
k31	DMSP consumption rate by B		
γ	Photoplankton S (DMSP):N ratio		
No=P+Z+N	Total nutrient		

Phytoplankton in Arctic Ocean is exposed to strong seasonal variations of day length, solar radiation and sea ice coverage [9]. In general, phytoplankton growth is affected by the availability of light, temperature and nutrient. The nutrient uptake rate is defined by (Platt et al. 1977):

$$\mu(t) = V_N(t)R_L(t)R_T(t) \tag{6}$$

where V_N is the nutrogen-specific nutrient uptake rate described by Michalis -Menten kinetics. R_L and R_T are dimensionless light and temperature limitation coefficients in the range of (0,1). They are defined by follows (equations (7) and (8)):

$$R_L = P / P_{\text{max}} = (I / I_k) (1 + (I / I_k)^2)^{-0.5}$$
(7)

where P is the gross phytosynthetic rate and P_{max} is the maximum phytosynthetic rate. I is the irradiance at a particular depth, I_k is the saturating irradiance that was measured from incubation experiment at each station.

$$R_T = e^{0.063(T - T_{\max})} \tag{8}$$

where T is the mean mixed layer temperature (Celsius) and $T_{\rm max}$ is the maximum temperature. Equation (8) is used originally by Eppley (1972) [11], where excluded temperature below zero. However, in Arctic Ocean, it is common to have temperature below zero. This equation is still valid for the Arctic Ocean.

The production of DMS in ocean could be described by equation [12]:

$$\frac{dDMS}{dt} = F_P + F_{DMSP} - F_B - F_{photo} - F_{air}$$
(9)

Where F_P is the release of DMS from phytoplankton cells; F_{DMSP} is the production of DMS from DMSP; F_B is the loss of DMS due to bacterial consumption; F_{photo} is the loss of DMS due to the photolysis; F_{air} is the loss of DMS due to emission to the atmosphere. The ventilation of DMS to the atmosphere was calculated by production of DMS mixed layer concentration $\Delta C(=C_O - C_A)$ and DMS sea-to-air transfer velocity K_w (Liss and Merlivat, 1986), where C_0 and C_A are the DMS concentration from the ocean and from the atmosphere respectively. As the atmospheric concentration of DMS (C_A) is very small comparing to C_0 [13], the sea-air flux of DMS can be written as

$$F_{air} = K_w C_O \tag{10}$$

where transfer velocity K_w is mainly dependent sea surface temperature (*SST*) and wind velocity (10 metres above the sea surface). Gabric et al. (1995) [14] has rescaled for DMS and given as following:

$$K_{w} = 0.17(600/Sc)^{2/3}w \qquad \text{for } w \le 3.6$$

$$K_{w} = (600/Sc)^{1/2} (2.85w - 10.26) + 0.612(600/Sc)^{2/3}$$

$$\text{for } 3.6 \le w \le 13$$

$$K_{w} = (600/Sc)^{1/2} (5.9w - 49.91) + 0.612(600/Sc)^{2/3}$$

$$\text{for } w > 13$$
(11)

where *Sc* is the temperature-dependent Schmidt number given by Erickson et al. (1990):

$$Sc = 2674.0 - 147.12 * SST + 3.726 * SST^{2} - 0.038 * SST^{3}$$
(12)

Although the DMS transfer velocity by Liss and Merlivat (1986) is widely used by many researchers, the DMS flux predicted from the relationship of Liss and Merlivat (1986) may be under-estimated by as much as 30% (Archer et al., 2002). It should be noted that the DMS ventilation can only occur in ice-free waters. Thus, in Arctic Ocean covered with large area of ice, the computed DMS transfer velocity should be scaled by the percentage of ice-free waters [5].

III. METROLOGICAL AND SATELLITE DATA FOR DMS FORCINGS

The study region is located in Barents Sea in east Arctic Ocean (30-35E, 708-80N). Before starting the calibration process, the mean time series of metrological and satellite data are obtained and calculated. Sea Surface Temperature (SST) (1998-2002) were obtained from Reynolds/NCEP (monthly time series spatial average in the study region). Surface wind speed was from QuikSCAT daily spatial average calculations based on HDF data files (http://podaac.jpl.nasa.gov/quikscat, Level 3). Mixed layer depths (MLD) are from the Levitus World Ocean Atlas (WOA94) based on long-term monthly history data (Boyer and Levitus, 1994). The ice cover is derived from NCDC Special Sensor Microwave Imager (SSMI) satellite 1.0-degree data. The cloud cover is calculated from Data Support Section, NCAR/SCD (http://www.dss.ucar.edu/datasets/ds540.9).

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IV. DMS MODEL CALIBRATION USING GENETIC ALGORITHM

The DMS is used (see equation $1\sim5$) and the satellite and metrological data SST, Wind Speed, Cloud Cover and MLD were calculated before the model simulations.

The new version of Genetic Algorithm (GA) calibration for the DMS model is developed based on the FORTRAN program provided by David L. Carroll in CU Aerospace, IL. This code initializes a random sample of individuals with different parameters to be optimized using the genetic algorithm approach, i.e. evolution via survival of the fittest. The selection scheme used is tournament selection with a shuffling technique for choosing random pairs for mating. The simplified DMS model is placed as a subroutine of the program and the fitness function is updated by using negative value with maximum optimization rule applied.

CHL Calibration

The most sensitive 6 parameters were calibrated based on CHL satellite SeaWiFS data. They are: k4, k19, k20, k23, I_k and No (=P+Z+N). DMS model simulations were run for one year starting from Julian day 1. Actually CHL were only available from 12th March to 27th September in SeaWIFS. The time square root fitness function is used for every 7-days output. Hence the weekly satellite data is used for SST and wind speed. The monthly meteorological data (cloud cover, ice cover and MLD) were all converted to weekly data.

The reference values in Barents Sea from Gabric et al. (1999) [5] station 1 and 2 were used for the first instance. The initial values were adjusted one at a time after comparing with the SeaWiFS CHL data. The total number of nutrient was set reasonable large (between 500-1000) in order to generate a force for initial spring bloom (this is based on Table 2, [5]). Two parameters I_k and k4 are the most sensitive parameters. It was found that the smaller the k4 value is, the higher the bloom peak is; the smaller the saturating irradiance value I_k is, the earlier the bloom peak would appear.

DMS Calibration

Based on CHL calibration for the 6 parameters, DMS model is calibrated for another 5 most sensitive parameters: γ , k27, k28, k29, k31 [5]. The initial DMS and DMSP values were all set to zero [5]. There are limited resources for DMS calibrations. The monthly DMS data from Kettle and Andreae(1999) in Arctic area was firstly compared with the DMS generated by calibrated DMS model using SeaWiFS satellite data. It shows mismatches for the bloom patterns although the peak periods are all in July. The large differences on its time scale, spatial scale and large area ice cover could be all the reasons causing the mismatches. Three cruises launched in our study region in March, May 1998 and June, July 1999 ([6]) provided some useful DMSPd field data for DMS calibrations.

The mean algal cell S: N ratio γ is one of the most sensitive parameter for DMS and DMSP productions. The range of γ value was estimated by comparing the model DMSP results

and the field data. $\gamma = 0.3$ is used for the rest of years while $\gamma = 0.06$ is used for year 1999. DMSP-DMS conversion rate k27 is set to 0.1 which is much lower than the previous setting as 0.5 by Gabric et al. (1999). According to Bouillon et al.[17], the DMSP is almost 3~5 times higher than DMS in the Northern water in 1998. Kettle et al. ([16]) provided DMS in ARCT and SARC regions (monthly data) with the highest of 20 nM in June, while the DMSPd field data reached to more than 70nM in May 1998 in our study region. Hence, based on the limited knowledge of DMS in Arctic Ocean, k27 valued was set as 0.1 in the DMS model, in order to make similar peak value of DMS based on Kettle's data. DMS consumption rate k28 is set to 0.2 (the value between station 1 and 2 in Gabric et al. 1999). However, in order to match the DMSP field data, the maximum DMS photo-oxidation rate has to be reduced to 0.1 and DMSP consumption rate by B has to be reduced to 0.2 in 1999 and 0.1 in the other years.

V. RESULTS

A. GA Calibration in Barents Sea

According to the adjusted parameter values based on Gabric et al. (1999) and SeaWiFS CHL satellite data, the Genetic Algorithm program was used for searching the best-fit values for the 6 parameters: k4, k19, k20, k23, I_k , No(=P+Z+N). The mean CHL SeaWiFS data was used for the calibrations. Fig. 4 shows the comparisons for the calibrated model results and the original SeaWiFS data for year 1998-2002. The fitness=-0.76 which is excellent fit (the more close to zero the better fitness result).We used GA Calibration: 50 population, 80 generation for 1998-2002 mean CHL. The parameter values are shown in Table 3.

TABLE III. GA CALIBRATION RESULTS FOR THE SENSITIVE PARAMETERS

PAR.	1998 fitness=-2.9	1999 fitness=-4.1	Mean for 1998-2002 fitness=-0.76
k4	0.00002112	0.00002127	0.000055
k19	0.084	0.0041	0.0424
k20	0.0188	0.3101	0.1381
k23	0.3186	0.3658	0.4964
Ik	17.5693	9.5739	11.3997
No	453.65	440.32	532.88
k27	0.2751	0.1030	0.2751
k28	0.1115	0.1519	0.1115
k29	0.4421	0.0329	0.4421
k31	0.2541	0.0541	0.2541
γ	0.6943	0.0758	0.6943



Fig. 1. GA Calinration for 1998-2002 mean CHL for zonal 70-80N.

B. The Distribution of DMS and DMS Flux

Based on the calibrated DMS model, the inter-annual concentrations of DMS were calculated (Fig. 2). The DMS concentrations were low in winter and gradually increased to its peak in later spring. The first DMS bloom was always happened a few days (5-6 days) after the CHL spring bloom (not shown in figure). The double peak of DMS appeared in most of the years, triple peaks happened in year 2002. The duration of the two peaks is increased from 40 days in 1998 to 66 days in 2002 (first two peaks in 2002). Year 2002 DMS peak time lasted more than 3 month from day 124 to 220. The DMS spring blooms were shifted from late April to early April in the 5 years. For the other less productive years (1999 and 2000) with less radiation in spring, the DMS concentrations are also relatively lower. Year 2002 is the most productive year with its peak value of over 30 nM in early April and year 1999 is the least productive year with its peak DMS of 4.6 nM in late April. We noticed that a small DMS bloom always happened in autumn (late Oct. to early November), this is followed by a small CHL bloom in September (more obviously in 2001 and 2002).



Fig. 2. 5 years DMS (nM) comparison in the study region.

As there is an empirical relation between DMS flux, F_{DMS} and the concentration of CCN (Cloud condensation nuclei) (Lawrence, 1993):

$$CCN = 29F_{DMS} + 45 \tag{13}$$

Hence, it is crucial to quantify the flux of DMS from the oceans to investigate its impact on atmospheric chemistry and radiative transfer [16]. The DMS flux is related with the SST and the wind speed. Hence, the changing on temperature or wind speed could cause significant changes of the regional DMS flux.

The DMS flux is calculated in the ice-free water. 5 vears DMS flux time series was calculated according to the parameters in Table 3 (Fig. 3). It is clear that the year 2002 was the most DMS emission year and year 1999 was the least DMS emission year. The inter-annual variability of DMS Flux was high in the study region. It is proved that the high interannual variability in DMS flux could occur at high latitude [16]. The high inter-annual variability of DMS flux could be caused by high inter-annual variability of CHL as well as the wind speed and SST records. We notice that year 1998 was the second DMS productive year next to year 2002. Considering the SST and wind speed had not had significant increase in year 1998, the higher production of DMS flux may be related to the fact that more and larger area of ice cover in the southern part of the region in that year[19]. The important source of DMSP and DMS could come from larger area of ice algae in 1998.



Fig. 3. Monthly Mean DMS Flux in Ice Free Water for Year 1998-2002 in the Study Region.

VI. CONCLUSIONS

A developed Genetic Algorithm was used in calibrating the DMS model parameters. Satellite data and field data sets were used for calibrating a regional DMS production model. The GA proved an efficient tool in the multiple-parameter calibration task. Model simulations indicate significant interannual variation in the CHL amount leading to significant interannual variability in the observed and modeled production of DMS in the study region.

The Arctic Ocean circulations and its special characteristic of ice cover, low temperature and long dark winter made the unique marine biological cycle and hence its unusual effect on the marine sulphur cycle. The large area of Arctic ice melting in spring could influence the sea level, ocean circulation and nutrient-rich euphotic zone, hence the significant spring vernal bloom happened right after ice cover started melting. The icealgae contributed high DMSP content and high biomass of

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Phaeocystis sp. and *Emiliania huxleyi*, could lead to subsequent production of large quantities of DMS. The DMS is low in the winter and high in summer could be cited as indication of a negative feedback in the Charlson et al. (1987) hypothesis. The maximum DMS production takes place during the declining phase of algal blooms. The high inter-annual variations of CHL led to high inter-annual variation of DMS flux (to air). The relative higher production of DMS flux and earlier DMS spring bloom in year 1998 could be related to the fact of the more ice cover (hence more ice algae) in southern part of the study region. The significant decrease of ice cover from August to October is the main reason of increasing DMS flux. This would contribute great impact on global warming.

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