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- Jennie Thomas: Question for Antoine, what is the main impact of your figure on slide 6?
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| ****************** 3rd CATCH Open Science Workshop 9-13 May 2022 |
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Day 1 - 9 May 2022: Linking biogeochemistry to aerosol-cloud interactions in the Southern Ocean and Antarctic (Marc Mallet & Ruhi Humphries & Sonya Fiddes):

PICCAASO (Partnerships for Investigations of Clouds and the biogeoChemistry of the Atmosphere in Antarctica and the Southern Ocean) aims to take a community approach to understanding links between ocean and ice biology up to clouds around Antarctica. This session will have presenters with recent key findings as well as discussions about upcoming observational and modelling work.

Please use this etherpad "chat" to leave your general comments and specific questions to speakers. This way we'll keep a record of your contributions and discussion across all three session of today.

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CHECK OUT THE PICCAASO WEBSITE HERE!! <a href="https://www.piccaaso.org/">https://www.piccaaso.org/</a>

- Follow us on Twitter: @piccaaso\_tweets
- Let us know if you wish to add projects, papers or ideas

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Session 1 - 0600-0800 UTC+2

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# <u>Introductions and welcome - Marc Mallet</u>

Sonya Fiddes: Don't forget our posters here:

https://app.gather.town/app/ueKHvojBKqY9wBgq/Catch%20Science

Julia: To Jennie's comment on having communities work together on the science case for chemical measurements: we need to think more about time scales as well since not all is converted instantly in the atmosphere, so there is more and important gaps to be tackled, where it would be great to have CATCH and BEPSII. Markus' question on the sea ice as a source was critical and we can't answer this. So what about an MIZ study?

Jennie @Julia -> Good point about timescales & MIZ. How can we do this?

<u>Keynote: A circum-Antarctic perspective on aerosol properties and processes: What we know and what we wish we knew - Julia Schmale</u>

Sonya Fiddes: The size distribution clusters are really interesting - how were they defined?

Julia: Thanks Sonya. Very nice CMIP6 overview! The size distributions were clustered using k-means simply. I showed the normalized versions (normalized to the average).

Sonya: Interesting - have you been able to look at any other properties (eg. composition, or met) associated with the clusters? OR should I just wait for the paper!?

Julia: We're working on the paper :-)

Sonya Fiddes: The tethered balloon is a really exciting prospect! How do

you anticipate that's going to go in the SO? Is there a max wind speed at which you can fly? Do you anticipate a lot of downtime?

Julia: Marc, Ruhi and Petra are organizing the MIZ voyage, where we try to have it on the ship. Max wind speed is 13 m/s. Downtime depends on weather and what the captain allows or might not...

Charel Wohl: Awesome work! I liked the importance of organics in influencing aerosol properties. Do we have any idea where these organics come from? Sea surface microlayer vs direct air sea exchange? Oxidation of precursurs from terrestrial emissions? Thank you.

Maija Peltola: Thanks for an excellent talk Julia! I was curious if you saw any interesting organic compounds in the CIMS data?

Sakiko Ishino: Thanks for a really exciting talk Julia. I'm interested in the role of MSA (as always!). You showed there are two significant regions with high MSA and high CCN number. Does high MSA mean high DMS emission there or is there specific oxidation processes preferencially producing MSA, such that BrO or aq-phase reactions? I'm curious if the oxidants are also important factors to produce HOMs that leads to low kappa values... Julia: Hi Sakiko, great questions. It think we should have a dedicated discussion on this over a coffee in Sion :-)

<u>Keynote: New findings from Southern Ocean Cloud-Aerosol-Precipitation-</u>
<u>Radiation Field Campaigns in 2017-18 and Needs for Future Observations -</u>
<u>Greg McFarquhar</u>

Sonya: The role of generating cells is quite interesting. Were they observed throughout the SO or were they more common at certain latitudes?

Jennie: @Greg - how can we get the atmopsheric chemistry community behind your strategy to ensure there is aerosol measurements in the mix for the next aircraft experiments?

### Discussion:

What are the grand challenges?

What would you like to see on the website (www.piccaaso.org)?

Do you have an update on an upcoming project you'd like to share? What gaps and overlaps do we have in measurements? Ambient vs laboratory measurements. How do we make quantitative links between biology and the atmosphere? Is vertical profiling part of your measurement? Charel Wohl: I have used it for making some guesses on the dominant biogeochemical production mechanism in seawater e.g. https://bg.copernicus.org/articles/19/1021/2022/ (Arctic sea ice zone). I also discuss some depth profiles from 60° S, Atlantic sector of DMS, isoprene, acetone, acetaldehyde and methanol in my thesis: https://ueaeprints.uea.ac.uk/id/eprint/84213/ Happy to share data if anyone is interested. How do we incorporate our observations and knowledge into model improvement? How do we incorporate our observations into upcoming satellite missions (e.g. PACE)? What opportunities are there for collaboration (especially PhD students and ECRs)? How should we coordinate in the future via workshops/conferences? Session 2 - 1200-1400 UTC+2

Welcome and recap of Session 1 - Marc Mallet

Flux measurments of DMS and MESH during Sea2Cloud - Manon Rocco

Sonya Fiddes: Were you able to find any similarly strong relationships between oceanic DMS and the phytoplankton population? If this were to be converted to improved DMS parameterisations for models, the relationship with oceanic DMS would be most helpful!

Manon Rocco : Similar strong relationship has been found with DMS measured in seawater and nanophytoplankton population for both ASITs.

## New particle formation around the Antarctic Peninsula - James Brean

Jennie Thomas: @James It is really a bit of a concern for me how many results/ conclusions come from air trajectories, which are most likely quite limited in the ability to predict sea ice-air contact in stable boundary layers (over ice and snow). I know we have nothing else, but I also think we should try to talk about this a bit as a community given how important these conclusions are.

Sonya Fiddes: Jennie you have read my mind! I have a discussion loosly around this tomorrow/later today organised! (the last session of this set of talks!)

Marc Mallet: @ James How can we hope to model these processes?

James Brean: Great question. I think first we need to know where the amines truly come from (i.e., if it's sea ice, is it just sea ice near our measurement site?). This will be answered hopefully by upcoming measurements. Different mechanisms of new particle formation have been input into global models with quite some success (i.e., Dunne et al 2016), but I'm not sure how well these behave over the Antarctic

Charel W: Best probably to measure directly the amines dissolved in seawater. I tried, but not managed. Fantastic talk James! Thanks Charel, great to see you last week :)

Nicolas Faure: Hi James, thank you for this very interesting presentation. From a perspective of surfactant activity of these alkylamine molecules, I am wondering if you have any idea about the carbon chain length of these molecules? Hi Nicolas! If we presume that we have no molecules with more than 1 nitrogen molecule (which I think is reasonable), then we only have C1-C4 alkylamines. We have some clusters with formulae like C8H22N2 H2SO4HSO4-. C8H22N2 is, however, likely the sum of two C4 amines (i.e., two butylamines). Some data are presented at the

bottom of the extended data of the paper (<a href="https://doi.org/10.1038/s41561-021-00751-y">https://doi.org/10.1038/s41561-021-00751-y</a>) A rather small tail, perhaps they can act more as a cosurfactant then. Thank you!

<u>Evaluation of ocean dimethylsulfide concentration and emission in CMIP6</u> <u>models - Roland Séférian</u>

Roland: the reference of the paper is

https://bg.copernicus.org/articles/18/3823/2021/bg-18-3823-2021.html

Sonya F: The Lana climatology appears to be really large over the SO, compared to the other observational products and the modelled products. (although the agreement in the polar biomes is interesting).. Do we rely too much on this data set? Do you think better DMS parameterisations, informed by results such as those that Manon discussed could do a better job?

Roland: To be honest I've been suprised by such an disagreement between observations.

ML-based data product are not perfect neither because we don't know how the gaps are filled. Nonetheless, Wang et al. (2020) dataset include more measurements than Lana's...

Regarding the model parameterization, It might be interesting to test them. In my opinion, it might be even more interesting to make use of observations (ocean, fluxes and atm) within a really constrained 1D modelling framework to test various parameterization.

Sonya F: Do any of the parameterisations include any sea ice processes? Roland: (answered) NO but its impact on climate spatiotemporal scales is expected to be small. Nonetheless I see an added value of this knowledge to better understand the response of open-ocean vs sea-ice DMS cycling

Sonya F: Do you think we need to lean more towards prognostic or diagnostic parameterisations?

Roland: if brief, prognostic model do simulate DMS concentration interactively (the represent driving process, at least the mechanisms) whereas the diagnotics model do use priors such as surface chlorophyll. In my opinion, diagnostics model are oversimplified esp because they are overfitted in drivers (chlorophyll and mixed-layer depth) which is not 100% consistent with our latest understanding

Jennie T: Any thoughts on if this is better for the Arctic: https://bg.copernicus.org/articles/14/3129/2017/

I know this is an Antarctic session, but I am still interested in this.

Roland: It is indeed, CanOE/CanESM5-CanOE wasn't available at the time of our multi-model study

@Roland (Jennie here): The CanOE/CanESM5-CanOE team is currently work with us on a Polar modeling project. I think we could stay in touch with you about that if you would like.

Louis M: Do we have any idea which of these DMS climatologies is more accurate/realistic? Like many atmopsheric modelers I use Lana11 but already realized the atmospheric DMS (and further down the line SO2 and sulfate) are often overestimated in the Arctic with Lana11 as input (this is maybe the same question than Sonya F)

Roland: have a look at Figure 6 in

https://bg.copernicus.org/articles/18/3823/2021/bg-18-3823-2021.html you will see how far available dataproduct for DMS flux different between each other. Thank you! We use Nightingale+Lana which really seems to be an extreme setup

# <u>Updates to sulfur chemistry in the UM - Laura Revell</u>

Matt W: A range of interesting work! Sonya F and I are (still) working on including your MSA chemistry developments into ACCESS. We would like to explore the aerosol fate of MSA/MSIA. Have you done any further work along those lines? We could potentially investigate the MSA re-evaporation question also.

Sonya F: How do we prioritise which 'new' chemistry mechanisms, that we observe to be important, to add to the model? Do we need to be able to 'lump' some of these processess perhaps to save computational costs?

Matt W: Perhaps a more general query... is Chl-a the right quantity to focus on when we are talking about marine biogenic influence on gas-phase, aerosol...? Is a more useful quantity biomass concentration?

Andrea B: the main point concerning MSA is to treat it as a semivolatile and consider the effect of particle acidity on its partitioning. Hodshire

| et al., made an interesting modelling study looking at this ( <a href="https://www.atmos-chem-phys.net/19/3137/2019/">https://www.atmos-chem-phys.net/19/3137/2019/</a> ), but there is still so  |
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| much to do!   |
| James Brean: Hey Andrea! Do you know of any estimates of the saturation vapour pressure of MSA? I know there's some attention being given to it   |
| right now at CLOUD  |
| Andrea B: that's very much acidity dependent, you can have a look at Fig1. of Hodshire et al., 2019 to get an idea But the real picture is certainly more complex, in my opinion we are also missing some good measurements of MSA Henry's law constant (you can find values spanning 4-5 orders of magnitude between different studies). |
| Jennie T. for Laura: what tropospheric halogen chemistry emissions/schemes do you use for DMS oxidation in your current version? Sorry if I missed  |
| that.   |
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| Discussion  |
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| What are the big picture questions that we need to address as a community?  |
| What opportunities are there for collaboration?   |
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| Markus F.: Note during Friday's session 2 there will be a discussion on Joint Field Campaign Planning how to address cross-disciplinary questions regarding the sea-ice/ocean/atmosphere system (1520-1620 CEST)  |
| How can we ensure new observations really guide model development?  |
| What are our modelling grand challenges and priorities?   |
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Welcome and recap of Session 1 and 2 - Sonya Fiddes

Session 3 - 2100-2300 UTC+2

<u>Evaluation of methods to estimate dry marine aerosol surface area from</u> <u>bulk optical measurements over the Southern Ocean - Kathryn Moore</u>

Sonya F: Do you have the data needed to test your hypothesis about NPF for the CAP2 campaign?

Kathryn Moore: @Sonya I do not, but the data exists, and if anyone has identified NPF events in the CAP2 dataset, I'd be very interested.

Marc Mallet: @Kathryn How much variability is there with height? Are surface measurements representative of what's happening higher up? This is is very important for condensation sinks for all the gases that might be emitted from the ocean/sea ice regions. Could this method also be useful for wind blown snow and sea salt emitted via that process? (answered already but put here for records :))

Kathryn Moore: @Marc The MBL is fairly well-mixed up to a point (depends on the individual profile what height that is exactly). But in general,

on the individual profile what height that is exactly). But in general, surface measurements are representative of what's happening up to at least 600m. Caveat: the lidar profiles I used for this study were limited to being well mixed, clear up to >3km, and have a strong inversion, so this may not be true when clouds are present. The angstrom exponent is sensitive to the overall shape of the size distribution and the aerosol number in different categories/sizes. I think it could be applied to wind blown snow, but you might struggle to see the signal if you have a large nucleation and/or Aitken mode at the same time as a wind blown snow event.

Susannah Burrows: @Kathryn, I think you went through this but I missed it: are you finding that both the nephelometer method and the lidar method produced overestimates of the aerosol surface area in this dataset? Or is it only the lidar method that is overestimating surface area (and N500)? Kathryn Moore: @Susannah Specifically for the DeMott et al. 2016 nephelometer method, for distributions with angstrom exponent<1 (majority of cases) D16 does a good job. However, for distributions with angstrom>1, D16 underestimates the aerosol surface area by ~2x. Only the lidar (Mamouri and Ansmann 2016) method I tested overestimates the surface area, but by a large factor (3-5x) for the CAP2 dataset. It also overestimates

N500, but by a smaller amount (1.5-2x). I don't know of any studies that have tried to estimate N500 from nephelometer data. Thanks Kathryn

# Importance of remote marine aerosol - Leighton Regayre

Sonya F: What types of observations are needed now to further constrain the model uncertainty?

Leighton Regayre: @Sonya, that's a really important question. For us, we've yet to tightly constrain natural aerosol in our current ensemble. Using ACE-SPACE measurements will help with that. But, the emission flux uncertainties compensate with removal rate uncertainties. So, it would be really useful to constrain deposition rates using measurements of these fluxes. Also, droplet activation is highly uncertain due to updraft velocity uncertainties. We're suggesting making maps of the remaining uncertainty, after constraint, to identify where and what type of measurements could be most useful as additional constraints.

Markus F: Related to the above, which areas & season would you suggest

Markus F: Related to the above, which areas & season would you suggest observers should go next around the Antarctic? Was there any particularly large uncertainty associated with sea ice or the marginal sea ice zone, which needs to be addressed?

Leighton Regayre: @Markus, our model ensemble mean CCN is certainly biased very low near the Antarctic continent as you suggest. But, I think there are probably many sources and perhaps local processes missing from our model. Measurements in those regions would improve our process-based understanding, but not models that don't include sufficient detail. From my perspective of trying to constrain aerosol forcing, the largest aerosol-cloud-radiation interactions are further from the poles, so immediately near the continent may not help in my constraint effort. Kathryn Moore: @Leighton, the SOCRATES dataset may be useful in constraining vertical velocities. As mentioned during the discussion, it was limited to north of 62S, but there are 1s (at least) 3D wind measurements below, in, and above cloud.

<u>Earth System models and biogeochemistry to clouds - Susannah Burrows</u>
Sonya F: If you were to have an unconservative method of INP formation, what you incldue in the model parameterisation?

Answered online

Kathryn Moore: @Susannah, what would be your ideal set of BGC measurements for lab/mesocosm measurements? The issue with a lot of those measurements

is the water you are using is coastal, with more anthropogenic influences and a different seasonal cycle than, ie, the Southern Ocean. Whereas field measurements target areas of potentially higher interest and relevance, but you are limited to the oceanographic and meteorological conditions during the campaign, and SSA generation techniques that are smaller and portable (if used at all). These are combined with the problem that many model quantities are not directly physically observable.

Answered online

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# **Discussion**

What are the big picture questions that we need to address as a community?

What opportunities are there for collaboration?

How can we ensure new observations really guide model development?

What are our modelling grand challenges and priorities?