PROCESS ROUTE SELECTION FOR INHERENTLY SAFER DESIGN BASED ON CONSEQUENCES ANALYSIS

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Mardhati Zainal Abidin[1] and Mohd Sobri Takriff [2]
[1,2] Department of Chemical and Process Engineering,
Faculty of Engineering and Built Environment
Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor
E-mail: [2]sobri@eng.ukm.my

ABSTRACT

Increased public awareness of safety and stringent requirements by the authority has led to the consideration of inherent safety in the design of processing plants. Inherent safety approach ensures the safety of a process by eliminating or minimizing the hazard from a process rather than implementing engineering control to manage the hazard. The opportunity for such an approach is the highest at the early stages of the design. In addition, the effectiveness of the hazard reduction measures by employing the inherent safety principles must also be assessed at the early stages of the process design so that the design engineers can make an informed decision on the process design. This paper describes the methodology for integrating the assessment of fire hazards with process simulation at the early stage of process design. The methodology was illustrated by comparing process routes for dimethyl ether (DME) production plant using substitution principle. The process design simulation was carried out in iCON® process simulator, while assessment of the fire hazards was carry out in Excel® using a seamless two-way data transfer facility that is available in iCON®. The results from the case study showed that the potential consequences of a fire can be reduced by employing the substitution principle of inherent safety. The methodology that has been developed in this work enables simultaneous technical and safety assessments at the early stages of the process design.

Keywords: *Consequence Analysis, Inherent Safety, Process Design, Simulation, Synthesis Gas*

1.0 INTRODUCTION

Optimisation of process design according to economics, operational, environmental and safety requirement is the origin to an economical, safer and environmentally benign process throughout the whole lifetime of the plant. In addition, due to general society expectation, company image and economic reasons, safety of a processing plant should achieve a common acceptable level [1]. For instance in Malaysia, the Occupational Safety and Health act 1994 [2] states that, it is the responsibility of the company to ensure safety and well being of its workers and the general public. The rapid growth in the use of hazardous chemicals in the industry has brought significant risk to both workers and general public, whose well being could be endangered at any time by accident involving these chemicals. For the above reasons, the inherent safety principles since its introduction by Trevor Kletz in has gained popularity as an approach for safety improvement in the design of processing plants[3]. Inherent safety strives to enhance process safety by introducing fundamentally safer characteristics into process design as well as selecting and designing the process to eliminate or minimise hazards rather than accepting the hazards and implementing add-on systems to control it [4]. One of the principles of inherent safety is substitution. This can be accomplish by using alternative chemistry that allows the use of less hazardous materials or less severe processing conditions [5,6].

The opportunity for incorporating inherent safety features decreases exponentially from conceptual design stage to operational stage as illustrated in Figure 1 [5]. Thus, it is best to apply inherent safety principles and to assess their effectiveness in improving process safety at early stages of process design. In order to apply inherent safety principles successfully at the early stages of process design, a systematic assessment methods and tools must be available to assist the implementation. One possible option is to integrate safety assessment with the process simulation. Numerous process simulation software are used by process design engineers such as Aspen Plus® [7], HYSYS® [8] and the locally developed iCON® [9]. Each software has its own strength and unique features. However, to integrate safety assessment with process simulation, the latter should have features that allow for interfacing with other readily available and accessible softwares.

Most existing safety assessment methods focus on existing plants or later phases of process design, where most of the process engineering details are known [1]. For example, the conventional risk assessment is typically done at the detailed engineering stage. Hence, the effects of changes in process synthesis route and operating conditions on the potential consequence and risk level cannot be studied in a timely manner during the design stages [10]. At the process simulation stage, adequate data are available for safety assessment using the *consequence analysis technique*. However, a methodology that automatically extracts data from process simulation and carries out the consequence analysis is currently not available. Without an automated methodology, the consequence analysis will be a tedious process, requires manual extraction of data and is very time consuming. Such a situation makes the effort to assess the effectiveness of inherently safer design at process simulation stage an unattractive option when the designs engineers are under pressure to meet the scheduled target. This paper discusses the integration of consequence analysis with process simulation at preliminary design stage. The method enables process design decision making takes into account the potential consequence of the process accidents by considering the selection of process synthesis route and process conditions.

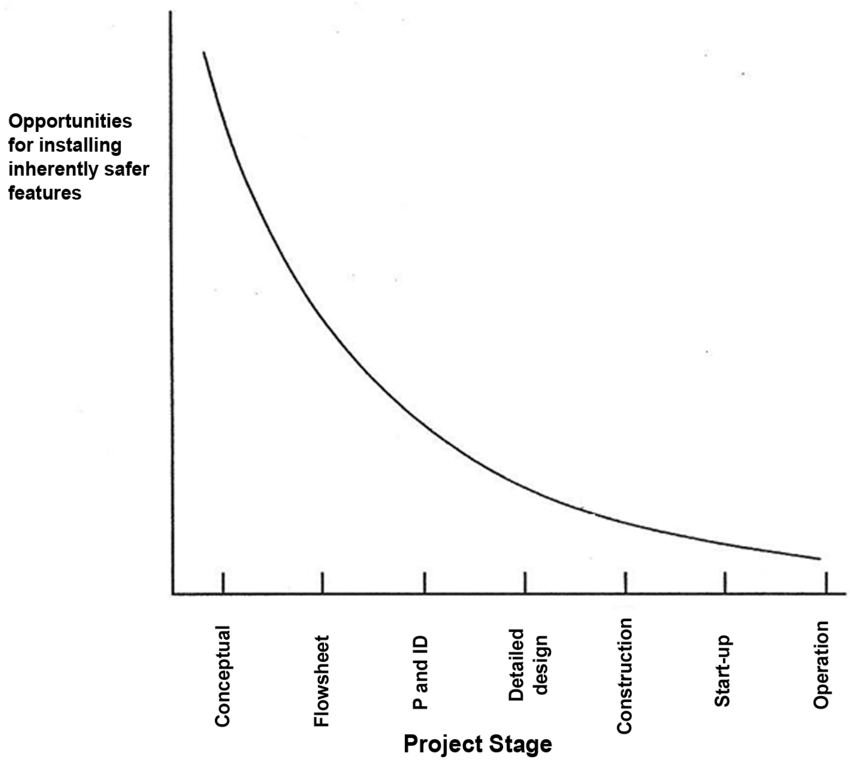

Figure 1: Opportunity for implementing inherent safety features [5]

2.0 INTEGRATING CONSEQUENCE ANALYSIS WITH PROCESS SIMULATION

Figure 2 shows the framework for integrating consequence analysis with process simulation in iCON®. The first step is to simulate a base design case using iCON® process simulator that was later used as a basis for comparison. A unit operation was then selected for assessment based on consequence analysis. The Excel® worksheet is then call upon using the worksheet option that is provided in iCON®. The required input variables from process simulation were identified and the necessary equations for consequence analysis for fire effects were then set-up in the worksheet. All major equipment in the plant should be considered and consequence analysis was done for all process routes that were considered before selecting the best process route for detailed design.

iCON® provides a seamless two way data transfer with Excel® allowing a user to link Excel® spreadsheets directly to iCON®. Any changes that is made either on iCON® or through Excel® is immediately captured and new set of process simulation and consequence analysis calculations are triggered automatically in the other software. Such features allows a user to manipulate any process parameter from either iCON® or Excel® to meet the required safety criteria. The available process data from simulation at early stage of process design are adequate for consequence analysis purposes. Data needed for consequence analysis such as process conditions, physical properties, flammability data and others were transferred from the process simulator to the Excel® worksheet using the import/export features available on iCON®. These data are used as input in modeling the potential consequence of various unwanted events such as fires, and in generating useful data such as thermal

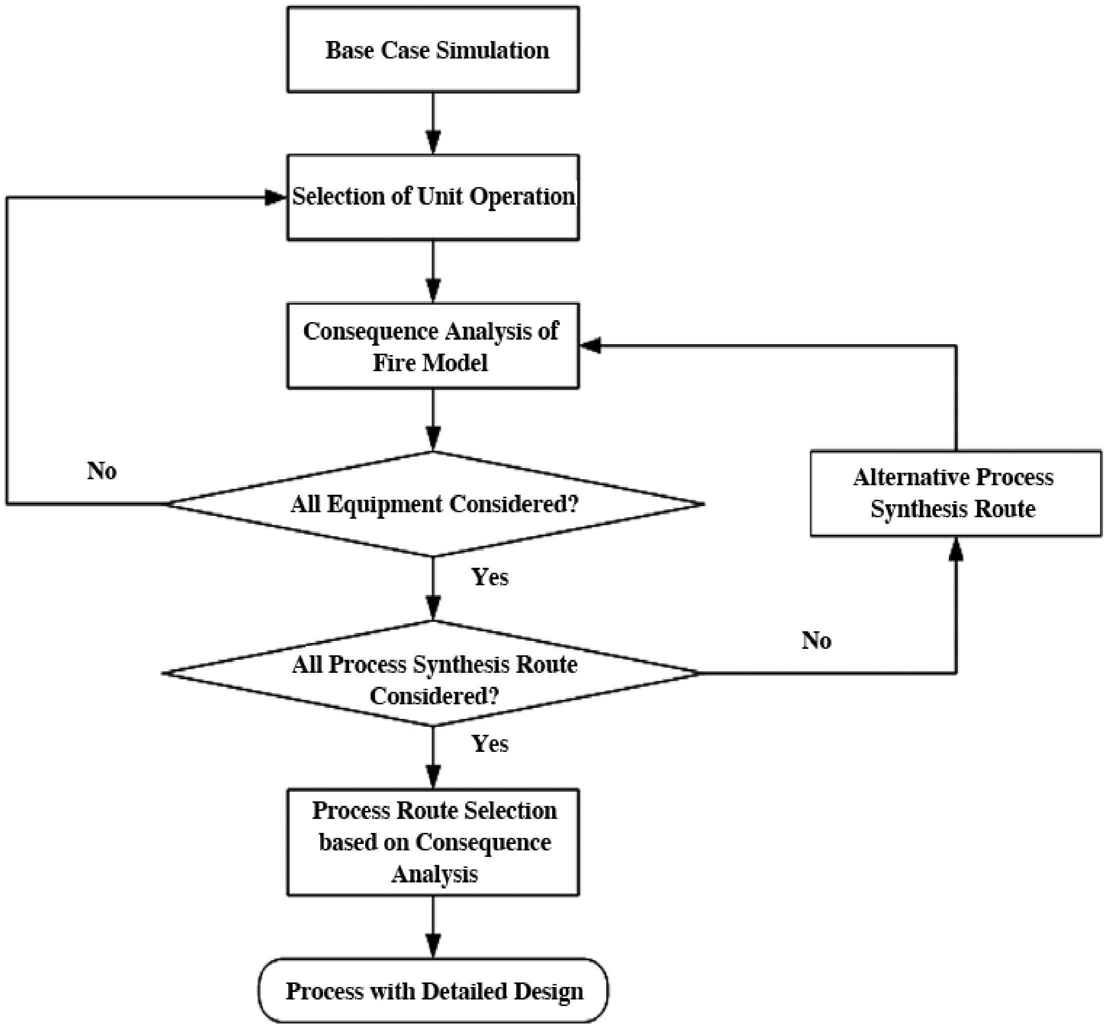

Figure 2: Consequence analysis approach for fire analysis in inherently safer design

radiation intensity versus distance. The consequences onto various receptors such as human is then determined using the vulnerability model [11]. The results of assessment can then be used as indicators on the potential consequence of accidents in the plant, which provides a basis for selecting process synthesis route or the operating conditions that will meet the safety requirements.

3.0 CASE STUDY: FIRE MODEL IN A DIMETHYL ETHER PLANT

The assessment of two alternative process synthesis routes for dimethyl ether (DME) production was selected as a case study. In this case study, the substitution approach can be accomplished by using alternative process chemistry with different catalyst that allows process to be carried out at less severe processing conditions and less severe potential consequence of accidents at the plant. In the first route, DME was synthesis from syngas using Cu-based catalyst and γ-Al2O3 catalyst and the stoichiometric equations are presented in equations (1) through (3) [12].

$$CO + 2H_2 \rightarrow CH_3OH \quad (1)$$

$$2CH_3OH \rightarrow CH_3COH_3 + H_2O \quad (2)$$

$$CO + H_2O \rightarrow CO_2 + H_2 \quad (3)$$

In the second route, DME was produced from the dehydration of methanol over acid-zeolite catalyst [13] as shown in equation (4).

$$2CH_3OH \rightarrow (CH_3)_2\ O + H_2O \quad (4)$$

The simulation flowsheet for the two DME plants are presented in Figures 3 and 4, respectively. The occurrence of a major jet fire at the reactor and absorber as well as pool fire at the distillation columns were selected as illustrations in using consequence analysis as a basis for process route selection. The DME plant employing the syngas reaction was used as a base case design. The simulation flowsheet for the base case design with excel® worksheet interface is shown in Figure 5.

A jet fire occurs when there is a loss of containment of pressurized flammable gas that is immediately ignited. Detailed description on modeling the consequence of a jet fire may be obtained from the AIChE Guideline [11]. The main equations and brief description in modelling a jet fire are presented in Table 1. For estimation of potential consequences due to a jet fire, several input data are needed, *e.g.* release diameter for calculation of mass flow rate of flammable gas, combustion reaction for flammable gas leak, height above ground and receptor distance from the flame. The release diameter used in this work was 100 mm, as recommended by the AIChE Guideline [11].

A pool fire occurs when there is a loss of containment of liquid phase of flammable substance that is immediately ignited [10]. A pool fire model for the estimation of incident thermal radiation is shown in Table 2. Detailed description on the modeling of the consequence of a pool fire may be obtained from the AIChE Guideline [11]. The main equations with a brief description for the modeling of a jet fire are presented in Table 2. For estimation of potential consequences due to a pool fire, several input data are needed, *e.g.* release diameter for the calculation of mass flow rate of flammable substance, heat of combustion, heat of vaporisation, *etc*.

The damaging effect of fire model is from its thermal radiation and the consequence that is experienced by a receptor, depending upon the intensity of thermal radiation and the exposure duration. Longer exposure durations, even at a lower thermal radiation level, can produce serious physiological effects. The consequence of thermal radiation onto a human receptor was estimated using the probit analysis [11,14]. The probit variable, *Y*, for heat radiation lethality is given by Equation (20) and the conversion from probit value to percentage of fatalities is given by Equation (21), respectively.

$$Y = 1.49 + 2.56\ in\left(\frac{t1^{4/3}}{10^4}\right) \tag{20}$$

$$P = 50\left[1 + \frac{Y-5}{|Y-5|}\, erf\left(\frac{|Y-5|}{\sqrt{2}}\right)\right] \tag{21}$$

where *Y* is the probit variable (unitless), *t* is the duration of exposure (s), *I* is the thermal radiation intensity (W/m2), *P* is fatalities percentage (%) and "*erf*" is the error function.

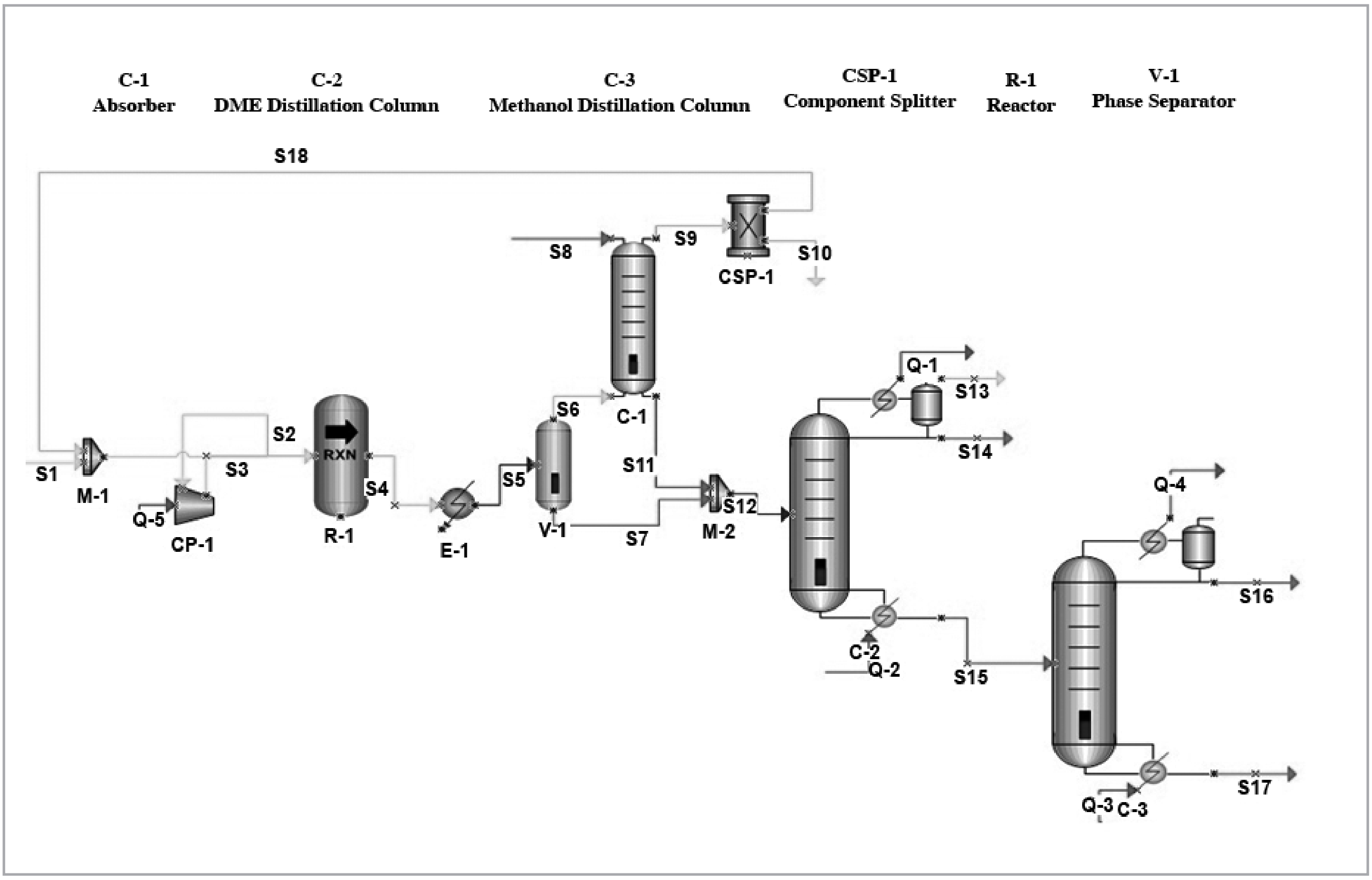

Figure 3: Preliminary simulation flowsheet for the production of DME from syngas

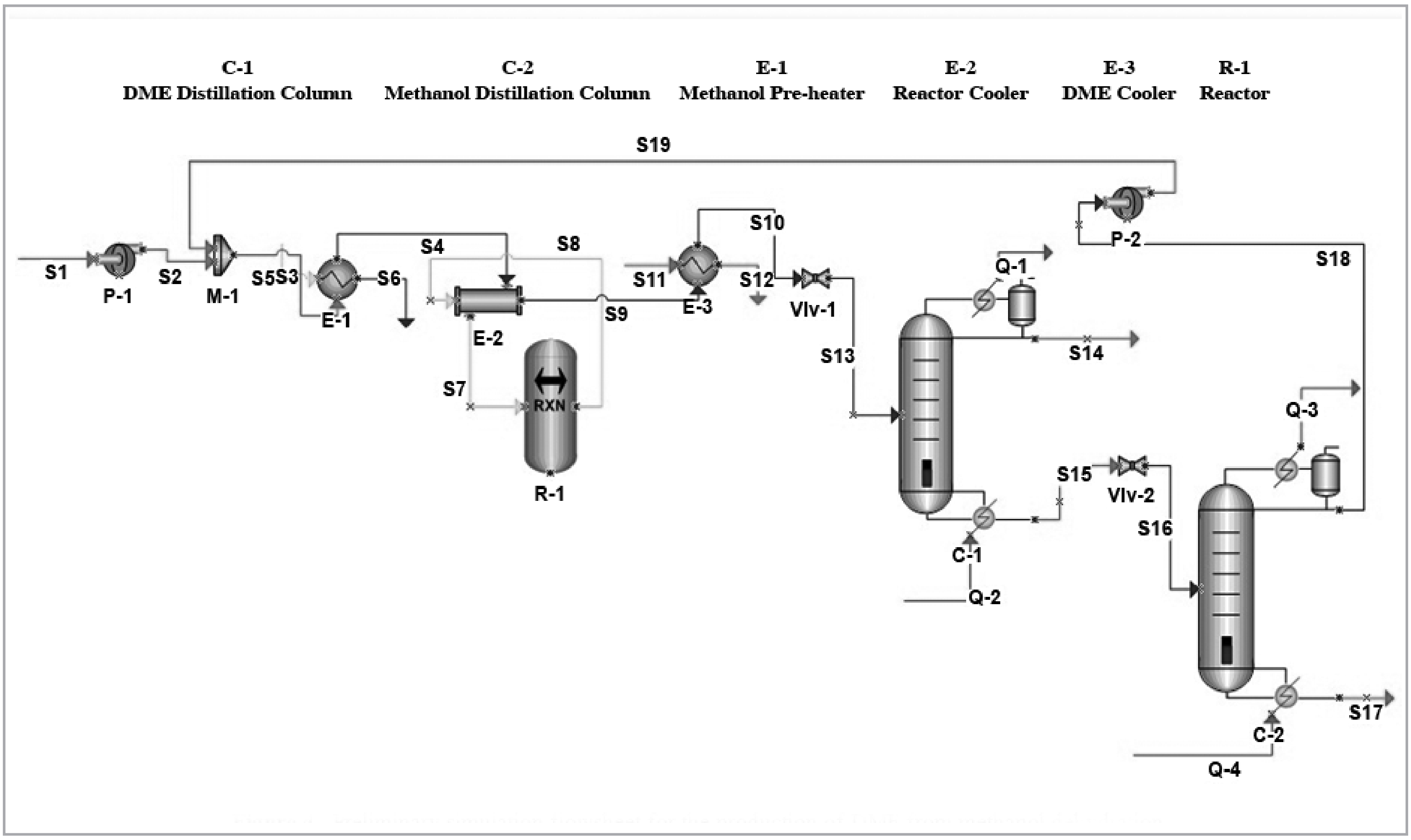

Figure 4: Preliminary simulation flowsheet for the production of DME from methanol dehydration

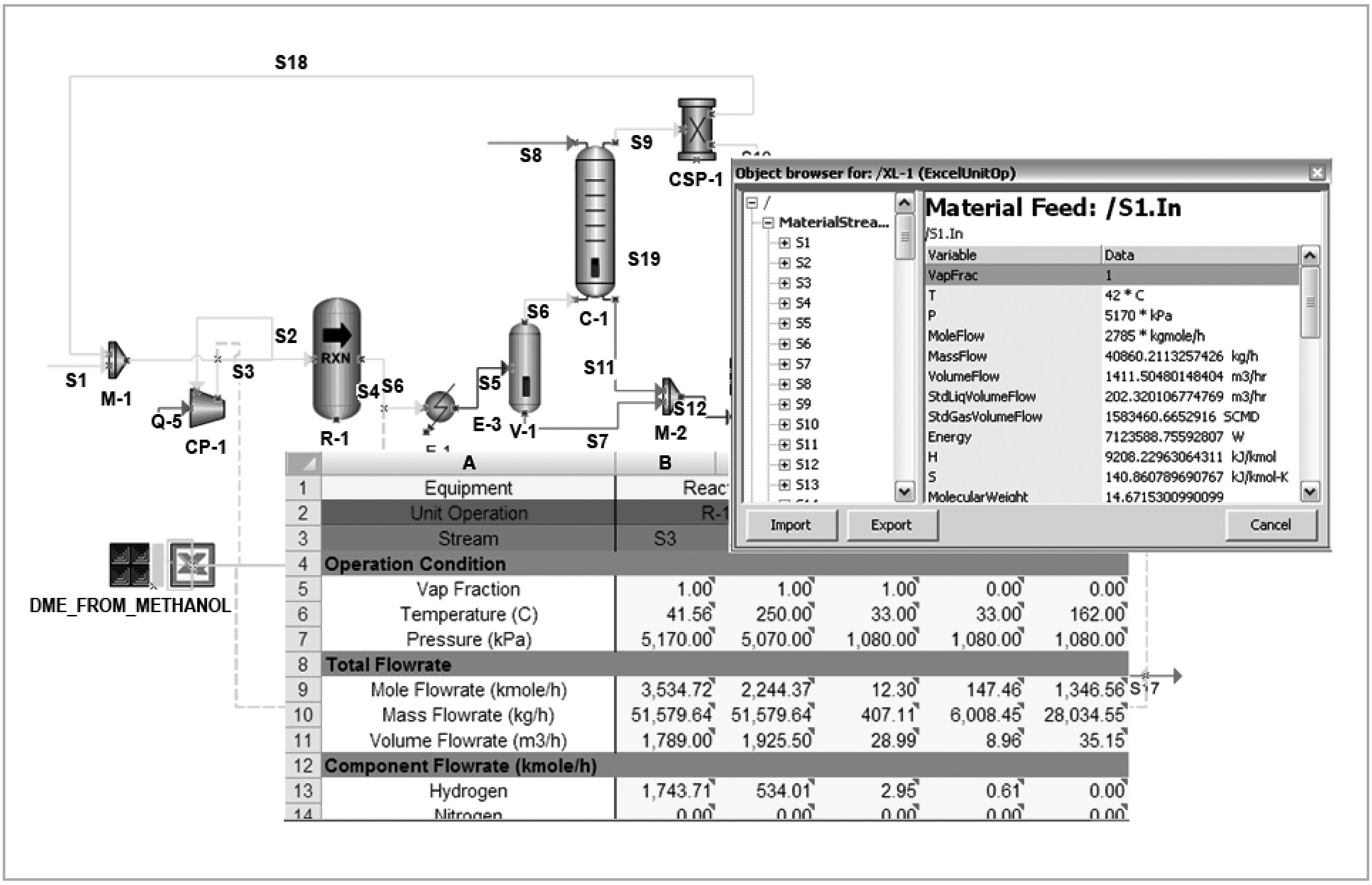

Figure 5: Simulation flowsheet for base case design with Excel® interface

Table 1: Consequence model for jet fire [10]

Item	Description
Source Model	$$\boldsymbol{m}_{choked} = C_D A P_1 \sqrt{\frac{k g_c M}{R_g T_1}\left(\frac{2}{K+1}\right)^{(k+1)(k-1)}} \quad (5)$$ ***m*** is mass flow rate of gas through the hole (kg/s), A is area of the hole (m^2), C_D is discharge coefficient (unitless), g_c is the gravitational constant (kg m/s²), P_1 is pressure upstream of the hole (*Pa*), k is heat capacity ratio, C_p/C_v (unitless), M is molecular weight of the gas (kg/kgmole), R_g is ideal gas constant (Pam³/kgmole.K) and T_1 is initial upstream temperature of the gas (K).The equation representing mass flow rate for sonic, or choked case. The pressure ratio required to achieve choking is given by; $$\frac{P_{choked}}{P_1}\left(\frac{2}{K+1}\right)^{k/(k-1)} \quad (6)$$ Equation (2) demonstrates that choking conditions are readily produced – an upstream pressure of greater than 13.1 psig for an ideal gas is adequate to produce choked flow for a gas escaping to atmospheric. For real gases, pressure of 20psig is typically used.
Jet Fire Model	$$\frac{L}{d_j} = \frac{15}{C_T}\sqrt{\frac{M_a}{M_f}} \quad (7)$$ ***L*** is the length of the visible turbulent flame measured from the break point (m), *dj* is the diameter of the jet, that is, the physical diameter of the nozzle (m), C_T is fuel mole fraction concentration in a stoichiometric fuel-air mixture (unitless), M_a and M_f are molecular weight of air and fuel (kg/kgmole). $$F_p = \frac{1}{4\pi\pi^2} \quad (8)$$ F_p is the point source of view factor (m^{-2}), x is the distance from the point source to the target (m) which can be obtained using the hypoteneous of a right triangle and π is a mathematical constant = 3.142 (unitless). $$E_r = \tau_a \eta \boldsymbol{m} \Delta H_c F_p \quad (9)$$ where *Er* is the radiant flux at the receiver (kW/m²), τ_a is the atmospheric transmissivity (unitless), η is the fraction of total energy convert ed to radiation (unitless), *m* mass is flow rate of the gas through the hole (kg/s), ΔH_c is energy of combustion of the fuel (kJ/kg) and F_p is the point source of view factor (m^{-2}).

Table 2: Consequence model for pool fire [10]

Item	Description
Source Model	$$\frac{g_c (P_2 - P_1)}{\rho} + g(z_2 - z_1) + \frac{1}{2} v_2^2 + g_c \sum e_f = 0 \quad (10)$$ where ρ is the density of the fluid (kg/m³), g_c is the gravitational constant (kg m/s²), P_1 is the pressure upstream of the hole (Pa), P_2 is the pressure downstream of the hole (Pa), g is the acceleration of gravity (9.81 m/s²), z_1 and z_2 is initial and final reference point (m), v_2 is fluid velocity (m/s) and $\sum e_f$ is the frictional loss term given by equation (11); $$\sum e_f = \sum K_f \frac{v_2^2}{2g_c} \quad (11)$$ where $\sum e_f$ is the frictional loss term(m/kg), $\sum K_f$ is the excess head loss due to the pipe or pipe fitting (unitless), v_2 is fluid velocity (m/s) and gc is the gravitational constant (kg m/s²). $$\boldsymbol{m} = \rho v_2 A \quad (12)$$ where ***m*** is the liquid discharge rate (kg/s), ***A*** is the area of the hole (m²), v^2 is fluid velocity (m/s) and ρ is the density of the fluid (kg/m³).

Pool Fire Model	$y_{max} = 1.27 \times 10^{-6} \dfrac{\Delta H_c}{\Delta H^*}$ (13) where y_{max} is the vertical rate of liquid decrease (m/s), ΔH_c is the net heat of combustion (kJ/kg) and ΔH^* is the modified heat of vaporization (kJ/kg) at the boiling point of the liquid given by equation (12) $\Delta H^* = \Delta H_v + \int_{T_a}^{T_{BP}} C_p dT$ (14) where T_{BP} is the boiling point temperature of the liquid (K), T_a is the ambient temperature (K) and C_p is the heat capacity of the liquid (kJ/kg.K). $m_B = y_{max} \times \rho$ (15) where m_B is the mass burning rate (kg/m^2 s) and ρ is the liquid density (kg/m^3) $\dfrac{H}{D} = 42 \left(\dfrac{m_B}{\rho_a \sqrt{gD}}\right)^{0.61}$ (16) where H is the visible flame height (m), D is the equivalent pool diameter (m), m_B is the mass burning rate (kg/m^{2}s), ρ_a is the air density (1.2 kg/m^3), g is the acceleration of gravity (9.81 m/s^2). $D_{max} = 2 \sqrt{\dfrac{V_L}{\pi y}}$ (17) where D_{max} is the equilibrium diameter of the pool (m), V_L is the volumetric liquid spill rate (m^3/s), and y is the liquid burning rate (m/s) and π is a mathematical constant = 3.142 (unitless). $F_p = \dfrac{1}{4\pi\pi^2}$ (18) F_p is the point source of view factor (m^{-2}), x is the distance from the point source to the target (m) which can be obtained using the hypoteneous of a right triangle and π is a mathematical constant = 3.142 (unitless). $E_r = \tau_a \eta m_B \Delta H_c A F_p$ (19) where E_r is the radiant flux at the receiver (kW/m^2), τ_a is the atmospheric transmissivity (unitless), η is the fraction of total energy converted to radiation (unitless), m_B is the mass burning rate (kg/m2s), ΔH_c is energy of combustion of the fuel (kJ/kg), A is the total pool area and F_p is the point source of view factor (m^{-2}).

For simplification purpose, from this point forward, production of dimethyl ether from syngas referred as process route 1 and production of dimethyl ether from methanol referred as process route 2. The results of the consequence analysis are presented in Tables 3 and 4, whilst Table 5 [14] presents various levels of damages as a result of exposure to thermal radiation. The results of the consequences analysis of a jet fire that has the potential to occur at the two alternative process routes along with the potential fatal consequences onto human receptors are presented in Table 3. Based on Table 3, the impact zone as well as the potential for fatal consequence as a result of the occurrence of jet fire at reactor was higher for process route 1. As shown, zero fatality is expected at a distance more than 50 m for process route 1. On the other hand, zero fatality is expected at a distance more than 25 m for process route 2. In addition, the distance of radiation limit that can cause pain to workers who are unable to reach for a cover in 20 seconds are more than 65 m and 35 m for process routes 1 and 2, respectively. The results of consequence analysis of a jet fire that has the potential to occur at the absorber at the plant using process route 1 shows that zero fatality is expected at a distance almost more than 37 m. Based on Table 5, the distance of radiation limit effects from potential jet fire at absorber that can cause pain to worker who are unable to reach for a cover in 20 seconds is more than 55 m.

The potential effects of thermal radiation from pool fire at distillation columns at the two alternatives routes are presented in Table 4a and b. Based on the results, thermal radiation effect from pool fire at DME distillation in both routes will cause zero fatality at more than 25m distance. However, longer exposure durations can produce serious physiological effects to the receiver. The impact zones for the methanol distillation columns in both routes are much smaller compare to the DME distillation column. Based on the assessment results for main components as presented in Tables 3 and 4, process route 2 is safer compared to process 1, thus process route 2 should be selected for the subsequent stages of the design of the DME production plant.

Table 3: Consequence of a jet fire at several distances for both process routes

Process Route	Process Route 1				Process Route 2	
Equipment	*Reactor*		*Absorber*		*Reactor*	
Distance (m)	*Flux (kW/m²)*	*Fatalities Percentage (%)*	*Flux (kW/m²)*	*Fatalities Percentage (%)*	*Flux (kW/m²)*	*Fatalities Percentage (%)*
25	32.78	76.39	29.25	62.95	8.66	0.01
27	28.95	61.60	21.95	25.76	7.64	0.00
30	24.26	37.88	16.90	6.14	6.41	0.00
33	20.55	19.08	13.32	0.93	5.43	0.00
35	18.50	10.88	10.73	0.10	4.89	0.00
37	16.73	5.74	8.79	0.01	4.42	0.00
40	14.49	1.94	7.32	0.00	3.83	0.00
45	11.61	0.24	6.18	0.00	3.07	0.00
50	9.48	0.02	5.28	0.00	2.50	0.00
55	7.88	0.00	4.56	0.00	2.08	0.00
60	6.63	0.00	3.97	0.00	1.75	0.00
65	5.66	0.00	3.49	0.00	1.49	0.00

Table 4a: Consequence of a pool fire at several distances for both process routes

Process Route	Process Route 1		Process Route 2	
Equipment	*DME Distillation Column*			
Distance (m)	*Flux (kW/m²)*	*Fatalities Percentage (kW/m²)*	*Flux (kW/m²)*	*Fatalities Percentage*
5	15.56	3.41	15.70	3.64
10	13.55	1.08	13.64	1.15
15	11.89	0.31	11.95	0.32
20	10.51	0.08	10.55	0.08
25	9.35	0.02	9.37	0.02
30	8.36	0.00	8.37	0.00
35	7.52	0.00	7.52	0.00
40	6.80	0.00	6.79	0.00
45	6.17	0.00	6.16	0.00
50	5.63	0.00	5.61	0.00
55	5.15	0.00	5.13	0.00

Table 4b: Consequence of a pool fire at several distances for both process routes

Process Route	**Process Route 1**		**Process Route 2**	
Equipment	***Methanol Distillation Column***			
Distance (m)	***Flux (kW/m²)***	***Fatalities Percentage (kW/m²)***	***Flux (kW/m²)***	***Fatalities Percentage***
5	13.65	1.16	13.61	1.13
10	11.76	0.27	11.72	0.26
15	10.21	0.06	10.18	0.05
20	7.02	0.00	6.99	0.00
25	7.90	0.00	7.87	0.00
30	7.02	0.00	6.99	0.00
35	6.27	0.00	6.25	0.00
40	5.64	0.00	5.61	0.00
45	5.09	0.00	5.07	0.00
50	4.62	0.00	4.60	0.00
55	4.21	0.00	4.19	0.00

Table 5: Thermal radiation limit [14]

Thermal Intensity (kW/m²)	**Exposure Limit**
37.5	Intensity at which damage is caused to process equipment
15.6	Intensity on structures where operators are unlikely to be performing and where shelter is available.
9.5	Intensity at design flare release at locations to which people have access and where exposure would be limited to a few seconds for escape
6.3	Intensity in areas where emergency actions lasting up to one minutes may be required without shielding but with protective clothing
4.5	Intensity sufficient to cause pain to personnel unable to reach for covers in 20 seconds, though blistering of skin (first degree burn) unlikely
1.6	Intensity insufficient to cause discomfort for long term exposure

4.0 DISCUSSION

The methodology that has been developed in this work links and automates the consequence analysis of fire hazards at process simulation stage using a standard process simulator and readily available Microsoft Excel® software. It enables the assessment on the selection of process synthesis route based on the potential impact of process accidents in addition to technical and economical criteria. The framework that has been presented in Figure 2 can be extended further to include other possible incident outcomes such as explosion and dispersion of toxic gas for a more comprehensive assessment on the selected process route.

The above case study illustrated the implementation of the methodology that has been developed in this work.

It allows for assessment of the effectiveness of the implementation of the inherent safety at the process simulation stage. The results of the consequence modeling of fire can be a useful input in the management decision making process. By knowing the thermal radiation vs. distance, the plant layout of a new plant can be designed such that the spacing between unit operations satisfy the exposure limit and adequate safe distance is provided for evacuation purpose. For modification or expansion of an existing plant, the information on thermal radiation vs. distance is very useful to determine the location of the new unit operations so that the necessary spacing distances are fulfilled.

5.0 CONCLUSION

A tool that integrates the consequence analysis of fire hazards with process simulation was successfully developed and demonstrated. It automatically extracts the required data from the process simulator to carry out the consequence analysis and generate useful data such as thermal radiation versus distance as well as consequences onto various receptors. The tool can be used to carry out safety assessment on process route selection based on inherent safety principles. With simultaneous technical and safety assessments are done at early stage of the process design, the process designers are provided with better information to make an informed decision on the process design.

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PROFILES

MARDHATI ZAINAL ABIDIN
Mardhati Zainal Abidin received her Bachelor of Engineering in Chemical Engineering from University Kebangsaan Malaysiain 2008. She is currently a Master student in area of process safety at the Department of Chemical and Process Engineering, Faculty of Engineering and Built Environment, UKM.

DR MOHD SOBRI TAKRIFF
Dr Mohd Sobri Takriff is a Professor and a Deputy Dean at the Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia. He received his PhD from the University of Arkansas in 1996. His research interest include fluid mechanics, multiphase flow, process safety and bioprocesses