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Sustainability assessment framework for chemical production pathway: Uncertainty analysis

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ABSTRACT

The sustainability level of a chemical production pathway is an important element that requires to be assessed when developing a new process. Note that the typical sustainability assessment is normally emphasised on economic and technological development. In order to ensure more comprehensive level of sustainability, the protection on human health and preservation of the environment should be considered. This paper presents a systematic framework for assessment of chemical production pathway based on multi-sustainability criteria, i.e., inherent safety, health and environment (SHE) and economic performance (EP). In order to generate an optimal design solution, uncertainty analysis is also incorporated in this framework. Two optimisation approaches are adapted into this framework, i.e. fuzzy optimisation is used for multi-objective analysis, while multi-period optimisation is applied to address the multiple operational periods with presence of uncertainty. To illustrate the proposed framework, assessment on biodiesel production pathway based on enzymatic transesterification using waste oil is conducted. In the case study, three periods (low, medium and high demand period) of demand for biodiesel are considered, whereby each period is subjected to uncertainties, i.e. waste oil flow rate, waste oil price and enzyme price. To accommodate the uncertainties, sensitivity analysis is performed to determine the feasible operating condition, i.e. *tert*-butanol concentration and reactor residence time, as well as the appropriate sizing of the process modules (or known as unit operations).

1. Introduction

Production pathway design appears as an important task during the chemical process design to achieve sustainable development [16]. Typically, chemical process design is performed in stages, which starts from the research and development (R&D), followed by preliminary engineering and basic engineering stage [11]. During these early design stages, the pathway design can be enhanced through various assessments [19]. In assessment, it is critical to consider the criteria which contribute to sustainability of the production pathway [35]. In terms of sustainability, it is essential to prioritise on the protection of human and conservation of the environment [20]. This is supported by a significant number of undesired events involving chemical plant industries that had took place in the past, e.g. Bhopal disaster, 1974, Piper Alpha disaster, 1988, Texas city refinery explosion, 2005, etc. Those accidents have caused great losses in terms of disastrous impacts on human life and the environment. In relation to this, the demand from the public and voluntary initiatives to improve the safety, health and environmental (SHE) performance in chemical production has gradually increased [12].

For the improvement of SHE, it is important to adopt the inherent safety (IS) principle during the early process design stages. The IS principle basically emphasises on the reduction or elimination of hazard by intrinsic mean, without the application of external add-on system or procedures [15]. In addition, it is highly recommended to perform the IS assessment during early process design stages due to the benefits of having higher degree of freedom for performing engineering modification with much lower cost [13]. Apart from considering the IS aspect, Kletz [15] also suggested to apply the IS principle to health and environmental aspects to promote more comprehensive protection on human and conservation of the environment. Therefore, the objective of

Abbreviations: EP, economic performance; HQI, health quotient index; IBI, inherent benign-ness indicator; IE, inherent environment; IH, inherent health; IS, inherent safety; R&D, research and development; SHE, safety, health and environment; WAR, waste reduction algorithm.

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Nomenclatures

Sets

j	Process stream
k	Chemical
l	Process module
ldc	Distillation column
lhe	Heat exchanger
lpv	Pressure vessel
lpvd	Decanter vessel
lpvr	Reactor
lpvt	Storage tank
n'	Non-product outlet stream

Parameters

c_k^{EL}	Exposure limit for chemical *k* in air
$COEF^{Dist}$	Coefficient for tray spacing and liquid surface tension
$COST_l^{Unit-CW}$	Unit cost of cooling water for process module *l*
$COST_l^{Unit-Elec}$	Unit cost of electricity for process module *l*
$COST_m^{Unit-Feed}$	Unit cost of raw material *m*
$COST_l^{Unit-LPS}$	Unit cost of low pressure steam for process module *l*
$COST_l^{Unit-MPS}$	Unit cost of medium pressure steam for process module *l*
$COST_n^{Unit-Prod}$	Unit price of product *n*
ft_{lhe}^{Pres}	Pressure factor for heat exchanger *lhe*
ft_{lhe}^{Mat}	Material factor for heat exchanger *lhe*
ft_{lhe}^{Len}	Tube-length correction factor for heat exchanger *lhe*
HY	Annual operating hour
I_0	Base CE index
I_1	Latest CE index
Inc^{Tax}	Income tax rate
RR_{ldc}^{Dist}	Reflux ratio for distillation column *ldc*
SP_{ldc}^{Dist}	Spacing of plate for distillation column *ldc*
$th_{ldc}^{Dist-Shell}$	Thickness of shell for distillation column *ldc*
$th_{lpv}^{Ves-Shell}$	Shell thickness for pressure vessel
U_{lhe}^{HEX}	Overall heat transfer coefficient for heat exchanger *lhe*
X_p^U	Upper fuzzy limit for period *p*
X_p^L	Lower fuzzy limit for period *p*
α_p	Occurrence probability for period *p*
ψ_k	Standard potential environmental impact value for chemical *k*

Variables

A_{lhe}^{HEX}	Heat transfer surface for heat exchanger *lhe*
c_k	Concentration of chemical *k* in air
c_{lpr}^{TB}	*tert*-butanol concentration in reactor *lpr*
$COST^{CFC}$	Contractor's fee and contigency
$COST^{DFC}$	Total depreciable capital
$COST^{Feed}$	Total cost of feedstock
$COST_{ldc}^{PM}$	Total cost of distillation column *ldc*
$COST_{lhe}^{PM}$	Total purchase cost for heat exchanger *lhe*
$COST_{lpv}^{PM}$	Total cost of pressure vessel *lpv*
$COST^{Prod}$	Annual production cost
$COST^{TCI}$	Total capital investment
$COST^{TPC}$	Total plant cost
$COST^{TPDC}$	Total plant direct cost
$COST^{TPEC}$	Total purchase cost for all process modules
$COST^{TPEC-PM}$	Total capital investment based on process modules
$COST^{TPIC}$	Total plant indirect cost
$COST^{Util}$	Total utility cost
$CONS_l^{Util-CW}$	Consumption of cooling water for process module *l*
$CONS_l^{Util-LPS}$	Consumption of low pressure steam for process module *l*
$CONS_l^{Util-MPS}$	Consumption of medium pressure steam for process module *l*
$CONS_l^{Util-Elec}$	Consumption of electricity for process module *l*
$COST^{WC}$	Working capital cost
$COST_{lpv}^{Ves}$	Cost of pressure vessel *lpv*
$COST_{ldc}^{Dist-PL}$	Cost of platform and ladder for distillation column *ldc*
$COST_{lpv}^{Ves-PL}$	Cost of platform and ladder for pressure vessel *lpv*
D_{ldc}^{Dist}	Diameter for distillation column *ldc*
D_{lpr}^{Ves}	Internal shell diameter for reactor *lpr*
D_{lpv}^{Ves}	Internal shell diameter for pressure vessel *lpv*
$D_{n,lpvt}^{Ves}$	Diameter of storage tank vessel *lpvt* for product *n*
Eco	Scoring index for economic performance
E'	Scoring index for explosiveness
F'	Scoring index for flammability
F_{ldc}^{Dist-D}	Distillate flow rate for distillation column *ldc*
F_m^{Feed}	Flow rate of raw material *m*
$F_{n'}^{Non-Prod-O}$	Flow rate of non-product outlet stream *n'*
F_n^{Prod}	Flow rate of product stream *n*
$F_{j,lpr}^{Re-In}$	Flow rate of inlet process stream *j* to reactor *lpr*
$FE_{j,l}^{PM}$	Standard fugitive emission rate based on process stream *j* connected to process module *l*
FE_k^{Total}	Total fugitive emission for chemical *k*
G_{ldc}^{Dist}	Allowable vapour velocity for distillation column *ldc*
H_{ldc}^{Dist}	Height of distillation column *ldc*
H_{lpr}^{Ves}	Height for reactor *lpr*
H_{lpv}^{Ves}	Shell tangent-to-tangent height for pressure vessel *lpv*
$H_{n,lpvt}^{Ves}$	Height of storage tank vessel *lpvt* for product *n*
HQI^{Total}	Total health quotient index value for all chemicals
HQI_k	Health quotient index for chemical *k*
I'	Scoring index for chemical inventory
IE	Scoring index for inherent environment
IH	Scoring index for inherent health
IS	Scoring index for inherent safety
$PEI^{Non-Prod-O}$	Potential environmental impact resulted by all non-product outlet streams
P'	Scoring index for pressure
Q_{lhe}^{HEX}	Heat transfer rate for heat exchanger *lhe*
R'	Scoring index for reactivity
REV	Annual sales revenue
ROI	Return on investment
q_{ldc}^{Dist}	Number of plates in distillation column *ldc*