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Identification of Research Trends in Chemical Process Design: A Review

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Abstract : The purpose of the study is to identify the research trends or developmentsin the chemical process design based on the analysis of a literature review for the period 1980-2015.The research problems or limitations or gaps in process design are the key sources for the research developments or research trends to the present world.In this study, we have identified and reported the research trends or developments in the chemical process design.Some of the research developments or trends are: *1) Mitigation of environmental hazards by calculating the environmental potential impacts WAR* (Waste Reduction Algorithm) techniques, *2) Effectively control of process hazards such as higher temperatures and higher pressures by using ASPEN DYNAMICS simulators,3) Waste heat recovery using process integrationwith pinch technology and 4) Zero waste discharge or at least minimise the waste hazards by using WARwith processmodification.*This study will be an attractive and useful for researchers in field of chemical process designto save their research time to investigate the research developments for further work.
Keywords: Process Simulation, process design, environmental pollution control, ASPEN PLUS, WAR, process integration, process intensification, research trends.

1. Introduction

The growth of human civilisation needs the development of chemical process industries and allied sectoracross the world wide today. Distillation process is the crucial role in the separation of highly non-ideal components in chemical process industries. Effective process design could be possible with process simulation particularly in the design and control of distillation process.Process simulation has been applied and studied successfully for various types of distillation process such as reactive distillation (RD), extractive distillation (ED), azeotropic distillation (AZD), wall column distillation (DWC) and pressure swing distillation (PSD) associated with thermally coupled systems.Previous research limitations or problems in process design are the key sources for the research developments or research trends to the present world. Today's research problems will be the future sources for research developments in the process design era. Process simulation era started in the design and control of various distillation process effectively in year 1990 onwards. At the early stage of process design focused on partial control of the process plants with an objective functions of energy savings and minimisation of total annual cost (TAC).However, partial studies have been studied about process safety and waste minimization in chemical process plants during 2005-2010. Moreover, no studies reported the mitigation and control of waste hazards and at the same time driving distillation process profitably during 2000-2015.Improper operations in industrial processes may cause economic loss, harm the environment, or even threaten human health[1,2].It is particularly important to supplement them with an imaginative anticipation of hazards with new technology[3,4].

This paper is provided the previous and recent literature on the chemical process design in the design and control of chemical process industries for the period 1980-2015. In this study, we have identified and reported the research developments or trends in the design of distillation process plants. This study will be an attractive for researchers in the field of chemical process design.

2. Chemical Process Design

2.1. Inherently safer design (ISD)

The safety requirements are extremely serious because most of the chemical process involves critical exothermic reactions at high temperature and high pressure, whose failure may cause catastrophic personal injury, severe air pollution, and tremendous economic loss[1]. Recently, new inherently safer design (ISD) has been introduced to address the risks of hazardous chemicals to human, environment, process plant during design and manufacturing phases of a process. The spirit of which is to mitigate hazards within the process during design phase[5,6].

2.2. Process Simulation

The role and responsibility of chemical engineers are mainly in providing reliable operation, optimization of material and energy consumption in the production and to minimize losses due to accidents[5]. Process simulation methods can be used to design, operate and secure the operations by simulating and evaluating process behaviour under various disturbances. It employs plant-wide dynamic simulations to virtually test the start-up safety by systematically examining plant dynamic behaviours and transient responses of critical parameters with enhanced the safety considerations[3]. Dynamic simulations of chemical processes are widely used to develop effective plant wide control structures and analysis of safety problems in the event of emergency situations[7].

2.3. Steady state and dynamic simulations

Simulation can be broadly classified into two categories, Steady state simulation and dynamic simulation.

2.3.1. Steady state simulation

Steady state simulation is the state of system with independent of time. Chemical plants and various units are operated in a continuous mode, usually under steady conditions. A steady state operation allows us to control the system efficiently and elegantly at a desired set-point. The behaviour and performance of such system is analysed by steady state simulation. Initially process simulation is used to simulate steady state processes. Steady-state models perform a mass and energy balance of a stationary process[8].

2.3.2. Dynamic simulation

Dynamic simulation is the state of system with dependent of time. This finds application in the study of batch operations and other transient phenomena associated with start-up and shut-down of plants. The dynamic mode of operation of plant is sometimes preferred as it can maximize selectivity in a reactor and productivity in a plant[8].

2.3.3. Role of steady state and dynamic simulation in chemical processes industry (CPI)

The goal of a process simulation is to find optimal conditions for an examined process and increase the separation efficiency of process systems[9], includes designing the controls for a new process[10], improving the process design[11] trouble-shooting the performance of an existing process, testing the effectiveness of a new advanced control application[12], and building the business case for the value of process control improvements[13]. Dynamic process modelling plays a vital role in plant design and operation[14].

Modern dynamic simulators are applied and studied for various types of distillation process such as reactive distillation, extractive distillation, and pressure swing distillation associated with thermally coupled system[15-21]. It was found that extractive distillation is economically feasible for various systems compare to others[22-25]. Most of the research work done on extractive distillation process for various systems and revealed that it is easy separation of components and economically good[20, 26-37]. Both Steady state and dynamic simulation have been successfully used in the separation of azeotropes without adding any third component i.e pressure swing distillation (PSD)[23, 35-37]. Total annual cost (TAC) of both energy and capital cost is minimized with use of steady state simulation in the design of distillation wall column process (DWC)[38-41]. Although significant research has been done regarding the steady state design of individual process units like recycle stream systems, reactors, distillation columns, plant wide design of multi-unit processes etc. The literature in extractive distillation has grown rapidly in recent years and steady state simulation is considered in many papers for the design of extractive distillation process[42-62]. A few authors have studied the dynamic behaviour and the control of extractive distillation process[63-65]. Table 1, Illustrates the steady state and dynamic simulations used in the chemical process design for the period 1980-2015.

Table 1.Literature review report on process simulation for the period 1980-2015

Author	Year	Process Simulation	Simulator	Chemical Process type	Objective function
Gilles et al.[15]	1980	Simulation – Control	Not reported	Extractive	N/A
Abu–Eisah et al.[16]	1985	Optimization-Steady state	Not reported	Azeotropic	Energetic
Rovaglio et al.[17]	1990	Simulation-Dynamics	Not reported	Azeotropic	N/A
Tyreus TD *et al.*[66]	1993	Simulation – Control	Not reported	Extractive	N/A
Filho R Maciel et al.[11]	1996	Optimization-Steady state	HYSIM simulator	Reactive	Zero pollution
Dimian AC, et al.[67]	1997	Simulation-Dynamics	Aspen plus & speedup	Recycle	Recycle control
Cao Yi, et al.[68]	1998	Dynamics control	Speedup via aspen technology	Reactive	Comparison of dynamic and original model
Lee D, et al.[10]	2002	Steady state & dynamics Simulation	Aspen Plus 7 & Aspen Dynamics 8	Conventional	Controllability of real plant
Kwo-Liang Wu et al.[69]	2002	Simulation-control	Heuristic approaches	Reactive	Plant wide control
Muhamman A.Al-Arfaj et al.[70]	2002	Simulation-control	Heuristic approaches	Reactive	N/A
Muhamman A.Al-Arfaj et al.[71]	2002	Simulation-control	Heuristic approaches-literature	Reactive	Minimum TAC
Robert K Cox, et al.[13]	2004	Dynamic simulation	TMODS™ package	Overall process	-
Chien I. Lung, *et al.*[14]	2004	Steady state & Dynamics simulation	aspen plus and dynamics	Azeotropic	Temperature control
Luyben WL, et al.[72]	2004	Steady state &dynamics	aspen plus and dynamics	Reactive	Economical
William L.Luyben[22]	2005	Steady state & dynamics simulation	Aspen plus	Reactive	N/A
A.Kanna et al.[33]	2005	Steady state & dynamics simulation	HYSIS	Azeotropic	N/A
Weiyu Xu et al.[52]	2005	Steady state simulation	Aspen plus	Azeotropic	N/A

Sasmita Pradhan et al.[26]	2005	Steady state simulation	JAVA code & Aspen plus	Extractive	N/A
I-Lung Chien et al.[50]	2006	Steady state & dynamics simulation	Aspen plus	Azeotropic	N/A
Lina M.Rueda et al.[32]	2006	Steady state & dynamics simulation	HYSIS/Aspen	Azeotropic	N/A
Krajnc Majda, et al.[73]	2006	Pinch analysis method	Aspen plus 10.1	Conventional	Energy savings
Devrim B.Kayamak et al.[74]	2006	Simulation-dynamics	Aspen plus	Reactive	Temperature control
A.Vincent Orchilles et al.[48]	2007	Experimental	Not reported	Extractive-ILS	N/A
Berenda P.Guedes et al.[34]	2007	Steady state & dynamics simulation	Aspen simulator v11.1	Azeotropic	Reduce energy consumption in real plant
Vincente Gomis et al.[49]	2007	Steady state design	Chemcad V	Azeotropic	N/A
Araujo Antonio, et al.[12]	2008	Steady state and dynamics simulation	Aspen plus and dynamics	Reactive	Comparison of two control models
William L.Luyben[31]	2008	Steady state & dynamics simulation	Aspen plus	Extractive & azeotropic	N/A
William L.Luyben[27]	2008	Steady state & dynamics simulation	Aspen plus	Extractive	N/A
William L.Luyben[23]	2008	Steady state & dynamics simulation	Aspen plus	Extractive & PSD	Capital cost
Devrim B.Kayamak et al.[75]	2008	Steady state-dynamics	Aspen plus	Reactive	Comparative dynamics
Iva stn D.Gil et al.[28]	2009	Steady state simulation	Aspen plus	Extractive	Minimum energy
Roberto Gutierrez-Guerra et al.[30]	2009	Steady state design	Not reported	Extractive	TAC/Co_2 emission
Zheng-Hong Luo, et al.[76]	2009	Simulation-Control	Polymers plus &aspen dynamics	Reactive	N/A
Tokos Hella, et al.[77]	2010	Mathematical based	N/A	Heat exchanger	Energy savings-live plant
M.A.S.S.Ravagnani et al.[29]	2010	Steady state simulation	HYSIS simulator	Extractive	N/A
San-Jang Wang et al.[24]	2010	Steady state design & temperature control	Chemcad/ aspen plus	RD/ED/PSD Thermally	Energy efficiency
Singh	2011	Pinch design method	Aspen hysis,	Heat	Energy savings

Kamel, et al.[78]			energy analyzer	exchanger	
Barreto et al.[21]	2011	Optimization-Dynamics(Stochastic)	Matlab®	Batch Extractive	Profit
LI Shaojun et al.[55]	2011	Steady state-Simulation	Aspen plus	Azeotropic	N/A
Marcella Feitosa et al.[56]	2011	Steady state-Simulation	Aspen plus	Extractive	N/A
Lan-Yi Sun et al.[38]	2011	Steady state -Simulation	Aspen plus	DWC &CHADS	Lowest TAC
Rodolfo Murrieta et al.[25]	2011	Genetic algorithm	Aspen plus	Reactive& Extractive	N/A
William L.Luyben [51]	2012	Steady state -Simulation	Aspen plus	Azeotropic	TAC saving
William L.Luyben [9]	2012	Steady state -dynamics	Aspen plus	Simple	Process Safety
William L.Luyben [7]	2012	Dynamics control	Aspen plus & dynamics	Reactive	Safety process
Younghoon Kim et al.[42]	2012	Optimization-Steady state	Aspen Plus®	Extractive	N/A
Anton A.Kiss et al.[39]	2012	SQP Method	Aspen Plus®	E-DWC	N/A
Mark T.G. et al.[43]	2012	Steady state Simulation	Aspen Plus V7.2	Extractive	Ionic liquids role
Xiong Zou et al.[54]	2012	GAMS-Optimization	Aspen plus	Zeotropic	TAC saving
Anton A.Kiss et al.[40]	2012	SQP- Optimization	Aspen plus	E&A-DWC	Energy saving
Qiaoyi Wang et al.[61]	2012	Simulation -Control	Aspen plus	Extractive	N/A
Gaungzhong Li et al.[57]	2012	Steady state-Simulation	Aspen plus	Extractive	N/A
Manuel Andres Ramos et al.[60]	2013	Optimization-Dynamics(Deterministic)	GAMS/IPOPT	Extractive	Profit
Anton A.Kiss et al.[41]	2013	Steady state-Simulation	Aspen plus	A&E-DWC	N/A
E.Quijada-Maldonado et al.[44]	2013	Steady state-Simulation	Aspen Radfrac	Extractive	Ionic liquids effect
Xiuhui Huang et al.[46]	2013	Steady state-Simulation	Aspen plus	Azeotropic	N/A
Cornelia Pienaar et al.[47]	2013	Steady state-Simulation	Aspen plus	Azeotropic	N/A
William L.Luyben [62]	2013	Steady state -dynamics	Aspen plus	Azeotropic	Economical

Lekan Taofeck Popoola et al.[79]	2013	Design-review	ANN/GA/ Fuzzy	CDU	Error minimal
Kai Cheng et al.[53]	2013	Steady state simulation	Aspen plus	Reactive/ Thermally CD	TAC
Luyben William L. et al.[66]	2013	Steady state&dynamics	Aspen simulations	conventional	Economy
P.Vega et al.[80]	2014	optimization &control methods	review	Overall process	N/A
Nagamalleswara Rao K,et al.[81]	2014	Simulation -Control	Aspen plus	Extractive	Plant wide control
Eda Hosgor et al.[35]	2014	Steady state & Dynamics simulation	Aspen plus	Extractive PSD	Alternative process
William L.Luyben [37]	2014	Steady state -simulation	Aspen plus	Azeotropic PSD	Energy saving
Zhaoyou Zhu et al.[36]	2015	Steady state & Dynamics simulation	Aspen plus	Azeotropic PSD	TAC
Shenfeng Yuan et al.[45]	2015	Steady state-Simulation &experiments	Aspen plus	CED	N/A
Jun Li et al.[58]	2015	Steady state-Simulation	Aspen plus	CED	Reduce energy
William L.Luyben [59]	2015	Steady state -dynamics	Aspen plus	Batch	N/A
Nagamalleswara Rao K, et al.[82]	2015	Steady state-dynamic simulation Pinch analysis	Aspen energy analyser	Reactive	Energy savings

3. Research Trends or Research Developments

3.1. Recent Relevant literature

a) A. Amelio et. al. (2016):This study investigated the energy concept for use in chemical engineering applications, and compares the energy and energy methodology for the production process of biodiesel. The process for biodiesel production was simulated using ASPEN PLUS and ASPEN ENERGY ANALYZERsimulating tools**.** A largest energy losses are identified and integrated with in the process in the reaction process of biodiesel production[83].

b) Nagamalleswara Rao et. al. (2015): studied "Design and Control of Ethyl Acetate Production Process" using ASPEN PLUS and ASPEN ENERGY ANALYZERsimulating tools**.** In this study ethyl acetate production process is designed and studied. A plant wide control structure is developed and demonstrated to provide effective control for large disturbances. The selection of the tray for temperature control is identified and a temperature control loop is designed. Finally process integration studies are performed using ASPEN ENERGY ANALYZER and retrofit studies are performed[84].

c) William L.Luyben (2015): Studied "Aspen Dynamics simulation of a middle-vessel batch distillationprocess" using ASPEN PLUS simulating tool. This study investigated the dynamics of a batch process. The example studied is a middle-vessel batch distillation systemfor separating a ternary mixture.

Alternative control strategies are also discussed by using the large library of control functions to the batch process[85].

d) Nagamalleswara Rao et. al. (2015):Studied "Design and Pinch Analysis of Methyl Acetate Production Process using ASPEN PLUS and ASPEN ENERGY ANALYZER". In this study design and heat integration of methyl acetate production process is discussed. Initially, methyl acetate production process is designed using ASPEN PLUS. Methyl acetate obtained is 99.99% pure. For the developed process plant, pinch analysis is applied using ASPEN ENERGY ANALYZER. Improved heat exchanger networks (HEN) is obtained with retrofit analysis of the process plant. The retrofit design saves the energy of the process by minimizing the operating costs and with less payback period of 0.9 years[86].

e) Nagamalleswara Rao et. al. (2014): Studied "Design and Control of Acetaldehyde Production Process" using ASPEN PLUS simulating tool. This work presented a realistic steady state model and a plant wide control structure for the production of acetaldehyde. Effect of various process parameters on acetaldehyde production is discussed. The purity of the acetaldehyde product is maintained despite the large disturbances present in the process[87].

Table 2: Research trends/developments identified in chemical process design for the period 1980-2015

Duration	Chemical Process Design	Research findings	Limitations
1980-1985	Modelling, simulation & control of the distillation	Introduced 2-AZD	No simulators
1986-1990	Steady state design of AZD	Het.AZC separated.	No simulators
1991-1995	Steady state & dynamic simulation of EXD	Recycle streams Introduced.	Partial use of simulators.
1996-2000	Modelling, simulation & control of RD	Multi-Recycle streams controlled	Partially Pollution control.
2001-2005	Modelling, simulation & control of R-AZD	Minimized the TAC.	Partially plant wide control. No studies on waste heat recovery,
2006-2010	Modelling, simulation & control of R-AZ-EXD	Energy savings, ISD used.	Partially concerns with process safety.
2011-2015	RD, AZD, EXD, (PSD), (DWC)etc.	Process intensification	Environmental & Process Hazards are not controlled. Waste hazards not controlled.

3.2. Today's Research Trends

In this study, we have identified the research developments or research trends in the design of distillation process based on the analysis of broad literature review over process simulation design as described in Table 2. Most of the previous and present process simulation has been applied and studied successfully for various types of distillation process with an objective functions of energy savings and minimization of total annual cost (TAC). However, partial studies have been studied about process safety and waste minimization in chemical process plants during 2005-2010. Moreover, no studies reported the mitigation and control of waste hazards and at the same time driving distillation process profitably during 2000-2015. This study will be certainly useful for researchers in the chemical process design to save their research time to investigate the research developments for further work. Research developments or trends are reported in the distillation process will be an attractive for researches in field of chemical process design.

Previous and present research limitations or problems in process design are the key sources for the research developments or research trends to the present or future research world. The list of research trends or developments are identified and reported here:

- Mitigation of environmental hazards by calculating the environmental potential impacts based on the following parameterswith WAR (Waste Reduction Algorithm) techniques

a. Human Toxicity Potential by Ingestion(HTPI),
b. Human Toxicity Potential by Exposure(HTPE),
c. Aquatic Toxicity Potential(ATP),
d. Terrestrial Toxicity Potential(TTP),
e. Global Warming Potential(GWP),
f. Ozone Depletion Potential(ODP),
g. Smog Formation Potential(PCOP),
h. Acidification Potential(AP)

- Effective control of process hazards such as higher temperatures and higher pressures by using advanced process dynamics simulators like ASPEN DYNAMICS
- Heat integration or waste heat recovery using process integration and advanced pinch technology methods
- Zero waste discharge or at least minimise the waste hazards by using waste reduction algorithms WAR (Waste Reduction Algorithm) with process modification studies forchemical process plants.

This study will be an attractive and useful for researchers in field of chemical process design to save their research time to investigate the research developments for their further work.

4. Conclusion

This paper reported the previous and recent literature on the process simulation used in the design and control of chemical process industries for the period 1980-2015 as shown in Table 1. Research developments or trends have been identified and reported in the chemical process design for the period 1980-2015 as shown in Table 2. Most of the research work done on the plant wide control and dynamic studies with an objective functions of energy savings and profit point of view. A few studies partially concerns with aim of pollution control and safety process design. Moreover, no studies reported the mitigation and control of waste hazards and at the same time driving distillation process profitably during 2000-2015. This study will be certainly useful for researchers in the chemical process design to save their research time to investigate the research developments for further work.

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