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ANALOGIES BETWEEN CHEMICAL REACTIONS AND QUALITY OF WORKPLACE ENVIRONMENT

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Abstract. Analogies are useful to deepen understanding of the object of study. Chemical reactions have an interesting behaviour, for a better comprehension they could be related with the real live situations. Thinking about the work organization problems is an important part of the learning. We try to find a connection between these two areas.

Keywords: continuing education; public understanding; analogies/transfer; reactions

The meeting of two personalities is like the contact of two chemical substances: if there is any reaction, both are transformed.

Carl Jung (1933)

Introduction

Analogies are comparisons between two domains (Orgill et al. 2015) that are considered a useful procedure to explain concepts or processes, introducing a new point of view. For example, Fuster and Sampedro (2008) compared the circulation problems that lead to myocardial infarction with traffic jams.

Chemical Engineering makes an extensive use of analogies, for example between the different kinds of transport phenomena, these analogies correspond to a similarity between the mechanisms of these processes resulting in virtually identical mathematical models. Thus, the solution and the understanding of one of these phenomena serves and assists in the solution and the understanding of another (Bird et al. 2002). In this case, the relationship between these domains is very deep.

Sometimes, to facilitate the teaching, the analogy is established between one process and an everyday situation (Fernandez-Torres 2005) with which the similarity may be casual or of a lower level. An interesting example could be the name of some enzymatic reactions," lock and key" is an image that helps to understand this mechanism (Fogler 2017). It could be a way to introduce a transversal subject in the regulated teaching.

Chemical reactors and chemical reactions have a special behaviour, in part because of possible non-linear kinetic model. In spite of this, analogies can be found with some processes with sharing a mathematical representation. Thus, Henda (2001) proposed that reactive systems can be simulated by hydrodynamic models and Hsu *et al.* (2001) examined the reactions of the Michaelis-Menten type with a predator-prey system. The general form of chemical reactions kinetics has been recognized by economists in the famous Cobb-Douglas production function (Hannon, 1997); they proposed an analogy between biology and economics and pointed out that "analogy seems to be the lifeblood of the creative scientist". In our days, we can highlight the use of reaction networks to simulate the dynamics of the spread of a virus (Peter et al., 2019).

The use of analogies has some problems related to a non-appropriate extension. As an example of these extensions, Mans (2014) analyzed the use of LEGO pieces to model the molecules taking part in a chemical reaction for very young students; these pieces can be connected in a good order (H-O-H, for example) or in one unreal (H-H-O).

In this article, we try to find similarities between reactive systems and some problems of the workplace (poor organization, stress, harassment, burning sensation, etc.). Thus, we show some examples to illustrate the reaction processes and, at the same time, we propose to the students a way of visualizing the effects of these problems on the work process.

Presentation

Problems in the workplace

The working environment is a broad term and means all the physical and human circumstances in which the job is conducted. The problems that appear are for both physical-chemical (lighting, ergonomics, pollution, etc.) or organizational (relationships, stress, harassment, etc.). This can ultimately result in a degradation of the work process and workers' health, negative company image and workers' reduced commitment and satisfaction (Steffgen et al. 2015).

To be healthy, a job must be alive, that is, it should provide personal growth through the incorporation of new knowledge and methods. The negative effects of poor work organization are obvious and generally accepted, but people are often unaware of the damage caused by it. It is interesting to prevent these problems, and education is a good way to achieve this prevention.

This subject could be a transversal one to be introduced in several lectures. To do that, we need a way to highlight view them. Perhaps reactive processes can help to make them more visible. Some examples of different degrees of complexity will be proposed.

General situation

The development of the work process and associated issues as personal growth can be compared to the progress of a chemical reaction. Just as a responsible person has to direct the work in the most effective way, a reactor must also be run in the same way. For this, different options are available, the type of reactor, its thermal behaviour, the composition of the mixture, the use of inert, etc. We can consider an irreversible chemical reaction developed in an isothermal reactor. The evolution of the degree of conversion X with time is obtained from the application of material balance. This equation, for the simpler kinetics, is of the form:

$$\mathbf{X} = \mathbf{f} \left(\mathbf{D} \mathbf{a} \right) \tag{1}$$

where Da is the Damköhler module containing the product k t and a function of the initial concentration of the limiting reagent, where k is the kinetics constant and t the reaction time in a batch reactor or the spatial time in a continuous reactor. This is a very interesting way, in our opinion, to show the influences on the development of the reactions. This dimensionless module and this relation display the effect of temperature, composition, residence time and type of flowing. If the rule of thumb according to which k is doubled by increasing the temperature 10 centigrade degrees were true, this increase will permit to achieve the same degree of conversion in the half of the time. Likewise, workers satisfied with their work, sure of what they are doing, recognized and supported by their environment will yield more and will be happier. For them, the work will be a source of personal fulfilment.

In an analogy, an improvement of work environment could be represented by an increase in temperature. This increase represents better conditions to develop their job.

Similarly, a higher level of knowledge or a better training could be represented by a higher initial concentration of the reagent in an irreversible reaction with an order higher than one.

The characteristics of the mixture in the reactor affect the effectivity of the reactor. This fact is reflected in the form of equation (1). Figure 1 shows the evolution of the degree of conversion X with Da for a first order reaction and for three ideal reactors: CSTR (Continuous Stirred Tank Reactor), TLFR (Tubular Laminar Flow Reactor) and PFR (Plug Flow Reactor). The evolution of X with Da for a batch reactor is the same that of the PFR one. One can see that the effectivity of the reactors is very different between them. The selection of the reactor is important, in the same way the selection of the work conditions can improve the work environment and the yield.

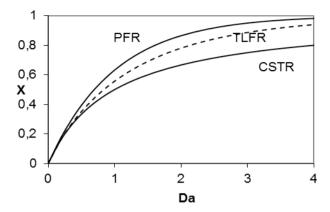


Figure 1. Evolution of the degree of conversion *X* for a first order reaction with *Da* for three kinds of reactors CSTR (Continuous Stirred Tank Reactor), TLFR (Tubular Laminar Flow Reactor) and PFR (Plug Flow Reactor). Adapted from Fogler (2017)

One of the main principles of the Industrial Hygiene is the adaption of the workplace to the workers (Sorensen 2017). In this analogy between reactions and work conditions, we can consider the selection of the reactor and conditions that have a better behaviour for a given reaction.

Similarly, it could be taken into consideration the situation in which workers are distracted from their work by various concerns related to their work environment, family, etc. This dispersion of interest could be represented by a decrease in initial concentration of the reagent. A perhaps more appropriate approach would be a system of multiple and competitive reactions: In this way, comparing the reaction

$$A \xrightarrow{k_1} B$$
 with the system of reactions

$$A \xrightarrow{k_1} B$$

$$A \xrightarrow{k_2} C$$

we can see that in the first case nothing distracts the reagent A to obtain the product B, but in the second case, the presence of a parallel reaction causes that a portion of the reagent A is wasted in obtaining the by-product C. Figure 2 shows the evolution of the concentration of B with the Damköhler module in both cases. To facilitate the construction of this graph has been considered that both reactions are elementary, and the kinetic constant is the same for both reactions. It can be appreciated that the production of B decreases due to the presence of the second reaction.

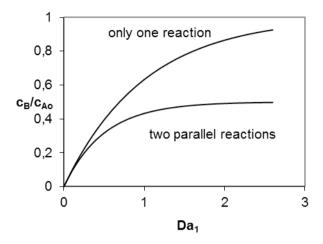


Figure 2. Evolution of the concentration of B with the Damköhler's module of the first reaction

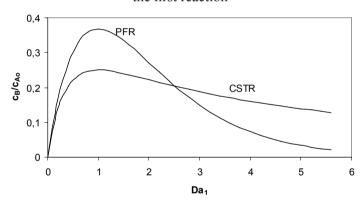


Figure 3. Evolution of the concentration of B with the Damköhler's module first reaction, Da_1 , of the first order series reactions $A \xrightarrow{k_1} B \xrightarrow{k_2} C$. To facilitate the calculation, it has been considered the case where $k_1 = k_2$

Another aspect to consider is the adequacy of the work environment to the process development. This can be analyzed by a famous example.

Consider the system of reactions: $A \xrightarrow{k_1} B \xrightarrow{k_2} C$. Figure 3 shows the concentration profile of species B over time (spatial time in the continuous reactors) in different ideal reactors. The batch and PFR reactors enable a higher level of concentration of B than the CSTR one.

In some cases the conditions of the process show natural limitations, for example chemical equilibrium; membrane reactors and reactive distillation are solutions proposed. On the one hand, two operations (reaction and separation) take place in the same equipment, and on the other hand, separation helps us to overcome these limitations. This case permits a deeper and better approach to the adaption of the workplace to the worker. The automation of some boring, difficult or dangerous tasks could be an example of this analogy.

The concepts enthalpy and entropy could be explained using the following analogy (adapted from Amjad and Stefan (2020)). A group of people is working together in the same department, and everyone has different motivation, capacity and responsibility. Workers confined in a small area, with little freedom to move, are most likely to suffer from anxiety disorders. An increase of the enthalpy could be related with the need for freedom. This anxiety could be explained as an increase of temperature and, in the same way, reducing the size of the workplace would be analogous to reducing workers' entropy. A similar situation could be found if the company is too bureaucratic, where permissions to carry out any initiative must be requested. Some motivated employees may not feel free to do their work and could feel frustrated and discouraged. This frustration may be represented as temperature. Their great energy and interest to start new projects could have a resemblance with the enthalpy. If the company loosens the requirements in terms of permissions, workers would have more flexibility to do their work; in thermodynamic terms, it can be interpreted as an increase of the entropy.

Discussion Mobbing

Mobbing, also known as occupational psychological harassment, occurs at work when an individual or several systematically and repeatedly engage in psychological violence against another individual or individuals. Mobbing can be between employees, from employees to the superior, from the superior to the employees or from the organization towards one of their workers. Mobbing not only affects work performance and causes serious conflicts; it can cause serious psychological problems in the person who suffers them. This is a problem that must be tackled once it is detected.

In recent years, the workplace harassment has been a subject of discussion. This assault on a worker results in serious damage to health and significant deterioration in relationships and work environment. We try to propose to represent these situations for a reaction that takes place with a serious decrease in temperature, or in the case of a reversible reaction in which the temperature changes leads the system to an area where reversibility is manifested, limiting the progress of the reaction in a very significant way. Some actions that are part of this mobbing can be represented by some reactions or

ways of developing them. Some examples: a typical attitude is a denial of the information needed to develop work or provide erroneous data, seeking to increase the difficulty or the mistake probability and with them the disrepute. This action can be simulated by changes in temperature or unfavorable reactor conditions (slowing reaction), changes in the reagents or catalyst (accelerating a reaction that competes with that of our interest, etc.).

The opposite attitude to mobbing could be a civilized collaboration among different people, groups, etc. A good example could be the coupling of exothermic and endothermic reactions in the same reactor (Ramaswamy, 2008). This reactor uses to be a tubular one similar to a concentric tube heat exchanger. Both fluids react and exchange heat. This creative arrangement permits to save money because a single reactor is needed, and heat exchange fluids are eliminated.

Some special reactions show an ability to simulate the complex relationships between people working in a toxic work environment. One of these reactions is the one that involves an inhibitor. This can happen in catalytic or enzymatic reactions, or microbial processes in the presence of an inhibitor or poison that can significantly reduce the speed of the process. A catalyst increases the reaction rate and an inhibitor decreases it. An enzyme inhibitor is a molecule that binds to an enzyme (a biologic catalyst) and decreases its activity.

Something similar can be found in polymerization reactions. The effect of the presence of this toxic element is also reflected in the rate of reaction and therefore in the production of the polymer, which affects significantly its quality. The polymer obtained could be contaminated by the unreacted reagents and be of shorter length or molecular weight, perhaps with greater polydispersity and lack the properties that correspond to the target characteristics. The effect of selecting the appropriate reactor for each of the polymerization reactions is analyzed in the book of Dotson et al. (1995). Figure 4 shows the distribution of chain lengths (j) for a polymerization of anionic addition in different reactors.

Polymerization is a very interesting and complex area that points out several complicated situations. One of this is the gel or Trommsdorff effect, which is a combination of several phenomena. The generation of polymer chains produces an increase of the system viscosity. This fact reduces, on one hand, the movement of chains that reduces in special the rate of the termination step, for this reason the living chains have more time to react and the global rate increases. On the other hand, this increase in the viscosity makes heat transfer difficult, and as a consequence, the gradient of temperature in the reactor contributes to the lack of homogeneity, leading to changes in the characteristics of the polymer and to a possible runaway. Figure 5 shows the change of the process rate due to the self-acceleration from the gel effect.

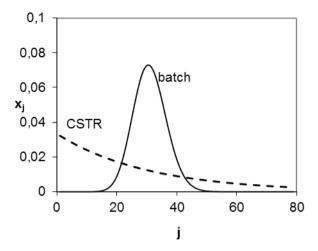


Figure 4. Distribution of chain lengths for a polymer of anionic addition in a CSTR and a Batch reactor (adapted from Dotson et al. (1995)

Stress

People use to say that, in small doses, stress has some advantages. It can help us to reach our objectives. But the dose makes the poison. An excess of stress can be harmful to our health.

The self-acceleration described previously (gel or Trommsdorff effect) can be related with the stress in the work. As a consequence of the increase of the viscosity, it could appear an increase in the rate of reaction. We can be interested in this phenomenon due to the faster rate of the process, but we must take care for the runaway risk. Figure 5 shows the evolution of the degree of conversion with the Damköhler's module in the expected way, and how in an intermediate state can appear an increase in the reaction rate.

Lack of teamwork

Teamwork is one of the skills most valued by recruiters, because when an employee works as a team, their creativity and learning improves, their stress level is reduced and performance and productivity increase. However, in cases where workers decide to go on their own and teamwork is not manifested in the company, it is possible that conflicts are generated.

This workplace problem can suggest an analogy in the chemical engineering reaction world. A series of reactors use to improve the yield in front of the parallel ordination.

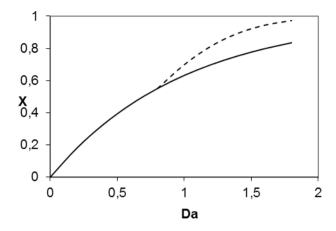


Figure 5. Change of the process rate due to the self-acceleration from the gel effect; continuous line represents the expected process, dashed line represents the increase on the rate due to the gel effect

Lack of communication

Lack of communication can cause serious conflicts at work, because when an employee or superior fails to communicate (or send the necessary messages) to other workers, problems can appear. Bad communication can occur as misinformation or bad information. In the first case, the information does not arrive; in the second case, the information arrives badly.

The loss of the process control can simulate this problem, the signal does not arrive to the control unit or its value is incorrect, and the decision is not adequate.

Toxic companions or boss

Toxic people create a bad environment where they go, especially at work. Toxic partners create conflicts where there are none. The boss, that can be a bad manager, arrogant, bad communicator, autocratic, inflexible, controlling or discriminatory, makes the workers' life impossible. Their effect is similar to an inhibition or poisoning.

Competitiveness

It is common for many companies to pay their employees based on the achievements. And while some companies distribute commissions among the members of a team, others reward employees individually: depending on the sales or objectives set, it is a person who receives the commission. This type of incentives can cause friction among workers, because the competitiveness that is created brings conflicts between workers. Parallel reactions compete similarly for the reactants.

Relationships between co-workers

These relationships can go from a romance to an intense hate. In some situations, these relationships at work can bring conflicts.

In the catalysis process, one can find the adsorption step (heterogeneous) or the complex catalyst-reactant formation (homogeneous). This step is necessary, but so bad is that this complex is too strong as too weak.

Colleagues who don't work well. Prejudices. Personality clashes

When a partner does not perform as he should render, the conflicts may appear. Companies and organizations are dynamic systems, and a delay in the deadline for submitting a project can cause all the general functioning of this "living organism" to suffer.

Prejudices are grounds for conflict in different spheres of life, and also at work. Partners who do not tolerate people from other places in the world or with other skin color, bosses who treat their employees in a sexist way, and so on. These are cases that may appear in the workplace. Sometimes the personalities simply do not fit, and a dispute could break out at anytime. In personal relationships, conflicts exist day by day as well. When such a conflict arises, it is best to solve the problem as soon as possible.

In a series of different types and sizes of reactors their order can affect the conversion degree obtained in the process, an incorrect order could be an example of bad co-work conditions.

Finally, considering the Planet as our workplace and paying attention to the climate change; when we observe the evolution of the temperature with time (an interesting figure can be found in the web page Earth Temperature Timeline (2020)), a similitude appears with the temperature evolution in a simulation of the Monsanto accident (Fogler 2017).

In both cases the temperature is maintained controlled, then, in a moment, a change in the environment produces a slight increase that with time becomes in an abrupt one, the runaway. Are we in time to avoid this situation?

Conclusion

In this paper, we propose different ways to represent problems with the organization that makes a work to be toxic to workers by simulating different reactive systems. This is intended, on the one hand, to make students aware of this pest, and on the other hand, to find real life examples that can illustrate some aspects of the engineering of chemical reactions as a help to understand the mechanisms governing these processes.

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