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Can we trust simple marine DMS parameterisations within complex climate models?

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Abstract

Dimethylsulphide (DMS) is a globally important aerosol precurser. In 1987 Charlson and others proposed that an increase in DMS production by certain phytoplankton species in response to a warming climate could stimulate increased aerosol formation, increasing the lower-atmosphere's albedo, and promoting cooling. Despite two decades of research, the global significance of this negative climate feedback remains contentious. It is therefore imperative that schemes are developed and tested, which allow for the realistic incorporation of phytoplankton DMS production into Earth System models. Using these models we can investigate the DMS-climate feedback and reduce uncertainty surrounding projections of future climate. Here we examine two empirical DMS parameterisations within the context of an Earth System model and find them to perform marginally better than the standard DMS climatology at predicting observations from an independent global dataset. We then question whether parameterisations based on our present understanding of DMS production by phytoplankton, and simple enough to incorporate into global climate models, can be shown to enhance the future predictive capacity of those models. This is an important question to ask now, as results from increasingly complex Earth System models lead us into the 5th assessment of climate science by the Intergovernmental Panel on Climate Change. Comparing observed and predicted interannual variability, we suggest that future climate projections may underestimate the magnitude of surface ocean DMS change. Unfortunately this conclusion relies on a relatively small dataset, in which observed interannual variability may be exaggerated by biases in sample collection. We therefore encourage the observational community to make repeat measurements of sea-surface DMS concentrations an important focus, and highlight areas of apparent high interannual variability where sampling might be carried out. Finally, we assess future projections from two similarly valid empirical DMS schemes, and demonstrate contrasting results. We therefore conclude that the use of empirical DMS parameterisations within simulations of future climate should be undertaken only with careful appreciation of the caveats discussed.

1 Introduction

Phytoplankton DMS production remains a hot topic in climate science despite the results of a number of recent studies suggesting that its impact within a changing climate is likely to be small (e.g., Gunson et al., 2006; Bopp et al., 2003). The reason why the hypothesis that phytoplankton DMS production may act as a negative feedback on climate (Charlson et al., 1987) remains in active debate two decades after its proposition, is that we still lack the evidence, observational, or in the form of robust models, necessary to confirm or reject its existence as an important component of the climate system. While this hypothesis remains in limbo, significant questions will surround our ability to interpret Earth System modelling results in the context of climate change. A recent expansion in the size of the global sea surface DMS database (http://saga.pmel.noaa.gov/dms/) allows us to assess the ability of empirical DMS parameterisations, incorporated into Earth System models, to predict observed seawater [DMS] recorded in a dataset independent from that used to create the parameterisations. From this starting point, we go on to assess whether we can be confident in the predictions of future sea surface [DMS] made using these schemes within fully coupled, physical-biogeochemical climate models, and therefore whether we are right to accept that the climatic impact of future changes in marine DMS production is likely to be small. This is a critical question to ask now, as we move towards the 5th assessment by the Intergovernmental Panel on Climate Change (IPCC), because for the first time, many of the climate models providing the basis for this report will attempt to include a wide range of earth-system processes, such as marine DMS production, within their climate projections.

We examine two empirical DMS parameterisations, one proposed by Anderson et al. (2001), and the second by Simo and Dachs (2002), (modified with Aranami and Tsunogai (2004), and both adapted for use with our Earth System model). We make a critical assessment of the ability of the two models to match observations and global features emerging from observations, then go on to explore whether or not we can apply these models with confidence when making predictions about the climate of the coming century.

2 DMS parameterisations

Both the Anderson et al. (2001), and Simo and Dachs (2002) DMS schemes derive surface ocean DMS concentration directly from basic biological and physical parameters. These DMS schemes therefore lend themselves ideally to incorporation into coupled physical-biogeochemical climate models without the need to implement a full marine sulphur cycle within these models. By avoiding the explicit modelling of the biological and chemical processes behind the emission of DMS, we avoid adding the uncertainty stemming from an incomplete understanding of these processes, and can produce models of a complexity suitable for examining centennial-scale climate change in a global context. The two parameterisations are outlined below.

2.1 Anderson et al. (2001) scheme

The Anderson et al. (2001) scheme (hereafter referred to as the Anderson scheme) correlates surface water DMS concentration (nM) with seawater chlorophyll concentration, daily mean shortwave irradiance and nitrate concentration:

$$[\mathrm{DMS}] = 2.29 \text{ where } \log_{10}(CJQ) \leq 1.72 \quad (1)$$

$$[\mathrm{DMS}] = 8.24[\log_{10}(CJQ) - 1.72] + 2.29 \text{ where } \log_{10}(CJQ) > 1.72 \quad (2)$$

Where C represents chlorophyll concentration (mg m^{-3}), J the mean daily shortwave irradiance (Wm^{-2}), $Q = \frac{N}{K_n+N}$, N the nitrate concentration (mmol m^{-3}) and K_n the half saturation constant for nitrate uptake by phytoplankton (mmol m^{-3}).

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2.2 Simo and Dachs (2002) scheme

The Simo and Dachs (2002) scheme (hereafter referred to as the Simo scheme) correlates DMS production with surface water chlorophyll concentrations and the corresponding mixed layer depth:

$$[\mathrm{DMS}] = -\ln(Z) + 5.7 \text{ where } \frac{C}{Z} < 0.02 \quad (3)$$

$$[\mathrm{DMS}] = 55.8\left(\frac{C}{Z}\right) + 0.6 \text{ where } \frac{C}{Z} \geq 0.02 \quad (4)$$

Where Z represents the depth of the mixed layer (m), and C the surface ocean chlorophyll concentration (mg m^{-3}). To prevent the model from simulating negative [DMS], when the mixed layer depth is exceptionally high ($Z > 182.5$ m) we have applied the relationship of Aranami and Tsunogai (2004):

$$[\mathrm{DMS}] = \left(\frac{90}{Z}\right) \text{ where } Z > 182.5 \quad (5)$$

3 Implementation

The schemes described above have been implemented within the biogeochemical component (Diat-HadOCC, a development of Palmer and Totterdell, 2001) of the fully coupled ocean-atmosphere Met Office Hadley Centre Earth System model HadGEM2-ES (at a developmental stage). Diat-HadOCC simulates nutrients, diatom and non-diatom phytoplankton, zooplankton and detritus, and within the physical model of HadGEM2, has access to all of the parameters required to separately calculate seawater [DMS] using the two described DMS parameterisations. Mixed-layer depth is the only parameter we are required to derive for these calculations. We define the base of the mixed layer as being the depth of the upper-most model level within which the temperature is at least half a degree cooler than that in the corresponding surface grid-box (Levitus, 1982). Both the Anderson (2001) and Simo (2002) schemes were developed at least in part using chlorophyll data from the SeaWiFS database (Yoder and Kennelly, 2005). As is the case with most global biogeochemical models, Diat-HadOCC has been developed to capture the broad function of the marine carbon cycle, rather then to accurately describe the ecosystem activity. Consequently, as we start to use these models to explore non carbon-cycle processes, we must be aware of the associated limitations. In the case of HadGEM2-ES, the interaction of the physical and biological models results in the majority of the biological production occurring in the model's surface layer, rather than in a deep-chlorophyll maximum. From a carbon-export perspective, the importance of the inaccuracy in the vertical production profile is of second order, however when applying a parameterisation based on surface ocean chlorophyll (as we are in this study), the near-surface vertical distribution of phytoplankton becomes crucial. To adjust for this, and in doing so provide additional information to the parameterisation, we have calculated surface ocean [DMS] using only one of the two phytoplankton functional types (excluding diatoms from the calculation because of their low DMS production, Yoch, 2002). Considering only non-diatom phytoplankton chlorophyll the model simulates a global mean surface chlorophyll concentration of 1.03 mg m^{-3}.

4 Results

4.1 Predictive capacity in the present ocean

Before investigating the model's predictive capacity, it is first important to understand the data to which we are comparing the model output. As with any database reliant on in-situ measurements, the available surface ocean [DMS] data covers only a small percentage of the global ocean, with sampling limited by resources and accessibility (e.g. few measurements have been made in the Southern Ocean during the Southern Hemisphere winter). For this reason, the construction of the Kettle et al. (2000)

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monthly DMS climatology (hereafter referred to as the Kettle climatology) was based on a large number of assumptions, notably the unadjusted extrapolation of values between areas considered to belong to similar biogeochemical provinces (Longhurst et al., 1995). The Kettle (2000) climatology therefore represents only a first order "model" of surface ocean [DMS]. Because the Kettle (2000) climatology is itself a model, we have avoided validating our results directly against this climatology. We have instead analysed the temporal (over an annual cycle) and spatial DMS production by our models, alongside this climatology, against DMS observations made since those used to construct the climatology and parameterisations. This approach allows us to subjectively assess whether running a present-day coupled ocean-atmosphere climate simulation with an interactive DMS scheme can capture present day DMS fluxes equally well, or better than, a model where DMS fluxes are calculated from the standard climatology. A greater than doubling of the surface ocean [DMS] database (http://saga.pmel.noaa.gov/dms/) volume since the year 2000, gives us confidence in undertaking such an analysis.

Both of the DMS schemes used within our model predict annual globally averaged seawater DMS concentrations similar to that calculated from the Kettle (2000) climatology (Kettle (2000)=2.23 nM, model using the Simo (2002) scheme=2.22 nM and the model using the Anderson (2001) scheme=3.35 nM). The remarkable, and to a large part coincidental, agreement between our global estimates based on the Simo (2002) scheme, and estimate using the Kettle (2000) climatology, although encouraging does not allow us to rule out the Anderson (2001) scheme. Because no rigorous estimate of the uncertainty exists for the Kettle (2000) climatology, it is not possible to say whether the high value we calculate using the Anderson (2001) parameterisation falls outside of any realistic range. While these results indicate we are on the right track, due to the short residence time of sulphate aerosols in the atmosphere (~1 day (Boucher et al., 2003)) and the importance of DMS in the stimulation of cloud formation being disproportionately high away from terrigenous/anthropogenic aerosol sources (Liss et al., 1992), simulating the spatial and temporal distribution of DMS production is as im-

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portant as correctly predicting the total global DMS production. We therefore present a range of analyses, including monthly global averaged model output normalised to observations, comparison of the seasonality of DMS production in the model and the Kettle (2000) climatology, assessment of the spatially resolved model and climatology surface ocean [DMS], an assessment of interannual variability in the models and observations, and a comparison of future ocean [DMS] simulated using the two different schemes.

We have stated that the global annual mean DMS production by both of the models agrees reasonably with that predicted by the climatology, however the monthly mean values fail to capture the seasonal range of DMS concentrations recorded in that climatology (Fig. 1). The failure of both models to match the amplitude of the seasonal cycle described by the climatology appears to reflect two major errors; one associated with the climatology, and one resulting from the interaction of the physical and biogeochemical model. The Kettle (2000) climatology contains atypically high values in the southern-summer Southern Ocean. These high values are now considered to be a product of an, at the time unrecognised, sampling bias (Lana et al., 2010). The failure of the model appears to result from its inability to simulate the Southern Ocean summer phytoplankton bloom and corresponding high [DMS] following sea-ice retreat (Smith and Nelson, 1986). By dividing model predicted and climatology predicted [DMS] values by mean observations made in the same month of the year and the same 1×1 degree latitude-longitude region as the predicted values, then taking the mean of these values weighted to account for the latitudinal dependence of a of a 1×1 degree region (Fig. 1b), we can examine how the skill of the two parameterisations (within our model) and the climatology compare throughout the year. We see that the Anderson (2001) based model, and the Kettle (2000) climatology perform similarly through the seasonal cycle, over-predicting the observed seawater [DMS] by three to five times in the winter and spring, and achieving the best correlation with data during the summer. Based on this assessment, the Simo (2002) scheme (within our model) performs considerably better than the Anderson et al. (2001) scheme and Kettle (2000) climatology at the start of the year, then performs similarly to those approaches from May to December.

Although the monthly mean analysis suggests that compared to the climatology, the models are performing well, it should be remembered that such a simplified view can hide the cancellation of errors occurring when averaging spatially varying data. We therefore examine the strength of correlation between observed [DMS] and model (or climatology) [DMS] from monthly gridded average values corresponding to locations where observational data has been collected between 2000 and 2009 (Fig. 2a–c). From the data presented in Fig. 2a–c we calculate Spearman's Rank correlation coefficients of 0.37, 0.39 and 0.39 for the Kettle, Simo and Anderson data versus observations (Table 1).

To understand why the climatology and models fail to correlate well with observations, we examine the spatial distribution of data where *predicted* values are greater than three standard deviations above *observations* (where the standard deviation of any grid-point value has been calculated as the global mean of the standard deviation in each "box" for each month over eight years of the model running the modified Simo (2002) scheme (chosen arbitrarily to provide a common platform for comparison), divided by the mean of each grid point over the same eight year period, multiplied by that grid-point value), or where *observations* are greater than three standard deviations above *predictions* (highlighted by the grey regions in the scatter plots Fig. 2a, b and c). The described data have been calculated for each of the two model-schemes ("model scheme" is used hereafter to refer to the DMS schemes used within the Earth System model HadGEM2-ES) and the climatology, for each month, and plotted in Fig. 2d, e and f, on-top of annual mean fields from the Kettle (2000) climatology, Anderson (2001) and Simo (2002) model-schemes respectively (black over-plotting represents where observations are >3 standard deviations above predictions, and white over-plotting represents where predictions are >3 standard deviations above observations). Figure 2g shows the location of all of the observations made between the 1 January 2000 and the 1 January 2009, therefore where black or white over-plotting exists in Fig. 2g, but not Fig. 2d–f, those model results have adequately represented the observations. Parts h and i of Fig. 2 then present how the Simo (2002) and Anderson (2001) DMS parameterisations perform using climatological fields for chlorophyll concentration (SeaWiFS, Yoder and Kennelly, 2005), mixed layer depth (de Boyer Montégut et al., 2004), shortwave radiation (Berry and Kent, 2009) and nitrate (Garcia et al., 2006). Note that the limited high-latitude coverage of SeaWiFS chlorophyll data prevents the calculation of DMS values in these regions. Comparison of Figs. 2e with h, and f with i (i.e. Simo (2002) and Anderson (2001) predictions using model variables and climatology variables respectively) highlights regions where the poor prediction can either be explained by inadequacies in the parameterisations, or by the observations being anomalous, and regions where the parameterisation is doing a good job, but the model is feeding it unrealistic physical or biological values. First looking at the Simo (2002) plots (Fig. 2e and h), the only areas which seem to fail badly as a result of the model's biological and physical simulation are the East Equatorial Pacific, and the west Pacific off Japan. The first of these disagreements can be explained by the overproduction of chlorophyll in the equatorial region, due to excess nutrient upwelling in the model, and the latter by a consistent local over-estimation of the mixed layer depth. The Anderson (2001) model-based and climatology-based plots (Fig. 2f and i), differ considerably more than the Simo (2002) model-based and climatology-based plots. The areas of under prediction common to Fig. 2f and i, are similar to those in the Simo (2002) predictions and climatology, suggesting either that these observations are anomalously low, or that they represent conditions not picked up in the pre year-2000 dataset and therefore not incorporated into the climatology or parameterisations. This observation supports the idea that given the recent considerable increase in the size of the global DMS database, there is significant value in developing an updated climatology, see Lana et al. (2010). Where the model output produced using the Anderson (2001) scheme deviates strongly from that based on climatological values (Fig. 2f and i) is in its Eastern Equatorial Pacific over prediction. Much of the over prediction by the Anderson et al. (2001) scheme can be explained by its setting of the lower limit for DMS concentrations to be 2.29 nM, however this can't explain the difference between

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Fig. 2f and i because the data shown in both are calculated using the same scheme. Instead, the disparity highlighted between Fig. 2f and i appears to be a response to the model's excessive surface chlorophyll simulation. Disagreement between the observations and the climatology (Fig. 2d) result from either the recent observations being atypical, the climatology being constructed from atypical data, or artifacts resulting from the techniques used to construct the climatology; the second option potentially explaining disagreement in the Southern Ocean and high North Atlantic.

Disagreement between the model data, obtained using the Simo (2002) parameterisation and observations appear to fall into three main categories; over-simulation resulting from excess model surface chlorophyll (equatorial regions), under-simulation resulting from an inability to capture phytoplankton blooms (e.g. the Southern Ocean summer ice-edge bloom), and poor-simulation in shelf-seas, a result of the model lacking coastal-specific processes. Disagreement between the Anderson (2001) data and the observed data occurs for the same reason as seen in the model when using the adapted Simo (2002) scheme, but also, due to the aforementioned high-bias in the model equations (illustrated by the employment of a 2.29 nM cutoff (Eq. 1) and discussed in Bell et al., 2006).

Considering now just the temporal accuracy of the simulations, although the amplitude of the seasonal cycle as described by the climatology is not reproduced by the models, the primary and secondary global peaks in DMS production, evident in both the data and the climatology, are captured (Fig. 1a). The model run using the Anderson (2001) scheme predicts the [DMS] peaks to occur in the month prior to that in which they are seen in the climatology, whilst the model run with the modified Simo (2002) scheme reproduces the peaks within the same months as does the climatology. A major criticism of many ocean DMS models is that they fail to satisfy the observation that peak DMS production generally occurs later in the season than the peak in phytoplankton biomass, the so called "summer paradox" (Simo and Pedros-Alio, 1999), it is therefore encouraging that using the Simo (2002) scheme our model can not be criticised in this way. To further evaluate the success of the model-schemes at cap-

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turing the spatially varying lag between the time of the phytoplankton bloom, and the time of peak DMS production, we have fitted sine-curves through the mean monthly [DMS] and [chlorophyll] values corresponding to each 1×1 degree latitude-longitude grid box in the models, and similarly using mean monthly [DMS] from the Kettle (2000) climatology, and SeaWiFS [chlorophyll]. The number of days of lag between the peak of the chlorophyll sine-curve, and the and the peak of the DMS sine-curve is represented visually in Fig. 3a–c. There are however large areas of the ocean where the assumption that the [DMS] or chlorophyll seasonal cycles can be described by a sinusoidal curve, breaks down. Where it has been possible to fit sine curves to the data, we see a strong relationship between the time lag calculated for the climatology (Kettle and Andreae, 2000), and that calculated for the Simo (2002) model-scheme. A similar relationship is seen between the climatology lag, and the Anderson (2001) lag in the Northern Hemisphere, but not seen in the Southern Hemisphere. Assuming the Kettle (2000) climatology is doing a reasonable job at capturing the seasonal cycle of [DMS], this observation lends support to the argument by Simo and Pedros-Alio (Simo and Pedros-Alio, 1999) that the mixed layer depth (or a related variable), represents an important process within the phytoplankton-DMS decoupling.

4.2 Predictive capacity in a future ocean

We have demonstrated that both the modified Simo (2002) and Anderson (2001) schemes simulate present-day surface ocean [DMS] (within the context of our model) with success similar to, and under some criteria better than, predictions from the standard climatology. Being able to reproduce present day seawater DMS concentrations with this degree of skill is valuable, in that it suggests that our model is simulating the required parameters appropriately, however it does not give us reason to trust the model under different climatic conditions. It is possible for example that the use of mixed layer depth values within the Simo (2002) scheme indirectly describes conditions which favour high DMS producing species (e.g. *Emiliania huxleyi*), yet moving into the future a parameter not considered by the scheme, (e.g. ocean chemistry), might play a dominant role in controlling the abundance of those species, having an opposite effect on surface ocean [DMS] than that which would be expected from changes in mixed layer depth. We must therefore be confident, not only that the model can adequately predict present ocean [DMS], but also that it will respond correctly to oceanic changes under future warming. Both DMS parameterisations we have tested are empirical, and although the variables making up the schemes were based (to some degree) on a mechanistic understanding of DMS production, they are far removed from those utilised in process based models such as Vogt et al. (2010).

When using empirical parameterisations to make projections of future change, one would ideally test the parameterisations over periods of past change. To our knowledge there are presently insufficient observations to quantify if/how phytoplankton DMS production has responded to changes in global temperature over the 20th and start of the 21st century, however there are enough data to start examining inter-annual variability of phytoplankton DMS production. If a model can capture variability promoted by changes internal to the system, then as those internal processes reorganise under an external forcing (i.e. changing greenhouse gas concentrations), we can have increased confidence in the model's ability to capture the change associated with those processes. It should however be noted that changes other than those involved in the Earth System's natural variability may play a role in future change. We perform such an analysis, in part to assess the two model DMS schemes, but also to test whether such an analysis is possible with the present DMS database, and to set out a potential framework by which similar empirical schemes might be tested in the future as more observational data become available.

We have first assessed the data available in the PMEL DMS database as of the first of January 2009, to see whether enough data exists to find statistically significant interannual variance. We do this by grouping data into season, and into biogeochemical province (Longhurst et al., 1995). We then perform a Kruskal-Wallis analysis (the non-parametric version of an Analysis Of VAriance, ANOVA) on data from different years, but the same season and biogeochemical province (Longhurst et al., 1995). We set

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our level of significance as ≤0.05 to show significantly different years, and ≥0.95 for significantly similar years. In those seasons and provinces which pass our criteria, we then calculate the standard deviation between the mean DMS concentrations from each year in which data exists (Fig. 4a–d). To compare the observed interannual variability with that simulated by the model, we calculate standard deviations using data selected from the same locations as those in which observational data exists, using the two different DMS parameterisations driven our Earth System model (Fig. 4e–f).

The first thing to note is that there are a, perhaps surprisingly, high number of biogeochemical provinces in which significant interannual variability is observed (those presented in colour, not white, in Fig. 4). An important caveat to note, and one which we have made no attempt to correct, is that a number of the cruises which have measured DMS concentrations will have targeted blooms, or accidentally come across blooms, which may have produced greatly elevated DMS concentrations. If this sampling bias occurs in some years but not others, and is not representative of that biogeochemical provinces' regime, we will have mistakenly identified the province as having statistically significant interannual variability. This aside, the picture that comes out of our analysis of the observations (Fig. 4a–d) shows rather nicely what we might expect; that the greatest variability exists in the mid to high latitudes, during the summer of that hemisphere. The rest of the ocean then shows lower, and remarkably consistent variability. Comparing the analysis of observations with that from the two different model-schemes, we see, again perhaps unsurprisingly, that the model underestimates the variability in all areas other then some of the equatorial provinces. The patterns of variability are very similar between the model runs using the Simo (2002), and Anderson et al. (2001) scheme, reflecting the important role of surface chlorophyll in both schemes, and the high spatial variability of that parameter. Contrary to its performance in other tests, the Anderson (2001) scheme generally shows interannual variability closer to that seen in observations, than does the Simo and Dachs (2002) scheme. Overall this analysis indicates that the model-schemes are underestimating the magnitude of change in DMS production in response to changes in the Earth System, and therefore might be considered to underestimate the change occurring under global warming scenarios. We believe analysis of this kind to be critical when using empirical schemes within future projections. We therefore encourage the observational community to put increased emphasis on making unbiased repeat measurements within those regions we have identified as potentially exhibiting significant interannual variability. Additional observations will dilute the impact of biased data, providing increased value from model validations of the sort performed here.

Given the limited conclusions we have been able to draw from our assessment of interannual variability, in an attempt to help us understand whether inclusion of DMS parameterisations of this sort into models of the Earth System adds to, or detracts from, our confidence in the ability of those models to predict future climate, we have looked at how our two model-schemes predict oceanic DMS production to evolve over the coming century (Fig. 5). This analysis has been undertaken offline by calculating surface water [DMS] retrospectively, following the two DMS parameterisations, using data from a Met Office Hadley Centre model HadCM3 climate simulation following the IPCC SRES 2a scenario. Because DMS calculations have been made off-line, this analysis does not include any potential feedbacks of changing DMS production on climate. In a spatial context, the differences between the trends predicted for surface ocean DMS using the two schemes are striking (Fig. 5). Focusing on the region where changing DMS concentrations are likely to have the greatest climatic impact, the Southern Ocean, using the Simo (2002) scheme we would predict a strong *increase* in DMS production, yet using the Anderson (2001) scheme we would predict a moderate [DMS] *reduction*. The change in local surface ocean and lower atmosphere temperatures resulting from these different DMS evolutions could be expected to cause significantly different responses in sea-ice cover, and therefore contrasting implications for global climate. The reason why we see such different DMS responses between the two models in this region essentially comes down to the inclusion of mixed layer depth as a parameter in the Simo (2002) scheme, but not in the Anderson (2001) scheme. Moving into the future, our model predicts a significant reduction in the southern ocean mixed layer depth (∼50 m over the 21st century), and consequently, using the Simo (2002) scheme, a significant increase in DMS production. Interestingly, the shallowing of the base of the mixed layer also contributes to the Anderson (2001) scheme reduction in [DMS] at this site, through its impact on photic zone nutrients and therefore chlorophyll concentration.

We have demonstrated in this paper that both of our model experiments, one using the Simo and Dachs (2002) and the other the Anderson et al. (2001) scheme, represent the present day surface ocean DMS concentration with skill similar to or better than that of the standard climatology (Kettle and Andreae, 2000) respectively, yet under a common future climate scenario both predict very different surface ocean [DMS] changes to occur. Given that one could equally well justify the use of either of these parameterisations, the contrasting implications for the predicted future climate highlights the danger of including poorly understood components into earth-system models. These results also remind us of the importance of the efforts being made to develop a complete process-based understanding of marine DMS production, and the continuing need to improve the global DMS dataset. In the light of our findings we would emphasise (as acknowledged by the studies themselves) that attempts to describe the likely future impact of changing DMS production on climate using empirical DMS schemes (e.g., Gunson et al., 2006; Bopp et al., 2003) are interpreted as valuable scientific exercises, rather than as robust predictions. Although we have specifically examined only two DMS schemes here, we expect many of the broad conclusions we arrive at to be applicable to the use of other empirical DMS schemes (e.g., Bopp et al., 2003; Vallina et al., 2007). We have attempted to derive a framework for testing empirical schemes within Earth System models which we hope will encourage the future development of improved schemes, as well as allow increased confidence in our application of these schemes.

5 Conclusions

From this study we can draw a number of conclusions. 1) In the context of the Met Office Hadley Centre's physical and biogeochemical global models, using the parameterisations of Simo and Dachs (2002) and Anderson et al. (2001) we can predict present day surface ocean [DMS] with a level of skill better than and similar to that of the Kettle et al. (2000) climatology respectively. 2) The aforementioned level of skill (for models and climatology), when assessed as the ability to predict values within an independent oceanic dataset is low (Spearman's rank correlation coefficients of 0.39 between the models and observations, and 0.37 between the climatology and observations). 3) Areas of poor [DMS] prediction in the two models, to a large degree correspond to inaccuracies in the biological simulation, and are therefore expected to improve as the biological model is improved. 4) Initial analysis of the ability of the models to predict changing [DMS] on an interannual scale indicate that the models underestimate the observed variability, suggesting that they may also underestimate the magnitude of change under future climate scenarios. 5) Further repeat surface ocean DMS observations within biogeochemical provinces already containing good data coverage, and within which significant interannual variability exists, are required to allow improved assessment of the ability of empirical DMS schemes to predict temporal change. 6) Given our present level of mechanistic understanding and the present scope for model validation, simple [DMS] parameterisations should be used within Earth-System models only with a careful understanding of the associated caveats, and when doing so care must be taken not to confuse greater complexity with greater confidence.

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Can we trust simple marine DMS parameterisations?

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Table 1. Spearman's rank correlation coefficients between predicted and observed surface ocean DMS concentrations, looking only at monthly data in one by one degree latitude-longitude regions where observations have been made. The observed value is the mean of all observations made at that one-by-one degree location during individual calendar months between the years 2000 and 2009.

	Model Spearman's rank correlation with observations	Spearman's rank correlation with observations calculating DMS values using climatologies
Kettle et al. (1999)	0.37	*n/a*
Simo and Dachs (2002)	0.39	0.47
Anderson et al. (2001)	0.39	0.36

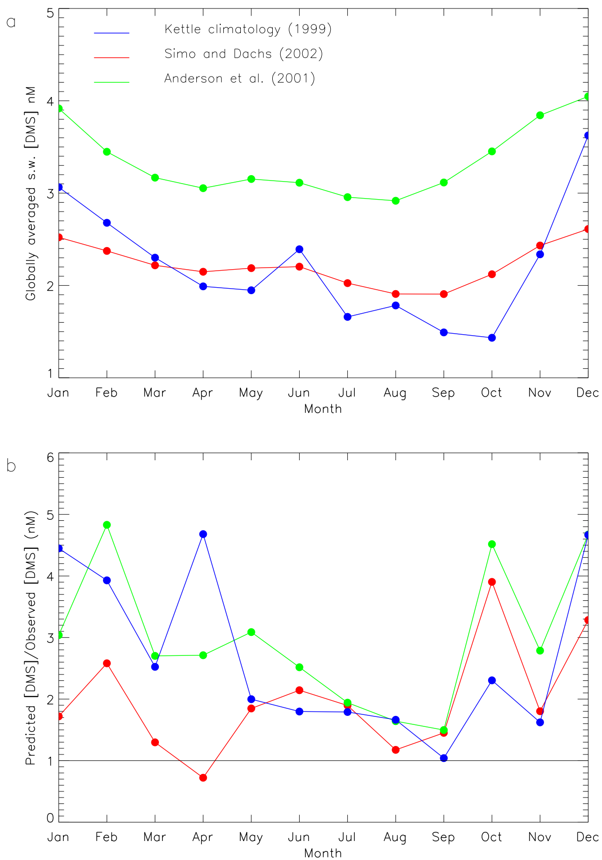

Fig. 1. **(a)** Monthly global mean surface ocean [DMS] from the Kettle et al. (2000) climatology (blue curve), mean of monthly global means from eight years of model data using the Anderson et al. (2001) scheme (green curve), and eight years of model output using the modified Simo and Dachs (2002) scheme (red curve). **(b)** Model and climatology predicted surface ocean [DMS] divided by observed [DMS] (averaged within 1×1 degree latitude-longitude grids), at locations where observations have been made between 2000 and 2009 (i.e. using data independent from that used to create the climatology and parameterisations, and averaged into 1×1 degree grid-boxes).

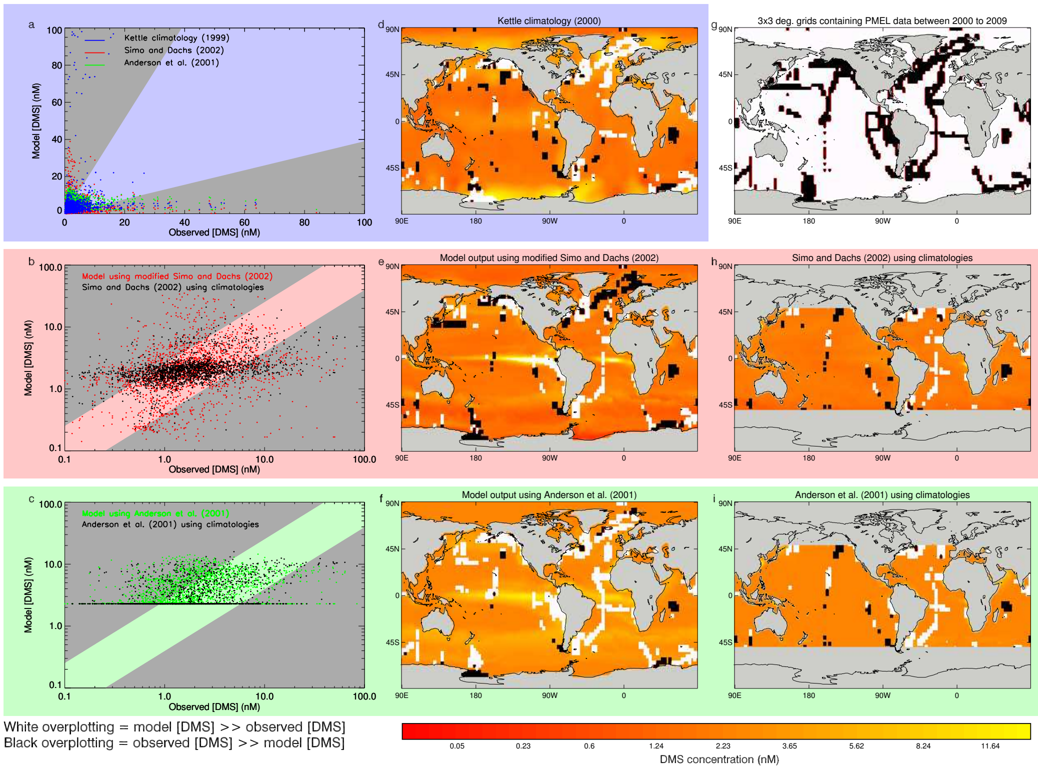

Fig. 2. Assessment of model and climatology success at predicting observed seawater [DMS] in a spatial context. **(a–c)** Model and climatology [DMS] predicted in monthly one degree grid-squares corresponding to (and plotted against) average observed values calculated for the same grid square in the same calendar month. Greyed areas represent regions where predicted values for a specific month are greater than three standard deviations above observations for that month (see main text for details), or where observations are greater than three standard deviations above predictions. Note that the axis limits artificially hide the extreme values, but were considered to best present the majority of the data. **(d–f)** Annually averaged present day fields for surface ocean [DMS] as predicted in the Kettle et al. (2000) climatology, using the Simo and Dachs (2002) scheme and the Anderson et al. (2001) scheme respectively (red-yellow shading). Plotted on-top of the annual average global fields are the locations of data, corresponding to those points highlighted in the grey regions of parts (a) (b) and (c), i.e. where predictions were more than three standard deviations above observations (white over-plotting) or where observations were more than three standard deviations above predictions (black over-plotting). **(g)** Plot showing the geographical location of all observations made between 2000 and 2009, and inputted into the PMEL database (http://saga.pmel.noaa.gov/dms/) by the start of January 2009. **(h and i)** As for (e) and (f) but where [DMS] has been calculated using climatological fields rather than model fields, using the Simo and Dachs (2002) and Anderson et al. (2001) parameterisations respectively. Note that all over-plotting has been done using a 3x3 degree grid (rather than the 1×1 degree grid used for all of the calculations) to make the results clearer to the eye.

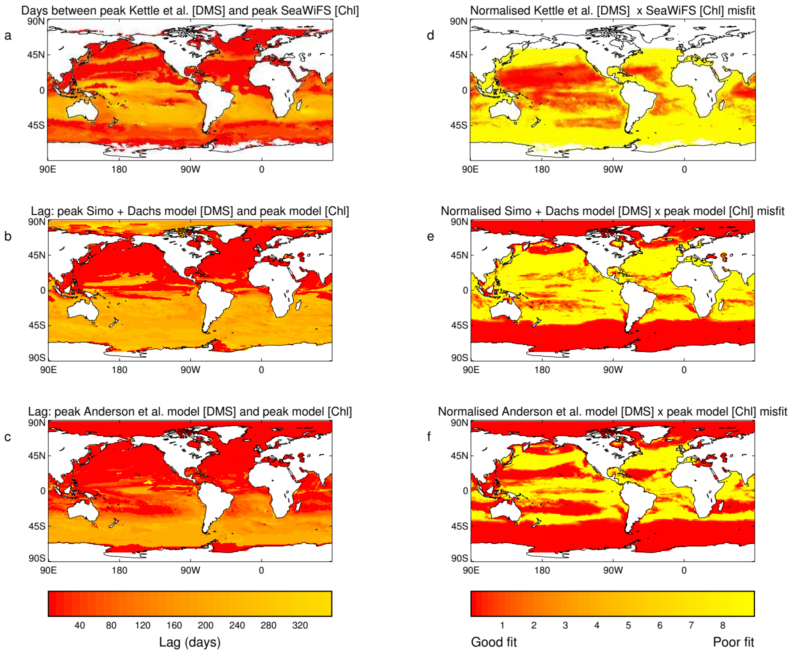

Fig. 3. **(a–c)** Lag (number of days) between peak chlorophyll and peak DMS concentrations, comparing; (a) SeaWiFS (Yoder and Kennelly, 2005) chlorophyll and Kettle et al. (2000) DMS, and model DMS and chlorophyll fields calculated using (b) the modified Simo and Dachs (2002) scheme and (c) the Anderson et al. (2001) scheme. Colours correspond to the number of days between DMS and chlorophyll concentration peaks. Peaks have been calculated by fitting a sine curve through an averaged 12 months of data at each grid point (or a minimum of six months of data in the case of SeaWiFS (Yoder and Kennelly, 2005)), and therefore assume a sinusoidal seasonal cycle. The colour correlation between the Kettle et al. (2000) – SeaWiFS plot (a) and the model plots (b, c) indicate the success of the model at reconstructing the non-linearity between primary production and DMS production, and allow us to examine the "summer paradox". **(d–f)** Quantification of the misfit between the calculated sine curves and the data, highlighting where the assumption of a sinusoidal seasonal cycle is (red), and is not appropriate (yellow). Colours represent the value of the average normalised DMS misfit at each point, multiplied by the average normalised chlorophyll misfit at each point. The multiplication of normalised misfit values for DMS and chlorophyll cause a strong polarisation between areas represented as demonstrating good fit (red) and areas demonstrating poor-fit (yellow).

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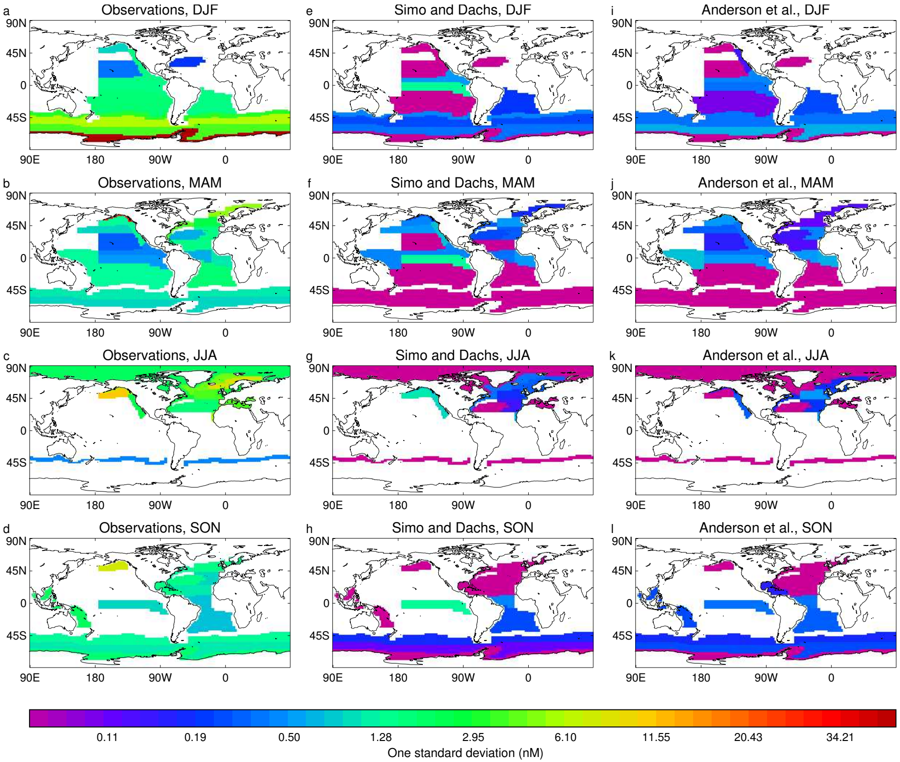

Fig. 4. Interannual variability in observations and model data. Colours represent the standard deviation of the mean values calculated for each biogeochemical province (Longhurst et al., 1995) for the named season in each year. Means were calculated using data from only the 1×1 degree grid-boxes which contain observational data. **(a–d)** Standard deviations calculated using data collected and input to the PMEL database between 1972 and 2009. **(e–h)** Standard deviations calculated using data generated by the model using the Simo and Dachs (**?**) parameterisation. **(i–l)** Standard deviations calculated using data generated by the model using the Anderson et al. (2001) parameterisation. Only biogeochemical provinces within which, statistically significant interannual variability (see main text for details), or significant lack of interannual variability can be demonstrated, are shown. DJF, MAM, JJA and SOC refer to the months of Northern Hemisphere winter, spring, summer and autumn respectively.

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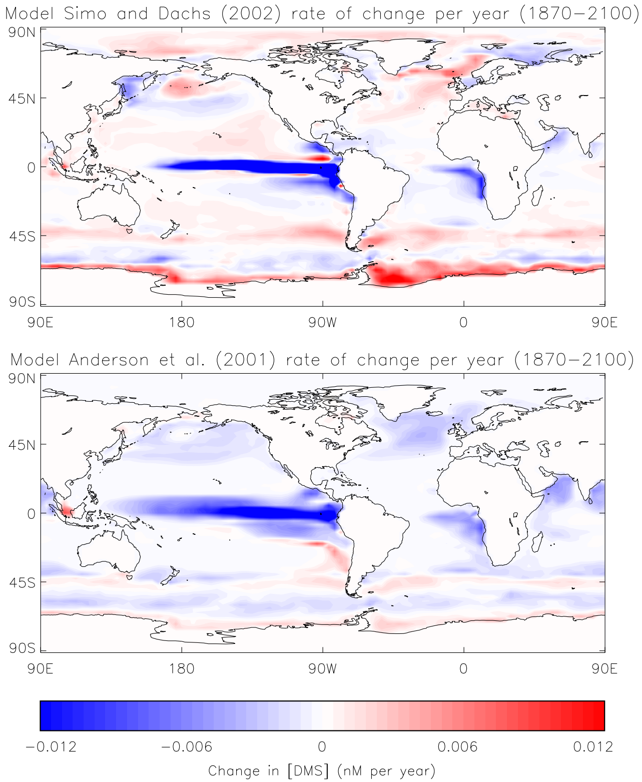

Fig. 5. Mean annual change in surface water [DMS] calculated using **(a)** the Simo and Dachs (2002) and **(b)** Anderson et al. (2001) parameterisations from fields produced by existing 20th and 21st century climate runs (following the IPCC's SRES 2a scenario) using the Met Office Hadley Centre's model HadCM3, with the HadOCC biogeochemical model (containing only a single phytoplankton group). Colours represent the gradient of a least squares regression through monthly mean data for each grid-point over the period 1870 to 2100.

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