Systematic Optimization-Based Integrated Chemical Product–Process Design Framework -
DTU Orbit (13/01/2019)

An integrated optimization-based framework for product and process design is proposed. The framework uses a set of
methods and tools to obtain the optimal product–process design solution given a set of economic and environmental
sustainability targets. The methods and tools required are property prediction through group contributions, unless
supported with a database, computer-aided molecular and mixture/blend design for generation of novel as well as existing
products and mathematical programming for formulating and solving multiscale integrated process–product design
problems. The application of the framework is demonstrated through three case studies: (i) refrigeration cycle unit for
R134a replacement, (ii) a mixed working fluid design problem for R134a replacement, and (iii) pure solvent design for
water-acetic acid LLE extraction. Through the application of the framework it is demonstrated that all solutions satisfy
product, process, economic, and environmental targets simultaneously. The solution is obtained through a direct
deterministic mathematical optimization strategy. The framework proposed in this work is generic and can be applied to a
wide range of problems where an integrated solution to process-product design is beneficial.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering
Centre, KT Consortium
Contributors: Cignitti, S., Mansouri, S. S., Woodley, J. M., Abildskov, J.
Pages: 677–688
Publication date: 2018
Peer-reviewed: Yes

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 57
Issue number: 2
ISSN (Print): 0888-5885
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.4 SJR 0.978 SNIP 1.203
Web of Science (2017): Impact factor 3.141
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.95 SNIP 1.155
Web of Science (2016): Impact factor 2.843
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 2.87 SJR 0.938 SNIP 1.145
Web of Science (2015): Impact factor 2.567
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.85 SJR 1.009 SNIP 1.287
Web of Science (2014): Impact factor 2.587
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.6 SJR 0.975 SNIP 1.232
Web of Science (2013): Impact factor 2.235
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.56 SJR 1.054 SNIP 1.32
Web of Science (2012): Impact factor 2.206