Supporting Information for

Kinetics and threshold level of 2,3,4,5-tetrachlorobiphenyl dechlorination by an organohalide respiring bacterium

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**PCB extraction and analysis.** PCBs were extracted from POM strips with a mixture of acetone:hexane (1:1) by shaking overnight on a wrist shaker at room temperature. The POM was re-extracted twice, then the pooled extracts were evaporated to ~1-2 mL using an N-EVAP 111 nitrogen evaporator (Organomation Associates). Volumes before and after evaporation were recorded, and the mass of each POM strip was determined after extraction. PCB 30 and 204 (80 ng from stock of 8 mg L<sup>-1</sup> in acetone) were added as internal standards to one mL extract prior to analysis with a HP 6890 GC-µECD (Agilent Technologies) equipped with a DB-1 capillary column (60 m × 0.25 mm × 0.25 μm; JW Scientific). Helium was used as the carrier gas at 128 kPa. The injector and detector temperatures were 225 and 300 °C, respectively. The oven program was as follows: gradient of 100 °C to 200 °C at 2 °C min<sup>-1</sup> followed by 10 °C min<sup>-1</sup> to 300 °C. PCB 61 and 23 were quantified with a 6- point calibration curve (5,000 to 5.10<sup>-2</sup> μg L<sup>-1</sup>). Surrogate congeners could not be used to estimate PCB loss during POM extraction from microcosms because trace contaminants interfered with the surrogate at the lowest concentrations. However, PCB loss during extraction independently tested with PCB 14 was negligible (av = 1 %, sd = 2 %, n = 3).

For PCB quantification from aqueous phase, one mL of culture was transferred to a Teflon-caped extraction tube with ten μL of the surrogate PCB 14 (1,000 μg L<sup>-1</sup>) and 5 mL of hexane. The tube was vigorously shaken for 10s, frozen at -20°C to separate phases and the supernatant was purified on pre-equilibrated florisil and copper. Volumes of sample collected before and after purification were recorded and 1mL of purified sample was analyzed. PCB<sub>aq</sub> measurements were performed in triplicate.
Calculation of PCB mole percentage. To quantify dechlorination of PCB 61 to PCB 23, the exact concentration of PCB 23 product detected over time in POM strips was converted to mol % by the following equation:

\[
P_C B\ 23\ \text{mol}\% = \frac{P_C B\ 23_{pom}}{(P_C B\ 23_{pom} + P_C B\ 61_{pom})} \times 100
\]

Eq. S1

Calculation of freely dissolved PCB concentration in the aqueous phase. The concentrations of PCB61 and PCB 23 in the aqueous phase (PCB 61_{aq} and PCB 23_{aq}, respectively) were estimated with equation S2:

\[
P_C B\ 23_{aq} = \frac{P_C B\ 23_{pom}}{K_{pom}}
\]

Eq. S2

The partition coefficient \(K_{pom}\) for PCB 61 and PCB 23 were calculated with the following equation:\(^1\):

\[
\log K_{pom} = 0.791 \log K_{ow} + 1.018
\]

Eq. S3

In this approach, the exchange rate between water and POM is assumed to be much faster compared to the rate of dechlorination which is a reasonable assumption based on the fast exchange kinetics reported by Hawthorne et al.\(^1\) in well mixed slurry systems with POM.

\(K_{ow}\) values used were from Hawker and Connell\(^2\): PCB 23, \(log K_{ow}=5.57\) and \(log K_{pom}=5.424\); PCB 61, \(log K_{ow}=6.04\) and \(log K_{pom}=5.796\).

Calculation of PCB dechlorination rate. The calculation of PCB dechlorination rate from a passively dosed system must take into account the buffering of PCB concentration in the aqueous phase as a result of the large reserve capacity in the polymer phase. Since the
dechlorination rate is limited to the bioavailable aqueous phase and is controlled by both the substrate concentration in the aqueous phase and population density, a larger buffering capacity in the solid phase (more POM or sediment) will reduce the apparent decline of the freely dissolved aqueous concentration. Thus, the ratio of buffering capacity vs. aqueous volume where dechlorination is taking place influences the overall rate of disappearance of PCBs observed and is incorporated into a model as described here:

\[
\text{(rate of mass loss from water)} + \text{(rate of mass loss from solids)} = \text{(rate of dechlorination)}
\]

\[
V_w \cdot \frac{d\text{PCB 61}_{aq}}{dt} + m_s \cdot \frac{d\text{PCB 61}_{solid}}{dt} = V_w \cdot r_{bio}
\]  
Eq. S4

where \(V_w\) is the volume of the aqueous phase and \(m_s\) is the mass of the solid phase, and \(r_{bio}\) is the rate of microbial dechlorination in the aqueous phase. 

\[
\text{PCB 61}_{aq} \quad \text{and PCB 61}_{solid} \quad \text{is the solid phase concentration (POM or sediment) of PCB 61. Assuming first order rate for dechlorination with respect to aqueous concentration:}
\]

\[
V_w \cdot \frac{d\text{PCB 61}_{aq}}{dt} + m_s \cdot \frac{d\text{PCB 61}_{solid}}{dt} = V_w \cdot \text{PCB 61}_{aq} \cdot k_b
\]  
Eq. S5

where \(k_b\) is the first order rate constant. Assuming that the solid phase is in equilibrium with the water phase at any time:

\[
\text{PCB 61}_{solid} = K_d \cdot \text{PCB 61}_{aq} \quad \text{or} \quad \frac{d\text{PCB 61}_{solid}}{dt} = K_d \cdot \frac{d\text{PCB 61}_{aq}}{dt}
\]  
Eq. S6

where, \(K_d\) is the partition constant between solid phase and aqueous phase. Substituting Eq. 6 into Eq. 5:

\[
V_w \cdot \frac{d\text{PCB 61}_{aq}}{dt} + m_s \cdot K_d \cdot \frac{d\text{PCB 61}_{aq}}{dt} = V_w \cdot \text{PCB 61}_{aq} \cdot k_b
\]  
Eq. S7
Dividing by $V_w$:

$$\frac{d \text{PCB 61}_{aq}}{dt} + \frac{m_s K_d}{V_w} \frac{d \text{PCB 61}_{aq}}{dt} = \text{PCB 61}_{aq} \cdot k_b$$

Eq. S8

$$\frac{d \text{PCB 61}_{aq}}{dt} \left( 1 + \frac{m_s K_d}{V_w} \right) = \text{PCB 61}_{aq} \cdot k_b$$

Eq. S9

Defining apparent dechlorination rate:

$$k'_b = \frac{k_b}{\left( 1 + \frac{m_s K_d}{V_w} \right)}$$

Eq. S10

The right term in brackets in the denominator is the buffering capacity of the solid phase that attenuates the observed rate of dechlorination by depressing the freely dissolved aqueous concentration and serving as a source:

$$\frac{d \text{PCB 61}_{aq}}{dt} = \text{PCB 61}_{aq} \cdot k'_b$$

Eq. S11

After integration the equation is:

$$\frac{\text{PCB 61}_{aq}}{\text{PCB 61}_{aq}} = e^{-k'_b t}$$

Eq. S12

Where, $\text{PCB 61}_{aq}$ is the aqueous concentration of PCB 61 at time zero. The first order dechlorination rate $k'_b$ is estimated by plotting PCB 61$_{aq}$ determined from measurement of PCB 61$_{pom}$ and calculated according to equation S2. The estimated value of $k'_b$ is then converted to the true aqueous phase dechlorination rate ($k_b$) using equation S10.
**Table S1. Growth rate of pelagic DF-1 in liquid medium.**

| PCB61 concentration (nM) | Growth rate in media (log total 16SrRNA gene copies day$^{-1}$) | y-intercept (log total 16SrRNA gene copies) | $r^2$ |
|--------------------------|---------------------------------------------------------------|------------------------------------------|------|
| 1.69                     | 0.0058                                                        | 7.73                                     | 0.77 |
| $3.23 \times 10^{-1}$    | -0.0004                                                       | 7.53                                     | 0.01 |
| $9.01 \times 10^{-2}$    | -0.001                                                        | 7.62                                     | 0.04 |
| $3.33 \times 10^{-2}$    | -0.0011                                                       | 7.64                                     | 0.29 |
| $8.56 \times 10^{-3}$    | -0.0004                                                       | 7.64                                     | 0.01 |
| $3.95 \times 10^{-3}$    | -0.0042                                                       | 7.61                                     | 0.73 |
| control                  | 0.0057                                                        | 7.31                                     | 0.48 |
Table S2. Growth rate of DF-1 on POM surface.

| PCB61 concentration (nM) | Growth rate on POM (log total 16SrRNA gene copies day$^{-1}$) | y-intercept (log total 16SrRNA gene copies) | $r^2$ |
|--------------------------|-------------------------------------------------------------|------------------------------------------|------|
| 1.69                     | -0.009                                                      | 6.71                                     | 0.93 |
| $3.23 \times 10^{-1}$    | -0.008                                                      | 6.69                                     | 0.96 |
| $9.01 \times 10^{-2}$    | -0.0044                                                     | 6.59                                     | 0.80 |
| $3.33 \times 10^{-2}$    | -0.0134                                                     | 6.52                                     | 0.88 |
| $8.56 \times 10^{-3}$    | -0.0066                                                     | 6.79                                     | 0.48 |
| $3.95 \times 10^{-3}$    | -0.0099                                                     | 7.44                                     | 0.81 |
| control                  | 0.007                                                       | 6.05                                     | 0.37 |
Table S3. Comparison of dechlorination rates in current and prior studies. Units normalized for comparison to µg L⁻¹ Cl removed week⁻¹ µmol L⁻¹ substrate and µg L⁻¹ Cl removed week⁻¹ µmol L⁻¹ Cl are highlighted. Average Cl per molecule of 3 and 4 were used, respectively, in calculations for Aroclor 1242 and Aroclor 1248.

| Rate of dechlorination | Units | Ref. |
|------------------------|-------|------|
| 2.70 x 10⁻²            | PCB23 nM day⁻¹ per nM PCB61 | This study |
| 6.95                   | PCB23 µg L⁻¹ day⁻¹ per µM PCB61 |
| 4.86 x 10⁻¹            | PCB23 µg L⁻¹ week⁻¹ per µM PCB61 |
| 6.70 µg L⁻¹ Cl removed week⁻¹ per µmol L⁻¹ substrate added |
| 1.34 µg L⁻¹ Cl removed week⁻¹ per µmol L⁻¹ Cl added |
| 3.78 x 10⁻²            | µmol L⁻¹ congener week⁻¹ per µmol L⁻¹ Cl added |
| 7.05 x 10⁻³            | µmol L⁻¹ congener week⁻¹ per µmol L⁻¹ Aroclor 1242 added |
| 1.80 x 10⁻³            | nmol g⁻¹ Cl removed day⁻¹ per µmol g⁻¹ Cl added |
| 1.80 x 10⁻⁶            | µmol g⁻¹ Cl removed day⁻¹ per µmol g⁻¹ Cl added |
| 1.26 x 10⁻⁵            | µmol g⁻¹ Cl removed week⁻¹ per µmol g⁻¹ Cl added |
| 3.78 x 10⁻²            | µmol kg⁻¹ congener week⁻¹ per µmol kg⁻¹ Aroclor 1248 added |
| 1.34 x 10⁻²            | µg kg⁻¹ Cl removed week⁻¹ per µmol kg⁻¹ Cl added |
| 4.47 x 10⁻³            | µg kg⁻¹ Cl removed week⁻¹ per µmol kg⁻¹ Cl added |
| min 6.00x10⁻³           | 9.00x10⁻³ |
| max 1.80x10⁻²           | 9.00x10⁻³ |
| av 6.00x10⁻³            | 1.80x10⁻² |
| min 6.00x10⁻³           | 9.00x10⁻³ |
| max 1.80x10⁻²           | 1.80x10⁻² |
| av 1.90x10⁻²            | 1.80x10⁻² |
| min 1.49                | 2.23 |
| max 4.47                | 4.47 |
| av 3.72x10⁻⁴            | 5.58x10⁻¹ |
| 1.12 µg kg⁻¹ Cl removed week⁻¹ per µmol kg⁻¹ Cl added |
| 7.70 x 10⁻³             | nmol g⁻¹ Cl removed day⁻¹ per µmol g⁻¹ Cl added |
| 7.70 x 10⁻⁶             | µmol kg⁻¹ Cl removed week⁻¹ per µmol kg⁻¹ Cl added |
| 5.39 x 10⁻⁹             | µmol kg⁻¹ Cl removed week⁻¹ per µmol kg⁻¹ Cl added |
| 1.91 x 10⁻⁴             | µg kg⁻¹ Cl removed week⁻¹ per µmol kg⁻¹ Cl added |
| 7.64 x 10⁻⁷             | µg kg⁻¹ Cl removed week⁻¹ per µmol kg⁻¹ substrate (Aroclor 1248) |
Figure S1: Dechlorination activity of PCB 61 in the aqueous phase at different concentrations, calculated from POM measurements with equation S2. (a) log PCB 61_{aq} (substrate) and (b) log PCB 23_{aq} (product) concentration measurements, data points fitted with a linear trendline. PCB 61_{aq} concentration in nM: (●):1.7, (■):3.2 × 10⁻¹, (▲): 9.9 × 10⁻², (+): 3.3 × 10⁻², (×) 8.6 × 10⁻³ (●): 3.4 × 10⁻³.
Figure S2. Rate of accumulation (M day\(^{-1}\)) of PCB 23\(_{aq}\) for indicated initial concentrations of PCB 61\(_{aq}\).
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