

VOL. 77, 2019





DOI: 10.3303/CET1977064

The Choice among Competing Technologies in Process Plants. Risk Based Approach

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Process industry is characterized by the existence of several, usually competitive, technical solutions that can be used to achieve a certain result. In this paper competing technologies for the treatment of lean VOC-air mixtures are compared on the basis of more relevant operational parameters: the energy consumption, the out-of-service time and monetary risk. Two systems has been compared in this paper: a catalytic fixed-bed reactor in which the heat recovery is guaranteed by a heat exchanger - traditional plant, and a "intensified" plant, where a catalytic reverse-flow reactor is installed, able to achieve and internal heat recovery through the periodical reversal of the flow direction. The decisions-making would require a full picture of the plant behaviour in regime conditions, but also during transients deviations following a failure and the related recovery actions. This picture can be obtained through the Integrated Dynamic Decision Analysis, that generates the full set of possible sequences of events that could result in plant unavailability, with their probability of occurrence and the effect on energy consumption. Results are expressed in terms of out-ofservices times, that for operatively sake have to be minimized of energy absorbed by each piece of equipment and cost for the VOC treatment. Outcomes evidenced the pros and cons of the two plants. The "traditional" plant guarantees a better continuity of service, but also higher operational costs. The "intensified" plant shows lower operational costs, but a higher complexity, with a need of more level of protection to obtain a comparable out-of-service time. The quantification of risks and benefits allows the comparison between competing technologies to be performed on a complete picture of the behaviour of the plants, promoting a more effective decision-making process.

1. Introduction

Process industry is known to offer multiple solutions to address different production and manufacturing requirements, continuously developing thanks to the technological and materials advancements. Considering, as an example, the Volatile Organic Compounds (VOCs) treatment, the available solutions include: combustion (homogeneous and catalytic), absorption (Chen and Liu, 2002), adsorption (Ruhl, 1993), etc. Some of the alternative available technologies could be discarded because of the process constraints, as feed composition, output requirements, etc. E.g., for a feed with low concentrations of VOCs (lower than 1%), the only possible approach is the catalytic combustion. Nevertheless, also to carry out the catalytic combustion of VOCs different competing technologies are available, as the more traditional fixed bed reactor, the reverse flow reactor (Fissore, et al., 2005), the monolithic reactor (Mazzarino and Barresi, 1993), and others.

Choosing the optimal solution among competing technologies is certainly a problem of costs of investments, but this aspect is more and more complemented with operational aspects related to the productivity (Comberti et al., 2019), as reliability, operational costs and, among them, the energy consumption.

For the catalytic combustion, depending on the catalyst uses and the chemical compounds to be removed, the combustion temperature may range between 200°C and 500°C. To reduce the energy consumption, some kind of energy recovery is required. In the heat recovery section of the plant, the feed is pre-heated at the reaction temperature trough part of the energy contained in the exhaust gases. The heat recovery is usually not complete and, thus. the energy efficiency is rarely higher than 70% (Barresi, Baldi, & Fissore, 2007).

Paper Received: 23 November 2018; Revised: 5 May 2019; Accepted: 13 July 2019

Please cite this article as: Baldissone G., Demichela M., Fissore D., 2019, The choice among competing technologies in process plants. Risk based approach, Chemical Engineering Transactions, 77, 379-384 DOI:10.3303/CET1977064

A more efficient technology, from this point of view, is represented by the reverse flow reactor, proposed by Cottrell (1938). In this type of reactor, the heat recovery occurs in the reactor itself: the heat of reaction heats up a solid layer inside the reactor, that, at the reactor inversion, cools down, heating the feed gases to the reaction temperature.

The reverse flow reactor was proposed and applied for catalytic combustion (Nieken and Eigenberger, 1994) and also in (Zufle and Turek, 1997) for air purification (Van de Beld and Westerterp, 1996) and in the case of the VOCs treatment (Fissore, et al., 2005). The reverse flow reactor is a flexible technology because it can easily manage variations of composition and concentration in the feed stream (Cittadini et al., 2001) also discussed in (Chen et al., 2011). To manage low concentration stream of VOCs it may require also an electrical heater in the center of the reactor (Barresi, Baldi, & Fissore, 2007).

The reverse flow reactor results to be more complex than the traditional fixed bed one, but despite its higher complexity, directly related to higher investment costs, it was proven to be more convenient than the fixed bed reactor plant for VOCs treatment (Baldissone, Fissore, & Demichela, Catalytic after-treatment of lean VOC–air streams: Process intensification vs. plant reliability, 2016). In fact, the reduction of the operational cost (e.g. catalyst cost, restoration cost,...) covers the higher costs due to the plant complexity.

The comparison made in (Baldissone, Fissore, & Demichela, Catalytic after-treatment of lean VOC-air streams: Process intensification vs. plant reliability, 2016) did not consider the energy consumption within operational parameters, that is instead shown in the present paper, as an optimization parameter to choose among competing technologies.

The energy consumption is evaluated at the design operating condition and in case of deviations in the feed composition or equipment fault. The expected value of energy consumption for the two plants is evaluated and compared, together with the expected value of the out of service time.

To compare the two alternatives on the basis of all the possible scenarios the system could undergo, taking into account also their probabilities, the Integrated Dynamic Decision Analysis (IDDA) is applied.

IDDA was developed by Remo Galvagni and proposed in the eighties of the twentieth century (Clementel and Galvagni, 1984) and in (Galvagni and Clementel, 1989). IDDA was then applied to different case studies to support the risk based decision making: an allyl-chloride production plant design (Turja and Demichela, 2011) and extended in (Demichela and Camuncoli, 2014), the LPG tank pressure test procedure optimization (Gerbec, Baldissone, & Demichela, 2016), the overflowing of a tank (Demichela and Piccinini, 2008), a formaldehyde plant modification (Demichela et al., 2017) and in (Baldissone et al., 2017).

The IDDA methodology joints a logical – probabilistic model and phenomenological model.

The phenomenological model is a mathematical description of the plant behavior in normal condition and in case of process deviations and/or equipment fault. The phenomenological model provides the process variables trends, and in the present case, the energy consumption in the different plant conditions.

The logical – probabilistic model is based on the logic analysis of the plant behavior. The logical analysis discloses all the possible sequences of events the plant could undergo, together with their probabilities of occurrence.

The connection between the logical – probabilistic model and the phenomenological model allows the riskbased decision making to be performed on a wider knowledge base that the one disclosed by traditional risk assessment techniques (Demichela and Piccinini, 2008) and updated in (Demichela and Camuncoli, 2014). In Section 2 the case study is described in detail. Then in Section 3 the results are discussed and analyzed.

2. Materials and Methods

2.1 Case study

The two plants under analysis treat 5000 Nm³/h of gas stream with 0.2% of VOCs (ethylene). The feed stream is at 230°C and 1.12 bar. In the output stream the VOCs concentration must not exceed 50 ppm. This feed corresponds to an inert stream in a polymerization plant, to be purified before recycling. For the combustion of the VOCs an oxidant has to be added, paying attention to the fact that the oxygen concentration in discharged stream must remain below 0.01%. In the fixed bed plant the operating temperature is around 350°C, and a catalyst based on Platinum (015%) and Palladium (0.15%) supported on alumina is used. The catalyst is in form of pellet, with diameter ranging between 2 and 4 mm. The reverse flow reactor operates at temperature around 430°C. With this temperature a metal oxide catalyst, Cooper (3.34%) and Manganese (5.44%) supported on alumina, is adapt. This catalyst is in form of pellets, with diameter from 4 to 6 mm.

For both plants a reactor with 1.5 m diameter and 0.6 length is used. In the fixed bed reactor, the reactor is filled of catalyst. In the reverse flow reactor, the reactor is divided in 3 layers. The central layer contains the catalyst, while the top and bottom layers are made of alumina, in spherical pellets with diameter similar to that of the catalyst (4 - 6 mm), acting as thermal flywheel.

Figure 1a shows a simple scheme of the fixed bed plant, while in Figure 1b the scheme of the reverse flow plant is given.



Figure 1: Plants schemes, (a) fixed bed plant, (b) reverse flow plant

Some sections and pieces of equipment are similar in the two plants:

- the blower (B-1), used for the gas feed;
- the oxygen feed line, and its control system;
- the filter (F-1), used to intercept possible solid particles contained in the gas.

The fixed bed plant includes also:

- a heat recovery device (H-1) used for preheating the feed gas through the heat of the discharged gas;
- the heater (H-2), an electrical heater used to bring the feed gas at the reaction temperature;
- the reactor (R-1) where the oxidation reaction occurs.

Instead, the reverse flow plant includes:

- the reactor (R-2), an intensified reactor where the oxidation reaction occurs together with the heat recovery;
- the heater (H-3), used to control the rector temperature and for the start-up phase (Fissore, et al., 2005);
- the valves (V-1, V-2, V-3, V-4, V-5) used to control the gas flow direction in the reactor. During the normal condition only two valves are opened at the same time, V1 and V4 (or V2 V3). Periodically, the couple of open valves is changed to reverse the flow direction of the gas. Valve V-5 is used only in case of an emergency, for cooling down the reactor.

In the two plants a series of alarm and protective devices are present.

2.2 Logical – probabilistic model

The logical – probabilistic model is a logical description of the plant behaviors, based on a functional analysis of the plant.

The logical model is based on a series of question and affirmation. Each question represents the possible events that can occur in the plant (e.g. equipment fault, operator error, ...). The answers to the questions represent the possible outcomes of the event. An occurrence probability is coupled to each outcome. The probability data were obtained by the literature (Mannan, 2005) and the plant management. For a correct comparison between the two plants, the same probability data were assigned to similar events.

The different events (questions and affirmations) are used to build a network of possible sequences describing the plant behavior.

The logical analysis is written in appropriate syntax, to allow the software IDDA 2.0 evaluating all the sequences of events the plant could undergo.

The evaluation of all sequences of events can require high computational resources. In order to control the necessary computational resources a cut-off value is used. It is a probability threshold below which the sequences are assumed to be negligible. The probability of the neglected sequences of events are collected in the residual probability. The cut-off value is thus chosen to optimize the computational resources and the residual probability.

For the fixed bed plant, a cut-off value of 10⁻¹⁶ was used: 3,901,910 sequences of events were evaluated, with a residual probability of 7.5×10⁻¹¹.

The sequences bringing to the discharge with high concentration of VOCs sum up to a probability of 8.37×10^{-3} (1,955,342 sequences of events).

For the reverse flow plant, 5,336,624 sequences of events were evaluated with a cut-off value of 10^{-12} and a residual probability of 2.9×10^{-6} . In this plant the discharge with high VOCs concentration have a probability of occurrence of 1.32×10^{-2} (1,134,625 sequences of events).

2.3 Phenomenological model

The phenomenological model was applied to the sequences of events bringing to a discharge with an excess of VOC, with 3 or less equipment fault.

For the fixed bed plant, the phenomenological model was applied to around 1,285,000 sequences of events, with the 99% of probability. These sequences of events were divided in 843 different possible dynamic scenarios. For the reverse flow plant, the phenomenological model was applied to 1640 different dynamic scenarios, collecting around 1,672,000 sequences of events, with a probability around the 85%.

In the phenomenological model plant dynamic models are used. The mathematical equations were solved with Matlab® software.

Several parts of the model are common to both plants, such as:

- Blower (B-1): The output pressure is evaluated to supply the pressure drop in the plant. The compression work is evaluated assuming an adiabatic compression (Green and Perry, 2008). Also the discharge temperature is evaluated assuming an adiabatic compression.
- Filter (F-1): In case of normal condition the flow throughout the filter is not modified. Instead, in case of the filter clogged the flow is modified.
- Oxygen input: the oxygen feed flow is evaluated on the basis of the oxygen concentration required in the discharged gas.

The specific equipment for the fixed bed reactor plant is modeled as the following way:

- Heat recovery device (H-1): The heat recovery device is modeled by the heat balance and heat transfer equation.A 30% reduction of the heat exchange transfer is assumed to model the case of heat exchanger malfunction because of dirtying.
- Heater (H-2): In the heater, the heat used to reach the reaction temperature is evaluated though the heat balance. In the model, also the heater malfunction is taken into account: in one case, the heater gives continuously the maximum value of heat (100 kW), whilein the other case the heater does not give any heat. In case of heater malfunction equation 6 allows evaluating the discharge temperature.
- Reactor (R-1): The reactor behavior is modeled though the energy and the mass balance. The energy balance is written for the gas phase and for the solid. In the mass balance, the chemical reaction is considered instantaneous and complete at the reaction temperaturewhere y_{VOC} is the VOC as fraction, y_{O2} is the oxygen mass fraction, M_{VOC} is the VOC molar mass and M_{O2} is the oxygen molar mass.

To model the equipment present only in the reverse flow reactor plant the following considerations were used: Reactor (R-2): the catalyst layer is modeled in the same way of the reactor R-1. The same model is used for the inert layer but in this case is not taken into account the reaction terms.

Heater (H-3): This heater is used only for control purposes: it takes into account only tree possible heat emissions, namely 0, 2 and 4 kW. The heat balance in the gas phase is evaluated.

2.4 Energy consumption and out of service time expected values

The comparison between the two plants is done comparing the expected value of the annual plant energy consumption in case of normal operational conditions and in case of equipment fault.

The energy consumption in the fixed bed reactor plant includes the energy used in the blower (B-1) and in the heater H-2. In the reverse flow plant, the energy consumption takes into account the blower (B-1) and the heater H-3, when required.

The expected value better describes the energy consumption with respect to the nominal energy consumption, because it takes into account also the malfunction conditions with their probability.

Intervention	Estimated time
Restore filter	3 h
Restore system of input of oxygen	2 h
Restore heat recovery	5 d
Restore heater	1 d
Restore blower	1 d
Restore valve of reactor	2 d
Restore heat control inside of reactor	3 d
Replace catalyst in traditional plant	7 d
Replace catalyst in intensified plant	7 d
Plant stop	1 d

Table 1. Summary of time loss

With respect to the out-of-service time, it is evaluated as the sum of the restoration times of the different pieces of equipment failed (Table 1). The restoration time is provided by the plant management.

3. . Results

On the basis of the results obtained with the IDDA methodology, for each year of activity (8760 h), the reverse flow plant shows an expected value of energy consumption around 136950 kWh, lower than the value of the fixed bed plant (around 713800 kWh). Nevertheless, with reference to the operational continuity, the fixed bed plant shows an expected value of out of service time lower (29.25 h) than the reverse flow reactor plant (76.9 h). In Figure 2a the probability and the energy consumption for a sample of 1000 sequences of events, those with the higher contribution to the energy use. The size of the dots represents the contribution of each sequence to the expected value.



Figure 2. Energy consumption: (a) for the reverse flow plant, (b) for the fixed bed plant

The more contributing sequences are those characterized by the transient with the filter clogged, that, before the cleaning operations, require more compression energy.

The more important sequence (1) represents the filter clogged. The next more important sequences of events represent the case where at the filter clogged is coupled, fault at the oxygen control (2) and fault at the blower flow control (3, 4, 5). All this sequences of events have mean energy consuming (around 161000 kWh). But there are more relevant because their have high probability of occurrence.

Figure 2b shows the data for the fixed bed plant.About the energy consumption, the more relevant sequences of events involve the filter clogging, in same case coupled with the fault of the devices of the oxygen control system (2, 3, 4). Despite they are less relevant from the energy consumption point of view with respect of those involving the failure of the heater H-2, their importance is increased by their higher probability of occurrence.

4. Conclusion

When choosing among competing technologies available in process plants to address a given production target, the operational constraints and the investment costs are certainly the first screening tools. But immediately after, the operational parameters play a central role to support the decision making. Among them, as they affect costs and productivity, energy consumption and out-service times are important reference parameters.

In this paper a case study about the selection between different available technologies for the treatment of process streams in which VOCs have to be removed has been investigated.

The results of the integrated analysis of the probabilities of occurrence of unwanted events and their impact on productivity and energy consumptions allows the following conclusions can be drawn.

Considering the benefits related to the minimization of the operational costs, the intensified plant appears to be the best option, since it can run with a less expensive catalyst and it requires less energy. In fact, it shows an expected value of energy consumption around 136950 kWh, lower than the value of the fixed bed plant (around 713800 kWh). Analyzing the time losses following a failure, the fixed bed shows an expected value of out of service time lower (29.25 h) than the reverse flow reactor (76.9 h). For both plants the more critical system from the energy point of view appears to be the filters and the oxygen input control, both systems that requires a particular attention during operations and inspections and maintenance.

The different expected values figures provide to the management a global view of the plant foreseeable behavior, allowing a more informed decision. This last will then depends on the final aim of the plant managers, that have in any case available the full picture of the behavior of the plant alternatives. The IDDA analysis, used to draw the foreseeable behavior of both the plants allows analyzing in a systematic way the plant performances in case of normal condition and in case of process deviation and/or equipment failure. It also allows to evaluate the occurrence probability of the unwanted outcomes, but also their expected values in a cost-benefit form.

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