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An optimization approach to the integration of inherently safer design and process scheduling

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This work introduces an optimization-based approach to the simultaneous consideration of process safety and process scheduling during the design phase. Expected variations in production schedule and associated environmental constraints are included early enough in the design phase. Additionally, safety metrics are used in screening and selecting design alternatives. The Dow Fire and Explosion Index is used as the safety-evaluation metric. An optimization formulation is developed to account for potential design and scheduling options while incorporating safety and environmental objectives. The proposed approach optimizes the process by establishing Pareto curves that demonstrate the tradeoff between the safety metrics and the economic objectives of the process. A case study on NO_x removal in a refinery is solved to illustrate the applicability of the devised procedure.

1. Introduction

The fluctuations in market demands for various products and availability of raw materials require adaptation in production schemes. Process scheduling is one of the most effective approaches to adjusting the type and quantity of products in response to the changes in market conditions. For instance, oil refineries must continuously adjust the product slate to account for seasonal changes in product demand (e.g., gasoline, diesel, heating oils, etc.). Therefore, it is beneficial to include process scheduling expectations in the design and retrofitting activities. In addition to the technical, economic, and environmental objectives of design, it is also imperative to consider process safety metrics for appropriate management of hazards. Unfortunately in some occurrences, lack of knowledge, technology, or implementation of process safety has led to tragic incidents. Examples are the Flixborough incident with 28 fatalities (Crowl & Louvar, 2002), the Bhopal incident with more than 2000 fatalities (Crowl & Louvar, 2002), the Pasadena-Texas explosion with 23 fatalities (Crowl & Louvar, 2002), and the more recent Texas City-refinery explosion, which cost the lives of 15 people are several regrettable examples. In addition to multiple fatalities and injuries, the consequences included capital loss, lawsuits, decreased stock price, ruined negative impact on image/brand, etc.

In order to understand what had happened, what to learn from those incidents and how to achieve future improvements, it is very important to comprehend the term hazard. Adapted from the Center for Chemical Process Safety (CCPS), hazard is defined as physical or chemical characteristic that has the potential for causing harm to people, the environment, or property (Crowl, 1996). It is an intrinsic and basic property of the material, situation, or conditions. For example, under the right conditions, 10,000 lbs of propane hold the same amount of energy, which could be released by 28 tons of TNT. This energy is inherent to propane and cannot be eliminated or changed. The release of that energy will lead to an incident.

There are various ways of accounting for process safety in design. While it may be impossible to completely eliminating risk, there is a significant need to develop systematic methodologies and strategies to manage risks. One of the strategies is to apply the concept of inherently safer design and to combine it with process design and optimization during the early stages of design where the degrees of freedom in process modification are still high (Heikkila, 1999). While several previous research efforts have considered integrating inherently safer design into process design and optimization, much less attention has been paid to the cases involving operational changes and process schedules (Edward & Lawrence, 1993).

The objective of this work is to introduce a procedure for the integration of inherently safer design techniques with process scheduling. Expected variations in production scheduling are included early enough in the design phase. Additionally, safety

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metrics are used in screening and selecting design alternatives. Safety level is measured by quantifying the process hazards using the Dow Fire and Explosion Index (F&EI) methodology. Tradeoffs are established between the safety metrics of the process and other process objectives such as the economic performance of the process. The following sections provide an overview of two important subjects: (a) inherently safer design and (b) Dow F&EI.

1.1. Inherently safer designs

The term "inherently safer design" started appearing in safety discussion after Trevor Kletz introduced this concept as an identifiable element of process safety in one of his most famous phrases "What You Don't Have Can't Leak". Inherently safer design infers the elimination of hazards as much as possible out of a chemical or physical process permanently as opposed to using layers of protection. There are four primary principles of inherently safer design concept proposed by Kletz (1991):

1. Intensification—to reduce the risk of chemicals by reducing the inventories of hazardous materials.
2. Substitution—to use less hazardous materials in the process.
3. Attenuation—to operate the process at more moderate/less dangerous process conditions (e.g., pressure, temperature, flow rate, etc.).
4. Limitation of effects—to undertake design changes subject to the hazards constraints and limits.

The key advantage of inherently safer design is that it provides a broad framework for undertaking design and operating changes. Nonetheless, it is worth noting a couple of disadvantages. While the concept will result in lower hazards and lower requirement for providing layers of protection, it also affects the production rate. Therefore, it is a challenge for engineers to establish tradeoffs between the technical and economic objectives of the design and inherent safety considerations (Khan & Amyotte, 2003). Additionally, there is a need to systematically generate alternatives for intensification, substitution, and attenuation. Therefore, inherently safer design must be supported by process synthesis and analysis tools.

1.2. Dow F&EI

The Dow F&EI is the most widely used hazard index and has been revised six times since 1967. The latest edition (7th edition), which was published in 1994, is employed in this work. The AIChE (1994) describes F&EI as the "quantitative measurements which are based on historical data, energy potential of the materials under evaluation, and the extent to which loss prevention practices are currently applied (AIChE, 1994)". The Dow F&EI is valuable as a guide to decide whether it is necessary for process designers to consider other less hazardous materials and/or other process routes (Etowa, Amyotte, Pegg, & Khan, 2002). Moreover, F&EI helps engineers to be aware of the hazards in each process unit while making important decisions in reducing the severity and/or the probability of the potential incident. The Dow F&EI relates process hazards to process information (i.e., process conditions, materials, type of equipment, and other characteristics of the process) in terms of "penalties" and how they impact the process hazard. Therefore, it is important to exercise careful judgment to address the "worst case" which means only the most hazardous material in the evaluated process are assessed at a time in a specific operational state (i.e., start up, shut down, and normal operation). For example, when a process unit has hazards posed by three different flammable liquids, the F&EI evaluation must be determined based on all flammable liquids. Then, the highest F&EI among the three evaluations is used as the worst case and is considered as the characteristic hazard of the process. This is due to the fact that while the worst case might not be the first event during the incident, any initiating event may lead to conditions whereby the worst case may happen. This concept helps the designers and decision makers to prepare for the worst case (Khan, Sadiq, & Amyotte, 2003). The details of procedures, guidelines, and equations to determine the penalties and the method is provided in *Dow's Fire and Explosion Hazard Classification Guide* 7th Edition which was published in 1994 by American Institute of Chemical Engineers (AIChE). The Dow F&EI requires the following documents (AIChE, 1994):

1. Plot of the plant/process and/or process flow sheet.
2. Replacement cost data for the installed process equipment under study.
3. Fire and Explosion Index Hazard Classification Guide, 7th Edition.
4. Fire and Explosion Index, Loss Control Credit Factors, Process Unit Analysis.
5. Summary, and Manufacturing Unit Risk Analysis Summary Form.

The method starts with the selection the process unit to be evaluated. The process unit that could pose a significant impact in a potential incident should be overlooked. Therefore, these important factors must be considered when selecting the process units under evaluation (AIChE, 1994):

- Chemical energy potential (material factor).
- Quantity of hazardous material.
- Business interruption and capital density (dollars per ft^2).
- Operating pressure and temperature.
- History of fire and explosion incident related to the same type of process unit.
- The importance of the process unit to the whole process.

The Dow F&EI has two major components, Process Unit Hazards Factor (F_3) and Material Factor (MF). F_3 consists of General Process Hazards (F_1) and Special Process Hazards (F_2). AIChE (1994) defines those terms as the following:

- Material factor is the intrinsic rate of potential energy release caused by fire or explosion produced by combustion or chemical reaction F_3 consists of General Process Hazards (F_1) and Special Process Hazards (F_2).
- General process hazard items have historically played an important role in determining the magnitude of potential incidents, and are applicable to most process conditions.
- Special process hazards are the factors that play an important role in increasing the probability of a potential incident and comprise of the specific process condition that historically contribute to the major causes of fire and explosion incidents.

The Dow F&EI is determined by Eqs. (1) and (2) (AIChE, 1994):

$$F_3 = F_1 \times F_2 \tag{1}$$

$$\text{F\&EI} = \text{MF} \times F_3 \tag{2}$$

More information on the Dow F&EI and safety metrics can be found in literature (AIChE, 1994; Etowa et al., 2002; Khan et al., 2003; Mansfield & Cassidy, 1994; Suardin, Sam Mannan, & El-Halwagi, 2007).

Suardin et al. (2007) integrated inherently safer design concept into process design and optimization using well-accepted hazard identification method. The integration was conducted at the early design stages where it is most effective since there are typically numerous degrees of freedom for making changes.

As stated earlier that the objective of this work is to introduce a procedure for the integration of inherently safer design techniques with environmental objectives and process scheduling. Expected variations in production scheduling are included early enough in the design phase. Additionally, safety metrics are used in screening and selecting design alternatives. Safety level is measured by quantifying the hazards of the process using the Dow F&EI. An optimization approach is developed to account for potential design and scheduling options while incorporating safety and environmental objectives. The proposed approach will optimize the process by establishing a pareto curve that demonstrates the tradeoff between the inherently safer design and various production and operation scheduling.

2. Problem statement

The problem to be addressed by this work is stated as follows: Given a continuous process with:

- A set of unit operations $U = \{u|u = 1,2,\ldots,N_u\}$. Each process unit, u, has a set of input streams $\mathrm{INPUT}_u = \{i_u|i_u = 1,2,\ldots,N_u^{\mathrm{in}}\}$ and a set of output streams $\mathrm{OUTPUT}_u = = \{j_u|j_u = 1,2,\ldots,N_u^{\mathrm{out}}\}$. An input stream, i_u, has a flowrate, F_{i_u}, and the composition of component q, $X_{i_u,q}$, while an output stream, j_u, has a flowrate, G_{j_u}, and the composition of component q, $Y_{j_u,q}$.
- A set of environmental discharges for the process: $\mathrm{WASTES} = \{w|w$ is a waste stream leaving the process and is subject to environmental regulations$\}$.
- A set of environmental regulations governing the composition and/or load of the pollutants leaving the plant, i.e.

$$Z_{w,q} \leqslant Z_{w,q}^{\mathrm{env}} \tag{3}$$

  and

$$W_w Z_{w,q} \leqslant \mathrm{Load}_{w_u q}^{\mathrm{env}} \tag{4}$$

  where $Z_{w,q}$ is the composition of the qth pollutant in the wth waste stream and W_w is the flowrate of the wth waste stream.
- A set of candidate environmental technologies (environmental management units: "EMUs"): $\mathrm{EMU} = \{v|v = N_u+1,\ N_u+2,\ldots,N_u+N_v\}$ that may be added to the process to reduce environmental impact and comply with environmental regulations of the process.
- Safety metrics that is used to evaluate various design options to control the wastes to comply with the environmental regulations. The safety metrics designate each EMU options with respect to safety by safety index. The value of the safety index provides the design another dimension to consider simultaneously with the scheduling of process operation, choice of EMU and process safety. F&EI is used to quantify the safety metrics of the process where the expected schedules have designated values of F&EI based on operation mode and design of the process.
- A given decision-making time horizon (t_{h}). Within this horizon, the variations in the market conditions are anticipated and expressed in terms of time-dependent changes in quantities and prices of supply (e.g., feedstocks, utilities, etc.) and demand (e.g., products and byproducts).

It is desired to develop a systematic procedure that can determine production schedules, process modifications, and EMUs selection and design so as to maximize the process profit. On the other hand, this procedure goes along simultaneously with consideration of changes in process safety. The final decisions related to process scheduling, design, process modifications, EMUs selection and design is linked with inherently safer design simultaneously to have the proper tradeoff between all multi-objectives mentioned above.

3. Approach

To simplify the problem, the following assumptions are introduced:

- The decision-making time horizon is discretized into N_t periods leading to a set of operating periods: $\mathrm{PERIODS} = \{t|t = 1,2,\ldots,N_t\}$. Within each time period, the process operates in steady-state mode. Also, it is only allowed to have intra-period integration (i.e., no streams are stored, integrated, and exchanged over more than one period). In selecting the number and duration of the periods, one has to strike proper balance between capturing the market variations, significance to the process, and computational efforts.
- Process modifications will be limited to two alternatives:
  - o Manipulation of certain design and operating variables for each unit within permissible ranges, i.e.,

$$d_u^{\min} \leqslant d_u \leqslant d_u^{\max} \tag{5}$$

    and

$$o_u^{\min} \leqslant o_u \leqslant o_u^{\max} \quad \forall u. \tag{6}$$

    This assumption implies that the design of the current process is flexible enough to produce any of the anticipated production schedules and that there is no economic incentive to add a process unit or reroute process streams.
  - o Addition of new EMUs (whose number, design, and placement will be determined as part of the solution procedure).

3.1. Structural representation

In order to embed potential configurations of interest, a source-sink structural representation of the problem is adopted. Outputs from process units are split into fractions and assigned to inputs of the EMUs. Each EMU discharges several outputs. An output from the EMU is split and distributed into fractions; some of which are discharged as wastes while the others return back to the process to be assigned to process inputs. The flows from process units to EMUs and from EMUs to wastes and back to the process are unknown and to be determined as part of the solution. Fig. 1 provides a schematic of the structural representation.

Now, we proceed with the modeling aspects. The mass balance equation for unit u during period t is given by

$$\sum_{j_u} G_{j_u,t} = \sum_{i_u} F_{i_u,t} \quad \forall u,t \tag{7}$$

and the qth component balance for unit u during period t is expressed as

$$\sum_{j_u} G_{j_u,t} Y_{j_u,q,t} = \sum_{i_u} (F_{i_u,t} X_{i_u,q,t} + \mathrm{Net\_Gen}_{u,q,t}) \quad \forall q,u,t \tag{8}$$

where the additional index, t, in the flowrates and compositions refers to the time period over which these flowrates and compositions are considered. Additionally, the performance model for unit u at period t is expressed as by a set of algebraic

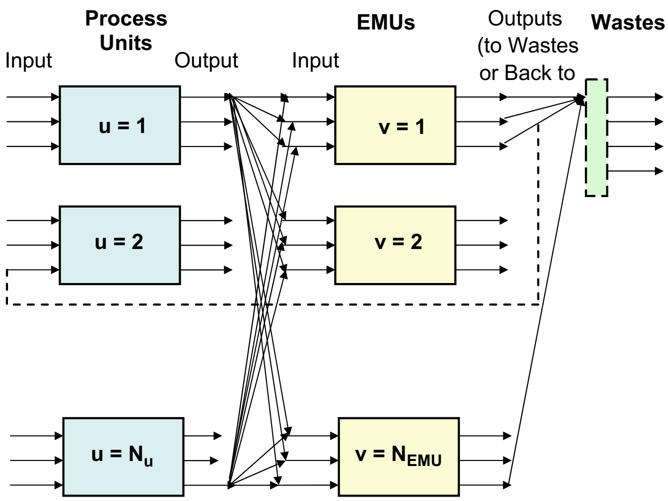

Fig. 1. Structural representation of the problem.

equations represented by

$$(G_{j_u,t}, Y_{j_u,q,t} : j_u = 1,2,\ldots,N_u^{\text{out}} \text{ and } q)$$
$$= f_u(F_{i_u,t}, X_{i_u,q,t} : i_u = 1,2,\ldots,N_u^{\text{in}} \text{ and } q, d_{u,t}, o_{u,t}) \quad (9)$$

Let the flowrate assigned from source j_u to destination i_v during period t be referred to as g_{j_u,i_v}. The flowrate from the j_uth source goes to other units, to EMUs, and to final product streams. Therefore, the material balance for the splitting of source j_u is given by

$$G_{j_u,t} = \sum_u \sum_{i_u} g_{j_u,i_u,t+} \sum_v \sum_{i_v} g_{j_u,i_v,t+} \sum_p P_{j_u,p,t} \quad \forall u, j_u, t \quad (10)$$

where $p_{j_u,p,t}$ is the flowrate assigned from j_u to the pth product stream.

The flowrate of the pth product in period t is described by

$$P_{p,t} = \sum_u \sum_j p_{j_u,p,t} \quad \forall p, t \quad (11)$$

Then, for the mixing of the split flowrate before the i_vth input to the vth EMU, the material balance and the qth component balance during period t are given by

$$F_{i_v,t} = \sum_u \sum_{j_u} g_{j_u,i_b} \quad \forall v, i_v, t \quad (12)$$

$$F_{i_v,t} X_{i_v,q,t} = \sum_u \sum_{j_u} g_{j_u,i_b} Y_{j_u,q,t} \quad \forall v, i_v, q, t \quad (13)$$

The mass balance equation for EMU, v, during period t is given by

$$\sum_{j_v} G_{j_v,t} = \sum_{i_v} F_{i_v,t} \quad \forall v, t \quad (14)$$

The qth component balance for EMU, v, during period t is expressed as

$$\sum_{j_u} G_{j_u,t} Y_{j_v,q,t} = \sum_{i_v} (F_{i_v,t} X_{i_v,q,t} + \text{Net\_Gen}_{v,q,t}) \quad \forall q, v, t \quad (15)$$

and the unit performance equation for the vth EMU is expressed as

$$(G_{j_v,t}, Y_{j_v,q,t} : j_v = 1,2,\ldots,N_v^{\text{out}} \text{ and } q = 1,2,\ldots N_{\text{Components}})$$
$$= f_v(F_{i_v,t}, X_{i_v,q,t} : i_v = 1,2,\ldots,N_v^{\text{in}} \text{ and}$$
$$q = 1,2,\ldots,N_{\text{Components}}, d_{v,t}, o_{v,t}) \quad \forall v, i_v, q, t \quad (16)$$

There are N_w waste streams leaving the process. Each output stream, j_v, from an EMU unit is split into several flowrates; some are assigned to waste outlets and some are recycled back to the process to enter process units. The flowrate assigned to the wth waste stream is referred to as $w_{j_v,w,t}$ and the flowrate recycled back to the process to the i_uth input of the uth unit is described by $r_{j_v,i_u,t}$. Therefore, the material balance for the splitting of the j_vth stream is given by

$$G_{j_v,t} = \sum_w w_{j_v,w,t} + \sum_u \sum_{i_u} r_{j_v,i_u,t} \quad \forall v, j_v, t \quad (17)$$

The flowrate of the wth waste stream during the tth period is given by

$$W_{w,t} = \sum_v \sum_{j_v} w_{j_v,w,t} \quad \forall w, t \quad (18)$$

and the qth component material balance for the wth waste stream is given by

$$W_{w,t} Z_{w,q,t} = \sum_v \sum_{j_v} w_{j_v,w,t} Y_{j_v,q,t} \quad \forall w, q, t \quad (19)$$

The environmental regulations for the wth waste stream and the qth pollutant are described by

$$Z_{w,q,t} \leqslant Z_{w,q,t}^{\text{env}} \quad (20)$$

and

$$W_{w,t} Z_{w,q,t} \leqslant \text{Load}_{w,q,t}^{\text{env}} \quad (21)$$

The design and operating constraints for the process units and the EMUs are:

$$d_u^{\min} \leqslant d_{u,t} \leqslant d_u^{\max} \quad (22)$$

$$d_v^{\min} \leqslant d_{v,t} \leqslant d_v^{\max} \quad (23)$$

$$o_u^{\min} \leqslant o_{u,t} \leqslant o_u^{\max} \quad (24)$$

and

$$o_v^{\min} \leqslant o_{v,t} \leqslant o_v^{\max} \quad (25)$$

The product demand and composition constraints are expressed as

$$P_{p,t} \leqslant P_{p,t}^{\text{Demand}} \quad (26)$$

The flowrate and composition constraints for the i_uth input to the process unit are given by

$$F_{i_u}^{\min} \leqslant F_{i_u,t} \leqslant F_{i_v}^{\max} \quad (27)$$

and

$$X_{i_u,q}^{\min} \leqslant X_{i_u,q,t} \leqslant X_{i_u,q}^{\max} \quad (28)$$

The flowrate and composition constraints for the i_vth input to the vth EMU are given by

$$F_{i_v}^{\min} \leqslant F_{i_v,t} \leqslant F_{i_v}^{\max} \quad (29)$$

and

$$X_{i_v,q}^{\min} \leqslant X_{i_v,q,t} \leqslant X_{i_v,q}^{\max} \quad (30)$$

The objective function is given by

$$\text{Maximize gross profit} = \sum_t \sum_p C_{p,t}^{\text{product}} P_{p,t} - \sum_t \text{POC}_t - \text{TAC}^{\text{EMU}} \quad (31)$$

where $C_{p,t}^{\text{product}}$ is the unit selling price of product p during period t, POC_t represents the plant operating cost (e.g., feedstocks, utilities, etc.) during period t, and the term TAC^{EMU} is the total annualized cost of the environmental management system which is defined as the sum of the annualized fixed costs (AFC) and the environmental annual operating cost (EOC) and is expressed as

$$\mathrm{TAC}^{\mathrm{EMU}} = \sum_{v} I_v\,\mathrm{AFC}_v + \sum_{t}\sum_{v} \mathrm{EOC}_{v,t} \tag{32}$$

where I_v is a binary integer variable designating the presence or absence of the vth EMU and is determined through the following constraint:

$$\sum_{i_v} F_{i_v,t} \leqslant F_v^U\, I_v \quad \forall t \tag{33}$$

where $F_v{}^U$ is an upper bound on the allowable flowrate to unit v. When the flowrate entering unit v is positive, the value of I_v is forced to be one. Otherwise, it takes the value of zero.

The foregoing expressions constitute the mathematical program for the problem. It is a mixed-integer nonlinear program (MINLP), which can be solved to identify the optimal scheduling, process modifications, and selection as well as design of the EMUs.

On the other hand, F&EI is used to quantify the safety metrics of the process. In this work, F&EI is the measurement of inherently safer design of the process with respect to the various scheduling alternatives that provide environmental impact minimization. The calculations and related procedures of F&EI were introduced earlier. Fig. 2 illustrates the procedure of simultaneous inherently safer design and process scheduling. First, a process model is developed in the form of path equations that characterize process performance in terms of the targeted design and operating variables. Next, the optimization formulation is developed as described by Eqs. (7)–(33). The optimization is carried out for the process and the EMUs to get a number of alternative solutions

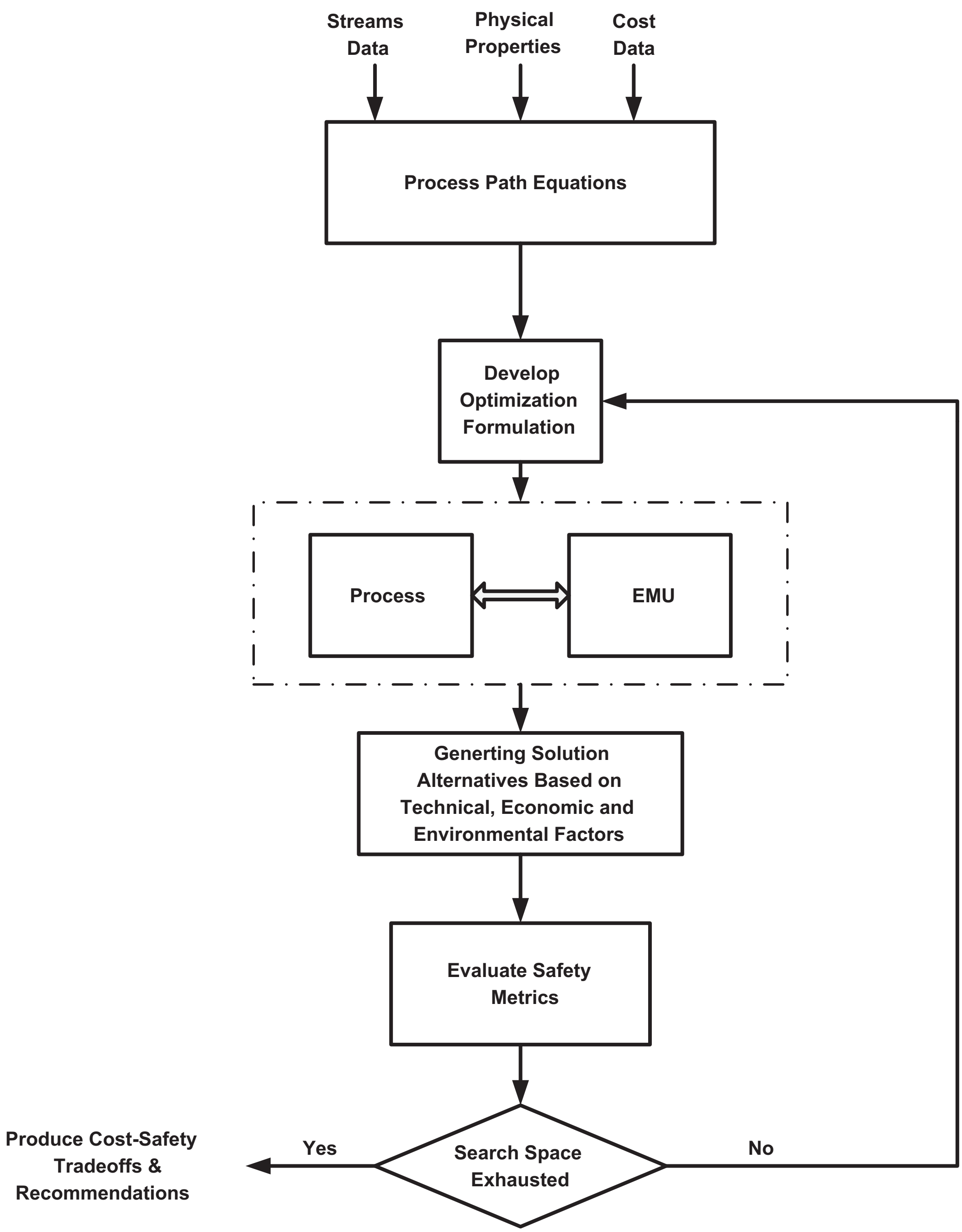

Fig. 2. Flowchart of process scheduling, environmental control and inherently safer design.

that are ranked in terms of their economic and technical performance. Next, the Dow F&EI calculations are undertaken for each alternative and a tradeoff (Pareto) curve is generated.

4. Case study: scheduling and safety for a NO_x management system of a refinery

Scheduling is an important activity in refineries. Most of the research contributions in refinery scheduling have focused on responding to market demands to maximize profit. For instance, in the US, the demand for gasoline usually increases during summer while the demand for diesel typically increases in winter. Various process units (e.g., the fluid catalytic cracker FCC) are operated differently along with pooling and blending to obtain the desired products. It is worth noting as the refinery is operated differently; its environmental emissions will also change. Here, we expand the scope of scheduling to include the need for compliance with environmental regulations including NO_x emissions. We also allow for the addition of NO_x removal units as needed. There are several technologies that can reduce NO_x emissions. Selective catalytic reduction (SCR) units may be installed in oil refineries in order to assure that NO_x is within the acceptable environmental range. NO_x emissions fluctuate depending on the mode of operation, product demands or crude properties. Therefore, the design and operation of the SCR is tied to scheduling decisions and vice versa. In this case study, there is an anticipated profile for market demands. The objective is to determine the optimal refinery scheduling along with any process modifications and the number and design and the EMUs (SCR in this case).

Process safety is another of the important parameter in process design. The control of NO_x is considered in this study with the process modifications along with different operations of FCC-SCR due to process or environmental regulations changes. The hazards in the control of NO_x process is quantified by applying F&EI as the safety metrics. Based on the process conditions, chemical types, reaction types, and inventory involved, a range of F&EI values as a function of flammable material inventory involved in NO_x control (Ammonia and ethanol) is provided. This provides additional information for the decision maker about the hazards involved in the process under evaluation. The next step could include the selection of process with lower hazards or to accept higher hazards with addition cost for mitigation systems, all without sacrificing the business and environmental objectives at the same time. This adds one more layers is to the control of NO_x where safety metrics (F&EI) values are considered here with the process modifications along with different operations of FCC-SCR due to process or environmental regulations changes to have inherently safer design as well. The modeling aspects of FCC-SCR are given in Appendix I. Here, the main emphasis is upon showing the competition between FCC production schedules, SCR performance and NO_x removal efficiency and all of that is linked with the safety of the process. Two SCR systems are considered using two different mass separating agents: ammonia and ethanol (Dong et al., 2008; He & Yu, 2005).

A Pareto chart is constructed to show the tradeoffs for each scenario. Fig. 4 illustrates the effect of variable scheduled production on the safety metrics for the ammonia SCR system. The figure shows as production increases, the need for NO_x removal increase and, consequently, more ammonia is used in the SCR, which leads to increased hazard. Although more net profit is achieved due to higher scheduled productions, the hazards of the process (quantified by F&EI) also increase as shown in Fig. 3. This is due to the fact that the ammonia (which is flammable) poses hazard in terms of energy that can be released at a certain condition and could lead to an incident. This energy is increased as the usage of ammonia increases which leads to increased ammonia inventory.

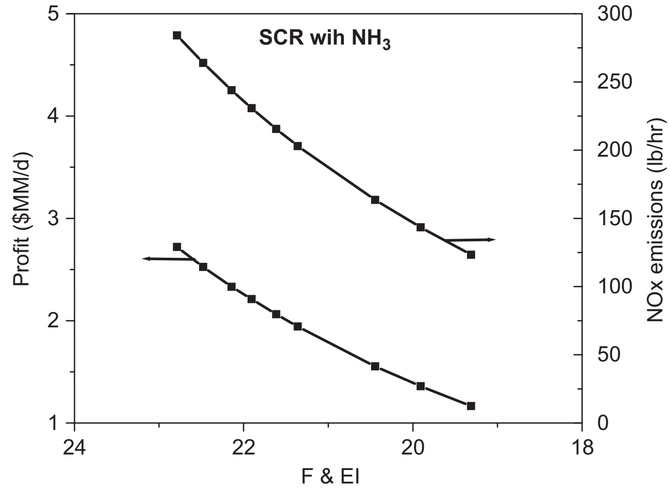

Fig. 3. Pareto curve for the ammonia–SCR system.

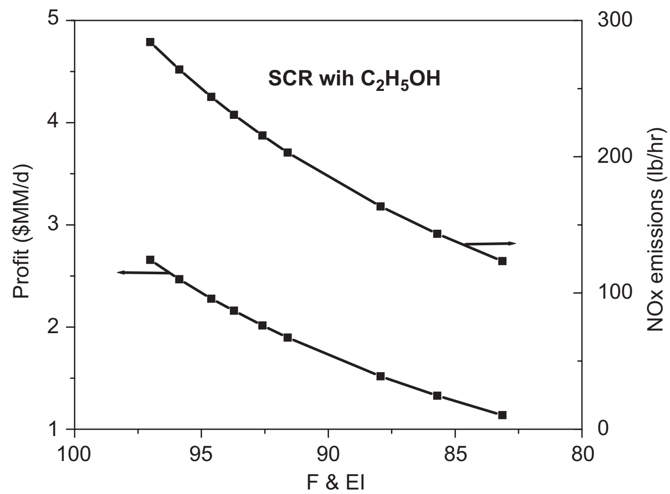

Fig. 4. Pareto curve for the ethanol–SCR system.

Similar trends are observed for ethanol–SCR technology as shown in Fig. 4. But, the hazards in this case are much higher than ammonia–SCR technology as a result of the higher energy content of ethanol and its associated flammability hazards.

Instead of recommending a single operating point that works for all companies, the Pareto curves should be presented to the decision makers of the company as tradeoff curves. As such, a selection is made by considering the economic, environmental, and safety objectives of the company.

5. Conclusions

A new approach is introduced to consider both the inherently safer design and expected process scheduling. An optimization formulation is developed to generate design alternatives for addressing scheduling needs while accounting for technical, economic, and environmental aspects of the process. Dow F&EI index is used as a safety metric to assess design alternatives. The tradeoff between the inherently safer design and scheduling of production objectives is accomplished by a mathematical formulation of the process design. A case study on NO_x removal in a refinery was considered. Two systems are considered for NO_x removal: (a) ammonia–SCR system and (b) ethanol–SCR system. Pareto curves are shown for both technologies and comparisons between the inherently safer designs for them were graphically shown. It can be shown that the integration of process scheduling and F&EI can be performed. The results obtained provided clearer picture regarding the process under evaluation. Decision makers and/or engineers could benefit from this information, especially when this methodology is performed at early stages of design or during process retrofitting.

Appendix I

The model for gasoline yield (wt%) in fluid catalytic cracking unit is:

$$\text{Gasoline} = a\left(\frac{H}{C+S} + \log f_c T\right) + b(M_{\text{eff}}) + c(N_B) + d(C/O) + e(T) + f(\text{Conversion})$$

with the following coefficients: $a = 9.0428$, $b = -2.0002$, $c = 0.2008$, $d = 0.4906$, $e = -0.0171$, $f = 0.5983$

Coke yield calculations from modified Amoco model:

$$Coke = (C/O)^a (\text{WHSV})^b \exp(E/RT)$$

The coefficients' values are: $a = 0.325$, $b = -0.198$, activation energy $= E = 6303$ Btu/lb mol.

Cycle oils products are given by

$$\text{LCO} = 59.73 - 0.55(\text{Conversion})$$
$$\text{HCO} = 100 - \text{LCO} - \text{Conversion}$$

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