KEYNOTE SPEAKER

1. Prof. Akihiko Chiba
   (Institute for Materials Research, Tohoku University, Japan)
2. Assoc. Prof. Dr. Yan Mulyana
   (Tokyo Metropolitan University, Japan)
3. Prof. Dr. Djarwani S. Soejoko
   (University of Indonesia, Depok, Indonesia)
4. Prof. Dr. Hassan Y. Aboul-Enein
   (National Research Centre, Cairo, Egypt)
5. Roy Andreas, Ph.D
   (Jenderal Soedirman University, Purwokerto, Indonesia)

INVITED SPEAKERS

1. Assist. Prof. Dr. Warakorn Limbut
   (Prince of Songkla University, Thailand)
2. Dr. Apon Numnuam
   (Prince of Songkla University, Thailand)
3. Ir. Basril Abbas, M.Si
   (BATAN, Indonesia)
4. Prof. Deni Noviana, Ph.D
   (IPB, Bogor, Indonesia)
5. Pratama Jujur Wibawa, Ph.D
   (Diponegoro University, Semarang, Indonesia),
6. Dr. Mukhammad Asy'ari
   (Diponegoro University, Semarang, Indonesia)
7. Dr. rer.nat. Maulidan Firdaus, M.Sc
   (Sebelas Maret University, Surakarta, Indonesia)
8. Dr.rer.nat. Witri Wahyu Lestari
   (Sebelas Maret University, Surakarta, Indonesia)
9. Uyi Sulaeman, Ph.D
   (Jenderal Soedirman University, Purwokerto, Indonesia)
10. Dr. Hartiwi Diastuti, M.Si
    (Jenderal Soedirman University, Purwokerto, Indonesia)
11. Dr. Jumaeri, M.Si
    (Semarang State University, Indonesia)
12. Dr. Sri Wardani, M.Si.
    (Semarang State University, Indonesia)

REGISTRATION FEE

	Early Bird (up to August 17th, 2016)	Normal (until September 8, 2016)
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• Presenter	100 USD	125 USD
Indonesian		
• Participant		
• Student	550.000 IDR	650.000 IDR
• Non student	600.000 IDR	700.000 IDR
• Presenter	900.000 IDR	1.000.000 IDR
Proceeding (IOP Conference Series:MSE)		1.000.000 IDR
Proceeding Non IOP		200.000 IDR

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IMPORTANT DATES

Abstract Submission (1st)	:	June 30, 2016
Abstract Submission (2nd)	:	July 31, 2016
Abstract Acceptance Notification	:	August 15, 2016
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Full Paper Submission	:	September 7, 2016
Normal Registration	:	September 8, 2016
Conference Days	:	September 15-16, 2016
Manuscript Review Process	:	December 31, 2016
Proceeding Available Online	:	March 2017

PROCEEDING

Submitted full papers will be reviewed and published in:
A periodical publication which is indexes by SCOPUS
(IOP Conference Series:MSE)

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11th Joint Conference on Chemistry 2016

in conjunction with

The 4th Regional Biomaterials Scientific Meeting 2016

15 - 16 September 2016
Horizon Hotel
Purwokerto - Indonesia

"Material Chemistry Development for Future Medicine, Industry, Environmental and Biomaterial Application"

Organized by:
Jenderal Soedirman University (UNSOED)
Diponegoro University (UNDIP)
Sebelas Maret University (UNS)
Semarang State University (UNNES)
Satya Wacana Christian University (UKSW)
Indonesian Biomaterials Society

SECRETARIAT

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Jenderal Soedirman University
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BACKGROUND

The advancement of chemistry, chemical science and engineering research in Indonesia need more acceleration to be in line with the state of the art of world research to so that it can contribute to create a better world to live. The materials and biomaterials field, as example, has been expanding rapidly over the past decade. This growth is due to many factors, including medical needs, new biosynthetic and synthetic chemistries, and new technological innovations. The need to improve tailoring of materials chemistry, control of structure and morphology of materials, and new insight into biological interactions with materials underlies the field, particularly when considering biological interfaces as dynamic environments that can be navigated and utilized in a proactive way.

Scientists who dedicate their research activities to materials and biomaterials pass through the typical dichotomy that often characterizes the basic research. On one side is the wish of exploring new frontiers of chemistry, physics, biology, engineering, medicine, pharmaceutics and all other disciplines to which materials and biomaterials can be applied. The constantly improving scientific knowledge would feed the freedom of attempting new strategies for producing materials with greater tailored and improved characteristics.

The design, synthesis, and modification of novel materials and biomaterials allow for enhanced performance for industrial and environmental related applications. In the meantime, the research and development in the past five years has been increasing, involving researchers from government institutions and academia from many universities all over the world. To support the acceleration and the integration, it is necessary to provide a forum which gathers all national stake holders to build mutual understanding, to share information, resources and roles, and to go with national development direction to the final goal of welfare of the nation and worldwide in general.

PROGRAM CONFERENCE

The 2-days conference (September 15-16, 2016) will consist of plenary lectures and poster session, given by outstanding scientists and whose exceptionally creative work opens up new frontiers for chemistry, chemical sciences and education, engineering, biomaterials science and industrial applications. Both oral and poster presentation will cover the whole topics in Chemistry, Chemical Sciences and Education, Biomaterials Science and Technology.

SCOPE / TOPICS

Topics of the conference include:

- ☑ Theoretical chemistry and environmental chemistry
- ☑ Material synthesis for energy and environment
- ☑ Isolation, purification and modification of molecular biomolecules and their application
- ☑ Design development and validation of analytical methods
- ☑ Synthesis of Hydroxyapatite based on natural resources.
- ☑ Biodegradable materials.
- ☑ Metal, polymer, ceramic and composite as material implant
- ☑ Simulation and modelling of biomaterials
- ☑ Soft tissue biomaterials.
- ☑ Development of In vitro and in vivo method.
- ☑ Biomaterials as wound healing.

THE ORGANIZATION

The 11th Joint Conference on Chemistry 2016 in conjunction with The 4th Regional Biomaterials Scientific Meeting 2016 is organized by Universitas Jenderal Soedirman (UNSOED), Diponegoro University (UNDIP), Sebelas Maret University (UNS), Semarang State University (UNNES), Satya Wacana Christian University (UKSW), Badan Pengkajian dan Penerapan Teknologi (BPPT), Indonesian Biomaterials Society (MBI). This event is also supported by Badan Tenaga Nuklir Nasional (BATAN).

PURPOSE

The purposes of the conference are:

- ☑ to provide a forum for scientific discussion, professional networking, research collaboration, education, and dissemination of scientific research, innovation and industrial products.
- ☑ to increase the quality of research and development in biomaterials science and technology for local, regional and international scientists or academia.
- ☑ to encourage the local and regional young scientists to attend and present their works at the regional/international level of biomaterials conference.

VENUE

The venue of the Conference will be at Horison Hotel, Jl. Dr. Angka, Purwokerto, Jawa Tengah, Indonesia.

11th Joint Conference on Chemistry 2016

in conjunction with

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organized

INTERNATIONAL CONFERENCE

on

"Material Chemistry Development for Future Medicine, Industry, Environmental and Biomaterial Application"

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Conference Dates : September 15 & 16 2016

IOP Conference Series: Materials Science and Engineering

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The Effect of Temperature on the Production of Nitrobenzene

2017 IOP Conf. Ser.: Mater. Sci. Eng. 172 012045

(http://iopscience.iop.org/1757-899X/172/1/012045)

The Effect of Temperature on the Production of Nitrobenzene

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Abstract. Nitrobenzene is a compound derived from benzene and quite fundamental in the petrochemical industry. One of which is in the manufacture of aniline. Aniline has an important role as dyes, synthetic rubber materials, rocket fuels and pharmaceuticals. Nitrobenzene can be synthesized by the nitration reaction of benzene. The purpose of the research is to design synthesis process of nitrobenzene by using Aspen Hysys simulator. The effect of changes in operating condition on nitrobenzene will be investigated. The benefits of the research are to obtain the optimum operating temperature for nitrobenzene production so that the use of utility can be minimized.

1. Introduction

Nitration reaction is important because it is the most general process for the preparation of aromatic nitro compounds. This reaction plays a role in the development of theoretical organic chemistry. It is of interest because of its characteristics as an electrophilic substitution [1]. Nitration of aromatics is a large scale industrial process with global production of about 4-5 million tons of commercially valuable chemicals (nitrobenzene, nitrotoluene, 2,4-dinitrotoluene) per year [2].

Nitrobenzene has been produced commercially since 1856 when Simpson, Maule and Nicholson started operation in England [3]. It was first synthesized in 1834 from benzene and fuming nitric acid. Since then the nitration of aromatic hydrocarbons has been the subject of numerous investigations, however, only a few investigators have determined data which are useful for engineering applications [4].

Nitrobenzene is produced by reacting benzene with a mixture of nitric acid and sulphuric acid at a temperature not exceeding 50°C, to avoid getting more than one nitro group [5]. The mixture is held at this temperature for about half an hour. The sulphuric acid is acting as a catalyst. Yellow oilly nitrobenzene is formed. The reaction is as follows:

$$C_6H_6 + HNO3 \rightarrow C_6H_5NO_2 + H_2O \quad (1)$$

or

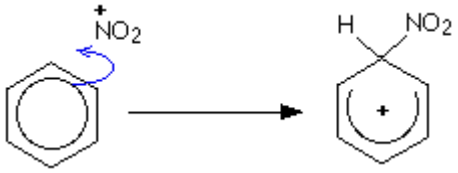
(2)

The electrophile is the nitronium ion or the nitryl cation, which is formed by reaction between nitric acid and sulphuric acid:

$$HNO_3 + 2H_2SO_4 \rightarrow NO_2^+ + 2HSO_4^- + H_3O^+$$

The mechanism of electrophilic substitution are as follows:

Stage 1:



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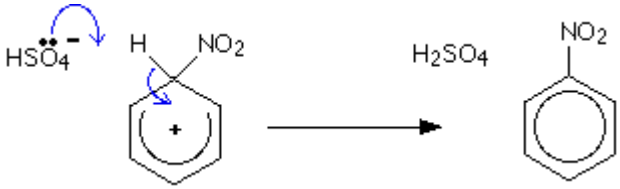
Stage 2:



(4)

Chemical engineering research on nitration process of benzene has achieved many valuable improvements including better energy management of modern nitration plants and various clean nitration approaches focused on dispensing the use of sulphuric acid [6]. The catalyst (sulphuric acid) were costly to recycle and generated environmental problems making nitration of benzene as one of the most hazardous industrial processes. Therefore many researches focuss on the use of other material as catalyst [1,6-8].

Quadros et al [9] constructed a pilot plat for the continuous nitration. The following equations correlate E_a and k_o to sulphuric acid weight fraction S:

$$E_a = (-283.88S + 263.37) \times 1000 \quad (5)$$

$$k_o = \exp\left[166.64S^2 - 254.36S + 113.79\right] \quad (6)$$

By the availability of process simulator like Aspen Hysis, process design can be done more easily, since the derivation of the mathematical model for the process were difficult. The aim of this research is to simulate the nitration reaction of benzene at various temperature. The scope is mainly for the nitration reactor. The percentage of conversion will be shown over temperature for a specific loading duty in the reactor.

2. Method

In this study, Aspen Hysis were used to simulate process flow diagram for nitrobenzene production. Figure 1 shows the methodology framework.

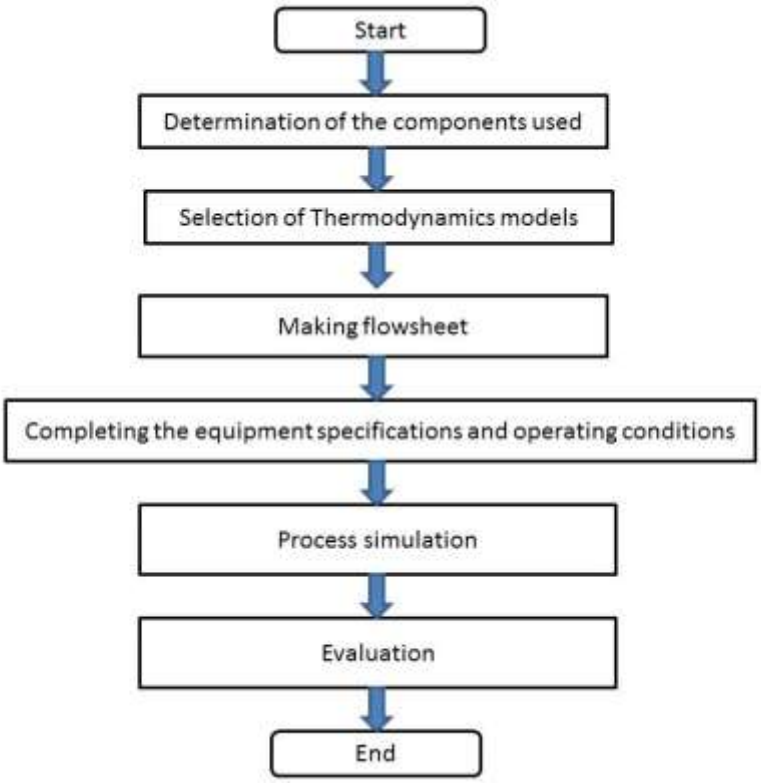


Figure 1. Methodology framework

Isothermal CSTR is used, and Table 1 shows the operating condition of the simulated system. Process Flow Diagram of the production system of nitrobenzene is shown in Figure 2.

Table 1. Operating conditions

Operating conditions	**Values**	
Mass flow benzene	1000	kg/h
Concentration of benzene	89.99	%
Mass flow of nitric acid	1173	kg/h
Concentration of nitric acid	65	%
Mass flow of sulphuric acid	2561	kg/h
Concentration of sulphuric acid	89	%
Reactor diameter	1.221	m
Reactor height	1.832	m
Pressure	101.3	kPa
Liquid volume in the reactor	80	%

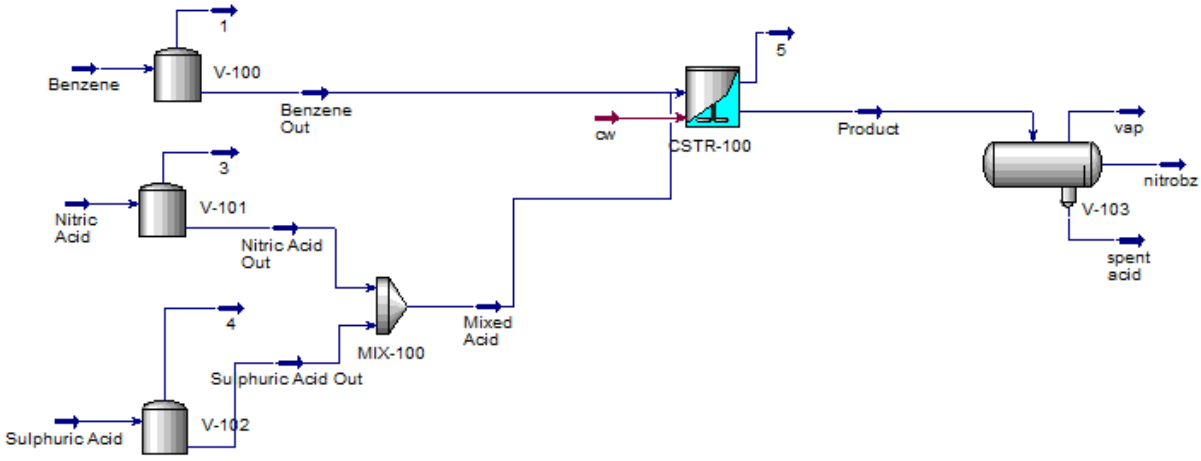


Figure 2. Simplified Nitration Process Flow Diagram

3. Results and Discussion

Figure 3 shows plot of benzene conversion as a function of temperature.

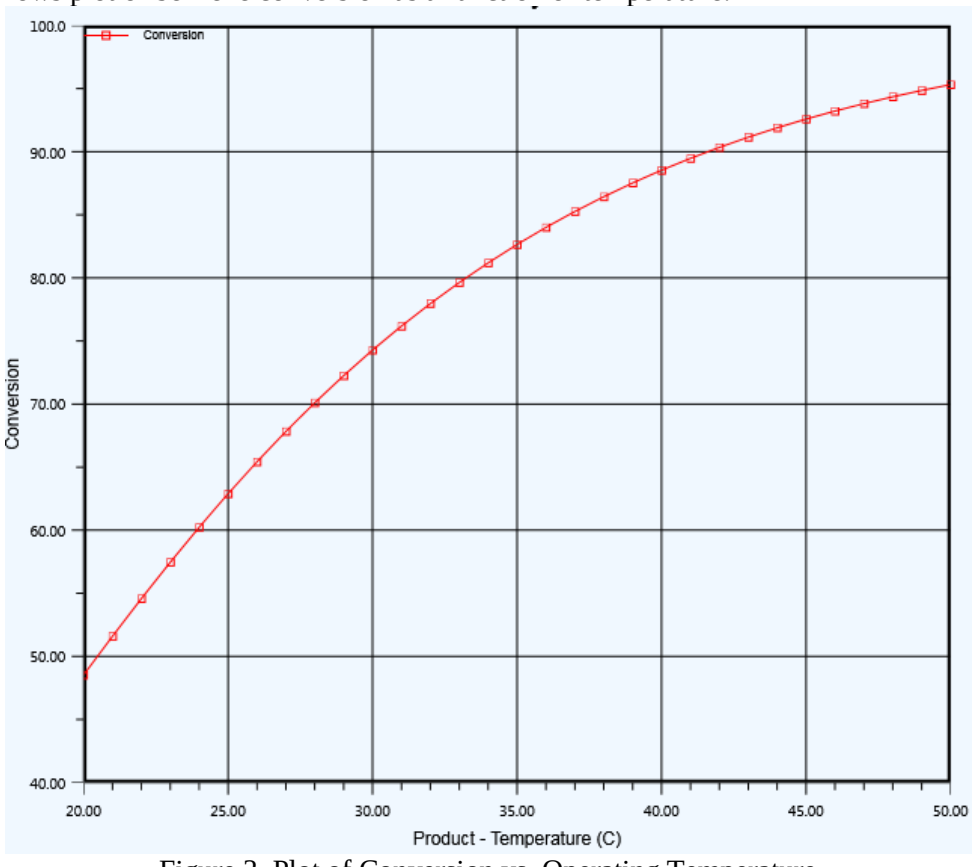


Figure 3. Plot of Conversion vs. Operating Temperature

These results were obtained while the physical properties of products were calculated automatically in Hysis as shown in Table 2. Properties of other streams can also be found.

It can be seen from Figure 3 that the conversion can reach 95.32% at 50°C and as low as 48.54% at 20°C. These conversions were obtained based on the loading given. The most crucial point in the simulation is the value of E_a and k_o used. Here, the parameter values provided by Quadros (2005) were used.

Table 2. Physical properties of the product

Name	Values	
Molecular Weight	52.11	
Molar Density	26.82	Kmole/m^3
Mass Density	1398	kg/m^3
Act. Volume Flow	3.387	M^3/h
Mass Enthalpy	-7169	kJ/kg
Mass Entropyc	0.8385	kJ/kg°C
Heat Capacity	100.5	kJ/kmole.°C
Mass Heat Capacity	1.929	kJ/kg.°C
Viscosity	2.309	cP
Thermal Conductivity	0.3902	W/mK
Viscosity Index	9.394	

4. Conclusions

Simulations have been conducted for the nitrification reaction of benzene at various temperatures by using Aspen Hysis software. The results are useful for process and energy optimization in the petrochemical industries. The possibility to explore the influence of residence time (hence the dimension of the reactor), ratio of sulphuric acid to nitric acid, and ratio of benzene to mix acid are open for further research.

5. References

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