An integrated platform of chemically reacting modeling into dynamic probabilistic risk assessment

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Abstract
An integrated platform of dynamic risk assessment using the Theory of Stimulated Dynamics (TSD) is developed for chemical and petrochemical industrial facilities. The methodology has been applied to perform the nuclear protection engineering with good assessment capabilities. The probabilistic modeling part of TSD aims to identify the risk space with the objective of obtaining an estimation of the exceedance frequencies of specified safety limits. The calculation of the exceedance frequency of a given safety limit consists of a two-fold tasks: (1) identification of the damage domain of all the possible transients grouped in the sequence by using the adaptive search algorithm, and (2) the calculation of the collective frequencies of all those transients with the Q-Kernel frequency density function.

The Probabilistic analysis with these two tasks can be coupled with the deterministic analysis based on thermodynamic and chemical reactions modeling which aims to evaluate the transient behavior of chemically reacting system inside containment. Both probabilistic and deterministic risk analysis provide a framework to evaluate the dynamic safety in chemical and petrochemical industries. To illustrate the dynamic risk analysis study, we present a simplified case of Methyl-Isocyanate explosion scenario inside the storage tank 610 of the Bhopal plant.

Keywords: TSD; exceedance frequency; damage domain; adaptive search algorithm; Q-Kernel function

1. Introduction

Dynamic Reliability is today a mature approach to risk assessment in environments where the dynamic evolution of process variables is of high complexity and discrete stochastic events may continuously change the plant dynamic behaviour [1]. In addition, it provides next step improvements by relaxing some of the restricting assumptions within traditional methods, and establishing a closer link between the plant dynamic behaviour, and the calculation of the frequency of damage under any credible event.
A new integrated platform based on dynamic reliability using the Theory of Stimulated Dynamics (TSD) has been applied for severe accidents in nuclear power plants with good assessment capabilities. The objective of this work is to study how to apply the TSD methodology to a key issue of any severe accident in chemical/petrochemical industrial facilities, and to identify the abilities and weaknesses of this methodology for the simplified case of Methyl-Isocyanate explosion scenario inside the storage tank 610 of the Bhopal plant. No attempt is made to actually reproduce the Bophal scenarios, rather to show how the approach may handle events of its kind. Probabilistic and deterministic analysis provide a framework to evaluate the dynamic risk for the simplified case of tank 610. Deterministic analysis based on thermodynamic and chemical reactions modeling aims to evaluate the transient behaviour of chemically reacting system inside storage tank 610. The TSD methodology as part of the probabilistic analysis integrates damage due to accident scenarios with scenario frequency by formulating equations for the frequency exceeding of a given damage. The calculation of the exceedance frequency of a given safety limit in the context of TSD consists of a two-fold tasks: (1) identification of the damage domain of all the possible transients grouped in the sequence by using the adaptive search algorithm, and (2) the calculation of the collective frequencies of all those transients with the Q-Kernel frequency density function.

2. Use of TSD Methodology to Assess the Risk

2.1 TSD versus PSA

The development of TSD is designed to establish a closer relationship with the usual PSA methods and tools [2]. Both FT/ET tools and of the accident dynamics, may continue to be part of the TSD methodology. The essence of the treatment is:

1) To be able to compute the path frequency density to be used as a weighting factor of the paths in the sequence frequency aggregate.

2) To be able to filter-in only those paths that activate damage conditions and consistent calls for headers system intervention.

2.2 Calculation of Damage Exceedance Frequency

Damage exceedance frequency may be written as integral equations representing the solution of the semi Markov system for the frequency of entering state *j*,

$$Q_j^{seq\,\vec{j}}(t/\vec{\tau}_n) = q_{j,j_n}(t,\tau_n)q_{j_n,j_{n-1}}(\tau_n,\tau_{n-1}).....q_{j_2,j_1}(\tau_2,\tau_1)$$
$$\tau_1 < ... < \tau_{n-1} < \tau_n < t \qquad \vec{\tau}_n \equiv (\tau_1,\ldots,\tau_n) \tag{1}$$

$Q_j^{seqj}(t, \tau_n)$ is called the path *Q*-kernel. Thus the frequency becomes an aggregate of path contributions, each being a product of factors that carry the influence of each sequence header.

2.3 Damage Domain Searching

The adaptive search algorithm is an ultimate tool able to precisely define the size of the damage domain within the sequence domain, in order to multiply it by the 'weighting factors' given by the Q-kernels of each path. The algorithm is formed by one initial stage and an adaptive search stage divided in three parts:

- Initial stage: an initial mesh grid is defined and points within that grid are sampled and analyzed, via the simplified dynamic models, to determine whether if they are a damage, success or impossible path.

- Adaptive search stage: a loop is performed with successively higher scales 2, 3, 4, etc. until a stopping criterion is reached. This stage has the following parts:

  - Refining stage: when entering a higher scale, the new time step for the sampling process is half the previous one, *dt*/2.

  - Seeding stage: an alleatory seeding of new sampling points along the whole domain has been included here, in order to discover new damage zones separated from the previous ones.

  - Growing stage: at this stage, the algorithm extends the sampling through all the interior zone of the damage domain.

3. Deterministic Modelling

3.1 Thermodynamic Modelling

To determine the complete thermodynamic properties requires the sum of the ideal gas properties contribution and the residual correction for non-ideal behaviour [3]. The following generalized cubic equation of state used to describe the behaviour of pressure can be written as:

$$p = \frac{RT}{V-b} - \frac{a_c m(T)}{V^2 + c_1 V + c_0} \tag{2}$$

3.2.1. Pressure Calculation

In this work, the Peng-Robinson equation of state has been applied to a pure fluids for both liquid and vapour phases. It is given by:

$$p = \frac{RT}{V-b} - \frac{a(T)}{V(V+b)+b(V-b)} \tag{3}$$

3.2.2. Calculation of Residual Properties

A residual quantity is the difference between a property of a real fluid and the same property of an ideal gas at the same density and temperature. The residual Helmholtz free energy $A^r(T,V)$ is obtained as follows:

$$(8-T'-p')\xi^3 + (2T'+3p'-8)\xi^2 + (T'-p')\xi - p' = 0 \tag{4}$$

From the residual Helmholtz free energy:

$$\frac{G^r}{RT} = \frac{A^r}{RT} + Z - 1 \tag{5}$$

Also, the residual internal energy can be written as:

$$\frac{U^r}{RT} = -T\left(\frac{\partial\left(A^r/RT\right)}{\partial T}\right)_V \tag{6}$$

The residual enthalpy can then be written as:

$$\frac{H^r}{R} = \frac{U^r}{RT} + Z - 1 \tag{7}$$

The residual isochoric and isobaric heat capacities can be written as:

$$\frac{C_V^r}{R} = -2\left(\frac{\partial\left(A^r/RT\right)}{\partial T}\right) - T\left(\frac{\partial^2\left(A^r/RT\right)}{\partial T^2}\right); \tag{8}$$

And:

$$\frac{C_P^r}{R} = \frac{C_V^r}{R}\frac{\alpha_p^2}{\kappa_T} - 1 \tag{9}$$

3.2.3. Calculation of Ideal Gas Properties

The ideal isobaric heat capacity is obtained by using a polynomial form of the Shomate equation [4]:

The ideal isochoric heat capacity can be written as:

$$C_V^{id} = C_p^{id} - R \tag{10}$$

To calculate the ideal enthalpy, we use the standard equation. For instance:

$$H^{id} = \int_{T_{ref}}^{T} C_p^{id}\, dT \tag{11}$$

3.3 Chemical Reactions Modelling

The reaction rate is given by:

$$q_k \equiv K_k^{dir} \prod_{m=1,\ldots S_{kdir}} [X]_{m,k}^{\beta^k_{m,in}} - K_k^{rev} \prod_{m=1,\ldots S_{krev}} [X]_{m,k}^{\beta^k_{m,out}} \tag{12}$$

Any reaction is supposed to take place during a time τ_k, and generates during it an energy rate:

$$\dot{Q}_k = V_k q_k \Delta h_k \qquad (13)$$

4. Description of Dynamic Risk Assessment Methodology

4.1. Deterministic Assessment (Block 1)

As shown in Figure 2, at the beginning we select the cubic equation of state with its parameters.

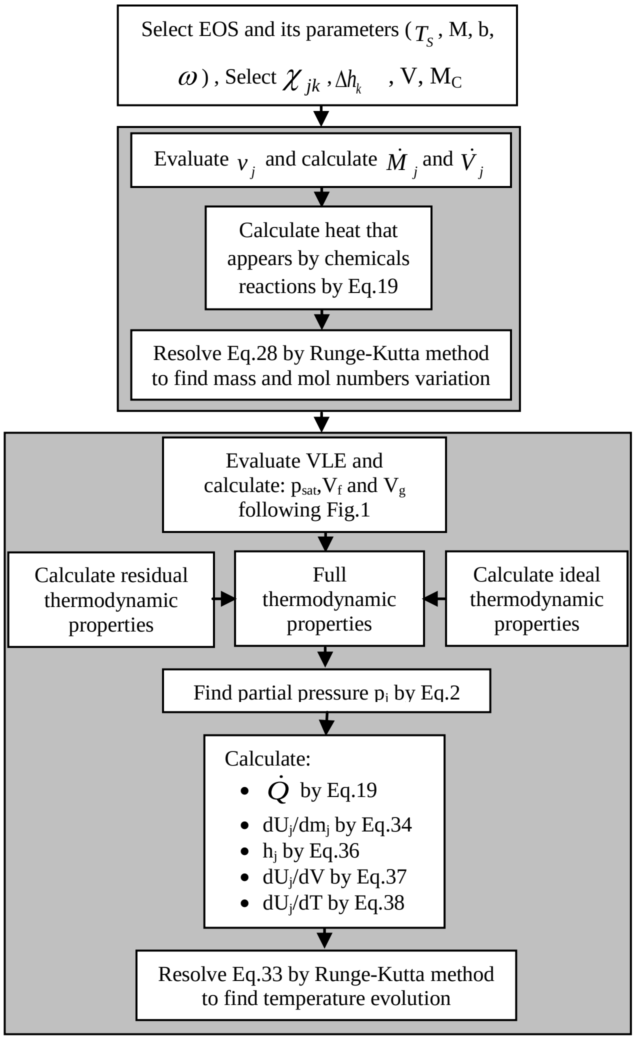

Fig. 1 Diagram of Thermal-Hydraulic Analysis

4.1.1. Mole (Mass) Variation Calculation

In addition to accounting for the sources of species as a result of the chemical reactions, mass transport is important when there is material transfer across the volume surface. Then, a typical mole conservation equation is of the form:

$$\frac{dN_j}{dt} \equiv \sum_r \left[\frac{\varepsilon_{jr}\rho_j^{in} j_r^{in}}{M_j} - \frac{\varepsilon_{jr} N_j}{V} j_r^{out} \right] + \sum_k \chi_{jk} q_k(t)\theta(t - \tau_{stark})\theta(\tau_{startk} + \Delta_k - t) \qquad (14)$$

4.1.2. Temperature Evolution Calculation

By applying thermodynamic laws we obtain the following temperature differential equation:

$$\frac{dT}{dt} = \frac{\dot{Q} + \sum_j (\dot{m}h_{in})_j - \sum_j \left[\frac{\partial U_j}{\partial V} + p_j\right] dV/dt - \sum_j \frac{\partial U_j}{\partial m_j}\frac{dm_j}{dt}}{M_C + \sum_j \frac{\partial U_j}{\partial T}} \tag{15}$$

4.2.Probabilistic Assessment with TSD (Block 2)

While deterministic analyses may be used to verify that acceptance criteria of protection design are met, probabilistic safety analyses may be used to determine the probability of damage for each protection barrier. Probabilistic safety analysis may thus be a suitable tool to compute the exceeding frequency for the sequences created from a common initiating event. As shown in Figure. 2, the global simplified diagram for probabilistic analysis methodology computes the exceeding frequency of sequences created from the evolution of process variables (temperature, pressure and mass) given by the deterministic analysis. The computing process consists on the following steps:

1. Dynamic sequences generation: the objective is to generate the dynamic event trees (DET) through all possible scenarios, delineates each sequence of DET stemming from an initiating event. For each sequence, the corresponding times and probabilities are provided.

2. Sequence analysis: aims to identify the damage domain of all paths which constitute one sequence. Each sequence is characterized by a set of times and a set of sensitive parameters, such that for certain combinations of them damage affected to each path may be generated. Thus, the damage domain is a volume in the multi-dimension space of times and parameters, each point in it representing a different transient. Each point should be evaluated by using the information of process variables evolution given by the deterministic analysis.

3. Risk assessment: Once the damage domain has been identified, the analysis may proceed with the calculation of the exceeding frequency of the contribution of all paths within the sequence. Each transient belonging to the damage domain is revisited in order to identify the information needed for the calculation of the frequency density. Numerical integration of the exceeding frequency will then consist in computing the *Q*-kernel on the damage points inside the sequence sampling domain by summing up all the contributions.

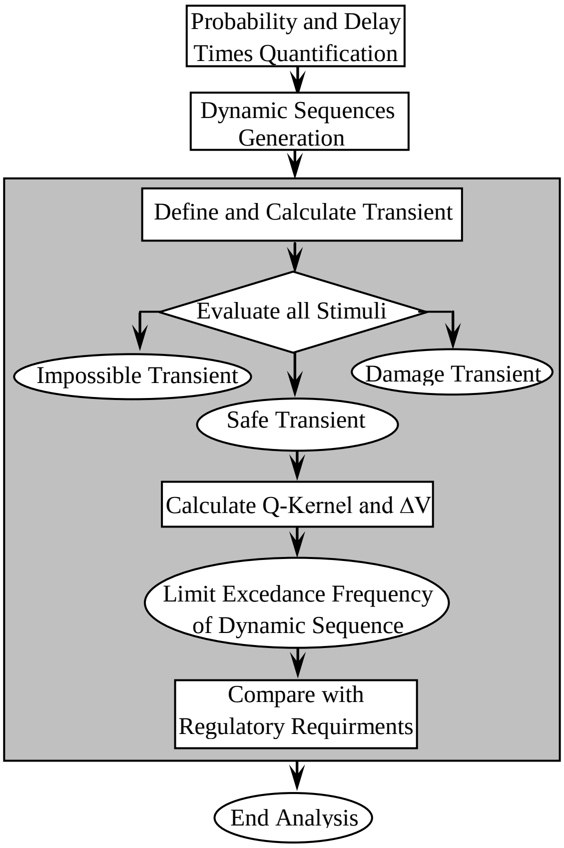

Fig. 2 Probabilistic Assessment Organigramm

5. Results and Analysis

- **Mass Variation Inside the Tank**

At the beginning of the reaction between steam water, and Methyl-Isocyanate at 0 second, the mass of reactants composed of Methyl-Isocyanate and steam water decrease gradually. In addition, the mass of product composed of the Methylamine and the CO_2 decrease. During simulation the mass of product increases and the mass of reactants decreases.

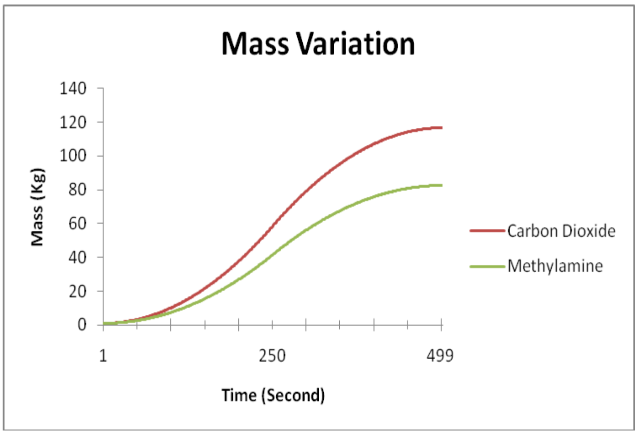

Fig. 3 Mass Variation of Methylamine and Carbon Dioxide

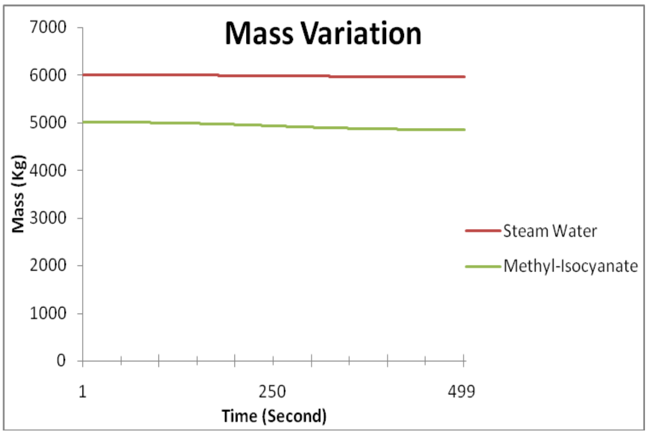

Fig. 4 Mass Variation of Steam and Methyl-Isocyanate

- **Temperature and Pressure Evolution Inside the Tank**

Figures.5 and 6 show the temperature and the pressure evolution inside the tank. At 0 second, the exothermic reaction between steam water and Methyl-Isocyanate takes place. We can observe that the temperature and the pressure increase.

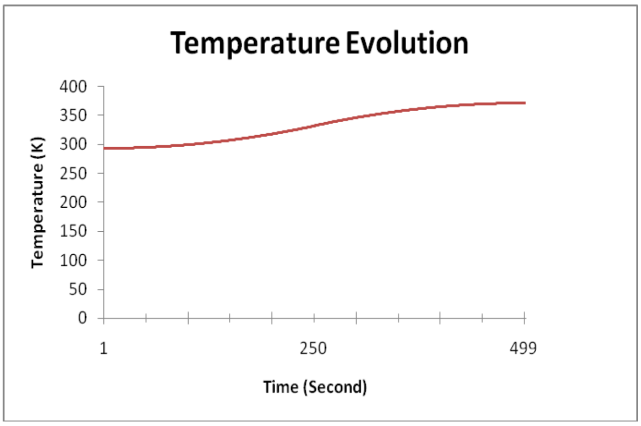

Fig.5 Temperature Evolution Inside the Tank

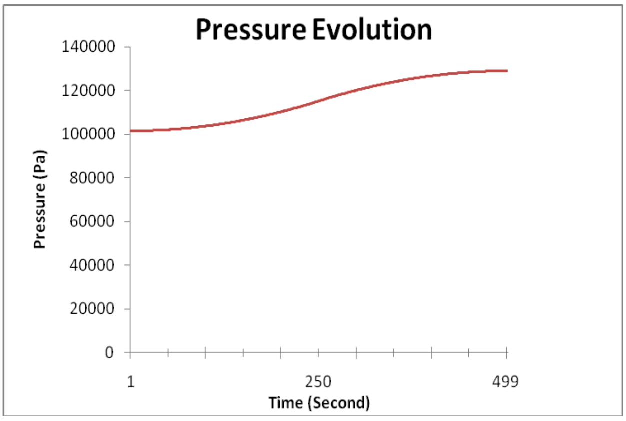

Fig.6 Pressure Evolution Inside the Tank

5.2. Probabilistic Analysis

5.2.3. Numerical Results

Tables 1 and 2 present the results of our simulation with pressure and temperature accumulations. Several comments can be made out from the results:

The first part of the simulation, as shown in table 1, computes the exceedance frequency of the runway exothermic reaction damage stimulus.

Table 1
Damage domain results with activation of runway exothermic reaction damage stimulus

Sequence	Damage paths	Safe paths	Impossible paths	Total paths	Damage frequency
[1]	0	1	0	1	0
[1 2]	30	4	0	34	0.3448
[1 2 3]	343	7	149	499	0.0243
[1 3]	19	15	0	34	0.1357
[1 3 2]	846	15	143	1004	0.0543
TOTAL	1238	42	292	1572	0.5591

The second part of the simulation as shown in table 2 computes the exceedance frequency of the safety disc rupture damage stimulus for each possible sequence.

Table 2
Damage domain results with activation of safety disc rupture damage stimulus

Sequence	Damage paths	Safe paths	Impossible paths	Total paths	Damage frequency
[1 2 4]	669	0	2331	3000	2.49e-003
[1 2 4 3]	324	0	3140	3464	5,48e-04
[1 2 3 4]	15621	1745	3009	20375	0.0209
[1 3 4]	1494	420	1506	3420	2.74e-003
[1 3 4 2]	474	220	2151	2845	6,01e-04
[1 3 2 4]	16995	0	2946	19941	0.1261

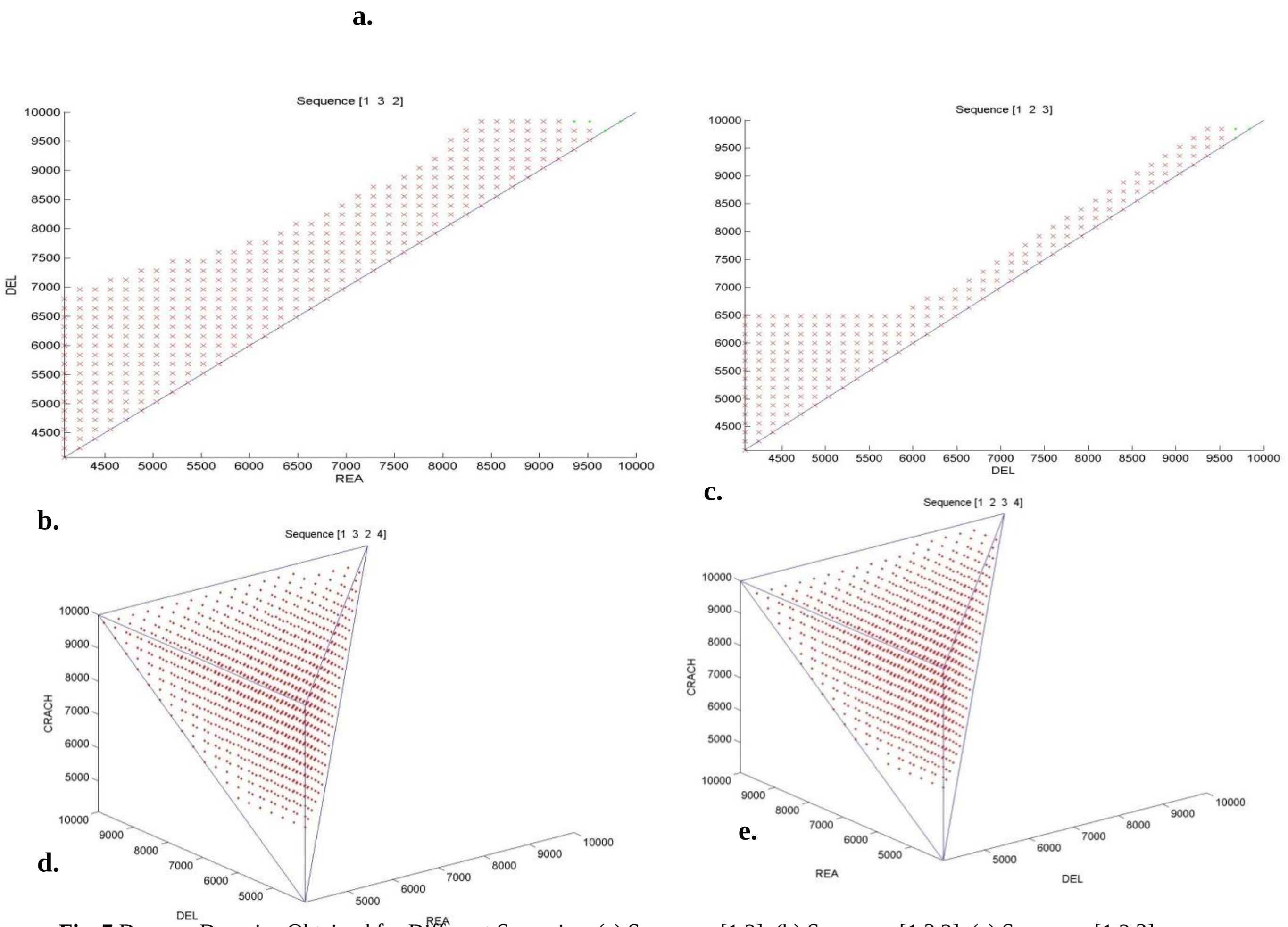

Fig. 7 Damage Domains Obtained for Different Scenarios: (a) Sequence [1 2], (b) Sequence [1 3 2], (c) Sequence [1 2 3] , (d) Sequence [1 3 2 4] , (e) Sequence [1 2 3 4]

Several comments can be made out from the results:

- There are some impossible paths within each sequence, what means that sequences have physical meaning only in a narrow timeframe of headers occurrence times. This is in part a nice feature of the TSD method and in part an inefficiency coming out of the fact that in this early prototype of the risk assessment method every sequence has been treated separately without considering the implications of results obtained in the damage domain analysis of prior precursor sequences. As it is shown below, properly accounting for the relation between them will result in that most impossible sequences should have never been considered. This is an improvement already on the way and it will be tested in the second stage.

- The high ratio of damage paths with respect to the success paths is just the result of the damage domain refinement algorithm. The sampling has no relation with the delay pdf's of the events, as they are already taken into account in the TSD formulae. Instead, the sampling process focuses in the damage domain areas, what implies that for the same number of total sampled paths, more damage paths are detected, and therefore the computation of the exceedance frequency is much more efficient and precise.
- The worst sequences are the [1 2 4], the [1 2 3 4], the [1 3 4] and the [1 3 2 4], which together account for the 99,3% of the total damage exceedance frequency.

Conclusions about the establishment of setpoints for the different safeguards should be obtained from any reliable safety assessment. Damage domains can reflect the influence of the stimuli setpoints on safety and through them, the influence of the design of the protection system. The damage domain obtained for safety disc rupture damage reflects the violation of the rupture threshold.

It is important to mention that the total damage domain obtained for all possible sequences as shown in table 2 is more important than the total damage domain obtained in table 1 when the TMR_{ad} was elapsed and the TNR was reached. Deluge or spray system are activated after the runway exothermic reaction event observing then how the damage domain is reduced progressively for the sequence [1 2 4 3] and [1 3 4 2] compared with the sequence [1 2 4] and [1 3 4].

6. Conclusions

We have developed an adequate platform to transfer some Thermal Hydraulic features modelling from the nuclear industry into the simulation of similar scenarios in chemically reacting facilities, necessary when the risk related decision making requires the performance of a large number of scoping deterministic analysis. Because of the relation of deterministic and probabilistic safety approaches, the both are connected, as a practical specific module with the objective of assessing the safety space. The safety space in the context of probabilistic safety can be understood as an extension of the PSA event trees and the uncertainty analysis methods, aimed at obtaining an estimation of the exceedance frequencies of specified safety limits.

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