Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supporting information for

Investigating the dynamics of methylmercury bioaccumulation in the Beaufort Sea Shelf food web: a modeling perspective

1. Calculations of model parameters

1.1. Direct absorption rate (DAR) of MeHg from seawater

- Primary producers

$$U = t\frac{0.118S_A}{V}e^{-0.008DOC}$$ Eq.1 from Schartup et al. 2017[1]

$$DAR_P = U * C_W/C_W^{'}$$ Eq.2

Parameter	Units	Description	Equation or value
DAR_P	$km^2 \cdot t^{-1} \cdot year^{-1}$	Direct uptake rate of producers	Calculated based on Eq.2
C_W	pg L^{-1}	Seawater concentration	53[2]
$C_W^{'}$	$t \cdot km^{-2}$	Unit converted seawater concentration assuming 200m depth of Beaufort Sea	0.0000106
U	amol μm^{-3}nM	Empirical relationship between net MeHg uptake rate and cell surface to volume ratio	Calculated based on Eq.1
t	hour	Uptake time to reach equilibrium between cells and seawater	4 hours[1]
S_A/V	μm^{-1}	Assumed surface area to volume ratio of model species of interest (spherical)	$S_A/V = 3/r$
r	µm	Radius of cell	*r* = 1 and 10 for small and large phytoplankton groups, respectively. r= 4 and 20 for ice algae (e.g., N. frigida[3]) and benthic plants, respectively.
DOC	µM	Dissolved organic carbon concentration in seawater	120 µM[4]

- Zooplankton

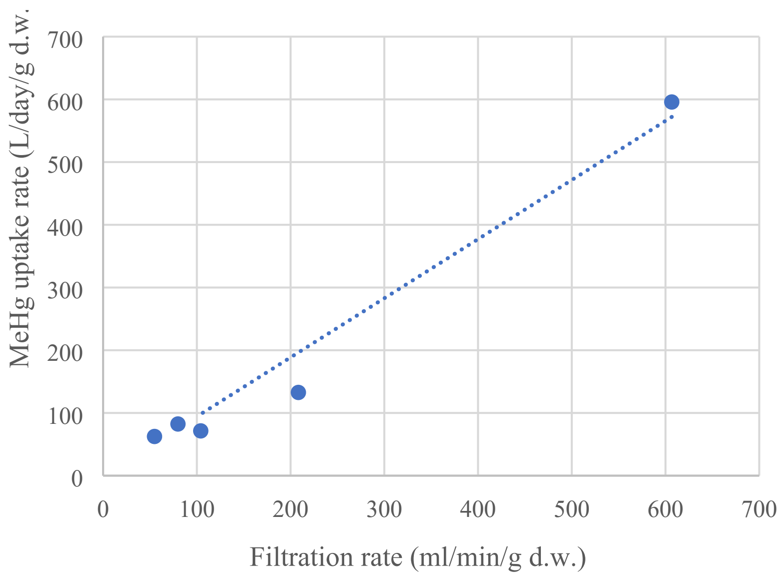
$DAR_{ZOO} = A_{EW}\frac{F}{M_Z} C_W / C_W^{'}$ Eq.3 modified from Schartup et al. 2017 [1]

$F = 1.777 \cdot e^{0.234T} \cdot (0.002 \cdot M_c)^{0.681e^{0.0199T}} \cdot 0.024$ Eq.4 [5]

Parameter	Units	Description	Equation or value
DAR_{ZOO}	$km^2 \cdot t^{-1} \cdot year^{-1}$	Direct uptake rate of zooplankton	Calculated based on Eq.3
A_{EW}	unitless	Absorption efficiency from seawater	$(1.87 + \frac{155}{K_{OW}})^{-1}$
C_W	pg L^{-1}	Seawater concentration	53 [2]
C_W'	$t \cdot km^{-2}$	Unit converted seawater concentration assuming 200m depth of Beaufort Sea	0.0000106
F	L d^{-1}	Clearance rate	Calculated based on Eq.4
K_{OW}	unitless	Octanol-water partition coefficient for CH_3HgCl	1.7 [6]
M_Z	g	Zooplankton mass (wet)	17.2 for macro-zooplankton; 0.00052 for medium copepod; 0.03 for large copepods; 0.0042 for other meso-zooplankton; and 0.0000082 for micro-zooplankton, based on Schartup et al. 2017 [1]
M_C	µg C	Zooplankton mass (wet)	$M_C = M_Z \cdot 10^5$
T	°C	Seawater temperature	Assumed 1°C

- Bivalves

We derived a linear relationship between MeHg absorption rate and filtration rate based on experimental results of various bivalves species at room temperature (see figure below, data from Pan and Wang 2011[7]). Using this relationship, we estimated that the theoretical direct absorption rate (K_u) of Arctic bivalves is 4.7 to 17.0 L/day/g d.w. (0.94 to 3.4 L/day/g w.w., assuming 80% moisture content) at room temperature, based on their filtration rate 5-18ml/min/g[8]. Tsui and Wang 2004[7] showed a strong temperature effect on K_u of *D. magma* and the MeHg uptake rates at lower temperature (14°C) are about three times lower than that at 24 °C given the same filtration rate. We thus consider the K_u for Arctic bivalves at ~1 °C is least three time lower than that is room temperature. Thus we adjusted final K_u for Arctic bivalves as 0.3 to 1.1 L/day/g w.w.



$DAR_{BV} = A_{EW} K_u C_W / C_W^{'}$ Eq.5

Parameter	Units	Description	Equation or value
DAR_{BV}	$km^2 \cdot t^{-1} \cdot year^{-1}$	Direct absorption rate of bivalves	Calculated based on Eq.5
A_{EW}	unitless	Absorption efficiency from seawater	0.5 [7]
K_u	L/hour/g w.w.	Empirically derived MeHg absorption rate	0.3 to 1.1
C_W	pg L^{-1}	Seawater concentration	53 [2]
$C_W{'}$	$t \cdot km^{-2}$	Unit converted seawater concentration assuming 200m depth of Beaufort Sea	0.0000106

1.2. Elimination rate (K_E)

- Zooplankton

$K_E = 0.00335\, M_Z^{\,-0.195} \cdot e^{(0.0066T)}$ Eq.5 from Schartup et al. 2017 [1]

where K_E is the elimination rate (per day), M_Z is the zooplankton biomass (see table above for details), and T is temperature 1°C.

- Fish

$ln(K_E) = 0.066T - 0.2 lnW - 5.83$ Eq.6 from Trudel et al. 1997 [9] where T is temperature (1 °C) and W is fish weight (g) that we obtained by searching common weight of typical species of each functional group on fishbase[10].

Functional group	Typical species	W (g)	$Ln(K_E)$	K_E (day^{-1})	K_E ($year^{-1}$)
Char & Dolly Varden	arctic char	518	-7.014	0.0009	0.328
Ciscos & Whitefish	cisco	298	-6.903	0.0010	0.367
Salmonids	arctic grayling	311	-6.912	0.0010	0.363
Small Nearshore Forage Fish	pacific herring	160	-6.779	0.0011	0.415
Arctic & Polar Cods	arctic cod	107	-6.699	0.0012	0.450
Capelin	capelin	19	-6.353	0.0017	0.636
Flounder & Benthic Cods	starry flounder	2990	-7.365	0.0006	0.231
Small Benthic marine Fish Other fish	saffron cod (30cm)	225	-6.847	0.0011	0.388

Table S1. Modeled and literature values of the MeHg concentrations (μg/g wet weight) in Beaufort Sea, supplemented by trophic level (TL), production-biomass ratio (P/B; an indicator for population turnover rate), and description of major species in each functional group. The model simulates steady-state MeHg concentration in each group in early 2010s.

Functional group	Typical species or family[a]	TL	P/B	Modeled conc.	Avg. Obs. conc.	M/O ratio [b]	Normalized mean bias	Obs. conc.[c]	SE	Notes and data sources
Beluga	Eastern Beaufort Sea Beluga stock (*Delphinapterus leucas)*	4.25	0.05	2.1E+00	1.2E+00	1.7	0.7	1.4E+00	1.5E-01	Collected in 2005[11]
								1.3E+00	1.1E-01	Collected in 2006[11]
								1.2E+00	1.5E-01	Collected in 2007[11]
								1.2E+00	1.3E-01	Collected in 2008[11]
								9.7E-01	1.5E-01	Collected in 2009[11]
								1.1E+00	1.4E-01	Collected in 2010[11]
								1.2E+00	1.5E-01	Collected in 2011[11]
								1.3E+00	1.3E-01	Collected in 2012[11]
Bowhead	Bering-Chukchi-Beaufort Bowhead stock *(Balaena mysticetus)*	3.37	0.02	2.3E-02	2.0E-02	1.2	0.2	2.0E-02	NA	collected in 2002-2003, Barrow, Alaska[12]
Ringed Seal	*Pusa hispida hispida*	3.87	0.50	2.7E-01	3.7E-01	0.8	-0.2	2.1E-01	5.0E-02	Collected in 2005[13]
								5.2E-01	1.4E-01	Collected in 2010[13]
Bearded Seal	*Erignathus barbatus*	3.84	0.20	5.7E-01				NA	NA	
Char & Dolly Varden	Arctic char and dolly varden	3.64	0.71	3.2E-02	7.5E-02	0.4	-0.6	7.5E-02	4.8E-02[d]	Collected in Shingle point, Yukon[14]
Ciscos & Whitefish	Various species in coregonids: arctic cisco, least cisco, and lake, broad and round whitefish	3.25	0.95	1.6E-02	2.3E-02	0.7	-0.3	2.0E-02	6.0E-03	Arctic cisco[15]
								2.5E-02	1.8E-03	Least cisco[15]
Salmonids	Arctic grayling and Inconnu	3.59	0.85	8.6E-02	NA	NA	NA	NA	NA	
Small Nearshore Forage Fish	Pacific herring, northern and pacific sand lance, rainbow smelt.	3.12	1.5	1.1E-02	2.7E-02	0.4	-0.6	3.3E-02	1.8E-03	Rainbow smelt[15]
								2.2E-02	6.0E-04	Pacific herring[15]
Arctic & Polar Cods	Arctic cod and polar Cod	3.50	0.81	2.7E-02	3.2E-02	0.9	-0.1	3.2E-02	1.6E-03	Arctic cod[15]

Capelin	Capelin	3.50	0.97	2.3E-02	NA	NA	NA	NA	NA	
Flounder & Benthic Cods	Starry flounder, arctic flounder, bering flounder, saffron cod, burbot, greenland cod	3.36	0.76	2.9E-02	4.9E-02	0.6	-0.4	4.6E-02	1.8E-02	Starry flounder[15]
								4.7E-02	1.1E-02	Arctic Flounder[15]
								5.5E-02	1.6E-03	Saffron cod[15]
Small Benthic Marine fish	sculpins and zoarcids, with fourhorn sculpin most common	3.20	1.07	2.4E-02	1.1E-01	0.2	-0.8	1.1E-01	9.2E-03	Fourhorn sculpin[15]
Other Fish	Arctic lamprey, threespine and niniespine stickleback, longnose sucker, northern pike	3.08	0.53	1.7E-02	NA	NA	NA	NA	NA	
Arthropods	Amphipoda, Isopoda, Decapoda, Pycnogonida, and Maxillopoda	2.22	0.76	2.0E-02	1.8E-01	0.1	-0.9	3.2E-02	1.7E-02	*Acanthostepethia & Anonyx spp*[15]
								3.3E-01	3.7E-02	*S. ferox*[16]
Bivalves	Bivalvia	2	0.61	5.31E-03	NA	NA	NA	NA	NA	
Echinoderms	Ophiuroidea, Asteroidea, Holothuroidea, Echinoidea, and Crinoidea	2.23	0.55	9.1E-03	NA	NA	NA	NA	NA	
Mollusks	All mollusks except bivalves: Gastropods, Polyplacophora, Scaphopoda, Cephalopod, and Caudofovaeta	2.00	0.86	4.0E-03	9.1E-03	0.4	-0.6	3.8E-03	1.4E-03 [d]	*Limacina helicina*[17]
								1.4E-02	9.0E-03 [d]	*Clione limacine*[17]
Worms	All worms from various phyla: primarily Annelids (segmented worms: Polychaetes and Ciltellata), but also from Entoprocta, Nematoda, Nemertea, and Priapulida	2.07	0.96	5.1E-03	1.0E-02	0.5	-0.5	1.0E-02	5.6E-03	*A.malmgremi* [15]
Other Benthos	Cnidarians (Anthozoa: sea anemones and Hydrozoa), Ascidiacea, brachiopods, and bryozoa	2.08	0.76	6.9E-03	NA	NA	NA	NA	NA	
Jellyfish	ctenophores, cnidarians (Scyphozoa, Hydrozoa), and larvaceans	2.34	23.59	7.1E-04	NA	NA	NA	NA	NA	
Macro-Zooplankton	size>20mm: including krill, shrimp, mysids, amphipods,	2.69	9.36	1.8E-03	2.1E-02	0.1	-0.9	6.4E-03	2.6E-03	Mysids[15]
								3.2E-03	1.8E-03 [d]	*Thysanoessa spp.*[17]

	and chaetognaths							3.8E-03	1.6E-03 [d]	*Parasagitta spp.*[17]
								1.3E-02	4.0E-04	*T.Libellula*[15]
								1.8E-02	8.0E-04	chaetognaths[18]
								6.5E-02	1.0E-02	*Eualus gaimardiil*[16]
								4.6E-02	5.2E-03	*Eualus spp.*[15]
								1.2E-02	5.2E-03[d]	*Themisto spp.*[17]
Medium Copepods	medium sized copepod species: *Pseudocalanus spp., O. simils, and L. macrurus*	2.14	20.76	5.5E-04	NA	NA	NA	NA	NA	
Large Copepods	*C. hyperboreus, C. glacialis and M. longa*	2.38	5.8	1.2E-03	1.5E-03	0.8	-0.2	1.8E-03	8.0E-04 [d]	*C. hyperboreus & C. glacialis*[17]
								1.4E-03	2.0E-04	*Calanus spp.*[15]
								1.4E-03	2.0E-04 [d]	*C. hyperboreus & C. glacialis*[19]
								1.4E-03	2.0E-04 [d]	*C. hyperoboreus*[18]
Other Meso-Zooplankton	Size 0.2-20mm: *C. glacialis, C. hyperboreus, M. longa, and Pseudocalanus spp*	2.36	26.29	7.1E-04	8.5E-04	0.8	-0.2	8.5E-04	3.9E-04 [d]	Zooplankton > 0.153 mm[20]
Micro-Zooplankton	Zooplankton with size <0.2mm	2.00	61.94	6.0E-04	8.5E-04	0.7	-0.3	8.5E-04	3.9E-04 [d]	Zooplankton > 0.153 mm[20]
Large Phytoplankton	Phytoplankton with size> 5 µm	1.00	42.33	6.0E-05	1.2E-04	0.5	-0.5	1.2E-04	1.1E-04 [d]	Phytoplankton >20 µm[20]
Small Phytoplankton	Phytoplankton with size < 5 µm	1.00	83.86	3.0E-04	NA	NA	NA	NA	NA	
Ice Algae	living organisms that are frozen into sea ice	1.00	36.28	1.8E-04	NA	NA	NA	NA	NA	
Benthic Plants	Arctic kelp	1.00	10.00	1.3E-04	NA	NA	NA	NA	NA	
Pelagic detritus				3.4E-04						
Benthic detritus				2.6E-04						

a. Details can be found in Ehrman et al 2021[21] and Hoover et al. 2021.[22]

b. The ratio of Modeled concentration to average observed concentration.

c. Literature values from each study were selected based on available MeHg data in the Beaufort Sea coastal region. If the dry weight-based concentration was provided, it is converted to wet weight based concentration, assuming 80% moisture content in the sample. Concentration of fish and marine mammal are from analyses of their muscle tissues. We choose the total Hg data between 2005 and 2015 for species that have temporal trends of Hg (ringed seal and beluga), and assume 100% Hg in muscle tissue is MeHg in these mammals.

d. Only standard deviation was reported.

Table S2. Sensitivity coefficients of toxicokinetic input parameters (DAR - direct absorption rate, K_E -elimination rate, AE - assimilation efficiency). The sensitivity analysis was conducted by increasing (+) or decreasing (-) 10% of the input parameter. If the absolute value of sensitivity coefficient <0.01, it is illustrated as 0, which indicates that the MeHg concentration in the specified functional group is not sensitive to the parameter change. The further the sensitivity coefficient is from 0, the higher the sensitivity coefficient is of the MeHg concentration in the specified functional group.

	DAR						K_E		AE							
	Benthos		zooplankton		producers		Mammals		Mammals		Fish		Benthos		Zooplankton	
Groups	(+)	(-)	(+)	(-)	(+)	(-)	(+)	(-)	(+)	(-)	(+)	(-)	(+)	(-)	(+)	(-)
Beluga	0.72	0.71	0.08	0.07	0.18	0.18	-0.61	-0.7	0.18	0.17	0.36	0.34	0.12	0.11	0.12	0.1
Bowhead	0.02	0	0.39	0.38	0.59	0.58	-0.74	-0.89	0.18	0.17	0.01	-0.01	0.01	-0.01	0.51	0.47
Ringed seal	0.79	0.76	0.07	0.04	0.18	0.14	-0.31	-0.36	0.19	0.16	0.29	0.26	0.14	0.11	0.09	0.06
Bearded seal	0.82	0.81	0.04	0.03	0.14	0.12	-0.52	-0.59	0.18	0.17	0.25	0.24	0.13	0.12	0.06	0.05
Char & dolly varden	0.80	0.78	0.06	0.04	0.16	0.13	0.01	-0.01	0.01	-0.01	0.39	0.35	0.14	0.11	0.08	0.05
Ciscos & whitefish	0.75	0.71	0.1	0.05	0.19	0.16	0.02	-0.02	0.02	-0.02	0.29	0.24	0.14	0.09	0.13	0.08
Salmonids	0.79	0.78	0.06	0.05	0.15	0.14	0	-0.01	0	0	0.39	0.36	0.12	0.11	0.08	0.07
Small Nearshore Forage Fish	0.70	0.70	0.08	0.08	0.18	0.2	0	0	0	0	0.3	0.29	0.12	0.11	0.13	0.11
Arctic & polar cods	0.70	0.68	0.1	0.08	0.22	0.19	0.01	-0.01	0.01	-0.01	0.42	0.39	0.12	0.1	0.14	0.11
Capelin	0.71	0.67	0.11	0.07	0.21	0.19	0.02	-0.02	0.02	-0.02	0.43	0.38	0.13	0.09	0.14	0.1
Flounder and benthic cods	0.86	0.83	0.04	0.01	0.14	0.1	0.01	-0.01	0.01	-0.01	0.3	0.27	0.15	0.12	0.05	0.02
Small benthic marine fish	0.87	0.85	0.03	0.01	0.12	0.09	0.01	-0.01	0.01	-0.01	0.23	0.21	0.15	0.13	0.04	0.02
Other fish	0.78	0.77	0.06	0.05	0.17	0.15	0.01	-0.01	0.01	-0.01	0.18	0.17	0.12	0.11	0.08	0.06
Arthropods	0.9	0.94	-0.02	0.02	0.05	0.08	-0.02	0.02	-0.02	0.02	-0.02	0.02	0.09	0.12	-0.02	0.02
Bivalves	0.89	0.87	0.01	-0.01	0.11	0.09	0.01	-0.01	0.01	-0.01	0.01	-0.01	0.08	0.06	0.01	-0.01
Echinoderms	0.9	0.91	0	0	0.08	0.08	0	0	0	0	0	0	0.29	0.29	0	0.01

Mollusks	0.82	0.84	0	0.02	0.13	0.15	-0.01	0.01	-0.01	0.01	-0.01	0.01	0.09	0.11	0	0.02
Worms	0.83	0.84	0	0.01	0.14	0.15	-0.01	0.01	-0.01	0.01	-0.01	0.01	0.28	0.28	0	0.02
Other benthos	0.84	0.84	0.01	0.01	0.13	0.13	0	0	0	0	0	0	0.14	0.14	0.01	0.01
Jellyfishes	0.02	0	0.25	0.23	0.74	0.73	0	-0.01	0.01	-0.01	0.01	0	0.01	0	0.5	0.47
Macro zooplankton	0	0.03	0.32	0.35	0.61	0.65	-0.02	0.01	-0.01	0.02	-0.01	0.02	-0.01	0.02	0.66	0.65
Medium copepods	0.02	0	0.45	0.43	0.55	0.53	0.01	-0.01	0.01	-0.01	0.01	-0.01	0.01	-0.01	0.61	0.57
Large copepods	0.03	-0.02	0.42	0.37	0.59	0.56	0.02	-0.03	0.02	-0.02	0.03	-0.02	0.03	-0.02	0.44	0.38
Other meso zooplankton	0.01	0.01	0.35	0.34	0.63	0.63	0	-0.01	0	0	0	0	0	0	0.91	0.86
Micro zooplankton	0.01	0	0.39	0.39	0.59	0.59	0	0	0	0	0	0	0	0	0.42	0.42
Large Pelagic Producers	0	0	0	-0.01	0.98	0.99	0	0	0	0	0	0	0	0	0	-0.01
Small Pelagic Producers	-0.01	0.01	-0.02	0.01	0.97	1	-0.01	0.01	-0.01	0.01	-0.01	0.01	-0.01	0.01	-0.02	0
Ice algae	-0.02	0.02	-0.02	0.01	0.98	1.01	-0.02	0.02	-0.02	0.02	-0.02	0.02	-0.02	0.02	-0.03	0.01
Benthic plants	0	0	-0.01	0	0.98	0.99	0	0	0	0	0	0	0	0	-0.01	0
Pelagic detritus	0.05	0.07	0.17	0.2	0.74	0.75	-0.03	-0.01	-0.01	0.02	0.01	0.04	0	0.02	0.25	0.27
Benthic detritus	0.04	0.05	-0.01	0	0.94	0.94	0	0	0	0	0	0	0.01	0.01	-0.01	0

Table S3. Comparison of MeHg concentrations (μg/g wet weight) in beluga prey species from Beaufort Sea vs. Bering/Chukchi Sea. Only samples collected within the wintering range of beluga in Bering and Chukchi Sea are chosen (i.e., north of St Matthew Island, Alaska).

	Beaufort Sea [a]		**Bering/Chukchi Sea** [b]		
Species	Mean conc.	SE	Mean conc.	SE	**Ratio** between Beaufort and Bering/Chukchi Sea
Starry flounder	5.54E-02	1.46E-02	2.8E-02	2.1E-02	2.0
Arctic Flounder	5.10E-02	8.80E-03	2.0E-02	2.0E-03	2.6
Saffron cod	6.16E-02	5.80E-03	2.3E-02	8.0E-03	2.7
Fourhorn Sculpin	1.17E-01	1.52E-02	5.1E-02	2.2E-02	2.3
Arctic cod	3.26E-02	5.80E-03	1.5E-02	3.2E-03	2.1

a. Data are from Loseto et al. 2008 [23].
b. Data are from State of Alaska Department of Environmental Conservation Fish Monitoring Program https://dec.alaska.gov/eh/vet/fish-monitoring-program/fish-tissue-mercury.aspx.html except for Arctic cod, of which data is published in Fox et al. 2017[24].

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