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## Dynamic metabolic control analysis on *Cupriavidus necator* predicts effects of environmental conditions on PHB production from glycerol

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**S**tatement of the Problem: Utilisation of glycerol from the ever-expanding biodiesel industry is deemed as a promising solution for the sustainable manufacturing of value-added chemicals. In one such novel fermentation processes, glycerol is utilised by bacterial strain. *Cupriavidus necator* DSM 545 to synthesise poly(3-hydroxybutyric acid), a bioplastics with the potential to replace its petrochemical counterparts in many applications. To improve PHB batch production via means of model-guided process or genetic engineering, insights into the behaviour of cellular metabolism under dynamic fermentation environments is essential. The purpose of this research is, therefore, to demonstrate how metabolic fluxes can be reconfigured in response to environmental or genetic changes. Methodology & Theoretical Orientation: A dynamic flux control analysis (DMCA) approach was used in this study. It comprises generation of time-series flux distributions over batch fermentation using dynamic flux balance analysis (DFBA), a constraint-based stoichiometric modelling approach. Based on the flux distributions profiles, metabolic control analysis (MCA) calculated flux control coefficients to quantify the relative changes of metabolic fluxes in response to changes in system variables such as enzyme activities and metabolite concentrations. Findings: We calculated control coefficients of PHB flux with respect to factors such as TCA activity, glycerol concentration and oxygen level. The degree of control of PHB synthesis fluxes was not fixed, but rather changed with metabolic state and environmental condition during the fermentation. Furthermore, the control coefficients were able to provide qualitatively correct predictions of the change of PHB synthesis in response to perturbation in oxygen level during the fermentation. Conclusion and significance: DMCA could generate quantitative description of the interaction between PHB synthesis pathway and system variables. We envisaged the possibility of developing a process control scheme for PHB production based on metabolic control coefficients.

### Biography

Chenhao Sun joined Professor Konstantinos Theodoropoulos's research group in 2013 and has since been working on PHB production using *Cupriavidus necator* DSM 545 from glycerol. His research focused on using combined computational-experimental approaches to gain an in-depth understanding of the metabolism of the strain associated with PHB synthesis, and hence providing hints as to how PHB productivity can be improved via genetic or process engineering means. He has created Matlab programs to perform dynamic flux balance analysis and dynamic flux control analysis on bioreactor experiment data and yielded positive results.

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### Notes: