Multi-scale exploration of the technical, economic, and environmental dimensions of bio-based chemical production - DTU Orbit (25/12/2018)

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In recent years, bio-based chemicals have gained traction as a sustainable alternative to petrochemicals. However, despite rapid advances in metabolic engineering and synthetic biology, there remain significant economic and environmental challenges. In order to maximize the impact of research investment in a new bio-based chemical industry, there is a need for assessing the technological, economic, and environmental potentials of combinations of biomass feedstocks, biochemical products, bioprocess technologies, and metabolic engineering approaches in the early phase of development of cell factories. To address this issue, we have developed a comprehensive Multi-scale framework for modeling Sustainable Industrial Chemicals production (MuSIC), which integrates modeling approaches for cellular metabolism, bioreactor design, upstream/downstream processes and economic impact assessment. We demonstrate the use of the MuSIC framework in a case study where two major polymer precursors (1,3-propanediol and 3-hydroxypropionic acid) are produced from two biomass feedstocks (corn-based glucose and soy-based glycerol) through 66 proposed biosynthetic pathways in two host organisms (Escherichia coli and Saccharomyces cerevisiae). The MuSIC framework allows exploration of tradeoffs and interactions between economy-scale objectives (e.g. profit maximization, emission minimization), constraints (e.g. land-use constraints) and process- and cell-scale technology choices (e.g. strain design or oxygenation conditions). We demonstrate that economy-scale assessment can be used to guide specific strain design decisions in metabolic engineering, and that these design decisions can be affected by non-intuitive dependencies across multiple scales.

General information
State: Published
Organisations: Novo Nordisk Foundation Center for Biosustainability, Global Econometric Modeling, Research Groups, iLoop
Contributors: Zhuang, K., Herrgard, M.
Number of pages: 12
Pages: 1-12
Publication date: 2015
Peer-reviewed: Yes
Early online date: 2015

Publication information
Journal: Metabolic Engineering
Volume: 31
ISSN (Print): 1096-7176
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.95 SJR 3.337 SNIP 1.787
Web of Science (2017): Impact factor 7.674
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.33 SJR 3.626 SNIP 1.865
Web of Science (2016): Impact factor 8.142
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 8.2 SJR 3.6 SNIP 1.809
Web of Science (2015): Impact factor 8.201
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 7.23 SJR 3.395 SNIP 2.009
Web of Science (2014): Impact factor 6.767
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 8.43 SJR 4.036 SNIP 2.164
Web of Science (2013): Impact factor 8.258
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 6.72 SJR 2.989 SNIP 1.847
Web of Science (2012): Impact factor 6.859
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 6.75 SJR 3.049 SNIP 2.038
Web of Science (2011): Impact factor 5.614
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.375 SNIP 1.786
Web of Science (2010): Impact factor 5.512
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.621 SNIP 1.4
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.789 SNIP 1.03
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.508 SNIP 1.182
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.28 SNIP 0.897
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.069 SNIP 1.042
Scopus rating (2004): SJR 1.688 SNIP 1.255
Scopus rating (2003): SJR 1.177 SNIP 0.869
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.702 SNIP 1.068
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.925 SNIP 0.755
Scopus rating (2000): SJR 0.724 SNIP 0.9
Original language: English
Keywords: Industrial biotechnolog, Sustainability, Biochemicals, Multi-scale modeling, Optimization
DOIs:
10.1016/j.ymben.2015.05.007
Source: PublicationPreSubmission
Source-ID: 112568940
Research output: Research - peer-review › Journal article – Annual report year: 2015