INHERENT SAFETY, HEALTH, ENVIRONMENT AND ECONOMIC ASSESSMENT FOR SUSTAINABLE CHEMICAL PROCESS DESIGN: BIODIESEL CASE STUDY

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ABSTRACT

Chemical process design involves the development of chemical route that converts the feedstock to the desired product. During chemical process design, the sustainability features, i.e. safety, health and environmental (SHE), and economic performance (EP) should be established through assessment. However, at present, no relevant assessment framework with simultaneous consideration of SHE and EP is reported in literature. As improvement to the mentioned shortfall, this thesis presents four systematic frameworks for chemical process design based on multiple objectives of inherent SHE and EP. These frameworks are specifically dedicated for three design stages of (1) research and development, (2) preliminary engineering stage, and (3) basic engineering stage, and lastly (4) uncertainty analysis with the presence of multiple operational periods. Following the proposed frameworks, the mathematical optimisation models were developed for the assessment. Besides, multi-objective optimisation algorithm (fuzzy optimisation) and multi-period optimisation approach were also integrated into the frameworks to address the multiple objectives, uncertainties and multiple operational periods. To illustrate the frameworks proposed in this thesis, the assessments on biodiesel production pathway in different design stages were solved. Prior to the assessment, eight alternative biodiesel production pathways were identified based on literature. Through the evaluations and assessments in each design stage using the proposed frameworks, a final optimum biodiesel production pathway, i.e. enzymatic transesterification using waste vegetable oil, was designed through assessment. This pathway was further assessed and improved via assessment in basic engineering stage and uncertainty analysis. Following the assessments, several inherent SHE improvement strategies for all the three highlighted design stages were also suggested. Lastly, it can be concluded that the developed frameworks provide simplified yet effective ways for chemical process design based on the multi-objective of inherent SHE and EP.

ABSTRAK

Reka bentuk proses kimia melibatkan pembangunan laluan kimia yang menukarkan bahan mentah ke produk yang diperlukan. Dalam reka bentuk proses kimia, ciri-ciri kemampanan dari segi keselamatan, kesihatan dan alam sekitar (SHE) yang wujud, serta prestasi ekonomi (EP) perlu diwujudkan melalui penilaian. Walau bagaimanapun, setakat ini, tiada rangka kerja penilaian yang berkaitan didapati dalam bahan literatur sedia ada. Untuk penambahbaikan, tesis ini mengemukakan empat rangka kerja sistematik untuk reka bentuk laluan pengeluaran kimia semasa peringkat awal berdasarkan prinsip SHE yang wujud dan EP sebagai objektif. Rangka kerja tersebut adalah direka untuk tiga reka bentuk peringkat awal, iaitu (1) penyelidikan dan pembangunan, (2) kejuruteraan awal, (3) kejuruteraan asas, serta (4) analisis ketidakpastian dengan mengambil kira tempoh operasi berganda. Dalam rangka kerja tersebut, model pengoptimuman matematik telah direka untuk kerja penilaian. Selain itu, kaedah pengoptimuman pelbagai objektif (cara pengoptimuman kabur), dan pengoptimuman pelbagai tempoh telah digunakan dalam rangka kerja untuk analisis atas pelbagai objektif, sensitiviti dengan kehadiran ketidakpastian serta tempoh operasi berganda. Untuk menggambarkan rangka kerja yang dikemukakan dalam tesis ini, penilaian ke atas laluan pengeluaran biodiesel dalam beberapa peringkat reka bentuk telah diselesaikan. Sebelum kerja penilaian, sebanyak lapan laluan pengeluaran biodiesel telah dikenalpasti melalui kajian literatur. Melalui penilaian dengan menggunakan rangka kerja yang direka, laluan pengeluaran biodiesel yang paling optimum telah direka, iaitu transesterifikasi berenzim dengan minyak sayuran sisa. Laluan pengeluaran ini telah dinilai dan dipertingkatkan melalui penilaian di peringkat kejuruteraan asas serta analisis ketidakpastian. Melalui penilaian, beberapa strategi peningkatan SHE yang wujud untuk tiga peringkat awal reka bentuk process telah dicadangkan. Sebagai kesimpulan, rangka kerja yang dicadangkan telah menunjukkan cara yang mudah dan efektif untuk mereka bentuk proses kimia berdasarkan objektif berganda iaitu prinsip SHE yang wujud dan EP.

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LIST OF ABBREVIATION

AHI	-	Atmospheric Hazard Index
AHP	-	Analytical Hierarchical Process
EHI	-	Environmental Hazard Index
EHS	-	Environmental, Health and Safety Analysis Method
ESD	-	Engineering Sustainable Development
EP	-	Economic Performance
FAME	-	Fatty Acid Methyl Esters
FMEA	-	Failure Modes and Effects Analysis
GA	-	Genetic Algorithm
GHG	-	Greenhouse Gases
GREENSCOPE	-	Gauging Reaction Effectiveness for the Environmental Sustainability of Chemistries with a Multi-Objective Process Evaluator
HAZOP	-	Hazard And Operability Study
HQI	-	Health Quotient Index
I2SI	-	Integrated Inherent Safety Index
IBI	-	Inherent Benign-Ness Indicator
IE	-	Inherent Environment
IEI	-	Integrated Environmental Index
IETH	-	Inherent Environmental Toxicity Hazard
IH	-	Inherent Health
INSET	-	Inherent SHE Evaluation Tool

IOHI	-	Inherent Occupational Health Index
IS	-	Inherent Safety
ISD	-	Inherently Safer Design
ISI	-	Inherent Safety Index
KPI	-	Key Performance Index
LCA	-	Life Cycle Assessment
LFL	-	Lower Flammability Limit
LOP	-	Layers of Protection
MCA	-	Multi-Criteria Analysis
MILP	-	Mixed Integer Linear Programming
MINLP	-	Mixed Integer Nonlinear Programming
OAT	-	One-At-a-Time
OHHI	-	Occupational Health Hazard Index
OHI	-	Occupational Health Index
P&ID	-	Piping and Instrumentation Diagram
PEI	-	Potential Environmental Impact
PFD	-	Process Flow Diagram
PHA	-	Preliminary Hazard Analysis
PIIS	-	Prototype Index of Inherent Safety
PP	-	Production Pathway
PRHI	-	Process Route Healthiness Index
PRI	-	Process Route Index
PSE	-	Process System Engineering
QRA	-	Quantitative Risk Assessment
R&D	-	Research And Development
RAM	-	Risk Assessment Matrix
SHE	-	Safety, Health And Environment

SIS	-	Safety Interlock System
SWeHI	-	Safety Weighted Hazard Index
SREST	-	Substance, Reactivity, Equipment and Safety-Technology
TLV-STEL	-	Threshold Limit Value - Short-Term Exposure Limit
UFL	-	Upper Flammability Limit
WAR	-	Waste Reduction Algorithm

LIST OF SYMBOLS

Sets

cv	-	Alternative types of control valves
e	-	Environmental impact category
gk	-	Alternative types of gaskets
gkc	-	Alternative types of gaskets for control valve
gkmb	-	Alternative types of gaskets for big size manual valve
gkms	-	Alternative types of gaskets for small size manual valve
i	-	Production pathway
j	-	Process stream
k	-	Chemical
l	-	Process module
ldc	-	Distillation column
lhe	-	Heat exchanger
lp	-	Process pump
lpv	-	Pressure vessel
lpvd	-	Decanter vessel
lpvr	-	Reactor
lpvt	-	Storage tank
m	-	Feedstock stream
mbv	-	Alternative types of big size manual valve
msv	-	Alternative types of small size manual valve

n	-	Product stream
n'	-	Non-product outlet stream
oc	-	Location of control valve for the case of chemical leakage
oc'	-	Location of big size manual valve for the case of fugitive emission
of	-	Location of flange for the case of chemical leakage
of'	-	Location of flange for the case of fugitive emission
omb	-	Location of big size manual valve for the case of chemical leakage
omb'	-	Location of big size manual valve for the case of fugitive emission
oms	-	Location of small size manual valve for the case of chemical leakage
oms'	-	Location of small size manual valve for the case of fugitive emission
pc	-	Alternative types of piping connections
pcmb	-	Alternative types of piping connections for big size manual vale
pcms	-	Alternative types of piping connections for small size manual valve
ps	-	Alternative pipe sizes
s	-	Types of selection
ss	-	Alternative types of process pump shaft seals
vr	-	Alternative types of control valve ratings

Parameters

$COST_m^{Unit\text{-}Feed}$	-	Unit cost of feedstock *m*
$COST_n^{Unit\text{-}Prod}$	-	Unit price of product *n*
C_k^{EL}	-	Exposure limit for chemical *k* in air

C_p	-	Specific heat capacity
$COEF^{Dist}$	-	Coefficient for tray spacing and liquid surface tension
$COST_l^{Unit\text{-}CW}$	-	Unit cost of cooling water for process module *l*
$COST_l^{Unit\text{-}LPS}$	-	Unit cost of low pressure steam for process module *l*
$COST_l^{Unit\text{-}MPS}$	-	Unit cost of medium pressure steam for process module *l*
$COST_l^{Unit\text{-}Elec}$	-	Unit cost of electricity for process module *l*
D_{lp}^{Pip}	-	Diameter of discharge pipe for process pump *lp*
D_{ldc}^{Dist}	-	Diameter for distillation column *ldc*
D_{lpv}^{Ves}	-	Internal shell diameter for pressure vessel *lpv*
$D_{n,lpvt}^{Ves}$	-	Diameter of storage tank vessel *lpvt* for product *n*
Dis	-	Discharge coefficient
DISC	-	Discount rate
E_{lp}^{Pump}	-	Efficiency of process pump *lp*
f_{lp}	-	Friction factor for process pump *lp*
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*
g	-	Gravitational constant
$H_{ldc}^{Dist\text{-}Weir}$	-	Weir height for 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*
HY	-	Annual operating hour

I^B	-	Base CE index
I^L	-	Latest CE index
Inc^{Tax}	-	Income tax rate
L_{lp}^{Pip}	-	Length of discharge pipe for process pump *lp*
LC_1	-	Lethal concentration with 1% of animal killed
LC_{50}	-	Lethal concentration with 50% of animal killed
LD_{50}	-	Lethal dose with 50% of animal killed
LS^{Max}	-	Operation lifespan
MW	-	Molecular weight
MW_k	-	Molecular weight for chemical *k*
n^B	-	Number of bolt at flange
n^{CV}	-	Quantity of control valves
n^{MB}	-	Quantity of big size manual valves
n^{MS}	-	Quantity of small size manual valves
n^{FLG}	-	Quantity of flanges
n^{SS}	-	Quantity of process pump shaft seal
$PEI_{k,e}$	-	Potential environmental impact value for the individual chemical *k* under environmental impact category *e*
r	-	Separation ratio
RR_{ldc}^{Dist}	-	Reflux ratio for distillation column *ldc*
SP_{ldc}^{Dist}	-	Spacing of plate for distillation column *ldc*
$th_{ldc}^{Dist\text{-}Shell}$	-	Thickness of shell for distillation column *ldc*
$th_{lpv}^{Ves\text{-}Shell}$	-	Shell thickness for pressure vessel *lpv*
th^{Gas}	-	Thickness of gasket
TFI	-	Daily fluid/food intake

X^{L}	-	Lower fuzzy limit for objective *X*
X^{U}	-	Upper fuzzy limit for objective *X*
X_i^{L}	-	Lower fuzzy limit for objective *X* and production pathway *i*
X_i^{U}	-	Upper fuzzy limit for objective *X* and production pathway *i*

Variables

A_{lhe}^{HEX}	-	Heat transfer surface for heat exchanger *lhe*
A^{Leak}	-	Area of leakage
A_{o}^{Leak}	-	Area of leakage at location *o*
A_{oc}^{Leak}	-	Area of leakage at control valve at location *oc*
A_{of}^{Leak}	-	Area of leakage at flange at location of *of*
A_{omb}^{Leak}	-	Area of leakage at big size manual valve at location *omb*
A_{oms}^{Leak}	-	Area of leakage at small size manual valve at location *oms*
$A_{oc,ps,gkc}^{\mathrm{LeakCV}}$	-	Area of leakage at control valve location of *oc* with subject to pipe size, *ps* and types of gaskets, *gkc*
$A_{of,gkf}^{\mathrm{LeakFlg}}$	-	Area of leakage at flange location of *of* with subject to the types of gaskets, *gkf*
$A_{omb}^{\mathrm{LeakMB\text{-}FC}}$	-	Area of leakage for flange connection at big size manual valve location of *omb*
$A_{omb,gkmb,ps}^{\mathrm{LeakMB\text{-}FC}}$	-	Area of leakage for flange connection at big size manual valve location of *omb* with subject to types of gaskets, *gkmb* and pipe size, *ps*
$A_{oms}^{\mathrm{LeakMS\text{-}FC}}$	-	Area of leakage for flange connection at small size manual valve location of *oms*
$A_{oms,gkms}^{\mathrm{LeakMS\text{-}FC}}$	-	Area of leakage for flange connection at small size manual valve location of *oms* with subject to types of gaskets, *gkms*

A_{omb}^{LeakWC}	-	Area of leakage of welded connection at big size manual valve location of *omb*
A_{oms}^{LeakWC}	-	Area of leakage of welded connection at small size manual valve location of *oms*
AF	-	Annualised factor
C_k	-	Concentration of chemical *k* in air
$C^{\text{Cat-Re}}$	-	Catalyst concentration
C_{lpr}^{TB}	-	*tert*-butanol concentration in reactor *lpr*
CIR^{Int}	-	Internal circumference of pipe
$CONS_l^{\text{Util-CW}}$	-	Consumption of cooling water for process module *l*
$CONS_l^{\text{Util-LPS}}$	-	Consumption of low pressure steam for process module *l*
$CONS_l^{\text{Util-MPS}}$	-	Consumption of medium pressure steam for process module *l*
$CONS_l^{\text{Util-Elec}}$	-	Consumption of electricity for process module *l*
$CONV^{\text{Trigly}}$	-	Conversion of triglycerides (oil) through transesterification reaction
$COST^{\text{CFC}}$	-	Contractor’s fee and contigency
$COST^{\text{DFC}}$	-	Total depreciable capital
$COST_{gkc,ps,cv,vr}^{\text{CV}}$	-	Cost of control valve with subject to types of gaskets, *gkc*, pipe size, *ps*, types of control valves, *cv*, and valve rating, *vr*
$COST_{ldc}^{\text{Dist-PL}}$	-	Cost of platform and ladder for distillation column *ldc*
$COST^{\text{Feed}}$	-	Total cost of feedstock
$COST_m^{\text{Feed}}$	-	Purchase cost of feedstock *m*
$COST_{ps,gkf}^{\text{FLG}}$	-	Cost of flange at piping with subject to pipe size, *ps*, and types of gaskets, *gkf*
$COST_{gkmb,ps,mbv,pcmb}^{\text{MB}}$	-	Cost of big size manual valve with subject to types of gaskets, *gkmb*, pipe size, *ps*, types of manual valves, *mbv*, and piping connections, *pcmb*

$COST^{\mathrm{MS}}_{gkms,msv,pcms}$	-	Cost of small size manual valve with subject to types of gaskets, *gkms*, types of manual valves, *msv*, and piping connections, *pcms*
$COST^{\mathrm{PM}}_{ldc}$	-	Total cost of distillation column *ldc*
$COST^{\mathrm{PM}}_{lhe}$	-	Total purchase cost for heat exchanger *lhe*
$COST^{\mathrm{PM}}_{lpv}$	-	Total cost of pressure vessel *lpv*
$COST^{\mathrm{Prod}}$	-	Annual production cost
$COST^{\mathrm{SS}}_{ss}$	-	Cost of flange at piping with subject to pipe size, *ps*, and types of pump shaft seal, *ss*
$COST^{\mathrm{TCI\text{-}CV}}$	-	Capital cost of control valve
$COST^{\mathrm{TCI\text{-}FLG}}$	-	Capital cost of flange at piping
$COST^{\mathrm{TCI\text{-}MB}}$	-	Capital cost of big size manual valve
$COST^{\mathrm{TCI\text{-}MS}}$	-	Capital cost of small size manual valve
$COST^{\mathrm{TCI\text{-}Pip}}$	-	Capital cost of all pipe fittings
$COST^{\mathrm{TCI\text{-}SS}}$	-	Capital investment of process pump shaft seal
$COST^{\mathrm{TPC}}$	-	Total plant cost
$COST^{\mathrm{TPDC}}$	-	Total plant direct cost
$COST^{\mathrm{TPEC}}$	-	Total purchase cost for all process modules
$COST^{\mathrm{TPIC}}$	-	Total plant indirect cost
$COST^{\mathrm{Util}}$	-	Total utility cost
$COST^{\mathrm{Util}}_{cp}$	-	Utility cost for conversion process *cp*
$COST^{\mathrm{Util\text{-}Pip}}$	-	Utility cost incurred with association to pipe size
$COST^{\mathrm{WC}}$	-	Working capital cost
$COST^{\mathrm{Ves}}_{lpv}$	-	Cost of pressure vessel *lpv*
$COST^{\mathrm{Ves\text{-}PL}}_{lpv}$	-	Cost of platform and ladder for pressure vessel *lpv*
E	-	Explosiveness
E^{P}	-	Scoring index for explosiveness under method of PIIS

E'	-	Normalised scoring index for explosiveness
Eco	-	Scoring index for economic performance
F	-	Flammability
F^{P}	-	Scoring index for flammability under method of PIIS
F'	-	Normalised scoring index for flammability
$F_{ldc}^{\text{Dist-D}}$	-	Distillate flow rate for distillation column *ldc*
F_{m}^{Feed}	-	Flow rate of feedstock *m*
F_{n}^{Prod}	-	Flow rate of product stream *n*
$F_{j,lpr}^{\text{Re-In}}$	-	Mass flow rate of inlet process stream *j* to reactor *lpr*
F_j	-	Mass flow rate of process stream *j*
$F_{j,k}$	-	Flow rate of chemical component *k* in process stream *j*
F_{lp}^{Pump}	-	Mass flow rate at process pump *lp*
$F_{lp,ps}^{\text{Pump}}$	-	Mass flow rate at process pump *lp* based on pipe size *ps*
$FE_{oc',k}$	-	Fugitive emission at control valve location of *oc'* for chemical *k*
$FE_{omb',k}$	-	Fugitive emission at big size manual valve location of *omb'* for chemical *k*
$F_{j,l}^{\text{In}}$	-	Inlet flow rate of stream *j* for process module *l*
$F_{j,lpv}^{\text{In}}$	-	Inlet flow rate of stream *j* for pressure vessel *lpv*
$F_{j,l}^{\text{Out}}$	-	Outlet flow rate of stream *j* for process module *l*
$F_{n'}^{\text{Non-Prod-O}}$	-	Flow rate of non-product outlet stream *n'*
$F_{ldc}^{\text{Dist-Refl}}$	-	Reflux flow rate for distillation column *ldc*
$FE_{oms',k}$	-	Fugitive emission at small size manual valve location of *oms'* for chemical *k*

$FE_{oss',k}$	-	Fugitive emission at process pump shaft seal location of *oss'* for chemical *k*
$FE^{\mathrm{CV}}_{oc',k,cv,vr}$	-	Fugitive emission for chemical *k* at control valve location of *oc'* with subject to the types of control valves, *cv*, and valve rating, *vr*
$FE^{\mathrm{MB}}_{omb',k,mbv,pcmb}$	-	Fugitive emission for chemical *k* at big size manual valve location of *omb'* with subject to the types of valve, *mbv*, and piping connection, *pcmb*
$FE^{\mathrm{MS}}_{oms',k,msv,pcsb}$	-	Fugitive emission for chemical *k* at small size manual valve location of *oms'* with subject to the types of valve, *msv*, and piping connection, *pcms*
$FE^{\mathrm{PM}}_{oc'}$	-	Standard fugitive emission rate at location *oc'*
$FE^{\mathrm{PM}}_{omb'}$	-	Standard fugitive emission rate at location *omb'*
$FE^{\mathrm{PM}}_{oms'}$	-	Standard fugitive emission rate at location *oms'*
$FE^{\mathrm{PM}}_{oss'}$	-	Standard fugitive emission rate at location *oss'*
$FE^{\mathrm{SS}}_{oss',k,ss}$	-	Fugitive emission for chemical *k* at process pump shaft seal location of *oss'* with subject to the types of shaft seal, *ss*
FE^{Total}_{k}	-	Total fugitive emission for chemical *k*
FK_k	-	Number of fish killed due to chemical *k*
G^{Dist}_{ldc}	-	Allowable vapour velocity for distillation column *ldc*
G^{Leak}	-	Severity of chemical leakage
h^{Fr}_{lp}	-	Friction loss at process pump *lp*
$h^{\mathrm{Fr}}_{lp,ps}$	-	Friction loss at process pump *lp* based on pipe size *ps*
Haz	-	Hazard potential of chemical leakage
$H_{A,k}$	-	Atmospheric impact hazard for chemical *k*
$H_{T,k}$	-	Terrestrial impact hazard for chemical *k*
$H_{W,k}$	-	Aquatic impact hazard for chemical *k*
H^{Dist}_{ldc}	-	Height of distillation column *ldc*

$H_{j,l}^{\text{In}}$	-	Enthalpy of inlet stream *j* for process module *l*
$H_{j,l}^{\text{Out}}$	-	Enthalpy of outlet stream *j* for process module *l*
HQI_k	-	Health quotient index for chemical *k*
$HQI^{\text{NC-Total}}$	-	Chronic inhalation exposure risk for non-carcinogen
HQI^{Total}	-	Health quotient index value for all chemicals
I_{ldc}^{Dist}	-	Chemical inventory for distillation column *ldc*
$I_{ldc}^{\text{Dist-G}}$	-	Gas inventory for distillation column *ldc*
$I_{ldc}^{\text{Dist-L}}$	-	Liquid inventory for distillation column *ldc*
$I_{ldc}^{\text{Dist-RB}}$	-	Liquid inventory for reboiler of distillation column *ldc*
$I_{ldc}^{\text{Dist-RD}}$	-	Liquid inventory for reflux drum of distillation column *ld*
I_{lpv}^{Ves}	-	Chemical inventory of pressure vessel *lpv*
I	-	Chemical inventory
I'	-	Scoring index for chemical inventory
I_C	-	Scoring index for corrosiveness
IE	-	Scoring index for inherent environmental performance
I_{EL}	-	Scoring index for exposure limit
IH	-	Scoring index for inherent health performance
I_{HH}	-	Scoring index for health hazard
I_{IPPH}	-	Scoring index for physical and process hazard
I_{MS}	-	Scoring index for material phase
I_R	-	Scoring index for R-phrase
I^{P}	-	Scoring index for chemical inventory under method of PIIS
I_{PM}	-	Scoring index for mode of process

IS	-	Scoring index for inherent safety performance
I_T	-	Scoring index for temperature
I_V	-	Scoring index for volatility
m_k^{Leak}	-	Total leakage mass flow rate for chemical k
$m^{\text{Leak-Total}}$	-	Total leakage mass flow rate for all chemicals
NP_{ldc}^{Dist}	-	Number of plates in distillation column ldc
P	-	Pressure
P'	-	Normalised scoring index for pressure
P_l	-	Power consumption of process module l
pnr	-	Penalty value in inherent safety assessment
P_{oc}	-	Pressure of process stream at chemical leakage location oc
P_{omb}	-	Pressure of process stream at chemical leakage location omb
P_{oms}	-	Pressure of process stream at chemical leakage location oms
P_{oss}	-	Pressure of process stream at chemical leakage location oss
P^{P}	-	Scoring index for pressure under method of PIIS
PB_k	-	Probit value for chemical k
PEC_k	-	Predicted environmental concentration for chemical k
$PEI^{\text{Non-Prod-O}}$	-	Potential environmental impact value based on non-product outlet stream
PEI^{Total}	-	Potential environmental impact resulted by all leaked chemicals
$PSEC$	-	Predicted specific environmental concentration
Q_{lhe}^{HEX}	-	Heat transfer rate for heat exchanger lhe
R	-	Reactivity
R'	-	Normalised scoring index for reactivity

R_{mo}	-	Molar ratio of methanol-to-oil
REV	-	Total annual sales revenue
REV_n	-	Annual sales revenue for product *n*
ROI	-	Return on investment
S_c	-	Scoring index for chemical hazard
S_P	-	Scoring index for process hazard
S^{Leak}	-	Release condition of chemical
T	-	Temperature
T^{P}	-	Scoring index for temperature under method of PIIS
T'	-	Normalised scoring index for temperature
Tx^{P}	-	Scoring index for toxicity under method of PIIS
TAC	-	Total annualised cost
t^{Re}	-	Reaction duration
t_{lpr}^{Re}	-	Residence time for reactor *lpr*
t_{ldc}^{Dist}	-	Liquid hold-up time for distillation column *ldc*
t_{lpv}^{Re}	-	Residence time for pressure vessel *lpv*
t_n^{St}	-	Required storage duration for product *n*
T^{Re}	-	Reaction temperature
THI_k	-	Base impact of terrestrial toxicity hazard
$TYPE^{\mathrm{Cat}}$	-	Type of catalyst
U_{lhe}^{HEX}	-	Overall heat transfer coefficient for heat exchanger *lhe*
V^{Air}	-	Volumetric flow rate of air
Vel_{lp}^{Ave}	-	Average fluid velocity at discharge pipe of process pump *lp*
Vel_j^{Opt}	-	Optimum fluid velocity in pipe for process stream *j*

W_{ldc}^{Dist}	-	Weight of distillation column *ldc*
W_{lpv}^{Ves}	-	Weight for pressure vessel *lpv*
WHI_k	-	Base impact of atmospheric toxicity hazard
$x_{j,k}$	-	Composition of chemical *k* in stream *j*
$x_{n',k}$	-	Composition of chemical *k* in non-product outlet stream *n'*
$x_{oc,k}$	-	Stream composition of chemical *k* for chemical leakage location *oc*
$x_{oc',k}$	-	Stream composition of chemical *k* for fugitive emission location *oc'*
$x_{omb,k}$	-	Stream composition of chemical *k* for chemical leakage location *omb*
$x_{omb',k}$	-	Stream composition of chemical *k* for fugitive emission location *omb'*
$x_{oms,k}$	-	Stream composition of chemical *k* for chemical leakage location *oms*
$x_{oms',k}$	-	Stream composition of chemical *k* for fugitive emission location *oms'*
$x_{oss,k}$	-	Stream composition of chemical *k* for chemical leakage location *oss*
$x_{oss',k}$	-	Stream composition of chemical *k* for fugitive emission location *oss'*
X	-	Optimisation objective
Y	-	Process yield
Y'	-	Normalised scoring index for process yield
Y^{P}	-	Scoring index for process yield method of PIIS
$Y_{A,k}$	-	Atmospheric toxicity impact severity scale value for chemical *k*
$Y_{T,k}$	-	Terrestrial toxicity impact severity scale value for chemical *k*
$Y_{W,k}$	-	Aquatic toxicity impact severity scale value for chemical *k*

α_p	-	Occurrence probability for period *p*
β	-	Selection variable
β_{cv}	-	Selection variable for the types of control valve, *cv*
β_{gkc}	-	Selection variable for the types of gaskets at control valve, *gkc*
β_{gkf}	-	Selection variable for the types of gaskets at flange connection at piping, *gkf*
β_{gkmb}	-	Selection variable for the types of gaskets at big size manual valve, *gkmb*
β_{gkms}	-	Selection variable for the types of gaskets at small size manual valve, *gkms*
$\beta^{\text{MB-FC}}$	-	Selection variable for flange connection on big size manual valve
$\beta^{\text{MB-WC}}$	-	Selection variable for welded connection on big size manual valve
$\beta^{\text{MS-FC}}$	-	Selection variable for flange connection on small size manual valve
$\beta^{\text{MS-WC}}$	-	Selection variable for welded connection on small size manual valve
β_{mvb}	-	Selection variable for the types of big size manual valve, *mvb*
β_{mvs}	-	Selection variable for the types of small size manual valve, *mvs*
β_{pcmb}	-	Selection variable for the types of piping connection for big size manual valve, *pcmb*
β_{pcms}	-	Selection variable for the types of piping connection for small size manual valve, *pcms*
β_{ps}	-	Selection variable for pipe size, *ps*
β_s	-	Selection variable for selection set *s*
β_{ss}	-	Selection variable for the types of process pump shaft seal, *ss*
β_{vr}	-	Selection variable for the types of valve rating, *vr*
ρ_{ldc}^{Dist}	-	Material density for distillation column *ldc*

ρ_{ldc}^{L}	-	Density of liquid in distillation column *ldc*
ρ_{ldc}^{V}	-	Density of vapour in distillation column *ldc*
$\rho_{ldc}^{\mathrm{Ves}}$	-	Material density for pressure vessel *lpv*
ρ_j	-	Density of process stream *j*
ρ_{oc}	-	Density of process stream at chemical leakage location *oc*
ρ_{of}	-	Density of process stream at chemical leakage location *of*
ρ_{omb}	-	Density of process stream at chemical leakage location *omb*
ρ_{oms}	-	Density of process stream at chemical leakage location *oms*
λ	-	Sustainability indicator
λ_i	-	Sustainability indicator for production pathway *i*
$\lambda_{i,X}$	-	Sustainability indicator for production pathway *i* and objective *X*
λ_p	-	Sustainability indicator for period *p*
ΔH_R	-	Heat of reaction
$\Delta H_R'$	-	Normalised scoring index for heat of reaction
$\Delta T_{m,lhe}^{\mathrm{HEX}}$	-	Mean temperature driving force for heat exchanger *lhe*
ψ_k	-	Standard PEI factor for chemical *k*

LIST OF APPENDICES

CHAPTER 1

INTRODUCTION

1.1 Research Background

In early chemical process development, it involves several early design stages, which are known as research and development (R&D), preliminary engineering and basic engineering stage. During those design stages, chemical production pathway is designed to enable effective conversion of raw materials into the desired end products that meets the required specifications and other process performances (Seider et al., 2004). In specific, the screening and optimisation of production pathway are performed to generate the most optimum pathway amongst all alternatives. In this context, it is very important to ensure the developed chemical production pathway is sustainable (Zheng et al., 2012). According to World Commission on Environment and Development (1987), sustainability is defined as the development that meets the needs of the present without compromising the ability of future generations to meet their own needs. For chemical production, the typical objective is to maximise the economic performance (EP) subject to the technologically feasibility. Besides, in order to ensure the business sustainability, other elements, such as environment, social development, safety, etc., are also essential (Othman et al., 2010).

In fact, all business units should fulfil the corporate responsibility in promoting the social development, which is primarily being emphasised as the contribution on safety, health and environmental (SHE) aspect. In chemical process industries, there is a strong demand from the public, legislation (e.g. The European Agency for Safety and Health at Work (EU-OSHA, 2010) and voluntary initiatives (e.g. Responsible Care) for the chemical manufacturers to seriously consider the improvement of SHE performance in their companies (Hook, 1996). This demand is primarily resulted from the increased public awareness along with the past history of chemical accidents (e.g. Fertiliser plant explosion, Texas, 2013, etc.) that have caused great loss of human life, properties and environment. This demand grows stronger with the rapid growth of chemical production activities over the years. The risk of chemical plants accident should be minimised through various means including addressing the fundamental problems by eliminating or reducing the inherent hazards in the process down to the minimum level.

As an effort to improve the SHE performance, it is important to assess the hazards of chemical production pathway (Kletz, 1991). Sustainable chemical production enables the long-term protection of human health and preservation of the environment. Therefore, SHE aspects have become the important elements to be considered in process design, apart from the aspects of technical and economic feasibility (Koller et al, 1999). Besides, in order to ensure the sustainable features in chemical production, it is recommended to perform SHE assessment based on the principle of inherent safety (IS) or inherently safer design (ISD) during early process design stage (Kletz, 1984). This principle emphasises on hazard elimination or reduction using intrinsic means, rather than any external system (e.g. devices) or administrative control (Kletz, 1984). Since the performances of occupational health and environmental compliance are equally important, the IS principle should be applied for inherent health (IH) and environmental (IE) assessment as well (Koller et al., 1999). In principle, the inherently safe, healthy and environmentally friendly plant should not cause any harm to human and environment. Those three aspects should be considered simultaneously rather than in a single form to promote comprehensive assessment, and hence it is known as inherent SHE.

The inherent SHE assessment should be conducted during early design stages rather than the latter engineering stage, due to great benefits i.e. lower cost, effort and time for any required engineering modification. On the other hand, late assessment of inherent SHE could result in a higher risk that intrinsically exists in the process. Therefore, early assessment on inherent SHE brings more benefits to the chemical production pathway and it should be emphasised in process design. Apart from the perspective of inherent SHE, EP should also be assessed in order to ensure the economic feasibility of the business before making any major investment to implement to the entire project. Considering the aforementioned advantages of conducting the assessment on chemical production pathway during early process design stages, it is important to apply the systematic frameworks for the assessment. Therefore, this forms the main motivation of this work to develop the systematic frameworks for sustainability assessment of chemical production pathway. In the framework, it is desirable to include multi-objective, e.g. inherent SHE and EP, for the purpose of ensuring the sustainability in comprehensive perspectives. Apart from that, since more than one objective is involved in the assessment, the multi-objective optimisation approach is used for the multi-objective analysis.

Other than development of the frameworks, it is also aimed to perform assessment on the chemical production pathway in order to illustrate the function of the frameworks. In this thesis, biodiesel production pathway is selected for the assessment. Since the past decades, biodiesel has emerged as a source of renewable energy that has potential to reduce the total dependency on petroleum fuel, and reduce the mentioned environmental problem (Hideki et al., 2001). Because of its mentioned potential, the production volume of biodiesel in global stage is expected to continually increase at least for the next decade (OECD and FAO, 2014). In this case, it is apparently important to assess the sustainability of biodiesel production pathway in terms of inherent SHE and EP. In this thesis, the engineering work of optimisation, screening and ranking of alternative biodiesel production pathways optimisation is performed using the developed frameworks.

1.2 Problem Statement

For the sustainability assessment on chemical production pathway, there are several key challenges emerged, and they should be taken note and addressed accordingly. At first, the consideration of inherent safety principle should be implemented in the assessment on chemical production pathway due to its significance in reducing or eliminating the intrinsic hazard in chemical process. As highlighted in literature (Khan and Amyotte, 2002), the application of inherent safety principle should be continuously widened in chemical industries and several key concerns are noted, i.e. (1) lack of awareness, knowledge and experience by plant designer, (2) limited attention in regulation, (3) time and cost constraint during process development stage, and lastly (4) lack of systematic methodology or tool for application purpose. Based on the mentioned reasons, in order to enhance its application in industries, it is essential to develop the assessment framework, which shows the systematic and simplified steps to the users (Preston and Hawksley, 1997).

Apart from that, the multi-objective which could contribute to sustainability should indeed be considered rather than assessing only a single aspect. However, note that a single aspect, e.g. technological performance, economic criteria, etc., is normally emphasised in conventional process design methodology (Tanabe and Miyake, 2012). In general, the factor of EP should be assessed in process design in order to ensure the economic feasibility of the production pathway (Zheng et al., 2012). Besides, as discussed in previous section, it is also necessary to consider inherent SHE in assessment. Based on this fact, the multi-objective of inherent SHE and EP should be considered in the framework. Nonetheless, the relevant assessment framework involving the mentioned aspects has yet to be reported in any literature. Hence, it becomes a challenge in this thesis to develop the new assessment framework, which incorporates the multi-objective of inherent SHE and EP. In conjunction with the multi-objective in assessment, the suitable optimisation tool should be adapted into the framework for multi-objective analysis. In this case, the entire structure of the framework and its detailed approach should be developed.

For the design of chemical production pathway during early stages, it is often experienced with a common problem, i.e. lacking of process data and the information on process modules (Koller et al., 2000). In fact, the information developed in each design stage is different, and the information becomes more detailed when progressing from one stage to the subsequent stage. The detailed information of the piping, process modules, operating procedures, etc., is normally developed and finalised during the detailed engineering design stage in order to support the procurement work. In overall, due to the difference of the early design stages, it is more recommended to use a specific assessment method for the individual stage (Abbaszadeh and Hassim, 2014). This provides the benefit of preventing the dilemma of searching for information, which is not yet developed, because only the information available in the particular process design stage is needed.

Based on the aforementioned problem statements, some key summaries are concluded. Firstly, it is important to develop the simplified assessment frameworks, which are comprised of systematic and holistic approaches, and tools that are easy to be understood and used. This is because the simplified framework could facilitate the application in both industries and academic fields. Next, in order to promote more comprehensive assessment, several frameworks should be developed according to the specific design stage or design purpose. This means that an individual framework is developed according to the specific design need (e.g. subject to certain design stage), rather than one general framework, which is claimed to be applicable for all design stages. The detailed classification and the key features of those frameworks are further discussed in the following section.

1.3 Research Objectives

Based on the abovementioned problem statements, the objectives of this research work are summarised as following:

(a) To develop systematic frameworks for assessment chemical production pathway based on multi-objective of inherent SHE and EP according to:
    (i) Research and development stage
    (ii) Preliminary engineering stage
    (iii) Basic engineering stage
    (iv) Uncertainty analysis

(b) To apply the assessment frameworks on biodiesel production pathway as a case study to illustrate the developed frameworks. From the assessment, the ways of identifying the most optimum pathway and performing further process design through the developed frameworks are demonstrated.

1.4 Scope of the Research

As elucidated in previous section, this thesis is aimed to present the novel and systematic framework of synthesising the production pathway which is inherently safer, healthier, environmental-friendlier, and more economically feasible. Based on this key research objective, the scopes of research are summarised as below. Note that the listed scopes are explained according to the case study of biodiesel production.

(a) Literature review: Several important topics are reviewed, starting with the introduction of the principle of hazard analysis and ISD. Subsequently, the features of the early process design stages and the developed assessment methods of inherent SHE are discussed. As biodiesel production is applied as a case study for the assessment, its production technology and the relevant sustainability assessment are also reviewed. Besides, the typical framework used for the chemical production pathway assessment is studied in order to understand its concept. Lastly, the optimisation approach, i.e. multi-objective optimisation and multi-period optimisation, which are to be incorporated in the proposed framework (refer to item (b) as below), is included in this review.

(b) Development of four systematic frameworks for inherent SHE and EP assessment with the integration of optimisation approach: The first three frameworks are designed for assessment according to individual early process design stage, i.e. R&D, preliminary engineering and basic engineering stage. Besides those three frameworks, the framework for uncertainty analysis is also included in this thesis. In the uncertainty analysis, the sensitivity analysis is performed by considering multiple operational periods aiming to generate a robust design solution towards the external factors, e.g. uncertainties. Note that, by applying those frameworks, it is targeted to demonstrate that only the information available in each stage (rather than the more detailed data) is used for the assessment. This is an important initiative to tackle the issue of lacking of data in early process design stages.

For each developed framework, the holistic and step-by-step approach for conducting the assessment is described. Besides, the detailed approach for formulating the mathematical optimisation model is also discussed. Note that multiple and conflicting objectives are involved in which the fuzzy optimisation approach (El-Halwagi et al., 2006) is adopted as multi-objective optimisation tool for all four assessment frameworks. For the fourth framework, the multi-period optimisation approach is applied together with the multi-objective optimisation approach for the assessment with uncertainty analysis.

(c) Assessment on biodiesel production pathways (as case study) with the application of all developed frameworks: Prior to the assessment, the superstructure diagram is developed, and the alternative production pathways are identified for assessment. From the assessment, the production pathway screening, and optimisation of the pathway are performed.

(d) Recommendation on inherent SHE improvement strategies based on inherent safety principle for the case study of biodiesel production: The recommended strategies are defined according to the individual design stage. It should be taken note that the suggested strategies are served as references for general chemical production pathways.

1.5 Contribution of the Research

The main objective of this thesis focuses on the development of assessment frameworks for chemical production pathways, which are based on multi-objective of inherent SHE and EP. Those mentioned assessment frameworks have been developed, and applied on biodiesel production pathway as a case study. Besides, based on the work in this thesis, there are three key contributions presented, as described as item (a) to (c) below. Besides, general findings in this thesis can also be served as references particularly to the biodiesel manufacturers in Malaysia as more extensive development of biodiesel plant industries is expected very soon (Mukherjee and Sovacool, 2014).

(a) Development of four systematic frameworks for inherent SHE and EP assessment for chemical process design through the application of multi-objective (fuzzy optimisation) and multi-period optimisation approach. As discussed in the previous section, those frameworks are applicable to three process design stages, namely the R&D, preliminary engineering and basic engineering stage, as well as for the uncertainty analysis with the presence of multiple operational periods.

(b) Application of the assessment frameworks on the case study of biodiesel production in order to illustrate the functionality of the frameworks, and identification of the most optimum and sustainable pathway.

(c) Recommendation of inherent SHE improvement strategies on biodiesel production pathway with specific to each stage's early process design through application of ISD principle

Based on the above-mentioned research contributions, as first author, five manuscripts have been prepared. The scopes of those five manuscripts are described as below.

(a) Manuscript 1: Literature review on evolution, production technologies and sustainability assessment for biofuel. This study is aimed to understand the development of biofuel and its relevant assessments.

(b) Manuscript 2, 3 and 4: Development of sustainability assessment frameworks for chemical production pathway during early process design stage of R&D, preliminary engineering and basic engineering stage respectively. Through the developed framework, biodiesel production is assessed as a case study.

(c) Manuscript 5: Uncertainty analysis with the consideration of multiple operational periods. Based on the developed framework, the simplified approach of determining the optimal design variables is elaborated in detail.

As outlined in Table 1.1, three of those manuscripts have been published in Journal with impact factor, while the other two manuscripts have been submitted for review. The details of the journal papers can be referred to Appendix A to C.

Table 1.1: List of manuscripts and the journal acceptance status

No.	Title	Status	Impact Factor*	Journal
1	Review of evolution, technology and sustainability assessments of biofuel production	Published	3.844	Journal of Cleaner Production
2	Sustainability assessment for biodiesel production via fuzzy optimisation during research and development (R&D) stage	Published	1.934	Clean Technologies and Environmental Policy
3	Systematic framework for sustainability assessment on biodiesel production: Preliminary engineering stage	Published	2.587	Industrial and Engineering Chemistry Research
4	Systematic framework for sustainability assessment on biodiesel production: Basic engineering stage	Submitted for review	2.551	Process Safety and Environmental Protection
5	Sustainability assessment on biodiesel production: Uncertainties analysis	Submitted for review	1.054	Journal of Environmental Chemical Engineering

*Based on year 2014 and available in Thomson Reuters Journal Citation Report 2015.

Apart from the journal papers, the scope of Manuscript 1 has been integrated partially into a book chapter and contributed as a second author. This book chapter outlines the principle of inherent safety, which is followed by the latest development of inherent safety and health in biofuel production. The details of the book chapter is listed in Table 1.2.

Table 1.2: List of book chapter

No.	Book Title	Chapter Title	Publisher
1	Process design strategies for biomass conversion systems	Chapter 14 - Overview of safety and health assessment for biofuel production technologies	John Wiley & Sons, Inc

Apart from that, five conference papers (as first author) have been published, as outlined in Table 1.3. The general scopes of those five conference papers are summarised as following, whereas the detailed papers can be referred to Appendix D to H.

Table 1.3: List of conference papers (continued)

No.	Title	Conference
1	Fuzzy optimisation for screening of sustainable chemical reaction pathways	15th Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction (PRES) 2012
2	Review of evolution and sustainability assessment of biofuel production	International Conference on Process Systems Engineering (PSE ASIA) 2013
3	Screening of sustainable biodiesel production pathways during process research and development (R&D) stage using fuzzy optimisation	16th Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction (PRES) 2013
4	Sustainability assessment on biodiesel production during research and development (R&D) stage	Asia Biohydrogen and Biorefinery (ABB) Symposium 2014
5	Sustainability assessment on biodiesel production during preliminary engineering stage through a systematic framework	International Conference on Environment (ICENV) 2015

(a) Conference Paper 1: The methodological approach for screening chemical production pathways in R&D stage was discussed, and the case study based on synthesis of methyl methacrylate (MMA) was presented.

(b) Conference Paper 2: Summarised from Manuscript 1 (literature review).

(c) Conference Paper 3 and 4: Summarised from Manuscript 2 (sustainability assessment during R&D stage).

(d) Conference Paper 5: Summarised from Manuscript 3 (sustainability assessment during preliminary engineering stage).

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