A metabolic model for targeted volatile fatty acids production by cofermentation of carbohydrates and proteins

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Supporting Information

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E-supplementary data

Table S1. AA spectrum of gelatine used in the simulations (molar basis) and molecular weight of a C-mol of that protein.

Arg	4.7%
Ala	2.7%
Asp	6.3%
Lys	3.3%
Glu	5.0%
Ser	5.3%
Thr	11.0%
Cys	8.0%
Gly	11.6%
Pro	5.6%
Val	6.0%
Ile	3.3%
Leu	4.0%
Met	3.0%
Gln	9.6%
Asn	6.3%
His	4.3%
MW (g/C-mol)	29.0

Table S2. Mass balances for the different compartments of the reactor. S_i is the intracellular concentration, R_i and $R_{T,i}$ are, respectively, the reaction rate and intra-extra cellular transport rate, S_k is the extracellular concentration, D_{liq} is the liquid dilution rate, $S_{K,in}$ is the concentration on the inlet, S_X is the biomass concentration, R_{ana} is the anabolism rate, R_{decay} is the decay rate, G_m is the concentration, D_{gas} is the gas space dilution rate and $R_{T,m}$ is liquid-gas transport rate.

Compartment	Equation	Units
Intracellular compounds	$\frac{dS_i}{dt} = R_i + R_{T,i}$	mol L_x^{-1} h^{-1}
Extracellular compounds	$\frac{dS_k}{dt} = D_{liq} \cdot (S_{K,in} - S_k) + R_{T,k}$	mol L_{liq}^{-1} h^{-1}
Biomass	$\frac{dS_X}{dt} = -D_{liq} \cdot S_X + R_{ana} - R_{decay}$	mol L_r^{-1} h^{-1}
Gas compounds	$\frac{dG_m}{dt} = -D_{gas} \cdot G_m + R_{T,m}$	mol L_{gas}^{-1} h^{-1}

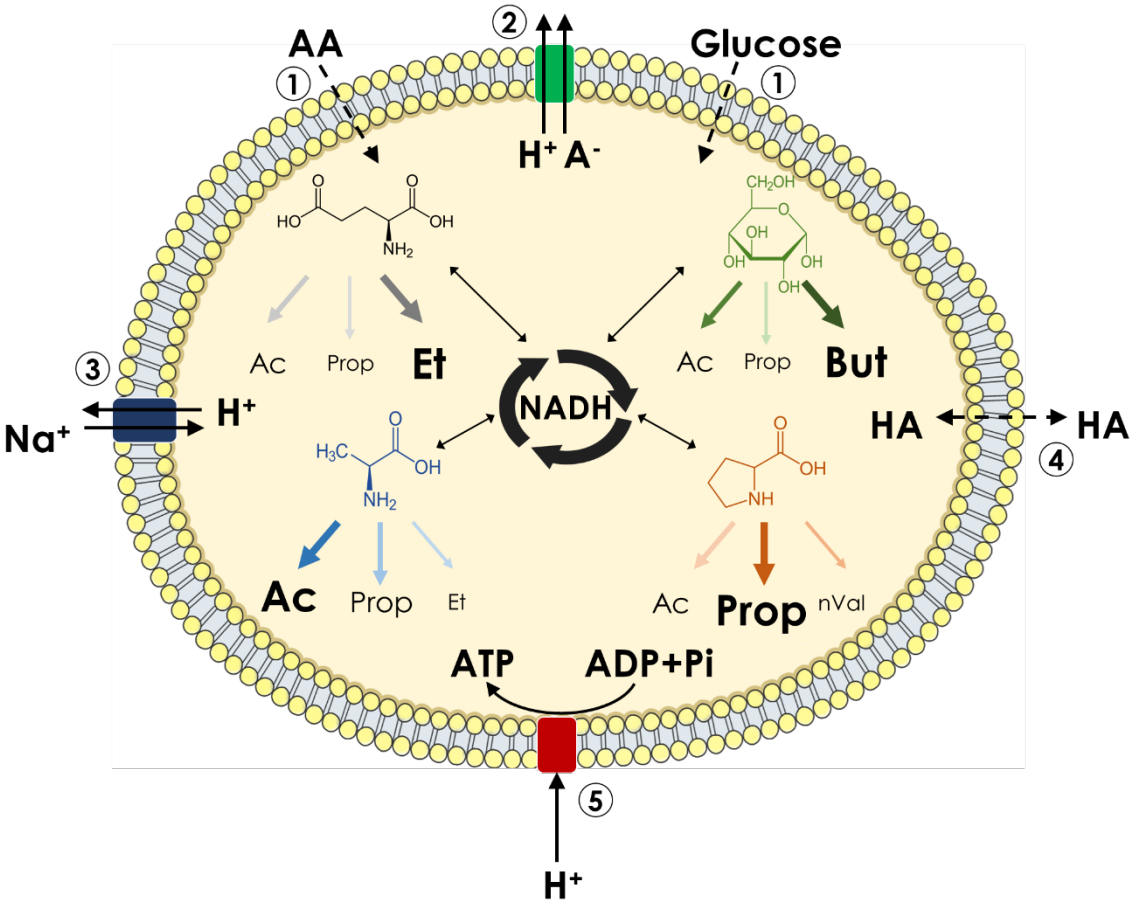

Fig. S1. Scheme of the processes considered in the model. 1: Passive transport of substrates is considered only to happen inwards the cell. 2: VFA active transport in a symport with protons. 3: Antiport transport of sodium and protons to regulate internal pH. 4: Passive transport of VFA is considered to happen in both directions. 5: Energy is stored in form of ATP in proton translocation processes (ATP synthase). The catabolism of the different substrates is determined in the optimisation part of the model. The substrates interact with each other through the NADH conservation as its production and consumption must be balanced at all times.

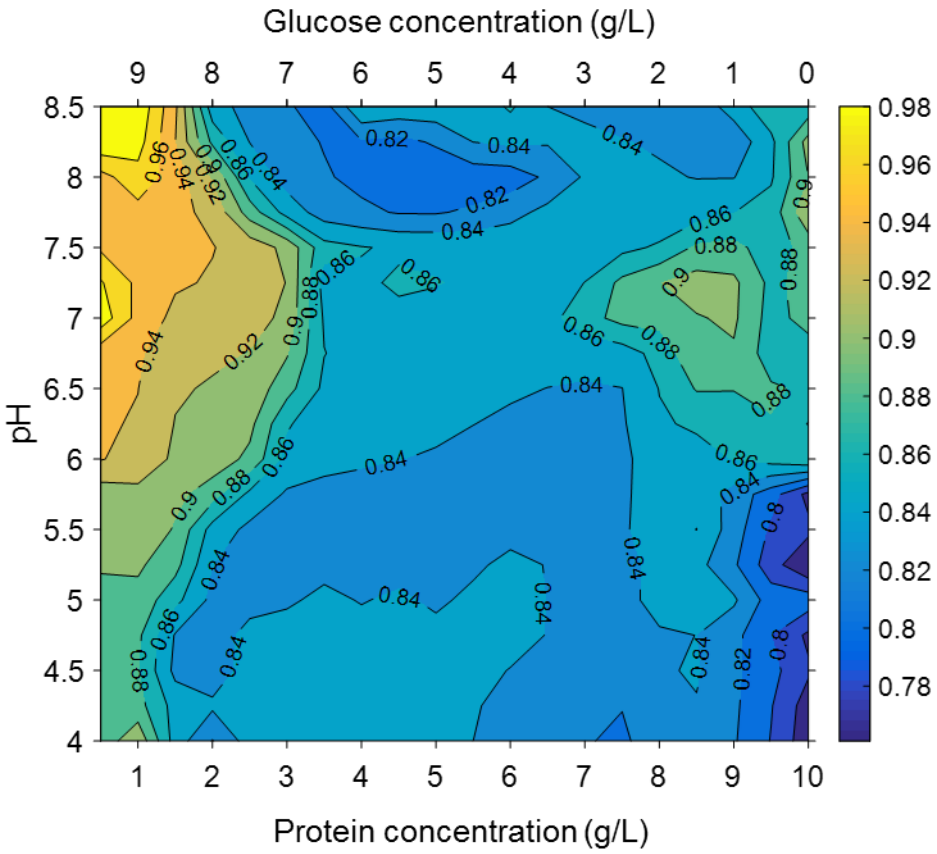

Fig. S2. Predicted protein conversion (g consumed/g feeding) at different pH values (vertical axis) and at different glucose and gelatine concentration in the feeding (horizontal axis).

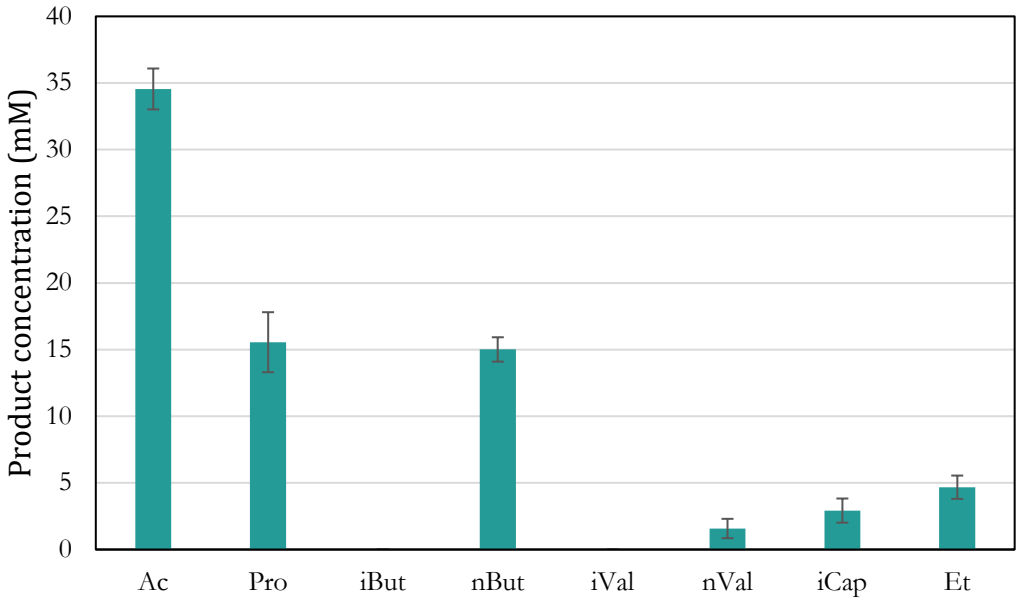

Fig. S3. Product variability due to different AA profiles. Model simulations at 5 g/L of glucose and gelatine and at pH 7 for 9 different gelatine AA profiles.