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Analysis of Thermal Runaway Scenarios in a Chemical Reactor

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In this paper we propose an analysis of different thermal runaway scenarios in a chemical reactor. We have chosen HAZOP method for the analysis of risk generated by chemical reaction, while FMEA method will be used in the analysis of risks linked to the functioning of chemical reactor. However, we should note the existence of interactions between the course chemical reaction and the behavior of the reactor; this leads us to develop a new analytical approach to this specific type of system, which based on methods combination (FMEA, HAZOP, Karnaugh Table). We obtain a simple final electrical schematic and simple equation that describes the occurrence of different thermal runaway scenarios in a chemical reactor.

1. Introduction

The analysis of past accident data confirms that sever accidents were caused by the release of decomposition products, more hazardous than those present in normal operating condition (Cozzani and Zanelli, 1999). A thermal explosion is the result of an uncontrolled temperature increase of exothermic reaction which is also refereed to as runaway reaction (Gustin, 1993).The runaway scenario can serve a basis for the assessment of thermal process (Eissen et al, 2003). Accident scenarios are also in the technique to select the top event of the emergency response plane (Dongwoon et al, 2003). In their work (Eissen et al, 2003) have described an impressive experimental and its background for demonstrating TMR_{ad} by presenting the catalytic decomposition of hydrogen peroxide with potassium lode. Also (Dongwoon et al, 2003) have developed systematic method of generation accident scenario and implemented software called yAGAS which generated automatically a list of accident event and generic hazardous situation. (Papadaki et al, 2005) have examined a number of runaway scenarios of the excess of hydrogen peroxide used during the N-oxidation of alkypiridine. Our contribution in this theme is to propose an approach for scenario, analysis, of thermal runaway in a chemical reactor; this approach is based on a combination of three methods, namely FMEA, HAZOP, and Karnugh Table. The originality of this work concerns the use of the Karnaugh Table which is generally used for the functional analysis of system, by applying it to dysfunctional analysis of system, it will allows us to represent these scenarios as a simple wiring diagram and a simple logic equation.

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2. Methodology

The proposed approach involves two steps, first steps: The combination of both methods FMEA and HAZOP for risk analysis of the system. We can see the existence of interaction between components of the tow subsystems but are not considered by the first stage where the insufficient of this combination FMEA-HAZOP alone and the need to introduce another method, which take into account these interactions, in this case thus the method of Karnaugh Table. This approach allows us to get a model of different thermal runaway scenarios form and an electrical circuit diagram which is translated by a simple logic equation.

2.1 FMEA

FMEA is a method of risk analysis that considers the system component failures, the cause of failure, its effect and criticality. (Villemeur, 1988).

2.2 HAZOP

This method is particularly applicable for analyzing the risks of operating systems for which thermal hydraulic parameters such as flow, temperature and pressure are particularly interesting for security (Salvi, 2003).

2.3 Karnaugh Table

The Karnaugh Table is a truth table; it is used to obtain the simple logical expression of the Boolean function (Jourlin, 2008)

2.4 Combinations

2.4.1 FMEA-HAZOP

The combination allows us to the complementarities between the results of both methods. However the existence of interactions between the two subsystems and which are not taken into account by combining the results FMEA/HAZOP reflects the insufficient of this combination.

2.4.2 FMECA-HAZOP-Karnaugh Table

The application of the Karnaugh Table allows us to configure the failures of the subsystem 1 (chemical reactor), that of Subsystem 2 (chemical reaction), but also the various interactions between the two subsystems which leads to the thermal runaway.

3. Case Study

3.1 System definition

A chemical reactor is composed of Subsystem 1 the chemical reactor itself consists of various elements such as the cooling system, agitator and so on, and the Subsystem 2, the chemical reaction which is characterized by several parameters such as temperature, concentration and reaction kinetics.

3.2 Application of FMEA to the Subsystem 1 (Chemical reactor)

The application of the FMEA method to the chemical reactor allows us to see that runaway scenario may be caused by the failure of some components such as the agitator, the cooling system, and so on thus the control ongoing operation of agitator, a regular maintenance of all these components, the verification and strict control of raw materials are necessary.

3.3 Application of HAZOP to the subsystem2 (chemical reaction)

The application of the HAZOP method on the chemical reaction demonstrates that runaway scenario can be envisaged on the basis of drift parameters such as temperature, concentration, or other.

3.4 Study of interactions

At this stage of our study we can establish the existence of different interactions between the two subsystems: -Increasing the Temperature **T** of the reaction environment **OR** -Increasing in pressure **P** of the reaction environment **OR** -Inappropriate loading of reagent **R OR** -Bad agitation **A.** On the other hand each of earlier disturbances may be the combination result of the reactor failure components and the drift parameters of the reaction, we can explain this by the following considerations:

T = Cooling system failure (**a) AND** increase the amount of heat of chemical reaction (**b**). **P** = Failure of the pumping system (**c**) **AND** accumulation of gas in the course of reaction (**d**). **R =** Inappropriate loading of reactants (**e**) **AND** presence of tow incompatible reactants (**h**) (a), (c), (e) are the failures related to the chemical reactor components. However, (**b**), (**d**), (**h**) are the drift of chemical reaction parameters.

Some causes leading to a disruption can be added to a cause leading to further disruption and thus increase the probability of occurrence thereof:

T = cooling system failure (**a**) **AND** load control system of reactant (**e**). **T** = increase of amount of heat of chemical reaction (**b**) **AND** accumulation of gas in the course of the reaction (**b**). **P** = accumulation of gas in the course of reaction (**d**) **AND** failure of pumping system (**c**) **AND** failure of the cooling system (**a**).

3.5 Application of Karnaugh table

3.5.1 Analogy with electricity

-In electricity a lamp (**L**) which is controlled by a contact (**a**) is on (**L** = **1**) if the contact is closed (**a** = **1**), it is off (**L = 0**) if (a) is open (**a = 0**).

-If **L** is controlled by two contacts (**a**) et (**b**) in series circuit, so we have **L** = **1** if **a** = **1 AND b** = **1;** -If **L** is controlled by tow contacts (**a**) and (**b**) in parallel circuit so we have **L** = **1** if **a** = **1 OR b** = **1;** -The **AND** function is translated the series circuit, while the **OR** function is translated by the parallel circuit.-In our work we will do the following assimilations: The runaway phenomenon is likened to a lamp **L**, L= 1, ie. the concurrency of runaway, **L** = **0**, i.e. the runaway phenomenon does not occur. The events, increase in temperature **T**, increase in pressure **P**, inappropriate loading of reactant **R**, and a poor agitation **A**, are treated as bobbins A, P, Q, A. The defects such as failure of the cooling system (a), increase the heat of reaction (b)…..are likened to contacts which control A, P, Q, A.

3.5.2 Application

A-Definition of the function T = f (**a**, **b**, **e**, **d**):

We note that **T** is a function of variables (**a**, **b**, **e**, and **d**).

Truth table for **T** (**a**, **b**, **e**, **d**): To establish the truth table of T we have 4 variables, so we have $2^4 = 16$ combinations. We note that **T** = **a** and **b**, **T** = **a** and **e**, **T** = **b** and **d**.

Table 1: Truth table for T(a,b,e,d)

a	b	e	d	T(a,b,e,d)
0	0	0	0	0
0	0	0	1	0
0	0	1	0	0
0	0	1	1	0
0	1	0	0	0
0	1	0	1	1
0	1	1	0	0
0	1	1	1	1
1	0	0	0	0
1	0	0	1	0
1	0	1	0	1
1	0	1	1	1
1	1	0	0	1
1	1	0	1	1
1	1	1	0	1
1	1	1	1	1

*Table 2: Simplification of **T(a,b,d,e)** equation*

a b / e d	00	01	11	10
00	0	0	1	0
01	0	1	1	0
11	0	1	1	1
10	0	0	1	1

T = ab + ae + bd (1)

B-Definition of the function P = f (**c**, **d**, **a**):
We note that **P** is a function of variables (**a**, **c**, **d**,).
Truth table for **P** (**a**, **c**, **d**): To establish the truth table of **P** we have 3 variables, so we have $\mathbf{2^3} = \mathbf{8}$ combinations. We note that **T** = **c** and **d**, **P** = **a** and **c** and **d.**
In this case we have one group which gives us: **P** (**a**, **c** ,**d**) = c d (2)

C-Definition of the function R = **f(e**, **f)**:
We not that **R** is a function of variables (**e**, **f**,).
Truth table for **R** (**e**, **f**): To establish the truth table of **R** we have 2 variables, so we have $\mathbf{2^2} = \mathbf{4}$ combinations. We note that **R** = **e** and **f.**
In this case we cannot simplify the equation because the boxes which containing 1 are separated so we have: **R** (**e**, **f**) = **e f** (3)

D-Definition of the function A = f (**g**, **h**):

We note that **A** is a function of variables (**g**, **h**,).

Truth table for **A** (**g**, **h**): To establish the truth table of **A** we have 2 variables, so we have $\mathbf{2^2} = \mathbf{4}$ combinations. We note that **A** = **g** and **h.**

so we have: **A** (**e**, **f**) = **e f** (4)

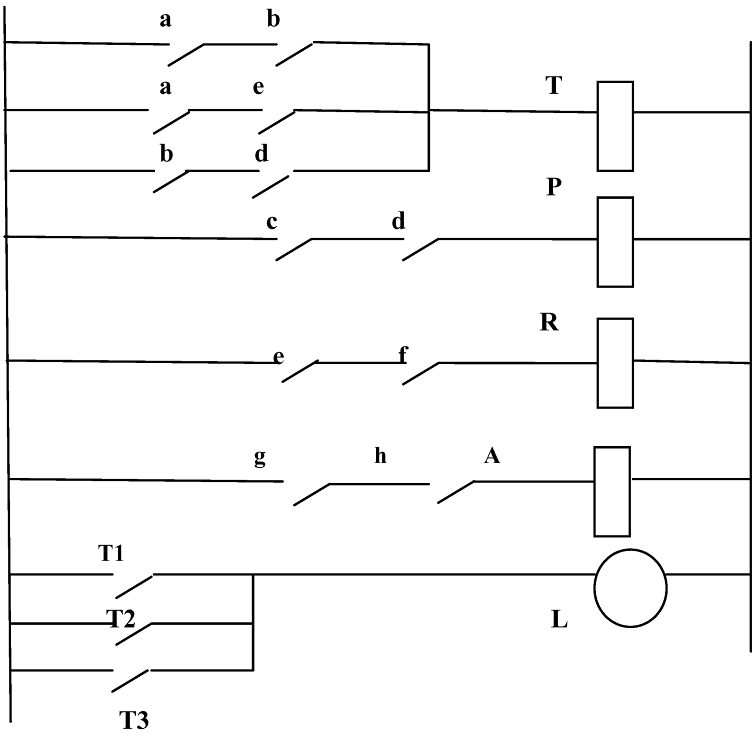

Figure 1: Model representing the scenarios of thermal runaway in a chemical reactor

Discussion

From the Figure 1 we can see that the runaway can occur (i.e. L=1) if the temperature increases (T = 1), as we have said previously that if the bobbin T is excited (T = 1) then it closes the contact T1, then lit the lamp L (L = 1), which reflects the accuracy of the thermal runaway. Similarly the Lamp (L= 1) if the pressure increase (P = 1), **OR** a bad agitation (A = 1), **OR** an inappropriate load control system (R = 1).

L = T + P + R + A (5)

On the other hand the application of Karnaugh table method allowed us to find the respective equation of the bobbins T, P, R, A. Therefore we can establish the final logic equation reflecting the occurrence of thermal runaway in our system (chemical reactor):

L = (a . b + a . e + b . d) + (c . d) + (e . f) + (g . h) (6)

Conclusion

In this work the problem of runaway scenario was discussed in another form, the proposed approach allowed us to present the various scenarios of thermal runaway under the form of electrical circuit diagram which is translated by a simple logic equation. We emphasize that the study of various defects related to the reactor or those related the chemical reaction was not complete because there are multitude of faults and failures that could generate another scenarios that were not considered in this work, because the increasing number of faults considered led to an increase in the number of variable which makes complicated the study to develop the truth table, or for development of Karnaugh table.

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