Modeling historical budget for β-Hexachlorocyclohexane (β-HCH) in the Arctic Ocean: A contrast to α-HCH


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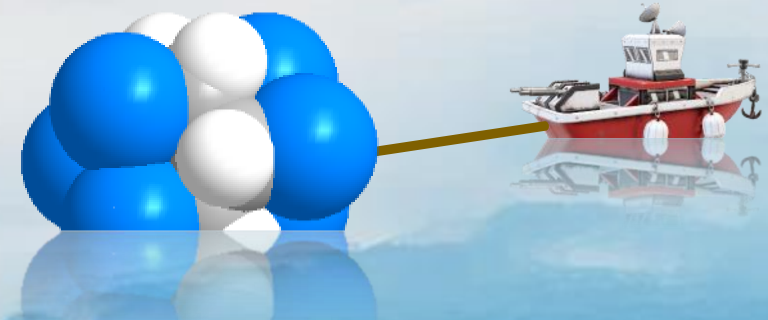
Pu-Fei Yang [a,b], Robie W. Macdonald [c,d], Hayley Hung [e], Derek C.G. Muir [f], Roland Kallenborn [g], Anatoly N. Nikolaev [h], Wan-Li Ma [a,b], Li-Yan Liu [a,b], Yi-Fan Li [a,b,i,*]

[c] Institute of Ocean Sciences, Department of Fisheries and Oceans, Sidney, BC, V8L 4B2, Canada
[d] Centre for Earth Observation Science, University of Manitoba, Winnipeg, R3T 2N2, Canada
[e] Air Quality Processes Research Section, Environment and Climate Change Canada, Toronto, Ontario, Canada
[f] Canada Centre for Inland Waters, Environment and Climate Change Canada, Burlington, Ontario, Canada



Pu-Fei Yang

Supervisor: Yi-Fan Li

2023/7/11

1

Background

1 Background

- Technical HCHs (tech-HCHs) are cheaply-produced organochlorine pesticides (OCPs), but caused environmental pollution;
- Tech-HCHs contains （Kutz, 1991）:
  - α-HCH (60-70%);
  - β-HCH (5–12%);
  - γ-HCH (10–12%);
  - σ-HCH (6–10%)。

Properties

β-HCH has stronger lipophilicity, hydrosolubility, and longer half-lives than α-HCH.

Xiao, 2004

Behavior

β-HCH was transported to the Arctic Ocean mostly by ocean current, not air

Li, 2002

2

Methods

2

Methods

Comparing with AMBBM 1.0

	AMBBM 1.0	**AMBBM 2.0**
Phases considered	Air, surface water, deep water	Air, surface water, deep water, snowpack, sea ice, and soil phases
Processes	gas–phase dry and wet depositions, particle-phase dry and wet depositions, volatilization, degradation, etc.	Add snowfall, melt & refreeze processes of snow and ice, etc.
Input data	Concentrations in the Arctic air, the seawater in the Bering Strait and the North-Atlantic Ocean, and the rivers to the Arctic Ocean	Monitoring data is no longer needed as the input data
Times step	One year	One day, but output data for every half year (six months)
Particle/gas (P/G) partitioning	Based on equilibrium theory (Harner-Bidleman Equation)	Based on the steady-state theory (Li-Ma-Yang Equation) [25]

2 Methods

Advection and mass transfer

Source zone

Source Zone

Gas phase

$$\frac{dM_{\mathrm{Air\_S}}}{dt} = -\begin{pmatrix} D_{\mathrm{Tran\_Air\_SA}} + D_{\mathrm{Deg\_Air\_S}} + D_{\mathrm{Air\_Seawater\_S}} \\ +D_{\mathrm{Air\_Soil\_S}} + D_{\mathrm{Rain\_S}} + D_{\mathrm{DD\_S}} + D_{\mathrm{WD\_S}} + D_{\mathrm{Air\_Strat\_S}} \end{pmatrix} \frac{M_{\mathrm{Air\_S}}}{V_{\mathrm{Air\_S}} Z_{\mathrm{Air\_S}}} + D_{\mathrm{Air\_Water}} \frac{M_{\mathrm{Seawater\_S}}}{V_{\mathrm{Seawater\_S}} Z_{\mathrm{Seawater\_S}}} + D_{\mathrm{Air\_Soil}} \frac{M_{\mathrm{Soil\_S}}}{V_{\mathrm{Soil\_S}} Z_{\mathrm{Soil\_S}}} + E_{\mathrm{Air}}$$

Seawater phase

$$\frac{dM_{\mathrm{Seawater\_S}}}{dt} = -\begin{pmatrix} D_{\mathrm{Tran\_Seawater\_SA}} + D_{\mathrm{Deg\_Seawater\_S}} \\ +D_{\mathrm{Seawater\_Sink\_S}} + D_{\mathrm{Air\_Water\_S}} \end{pmatrix} \frac{M_{\mathrm{Seawater\_S}}}{V_{\mathrm{Seawater\_S}} Z_{\mathrm{Seawater\_S}}} + \begin{pmatrix} D_{\mathrm{Rain\_Seawater\_S}} + D_{\mathrm{DD\_Seawater\_S}} \\ +D_{\mathrm{Air\_Water\_S}} + D_{\mathrm{WD\_Seawater\_S}} \end{pmatrix} \frac{M_{\mathrm{Air\_S}}}{V_{\mathrm{Air\_S}} Z_{\mathrm{Air\_S}}} + k_{\mathrm{Runoff}} D_{\mathrm{Runoff\_S}} \frac{M_{\mathrm{Soil\_S}}}{V_{\mathrm{Soil\_S}} Z_{\mathrm{Soil\_S}}} + E_{\mathrm{Seawater}}$$

Soil phase

$$\frac{dM_{\mathrm{Soil\_S}}}{dt} = -\left(D_{\mathrm{Deg\_Soil\_S}} + D_{\mathrm{Runoff\_S}} + D_{\mathrm{Air\_Soil\_S}}\right) \frac{M_{\mathrm{Soil\_S}}}{V_{\mathrm{Soil\_S}} Z_{\mathrm{Soil\_S}}} + \left(D_{\mathrm{Rain\_Soil\_S}} + D_{\mathrm{DD\_Soil\_S}} + D_{\mathrm{Air\_Soil\_S}} + D_{\mathrm{WD\_Soil\_S}}\right) \frac{M_{\mathrm{Air\_S}}}{V_{\mathrm{Air\_S}} Z_{\mathrm{Air\_S}}} + E_{\mathrm{Soil}}$$

Arctic zone

Arctic Zone

Gas phase

$$\frac{dM_{\mathrm{Air\_A}}}{dt} = -\begin{pmatrix} D_{\mathrm{Tran\_Air\_AS}} + D_{\mathrm{Deg\_Air\_A}} + D_{\mathrm{Air\_Strat\_A}} + D_{\mathrm{Air\_Soil\_A}} \\ +D_{\mathrm{Air\_Snowpack\_A}} + D_{\mathrm{Air\_Sea\_Ice\_A}} + D_{\mathrm{Rain\_A}} \\ +D_{\mathrm{Snow\_A}} + D_{\mathrm{DD\_A}} + D_{\mathrm{WD\_Rain\_A}} + D_{\mathrm{WD\_Snow\_A}} \end{pmatrix} \frac{M_{\mathrm{Air\_A}}}{V_{\mathrm{Air\_A}} Z_{\mathrm{Air\_A}}} + D_{\mathrm{Tran\_Air\_SA}} \frac{M_{\mathrm{Air\_S}}}{V_{\mathrm{Air\_S}} Z_{\mathrm{Air\_S}}} + D_{\mathrm{Air\_Water}} \frac{M_{\mathrm{Seawater\_A}}}{V_{\mathrm{Seawater}} Z_{\mathrm{Seawater}}} + D_{\mathrm{Air\_Soil}} \frac{M_{\mathrm{Soil\_A}}}{V_{\mathrm{Soil}} Z_{\mathrm{Soil}}} + D_{\mathrm{Air\_Snowpack}} \frac{M_{\mathrm{Snowpack\_A}}}{V_{\mathrm{Snowpack\_A}} Z_{\mathrm{Snowpack\_A}}} + D_{\mathrm{Air\_Sea\_Ice}} \frac{M_{\mathrm{Sea\_Ice\_A}}}{V_{\mathrm{Sea\_Ice}} Z_{\mathrm{Sea\_Ice}}}$$

Seawater Phase

$$\frac{dM_{\mathrm{Seawater\_A}}}{dt} = -\begin{pmatrix} D_{\mathrm{Tran\_Seawater\_AS}} + D_{\mathrm{Deg\_Seawater\_A}} \\ +D_{\mathrm{Seawater\_sink\_A}} + D_{\mathrm{Air\_Water\_A}} \end{pmatrix} \frac{M_{\mathrm{Seawater\_A}}}{V_{\mathrm{Seawater\_A}} Z_{\mathrm{Seawater\_A}}} + \begin{pmatrix} D_{\mathrm{Rain\_Seawater\_A}} + D_{\mathrm{Snow\_Seawater\_A}} \\ +D_{\mathrm{DD\_Seawater\_A}} + D_{\mathrm{Air\_Water\_A}} + D_{\mathrm{WD\_Seawater\_A}} \end{pmatrix} \frac{M_{\mathrm{Air\_A}}}{V_{\mathrm{Air\_A}} Z_{\mathrm{Air\_A}}} + (1 - k_{\mathrm{Runoff}}) D_{\mathrm{Runoff\_S}} \frac{M_{\mathrm{Soil\_S}}}{V_{\mathrm{Soil\_S}} Z_{\mathrm{Soil\_S}}} + D_{\mathrm{Tran\_Seawater\_SA}} \frac{M_{\mathrm{Seawater\_S}}}{V_{\mathrm{Seawater\_S}} Z_{\mathrm{Seawater\_S}}} + D_{\mathrm{Runoff\_A}} \frac{M_{\mathrm{Soil\_A}}}{V_{\mathrm{Soil\_S}} Z_{\mathrm{Soil\_A}}}$$

Soil Phase

$$\frac{dM_{\mathrm{Soil\_A}}}{dt} = -\left(D_{\mathrm{Deg\_Soil\_A}} + D_{\mathrm{Runoff\_A}} + D_{\mathrm{Air\_Soil\_A}}\right) \frac{M_{\mathrm{Soil\_A}}}{V_{\mathrm{Soil\_A}} Z_{\mathrm{Soil\_A}}} + \begin{pmatrix} D_{\mathrm{Rain\_Soil\_A}} + D_{\mathrm{Snow\_Soil\_A}} \\ D_{\mathrm{Air\_Soil\_A}} + D_{\mathrm{WD\_Soil\_A}} + D_{\mathrm{DD\_Soil\_A}} \end{pmatrix} \frac{M_{\mathrm{Air\_A}}}{V_{\mathrm{Air\_A}} Z_{\mathrm{Air\_A}}}$$

Seaice Phase

$$\frac{dM_{\mathrm{Sea\_Ice\_A}}}{dt} = -\left(D_{\mathrm{Deg\_Sea\_Ice\_A}} + D_{\mathrm{Air\_Sea\_Ice\_A}}\right) \frac{M_{\mathrm{Sea\_Ice\_A}}}{V_{\mathrm{Sea\_Ice\_A}} Z_{\mathrm{Sea\_Ice\_A}}} + \begin{pmatrix} D_{\mathrm{Rain\_Sea\_Ice\_A}} + D_{\mathrm{Sea\_Ice\_A}} \\ D_{\mathrm{Air\_Sea\_Ice\_A}} + D_{\mathrm{WD\_Sea\_Ice\_A}} + D_{\mathrm{DD\_Sea\_Ice\_A}} \end{pmatrix} \frac{M_{\mathrm{Air\_A}}}{V_{\mathrm{Air\_A}} Z_{\mathrm{Air\_A}}}$$

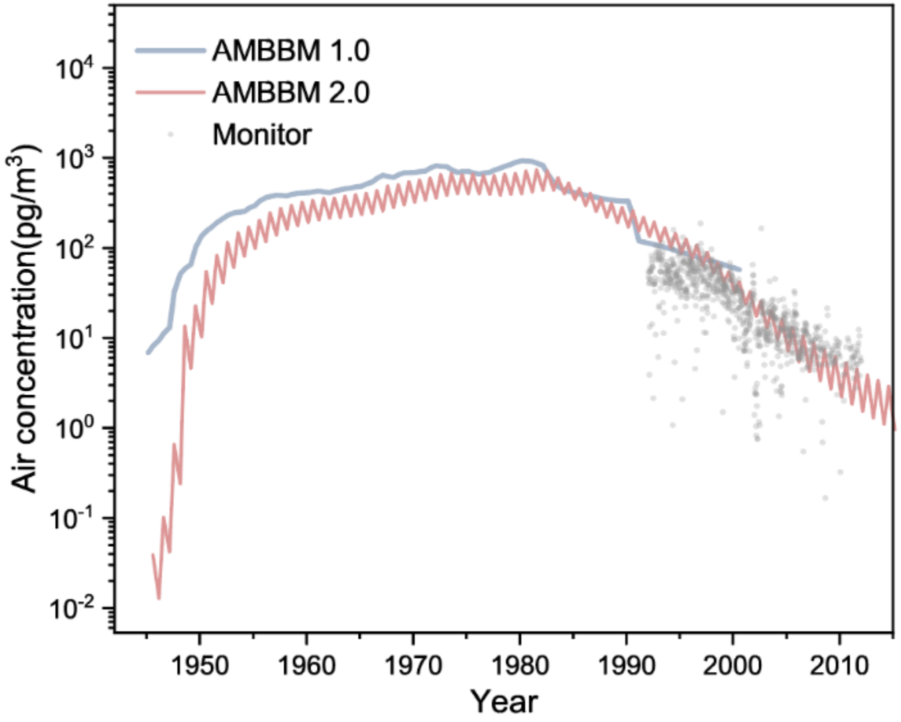
Snowpack Phase

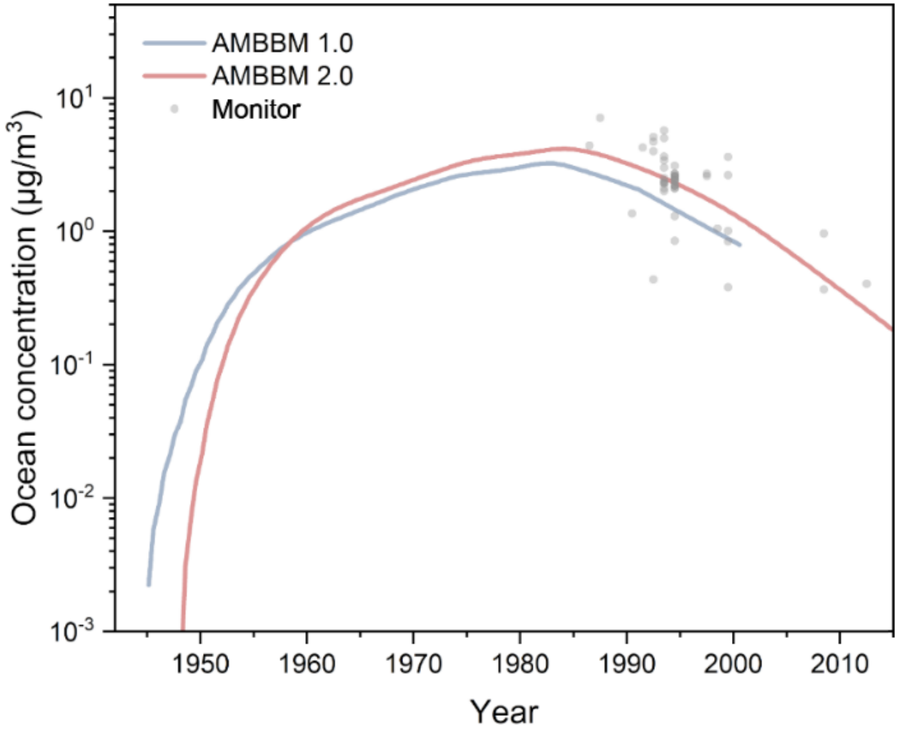
$$\frac{dM_{\mathrm{Snowpack\_A}}}{dt} = -\left(D_{\mathrm{Deg\_Snowpack\_A}} + D_{\mathrm{Air\_Snowpack\_A}}\right) \frac{M_{\mathrm{Snowpack\_A}}}{V_{\mathrm{Snowpack\_A}} Z_{\mathrm{Snowpack\_A}}} + \begin{pmatrix} D_{\mathrm{Rain\_Snowpack\_A}} + D_{\mathrm{Snow\_Snowpack\_A}} \\ D_{\mathrm{Air\_Snowpack\_A}} + D_{\mathrm{WD\_Snowpack\_A}} + D_{\mathrm{DD\_Snowpack\_A}} \end{pmatrix} \frac{M_{\mathrm{Air\_A}}}{V_{\mathrm{Air\_A}} Z_{\mathrm{Air\_A}}}$$

3 Model evaluation

Model evaluation

Air & ocean concentration





AMBBM 1.0 $RMSE_{\log}$ = 4.06

AMBBM 2.0 $RMSE_{\log}$ = 4.05

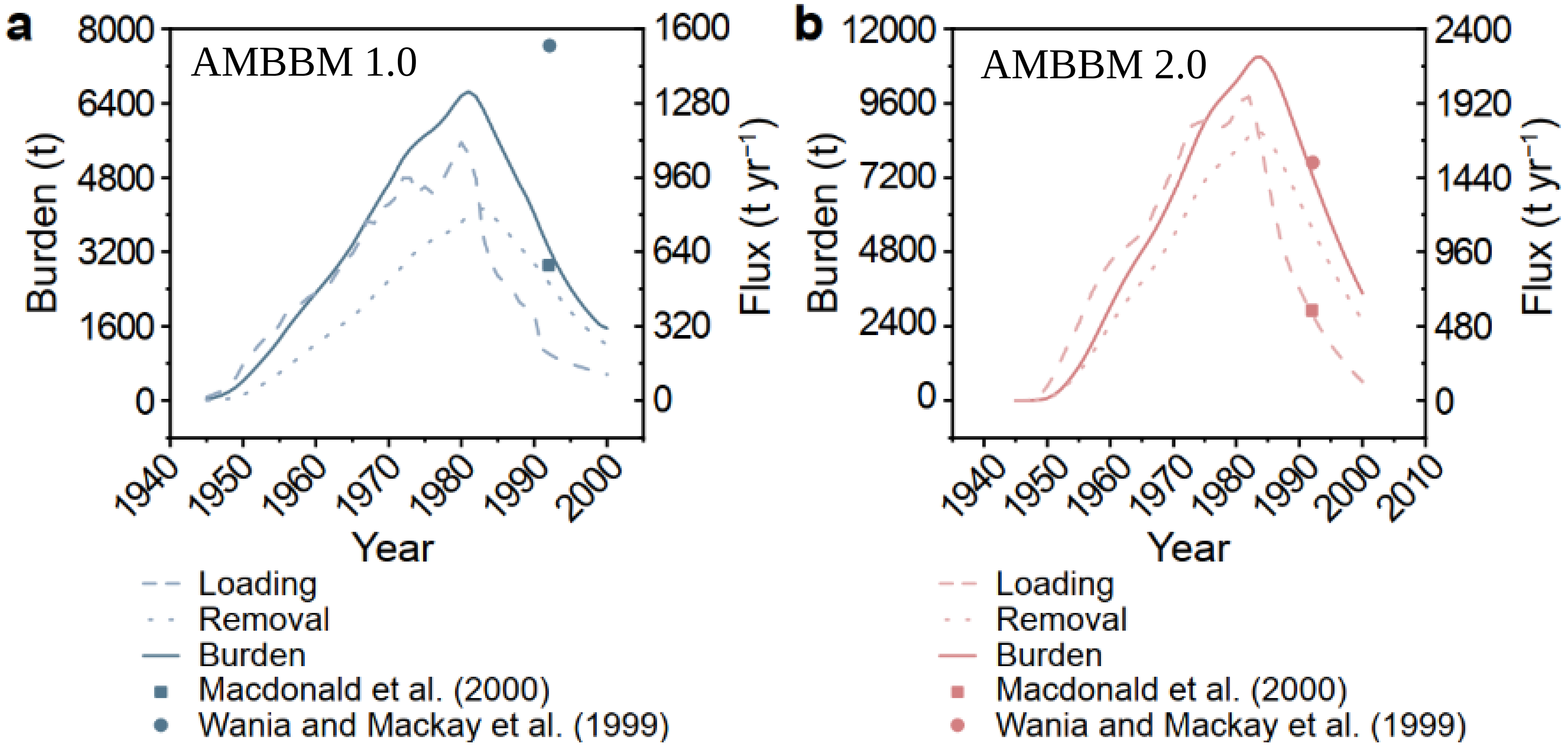
AMBBM 1.0 $RMSE_{\log}$ = 2.92

AMBBM 2.0 $RMSE_{\log}$ = 2.19

3

Model evaluation

Burden

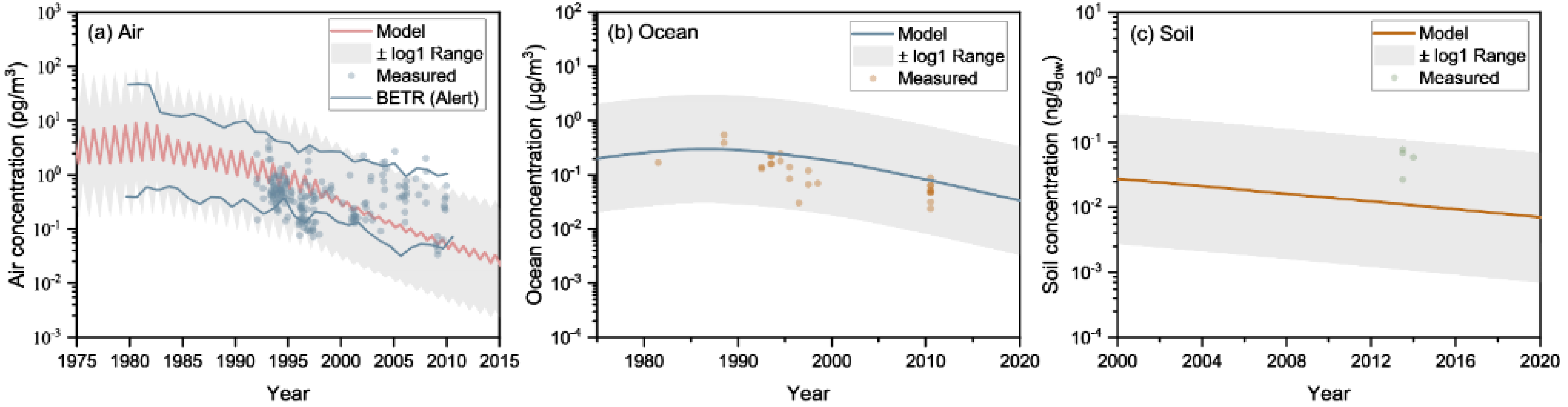


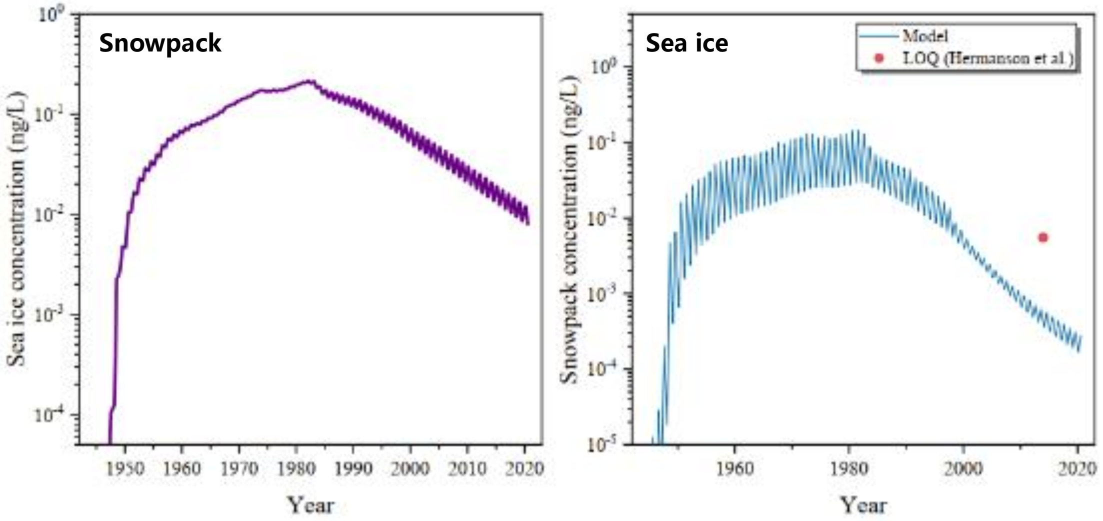
AMBBM 2.0 is about twice the burden of AMBBM 1.0 and is closer to the results of Wania and Mackay, 1999, while AMBBM 1.0 is closer to the results of Macdonald, 2000.

4 Result

4 Result

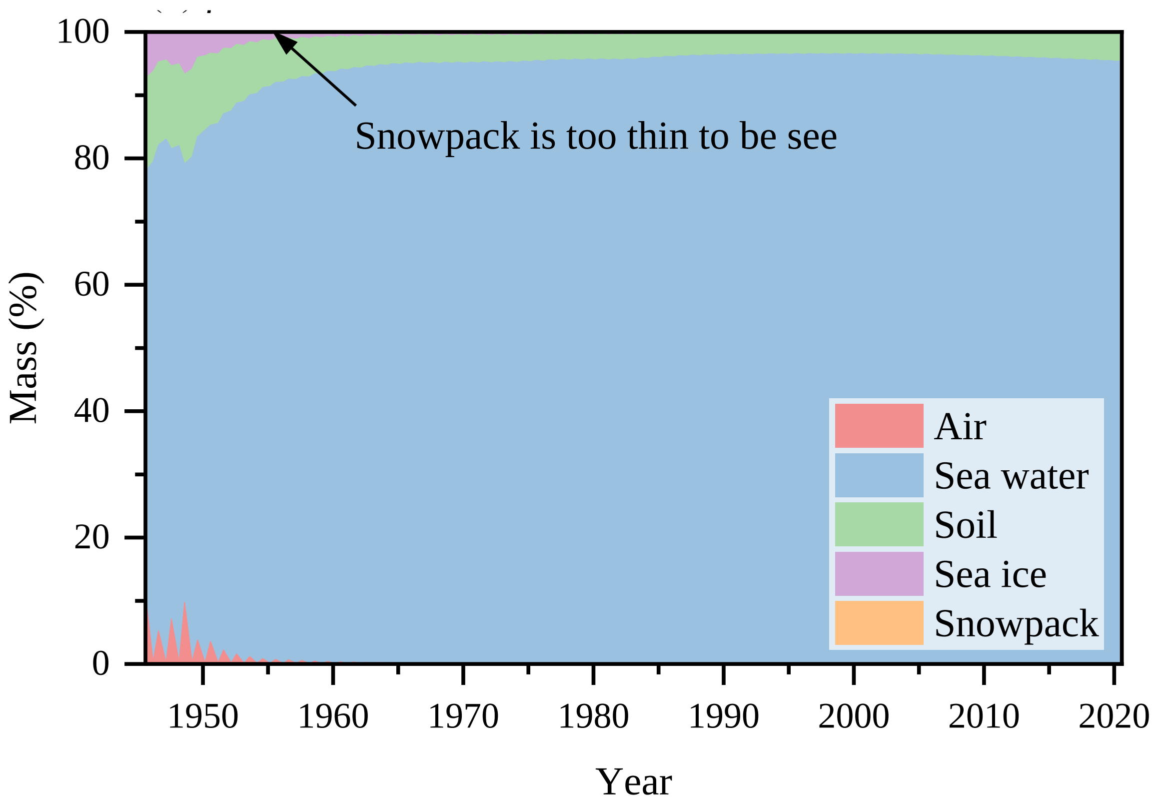
Concentration





4 Result

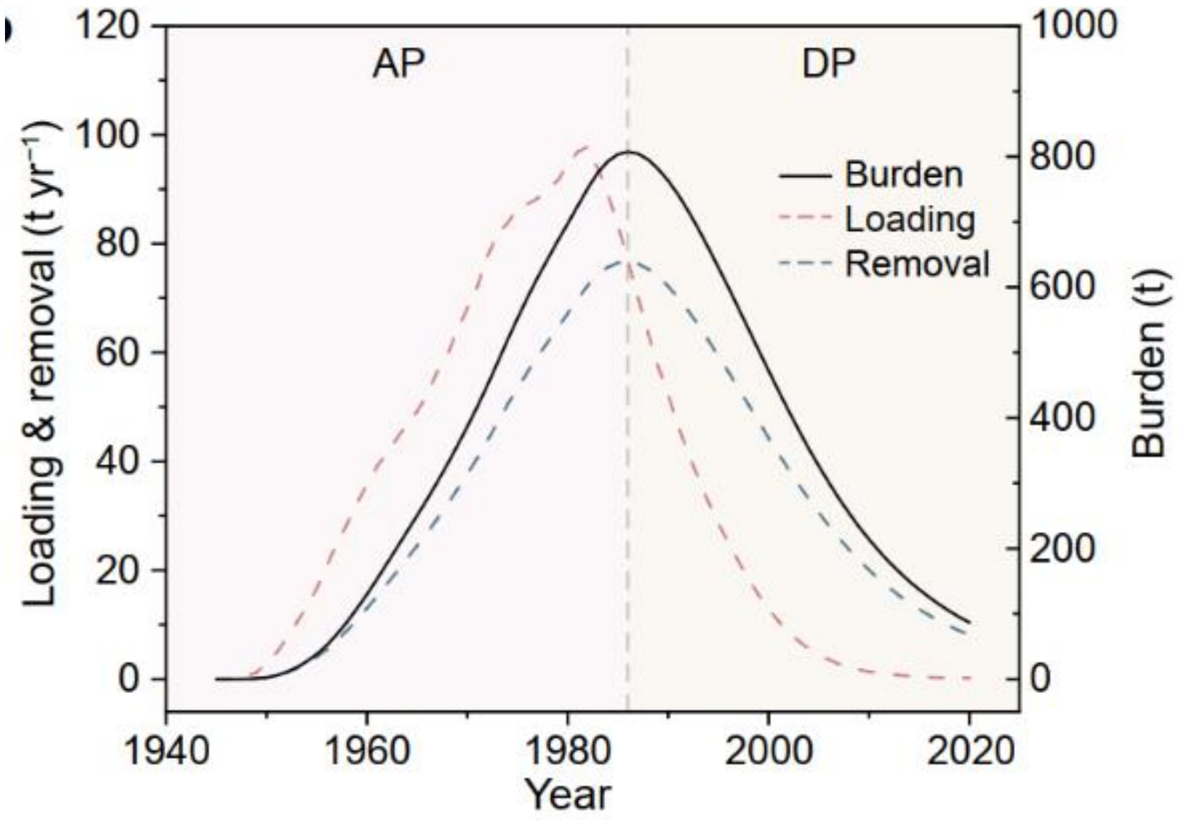
Burden



- Seawater stores most of the β-HCH;
- The atmosphere has a considerable amount in the early period, but the mass percentage is almost 0 in the middle and late period;
- The soil also stored a certain amount of β-HCH, and the proportion increased slowly in the later period;
- The proportion of burden in sea ice is high in the early stage and very low in the late period;
- The proportion of snow cover is negligible.

4 Result

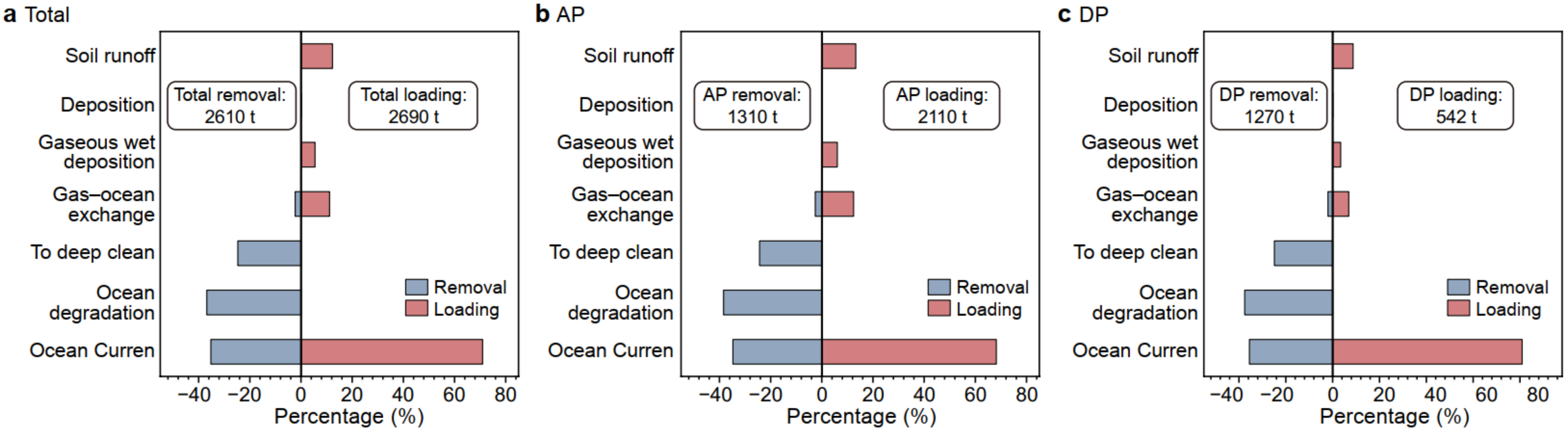
Burden



- Accumulation period（AP， 1945-1986）
- Decay period（DP， 1986-）

4 Result

Budget



Overall period

- Main loading： Ocean current
- Main removal： Ocean current，degradation、sink into deep sea

AP

- Effect of ocean currents are relatively weak
- Other processes are correspondingly stronger

DP

- Effect of ocean currents are relatively strong
- Other processes are correspondingly weaker

5 Discussion

5

Discussion

Loading to the Arctic Ocean

	α-HCH		β-HCH	
	Flux (t)	Percentage	Flux (t)	Percentage
Total	**52300**	**100%**	**2690**	**100%**
Gas–ocean exchange	30900	59%	301	11%
Gaseous wet deposition	5390	10%	147	5%
Deposition	11.7	0%	1.54	0%
Ocean current	11600	22%	1910	71%
River inflow	4420	8%	331	12%

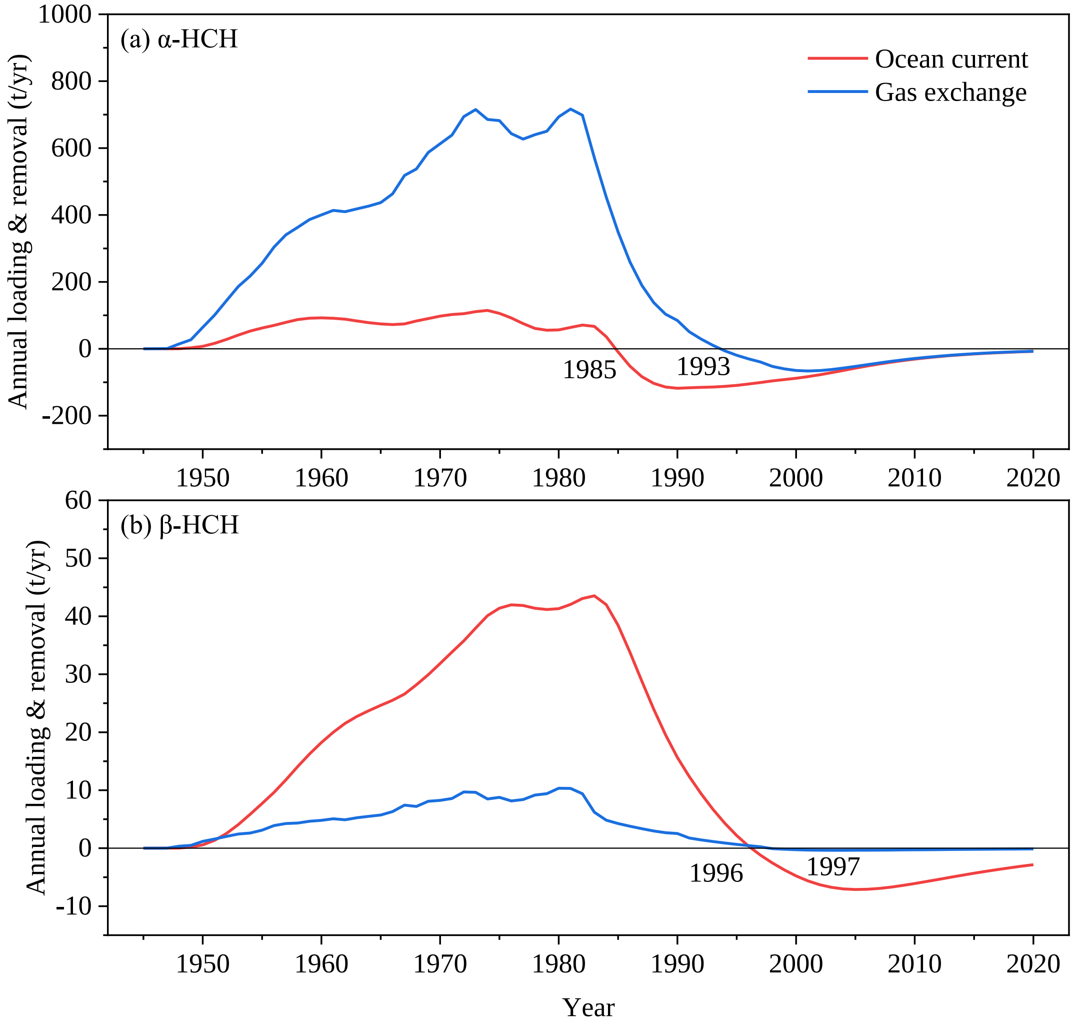
LRAT loading

LROT loading

- The total amount of α-HCH entering the Arctic is 20 times higher than that of β-HCH;
- For α-HCH and β-HCH, the sum of LRAT and LROT loading accounted for 92% and 88% of the total input;
- α-HCH，LRAT loading（69%）；β-HCH，LROT（71%）。

5 Discussion

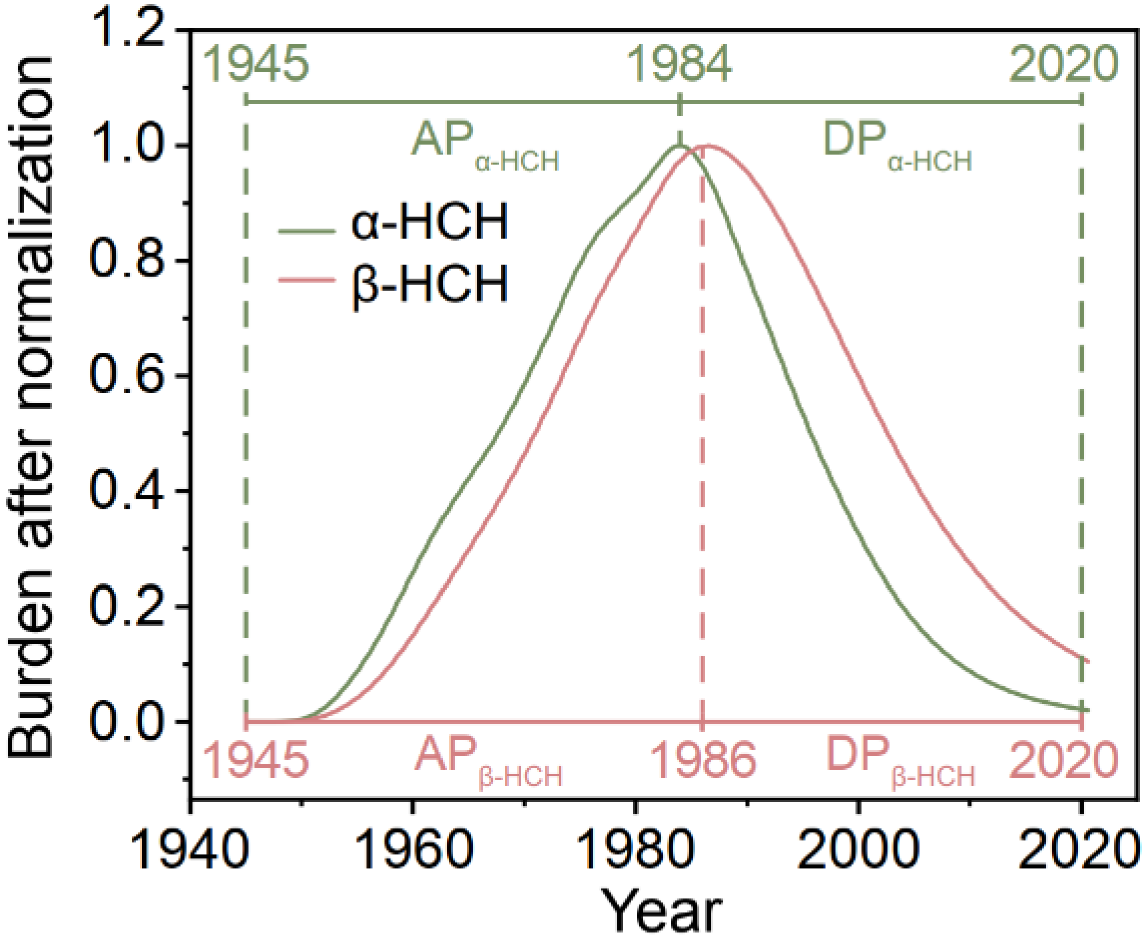
Re-emission



- In early period, both air-water exchange and the ocean current are important input pathways, but at a certain point, the direction changed.
- For ocean currents and air-water exchange, the switching points of α-HCH occurred in 1985 and 1993. β-HCH occurred in 1996 and 1997;
- Re-emission of α-HCH was mainly via LRAT (55%), and β-HCH was via LROT (94%).

5 Discussion

Burden

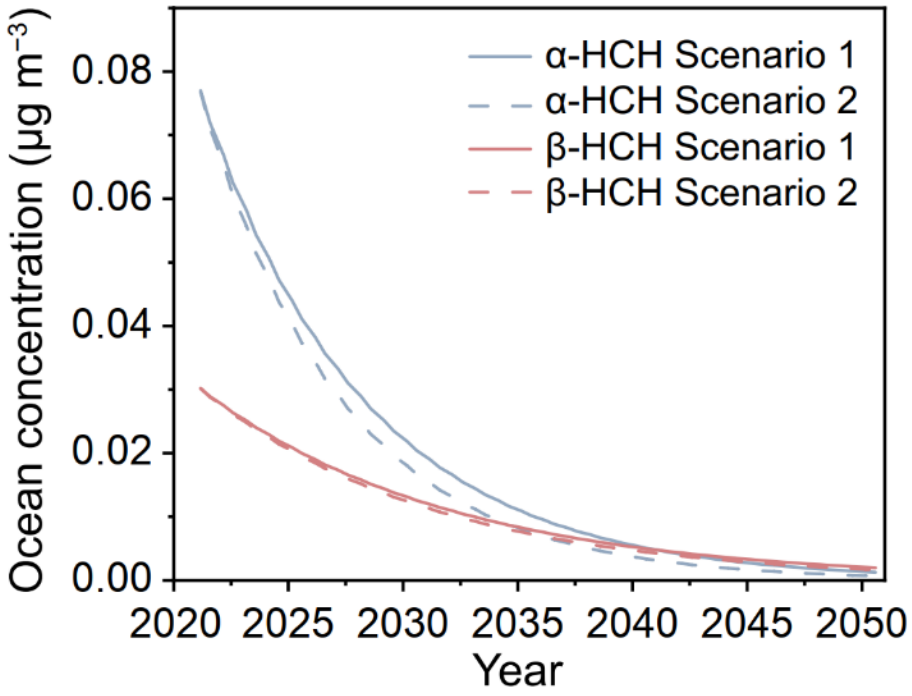


- In AP, the growth slopes of α- and β-HCH were similar, but β-HCH had a slower start.
- In DP, the decrease rate of β-HCH was slower than α-HCH.

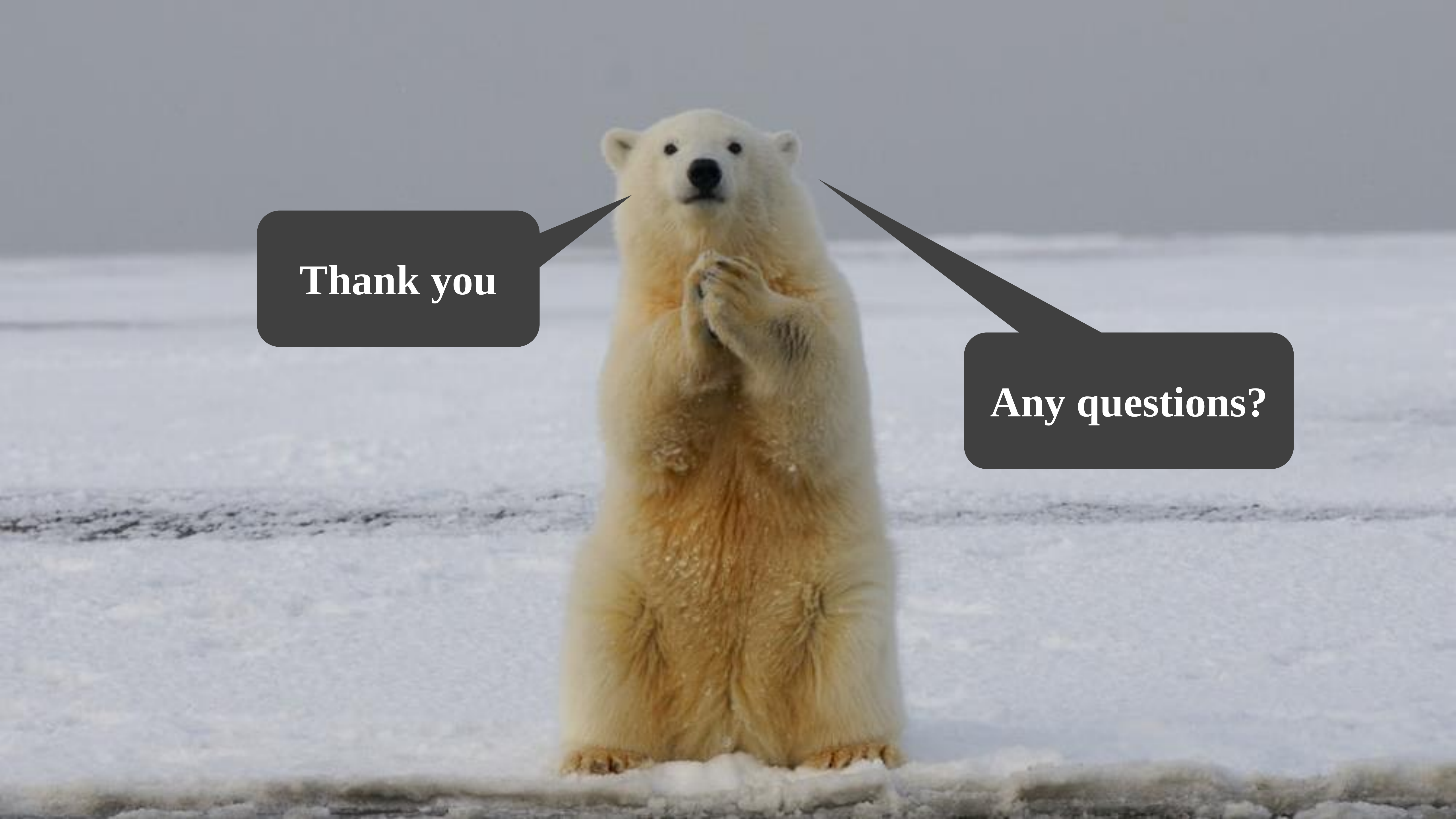
5 Discussion

Prediction and the Impact of Climate Change

- Scenario 1: Environmental parameters remain unchanged
- Scenario 2：RCP 8.5 assumptions (Carvalho, 2020; Overland, 2014; Bintanja, 2018; Shu, 2022)
  - Atmospheric temperature rises by 1K;
  - Ocean temperature increased by 2K;
  - 50% sea ice extent reduction;
  - Rainfall increases by 20%.



- Under the influence of climate change, the concentration of α-HCH is 1.5%-46% lower than scenario 1; the concentration of β-HCH is 0.3%-16% lower than scenario 1.
- In the future, the concentration of β-HCH will exceed that of α-HCH (2041, scenario 1; 2036, scenario 2).
- By 2050, β-HCH remains 4.4-5.3t, and α-HCH remains 1.8-3.4t.


Thank you
Any questions?