SUPPLEMENTARY MATERIAL

A. Detailed Mass Balances

General Reaction

$$\text{Glycerol (FC)} + \text{Ammonia (FN)} + O_2 \rightarrow X + P + CO_2 + H_2O + \Delta H_R$$

General Mass Balance Formulation

$$\text{Accumulation} = \text{In} - \text{Out} + \text{Generation} - \text{Consumption}$$

Batch Process: $F_{\text{in}} = F_{\text{out}} = 0$ and $V = \text{constant}$, thus:

$$\text{Accumulation} = \text{Generation} - \text{Consumption}$$

Biomass Balance

$$\frac{d}{dt}(X \cdot V) = \mu \cdot X \cdot V$$
$$\frac{dX}{dt} \cdot V = \mu \cdot X \cdot V$$
$$\frac{dX}{dt} = \mu \cdot X$$

Including the death rate constant k_d, the specific net growth rate becomes:

$$\frac{dX}{dt} = (\mu - k_d) \cdot X$$

Substrate and Product Balances

For any substrate or product S, assuming only microbial consumption or generation and constant volume V:

$$\frac{d}{dt}(S \cdot V) = -r_S \cdot V$$

The yield coefficient is defined as:

$$Y_{S/X} = \frac{r_X}{-r_S} = \frac{\mu X}{-r_S}$$

Therefore, the general expression becomes:

$$\frac{dS}{dt} = \pm \frac{\mu X}{Y_{S/X}}$$

where the sign depends on whether S is a substrate (negative) or a product (positive).

B. Ionic Balance

$$[\text{OH}^-] = \frac{K_{a6}}{[H^+]} \tag{8}$$

$$[\text{KHPO}_4^-] = \frac{\text{KH}_2\text{PO}_4^{\text{tot}}}{\left(1 + \frac{[H^+]}{K_{a1}}\right)} \tag{9}$$

$$[\text{C}_6\text{H}_5\text{O}_7^{3-}] = \frac{\text{C}_6\text{H}_8\text{O}_7^{\text{tot}}}{\frac{[H^+]^3}{K_{a2}K_{a3}K_{a4}} + \frac{[H^+]^2}{K_{a3}K_{a4}} + \frac{[H^+]}{K_{a4}} + 1} \tag{10}$$

$$[\text{C}_6\text{H}_6\text{O}_7^{2-}] = \frac{[H^+] \cdot [\text{C}_6\text{H}_5\text{O}_7^{3-}]}{K_{a4}} \tag{11}$$

$$[\text{C}_6\text{H}_7\text{O}_7^{-}] = \frac{[H^+] \cdot [\text{C}_6\text{H}_6\text{O}_7^{2-}]}{K_{a3}} \tag{12}$$

$$[\text{HCO}_3^-] = \frac{\text{CO}_2^{\text{tot}}}{\left(\frac{[H^+]}{K_{a7}} + 1\right)} \tag{13}$$

$$[\text{H}^+] = [\text{OH}^-] + [\text{KHPO}_4^-] + 3[\text{C}_6\text{H}_5\text{O}_7^{3-}] + 2[\text{C}_6\text{H}_6\text{O}_7^{2-}] + [\text{C}_6\text{H}_7\text{O}_7^{-}] + [\text{HCO}_3^-] - [I_{\text{ext}}]$$

C. Complementary Tables

TABLE II
MODEL PARAMETERS USED IN THE DYNAMIC SIMULATION OF *M. smegmatis* GROWTH

Parameter	Description	Value
t_{lag}	Lag phase duration [h]	7
k_C	Monod constant for glycerol [g/L]	0.3828
k_N	Monod constant for ammonia [g/L]	1.0027×10^{-4}
$Y_{X/C}$	Biomass yield on glycerol [g/g]	0.484
$Y_{X/N}$	Biomass yield on ammonia [g/g]	21.575
$Y_{X/CD}$	CO_2 yield [g/g]	0.3687
Y_{X/O_2}	O_2 yield [g/g]	1.352
X_{max}	Maximum biomass concentration [g/L]	1.4462
μ_{max}	Maximum specific growth rate [1/h]	0.19
k_d	Death rate constant [1/h]	0.001
pH_{LL}	Lower limit of pH tolerance	3.4687
pH_{UL}	Upper limit of pH tolerance	7.4
pH_{alk}	Alkalinity value	7.2
pK_{a1} to pK_{a9}	Acid dissociation constants [-]	See Table III
$[KH_2PO_4]$	Phosphate buffer (monobasic)	2.18
$[C_6H_8O_7]$	Citric acid (tricarboxylic acid)	2.00
I_{val}	pH inhibition shape parameter [-]	4.0413
$O_{2,\text{sat}}$	O_2 saturation concentration [g/L]	0.007267
k_La	Oxygen transfer coefficient [1/h]	86.26
k_O	Monod constant for oxygen [g/L]	0.0045

TABLE III
ACID DISSOCIATION CONSTANTS (pK_a) USED IN THE pH MODEL

Parameter	Chemical species or group	Value
pK_{a1}	KH_2PO_4 (phosphate buffer)	6.86
pK_{a2}	Citric acid ($C_6H_8O_7$)	3.13
pK_{a3}	Mono-deprotonated citric acid $(C_6H_7O_7)^-$	4.76
pK_{a4}	Di-deprotonated citric acid $(C_6H_7O_7)^{2-}$	6.40
pK_{a5}	Ammonium (NH_3)	9.25
pK_{a6}	Glycerol ($C_3H_8O_3$)	14.15
pK_{a7}	Carbon dioxide (CO_2)	6.35
pK_{a8}	Bicarbonate (HCO_3^-)	10.33
pK_{a9}	Water (H_2O)	14.00

TABLE IV
INITIAL CONDITIONS USED IN THE SIMULATION OF *M. smegmatis* GROWTH

Variable	Description	Initial Value
X_0	Biomass concentration [g/L]	0.223
C_0	Glycerol concentration [g/L]	5.922
N_0	Ammonium concentration [g/L]	1.027
$CO_{2,0}$	Carbon dioxide concentration [g/L]	0.000439
$O_{2,0}$	Dissolved oxygen concentration [g/L]	0.65

TABLE V
HIGHLY CORRELATED PARAMETER PAIRS ($|\rho| > 0.95$)

Parameter A	**Parameter B**	**Correlation**
t_{lag}	k_C	0.9712
t_{lag}	pH.UL	-0.9831
Y_{X/CO_2}	k_d	0.9877
Y_{X/O_2}	pH.LL	0.9988
Y_{X/O_2}	I_{val}	-0.9988
Y_{X/O_2}	k_{La}	-0.9998
pH.LL	I_{val}	-1.0000
pH.LL	k_{La}	-0.9995
I_{val}	k_{La}	0.9995
$O_{2,\text{sat}}$	k_O	0.9865

TABLE VI
t-VALUES OF ESTIMATED PARAMETERS

Parameter	**t-Value**
μ_{max}	12.94
pH$_{UL}$	300.29
$Y_{X/C}$	101.93
X_{max}	479.45
$Y_{X/N}$	355.84

D. Complementary Figures

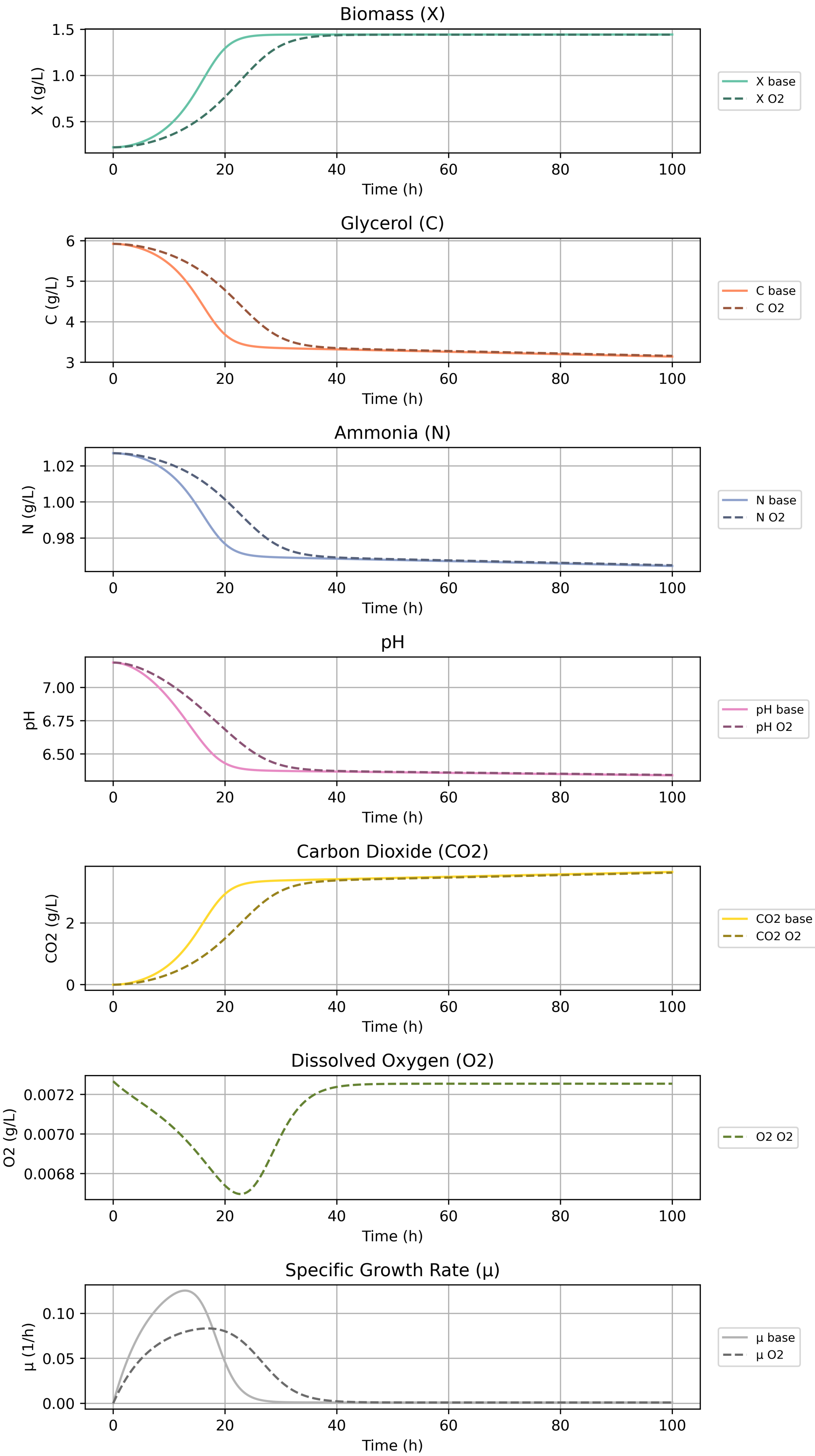

Fig. 1. Comparison between original model without oxygen, and the updated model with oxygen consumption on hypoxic conditions.

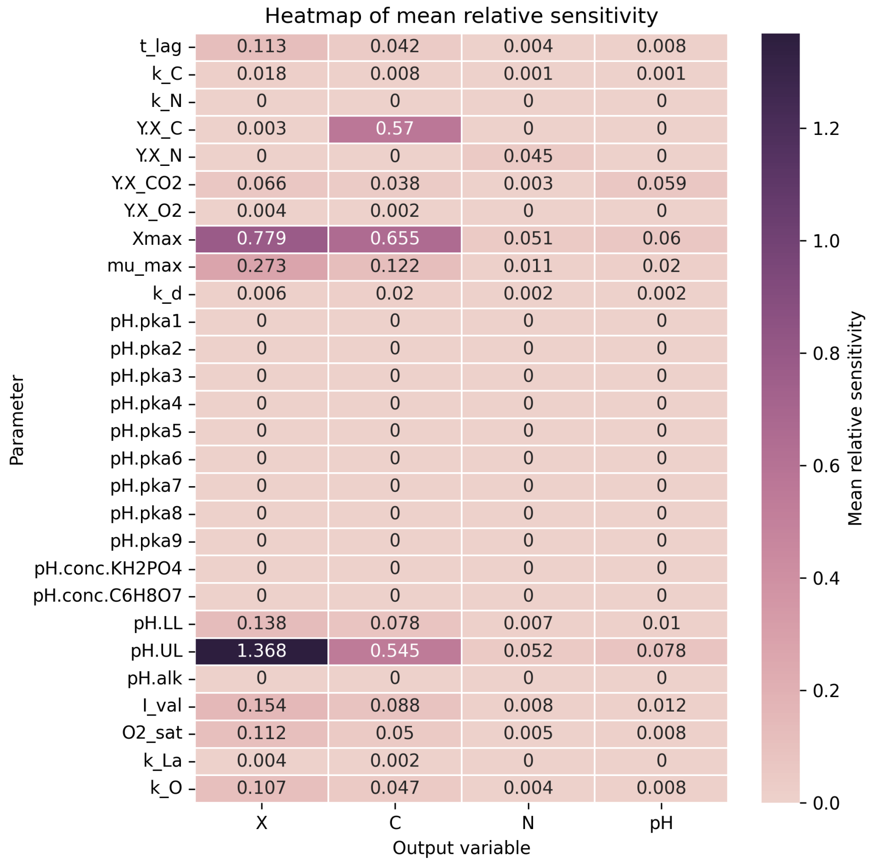

Fig. 2. Heatmap of the mean relative sensitivity of each parameter with respect to the model outputs.

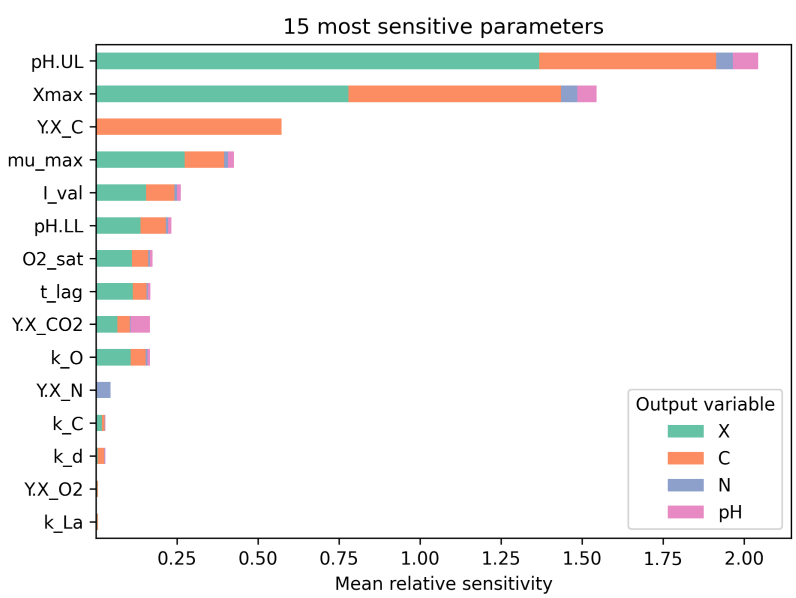

Fig. 3. Mean relative sensitivity of the 15 most influential parameters in the model, disaggregated by affected output variable. Each bar represents the cumulative sensitivity contribution of a parameter across all state variables.

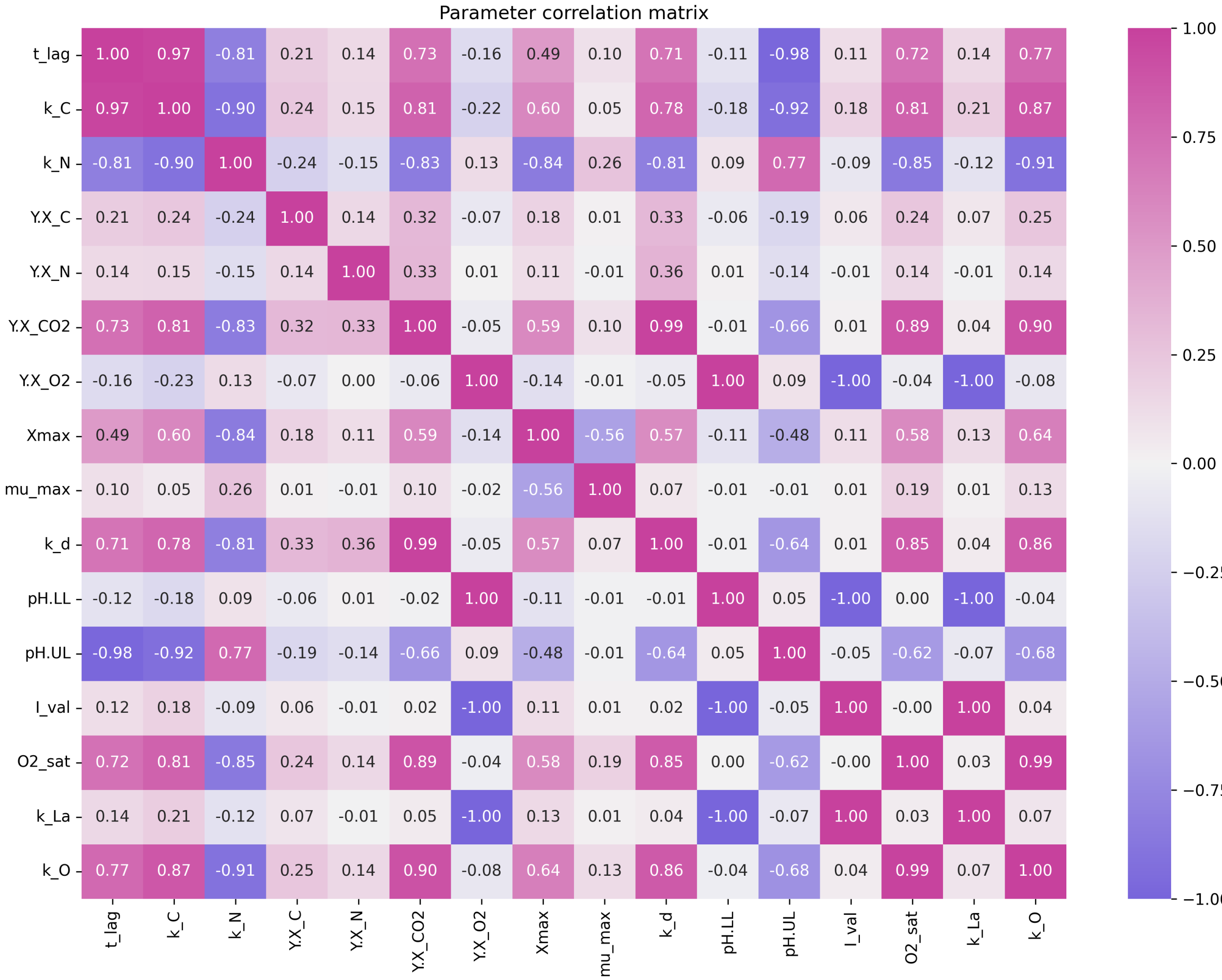

Fig. 4. Correlation matrix between the parameters retained after excluding non-identifiable pH-related terms.

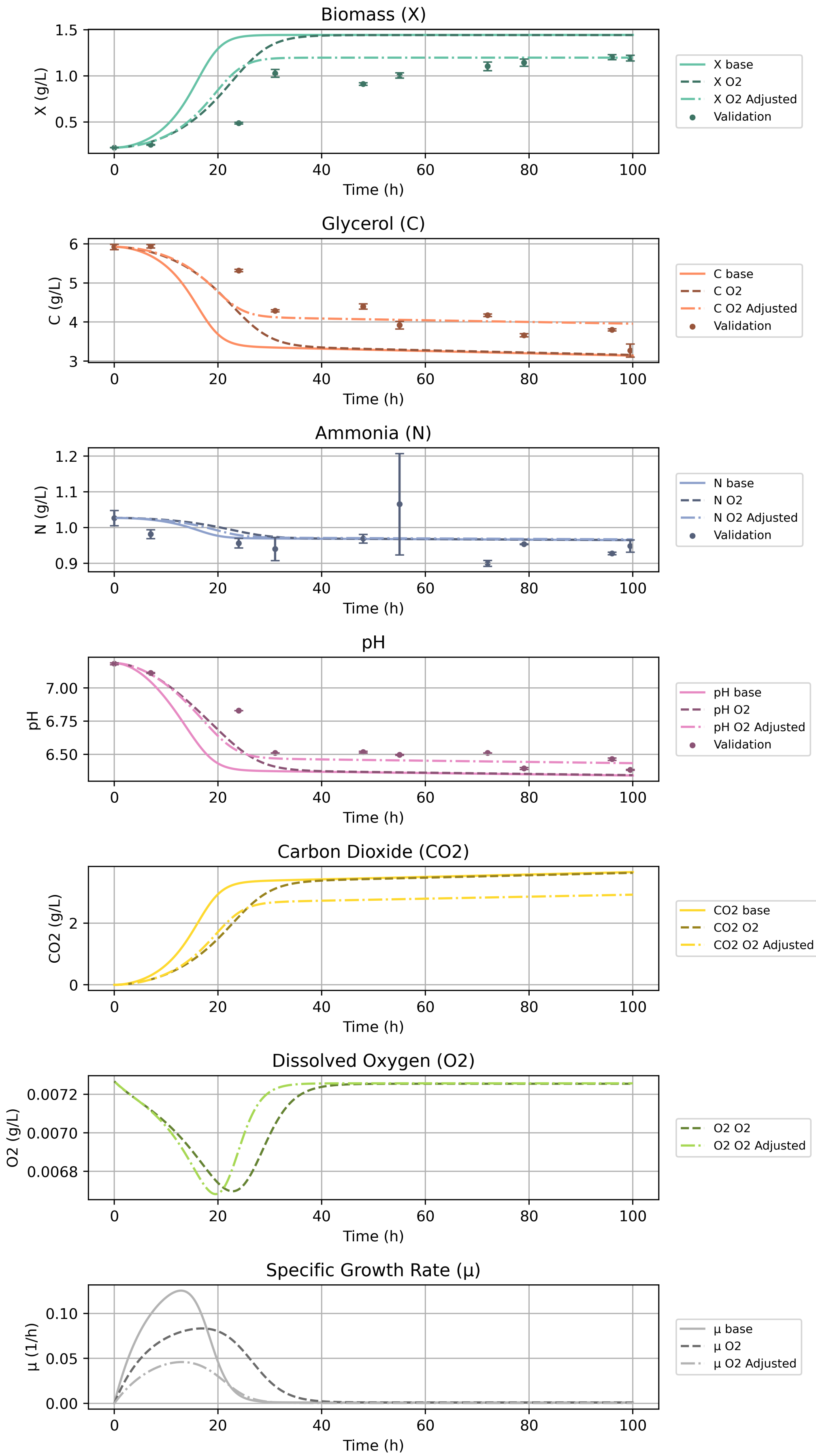

Fig. 5. Comparison between all the model tested, with the validation data. Error bars represent the relative deviation of experimental validation data.