

## Supplementary Information

# **Modelling and Feasibility Assessment of Mineral Carbonation Based on Biological pH Swing for Atmospheric CO<sub>2</sub> Removal**

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## Supplementary Data

### S1. Model parameters

Table S1. Model parameters for oxidation bioreactor.

NOTATIO N	PARAMETER	VALUE	UNIT	SOURCE
$\mu_{max}$	Maximum specific growth rate of <i>A. thiooxidans</i>	0.037	h <sup>-1</sup>	[1]
$k_d$	Decay rate of <i>A. thiooxidans</i>	0.003	h <sup>-1</sup>	Assumed
$K_S$	Half saturation constant	0.150	mg L <sup>-1</sup>	[1]
$K_O$	Kinetic constant of oxygen for microbial growth	1.100	mg L <sup>-1</sup>	[1]
$H_S$	Henry's law constant for H <sub>2</sub> S	0.427	-	[2]
$H_O$	Henry's law constant for oxygen	32.300	-	[2]
$N$	Impeller speed	1.667	rev s <sup>-1</sup>	Assumed
$D$	Impeller diameter	0.376	m	Assumed
$D_I$	Width of the impeller blade	0.075	m	Assumed
$V_L$	Liquid volume of reactor	1.000	m <sup>3</sup>	Assumed
$\mu_L$	Liquid viscosity	0.001	Pa s	-
$Y_{XS}$	Yield coefficient for oxidation	0.093	-	[1]
$M$	Molar mass of forsterite	1.41E+05	mg mol <sup>-1</sup>	[3]
$\rho_f$	Average density of forsterite particles	3.27E+09	mg m <sup>-3</sup>	[3]

Table S2. Model parameters for reduction bioreactor.

NOTATIO N	PARAMETER	VALUE	UNIT	SOURCE
$H_H$	Henry constant for hydrogen	1.364	-	[4]
$Y_{H_2S,S}$	Moles of sulphate ion would be needed to generate one mole of H <sub>2</sub> S ions	1	-	-
$Y_{S_2O_3,S}$	Moles of sulphate ion would be needed to generate one mole of S <sub>2</sub> O <sub>3</sub> <sup>2-</sup> ions	0.5	-	-
$H_C$	Henry's law constant for CO <sub>2</sub>	28.6651	atm L mol <sup>-1</sup>	[5]
$D_L$	Molecular diffusivities of CO <sub>2</sub> in liquid	1.92E-09	m <sup>2</sup> s <sup>-1</sup>	[6]
$\sigma$	Surface tension of liquid	0.072	N m <sup>-1</sup>	[7]
$K_{H_2S,aq}$	Equilibrium constant	10E+6.99	-	[8]
$K_{H_2S,g}$	Equilibrium constant	1.00E-07	-	[8]
$M_{MgCO_3}$	Molar mass for MgCO <sub>3</sub>	84.3139	g mol <sup>-1</sup>	[9]
$\rho_{MgCO_3}$	Density for MgCO <sub>3</sub>	2.96E+06	g m <sup>-3</sup>	[9]

### S2. Composition of the culture medium

To support the growth of *A. thiooxidans*, we prepared a medium and adjusted its pH to a range between 4.4 and 4.7. Subsequently, the medium was autoclaved at 121 Celsius degrees for 15 minutes. The composition of the medium is as follows:

Table S3. Composition of the medium prepared for *A. thiooxidans*.

Chemicals	Amount	Unit
KH <sub>2</sub> PO <sub>4</sub>	3	g
MgSO <sub>4</sub> x 7 H <sub>2</sub> O	0.5	g
(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	3	g
CaCl <sub>2</sub> x 2 H <sub>2</sub> O	0.25	g
Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> x 5 H <sub>2</sub> O	5	g
Distilled water	1000	ml

### S3. Minerals in the tailing

Table S4. Dissolution reactions and parameters for different mineral in the mine tailings [14].

Mineral Name	Dissolution reaction	A (mol m <sup>-2</sup> h <sup>-1</sup> )	E (J mol <sup>-1</sup> )	n (-)
Plagioclase	Plagioclase + 8H <sup>+</sup> ↔ 2Al <sup>3+</sup> + Ca <sup>2+</sup> + 2H <sub>4</sub> SiO <sub>4</sub>	9.29E+02	1.66E+04	1.41
Clinopyroxene	Clinopyroxene + 4H <sup>+</sup> ↔ Mg <sup>2+</sup> + Ca <sup>2+</sup> + 2H <sub>4</sub> SiO <sub>4</sub>	7.31E+07	8.80E+04	0.50
Orthopyroxene	Orthopyroxene + 2H <sup>+</sup> + H <sub>2</sub> O ↔ Mg <sup>2+</sup> + H <sub>4</sub> SiO <sub>4</sub>	3.60E+08	8.00E+04	0.60
Serpentine	Serpentine + 6H <sup>+</sup> ↔ 3Mg <sup>2+</sup> + 2H <sub>4</sub> SiO <sub>4</sub> + H <sub>2</sub> O	7.20E+05	7.35E+04	0.21
Mica	Mica + 8H <sup>+</sup> ↔ Al <sup>3+</sup> + K <sup>+</sup> + 3Mg <sup>2+</sup> + 3H <sub>4</sub> SiO <sub>4</sub>	4.51E+13	8.50E+04	0.7
Calcite	Calcite + H <sup>+</sup> ↔ Ca <sup>2+</sup> + HCO <sub>3</sub> <sup>-</sup>	3.13E+28	1.44E+05	1
Dolomite	Dolomite + 2H <sup>+</sup> ↔ Ca <sup>2+</sup> + Mg <sup>2+</sup> + 2HCO <sub>3</sub> <sup>-</sup>	4.93E+6	3.61E+04	0.5

Table S5. Abundance of minerals in the mine tailings.

Mineral	Formulae	Modal abundance (%)
Amphibole	Ca <sub>2</sub> (Mg,Fe,Al) <sub>5</sub> (Al,Si) <sub>8</sub> O <sub>22</sub> (OH) <sub>2</sub>	6
Calcite	CaCO <sub>3</sub>	1
Plagioclase	CaAl <sub>2</sub> Si <sub>2</sub> O <sub>8</sub>	17
Clinopyroxene	MgCaSi <sub>2</sub> O <sub>6</sub>	17
Orthopyroxene	MgSiO <sub>3</sub>	25
Quartz	SiO <sub>2</sub>	3
Chlorite	Mg <sub>5</sub> Al(AlSi <sub>3</sub> O <sub>10</sub> )(OH) <sub>8</sub>	6
Serpentine	Mg <sub>3</sub> (Si <sub>2</sub> O <sub>5</sub> )(OH) <sub>4</sub>	12

<b>Mica</b>	$Ca(Mg,Al)_3(Al_3Si)O_{10}(OH)_2$	4
<b>Talc</b>	$Mg_3Si_4O_{10}(OH)_2$	8
<b>Dolomite</b>	$CaMg(CO_3)_2$	1

#### S4. The initial conditions for simulations

Table S6. The initial conditions adopted for each simulation run in the oxidation bioreactor.

<b>Oxidation Bioreactor</b>				
	Forsterite (mg L <sup>-1</sup> )	$C_{LS}$ (mg L <sup>-1</sup> )	$C_{LO}$ (mg L <sup>-1</sup> )	Microbe density (mg L <sup>-1</sup> )
<b>H<sub>2</sub>S cycle</b>	200000	0	5.9	1000
<b>S<sub>2</sub>O<sub>3</sub> cycle</b>	200000	124050	5.9	1000

Table S7. The initial conditions adopted for each simulation run in the reduction bioreactor.

<b>Reduction Bioreactor</b>			
	Mg <sup>2+</sup> ions (mol L <sup>-1</sup> )	SO <sub>4</sub> <sup>2-</sup> ions (mol L <sup>-1</sup> )	Microbe density (mg L <sup>-1</sup> )
<b>H<sub>2</sub>S cycle</b>	0.5	0.5	20
<b>S<sub>2</sub>O<sub>3</sub> cycle</b>	1	1	20

#### S5. Sensitivity analysis

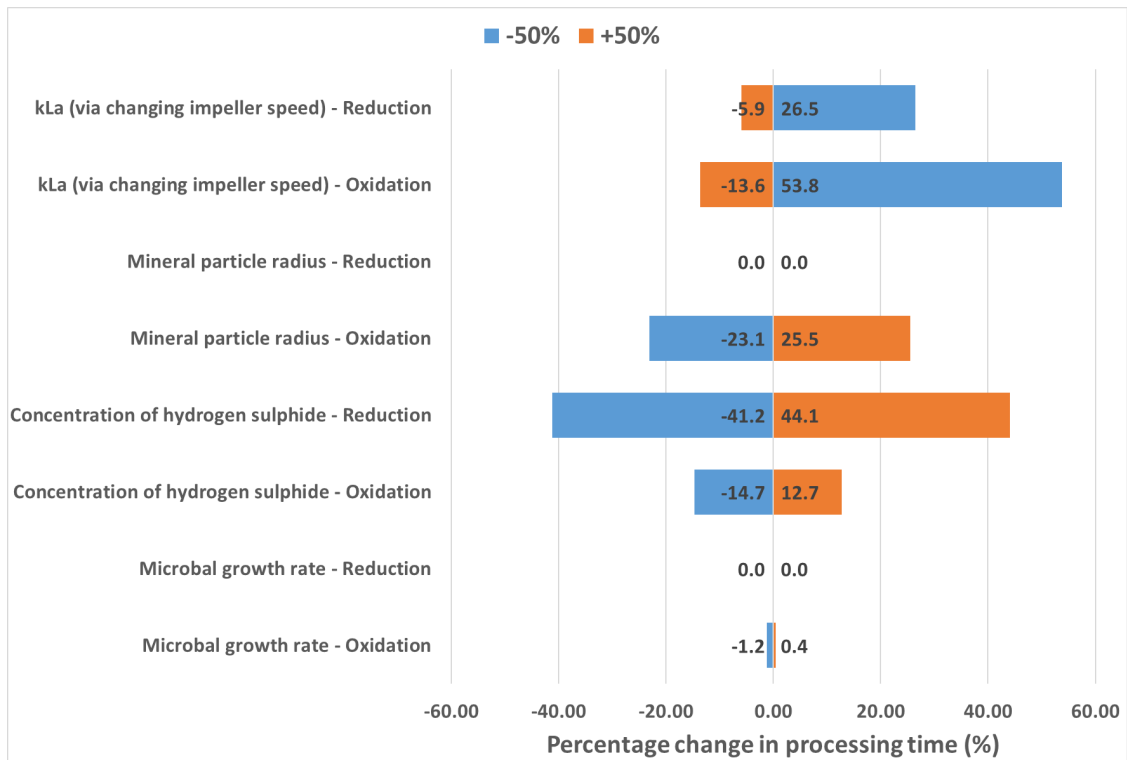


Fig. S1. Sensitivity analysis for mineral carbonation efficiency in hydrogen sulphide cycle.

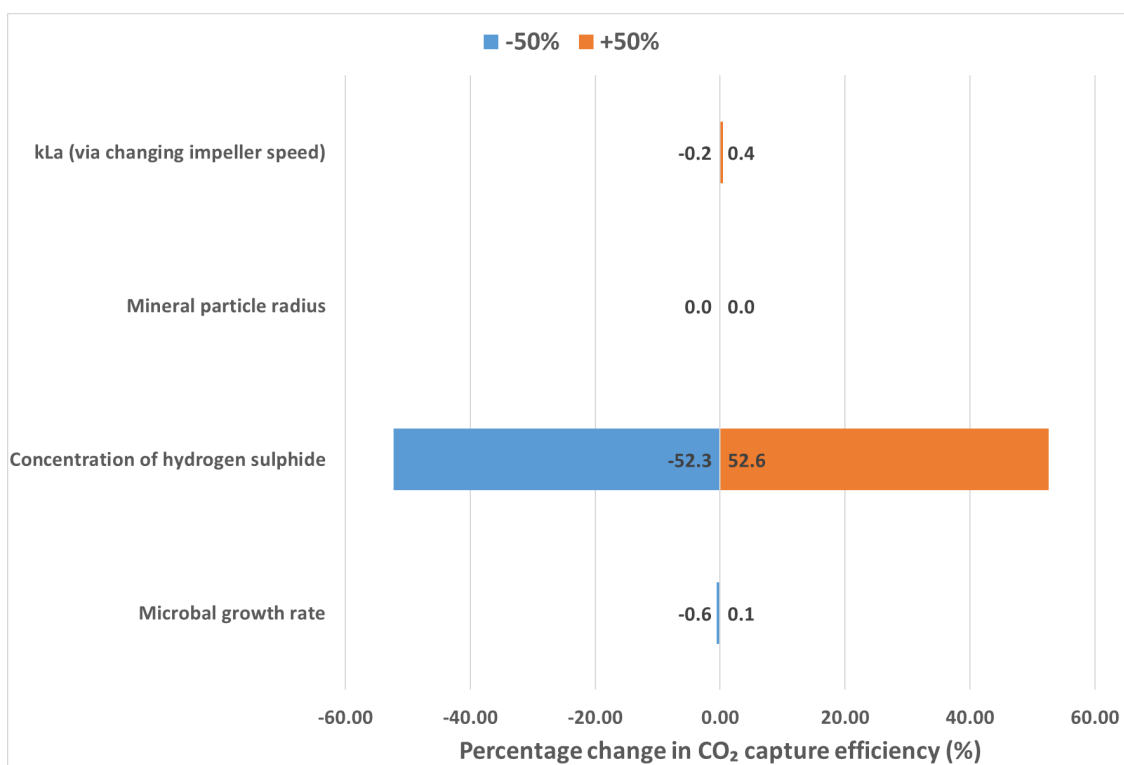


Fig. S2. Sensitivity analysis for CO<sub>2</sub> capture efficiency in hydrogen sulphide cycle.

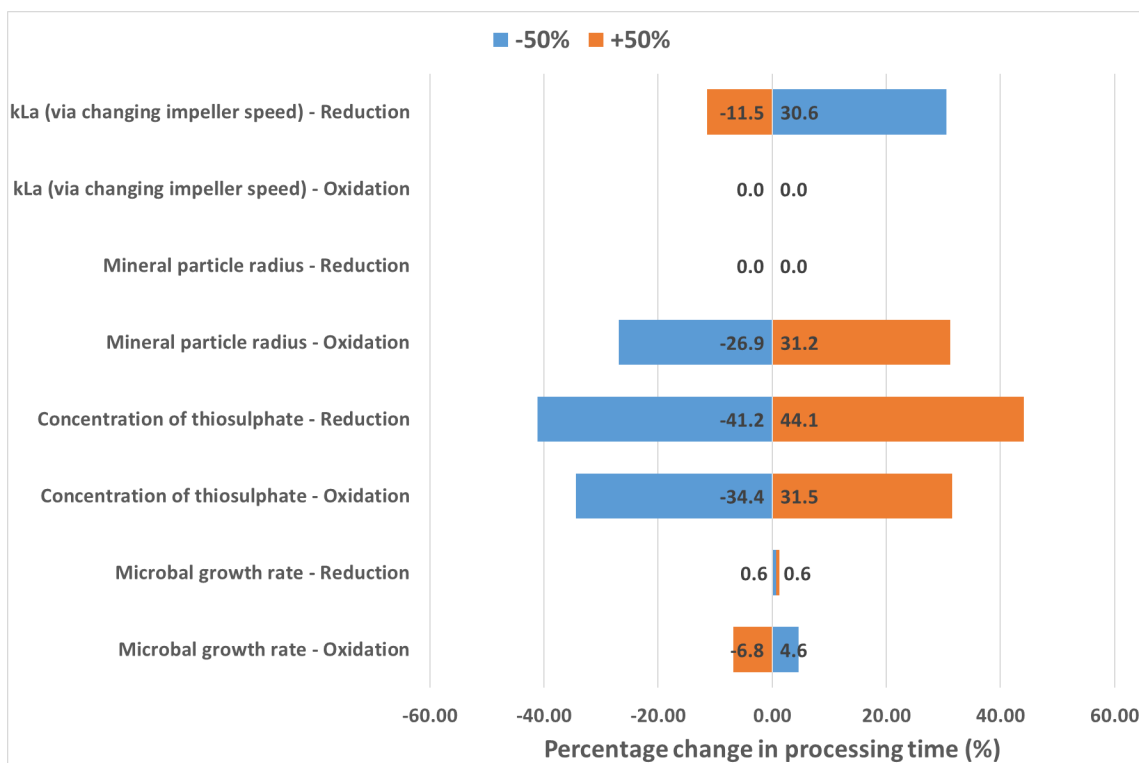


Fig. S3. Sensitivity analysis for mineral carbonation efficiency in thiosulphate cycle.

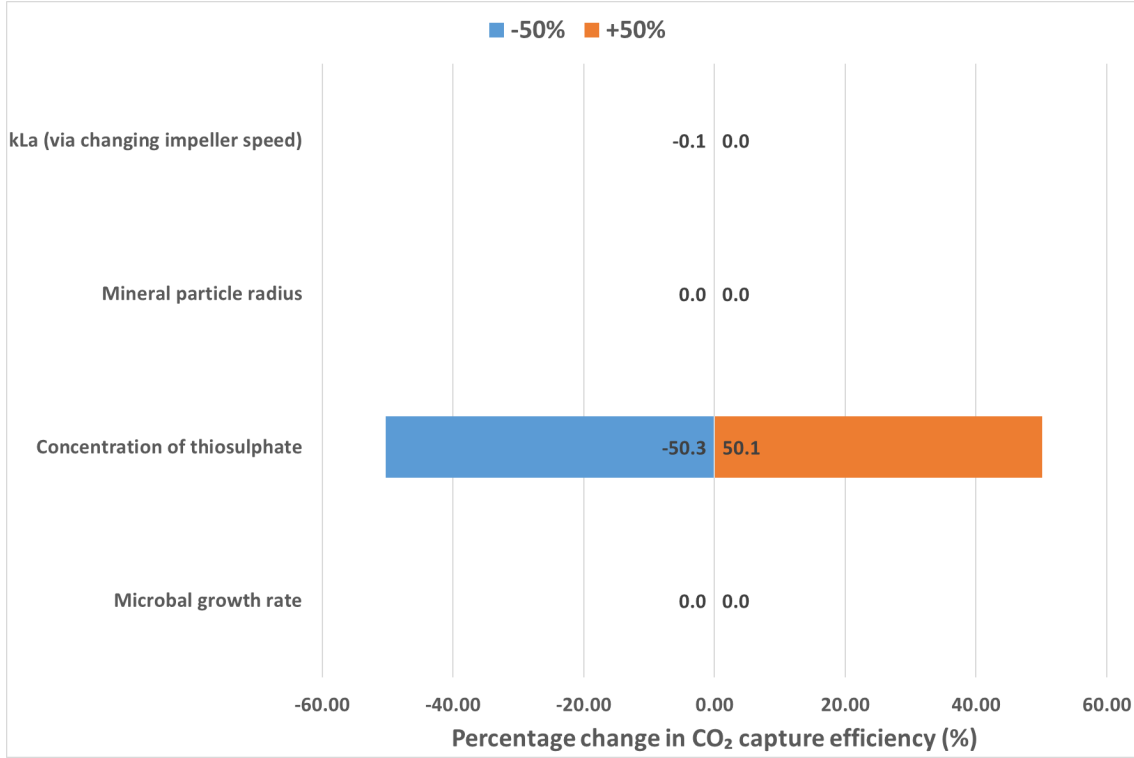


Fig. S4. Sensitivity analysis for CO<sub>2</sub> capture efficiency in thiosulphate cycle.

### S6. Calculation of $k_La$

$$k_La = 6.48 * \left(\frac{N}{N_{cd}}\right)^{1.44} * v_G^{1.12} \quad (S1)$$

$$N_{cd} = \frac{4 * Q_G^{0.5} * D^{0.25}}{D_I^2} \quad (S2)$$

As shown in Eqs. (S1) and (S2), we apply the method introduced by Smith to estimate the  $k_La$  value in stirred tank reactors [10, 11]. In these equations,  $N$  (rev s<sup>-1</sup>) refers to impeller speed,  $N_{cd}$  (rev s<sup>-1</sup>) refers to the minimum impeller speed for complete suspension of all the solid particles in stirred tank reactors,  $v_G$  (m s<sup>-1</sup>) is gas velocity,  $Q_G$  (L h<sup>-1</sup>) is volumetric gas flow rate,  $D$  and  $D_I$  (m) refer to diameters of the reactor and the impeller, respectively.

Note that for simulating the experimental oxidation reactor, as there was no active gas supply to the reactor, the gas phase mass balance for O<sub>2</sub> was excluded from the bioreactor model, while a modest  $k_La$  value (0.4 h<sup>-1</sup>) was assumed to approximate the mass transfer of oxygen into the culture medium at the top of the reactor.

### S7. Calculation of $\varepsilon_G$

$$\varepsilon_G = \frac{V_G}{V_R} = \left(\frac{1.98 * v_G}{1 + 40.9 * v_G}\right) * \left(\frac{P_G}{V_L}\right)^{0.21} \quad (S3)$$

$$P_G = 0.1 * P_0 * \left( \frac{Q_G}{N * V_L} \right) * \left( \frac{N^2 * D^4}{g * D_i * V_L^{\frac{2}{3}}} \right)^{-0.2} \quad (S4)$$

In Eq. (S3) and (S4),  $\varepsilon_G$  (-) refers to fractional gas hold up,  $P_G$  (W) refers to power consumption and  $P_0$  (W) refers to power consumption in absence of gas. We can calculate  $P_0$  by using following equations [12, 13]:

$$P_0 = \rho_L * N^3 * D^5 * N_p \quad (S5)$$

$$N_p = \min(19.5 * Re_L^{-0.3}; 24 * (Re_L * Fr_L)^{\frac{1}{3}}) \quad (S6)$$

$$Re_L = \frac{\rho_L * N * D^2}{\mu_L} \quad (S7)$$

$$Fr_L = \frac{D * N^2}{g} \quad (S8)$$

In Eq. (S5), (S6), (S7) and (S8),  $\rho_L$  (kg m<sup>-3</sup>) is density of liquid,  $N_p$  (-) is power number,  $Re_L$  (-) is Reynolds number,  $Fr_L$  (-) is Froude number,  $\mu_L$  (Pa s) is liquid viscosity and  $g$  (m s<sup>-2</sup>) is acceleration of gravity.

### S8. Calculation of $E$

$$E = 1 + \left[ \left( \frac{H_C * 1.67 C_{OH^-}}{2 C_{GC,in}} \right)^{-1.35} + \left( \frac{\sqrt{D_L k_2 C_{OH^-}}}{k_L \tanh \left( \frac{\sqrt{D_L k_2 C_{OH^-}}}{k_L} \right)} - 1 \right)^{-1.35} \right]^{-1.35} \quad (S9)$$

$$\log k_2 = 11.895 - \frac{2382}{T} + 0.221 I_c - 0.016 I_c^2 \quad (S10)$$

$$k_L = \frac{k_L a_{CO_2}}{1.38 * \left( \frac{g * \rho_L}{\sigma} \right)^{0.5} * \left( \frac{Q_G}{N * V_L} \right)^{\frac{1}{3}} * \left( \frac{N^2 * D^4}{g * D_i * V_L^{\frac{2}{3}}} \right)^{0.592} * \left( \frac{D_b * N^2 * D^4}{\sigma * V_L^{\frac{2}{3}}} \right)^{0.187}} \quad (S11)$$

$$D_b = \frac{5.5 * \sigma * \varepsilon_G^{\frac{1}{2}}}{g * \rho_L * \left( \frac{N^2 * D^3}{g * D_i * V_L^{\frac{2}{3}} * \left( \frac{P_G}{P_0} \right)^{\frac{2}{3}}} \right)^{\frac{1}{2}}} \quad (S12)$$

We apply Eq. (S9 – S12) to calculate enhancement factor  $E$ . In these equations,  $C_{OH^-}$  (mol L<sup>-1</sup>) refers to concentration of hydroxide in liquid,  $C_{GC,in}$  (atm) refers to concentration of CO<sub>2</sub> in supplied air,  $D_L$  (m<sup>2</sup> s<sup>-1</sup>) refers to molecular diffusivities of CO<sub>2</sub> in liquid,  $I_c$  (mol L<sup>-1</sup>) refers to ionic strength,  $\sigma$  (N s<sup>-1</sup>) refers to surface tension of liquid,  $D_b$  (m) refers to diameter of bubbles.

### S9. Liquid phase mass balance in the oxidation bioreactor

$$r_{G-L,S} = k_L a_S * \left( \frac{C_{GS}}{H_S} - C_{LS} \right) \quad (S13)$$

$$r_{G-L,O} = k_L a_O * \left( \frac{C_{GO}}{H_O} - C_{LO} \right) \quad (S14)$$

In Eqs. (S13) (only applicable to H<sub>2</sub>S, not to S<sub>2</sub>O<sub>3</sub><sup>2-</sup>) and (S14),  $r_{G-L,S}$  and  $r_{G-L,O}$  (mg L<sup>-1</sup>) refer to the rates of dissolution for H<sub>2</sub>S and oxygen;  $k_L a_S$  and  $k_L a_O$  (h<sup>-1</sup>) represent volumetric mass-transfer coefficient for H<sub>2</sub>S and oxygen;  $C_{GS}$  and  $C_{GO}$  (mg L<sup>-1</sup>) refer to the concentrations of H<sub>2</sub>S and oxygen in gas;  $H_S$  and  $H_O$  (-) refer to Henry's law constant for H<sub>2</sub>S and oxygen. The  $k_L a$  values are calculated using previously established correlations for aerated and agitated reactors; details are provided in the section S6.

Eqs. (S15) and (S16), supported by Eq. (S17), represent the rates of change in the concentrations of dissolved H<sub>2</sub>S and DO, respectively:

$$\frac{dC_{LS,H_2S}}{dt} = r_{G-L,S} * \frac{V_R}{V_L} - r_{S,H_2S} \quad (S15)$$

$$\frac{dC_{LO}}{dt} = r_{G-L,O} * \frac{V_R}{V_L} - r_O \quad (S16)$$

$$V_R = V_L + V_G \quad (S17)$$

$V_R$ ,  $V_L$  and  $V_G$  (L) represent the total reaction volume of the bioreactor (excluding the volume of the solid particles), liquid volume and gas volume, respectively.  $r_{S,H_2S}$  (mg L<sup>-1</sup>) refers to rate of H<sub>2</sub>S oxidation by *A. thiooxidans*, and  $r_O$  (mg L<sup>-1</sup>) refers to microbial consumption of oxygen in liquid, which could be calculated by the following Eqs. (S18) and (S19):

$$r_S = \frac{\mu_{max} * X * Y}{Y_{XS}} \quad (S18)$$

$$r_O = \frac{\mu_{max} * X * Y}{Y_{XO}} \quad (S19)$$

In these two equations,  $Y_{XS}$  (-) refers to the yield coefficient for oxidation of H<sub>2</sub>S or S<sub>2</sub>O<sub>3</sub><sup>2-</sup>. Unlike H<sub>2</sub>S, the supply of S<sub>2</sub>O<sub>3</sub><sup>2-</sup> ions do not involve gas-liquid mass transfer from gas to liquid; therefore, the change in concentration of S<sub>2</sub>O<sub>3</sub><sup>2-</sup> ions can be represented with following modified equation, as opposed to Eq. (S15):

$$\frac{dC_{LS,S_2O_3}}{dt} = -r_{s,S_2O_3} \quad (S20)$$

In this equation,  $C_{LS,S_2O_3}$  (mg L<sup>-1</sup>) refers to concentration of S<sub>2</sub>O<sub>3</sub><sup>2-</sup> ions, and  $r_{s,S_2O_3}$  (mg L<sup>-1</sup>) refers to rate of S<sub>2</sub>O<sub>3</sub><sup>2-</sup> oxidation by *A. thiooxidans*, which can be calculated by applying Eq. (S18) to thiosulphate.

### S10. Gas phase mass balance in the oxidation bioreactor

For mass balance in the gas phase, Eq. (S21) and (S22) correspondingly represent the rates of change in concentrations of gaseous H<sub>2</sub>S and oxygen:

$$\frac{dC_{GS,H_2S}}{dt} = \frac{Q_G * (C_{GS,in} - C_{GS,H_2S})}{V_G} - \frac{r_{G-L,S}}{\epsilon_G} \quad (S21)$$

$$\frac{dC_{GO}}{dt} = \frac{Q_G * (C_{GO,in} - C_{GO})}{V_G} - \frac{r_{G-L,O}}{\epsilon_G} \quad (S22)$$

In these equations,  $Q_G$  (L h<sup>-1</sup>) refers to gas flow rate in the bioreactor,  $C_{GS,in}$  (mg L<sup>-1</sup>) refers to concentration of H<sub>2</sub>S in feed gas,  $V_G$  (L) refers to effective gas volume, and  $\varepsilon_G$  (-) refers to fractional gas hold up; details of  $\varepsilon_G$  calculation are provided in section S7.

### S11. Liquid phase mass balance in the reduction bioreactor

For simplicity, the hydrogen supply in the reactor was assumed to be via a liquid phase that was in equilibrium with a hydrogen gas phase at 1 bar, using Eq. (S23) to simulate the concentration of aqueous hydrogen ( $C_{LH}$ ) in the reduction bioreactor:

$$C_{LH} = C_{GH} * H_H \quad (S23)$$

where  $C_{GH}$  (atm) refers to the concentration of H<sub>2</sub> in gas,  $H_H$  (mol L<sup>-1</sup> atm<sup>-1</sup>) refers to the Henry constant for H<sub>2</sub>. Note that the supply of hydrogen takes place at a stage different from (more precisely, earlier than) that for the supply of air and removal of H<sub>2</sub>S (in the sulphide cycle), thus the operation of the reactor does not involve mixing H<sub>2</sub> with any gas flow through the reactor and avoids the loss of H<sub>2</sub>.

For concentrations of reduced sulphur compounds ( $C_{LS}$ ), due to the different natures of hydrogen sulphide and thiosulphate, we apply separate equations to simulate the rates of change in concentrations:

$$\frac{dC_{LS,H_2S}}{dt} = -Y_{H_2S,S} * r_S - r_{L-G,H_2S} * \frac{V_R}{V_L} \quad (S24)$$

$$\frac{dC_{LS,S_2O_3}}{dt} = -Y_{S_2O_3,S} * r_S \quad (S25)$$

$$r_{L-G,H_2S} = C_{GS,H_2S} * Q \quad (S26)$$

where  $Y_{H_2S,S}$  and  $Y_{S_2O_3,S}$  (-) correspondingly refer to how many moles of H<sub>2</sub>S or S<sub>2</sub>O<sub>3</sub><sup>2-</sup> ions would be generated when one mole of sulphate ions are reduced,  $r_{L-G,H_2S}$  (mol h<sup>-1</sup>) refers to the rate of H<sub>2</sub>S gas released from liquid,  $C_{GS,H_2S}$  (mol L<sup>-1</sup>) refers to concentration of H<sub>2</sub>S in the gas phase, and  $Q$  (L h<sup>-1</sup>) refers to air flow rate in the reduction bioreactor. For simplicity, chemical and phase equilibria are assumed for the H<sub>2</sub>S-H<sub>2</sub>O system, which allows  $C_{GS,H_2S}$  to be determined based on the concentration of total dissolved H<sub>2</sub>S in the liquid phase,  $C_{LS,H_2S}$  (further explained in Section S12).

We use Eq. (S27) to simulate the change in liquid phase CO<sub>2</sub> concentration:

$$\frac{dC_{LC}}{dt} = r_{G-L,CO_2} * \frac{V_R}{V_L} - r_{cap} \quad (S27)$$

where  $r_{cap}$  (mol L<sup>-1</sup> h<sup>-1</sup>) refers to the rate of CO<sub>2</sub> capture. For the replenishment rate of CO<sub>2</sub> in the liquid phase,  $r_{G-L,CO_2}$  (mol L<sup>-1</sup> h<sup>-1</sup>), we apply Eq. (S28).

$$r_{G-L,CO_2} = k_L a_{CO_2} * E * \left( \frac{C_{GC}}{H_C} - C_{LC} \right) \quad (S28)$$

In this equation,  $k_L a_{CO_2}$  (h<sup>-1</sup>) refers to the volumetric mass-transfer coefficient value for CO<sub>2</sub>,  $C_{GC}$  (atm) and  $C_{LC}$  (mol L<sup>-1</sup>) correspondingly refer to the concentration of CO<sub>2</sub> in gas and liquid,  $H_C$  (atm L mol<sup>-1</sup>) refers to Henry's law constant for CO<sub>2</sub>,  $E$  (-) is the enhancement factor to account for the chemical effect on mass transfer [12, 15]. The details for calculating  $E$  are provided section S8.

### S12. Gas phase mass balance in the reduction bioreactor

H<sub>2</sub>S can be present in the reactor in both gaseous and dissolved states, with their ratio depending on the pH of the liquid phase. The split of H<sub>2</sub>S in the two phases is modelled based on phase and dissociation equilibria:

$$C_{LS,H_2S} = C_{H_2S,aq} + C_{HS^-} \quad (S29)$$

$$C_{H_2S,aq} = K_{H_2S,aq} * C_{HS^-} * 10^{-pH} \quad (S30)$$

$$C_{GS,H_2S} = C_{HS^-} * \frac{10^{-pH}}{K_{H_2S,g}} \quad (S31)$$

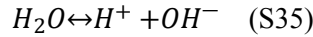
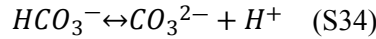
where  $C_{GS,H_2S}$  is the concentration of gaseous H<sub>2</sub>S,  $C_{HS^-}$  and  $C_{H_2S,aq}$  (mol L<sup>-1</sup>) refer to concentrations of HS<sup>-</sup> ions and H<sub>2</sub>S in solution,  $K_{H_2S,aq}$  and  $K_{H_2S,g}$  (-) refer to equilibrium constants for two reactions. The gaseous portion of H<sub>2</sub>S will be removed with the air flowing through the reactor; this gas mixture subsequently feeds into the oxidation bioreactor.

For CO<sub>2</sub>, we apply Eq. (S32) to simulate its gas phase concentration in reduction bioreactor:

$$\frac{dC_{GC}}{dt} = \frac{Q_G * (C_{GC,in} - C_{GC})}{V_G} - \frac{r_{G-L,CO_2}}{\varepsilon_G} \quad (S32)$$

### S13. Aqueous phase CO<sub>2</sub>-H<sub>2</sub>O equilibrium and charge balance

Complementary to the model equations introduced in sections 2.2 and 2.3, the model for each bioreactor further includes the following chemical reaction equilibria:



Finally, charge balance is included to complete the model, particularly to allow pH to be calculated:

$$\sum_i (C_{cation_i} * z_i) + \sum_j (C_{anion_j} * z_j) = 0 \quad (S36)$$

In this equation,  $C_{cation_i}$  and  $C_{anion_j}$  (mol L<sup>-1</sup>) refer to concentration of specific cation or anion respectively;  $z_i$  and  $z_j$  (C) refer to the charge number for the cation or anion.

## References

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