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1. Introduction

Process safety might be considered as the most important area to improve several aspects in the process industry design. Ways of dealing with hazards include means to either control them or totally remove them. Both control and removal ways can be applied during the design stage to produce inherently safer designs. There exist several practical examples where issues related to inherently safer designs have been explored (Kletz, 1984). Seven basic principles of inherently safer design have been identified from many application cases: intensification, substitution, attenuation, simplicity, operability, fail-safe design and second chance design, see for instance (Mannan, 2005). Indeed, the plant layout has been identified as a prominent feature for the second chance design, which means that it represents a second line of defence to guard against initial hazards or failures since the process has been already designed at this stage (Mannan, 2005).

Aids for the synthesis of inherently safer design are not well developed but some work has been done in process designs to conform into this principle. It is considered here that one way to avoid hazards is through safer designs that can be obtained for the process industry by appropriate plant layout designs. Plant siting and plant layout are considered as the last opportunity to enhance inherent safety during the design stage. The plant siting addresses finding a location for a plant as a part of a collection of plants and this task normally concerns with the safety for pupil surrounding the plants. The plant layout addresses the arrangement of units and equipment of each plant and it normally concerns with the safety for pupil inhabiting the plant (CCPS, 2003). In this work, the philosophy underlying the conceptual plant layout is considered applicable to virtually all aspects of siting. Plant layout is the term adopted in this work for both siting and plant layout where inherently safer designs should be the prime aim.

The plant layout problem includes thus accommodation not only of the process facilities but also of other facilities such as offices, parking lots, buildings, warehouses, storage tanks, utility areas, etc. It introduces a number of forms in which the results of any risk may be presented. A preliminary hazard screening will provide information to determine if the site provides adequate separation distances from neighbouring areas or among the process
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units. Experience has produced guidelines for facility siting and layout that can be used to estimate these distances (CCPS, 2003). However, there remains an inherent tendency to overdesign and any resulting preliminary plot area is never appropriately sized. A good model is required to estimate the risk related to eventually produce the optimal plot plan. A good plant layout will logically indicate a greater degree of inherent safety.

It has been indicated that 15-70% of total operational costs depends on the layout (Tompkins et al., 1996), and piping costs can be as high as 80% of the purchased equipment cost (Peters et al., 2003). It is also considered that a number of accidents can be reduced with an optimal process layout. Thus, the objective function must include sustainability factors to keep space for future expansions, environmental concerns, reliability, efficiency and safety in plant operations, land area and operating costs (Mecklenburgh, 1985).

Earlier plant layouts were based on common sense rules such as following the order in the process and separating adjacent units by sufficient distances to allow maintenance operations (Mecklenburgh, 1973; Moore, 1962). This procedure is not practical for optimization purposes and becomes particularly difficult to accommodate a large number of process units (Armour and Buffa, 1963). The complete problem is often partitioned to generate modules which are easier to solve in a sequence (Newell, 1973). This approach was improved through graph theory (Abdinnour-Helm and Hadley, 2000; Goetschalckx, 1992; Huang et al., 2007; Watson and Giffin, 1997) and fuzzy logic techniques (Evans et al., 1987).

The difficulty of solving the layout problem via programming techniques has been demonstrated in the arrangement of departments with certain traffic intensity which is a strongly NP-hard problem (Amaral, 2006). However, several efficient and systematic strategies have been developed to solve particularities of the layout problem. Several algorithms to solve the facility layout problem have been formulated as a quadratic assignment problem (QAP) (Koopmans and Beckmann, 1957; Pardalos et al., 1994; Sahni and Gonzalez, 1976). The QAP formulation is equivalent to the linear assignment with additional constraints (Christofides et al., 1980). Several QAP models were evolved into mixed integer programming (Montreuil, 1990; Rosenblatt, 1979; Urban, 1987). Another formulation was developed for facilities having fixed orientation and rectangular shape where the big-M method was applied to improve the numerical calculation (Heragu and Kusiak, 1991). Other MILP formulations solved different particularities of the layout problem through ad hoc methods or commercial packages (Barbosa-Póvoa et al., 2001; Barbosa-Póvoa et al., 2002; Guirardello and Swaney, 2005; Papageorgiou and Rotstein, 1998; Westerlund et al., 2007; Xie and Sahinidis, 2008). The layout of process units has been also formulated as a mixed-integer non-linear program (MINLP); however, the MINLP is converted to a MILP to ensure a numerical solution (Jayakumar and Reklaitis, 1996). A substantial improvement to the big-M formulation for the layout problem has been obtained with the convex-hull approach (Sherali et al., 2003). Stochastic techniques have shown their capability to produce practical solutions for the plant layout problem. Genetic algorithms are able to solve optimization problems containing non-differentiable objective functions thought the global optimum is not guaranteed (Castell et al., 1998; Martens, 2004; Mavridou and Pardalos, 1997; Wu et al., 2007). In addition, simulated annealing has been applied in the layout of manufacturing systems (Balakrishnan et al., 2003; McKendall and Shang, 2006).
The models to solve the layout problems cited above did not directly include safety issues. A new trend in designing plant layouts for the process industry consists of extending the layout formulations with safety issues. Though some MILP models have been proposed to reduce financial costs (Papageorgiou and Rotstein, 1998; Patsiatzis et al., 2004; Patsiatzis and Papageorgiou, 2002), modelling safety issues unavoidably end up in MINLP models. Inspired by the Flixborough and Bhopal accidents, the first paper on designing the plant layout incorporated financial risk and protection devices cost to the classical piping and land costs in the objective function (Penteado and Cric, 1996). The Mary Kay O’Connor Process Safety Center started a research to optimize the layout when some of the process units may release toxic gases. The following sections refer to the results of this research.

2. Overall Problem Statement

This work focuses at solving the layout when toxic release might occur in any process unit. The overall process layout consists on accommodating each process unit in a given land. The task can be divided in three parts: a) some units are grouped to remain as closed as possible among them with access for maintenance and fire-fighter actions to form facilities, b) all new facilities must be accommodated within a land where other facilities may exist and c) the pipe routing problem must be included in the two previous parts and it depends on the interconnectivity. Since toxic releases affects pupil and not to process units, it is convenient to describe the layout in terms of facilities where the control room becomes the most important facility to allocate. Furthermore, facilities typically have rectangular shapes. For the sake of simplicity, facilities and the available land are then considered to have rectangular shapes. Thus, the overall problem is established as follow:

Given:
- A set of already existing facilities \( I \);
- A set of new facilities for siting \( S \);
- A set of release types \( R \);
- A subset \( ri(i, r) \) of existing facilities \( i \in I \) having a particular release \( r \in R \), and displacement values, \( dx_i \) and \( dy_i \), to identify the exact releasing point with respect to the center of the releasing \( i \)-facility;
- A subset \( rs(s, r) \) of existing facilities \( s \in S \) having a particular release \( r \in R \), and displacement values, \( dx_r \) and \( dy_r \), to identify the exact releasing point with respect to the center of the releasing \( j \)-facility;
- The facilities interconnectivity for both types existing and new facilities;
- Length and depth of each new facility for siting, \( L_x \) and \( L_y \);
- Length and depth of each existing facility, \( L_x \) and \( L_y \), as well as their center point, \((x, y)\);
- Maximum length, \( L_x \) and depth, \( L_y \), of available land;
- Size of the street, \( st \);
Two approaches have been developed to solve the above problem. The dispersion of the toxic is important to calculate concentration and then the fatal effect for any toxic release scenario. Hence the wind effect is an important factor in this kind of scenarios. Since the wind behaves as a random variable for practical purposes, the first approach is referred as the stochastic approach where the wind speed, wind direction, and other factors are dealt through probabilistic models. In a second approach, the wind effect is modeled based on the worst scenario and this approach is referred to as the deterministic one. Both stochastic and deterministic approaches have different equations to evaluate the risk. However, they also have common constraints which are given in the following section.

3. Common Constraints

The common constraints are classified as land constraints, non-overlapping constraints and risk-related equations. In addition, the objective function contains also similar terms which are also presented below.

3.1 Land Constraints

Any new facility must be accommodated inside the available land having a street around it. The street size must be sufficient to facilitate the firefighting and emergency responses. Since it is considered that new facilities and the available land are described by rectangles, the center point for any new facility must satisfy:

\[
\frac{L_x}{2} + st \leq x_s \leq L_x - \left(\frac{L_x}{2} + st\right) \tag{1}
\]

\[
\frac{L_y}{2} + st \leq y_s \leq L_y - \left(\frac{L_y}{2} + st\right) \tag{2}
\]

For the sake of simplicity, the East direction is represented by the direction (0,0) to (∞,0) and the North by the direction (0,0) to (0,∞).

3.2 Non-overlapping Constraints

Simple common sense indicates that two facilities cannot occupy the same space, i.e. they must not overlap. A new facility s could be accommodated anywhere around another facility k provided there is sufficient separation to build a street between them, Fig. 1. These possibilities must be reproduced in a model without duplication or overlapping to avoid numerical difficulties in the optimization procedure. The following disjunction identifies four sections with respect to the facility k: left side, right side, north and south. It should be observed that the north-south is initially grouped but it is later disaggregated.
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Determine

- Each new facility center position \( (x_i, y_i) \),
- The occupied area out of the total land;
- The final cost associated with the optimal layout;

Two approaches have been developed to solve the above problem. The dispersion of the toxic is important to calculate concentration and then the fatal effect for any toxic release scenario. Hence the wind effect is an important factor in this kind of scenarios. Since the wind behaves as a random variable for practical purposes, the first approach is referred as the stochastic approach where the wind speed, wind direction, and other factors are dealt through probabilistic models. In a second approach, the wind effect is modeled based on the worst scenario and this approach is referred to as the deterministic one. Both stochastic and deterministic approaches have different equations to evaluate the risk. However, they also have common constraints which are given in the following section.

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\[
\begin{align*}
\left| x - x_s \right| & \leq \frac{L_x - D_{st}}{2} + st_1 \\
\left| y - y_s \right| & \leq \frac{L_y - D_{st}}{2} + st_2
\end{align*}
\]

where,

\[
D_{st}^{\text{min},x} = \frac{L_x + L_x}{2} + st
\]

and \( st \) is the street size and facility \( s \) refers to a facility to accommodate and facility \( k \) can be either a new or an already installed facility.

Since commercial optimization codes do not accept disjunctive formulations, equation (3) is reformulated as a MINLP. There are three methods to achieve this transformation: direct use of binary variables for each disjunction, the big-M and the convex hull (Grossmann, 2002).

The straightforward method of binaryzation generates new bilinear terms which are source of numerical difficulties (McCormick, 1982) whereas the main drawback of the big-M
formulation is that a bad selection yields poor relaxation (Grossmann, 2002). Thus the convex hull has been preferred in this conversion procedure (Vázquez-Román et al., 2009).

3.3 Risk-related Equations

The response vs. dose curves for single exposures is typically represented with the probit function as a straight-line (Finney, 1971):

\[ Pr = k_0 + k_1 \ln V \]  

(6)

where \( Pr \) is the probit variable, the dose \( V \) represents the causative factor, being the product of concentration and exposure time for toxic releases, and \( k_0 \) and \( k_1 \) are best-fitting values reported for several substances in several sources. The probit variable is related to the probability of death, \( P \), by:

\[ P = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{Pr} e^{-u^2/2} \, du \]  

(7)

The probit relationship transforms the typical sigmoid shape of the normal response versus dose curve into a straight line.

3.4 The objective function

The piping cost, \( C_{\text{piping}} \), is one of the important cost factors in the layout problem. It can be estimated by multiplying the separation distance, \( d_{ij} \), by the cost of the pipe, \( C_p \):

\[ C_{\text{piping}} = \sum (i,j) C_p d_{ij} \]  

(8)

In principle, the distance should include the equivalent distance because of all accessories such as elbows in changes of direction. For the sake of simplicity, the Manhattan and Euclidian distances have been used. The latter is preferred in this work because the derivative can be easily produced:

\[ d_{ij}^2 = (x_i - x_j)^2 + (y_i - y_j)^2 \]  

(9)

where \( d_{ij} \) is the separation Euclidian distance between facility \( i \) with coordinates \((x_i, y_i)\) and facility \( j \) with coordinates \((x_j, y_j)\).

The land cost, \( C_{\text{land}} \), represents the cost because of the area occupied by the overall layout. To easy this calculation, the process layout starts always in the origin \((0,0)\) and the area is considered as the minimum rectangle that includes all facilities:
where $c_i$ is the land cost per m$^2$, and $A_x$ and $A_y$ are the lengths in the x and y directions which can be calculated from:

$$A_x = \max(x_i + Lx_i / 2)$$
$$A_y = \max(y_i + Ly_i / 2)$$

Unfortunately the above formulation represents a non-convex function and it is not accepted in all optimization codes. Since the land cost and hence the area is minimized, a more convenient form can be used as follows:

$$A_s \geq x_i + Lx_i / 2$$
$$A_s \geq y_i + Ly_i / 2$$

where $s$ runs for all facilities. Next section describes the model developed where the stochastic effect of the wind is considered.

### 4. Stochastic Approach

Wind represents the main random factor in this stochastic approach developed to optimize the plant layout (Vázquez-Román et al., 2008; 2009). The main affected receptors in a given release scenario are those situated in direction of the wind but there is also a reduced effect on adjacent sectors. The occurrence of winds at any location are normally represented in the wind rose plot where speed, directions and frequency are indicated. In addition, atmosphere stability is also required in this approach. This information is estimated from other meteorological variables such as altitude, total cloud cover, and ceiling height. A procedure to incorporate meteorological data from several databases in the wind effect analysis is given elsewhere (Lee et al., 2009). Fig. 2 shows the wind rose and the cumulative probability versus wind direction for Corpus Christi obtained with this procedure.

A credible release scenario must be proposed to define the expected amount of toxic released material. The credible scenario depends on the size of pipes and process conditions (Crowl and Louvar, 2002). Once the stochastic behavior of wind direction, wind speed and atmospheric stability is characterised with cumulative probability curves and the release scenario is defined, a Monte Carlo simulation is applied where values for these stochastic variables are randomly selected. For this set of selected values, an appropriate model for the gas dispersion is used to estimate the concentration at all directions and several separation distances.

$$C_{land} = c_i A_x A_y$$

(10)
Ad hoc models can be developed to estimate concentrations of the toxic material in selected points. In addition, there exits several methods for different release scenarios such as liquid, dense gas or light gas (CCPS, 1996). The selected points must cover all possibilities in the available land so that the maximum separation between the first point and the last one in a given direction depends on the available land size. It is suggested to have intermediate neighbour points as close as possible without compromising the calculation time. A similar number of points must be used in each of several directions to get the concentration of the toxic gas at all possible directions. Thus the 360° are divided by direction-sectors to have a practical number of estimations. The Monte Carlo generates as many concentration values at each point as Monte Carlo runs and this number should be as large as practically possible. The concentration values can then be easily converted in risk of death values through the probit function. An exponential decay is assumed so that the probability of death at each $\alpha$ - direction, $P_{D_\alpha}$, is represented by the equation:

$$P_{D_\alpha} = a_\alpha e^{-b_\alpha d_{r,\alpha}}$$

(13)

where $d_{r,\alpha}$ refers to the distance from the release point in the $\alpha$ -direction to the point where the probability is estimated and $a_\alpha$ and $b_\alpha$ are fitted parameters.

For the sake of simplicity, it is suggested that the number of direction-sectors be a multiple of four. Thus each sector can be described by the initial and final angle of the sector and the following dinjunction is used to identify the sector in which an i-facility is being accommodated with respect to the s-facility that may release a toxic gas:
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... the number of direction-sectors whereas \( s_a^{\Delta x} \) and \( s_a^{\Delta y} \) are convenient vectors with either positive or negative ones to determine in which quadrant the facility \( i \) is positioned respect to facility \( s \). \( s_a^{\Delta x} \) contain positive ones in the elements referring to the first and fourth quadrants but negative ones in thouss referring to the second and third quadrants. \( s_a^{\Delta y} \) has positive ones in elements referring to the first and second quadrants and negative ones otherwise. The above disjunction is also converted to a MINLP via the convex hull technique.

The following risk term is incorporated into the objective function:

\[
C_{\text{risk}} = c_{pp} t_i \sum_i \sum_{r,(i,r)} f_{i,r} P_{i,r,s}
\]

where \( c_{pp} \) is the compensation cost per fatality, \( t_i \) is the expected life of the plant, \( f_{i,r} \) is the frequency of the type of release \( r \) in facility \( i \) and \( P_{i,r,s} \) is the probability of death in the facility \( s \) because of release type \( r \) in facility \( i \).

5. Deterministic Approach

It is often suggested that a better risk assessment for safety in chemical process plants should be based on what is called the worst scenario (Leggett, 2004). A more recent study (Díaz-Ovalle et al., 2009) ratifies that the worst scenario in a toxic release scenario correspond to that one where the wind remains in calm under stable atmospheric condition. Unfortunately, most of current models simplify the convective-diffusive dispersion equation to produce practical equations but these models tend to misbehave when the wind speed tends to zero. Models for both passive and dense dispersion phenomena produce higher concentrations when the wind speed is lower. An accepted value to be used for the wind speed in calm is 1.5 m/sec. Since the wind in calm can occur at any direction, then the risk becomes symmetric and contours having the same risk level have circular shape.

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A deterministic model based on the worst scenario is given in (Diaz-Ovalle et al., 2008). A threshold limit value (TLV) can be used to avoid exposures that may produce adverse effects to pupil. It is suggested that the concentration must not exceed the ceiling value, i.e. TLV-C, see for instance (Crowl and Louvar, 2002). Thus, the equation added to the general layout model described above consists in constraining the distance so that the calculated concentration cannot be superior to the TLV-C value. Otherwise and better than TLV, there are emergency responses planning guideline (ERPG) values that can be used with the same purpose in the layout determination. The objective function in the deterministic approach only contains the land and piping cost terms. The following section contains an analysis of the results obtained with both the stochastic and the deterministic approaches.

6. Discussion of Results and Future Research

The numerical difficulty of solving the layout problem even without toxic release has been clearly identified in (Vázquez-Román et al., 2009). An example considers two new facilities and the control room to be installed in a given land where there exist two installed facilities. While applying several optimization methods and using different initializations, three optima results were found. It should then be clear than increasing the number of units may produce more local optima and the question would remain about what is the best layout. The global optimum for this case was obtained through a global optimizer in GAMS (Brooke et al., 1998), but the time required to achieve the solution is too high and this time became unpractical when the number of facilities was increased.

To test the stochastic approach, a chlorine release was considered to occur in one of the installed facilities. All information required for the stochastic approach is provided in (Vázquez-Román et al., 2009). In this case two optimum layouts were detected with different GAMS solvers, Fig. 3. Though the global optimum was clearly identified, it was observed that it produced a small value in the cost associated to the financial risk whereas this cost became negligible in the other local optimum. Hence the question is again about what solution should be better to use. Another disadvantage of the stochastic approach is the time required to get the parameters of the exponential decay function for the probability of death. In principle, a high number of simulations should be used in the Monte Carlo procedure. The number of calculations could be reduced by reducing the number of direction-sectors but again a large number would produce more representative results. These results have been ratified with other examples in (Vázquez-Román et al., 2008).

Solving the layout with the deterministic approach tends to produce more conservative layouts (Diaz-Ovalle et al., 2008). However, when the toxic material is too toxic this approach may produce layouts occupying a large area. This was the case for the example used in (Vázquez-Román et al., 2009). This approach has the advantage that no extra calculation is required to incorporate the wind effect since calm conditions and hence symmetric effect is assumed. Thus the deterministic approach tends to enforce prevention, mitigation and removal of hazards to reduce the required land. This is typically achieved by inserting devices so that the final layout becomes more expensive than the one produced with the stochastic approach. This approach is justified by the fact that several severe accidents have occurred when calm conditions prevailed.
The two approaches are in effect an application of the principle of inherently safer design. In fact, an inherently safer design is easier to achieve during the plant layout design. However, more research is required to ensure convergence to the global optimum. We are considering the possibility of convexifying the equations so that any local optimization solver could achieve the global irrespectively of the initialization. Also, we are developing 3D-CFD programs to evaluate particular layouts such as each local optimum to detect if streams can form and potentially increase the risk of a given layout. Finally, other properties such as corrosiveness, flammability and explosibility; operating conditions such as pressure and temperature; reaction conditions such as phase, rate, heat release, yield and side reactions; and effluents and wastes must be incorporated in solving the layout problem.

7. Acknowledgements
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8. References


Parametric representation of shapes, mechanical components modeling with 3D visualization techniques using object oriented programming, the well known golden ratio application on vertical and horizontal displacement investigations of the ground surface, spatial modeling and simulating of dynamic continuous fluid flow process, simulation model for waste-water treatment, an interaction of tilt and illumination conditions at flight simulation and errors in taxiing performance, plant layout optimal plot plan, atmospheric modeling for weather prediction, a stochastic search method that explores the solutions for hill climbing process, cellular automata simulations, thyristor switching characteristics simulation, and simulation framework toward bandwidth quantization and measurement, are all topics with appropriate results from different research backgrounds focused on tolerance analysis and optimal control provided in this book.

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