Chemical Engineering Science 187 (2018) 223–244

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

A multistage stochastic programming formulation to evaluate feedstock/process development for the chemical process industry

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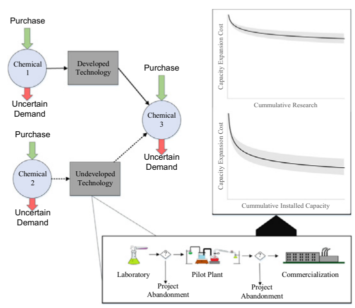
HIGHLIGHTS

- Feedstocks, products, and processes of chemical process industry (CPI) is changing.
- A new technology investment planning (NTIP) problem is defined for CPI.
- A multistage stochastic program (MSSP) is developed to solve NTIP problem for CPI.
- A relaxation approach is introduced to bound the MSSP formulation of NTIP problem.
- A biomass to ethylene production network is studied via the MSSP formulation.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 30 August 2017
Received in revised form 22 February 2018
Accepted 5 April 2018
Available online 22 April 2018

Keywords:
Multistage stochastic programming
Endogenous uncertainty
Exogenous uncertainty
Investment planning
Mixed integer non-linear programming

ABSTRACT

Industry trends suggest that the feedstock and product portfolios along with utilized technologies of chemical process industry (CPI) may grow and be quite different compared to today's in the near future. Incorporation of new feedstocks and technologies into the existing CPI infrastructure may require significant amounts of investments. Determining the investment decisions, i.e., how much to invest, which technologies to invest in, and when to invest in each technology for research and development and for capacity expansion, is a challenging task, because there are often many emerging technologies and the future performances of these technologies are uncertain. Here, we present a multistage stochastic programming (MSSP) formulation accounting for both endogenous and exogenous uncertain parameters associated with the new technology investment planning (NTIP) problem. The MSSP formulation is used to determine investment decisions for four case studies, including a biomass to ethylene production network. The solution for the biomass to ethylene case study suggests that, given the current market conditions, the investment in biomass technologies is not financially advantageous.

1. Introduction

An expanding middle class, urbanization, and a push for sustainability have driven growth in demand for chemicals, and the demand is expected to grow by 45% over the next 10 years (ExxonMobil, 2015). ExxonMobil is "progressing strategic investments that will capture low-cost feedstocks and increase premium product capacity to supply growing markets". DuPont plans to continue to drive innovation and accelerate growth in developing markets (DuPont, 2015). Bayer states that "being successful as a Life Science company requires a pronounced innovation culture that is the breeding ground for new ideas and facilitates their translation into successful products" (Bayer, 2015). These trends

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https://doi.org/10.1016/j.ces.2018.04.016
0009-2509/

Nomenclature

Indices/Sets

$i \in \boldsymbol{I}$ technologies
$sg \in \boldsymbol{SG}$ technology stages
$n \in \boldsymbol{N}$ chemicals
$t \in \boldsymbol{T}$ time periods
$s, s\prime \in \boldsymbol{S}$ scenarios
$np \in \boldsymbol{NP}$ partitions

Subsets

ϕ_k pairs of scenarios s and $s\prime$ which differ in the realized value of the uncertain parameter k

Parameters

$\gamma_{i,n,n'}$ stoichiometric ratio between component n and n' in technology i
p_s the probability that scenario s will occur
$MCst_{n,t}$ the per tonne purchase cost of chemical n at time t
INV^{Max} the maximum invest available for capacity expansion and research at each time period
$CC0_i$ the initial capacity expansion cost for technology i
β_i^0 the assumed value for the parameter β for technology i before investment
$\beta_{i,s}^1$ the realized value of β for technology i in scenario s
α_i^0 the assumed value for the parameter α for technology i before investment
$\alpha_{i,s}^1$ the realized value of α for technology i in scenario s
$D_{n,t,s}$ the demand of chemical n at time t in scenario s
$CX_{i,sg}^{Min}$ the minimum capacity of stage sg for technology i
$CX_{i,sg}^{Max}$ the maximum capacity of stage sg for technology i
$t_{s,s'}^{diff}$ the time of differentiation between scenarios s and s'
V^{α} the number of investments in research required to realize the true value of the parameter α
V^{β} the number of investments in capacity expansion required to realize the true value of β

Continuous variables

$CX_{i,t,s}$ the installed capacity of technology i at time t in scenario s
$RD_{i,t,s}$ the research investment in technology i at time t in scenario s
$F_{n,t,s}$ the amount of chemical n purchased at time t in scenario s
$M_{i,n,t,s}$ the amount of chemical n produced in technology i at time t in scenario s
$MatCst_s$ the total material cost for scenario s
$CapExCst_s$ the total amount spent on capacity expansion in scenario s
$RDCst_s$ the total amount spent on research in scenario s
ETC the expected total cost
$CC_{i,t,s}$ the capacity expansion cost of technology i at time t in scenario s
$X_{i,t,s}$ the capacity expansion of technology i at time t in scenario s
$\beta_{i,t,s}$ the elasticity parameter for capacity expansion for technology i at time t in scenario s
$\alpha_{i,t,s}$ the elasticity parameter for research expansion for technology i at time t in scenario s
$G_{n,t,s}$ the net production of chemical n at time t in scenario s
$\chi_{i,t,s}$ the yield of technology i at time t in scenario s

Binary variables

$NN_{i,t,s}^{\beta}$ takes a value of 1 if there have been V^{β} investments in capacity expansion for technology i at time t in scenario s, and 0 otherwise
$NN_{i,t,s}^{\alpha}$ takes a value of 1 if there have been V^{α} investments in research expenditure for technology i at time t in scenario s, and 0 otherwise
$N_{i,t,s}^{\beta}$ takes a value of 1 if there was an investment in capacity expansion in technology i at time t in scenario s and 0 otherwise
$N_{i,t,s}^{\alpha}$ takes a value of 1 if there was an investment in research expenditure for technology i at time t for scenario s and 0 otherwise
$Z_{i,sg,t,s}$ takes a value of 1 if technology i is in stage sg at time t in scenario s and 0 otherwise
$Y_{i,sg,t,s}$ takes a value of 1 if technology i has completed stage sg at time t in scenario s and 0 otherwise

suggest that the feedstock and product portfolios along with utilized technologies of the chemical process industry (CPI) may grow and be quite different compared to today's in the near future. As such, there is tremendous opportunity for investigating the impacts of these new technologies/feedstocks/products on the chemical process industry.

Determining which feedstock or technology to develop is a challenging task. Often there are many emerging feedstocks and processing technology alternatives. Incorporating new feedstocks and technologies into the CPI is an expensive and time consuming process. Beyond initial discovery, investments into new technology serve two purposes: (1) to improve the efficiency of the process, and (2) to expand the production capacity of the technology to meet market demands. Generally, the performance of a technology is not known with certainty until after the technology is fully developed. Large investments into technology projects do not guarantee successful development or favorable results. Often new technology projects are mishandled or mismanaged leading to investments without a return or loss of investment due to project abandonment (Cooper, 2007). Furthermore, the development of technologies is partially driven by product demand, which is not known with certainty at the time of the investments. Therefore, to incorporate new feedstocks and technologies into the existing CPI infrastructure, a systematic approach is necessary to answer the following questions: how much to invest, which new technologies to invest in, and when to invest in each technology for research and development (R&D) and for capacity expansions?

New chemical technologies start as ideas. Investments in these ideas lead to laboratory experimentation and if successful, pilot plant and commercial installations. Determining when and how much to invest in a new technology is a complicated decision, which relies on knowledge of the cost, yield, and the success of the new technology, as well as, the continued demand for the product that the technology produces. Fig. 1 provides a visual for the development and incorporation of new technologies into the CPI. The mini CPI depicted in Fig. 1 contains three chemicals (CHEM1, CHEM2, and CHEM3) and two technologies (TECH1 and TECH2). Each chemical can be purchased, produced (arrows connecting to technologies), and/or sold to meet demand. Technologies connected with solid lines represent established production routes. Connections between chemicals and technologies which appear as dashed lines are considered potential production routes. They