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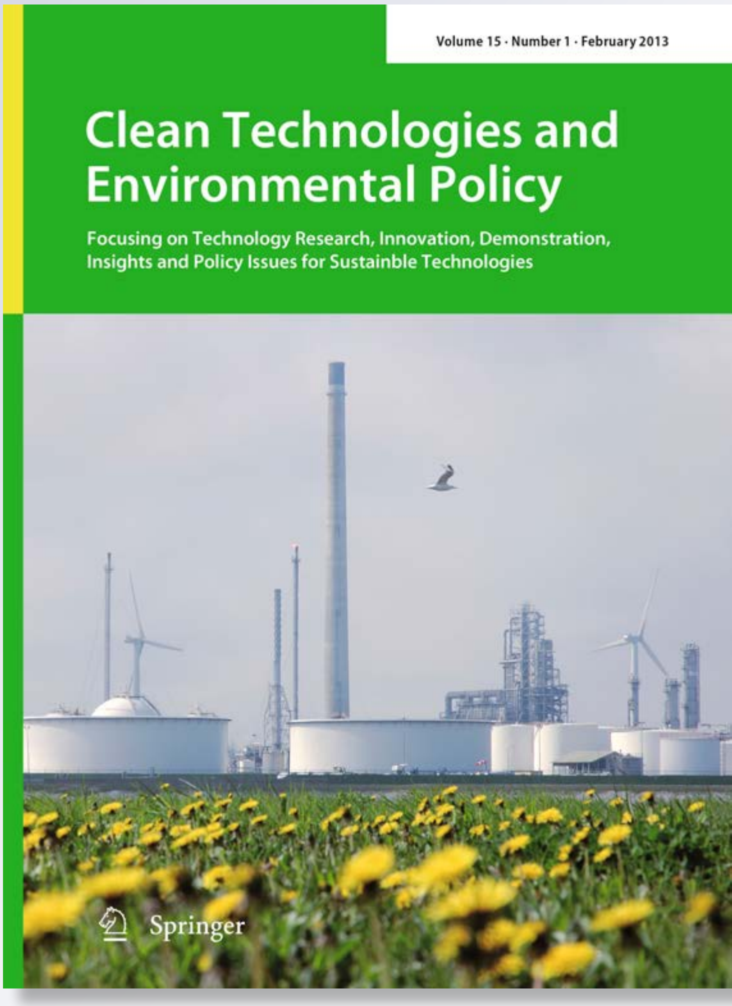

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ORIGINAL PAPER

Optimal integration of gaseous emissions from new industrial plants with the surroundings

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Abstract This paper presents a mathematical programming model for the optimal location of new industrial plants considering simultaneously the integration of the gaseous emissions and the environmental constrains for the surroundings by synthesizing recycle and reuse networks. The model considers different options to locate the new plant and to integrate it with the neighboring urban areas that may be affected by the installation of the new plant because of the gaseous emissions. Air quality conditions and targets for each city (e.g., wind direction, speed to calculate the dispersion parameters, regulations, etc.) are considered. The objective function minimizes the total annual cost needed for the installation of the new plant, the treatment of gaseous streams, and the fresh sources required by the process units. Three examples for the installation of new plants in Mexico are considered to show the applicability of the proposed model. The results show that the proposed model is capable of identifying the optimal integration inside and outside the plant for the gaseous streams. The model also identifies the governmental incentives required to install the new plant in a specific location. These incentives are based on economic aspects as well as social benefits characterized by the generation of jobs. In addition, the proposed model is useful to identify the set of Pareto solutions that trade off the economic and the environmental objectives.

Keywords Mass integration · Gaseous emissions · Optimal location of new plants · Environmental impact · Optimization · MINLP

List of symbols

Variables

$Conc_{p,c}$	Concentration for the component c, in the city p (ppm)
$dConc_{p,c,l}$	Disaggregated variable for the concentration for the component c, in the city p for location of the industry l (ppm)
$dEm_{c,l}$	Disaggregated variable for the total amount of emission discharged to the environment for each component c for location of the industry l (kg/h)
Em_c	Total amount of emission discharged to the environment for each component c (kg/h)
emission	Total flowrate discharged to the environment (kg/h)
F_r	Total flowrate of the fresh sources (kg/h)
$f_{r,j}$	Fresh flowrate sent to the process sinks (kg/h)
$g_{i,emission}^{int^1,\ldots,int^N}$	Exit flowrate from the interceptors and sent to environment (kg/h)
$g_{i,j}^{int^1,\ldots,int^N}$	Exit flowrate from the interceptors and sent to process sinks j (kg/h)
Q_m	Total amount of emitted gases using the Pasquill–Gifford model (kg/h)

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TAC	Total annual cost, \$/year
$w_i^{\text{int}^1}$	Flowrate sent to the interceptors of the first stage (kg/h)
$w_i^{\text{int}^1,\ldots,\text{int}^2}$	Flowrate sent to the interceptors of the second stage (kg/h)
$w_i^{\text{int}^1,\ldots,\text{int}^N}$	Flowrate sent to the interceptors for the stage N (kg/h)
Y_l	Boolean variable for the location of the new plant in option l
y_l	Binary variable for the location of the new plant in option l
z_i^{int}	Binary variable for the existence of interceptor *int* to treat streams i

Parameters

$CLand_l$	Annualized installation cost for the new plant in site p (\$/year)
$Conc_c^{\max}$	Maximum permissible concentration for the component c (ppm)
C_{op}^{int}	Interceptors operational cost (\$)
$CPG_{i,p,c}$	Pasquill–Gifford constants
$Em_c^{\max}$	Maximum amount of the emissions discharged to the environment (kg/h)
$EmPumpingC_i^{\text{int}}$	Unit pumping cost for the flowrate sent to the environmental emissions \$/kg
$EqPumpingC_{i,j}^{\text{int}}$	Unit pumping cost for the flowrate sent to the unit \$/kg
$FixC_{cap}^{\text{int}}$	Unit fix cost for the interceptors (\$)
$FreC_r$	Unit cost for the fresh sources (\$/kg)
$FshPumpingC_{r,j}^{\text{int}}$	Unit pumping cost for the fresh sources (\$/kg)
G_j	Total flowrate inlet to the process sinks (kg/h)
H_r	Height of the source (m)
H_Y	Operation time per year (h/year)
k_f	Factor used to annualize the capital costs
$MaxEmission$	Upper bound for the total emission (kg/h)
$TaxCredit$	Tax credit for the reduction of the emission (\$/kg)
$TPumpingC_i^{\text{int}}$	Unit pumping cost for the flowrate in the interception system (\$/kg)
u	Wind speed (m/s)
VaC_{cap}^{int}	Variable cost for the interceptors (\$/kg year)
W_i	Total inlet flowrate by the gaseous process sources (kg/h)
$w_i^{\text{int}MAX}$	Maximum flowrate to the interceptors (kg/h)
$w_i^{\text{int}MIN}$	Minimum flowrate to the interceptors (kg/h)
x	Wind direction
y	Ratio of dispersion (m)
z	Height of dispersion (m)
$z_{i,c}^{In}$	Concentration of process sources for the component c (ppm)
$z_{r,c}^{InFresh}$	Concentration of fresh sources for the component c (ppm)
$z_{j,c}^{InSink.LO}$	Lower limit for the concentration at the inlet to the sinks (ppm)
$z_{j,c}^{InSink.UP}$	Upper limit for the concentration at the inlet of the sinks (ppm)
$z_{j,c}^{Out,int}$	Concentration at the exit of the interceptors (ppm)
$z_{j,c}^{InSink}$	Inlet concentration to process sinks for the component c (ppm)

Greek symbols

$\alpha_c^{\text{int}^1,\ldots,\text{int}^N}$	Conversion factors for the interceptors
σ_y, σ_z	Dispersion parameters for the Pasquill–Gifford model
γ_c^{int}	Efficiency factor for the removal of the pollutant c

Superscripts

c	Component
i	Gaseous process sources
int	Interceptor
j	Process sinks
l	Location for the new plant
p	Nearby cities to the possible location of the new plant
r	Fresh sources

Introduction

The process and chemical industries generate large amounts of liquid and gaseous emissions. These emissions represent severe adverse impacts on the environment. Therefore, several environmental constraints have been imposed on the industrial emissions to promote sustainable processes. For the design of a new industry, the environmental constraints only impose limits to the concentration and discharges of the hazardous pollutants without considering the interaction with other emissions in the surroundings. End-of-pipe treatment units are typically needed to handle the gaseous emissions before environmental discharges. In addition, recycle/reuse strategies may be used to reduce or eliminate the extent of end-of-pipe treatment. In this context, several methodologies have been developed for recycling, reusing, and regenerating process streams to satisfy the process units requirements while reducing the consumption of fresh sources and the discharge of waste streams to the environment (see the paper reviews by Bagajewicz 2000; Dunn and El-Halwagi 2003;

Foo 2009). Unfortunately, most of the reported methodologies consider only liquid streams. Fewer methods have been reported for the reuse of the gaseous process stream in industry (see for example the works by Shonnard and Hiew 2000; Parthasarathy and El-Halwagi 2000; Hamad and Fayed 2004; El-Halwagi et al. 1996; Dunn and El-Halwagi 1994a, b; Gassner and Marechal 2010; Parthasarathy and Dunn 2003). Figure 1 shows a schematic representation of these recycle, reuse and interception schemes for the gaseous streams. It is worth noting that previous formulations only have considered the effects that happen inside the industrial facilities without accounting for the effect of the gaseous emissions on the surroundings. High levels of concentration of the gaseous pollutants affect the air quality of the surroundings, causing environmental and public health problems. To reduce the concentration of the pollutants emitted, it is needed to satisfy environmental constraints to insure proper air quality and to develop appropriate strategies for the processing and treatment of the gaseous streams inside the plant before they are discharged to the environment as well as at the exits of the plant. Recently, Lira-Barragán et al. (2011a, b) reported approaches to include water integration inside the industrial facilities together with the sustainability of the surrounding watershed. The models are based on material flow analysis models (MFA) (for details of MFA models see the works by Baccini and Brunner 1991; Brunner and Rechberg 2004; Lovelady et al. 2009) to track the effects of wastewater discharge over the surrounding watersheds while accounting for all the sources and users in the watershed. This holistic approach is much more conducive to sustainability than simple end-of-pipe regulations on discharges. Given the value of this holistic approach in water applications, it is expected that similar benefits can accrue as a result of adopting a similar approach for gaseous emissions.

The objective of this paper is to introduce a new approach for the allocation of new industrial facilities that takes into consideration to the management of industrial gaseous emissions by integrating in-plant modifications (e.g., recycle/reuse), end-of-pipe treatment, and interaction with the surroundings. The paper proposes a new mathematical programming model for the synthesis of recycle, reuse, and interception networks for gaseous streams associated with the installation of a new industrial facility while considering the interaction with their surroundings. The site location is to be determined as part of the optimization problem. The model also accounts for constraints for the gaseous emissions on the neighboring areas and the interaction with other sources of emissions. An atmospheric dispersion model such as the Pasquill–Gifford model (for details see Turner 1994; Barratt 2001) is used to consider the effect of the gaseous emissions on the surroundings. This Pasquill–Gifford model accounts for the dispersion of the emissions considering the air quality, speed, and direction of the wind. Therefore, the proposed model is based on the calculation of the dispersion parameters to determine the concentration of the pollutants at a certain distance from the point of emission to locate the industrial facility accounting for the surroundings.

This paper is organized as follows: the second section presents the outline of the proposed model, "Model formulation" section shows the proposed mathematical programming formulation, the application of the proposed model through the solution of three examples is presented in "Case studies" section, and finally the fifth section presents the conclusions of the paper.

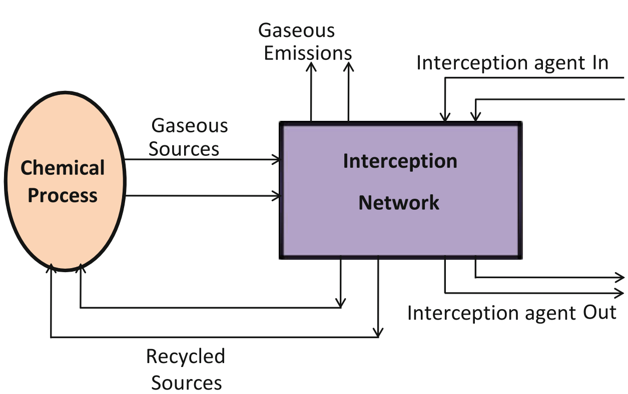


Fig. 1 Integration of gaseous emissions inside the plant

Outline of the proposed model

The problem addressed in this paper can be described as follows. Given a set of possible locations to install a new industrial plant ($L = \{l|l = 1,2,\ldots,N_l\}$), in each possible location l is assigned an installation cost ($CLand_l$); this cost includes the land cost, transportation of the raw materials, products, and services' costs. There are several nearby cities that can be impacted by the emissions from the new industrial plant ($P = \{p|p = 1,2,\ldots,N_p\}$); in each nearby city p, the effect of the emissions is evaluated by the dispersion model of Pasquill–Gifford, this model determines the concentration $Conc_{p,c}$ of each toxic compound ($C = \{c|c = 1,2,\ldots,N_c\}$) in each city taking into account the speed and direction of the wind. The Pasquill–Gifford model is based on the calculations of the concentrations like the MFA model for the liquid streams (see Lovelady et al. 2009). The estimation of the concentration by an emission point is given by the following Pasquill–Gifford equation:

$$\langle C\rangle(x,y,z) = \frac{Q_m}{2\pi\sigma_y\sigma_z u}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \times \left\{\exp\left[-\frac{1}{2}\left(\frac{z-H_r}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z+H_r}{\sigma_z}\right)^2\right]\right\} \quad (1)$$

where H_r is the height of the source, Q_m is the amount of the gases emitted, u is the wind velocity, x is the wind direction, y is the ratio of dispersion, z is the height of dispersion, and σ_y and σ_z are the dispersion parameters for the directions y and z, respectively. If the emissions source is found at $z = 0$, the Eq. (2) is obtained and it depends only on the ratio of dispersion as follows:

$$\langle C\rangle(x,y,0) = \frac{Q_m}{\pi\sigma_y\sigma_z u}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2 - \frac{1}{2}\left(\frac{H_r}{\sigma_z}\right)^2\right] \quad (2)$$

The concentration calculated by the Pasquill–Gifford model is used to determine the location of the plant considering the emissions of the new plant (Em_c). In this paper, the values obtained by the Pasquill–Gifford model are grouped into the Pasquill–Gifford constant ($CPG_{i,p,c} = \frac{1}{\pi\sigma_{y_{ip}}\sigma_{z_{ip}}u_i}\exp\left[-\frac{1}{2}\left(\frac{y_{ip}}{\sigma_{y_{ip}}}\right)^2 - \frac{1}{2}\left(\frac{H_{r_i}}{\sigma_{z_{ip}}}\right)^2\right]$) in a model reformulation to obtain one location for the new plant and also to consider what happens inside the plant. Inside the plant, there is a set of gaseous process sources ($I = \{i|i = 1,2,\ldots,N_i\}$) with composition $z_{i,c}^{In}$ and flowrate W_i, which can be segregated to be recycled and reused in the process sinks ($J = \{j|j = 1,2,\ldots,N_j\}$) with composition $z_{j,c}^{InSink}$ and flowrate G_j fixed by the process. To satisfy the requirements of the process sinks, there is available a set of fresh sources ($R = \{r|r = 1,2,\ldots,N_r\}$) with composition given $z_{r,c}^{InFresh}$ and the required flowrate F_r needs to be determined. Also, there is available a set of interceptors for the gaseous streams (*INT*). Each one of these interceptors has an efficiency to intercept the pollutants in the gaseous streams, and these efficiencies can be determined by simulation or by experimental data before the optimization process. The efficiency γ_c^{int} of each interceptor is a function of the configuration for the interceptor and the operating condition that are determined before the optimization process. In addition, each interceptor (according to the configuration and operating conditions) has associated a unitary cost that depends only on the manipulated flowrate. Therefore, the optimization must select the type of interceptor required and the intercepted flowrate.

To satisfy the environmental regulation after the installation of the new plant, a set of environmental constrains are stated to comply with the permissible limits for the amount of the emissions for the new plant and for the maximum permissible concentration in each nearby city.

The problem then consists of finding the optimal configuration for the treatment system for the gaseous emissions (involving recycle, reuse, and regeneration) inside the industrial facility considering the effects in the surrounding cities through the location of the new industrial facility and a new MFA model. The objective function consists of minimizing the total annual cost (*TAC*), which includes the installation cost for the new plant, the treatment for the gaseous process sources, the fresh sources cost, and the cost for the interceptors and pumping. Figure 2 shows a

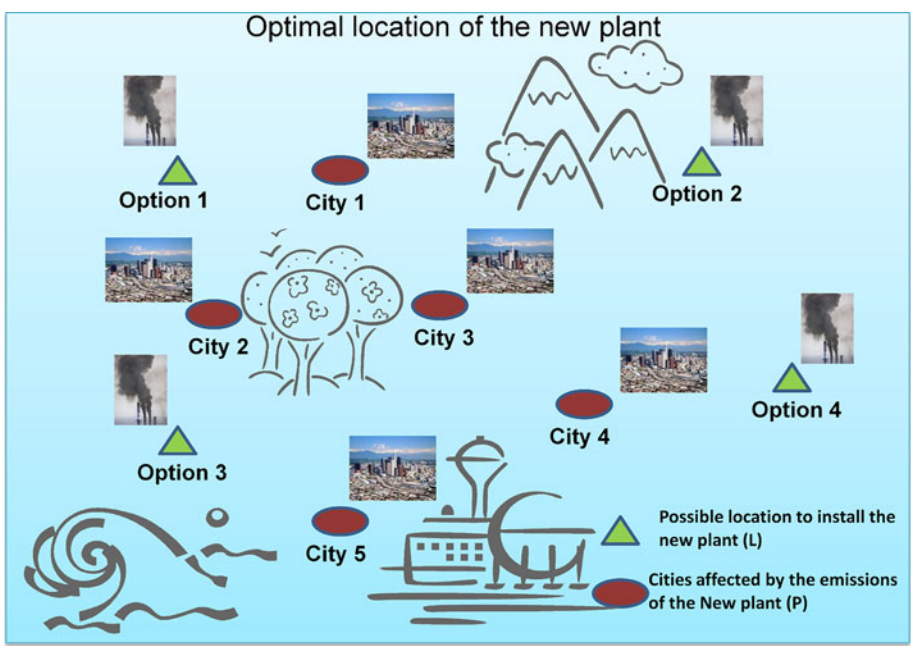


Fig. 2 Schematic representation for the integration of the industrial emissions and the surroundings

schematic representation to integrate the industrial emissions with the surroundings, where there are L possible locations to install the new plant and there are P neighboring cities that are affected by the emissions of pollutants from the new plant.

The dispersion parameters of the Pasquill–Gifford model are used to determine the influence by the dispersion of the contaminants discharged from the new plant in the surrounding air, where it is necessary to know the wind direction and speed; this way the model locates the new plant in the best option according to the air quality in each city. To satisfy the process, environmental and sustainability constraints, a recycle, reuse, and interception scheme is used. In this paper, the superstructure shown in Fig. 3 is used. The superstructure does not allow mixing of different process streams before discharge. This way, the relationships for the mass balances in the superstructure are linear. Avoiding mixing of different process streams before discharge yields linear relationships for the mass balances in the superstructure that can be manipulated properly in the optimization process; in this case, only the flowrates are variables, whereas the compositions are constants given by the process. On the other hand, allowing mixing of different process stream before discharge yields several bilinear terms in the model formulation. These bilinear terms result for the mixing of unknown flowrates of different process streams with unknown compositions and the multiplication of two variables in the mass balances (flowrate times' composition). The bilinear terms are nonconvex and pose a challenge in identifying global solutions (see Ponce-Ortega et al. 2010, Ponce-Ortega et al. 2012; Napoles-Rivera et al. 2010; Karuppiah and Grossmann 2006; Quesada and Grossmann 1995; Sherali and Alameddine 1992). In addition, there are available a set of interception units for different pollutants with different efficiencies and costs. There is included a fictitious interceptor to model the bypass streams (the last one for each set of interceptors). The optimization model must select the flowrate and the treatment technologies used to satisfy the process and environmental constraints.

Based on this outline of the problem addressed in this paper, next section presents the optimization model proposed on this paper for the optimal location of a new industrial facility integrating the gaseous streams inside and outside the plant.

Model formulation

The emissions discharged from the new plant that satisfy the constraints for the different surrounding cities depend on the location of the plant. Therefore, the model must consider the location of the new plant, the interception network inside the plant to satisfy the process, environmental and sustainability constraints as well as the relationships required to interconnect these models, minimizing the TAC.

Location of a new plant

To locate the new plant, there are l alternatives (see Fig. 2), and the Pasquill–Gifford model is used to evaluate the effects of the emissions in the p surrounding cities. For example, if the new plant is located in the position 1, the concentration of the pollutants and the emissions associated to this site and the effect in the surrounding cities can be determine by the Pasquill–Gifford model through the constants $CPG_{l,p,c}$ determined before the optimization process. This is modeled through the following disjunction:

$$\begin{bmatrix} Y_{l=1} \\ Conc_{p,c} = CPG_{l,p,c}Em_c \end{bmatrix} \vee \begin{bmatrix} Y_{l=2} \\ Conc_{p,c} = CPG_{l,p,c}Em_c \end{bmatrix} \vee \cdots \vee \begin{bmatrix} Y_L \\ Conc_{p,c} = CPG_{l,p,c}Em_c \end{bmatrix}, \quad \forall c \in C,\ p \in P$$

The Boolean variable Y_l is associated with the possible location of a new plant, $Conc_{p,c}$ is the concentration for the component in the emission discharged from the new plant to the neighboring city p, and Em_c is the total flowrate of the emission of the new plant. The Boolean variables Y_l are transformed into binary variables y_l to reformulate the disjunction as an algebraic problem (see Raman and Grossmann 1994 for example of disjunctive reformulations). The binary variables determine only one location for the new plant as follows:

$$\sum_{l \in L} y_l = 1 \tag{3}$$

Previous disjunction is modeled using the convex hull reformulation and the following algebraic relationships are obtained.

Disaggregate the continuous variables

The continuous variables that depend on the location of the new plan are disaggregated as follows:

$$\begin{aligned} Conc_{p,c} &= \sum_{l \in L} dConc_{p,c,l}, \quad \forall c \in C,\ p \in P \\ Em_c &= \sum_{l \in L} dEm_{c,l}, \quad \forall c \in C \end{aligned} \tag{4}$$

Relationships in terms of disaggregated variables

The concentration of a given component in a given position depends on the location of the new industrial facility, and this is calculated using the disaggregated variables as follows:

$$dConc_{p,c,l} = CPG_{p,c,l}\, dEm_{c,l}, \quad \forall p \in P,\ c \in C,\ l \in L \tag{5}$$

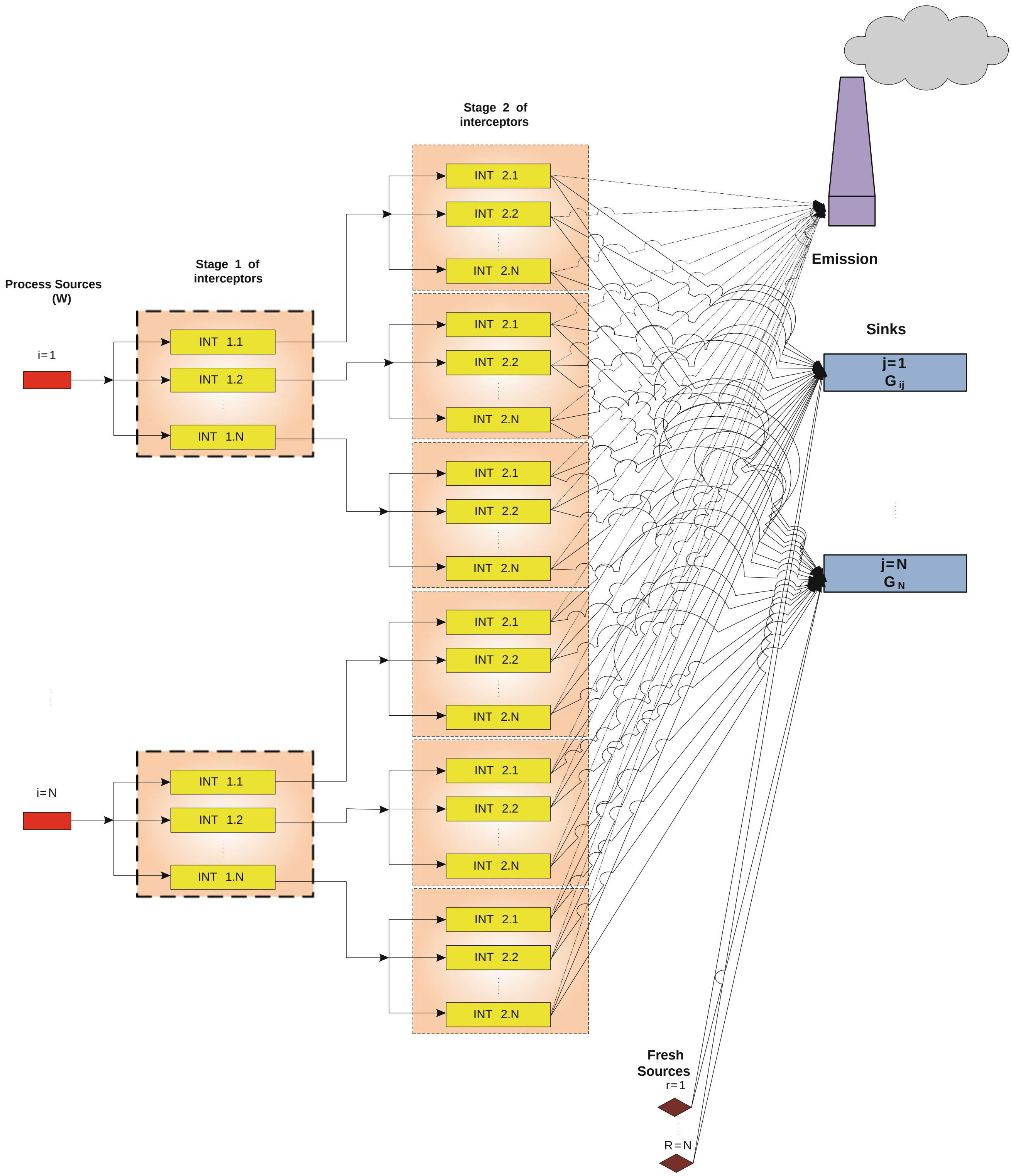


Fig. 3 Network to treat the gaseous emissions inside the plant

Upper limits for the disaggregated variables

There are required upper limits for the disaggregated variables to activate these variables only when the corresponding location is selected:

$$dConc_{p,c,l} \le Conc_c^{\max} y_l, \quad \forall p \in P, \ \ c \in C, l \in L$$
$$dEm_{c,l} \le Em_c^{\max} y_l, \quad \forall c \in C, \ \ l \in L \qquad (6)$$

Recycle and interception model inside the plant

The proposed model is based on the superstructure shown in Fig. 3, which shows the configuration for the interceptors and recycle network for the gaseous process streams. This superstructure is based on the one previously reported by Gabriel and El-Halwagi (2005) and Ponce-Ortega et al. (2010). The model for this superstructure is presented as follows.

Splitting of the fresh sources

First, fresh streams can be used to satisfy the process sink constraints, then different type of fresh sources can be used with different costs and compositions, and the model must select the amount of each type of fresh source selected to satisfy the process and environmental constraints at the minimum cost. Therefore, the superstructure allows splitting the fresh sources and sending them to the process sinks, which is modeled as follows:

$$F_r = \sum_{j \in J} f_{r,j}, r \in R \qquad (7)$$

where F_r is the total flowrate for the fresh source r and $f_{r,j}$ is the flowrate segregated from the fresh source r and directed to the process sink j. Notice that the fresh sources only are directed to the process sinks and these are not discharged to the environment.

Splitting of the process sources to the interceptors

The process sources in the interception network are segregated to avoid mixing different process streams; the mixing of different process streams is allowed only after the treatment and before inlet to the process sinks. If a gaseous process source does not require any treatment, a fictitious unit with effectiveness and cost equal to zero is used to model the bypass of this stream.

The flowrates for the gaseous process sources are segregated $w_i^{\mathrm{int}^1}$ and sent to the different interceptors to treat some pollutant as follows:

$$W_i = \sum_{\mathrm{int}^1 \in \mathrm{INT}^1} w_i^{\mathrm{int}^1}, i \in I \qquad (8)$$

To treat additional pollutants, the flowrates from each interceptor of the first stage are segregated $w_i^{\mathrm{int}^1,\mathrm{int}^2}$ and sent to the interceptors of the stage two.

$$w_1^{\mathrm{int}^1} = \sum_{\mathrm{int}^2 \in \mathrm{INT}^2} w_i^{\mathrm{int}^1,\mathrm{int}^2}, i \in I, \mathrm{int}^1 \in INT^1 \qquad (9)$$

Similar balances are required for the other stages required to treat different pollutants.

Splitting of the sources at the exit of the interceptors

Once the pollutants of the gaseous process sources are intercepted, the treated process sources are directed to the process sinks $g_{i,j}^{\mathrm{int}^1,\ldots,\mathrm{int}^N}$ and to the emissions discharged to the environment $g_{i,emission}^{\mathrm{int}^1,\ldots,\mathrm{int}^N}$:

$$w_i^{\mathrm{int}^1,\ldots,\mathrm{int}^N} = \sum_{j \in J} g_{i,j}^{\mathrm{int}^1,\ldots,\mathrm{int}^N} + g_{i,emission}^{\mathrm{int}^1,\ldots,\mathrm{int}^N}, i \in I, \mathrm{int}^1 \in INT^1, \ldots, \mathrm{int}^N \in INT^N \qquad (10)$$

Overall mass balance at the mixing point before any sink

The total flowrate inlet to any process sink G_j is given by the sum of the flowrates from the gaseous process source intercepted $g_{i,j}^{\mathrm{int}^1,\ldots,\mathrm{int}^N}$ and the flowrates from the fresh sources $f_{r,j}$:

$$G_j = \sum_{i \in I} \sum_{\mathrm{int}^1 \in \mathrm{INT}^1} \cdots \sum_{\mathrm{int}^N \in \mathrm{INT}^N} g_{i,j}^{\mathrm{int}^1,\ldots,\mathrm{int}^N} + \sum_{r \in R} f_{r,j}, j \in J \qquad (11)$$

Component balance at the mixing point before any sink

This balance is used to determine the composition of the pollutants at the inlet conditions of the process sinks $z_{j,c}^{InSink}$:

$$G_j z_{j,c}^{InSink} = \sum_{i \in I} \sum_{\mathrm{int}^1 \in \mathrm{INT}^1} \cdots \sum_{\mathrm{int}^N \in \mathrm{INT}^N} g_{i,j}^{\mathrm{int}^1,\ldots,\mathrm{int}^N} z_{i,c}^{Out,\mathrm{int}^1,\ldots,\mathrm{int}^N} + \sum_{r \in R} f_{r,j} z_{r,c}^{InFresh}, j \in J, c \in C \qquad (12)$$

Overall mass balance for gaseous emissions

The total flowrate of the gaseous emission discharged to the environment (*emission*) is given by the sum of the gaseous process sources from the interceptors emitted to the atmosphere $g_{i,emission}^{\mathrm{int}^1,\ldots,\mathrm{int}^N}$:

$$emission = \sum_{i \in I} \sum_{\mathrm{int}^1 \in \mathrm{INT}^1} \ldots \sum_{\mathrm{int}^N \in \mathrm{INT}^N} g_{i,emission}^{\mathrm{int}^1,\ldots,\mathrm{int}^N} \quad (13)$$

Component balance for the emission streams

This balance is needed to determine the amount of the gaseous stream emitted to the environment for each hazardous compound, Em_c:

$$Em_c = \sum_{i \in I} \sum_{\mathrm{int}^1 \in \mathrm{INT}^1} \ldots \sum_{\mathrm{int}^N \in \mathrm{INT}^N} g_{i,emission}^{\mathrm{int}^1,\ldots,\mathrm{int}^N} z_{i,c}^{Out,\mathrm{int}^1,\ldots,\mathrm{int}^N}, \quad \forall c \in C \quad (14)$$

The term Em_c is defined as the total amount of the emission for each hazardous compound c.

Equations to activate the fixed cost for the interceptors

The following relationships are required to determine the existence of the interceptor which depends on the maximum and minimum flowrates required to operate the treatment unit:

$$w_i^{\mathrm{intMIN}} z_i^{\mathrm{int}} \le w_i^{\mathrm{int}} \le w_i^{\mathrm{intMAX}} z_i^{\mathrm{int}}, \quad \forall i \in I, \ \mathrm{int} \in INT \quad (15)$$

Sink constraints

Each process sink includes a set of specific process constraints given in terms of the maximum $z_{j,c}^{InSink,UP}$ and minimum $z_{j,c}^{InSink,LO}$ compositions for the specific compound required to work properly:

$$z_{j,c}^{InSink,LO} \le z_{j,c}^{InSink} \le z_{j,c}^{InSink,UP}, \quad \forall j \in J, \ \ c \in C \quad (16)$$

Environmental constraints for the emission of the plant

The following constraint is required to specify that the plant is not allowed to discharge more emissions than the maximum constrained by the environmental regulation for the hazardous compounds $Em_c^{\max}$:

$$Em_c \le Em_c^{\max}, \quad \forall c \in C \quad (17)$$

Environmental constraints for the location of a new plant

These constrains determine the maximum permissible concentration for the hazardous compounds in each possible location $Conc_{p,c}^{\max}$.

$$Conc_{p,c} \le Conc_{p,c}^{\max}, \quad \forall p \in P, \ \ c \in P \quad (18)$$

Objective function

The objective function consists in minimizing the TAC, including the installation cost for the new plant ($CLand_l$), the cost for the fresh sources ($FreC_r$),operational costs for the interceptors (C_{po}^{int}) and cost for the treatment required ($FixC_{cap}^{\mathrm{int}}, VaC_{cap}^{\mathrm{int}}$), and the pumping cost for the different sections including the treatment ($TPumpingC_i^{\mathrm{int}}$), emission ($EmPumpingC_i^{\mathrm{int}}$), equipment ($EqPunpingC_{i,j}^{\mathrm{int}}$), and fresh sources ($FshPumpingC_{r,j}^{\mathrm{int}}$), minus the tax credit ($TaxCredit$) obtained for the reduction of the total emissions respect to a given maximum ($MaxEmission$). This way, the objective function is stated as follows:

$$\begin{aligned}
\min TAC = & \sum_{l \in L} CLand_l \, y_l + H_Y \sum_{r \in R} FreC_r \, F_r \\
& + H_Y \sum_{i \in I} \ldots \sum_{\mathrm{int} \in \mathrm{INT}} C_{op}^{\mathrm{int}} w_i^{\mathrm{int}} + k_f \\
& \times \left[\sum_{i \in I} \ldots \sum_{\mathrm{int} \in \mathrm{INT}} FixC_{cap}^{\mathrm{int}} z_i^{\mathrm{int}} + \sum_{i \in I} \ldots \sum_{\mathrm{int} \in \mathrm{INT}} VaC_{cap}^{\mathrm{int}} w_i^{\mathrm{int}} \right] \\
& + H_Y \left[\sum_{i \in I} \ldots \sum_{\mathrm{int} \in \mathrm{INT}} \left(TPipingC_i^{\mathrm{int}} w_i^{\mathrm{int}} + EmPipingC_i^{\mathrm{int}} g_{i,emission}^{\mathrm{int}} \right) \right. \\
& + \sum_{i \in I} \ldots \sum_{\mathrm{int} \in \mathrm{INT}} \sum_{j \in J} EqPipingC_{i,j}^{\mathrm{int}} g_{i,j}^{\mathrm{int}} \\
& \left. + \sum_{r \in R} \sum_{j \in J} FshPipingC_{r,j} f_{r,j} \right] \\
& - H_Y \, TaxCredit \, [MaxEmission - emission]
\end{aligned} \quad (19)$$

where H_Y represents the hours per year that operates the new plant, and k_f is the factor used to annualize the capital costs.

Interceptors' performance

The interceptors' performance is modeled through a conversion factor that is determined before the optimization process based on experimental data or simulation of given interception units (see for example Gabriel and El-Halwagi 2005; Ponce-Ortega et al. 2010). This way, the outlet concentration for the interceptors depends on the design and operating conditions for these units and these are fixed before the optimization process; therefore, the conversion factor $\alpha_p^{\mathrm{int}^1,\ldots,\mathrm{int}^N}$ is used to determine the concentration for the streams at the exit of the interception network as follows:

$$z_{i,c}^{Out,\mathrm{int}^1,\ldots,\mathrm{int}^N} = \alpha_c^{\mathrm{int}^1,\ldots,\mathrm{int}^N} z_{i,c}^{In}, \quad \forall i \in I, \ \ c \in C, \ \ \mathrm{int}^1 \in INT^1, \ldots, \mathrm{int}^N \in INT^N \quad (20)$$

Therefore, the model must determine the flowrate that is intercepted in each available unit (including the last one that is fictitious to model the bypass) to satisfy the process and environmental constraints.

The overall optimization model consists in minimizing (19) subject to (3–18), and this is a mixed integer non linear programming problem (MINLP).

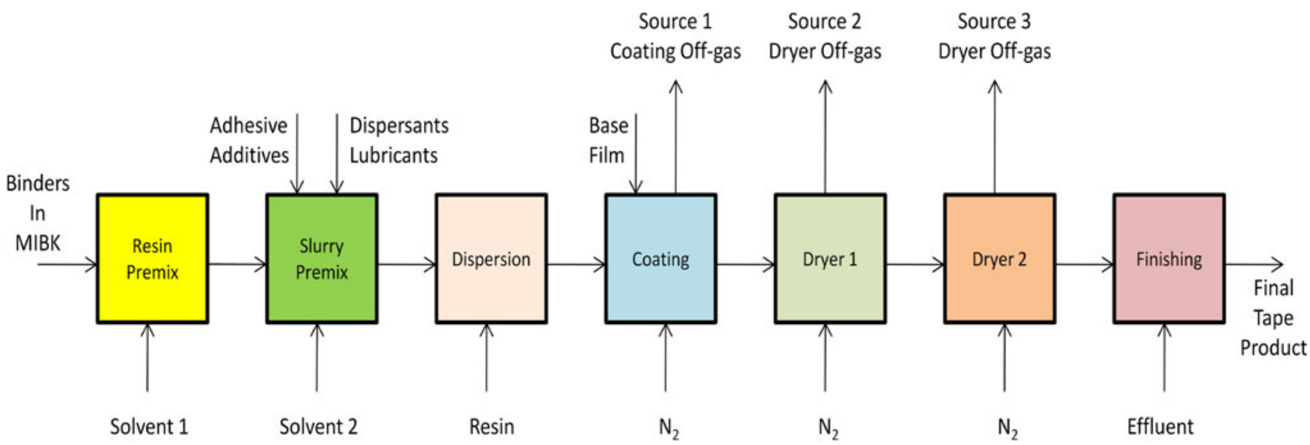


Fig. 4 Flowsheet for the process addressed in the Example 1

Table 1 Data for the gaseous process sources and the process sinks for the Example 1

Source	W_i (kg/h)	$z^{In}_{i,\text{MeOH}}$ (ppm)	Sink	G_j (kg/h)	$z^{InSink}_{j,\text{MeOH}}$ (ppm)
1	200	14	1	231	0.310
2	200	10	2	105	0.252
3	200	6			

Fig. 5 Optimal location for new plant for the Example 1

Case studies

Three examples are used to show the application of the proposed methodology. These examples consider the possibility to install a new industrial facility in the central part of Mexico, and different scenarios are presented to identify the best compromise between the costs and the environment. First, the general model formulation was programmed in the General Algebraic Modeling System (GAMS) and the solver DICOPT was used to solve the resulting MINLP problems (Brooke et al. 2010). For the examples presented, the tax credit used was zero.

Table 2 Pasquill–Giffort constants for the different locations for the Example 1

City	Option 1	Option 2	Option 3	Option 4
Guadalajara	3.19×10^{-8}	8.79×10^{-9}	3.52×10^{-8}	3.94×10^{-9}
Zacatecas	5.22×10^{-8}	1.20×10^{-8}	1.00×10^{-8}	3.28×10^{-9}
Aguascalientes	1.30×10^{-7}	3.04×10^{-8}	1.88×10^{-8}	4.69×10^{-9}
León	2.75×10^{-8}	9.77×10^{-8}	3.52×10^{-8}	7.77×10^{-9}
Querétaro	8.25×10^{-9}	2.64×10^{-8}	2.68×10^{-8}	2.45×10^{-8}
Morelia	7.98×10^{-9}	1.23×10^{-8}	1.26×10^{-8}	1.57×10^{-8}
Lázaro Cárdenas	3.98×10^{-9}	3.36×10^{-9}	4.82×10^{-8}	5.64×10^{-9}
Chilpancingo	2.28×10^{-9}	2.57×10^{-9}	1.27×10^{-8}	1.24×10^{-8}
Toluca	3.93×10^{-9}	6.10×10^{-9}	2.19×10^{-8}	1.45×10^{-7}
Distrito Federal	3.44×10^{-9}	5.38×10^{-9}	1.54×10^{-8}	7.19×10^{-7}

Table 3 Constraints for the emissions in each surrounded city for the Example 1

City	Environmental Constraints (ppm)
Guadalajara	0.00014
Zacatecas	0.00017
Aguascalientes	0.00016
Leon	0.00016
Queretaro	0.00015
Morelia	0.00018
Cd. Lazaro Cardenas	0.00019
Chilpancingo	0.00020
Toluca	0.00010
Distrito Federal	0.00005

Table 4 Installation cost for the locations of the Example 1

Option	Annualized installation cost ($/year)
1. Tabasco, Zacatecas	12×10^6
2. San Felipe, Guanajuato	11×10^6
3. Uruapan, Michoacán	13×10^6
4. Cuatitlan Izcalli, Mexico	14×10^6

Example 1. This example considers the recovery of volatile organic compounds (VOC) from adhesive tapes plant, the contaminants in this process are methanol (MeOH) and methyl-iso-butyl ketone (MIBK) due to the solvents used in the process of the adhesive tape manufacturing. The recovery of VOC is using condensation systems. In this case study, only the interception of the MeOH is considered. The mass integration for the VOC recovery was previously reported by Parthasarathy and El-Halwagi (2000) and Hamad and Fayed (2004); however, only the integration inside the industrial facility was considered previously, this means that the environmental problem for the pollutants emitted in the surrounding cities have not been considered properly. Figure 4 shows a schematic representation for the adhesive tape manufacturing process, where three process sources and two process sinks for the mass integration are identified. The data for the sources and sinks are shown in Table 1, which presents the characteristics of flowrates and compositions of the process sources. Table 1 also shows the conditions for the flowrates and compositions required for the process sinks. There is only one additional fresh source available to satisfy the process requirements and the unitary costs for this is $0.009/kg.

Table 5 Efficiency and costs for the interceptors for the Example 1

Interceptor	Efficiency α	Operation unit cost ($/kg)	Fixed interceptor cost ($/year)
INT^1	0.98	0.0065	1,500
INT^2	0.85	0.0033	1,300
INT^3	0.00	0.0000	0000

In this example, the central part of Mexico has been considered for the installation of the new industrial facility. Figure 5 identifies four possible options to install the new industrial plant and nine surrounding cities that may be affected by the gaseous emissions for the new plant. To consider the effect of the emissions in the surrounding cities, the conditions of the weather and direction and speed of wind are taken into account in each possible location. Table 2 shows the values for the constants of the Pasquill–Gifford model for each city depending on the option to locate the new plant. These values are necessary to calculate the dispersion parameters of the emissions and to know the concentrations in the nearby cities. These constants are calculated based on Eq. (2); notice that all the terms are constants except the total emission from each site, this way $z = 0$; $H_r = 11$ m, and the wind velocity u in

Fig. 6 Optimal solution for the interception system for the Example 1

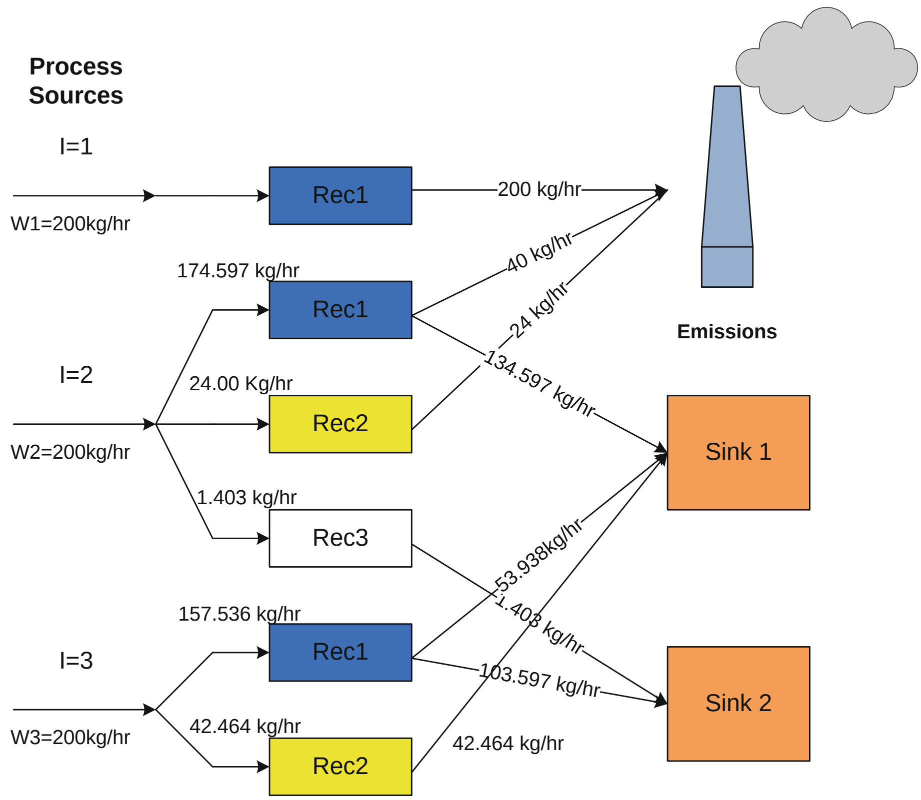


Table 6 Economic results for the location of the new plant for the Example 1

Location	Total annual cost ($/year)	Additional economic incentives required ($/year)
Option 1	12,353,770	999,998
Option 2	11,353,772	Optimal
Option 3	13,353,770	1,999,998
Option 4	14,353,770	2,999,998

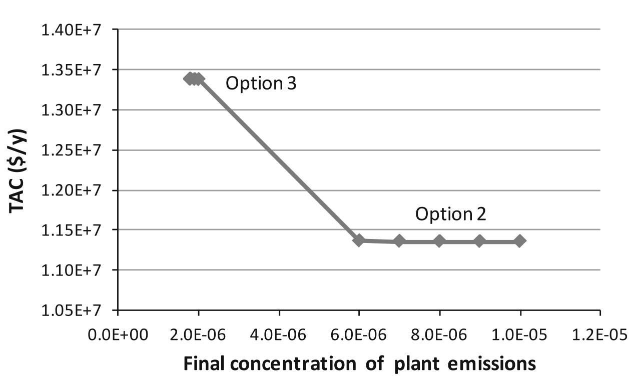


Fig. 7 Pareto curve for the Example 1

each location to install the new plant are obtained from meteorological information from web sites such as CONAGUA (2011), The Weather Channel (2011), and Meteored (2011) in the location, considering that the average wind velocity ranges from 1.0 to 5.0 m/s. The dispersion parameters are calculated as $\sigma_{y_{ip}} = 0.195x_{ip}^{0.90}$ and $\sigma_{z_{ip}} = 0.112x_{ip}^{0.91}$, where x_{ip} is the distance in meters from the possible option to locate the new plant i and the surrounding cities that will be affected by the installation of the new plant p. To obtain these distances, digital maps can be used (see for example Wanadoo 2011; Googlemaps 2011).

To consider properly the interactions between the processes inside the plant and the surroundings, it is necessary to include the environmental constraints for the emissions allowed in each location (see Table 3 for this case study). These environmental constraints are different in each city, and these depend on the environmental, geographic and weather conditions as well as the interactions with other emissions in the specific zone; therefore, these constraints are used to insure a sustainable process.

For each option to locate the new plant, there is a given installation cost that depends on the land cost, cost for transportation of raw materials and products, services, etc. Table 4 shows the installation cost for the locations identified in this example. The treatment system has different interceptors allowed to treat the gaseous process streams. Table 5 shows the operation and fixed costs and the efficiency to remove the hazardous compound for the interceptors allowed in this example.

Fig. 8 Optimal location for the new plant for the Example 2

Table 7 Data for the sources and sinks for the Example 2

Source	W_i (kg/h)	$z_{i,\mathrm{MeOH}}^{In}$ (ppm)	$z_{i,\mathrm{MIBK}}^{In}$ (ppm)	Sink	G_j (kg/h)	$z_{j,\mathrm{MeOH}}^{InSink}$ (ppm)	$z_{i,\mathrm{MIBK}}^{InSink}$ (ppm)
1	200	14	28	1	231	0.310	0.69
2	200	10	14	2	105	0.252	0.748
3	200	6	12				

Table 8 Constraints for the concentration in each city for the Example 2

City	Component 1 (ppm)	Component 2 (ppm)
Guadalajara	0.00014	0.00013
Zacatecas	0.00017	0.00016
Aguascalientes	0.00016	0.00015
Leon	0.00016	0.00015
Queretaro	0.00015	0.00014
Morelia	0.00018	0.00017
Cd. Lazaro Cardenas	0.00019	0.00018
Chilpancingo	0.00020	0.00019
Toluca	0.00010	0.00009
Distrito Federal	0.00005	0.00004
San Luis Potosi	0.00011	0.00010
Colima	0.00014	0.00013
Puebla	0.00016	0.00015
Celaya	0.00013	0.00012
Ciudad Valles	0.00018	0.00017

Table 9 Installation costs for the different locations of the Example 2

Option	Annualized installation cost (\$/year)
1. Tabasco, Zacatecas	12×10^6
2. San Felipe, Gto.	11.5×10^6
3. Uruapan, Michoacán	13×10^6
4. Cuatitlan Izcalli	14×10^6
5. Pachuca	13×10^6
6. Rio Verde	12×10^6
7. Ciudad Guzman	11×10^6
8. Tehuacan	14×10^6
9. Iguala	13×10^6

This example consists of 13 binary variables, 168 continuous variables, and 20 constraints, and it was solved in 0.094 s of CPU time. The solution of the optimization problem proposed in this paper yields the optimal location for the new plant in the option 2

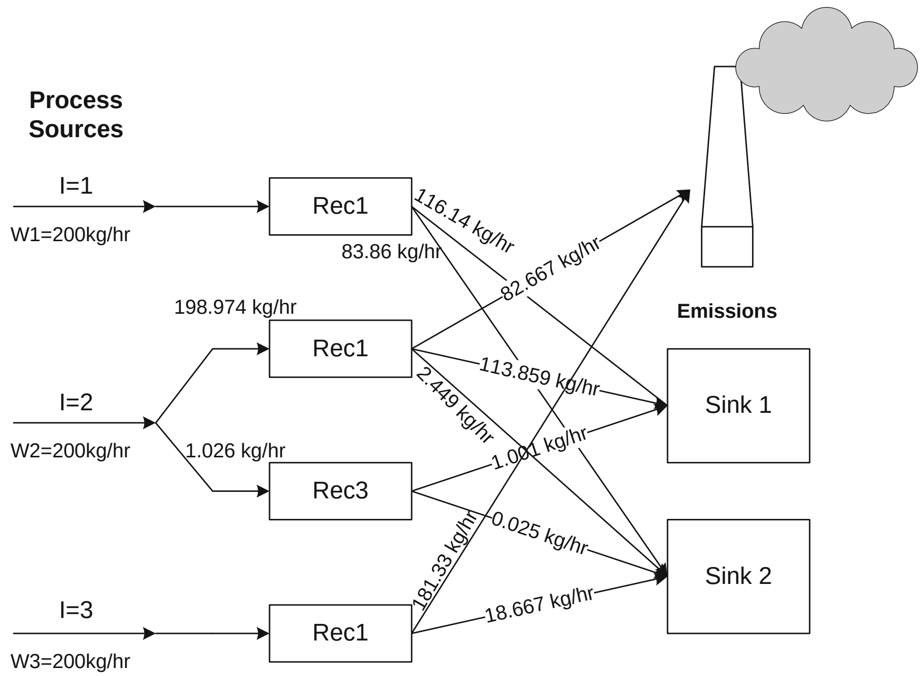


Fig. 9 Optimal solution for the treatment system for the Example 2

Table 10 Concentration in each city after the installation of the new plant of the Example 2

City	Component 1 (ppm)	Component 2 (ppm)
Guadalajara	7.73×10^{-6}	2.02×10^{-5}
Zacatecas	8.88×10^{-7}	2.32×10^{-6}
Aguascalientes	1.43×10^{-6}	3.74×10^{-6}
Leon	1.74×10^{-6}	4.55×10^{-6}
Queretaro	9.76×10^{-7}	2.55×10^{-6}
Morelia	1.81×10^{-6}	4.73×10^{-6}
Cd. Lazaro Cardenas	1.86×10^{-6}	4.86×10^{-6}
Chilpancingo	5.09×10^{-7}	1.33×10^{-6}
Toluca	7.04×10^{-7}	1.84×10^{-6}
Distrito Federal	5.59×10^{-7}	1.46×10^{-6}
San Luis Potosi	7.96×10^{-7}	2.08×10^{-6}
Colima	2.34×10^{-5}	6.13×10^{-5}
Puebla	3.9×10^{-7}	1.02×10^{-6}
Celaya	1.25×10^{-6}	3.29×10^{-6}
Ciudad Valles	4.28×10^{-7}	1.12×10^{-6}

corresponding to San Felipe, Gto (see Fig. 5) with a *TAC* of $11,353,772/year. The in-plant interception network is shown in Fig. 6, notice that several interceptors are required to eliminate the pollutant to satisfy the process and environmental constraints. Table 6 shows the solutions of the problem for the cases when the location for the new industrial facility is fixed (i.e., not optimized). This information is very useful to identify the governmental incentives required to install the new industrial facility in a location different to the optimal one.

Table 11 Total annual cost for each option of the Example 2

Location	Total annual cost ($/year)
Option 1	12,389,854
Option 2	11,889,854
Option 3	13,389,854
Option 4	14,214,059
Option 5	13,389,854
Option 6	12,389,854
Option 7	11,389,854
Option 8	14,389,854
Option 9	13,389,854

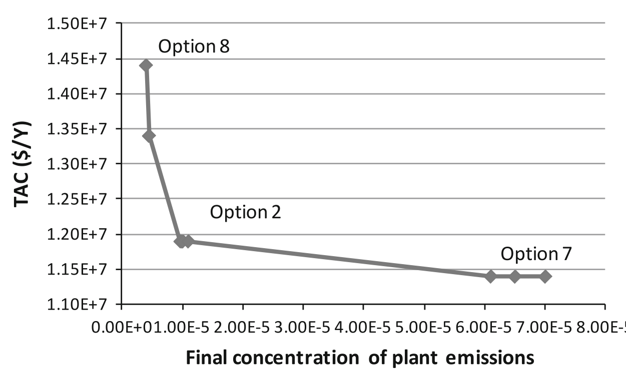


Fig. 10 Pareto curve for the Example 2

Table 12 Streams data for the Example 3

Source	W_i (kg/h)	$z_{i,Comp1}^{In}$ (ppm)	$z_{i,Comp2}^{In}$ (ppm)	Sink	G_j (kg/h)	$z_{j,Comp1}^{InSink}$ (ppm)
1	1,088	0.460	0.5	1	544	0.050
2	816	0.570	0.9	2	1,152	0.150
3	1,587	0.490	0.7	3	446	0.015
4	698	0.001	1.8	4	712	0.001
5	1,791	0.005	5.4	5	521	0.010
6	1,351	0.054	1.4	6	394	0.005

Table 13 Data for the interceptors for the Example 3

Interceptor	Efficiency *Comp1*	Efficiency *Comp2*	Operation unit cost ($/kg)	Fixed cost interceptor ($/year)
INT^1	0.98	0.90	0.0043	1,300
INT^2	0.85	1.00	0.0065	1,600
INT^3	0.95	0.90	0.0033	1,200
INT^4	0.00	0.00	0.0000	0000

Table 14 Constraints for the concentration for the cities for the Example 3

City	Compound 1 (ppm)	Compound 2 (ppm)
Guadalajara	0.00014	0.00013
Zacatecas	0.00017	0.00016
Aguascalientes	0.00016	0.00015
Leon	0.00016	0.00015
Queretaro	0.00015	0.00014
Morelia	0.00018	0.00017
Cd. Lazaro Cardenas	0.00019	0.00018
Chilpancingo	0.00020	0.00019
Toluca	0.00010	0.00009
Distrito Federal	0.00005	0.00004
San Luis Potosi	0.00011	0.00010
Colima	0.00014	0.00013
Puebla	0.00016	0.00015
Celaya	0.00013	0.00012
Ciudad Valles	0.00018	0.00017

Figure 7 shows the set of Pareto solutions for different concentrations of the pollutants emitted by the new plant. This Pareto curve is obtained by the constraint method (Diwekar 2008), notice that the solutions above the curve represent suboptimal solutions and that the solutions below the curve represent infeasible solutions. Two locations for

Table 15 Options to install the new industrial plant for the Example 3

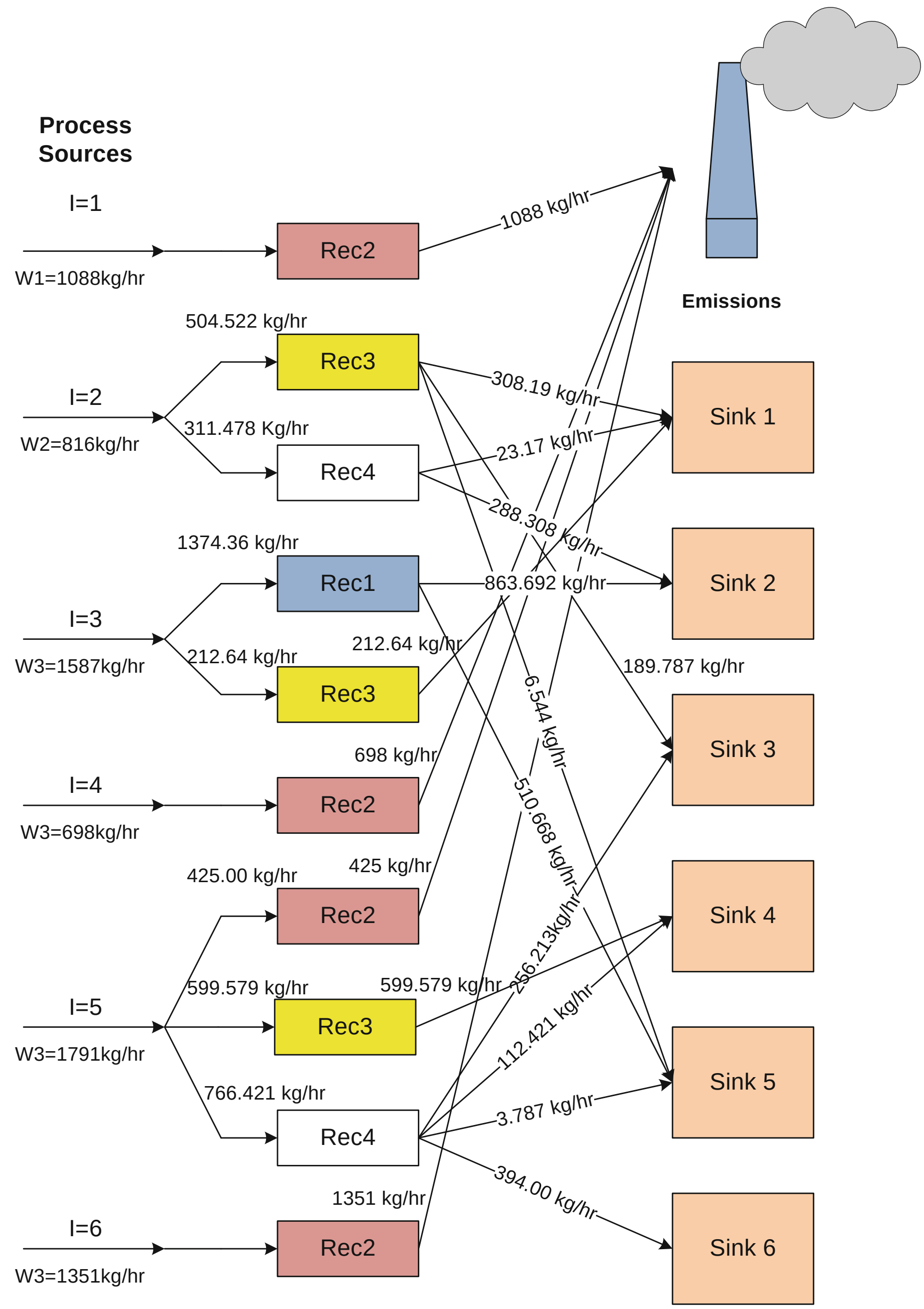
Option	Annualized installation cost ($/year)
1. Tabasco, Zacatecas	12×10^6
2. San Felipe, Gto.	14×10^6
3. Uruapan, Michoacán	13×10^6
4. Cuatitlan Izcalli	14×10^6
5. Pachuca	12×10^6
6. Rio Verde	12×10^6
7. Ciudad Guzman	11×10^6
8. Tehuacan	12×10^6
9. Iguala	13×10^6

Fig. 11 Optimal location for the Example 3

the new industrial facility are identified in this figure, location in option 3 (i.e., Uruapan, Michoacán) is selected for the low emissions and higher costs; whereas location in option 2 (i.e., San Felipe, Guanajuato) is selected for low cost but higher emissions. Figure 7 can also be used to determine the tax credit required for a given reduction in the concentration of the hazardous compounds in the new emission.

Example 2. This example problem considers the installation of a new industrial facility in Mexico, taking into account 15 cities that can be affected by the emission of the new plant and 9 possible locations to install this new plant like it is shown in Fig. 8. As in the previous case study, the VOC recovery process from adhesive tape plant is considered, also three sources and two sinks are considered,

Fig. 12 Optimal solution for the treatment system for the Example 3



but in this example two pollutants (MeOH and MIBK) are taken into account to increase the complexity of the problem. Table 7 shows the data for the process sources and sinks for this example. Table 8 shows the environmental constraints in each surrounding city for the pollutants considered in this example problem. Notice that there are different restrictions for each pollutant in each city, this is because of the interaction with other emissions and the environment. Table 9 shows the installation costs for the 9 possible options to locate the new industrial plant, this cost includes the land cost, cost for transportation of raw materials and products, and cost for services, between others.

This example consists of 18 binary variables, 383 continuous variables, and it was solved in 0.282 s of CPU time. In this case, the optimal solution to install the new plant is in the option 7 (see Fig. 8) and the *TAC* is \$11,389,854.11/year. Figure 9 shows the optimal interception network to satisfy the process and environmental constraints for the gaseous emissions. Notice in this figure that the interceptor 2 is required to treat some part of the flowrate of process source 1, whereas the interceptor 1 is required to treat the process source 3. The total

Table 16 Concentration in each city after the installation of the new plant of the Example 3

City	Compound 1 (ppm)
Guadalajara	1.746×10^{-6}
Zacatecas	2.005×10^{-7}
Aguascalientes	3.232×10^{-6}
Leon	3.933×10^{-6}
Queretaro	2.204×10^{-7}
Morelia	4.088×10^{-6}
Cd. Lazaro Cardenas	4.2×10^{-6}
Chilpancingo	1.149×10^{-7}
Toluca	1.59×10^{-7}
Distrito Federal	1.262×10^{-7}
San Luis Potosi	1.797×10^{-7}
Colima	5.298×10^{-5}
Puebla	8.816×10^{-7}
Celaya	2.843×10^{-6}
Ciudad Valles	9.681×10^{-7}

Table 17 Total annual cost for different options to install the new plant for the Example 3

Location	Total annual cost($/year)
Option 1	15,003,488
Option 2	17,003,488
Option 3	16,003,488
Option 4	17,065,264
Option 5	15,003,488
Option 6	15,003,488
Option 7	14,003,488
Option 8	15,003,488
Option 9	16,003,488

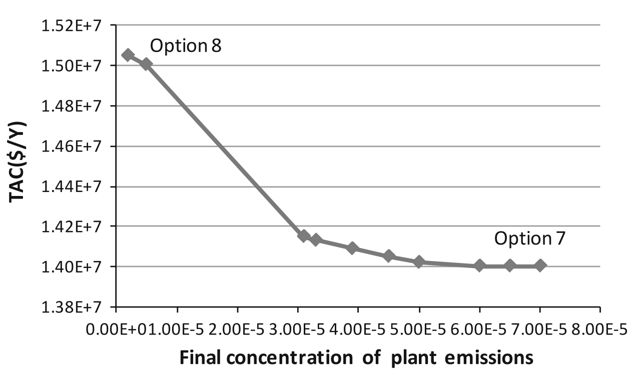


Fig. 13 Pareto curve for the Example 3

emissions discharged to the environment are 264 kg/h with flowrates for the pollutants 1 and 2 of 38.29 and 100 kg/h, respectively. Table 10 shows the concentration in the surrounding cities due to the emissions for the installation of the new plant.

To analyze different options, the location of the new plant is fixed to identify the governmental incentives required to install the new plant in these locations; this way, Table 11 shows the *TAC*s obtained for the different locations. Notice that option 2 requires an incentive of $500,000/year to be economically attractive; this means that the government of location 2 has to bring $500,000/year as incentives to the plant to generate additional jobs in that place, and a similar analysis can be done for the other locations.

Figure 10 shows the Pareto curve for the Example 2, this figure represents the compromise between the total cost and the emissions for the new plant; for higher emissions the costs increase, whereas for lower emissions the costs decrease. Notice also that the location for installing the new plant changes from location 8 (for lower emissions) to locations 2 and 7 for higher emissions. From Fig. 10 can be obtained the tax credit required for the reduction of the concentration in the plant emission.

Example 3. For this case study, six gaseous process sources and two toxic compounds were considered, and Table 12 shows the data for the process sources and sinks. Three interceptors are available to treat the process sources to satisfy the process and environmental constraints, and Table 13 shows the efficiency to remove the pollutants and the operational and fixed costs for each interceptor. Fifteen cities that may be affected by the emissions from the new plant were considered in this example. Table 14 shows the allowable limits for the emissions of each compound according to the environmental regulations. In addition, nine options are identified for the location of the new industrial facility and these are shown in Table 15.

The problem consists of 33 binary variables, 580 continuous variables, and 20 constraints, and the CPU time to solve this problem is 0.124 s. After solving the mathematical programming problem, location 7 is identified as the best option to install the new plant with a *TAC* of $14,003,488/year (see Fig. 11). The optimal location takes into account the environmental regulations for the emissions to consider the effect on nearby cities. Figure 12 shows the in-plant treatment system required to satisfy the process and environmental constraints, notice that several segregations and interceptors are required, the total emissions are 3,562 kg/h with flowrate for the hazard pollutant of 86.43 kg/h. For the nearby cities, this solution allows to have concentrations for the emission as shown in Table 16, which satisfies the sustainability constraints considering the interaction with other emissions.

Table 17 shows the results obtained when the location to install the new industrial facility is fixed. This information allows identifying that options 1, 5, 6, and 8 require incentives by $1,000,000/year to be economically attractive to install the new plant. This problem also allows to see that for this case the process constraint are dominant because for several locations the associated cost is the same.

Figure 13 shows the Pareto curve that compensates the total costs and the constraint for the emissions for the Example 3, this figure shows that for lower costs the location in site 7 is selected, whereas for lower emissions the location selected is in site 8. The information provided by Fig. 13 can be used to obtain the tax credit required for a given concentration of the hazardous compound in the emission discharged from the plant in a given location; for example, there is required a tax credit by one million dollars per year to yield a reduction of 77 % in the concentration of the emission of the plant changing the location from option 7 to option 8. These Pareto solutions allow to identify the tradeoffs between the considered objectives.

Conclusions

This paper has presented a new approach along with an optimization approach for including the impact of recycle/reuse of gaseous emissions as well as their interactions with the surroundings on the selection of site location for industrial facilities. The proposed model allows the management of gaseous emissions through in-plant recycle/reuse, end-of-pipe treatment, and dispersion into the surroundings while tracking the pollutants inside and outside the plant and satisfying environmental constraints within the plant and at various urban centers surrounding the facility. The model is driven by the objective of minimizing the total annualized cost which includes the plant installation, the fresh sources, and the interception devices to satisfy the process and environmental constraints. The model has also been used to identify the governmental incentives required to render a given location economically attractive while satisfying the environmental constraints. Three case studies have been solved. The results show the merits of this holistic approach and its ability to identify different options for managing the gaseous emissions in the plant and within the surrounding areas.

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