Simulating the physical air-sea disequilibrium of the glacial ocean

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Part I: Reconstructing past mean ocean temperature (MOT) with ice cores requires assumptions about the saturation state of Kr, Xe, and N_2 in the global ocean

- To first order, atmospheric Xe/N_2 and Kr/N_2 ratios track mean-ocean temperature assuming the whole ocean is in solubility equilibrium with the well-mixed atmosphere.
- By reconstructing these atmospheric ratios using ice cores, we can infer past changes in total ocean heat content.

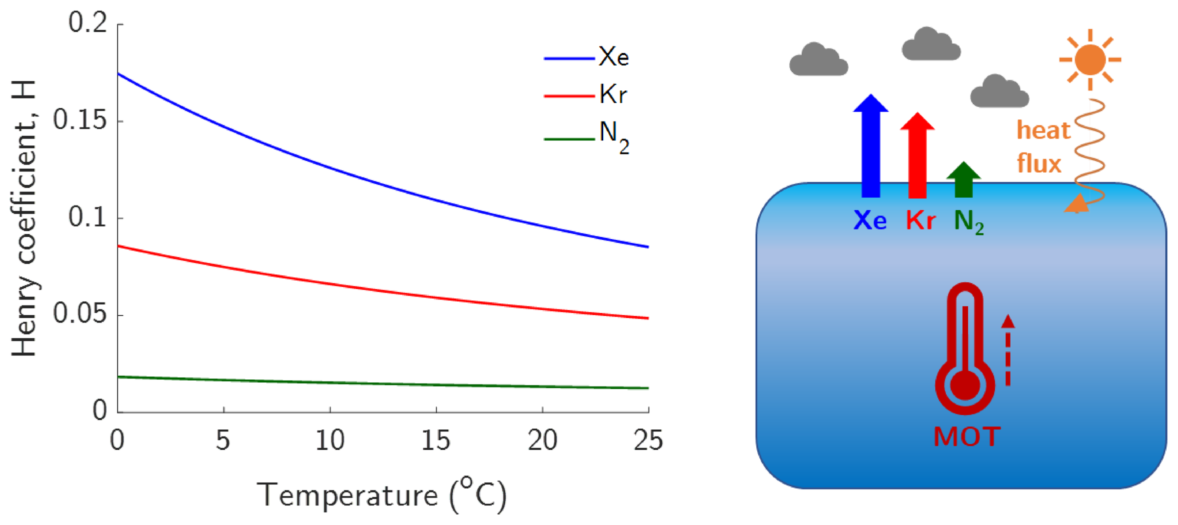

Figure 1: Changes in mean-ocean temperature (MOT) impact the ratios of Xe/N_2 and Kr/N_2 in the well mixed atmosphere due to the different solubility temperature dependences of these three gases.

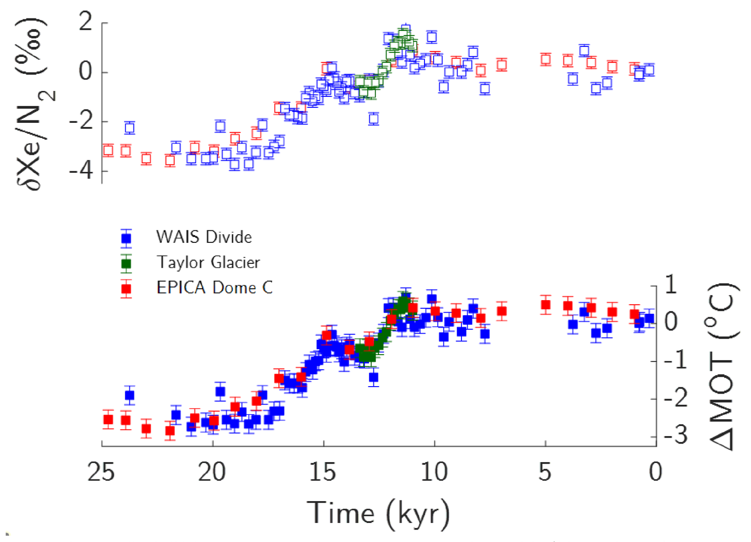

Figure 2: LGM-to-present change in atmospheric Xe/N_2 and implied change in MOT, assuming no change in global-ocean disequilibria. *(Data: Bereiter et al., 2018; Shackleton et al., 2019; Baggenstos et al., 2019)*

- But, the modern ocean is not in equilibrium with the atmosphere with respect to Xe, Kr, and N_2.
- Slight saturation anomalies (Δ) exist for all 3 gases at the order percent level.
- Could changes in ΔXe, ΔKr, and ΔN_2 between the modern the LGM oceans impact atmospheric ratios and, in turn, ice core MOT estimates? By how much?

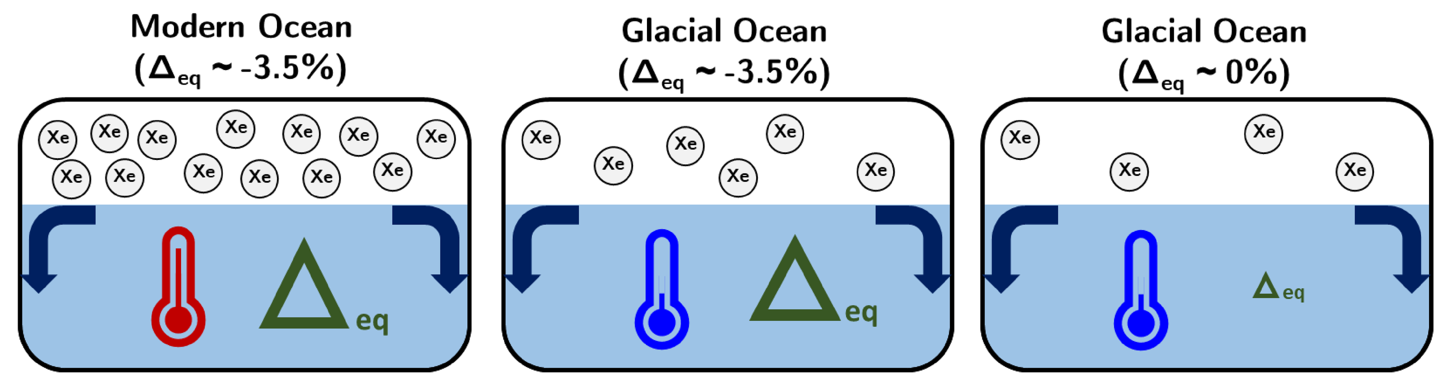

Figure 3: Simple illustrative example of how two possible changes (or lack thereof) in global-ocean Xe disequilibrium (ΔXe) between the LGM and present could lead to different atmospheric Xe concentrations in the LGM for the same amount of mean-ocean cooling (obviously not to scale...)

Part II: Can we precisely quantify - and accurately simulate - inert gas disequilibria in the modern ocean?

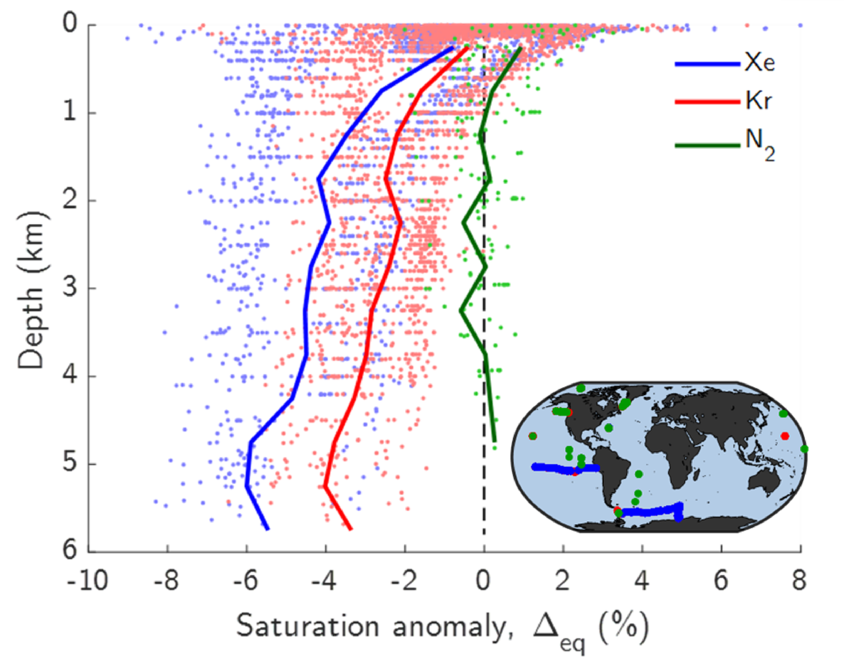

Figure 4: In the modern deep ocean (i.e., most of the ocean), Xe and Kr are undersaturated and N_2 is close to equilibrium. Some of the site-to-site scatter is due to barometric pressure differences between deep-water formation sites (and the assumption baked in the definition of Δ that air-sea exchange happens at 1 atm pressure). But, even gas ratio solubility anomalies (which are independent of pressure), show the same sense of disequilibrium (i.e., $Xe<Kr<N_2$). *(Data: Hamme et al., 2018 global database)*

- To simulate solubility disequilibria in the LGM ocean, we must first demonstrate that we can accurately reproduce disequilibria in the modern ocean.
- Here's our approach:
  - Introduce inert gas tracers (Ar, Kr, Xe, N_2, and their isotopes) into a GCM.
  - Measure these tracers in the deep ocean.
  - Compare data with model simulations to optimize physical gas exchange parameterization.
  - Use optimized model, with LGM boundary conditions, to simulate disequilibrium the LGM ocean.
- Some considerations and technical details:
  - We've used the UVic ESCM (pre-industrial/PI and last glacial maximum/LGM) and implemented tracers for offline equilibrium simulation (8000 years at 8-hr resolution) via the Transport Matrix Method (TMM; Khatiwala et al., 2005, 2007).
  - Diffusive and bubble-mediated gas exchange is parameterized using the Liang et al. (2013) model with the capacity to enhance bubble fluxes by a scalar *b*, following Emerson et al. (2019).
  - We measure and report gas and isotope *ratios* exclusively to eliminate barometric pressure effects.
  - All data used for model evaluation are from the deep ocean (>2 km) at the Bermuda Atlantic Time Series (BATS) site (32ºN)
  - We've added new isotope ratio and gas ratio measurements (May 2022, measured in Seltzer Lab at WHOI) to provide additional constraints with unique sensitivities.
  - Using the latest noble gas elemental and isotopic solubility functions (Jenkins et al., 2019; Seltzer et al., 2019)
  - Caveat #1: we use only the deep North Atlantic, because the Pacific reflects past deep-water formation conditions (e.g., Gebbie and Huybers, 2019; Jenkins et al., in review – see side panel)
  - Caveat #2: our model framework does not include the impact of submarine glacial ice melting (Loose et al., 2014, 2016)

Terminology and definitions

little δ = atmosphere normalized ratio

$$\delta \equiv \frac{(i/j)meas}{(i/j)atm} - 1 \quad \text{(in ‰)}$$

Big Δ = solubility anomaly

bulk concentration disequilibrium

$$\Delta C \equiv \frac{C}{C_{eq}(S,\theta)} - 1$$

reported in %, assuming 100% relative humidity and 1 atm pressure

ratio disequilibrium

(for isotope ratios IR or bulk gas ratios GR)

$$\Delta R \equiv \frac{C_i/C_{i,eq}}{C_j/C_{j,eq}} - 1$$

no pressure assumption needed!

Part II-a*: The deep Pacific as an archive of sea-level pressure change over the Common Era

*led by Bill Jenkins (associated publication currently in review)

- Related to our investigation of inert gas disequilibria in the modern ocean, recent high-precision measurements of Ne, Ar, Kr, and Xe along the GEOTRACES GP15 line (20 ºS to 56 ºN) have revealed coherent meridional shifts in Δ in the deep North Pacific
- The nearly identical shift in Δ across all four gases points to barometric pressure change (in the primary deep-water formation region around Antarctica) as the driver of this meridional trend
- We employ ^{14}C-calibrated inverse model to account for the impact of mixing of different-aged water masses.
- These results suggest a deepening (shift to lower pressure) of the circumpolar trough of 20 ± 6 mbar over the past two millennia

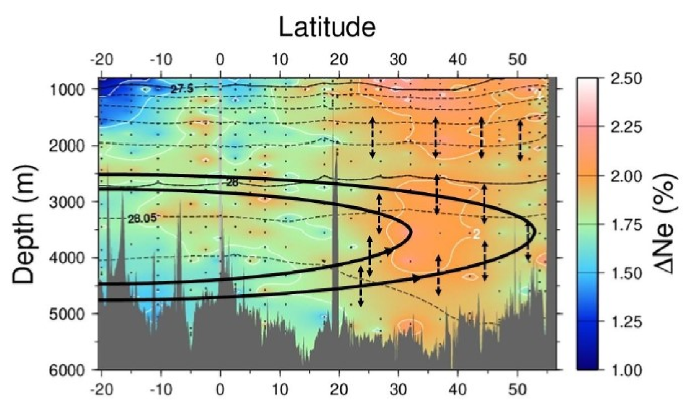

Figure 10: Contoured S-N section of neon supersaturation on the GP15 line through the central Pacific at ~152ºW. The seafloor is shown in gray, black dots represent sample locations, white contours show isopleths of saturation anomaly, think black contours show neutral density anomalies, thick black lines indicate schematic overturning from Holzer et al., 2021, arrows represent vertical mixing.

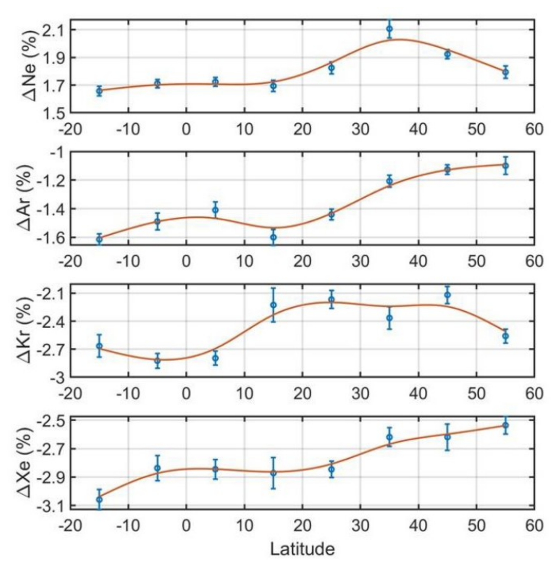

Figure 11: Binned latitudinal averages (10º) below the 28.05 kg m^{-3} neutral density anomaly.

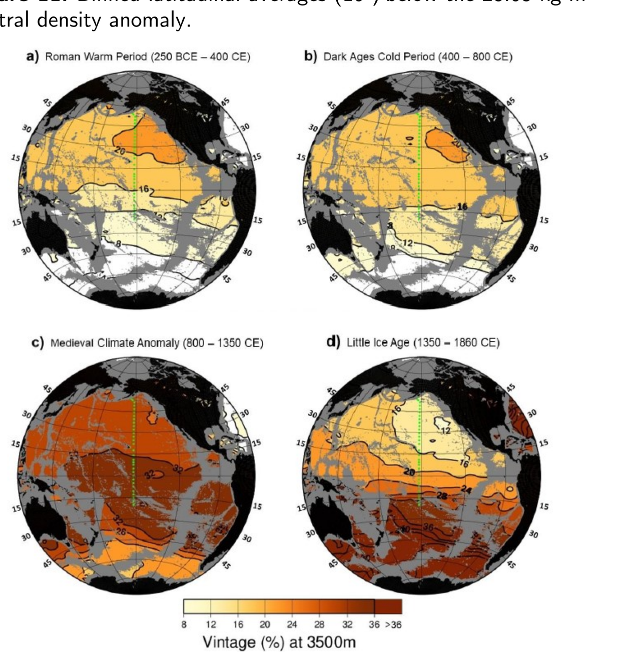

Figure 12: Water mass fraction distributions at 3500 m from inverse model (Gebbie and Huybers, 2010).

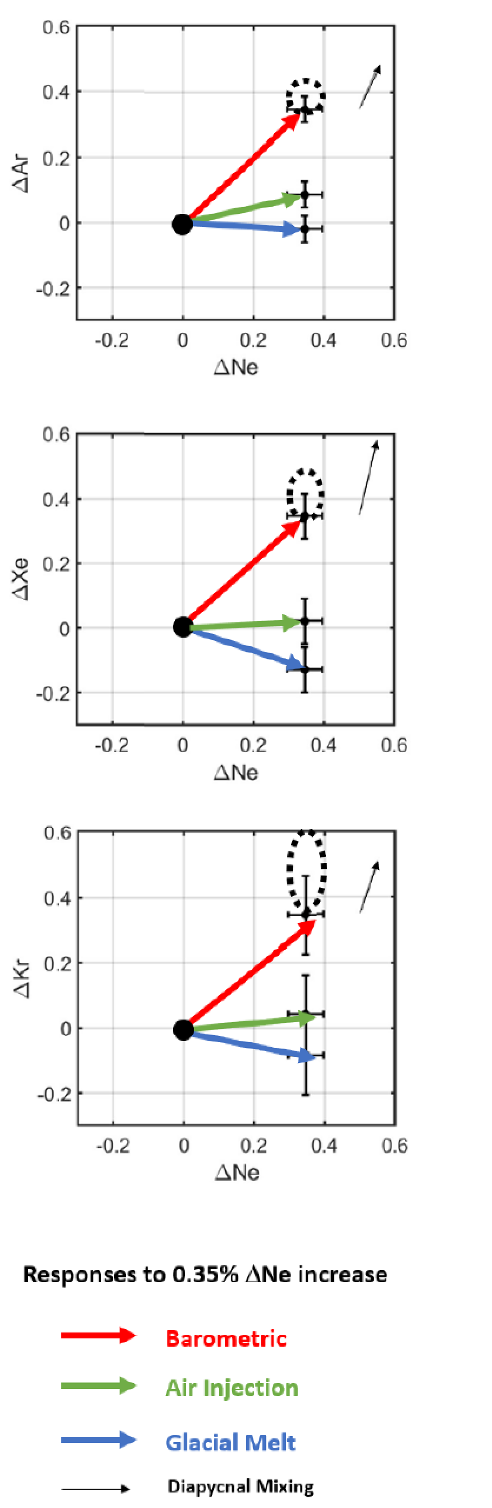

Figure 13: Schematic noble gas saturation anomaly responses corresponding to a ΔNe increase of 0.35% observed between the northern and southern regions. The black error bars indicate the approximate uncertainty in the projections while the different colored vectors indicate the changes due to the three candidate processes. The locations of the dotted black ellipses are the observed averaged gas differences between the regions and their axes are their respective standard errors. The narrow black vector to the right of the ellipse indicates the saturation anomaly tendency due to vertical mixing, whose length corresponds to a ΔNe enhancement of 0.05% (the uncertainty of the Δ Ne determination).

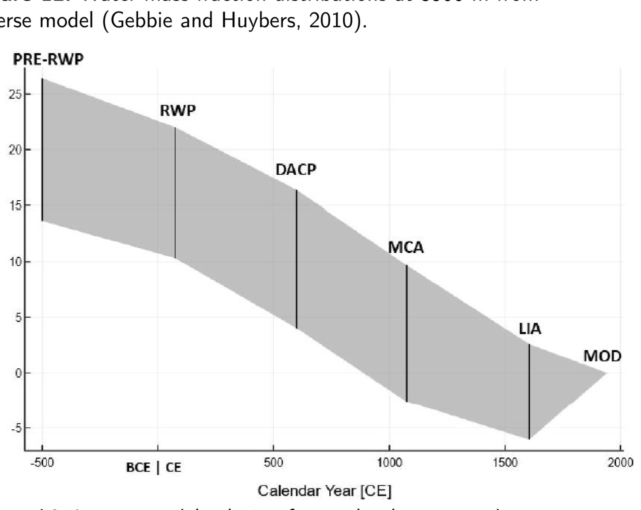

Figure 14: Inverse model solution for sea-level pressure change.

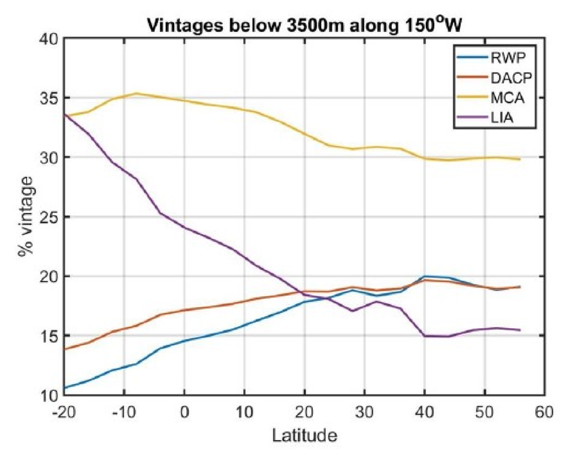

Figure 15: S-N changes in water mass vintage fraction from inverse model (below 3500m along 150ºW).

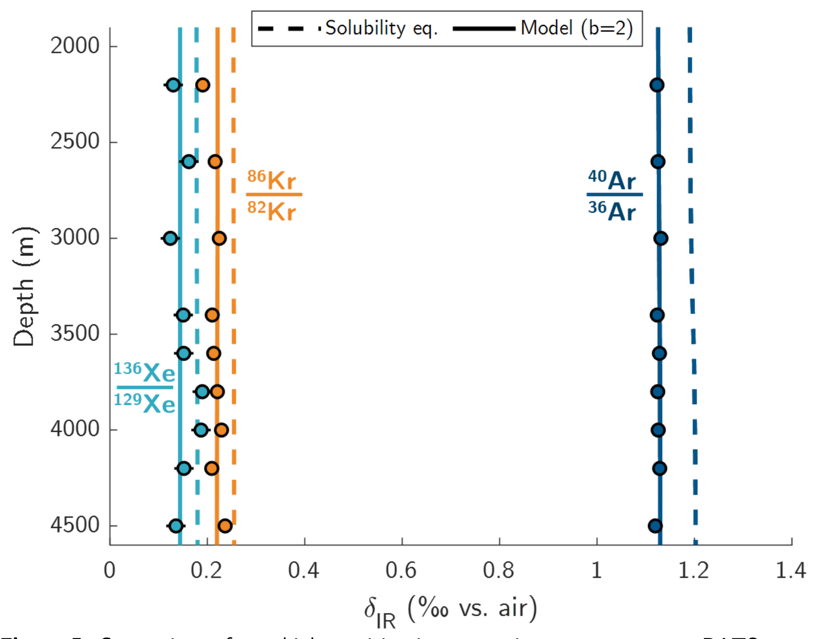

Figure 5: Comparison of new high-precision isotope ratio measurements at BATS to GCM predictions with enhanced bubble flux terms (Seltzer et al., in prep)

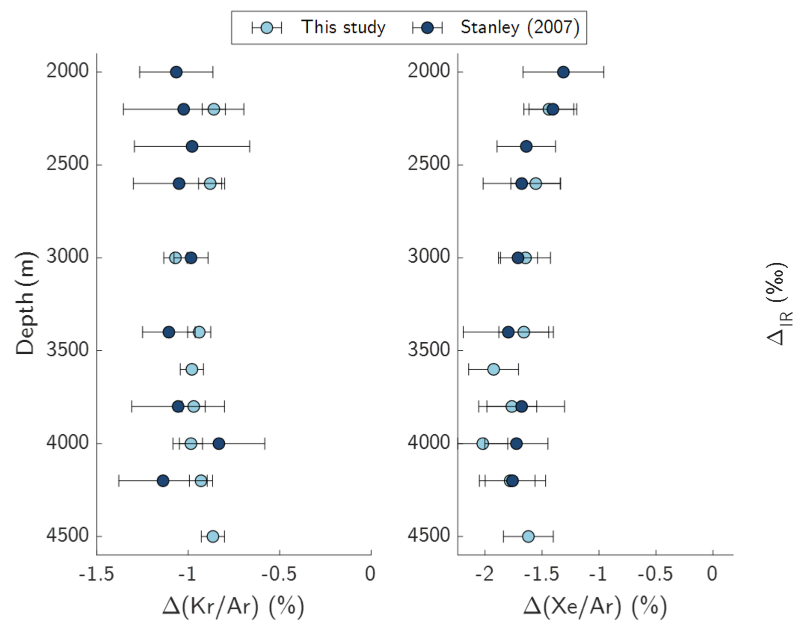

Figure 6: Persistent undersaturation of heavy noble gases in deep North Atlantic reproduced by two separate studies (Seltzer et al., in prep.; Stanley, 2007)

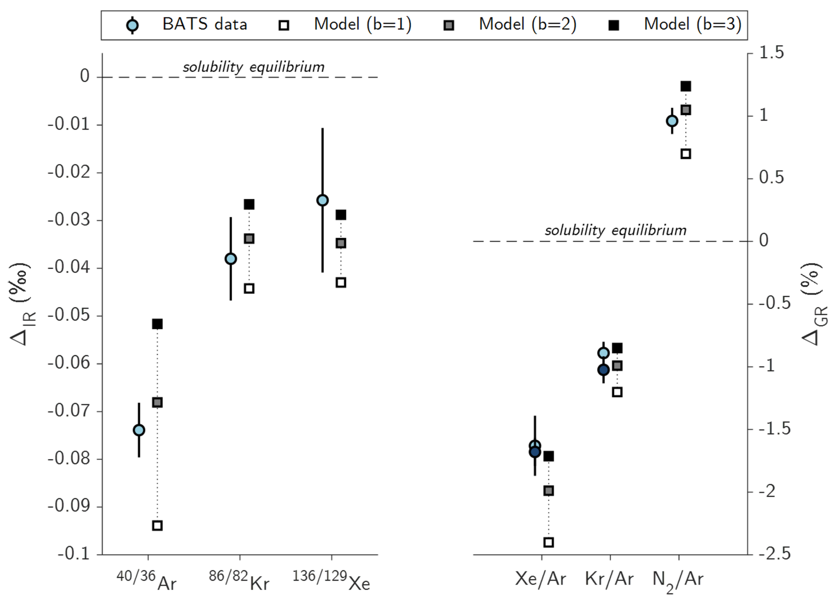

Figure 7: Comparison of BATS saturation anomalies with model simulations suggests b=2 gas parameterization is optimal (N_2/Ar data from Hamme and Emerson, 2013; dark blue Kr/Ar and Xe/Ar = Stanley '07, light blue = this study)

Part III*: Can we simulate LGM global-ocean disequilibria, and what is the impact on ice-core based MOT reconstruction?

*led by Perrin Davidson (MIT/WHOI PhD student)

- Using UVic ESCM, we have simulated N_2, Kr, and Xe in the LGM ocean using the above-mentioned optimized gas exchange parameterization. LGM ocean circulation transport matrices were extracted from the UVic ESCM as in Khatiwala et al. (2019)
- Here, we investigate changes in global-mean Δ between the LGM and PI for Xe, Kr, and N_2. We then implement these Δ estimates into a box model to solve for the impact of LGM-PI changes in disequilibrium on **atmospheric gas ratios** in the LGM atmosphere, accounting for different partitioning of these gases in the ocean-atmosphere system (e.g., 5% of Xe, but 0.5% of N_2, is in the ocean)
- With estimates for biases in atmospheric gas ratios, we can then determine the impact of LGM-PI changes in disequilibria on **mean ocean temperature reconstruction**, using scalings of approximately 0.73 and 1.83 ‰/ºC for Kr/N_2 and Xe/N_2, respectively (credit to Daniel Baggenstos for developing this box model)
- In total we carried out 11 LGM simulations: each simulation included the same LGM sea-ice, temperature, salinity, and circulation, but with modern (CORE-2) surface windspeeds at the high latitudes (>50º) increased or decreased by amounts ranging from -50 to +50%
- Using a likely PMIP3 high-latitude windspeed LGM-PI change of +0-30%, we suggest a bias in MOT of +0.05 to -0.44 ºC, where the negative sign indicates that MOT reconstruction neglecting changes in disequilibria would appear too cold.
- Please note that these findings are preliminary, and more experiments with different models and different sensitivity tests remain to be carried out. Nonetheless, we can preliminary suggest that changes in LGM winds lead to order 0.1ºC biases in ice core MOT estimates.

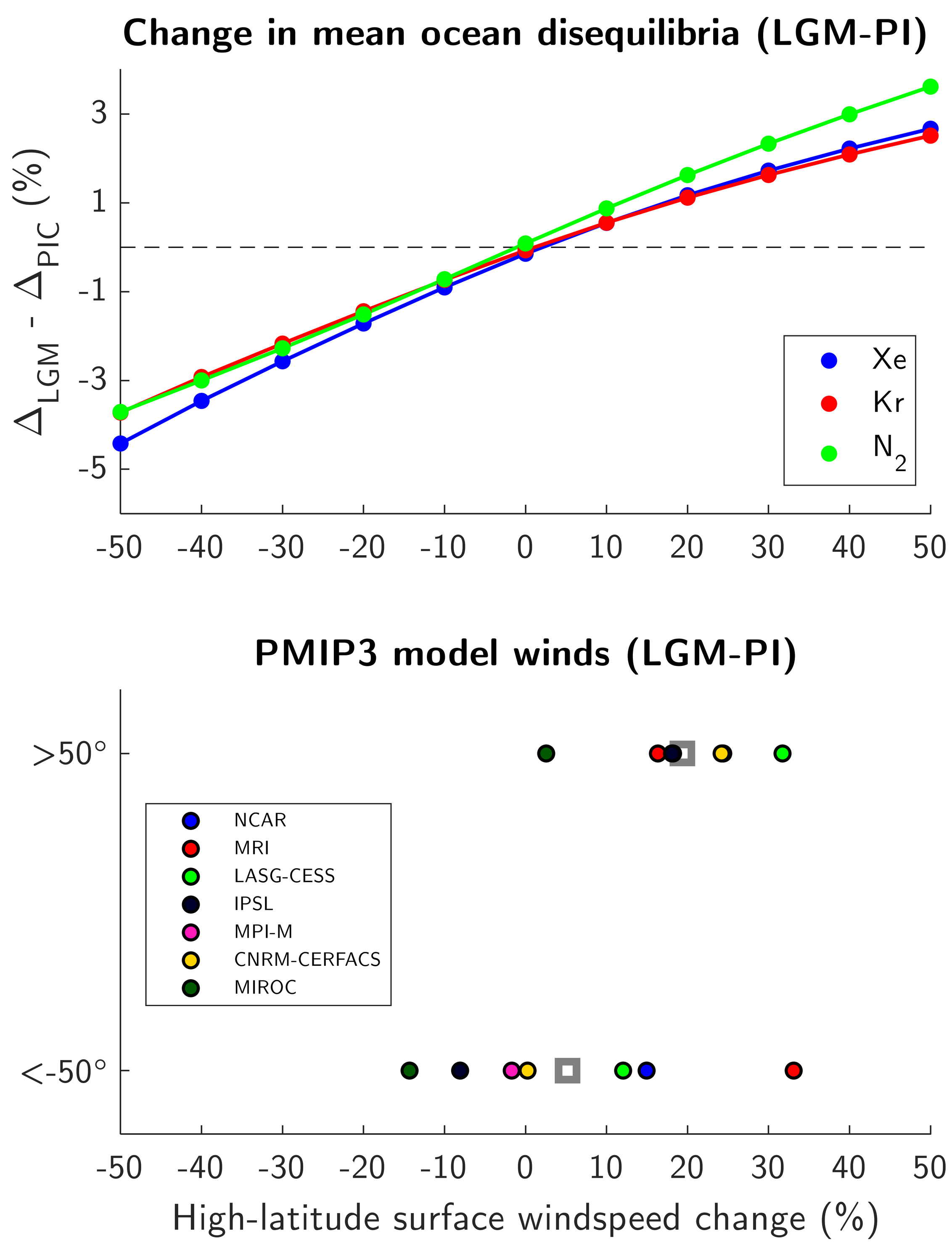

Figure 8: (Top) Change in global-mean ocean solubility disequilibria between LGM and pre-industrial period in UVic ESCM simulations with L13 gas parameterization (b=2) under different high-latitude windspeed experiments; (Bottom) Annual-mean surface wind speed changes (LGM-PI, in %) for 7 PMIP3 models, averaged over the high northern and southern latitudes.

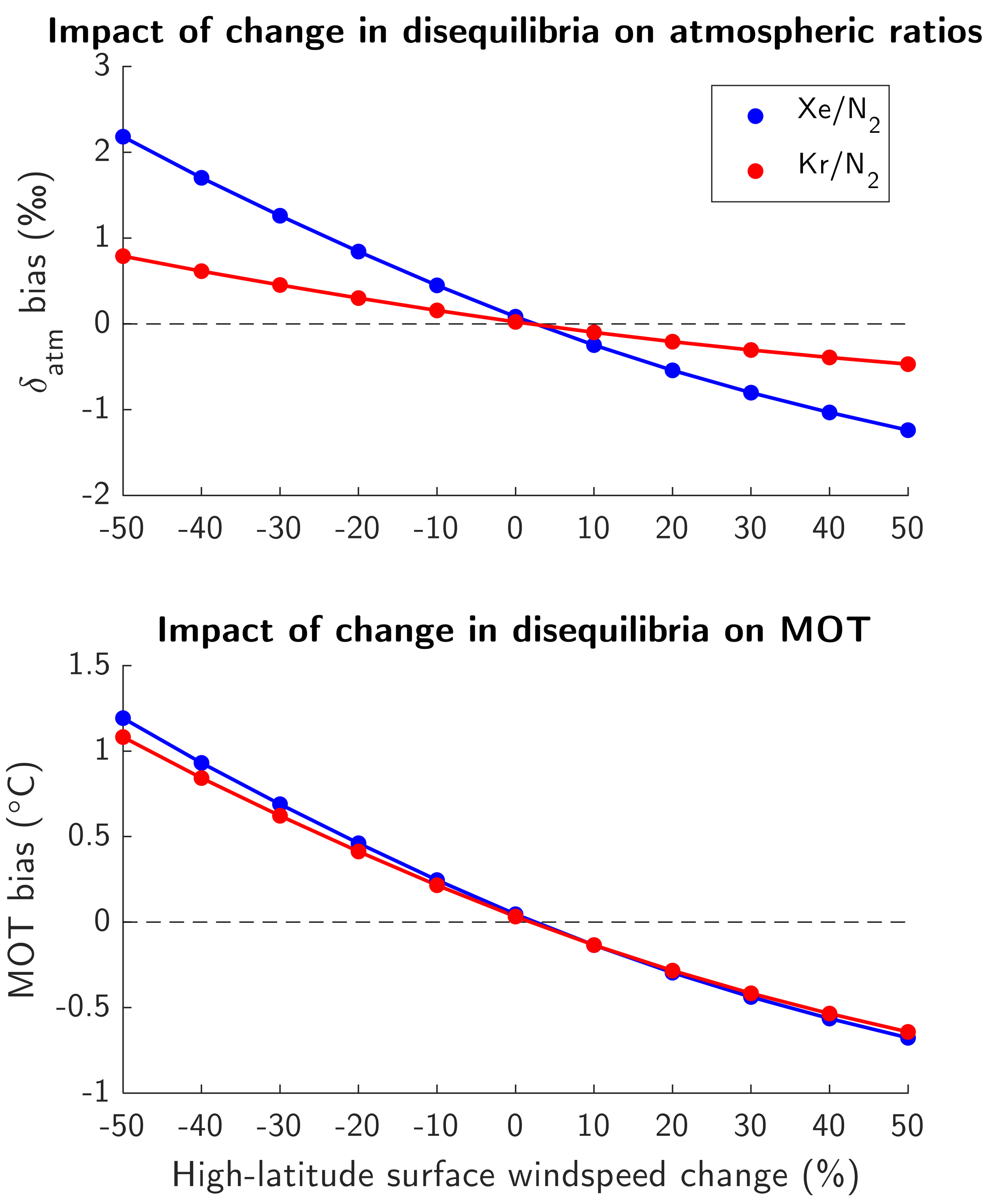

Figure 9: (Top) Impact on atmospheric gas ratios (Xe/N_2 and Kr/N_2) of LGM-PI changes in global-ocean disequilibria, relative to assumption of no LGM-PI change in disequilibria; (Bottom) Apparent bias in MOT due to assumption of constant disequilibrium between the LGM and PI for these 11 LGM UVic ESCM simulations.