Dynamic Risk Analysis Using Alarm Databases to Improve Process Safety and Product Quality: Part II—Bayesian Analysis

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Part II presents step (iii) of the dynamic risk analysis methodology; that is, a novel Bayesian analysis method that utilizes near-misses from distributed control system (DCS) and emergency shutdown (ESD) system databases—to calculate the failure probabilities of safety, quality, and operability systems (SQOSs) and probabilities of occurrence of incidents. It accounts for the interdependences among the SQOSs using copulas, which occur because of the nonlinear relationships between the variables and behavior-based factors involving human operators. Two types of copula functions, multivariate normal and Cuadras–Augé copula, are used. To perform Bayesian simulation, the random-walk, multiple-block, Metropolis–Hastings algorithm is used. The benefits of copulas in sharing information when data are limited, especially in the cases of rare events such as failures of override controllers, and automatic and manual ESD systems, are presented. In addition, product-quality data complement safety data to enrich near-miss information and to yield more reliable results. Step (iii) is applied to a fluidized-catalytic-cracking unit (FCCU) to show its performance. © 2011 American Institute of Chemical Engineers *AIChE J,* 00: 000–000, 2011
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Introduction

Despite the significant improvements in the reliability of instruments and safety practices in the chemical process industries (CPIs) over the last two decades, the potential for serious accidents has increased because of the operation of chemical plants at significantly higher production capacities. Consequently, there is an increased interest in improving risk-assessment techniques. This is especially challenging because accidents are rare events, having very low frequencies of occurrence. Normally, the probabilities of events or incidents are estimated using observed frequencies, but for rare events, data are too sparse.

Alternatively, estimates of the probabilities of the occurrence of accidents are computed using probabilistic risk analysis (PRA) based on Bayesian theory. Since the late 1970s

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and early 1980s,[1–4] this technique has received much attention, particularly in the nuclear industry.[5–19] A system (or plant) is decomposed into individual components—for example, power generators, pumps, and heat exchangers—and their failure probabilities are estimated using statistical analysis and expert knowledge. The latter is especially helpful when the data are limited.[20–23]

The dependencies among the systems in chemical plants are crucial. Often, there are direct causal relationships between the variables (e.g., temperature and pressure in a chemical reactor), or lurking variables governing interdependences (e.g., human operators or electrical power interrupts—affecting several adjacent equipment items). Consequently, to obtain more practical and reliable risk estimates, it is important to account for these dependencies. Clearly, the explicit modeling of some dependencies is difficult—especially as humans exhibit behavior-based factors that strongly influence their actions, especially during upsets or emergencies. Besides psychological factors, physiological factors (work conditions, weather, etc.) often play a significant role.[24]

The use of accident sequence precursor (ASP) data in PRA incorporates these dependencies among the component parts.[14,25–30] To facilitate this, copulas,[31,32] which are multivariate functions used to model the joint probability distribution of the random variables, have been utilized to model the dependencies among different components of the system.[25,26,33–36] The copula functions have many attractive features, as will be discussed in the subsections on SQOS Interactions and Copulas, Copulas, and Multivariate Normal and Cuadras–Augé Copulas—especially in permitting the combination of univariate marginal distributions from different distribution families through their correlations. Although widely used in banking and financial sectors, their use in the risk assessment of chemical and nuclear plants has been very limited. Yi and Bier[26] and Danaher and Smith[37] present excellent case studies on the benefits of copulas in modeling the dependences between the random variables in nuclear plants and marketing, respectively.

In our previous work,[25,33] Bayesian analysis using copulas was used for dynamic risk analysis to estimate the failure probabilities of various critical incident scenarios for chemical plants using hypothetical accident precursor data in response to abnormal events. Prior distributions were updated dynamically with incident consequence data to yield mean failure and incident probabilities (using Monte-Carlo integrations) for fixed correlation matrices.

This article, Part II, presents step (iii) of the three-step dynamic risk analysis methodology. First, in Part I, methods were introduced to transform the large distributed control system (DCS) and emergency shutdown (ESD) alarm databases into event-trees and set-theoretic formulations. In this part, a novel Bayesian analysis method using copulas is presented that utilizes the near-miss information in set-theoretic formulations, to yield risk levels in chemical plants and estimates for failure probabilities of the safety, quality, and operability systems (SQOSs) as well as their correlation matrix. The Bayesian model accounts for the interdependences among the SQOSs using copulas, which occur because of the nonlinear relationships between the variables and behavior-based factors involving human operators. As in Part I, the DCS and ESD databases for a large-scale fluidized-catalytic-cracking unit (FCCU) are utilized over a study period divided into 13 equal-time periods. The unit has about 150–200 alarmed variables and as many as 5000–10,000 alarm occurrences per day—as a result of 500–1000 abnormal events daily. For more specifics, see the Case Study 2 in Part I.

The organization of the remainder of this article is as follows. The section entitled Preliminaries introduces the Bayesian model and copulas. The elements of the Bayesian simulation using the multiple-block, Metropolis–Hastings algorithm are presented in the Bayesian Simulation using Random-Walk, Multiple-Block, Metropolis–Hastings Algorithm. Next, the section entitled Results includes a discussion on the selection of the copulas, and contrasting engineering and statistical perspectives, followed by the Conclusions.

Preliminaries

Classical methods, including maximum likelihood estimation,[38] focus on the calculation of point estimates. Often, they unreliably estimate the occurrence of rare events due to limited data. Alternatively, in PRA using Bayesian theory, estimates of incident frequencies (with uncertainties) are obtained. For every component, such as sensors and controllers, failure probabilities are estimated using failure data over many years and incident frequencies are modeled as a function of the failure rates of the individual components. But, because incidents normally involve interacting components, the failure probabilities of the individual components are normally inadequate to reliably estimate the probabilities of incidents. To be effective, PRA requires an explicit representation of the dependencies between components, which may not always be feasible, resulting in biases in the estimated incident frequencies.

Consequently, herein, in the Bayesian analysis, prior/expert knowledge is used and interactions of the SQOSs are modeled. In addition, vast amounts of near-miss data in DCS and ESD system databases, over extended periods of time, are utilized to obtain dynamic updates of the SQOS failure probabilities and more reliable probability estimates of rare incidents. As will be shown, the risks associated with low-probability, high-consequence incidents are predicted more accurately.

In this section, the basics of the Bayesian analysis are presented, beginning with a brief review of Bayesian theory, followed by the probability distributions for the SQOSs. The causal relationship between the SQOSs is outlined and the use of copulas is discussed. In addition, the likelihood, posteriors, and priors for the Bayesian model are presented.

Bayesian theory

Bayesian analysis is a statistical approach to reasoning under uncertainty. Herein, the uncertainty associated with the failure probability of a SQOS, $\boldsymbol{\theta}$, is modeled initially using a probability density function, $f(\boldsymbol{\theta})$, called the prior distribution. An improved failure probability distribution, $f(\boldsymbol{\theta}|\text{Data})$, called a posterior distribution (expressed in Eq. 1), is inferred using the near-miss data obtained from the DCS and ESD databases. On the basis of Bayes rule, $f(\boldsymbol{\theta}|\text{Data})$ is

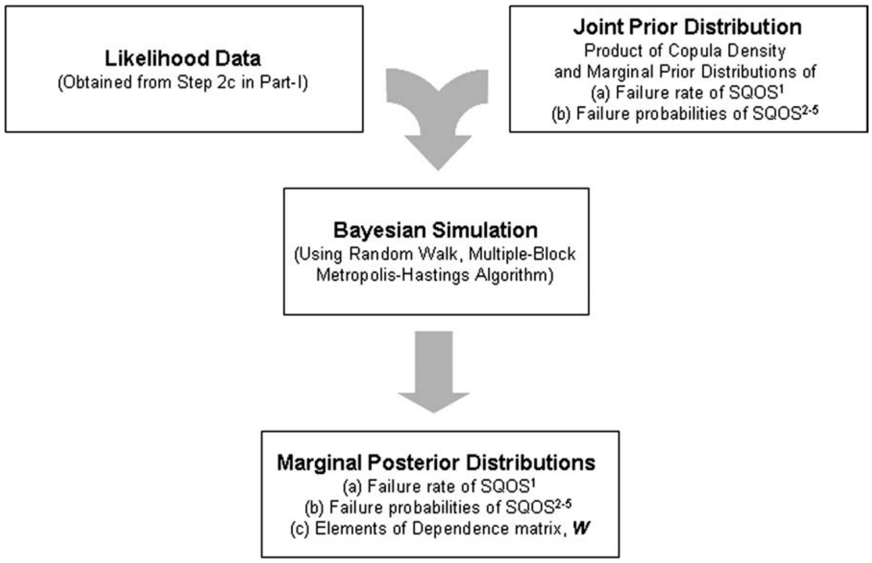

Figure 1. Overall schematic of the Bayesian analysis framework.

proportional to the distribution of data conditional on $\boldsymbol{\theta}$, $g(\text{Data}|\boldsymbol{\theta})$, the likelihood, multiplied by the prior distribution of $\boldsymbol{\theta}$, $f(\boldsymbol{\theta})$

$$f(\boldsymbol{\theta}|\text{Data}) = \frac{g(\text{Data}|\boldsymbol{\theta})f(\boldsymbol{\theta})}{\int g(\text{Data}|\boldsymbol{\theta})f(\boldsymbol{\theta})d\boldsymbol{\theta}} \tag{1}$$

In general, all Bayesian analyses begin with prior probability distributions for unobservable parameters (typically denoted as $\boldsymbol{\theta}$), normally based on prior or expert information. Then, using the data, the priors are updated to give posterior distributions. Clearly, as more data are added, the influence of the prior distribution on the resulting posterior distribution decreases.

Similarly, in the Bayesian analysis herein, the failure probabilities of the SQOSs are estimated with the help of prior knowledge and shared information from other SQOSs (using copulas). The near-miss data, in the set-theoretic formulation in Part I, are used to update the prior failure probabilities to obtain posterior failure probabilities. The latter probabilities permit a projection of the frequency of incidents. With more data points, estimates of their posterior failure probabilities become more accurate and certain.

Also, the method of conjugate priors is used to model the unobservable parameters. Their posterior distributions belong to the same family of distributions as their prior distributions. Here, the prior distributions are called conjugate priors to their likelihood distributions. For example, the Gamma distribution is a family of conjugate priors to the Poisson distribution. For more details on Bayesian theory, refer to Gelman et al.[39] and Bolstad.[40]

In addition, the posterior estimates of the correlation matrix of the SQOSs, denoted as $\boldsymbol{W}$, are computed herein. The Bayesian simulation to obtain the marginal posterior distributions for θs and $\boldsymbol{W}$ is carried out using the Metropolis–Hastings algorithm. The algorithm to implement these steps is shown in Figure 1. The results of the statistical analysis are obtained using the R and MATLAB packages.

Probability distributions for the SQOSs

As discussed in Part I, five SQOSs are defined for a typical chemical plant. They are (a) the basic process control system (BPCS) or SQOS^1, (b) operator (machine + human) corrective actions, level I, or SQOS^2, (c) operator (machine + human) corrective actions, level II, or SQOS^3, (d) the override controller, or SQOS^4, and (e) automatic ESD, or SQOS^5.

The number of abnormal events in a time period is the failure count of the first SQOS (i.e., the BPCS denoted as SQOS^1) in that period. Because the abnormal events in any period occur with an average rate, and independently of the last period, herein, the number of abnormal events in time period t, n_t, is assumed to follow a Poisson distribution with the (average) failure rate of SQOS^1 denoted as θ_1. That is

$$n_t \sim \text{Poisson}(\theta_1) \tag{2a}$$

and

$$f(n_t|\theta_1) \propto (\theta_1)^{n_t} \mathrm{e}^{-(\theta_1)} (\text{likelihood distribution}) \tag{2b}$$

Likelihood data on n_t can be the number of abnormal events for all the primary variables, n_T (see Table 5, Part I), or the number of abnormal events for $\text{p}P_1$, n_{pP_1} (see Table 6, Part I) or the number of abnormal events for all the primary process variables, $n_{\text{p}P}$ (see Table 7, Part I). As discussed above, the Gamma family of distributions is the conjugate family for Poisson observations (i.e., a Gamma prior when combined with Poisson likelihood leads to a Gamma posterior). Therefore, to simplify calculations, θ_1 is assumed to have a Gamma prior distribution with a_1 and b_1 as shape parameters

$$f(\theta_1) \propto (\theta_1)^{a_1 - 1} \mathrm{e}^{-b_1\theta_1} \tag{3}$$

For the other four SQOSs, as the outcomes of their actions on any abnormal event can have one of two possible outcomes, "success" and "failure," they are modeled as independent and identical Bernoulli trials with failure probabilities, θ_j, $j = 2,\ldots, 5$. The prior distributions for θ_j are assumed to be Beta distributions (conjugate priors) with the shape vector $[a_j, b_j]$, $j = 2,\ldots, 5$.

SQOS interactions and copulas

The interactions between the performances of the SQOSs (measured as failure rates or probabilities) are due to the following.

Nonlinear Relationships Between the Variables. As discussed in Part I and by Pariyani et al.,[41] because of the interdependent relationship between the variables of a process, the effects of the controlling actions of the SQOSs on variables/group of variables get channeled to other variables/groups of variables, thereby, influencing the controlling actions of the other SQOSs. For example, the impact of corrective actions of the override controllers on the primary variables get channeled to the secondary variables, which return the majority of the secondary variables to their green-belt zones (or normal operating ranges)—this clearly improves the failure probabilities of the corrective actions of the human operators.

Behavior-Based Factors. Stressor performance-shaping factors[24,41] associated with human operators are likely to influence the performances of human-operated SQOSs. These, in turn, influence other SQOSs through the nonlinear effects of their variables. For example, increases in the failure rates of the BPCSs, θ_1, are likely to deteriorate the performances of the operators (i.e., increase θ_2 and θ_3). These, in turn, could counter the corrective actions of $SQOS^1$ and $SQOS^4$. As $SQOS^5$, the ESD system, also involves human interventions, its failure probability, θ_5, is also likely to be influenced by changes in θ_1, θ_2, θ_3, and θ_4.

Herein, these causal relationships between the SQOSs are accounted for using a dependence matrix, which consists of pairwise interaction parameters.

Because the random variables, θ_k ($k = 1, 2,\ldots, 5$), are not independent, with their marginal distributions belonging to different families, copulas are used to describe their joint distribution. Note that for these multivariate distributions, given a parent parametric distribution function, the marginals are derived by integration. Consequently, the marginals are from the same family; for example, the marginals of a multivariate normal distribution are also normal. By contrast, with copula modeling, the marginals, which need not be from the same family, are combined and interactions between the random variables are accounted for using the dependence matrix.[31,37]

To describe the dependences between the related random variables, measures of dependences, such as rank-correlation measures (e.g., Spearman's ρ and Kendall's τ), which are insensitive to the marginal distributions of the raw data, must be used. For example, when random variables are not normally distributed, Pearson's or linear correlations (which assume normality) may no longer be meaningful measures of dependence. The important feature of copula modeling is that it permits the use of rank-correlation measures.

Another advantage of the dependence matrix is that it enables the random variables to interact among each other and share information. This is particularly important when data on random variables are limited; for example, associated with rare events. In such situations, information associated with other random variables is channeled through the elements of dependence matrix (i.e., interaction parameters). Clearly, the choices of copulas determine the dependences among random variables, as will be discussed in the sections entitled Copulas, Likelihood, Joint Posterior and Prior Distributions, and Multivariate Normal and Cuadras–Augé Copulas, and the Results.

Copulas

A copula is a function that links a multivariate cumulative distribution to its univariate cumulative marginals. Stated formally, according to the Sklar theorem,[42] given a joint cumulative distribution function (CDF), $F(\theta_1, \theta_2,\ldots, \theta_N)$, for the random variables, $\theta_1, \theta_2,\ldots, \theta_N$, with marginal CDFs, $F_1(\theta_1), F_2(\theta_2),\ldots, F_N(\theta_N)$), F can be written as a function of its marginals

$$F(\theta_1,\theta_2,\ldots,\theta_N) = C[F_1(\theta_1),F_2(\theta_2),\ldots,F_N(\theta_N)] \qquad (4)$$

where C is the copula (function). Given that F_k and C are differentiable, the joint density distribution, $f(\theta_1, \theta_2,\ldots, \theta_N)$, can be written as

$$f(\theta_1,\theta_2,\ldots,\theta_N) = c(F_1(\theta_1),F_2(\theta_2),\ldots,F_N(\theta_N)) \times \prod_{k=1}^{N} f_k(\theta_k) \qquad (5)$$

where $f_k(\theta_k)$ is the density distribution corresponding to $F_k(\theta_k)$ (denoted as u_k hereafter), and $c = \partial^N C/(\partial u_1 \ldots \partial u_N)$, ∂u_N is called the copula density distribution.

Therefore, when θ_k, $k = 1,\ldots, N$, are independent, $c = 1$ and $f(\theta_1,\theta_2,\ldots,\theta_N) = \prod_{k=1}^{N} f_k(\theta_k)$. Here, the copula is $C[u_1, u_2, \ldots, u_N] = u_1 u_2 \ldots u_N$, also known as the "independence copula." Note that no restrictions are placed on the marginal distributions; for example, a bivariate distribution can be constructed using beta and gamma distributions. The copulas do not impact the marginal distributions of the associated random variables and only model the dependences between them—they have no other role.

Several copula types have been reported.[31,32,43,44] Here, three types are reviewed:

Elliptical copulas are derived from common multivariate (elliptical) distributions, which can be extended to arbitrary dimensions. They have many parameters, which facilitate data regression. The Gaussian copula (derived from the multivariate normal distribution) and the *t*-copula (derived from multivariate Student's *t*-distribution) are two of the most common elliptical copulas. Compared with other copulas, the Gaussian copula has a nearly full range (-1, 1) of pairwise correlation coefficients—yielding a general and robust copula, which is used in most applications, including dependences between the SQOSs in the Results. The Gaussian copula, however, lacks the tail dependence; that is, the probability of observing extreme observations in all random variables at once. This limitation can be addressed by using *t*-copula or Archimedean copula.

Archimedean copulas are suitable for low-dimensional systems ($n \leq 2$) because of their simple closed functional forms. For n-dimensional distributions, serial iterates of Archimedean copulas are constructed, but these do not provide arbitrary pairwise correlations. Furthermore, restrictions on Kendall's τ limits reduce the usefulness of these copulas.[26] Examples include the Gumbel, Frank, and Clayton copulas.[31,32,43]

Marshall-Olkin copulas may be derived from a simple stochastic process model called a Poisson shock model, where components are subjected to fatal shocks, following Poisson processes.[32] One special copula in this family is the Cuadras–Augé copula[45] having an n-dimensional form capable of modeling arbitrary pairwise correlations.[26] It is used herein to model the dependences between the SQOSs.

Likelihood, joint posterior, and prior distributions

The joint likelihood distribution, $L(\text{Data}|\theta)$, is the product of likelihood distributions of the SQOSs

$$L(\text{Data}|\boldsymbol{\theta}) = (\theta_1)^{n_t} e^{-(\theta_1)} \prod_{j=2}^{Ns} (\theta_j)^{K_t^j} (1-\theta_j)^{L_t^j} \tag{6}$$

where Ns is the number of SQOSs (i.e., five for the FCCU), and K_t^j and L_t^j denote the failure and success counts for SQOS^j in time period, t. For the total study period, T, the K_T^j and L_T^j are the failure and success counts for all the primary variables, as given in Table 5, Part I, $K_{pP_1}^j$ and $L_{pP_1}^j$ are for pP_1 (Table 6, Part I), and K_{pP}^j and L_{pP}^j are for all the primary process variables (Table 7, Part I). Clearly, once data are added, the joint likelihood distribution is a function of the θs.

As shown in Figure 1, the joint posterior distribution (or target distribution), which is a function of the failure rate and probabilities of the SQOSs and their correlation matrix, is proportional to their joint prior distribution multiplied by their joint likelihood distribution

$$f(\theta_1, \theta_2, \ldots, \theta_{Ns}, \boldsymbol{W}|\text{Data}) \propto \underbrace{(\theta_1)^{n_t} e^{-(\theta_1)} \prod_{j=2}^{Ns} (\theta_j)^{K_j} (1-\theta_j)^{L_j}}_{\text{likelihood}} \times \underbrace{f(\theta_1, \theta_2, \ldots, \theta_{Ns}|\boldsymbol{W}) \times f(\boldsymbol{W})}_{\text{joint prior}} \tag{7}$$

where $\boldsymbol{W}$ is the Spearman rank correlation matrix between the failure rate and probabilities of the SQOSs, and Data is the set of success and failure counts for SQOS$^{1-5}$, as given in Tables 5–7 of Part I.

The joint prior distribution of θs, conditional on their correlation matrix, combines the marginal prior distributions of θs and their dependences using the copula density distribution, c, which is a function of the elements of the dependence matrix; that is

$$f(\theta_1, \theta_2, \ldots, \theta_{Ns}|\boldsymbol{W}) \propto c(F_1(\theta_1), F_2(\theta_2), \ldots, F_{Ns}(\theta_{Ns})) \times \prod_{k=1}^{Ns} f_k(\theta_k) \tag{8}$$

As discussed earlier, the prior distributions for the θs are

$$f_1(\theta_1) \propto (\theta_1)^{a_1-1} e^{-b_1\theta_1} \tag{9a}$$

$$f_j(\theta_j) \propto (\theta_j)^{a_j-1} (1-\theta_j)^{b_j-1}, \quad j = 2, \ldots, 5 \tag{9b}$$

where $\boldsymbol{a} = [a_1, a_2, a_3, a_4, a_5]^T$ and $\boldsymbol{b} = [b_1, b_2, b_3, b_4, b_5]^T$ are the shape-factor vectors. These vectors are selected to characterize the distributions before data are entered. They often reflect prior knowledge of the process or theoretical assumptions—and are especially important when few data points are available. Of course, expert knowledge or data for similar systems (or process units) should be used when available.

The prior distribution for the Spearman rank correlation matrix, $\boldsymbol{W}$, is taken as the Inverse-Wishart distribution

$$f_w(\boldsymbol{W}) \propto |S^{\text{init}}|^{v/2} |\boldsymbol{W}|^{-(v+n+1)/2} \exp(-0.5 \times \text{tr}(\boldsymbol{S}^{\text{init}}(\boldsymbol{W})^{-1})) \tag{10}$$

where $\boldsymbol{S}^{\text{init}}$ and v are the initial scale matrix and the number of degrees of freedom, respectively. Herein, the latter is assumed to be 10 because there are 10 different pairwise correlation coefficients for five SQOSs.

Multivariate normal and Cuadras–Augé copulas

Because of their abilities to model arbitrary pairwise correlations (both positive and negative) between the random variables, the multivariate normal and Cuadras–Augé copulas are used herein, with details provided in the next subsections.

Multivariate Normal Copula. The multivariate normal copula has been widely used in risk analysis.[31,32,35,37,43] Similar to multivariate normal distributions, it models dependencies (using pairwise correlations), but does so for random variables with arbitrary marginals.[31,35]

The multivariate normal copula density is

$$c(u_1, u_2, \ldots, u_5) = \exp[-\{\Phi^{-1}(u_1), \ldots, \Phi^{-1}(u_5)\}(\boldsymbol{R}^{-1} - \boldsymbol{I}) \times \{\Phi^{-1}(u_1), \ldots, \Phi^{-1}(u_5)\}^T/2]/|\boldsymbol{R}|^{1/2} \tag{11}$$

where $\boldsymbol{R}$, Φ^{-1}, and $\boldsymbol{I}$ are the product-moment correlation matrix, the normal inverse transformation, and the 5 × 5 identity matrix. The Spearman correlation matrix, $\boldsymbol{W}$, with elements w_{kq}, can be constructed from $\boldsymbol{R}$, with elements r_{kq}, using the following relationship[35,46]

$$r_{kq} = 2\sin(\pi w_{kq}/6) \tag{12}$$

This copula density applies for positive and negative correlations.

Cuadras–Augé copula. The Cuadras and Augé copula density for positive correlations is

$$c(u_1, u_2, \ldots, u_5) = \frac{\partial^5 C}{\partial u_1 \partial u_2 \partial u_3 \partial u_4 \partial u_5} = \prod_{k=1}^{5} \left(\prod_{h=1}^{5-k} (1-\alpha_{k-(k+h)}) u_k^{\left(\prod_{h=1}^{5-k}(1-\alpha_{k-(k+h)})-1\right)} \right) \tag{13a}$$

where

$$u_k \dot{\geq} \cdots \dot{\geq} u_n \tag{13b}$$

and

$$u_k = F_k(\theta_k) = \int_0^{\theta_k} f_k(\theta_k) d\theta_k, \quad k = 1, \ldots, 5 \tag{13c}$$

Note that $\dot{\geq}$ denotes $>$ or $\geq$, as appropriate. Here, the correlation coefficient, α_{k-q}, for interactions between θ_k and θ_q (k, $q = 1,\ldots, 5$, $k \neq q$) is related to the Spearman rank correlation coefficient, $w(\theta_k, \theta_q)$, by

$$w(\theta_k, \theta_q) = \frac{3\alpha_{k-q}}{4 - \alpha_{k-q}} \text{ for } k \neq q \tag{14}$$

High $w(\theta_k, \theta_q)$ indicates strong interaction between θ_k and θ_q—and zero indicates independence.

The constraint of Eq. 13b de-emphasizes the larger CDFs and ensures that u_k in Eq. 13a is sorted in descending order for each iteration of the M–H algorithm. For example, when $u_2 > u_3 > u_1 > u_5 > u_4$, the copula density is

$$\begin{aligned} c(u_1, u_2, \ldots, u_5) = {} & ((1-\alpha_{2-1})(1-\alpha_{2-3})(1-\alpha_{2-4}) \\ & (1-\alpha_{2-5})u_2^{(1-\alpha_{2-1})(1-\alpha_{2-3})(1-\alpha_{2-4})(1-\alpha_{2-5})-1}) \\ & \times ((1-\alpha_{3-1})(1-\alpha_{3-4}) \\ & (1-\alpha_{3-5})u_3^{(1-\alpha_{3-1})(1-\alpha_{3-4})(1-\alpha_{3-5})-1}) \\ & \times ((1-\alpha_{1-4})(1-\alpha_{1-5})u_1^{(1-\alpha_{1-4})(1-\alpha_{1-5})-1}) \\ & \times ((1-\alpha_{5-4})u_5^{(1-\alpha_{5-4})-1}) \end{aligned} \tag{15}$$

On the basis of the study of Cuadras and Augé,[45] the functional form of copula having negative correlation values is developed herein. When $\alpha_{k-q} < 0$, u_k is replaced with (1-u_k) and α_{k-q} is replaced with ($-\alpha_{k-q}$) in Eqs. 13a and 13b. Also, Eq. 14 becomes

$$w(\theta_k, \theta_q) = w_{kq} = \frac{3\alpha_{k-q}}{4 + \alpha_{k-q}} \text{ for } k \neq q \tag{16}$$

The resulting function defines the copula density for negative correlations. Note that the copula density is piecewise differentiable continuous on $w_{kq} \in [-1,1]$. It is continuous over the entire domain, but nondifferentiable at $w_{kq} = 0$.

Bayesian Simulation Using Random-Walk, Multiple-Block, Metropolis–Hastings Algorithm

As shown in Figure 1, the marginal posterior distributions of the θs and their correlation matrix, $\boldsymbol{W}$, are obtained using the Metropolis–Hastings (M–H) algorithm—a family of Markov chain simulation methods. These draw samples from approximate distributions (known as proposal or jumping distributions) and correct them to better approximate the target posterior distribution.

The powerful M–H algorithm produces a correlated sequence of draws from the target density that may be difficult to sample using independence sampling methods.[39,40,47,48] To define the algorithm, one needs to begin with a suitable starting point, $\boldsymbol{\theta}^{(0)}$, for which $f(\boldsymbol{\theta}^{(0)}|\text{Data}) > 0$; for example, maximum likelihood estimates (MLEs) of the failure rate and probabilities. For the next iteration, two steps are involved: (a) sample a proposal value, θ^*_1, from a proposal distribution, J_1^t (discussed in the subsection entitled Proposal Distributions for the Failure Rate and Probabilities of SQOSs) and (b) accept the proposal value as the next iterate in the Markov chain according to the probability, min(r_1, 1), where

$$r_1 = \frac{f(\theta_1^*, \theta_2^0, \ldots, \theta_5^0, \boldsymbol{W}^0|\text{Data})}{f(\theta_1^0, \theta_2^0, \ldots, \theta_5^0, \boldsymbol{W}^0|\text{Data})} \frac{J_1^t(\theta_1^0|\theta_1^*)}{J_1^t(\theta_1^*|\theta_1^0)} \tag{17}$$

More specifically, first a random number is obtained between 0 and 1. When $r_1 < 1$, the proposal value is accepted when that random number is less than r_1. Otherwise, the proposal value is rejected and the current θ_1 is retained. The ratio, r_1, is proportional to the relative change in the posterior distribution using the proposal value and indicates the goodness of the match of the proposal value to the target distribution compared with the previous value. This relative change is multiplied by $\frac{J_1^t(\theta_1^0|\theta_1^*)}{J_1^t(\theta_1^*|\theta_1^0)}$ to account for asymmetric jumping in the proposal distribution. When the proposal distribution is symmetric, this factor is unity.

For high-dimensional systems, such as the FCCU, a single block M–H algorithm that rapidly converges to the target density can be difficult to construct. In such cases, the variate space can be discretized into smaller blocks, with Markov chains constructed in the smaller blocks. This modified algorithm is referred to as the multiple-block, Metropolis–Hastings algorithm.[48] Note that the proposal distributions are chosen to be random-walk distributions with the mean at iteration t equal to the previous iteration value.

Using these two steps, a single iteration of the multiple-block, M–H algorithm is completed by updating each block sequentially, using the above probabilities of a move, given the current value for the other blocks. Many iterations are implemented until the initial state is indiscernible. Typically, the initial samples are not completely valid because the Markov chain has not been stabilized. These burn-in samples are discarded. The remaining values are accepted and represent samples from the posterior distribution. Note that samples are taken from regions where the posterior probability is high and the chains begin to mix in these regions. When effective, the proposal density matches the shape of the target distribution, which is usually unknown.

Next, a procedure is presented to carry out the Bayesian simulation to obtain the marginal posterior distributions of θ and $\boldsymbol{W}$.

Procedure for Bayesian simulation

In algorithmic form, the following recursive procedure is used to obtain simulated values:

(1) Specify initial values, $\boldsymbol{\theta}^{(0)}$ and $\boldsymbol{W}^{(0)}$.

(2) Repeat for $t = 1, 2,\ldots, M$ (number of iterations)

(a) Propose θ_1* using Eq. 18:

$$\text{Set } \theta_1^t = \begin{cases} \theta_1^* \text{with probability} \min(r_1, 1) \\ \theta_1^{t-1}, \text{otherwise} \end{cases}$$

with $r_1 = \frac{f(\theta_1^*,\theta_2^{t-1},\ldots,\theta_5^{t-1},\boldsymbol{W}^{t-1}|\text{Data})}{f(\theta_1^{t-1},\theta_2^{t-1},\ldots,\theta_5^{t-1},\boldsymbol{W}^{t-1}|\text{Data})}\frac{J_1^t(\theta_1^{t-1}|\theta_1^*)}{J_1^t(\theta_1^*|\theta_1^{t-1})}$

(b) Repeat for $j = 2,\ldots, 5$:

Propose $\theta*_j$ using Eq. 19:

Set $\theta_j^t = \begin{cases} \theta_j^* \text{with probability } \min(r_j, 1) \\ \theta_j^{t-1}, \text{ otherwise} \end{cases}$

with $_j = \frac{f(\theta_1^t,\ldots,\theta_{j-1}^t,\theta_j^*,\theta_{j+1}^{t-1},\ldots,\theta_5^{t-1},\boldsymbol{W}^{t-1}|\text{Data})}{f(\theta_1^t,\ldots,\theta_{j-1}^t,\theta_j^{t-1},\theta_{j+1}^{t-1},\ldots,\theta_5^{t-1},\boldsymbol{W}^{t-1}|\text{Data})}\frac{J_j^t(\theta_j^{t-1}|\theta_j^*)}{J_j^t(\theta_j^*|\theta_j^{t-1})}$

(c) Propose $\boldsymbol{W}*$ using Eq. 20:

Set $\boldsymbol{W}^t = \begin{cases} \boldsymbol{W}^* \text{with probability } \min(r_w, 1) \\ \boldsymbol{W}^{t-1}, \text{ otherwise} \end{cases}$

with $r_w = \frac{f(\theta_1^t,\theta_2^t,\ldots,\theta_5^t,\boldsymbol{W}^*|\text{Data})}{f(\theta_1^t,\theta_2^t,\ldots,\theta_5^t,\boldsymbol{W}^{t-1}|\text{Data})}\frac{J_w^t(\boldsymbol{W}^{t-1}|\boldsymbol{W}^*)}{J_w^t(\boldsymbol{W}^*|\boldsymbol{W}^{t-1})}$

(3) Save $\{(\boldsymbol{\theta}^{(1)}, \boldsymbol{W}^{(1)}), (\boldsymbol{\theta}^{(2)}, W^{(2)}),\ldots, (\boldsymbol{\theta}^{(M)}, \boldsymbol{W}^{(M)})\}$.

Next, the proposal distributions for θs and their correlation matrix, $\boldsymbol{W}$, are discussed.

Proposal distributions for the failure rate and probabilities of SQOSs

The proposal distribution for failure rate of SQOS[1] is taken to be

$$\theta_1^* \sim \text{Gamma}(A_1, B_1) \tag{18a}$$

with expected value

$$E(\theta_1^*) = \frac{A_1}{B_1} = \theta_1^{t-1} \tag{18b}$$

that is

$$\theta_1^* \sim \text{Gamma}\left(A_1, \frac{A_1}{\theta_1^{t-1}}\right) \tag{18c}$$

with the conditional proposal distribution

$$J_1^t(\theta_1^*|\theta_1^{t-1}) = \frac{\left(\frac{A_1}{\theta_1^{t-1}}\right)^{A_1}}{\Gamma(A)}(\theta_1^*)^{A_j-1}e^{-\left(\frac{A_1}{\theta_1^{t-1}}\right)\theta_1^*} \tag{18d}$$

and

$$\text{var}(\theta_1^*) = \frac{(\theta_1^{t-1})^2}{A_1} \tag{18e}$$

The proposal distributions for the failure probabilities of SQOS[2–5] are taken as

$$\theta_j^* \sim \text{Beta}(A_j, B_j), \quad j = 2, \ldots, 5 \tag{19a}$$

with

$$E(\theta_j^*) = \frac{A_j}{A_j + B_j} = \theta_j^{t-1}, \quad j = 2, \ldots, 5 \tag{19b}$$

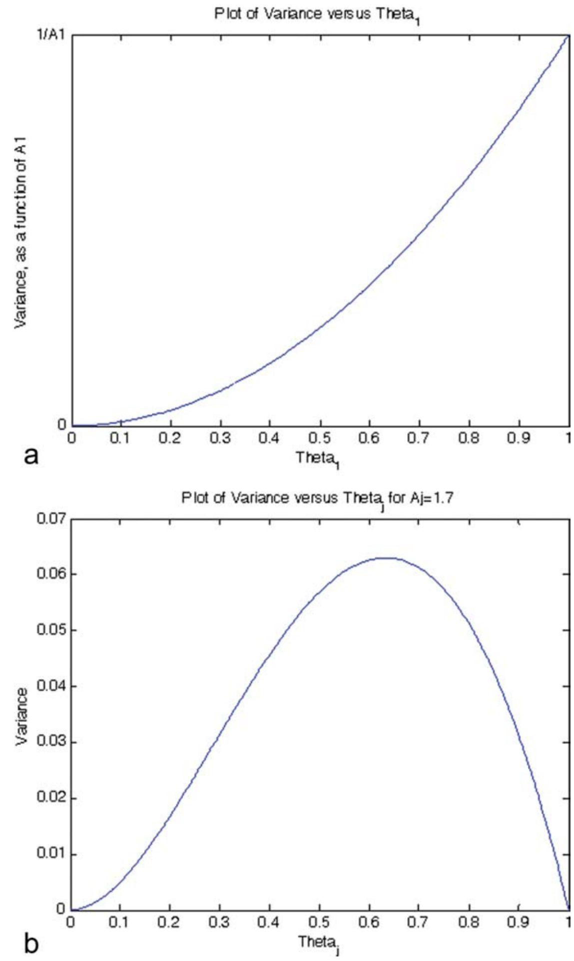

Figure 2. Variance of proposal distributions as a function of (a) failure rate (Eq. 18e), and (b) failure probabilities (Eq. 19e), with A_j = 1.7, j = 2, . . ., 5.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Therefore

$$\theta_j^* \sim \text{Beta}\left(A_j, A_j \times \left(\frac{1-\theta_j^{t-1}}{\theta_j^{t-1}}\right)\right), \quad j = 2, \ldots, 5 \tag{19c}$$

with the conditional proposal distribution

$$J_j^t(\theta_j^*|\theta_j^{t-1}) = \frac{\Gamma\left(\frac{A_j}{\theta_j^{t-1}}\right)}{\Gamma(A_j)\Gamma\left(A_j \times \frac{1-\theta_j^{t-1}}{\theta_j^{t-1}}\right)}(\theta_j^*)^{A_j-1}(1-\theta_k^*)^{A_j \times \frac{1-\theta_j^{t-1}}{\theta_j^{t-1}} - 1} \tag{19d}$$

and

$$\text{var}(\theta_j^*) = \frac{(\theta_j^{t-1})^2(1-\theta_j^{t-1})}{A_j + \theta_j^{t-1}} \tag{19e}$$

The variances of the proposal distributions are displayed as a function of the failure rate and probabilities in Figure 2.

Note that A_k, $k = 1,\ldots, 5$, are free parameters that determine the convergence and autocorrelation of the samples. From the above functional forms of the variances, some information regarding the A_k can be inferred. When the variances of the proposal distribution are very small (using high A_k), the acceptance rates of samples (i.e., the fraction of proposed samples accepted) are very high. However, these samples tend to move slowly about the space and/or become trapped in the vicinity of local minima, resulting in high autocorrelations when they are not well "mixed." On the other hand, when the variances are very high (using small A_k), the samples tend to experience jumps, resulting in less autocorrelation, but lower acceptance rates of the moves—because of the increased likelihood of jumping to regions having a lower probability density. In summary, the autocorrelations and acceptance rates of the moves are sensitive to A_k, with clear tradeoffs between them. For the simulation studies herein, the following $\boldsymbol{A}$ gave low autocorrelation and moderately high sample acceptance rates: $A_1 \in [30,40]$, $A_2 \in [35,45]$, $A_3 \in [15,25]$, $A_4 \in [1.5,2]$, and $A_5 \in [1.5,2]$.

Proposal distribution for the correlation matrix

The proposal distribution for the correlation matrix is chosen to be a random-walk, Inverse-Wishart distribution with its expected value at iteration t equal to its previous iteration value. Therefore

$$\boldsymbol{\Gamma}^* \sim \text{Inv} - \text{Wishart}_v(\boldsymbol{S}^{-1}) \tag{20a}$$

where $\boldsymbol{\Gamma}^*$ is the unconstrained correlation matrix (proposed), $\boldsymbol{S}$ is the scale matrix, and v is the number of degrees of freedom (assumed to be 10). The elements of $\boldsymbol{\Gamma}^*$ are scaled to obtain the scaled correlation matrix, $\boldsymbol{W}^*$

$$\boldsymbol{W}^* = \text{diag}((\boldsymbol{\Gamma}^*)^{-1/2})\boldsymbol{\Gamma}^*\text{diag}((\boldsymbol{\Gamma}^*)^{-1/2}) \tag{20b}$$

This transformation sets the diagonal elements of $\boldsymbol{\Gamma}^*$ to unity and scales the other elements to the range $[-1, 1]$.

Furthermore

$$E(\boldsymbol{W}^*) = (v - n - 1)^{-1}\boldsymbol{S} = \boldsymbol{W}^{t-1} \tag{20c}$$

Therefore

$$\boldsymbol{S} = (v - n - 1)\boldsymbol{W}^{t-1} = (10 - 5 - 1)\boldsymbol{W}^{t-1} = 4\boldsymbol{W}^{t-1} \tag{20d}$$

Thus, the probability density function is

$$J_w^t(\boldsymbol{W}^*|\boldsymbol{W}^{t-1}) \propto |S|^{v/2}|\boldsymbol{W}^*|^{-(v+n+1)/2}\exp(-0.5\text{tr}(S(\boldsymbol{W}^*)^{-1})) \tag{20e}$$

Note that the Inverse-Wishart distribution gives positive-definite samples (matrices)—a condition required for correlation matrices.[39,49]

Alternatively, elements of the correlation matrix can be sampled individually from different univariate proposal distributions (e.g., beta distributions)—without maintaining a positive-definite correlation matrix. Then, the sample elements that destroy the positive-definiteness of the matrix are rejected and re-sampled until the proposal matrix becomes positive-definite. The entire proposal matrix is accepted or rejected using the M–H algorithm. This individual sampling algorithm yielded a much lower acceptance rate for the correlation matrix than that obtained using the Inverse-Wishart distribution. In addition, the posterior variances of the elements were much higher, introducing more uncertainty and convergence problems. Hence, the random-walk, Inverse-Wishart distribution was used as the proposal distribution for the correlation matrix.

Results

Results for the simulation studies are presented next. Several Markov chains of 70,000 iterations for different priors and M–H starting points converged rapidly for θ_1, θ_2, and θ_3 (the differences between the means and variances of the posterior distributions for different priors and M–H starting points were found to be negligible). In addition, a low autocorrelation was found among the samples.

The results were obtained using "Jeffrey's priors" (noninformative prior distributions, invariant under reparameterization of the parameters) and "uniform priors." However, the Jeffrey prior for $SQOS^1$ yields $a_1 = 0.5$, $b_1 = 0$, which is improper (as $b_1 > 0$ for proper priors). Therefore, a_1 and b_1 are assumed to be equal to 0.01. For $SQOS^{2\text{–}4}$, the parameters (for Jeffrey's priors) for the beta distributions are a_2, a_3, a_4, b_2, b_3, $b_4 = 0.5$. For $SQOS^5$, a uniform prior is assumed; that is, $a_5 = 1$, $b_5 = 1$. Note that a Jeffrey prior for $SQOS^5$ led to significant autocorrelation among the $SQOS^5$ posterior samples. This does not occur when $b_5 > a_5 > 0.5$. In summary, $\boldsymbol{a} = [0.01, 0.5, 0.5. 0.5, 1]^T$ and $\boldsymbol{b} = [0.01, 0.5, 0.5. 0.5, 1]^T$ were used.

For the correlation matrix, the following prior value was used:[25]

$$\boldsymbol{W}^{\text{init}} = \begin{bmatrix} 1 & 0.8 & 0.7 & 0.6 & 0.5 \\ 0.8 & 1 & 0.8 & 0.7 & 0.6 \\ 0.7 & 0.8 & 1 & 0.8 & 0.7 \\ 0.6 & 0.7 & 0.8 & 1 & 0.8 \\ 0.5 & 0.6 & 0.7 & 0.8 & 1 \end{bmatrix} \tag{21}$$

$\boldsymbol{S}^{\text{init}}$ was assumed to be

$$\boldsymbol{S}^{\text{init}} = (v - n - 1) \times E(\boldsymbol{W}^{\text{init}}) = 4 \times \boldsymbol{W}^{\text{init}}$$
$$= 4 \times \begin{bmatrix} 1 & 0.8 & 0.7 & 0.6 & 0.5 \\ 0.8 & 1 & 0.8 & 0.7 & 0.6 \\ 0.7 & 0.8 & 1 & 0.8 & 0.7 \\ 0.6 & 0.7 & 0.8 & 1 & 0.8 \\ 0.5 & 0.6 & 0.7 & 0.8 & 1 \end{bmatrix} \tag{22}$$

Here, also, several prior matrices yielded rapid convergence to their posterior matrices.

Results for pP_1 using the multivariate normal and Cuadras–Augé copulas are presented next. Later, results for all the primary and primary process variables are compared to show the benefits of using quality data in dynamic risk

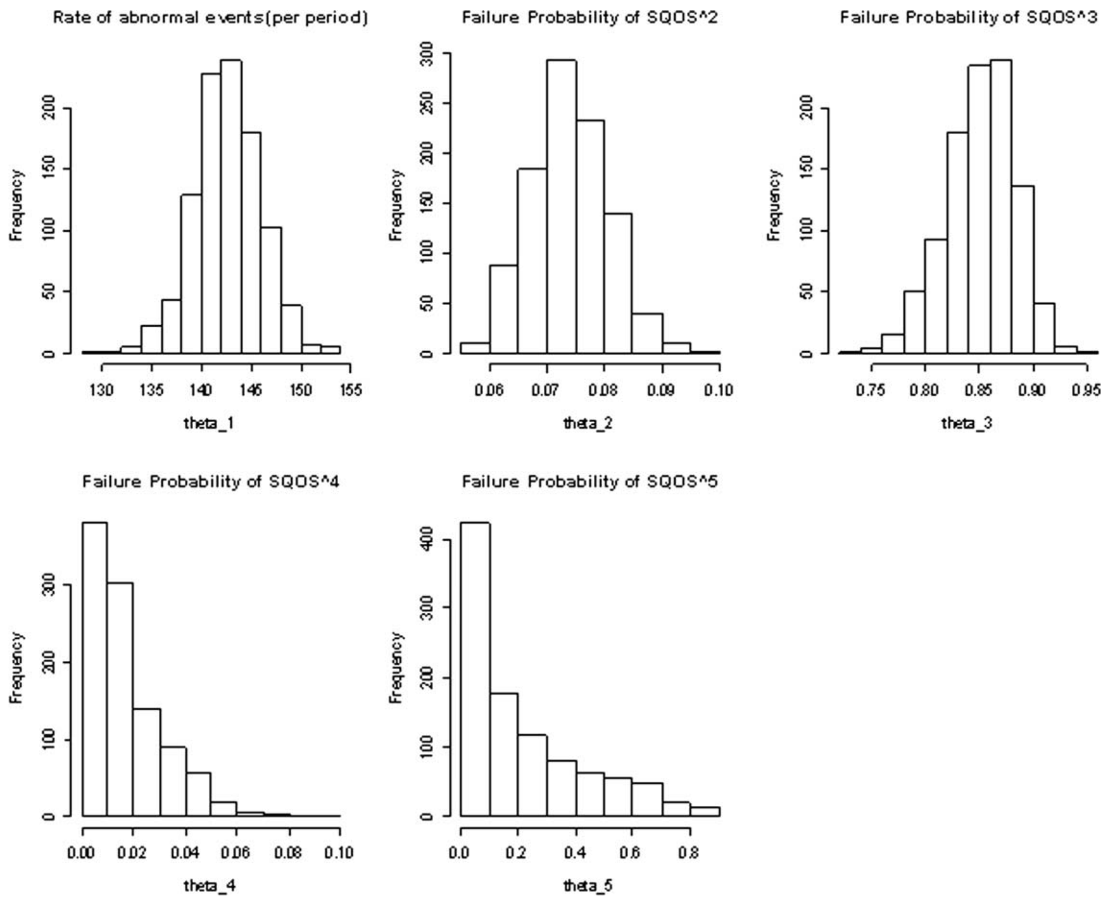

Figure 3. Marginal posterior distributions for θ using multivariate normal copula.

analyses. Finally, engineering and statistical perspectives on copula modeling are contrasted.

Results for pP_1 *using the multivariate normal copula*

On the basis of the likelihood data in Table 6, Part I, the histograms of the marginal posterior failure rate and probabilities of the SQOSs, $\boldsymbol{\theta}$, for pP_1 (over the entire study period, consisting of 13 equal periods), calculated using multivariate normal copula, are presented in Figure 3. Their 95% posterior intervals and means are

$\theta_1 = [135.781, 149.029]$, $E(\theta_1) = 142.624$
$\theta_2 = [0.061, 0.087]$, $E(\theta_2) = 0.074$
$\theta_3 = [0.782, 0.909]$, $E(\theta_3) = 0.851$
$\theta_4 = [0.001, 0.054]$, $E(\theta_4) = 0.017$
$\theta_5 = [0.0005, 0.719]$, $E(\theta_5) = 0.215$

Because of the availability of sufficient data for $SQOS^{1-3}$ (Table 6, Part I), the 95% posterior intervals and means for θ_1, θ_2, and θ_3 were insensitive to the prior values. However, for $SQOS^{4-5}$, because of far fewer data points, their failure probabilities vary significantly with the parameters of the prior distributions. For these results, $a_4 = b_4 = 0.5$ and $a_5 = b_5 = 1$, with prior means, $E(\theta_4) = E(\theta_5) = 0.5$, were used.

Over 13 periods, on average, 142 abnormal events occurred in each period. The mean posterior failure probability (and associated variance) of the operators level I corrective actions is fairly low [$E(\theta_2) = 0.074$]—indicating their robust performance. However, for operators level II corrective actions, the failure probability is abnormally high [$E(\theta_3) = 0.851$], indicating their difficulties in keeping the variables within their orange-belt zones. Stated differently, the probability that pP_1 moves from its yellow- to its orange-belt zone is just 7.4%, whereas the probability of moving from its orange- to its red-belt zone is 85%. Clearly, less-likely, moderately-critical abnormal events are very likely to propagate into most-critical abnormal events due to the ineffective level II control actions (i.e., $SQOS^3$). Hence, for the FCCU, to prevent the occurrence of most-critical abnormal events, it is important to prevent the occurrence of moderately-critical abnormal events.

The failure probability of the override controller is also quite low, $E(\theta_4) = 0.017$. However, its variance is high, as compared with that of $SQOS^{1-3}$. Also, the failure probability of the ESD system is relatively uncertain, due to the availability of few data points. In these cases, past performances (over several months and years) and/or expert knowledge regarding their failures, are desirable. The latter could be

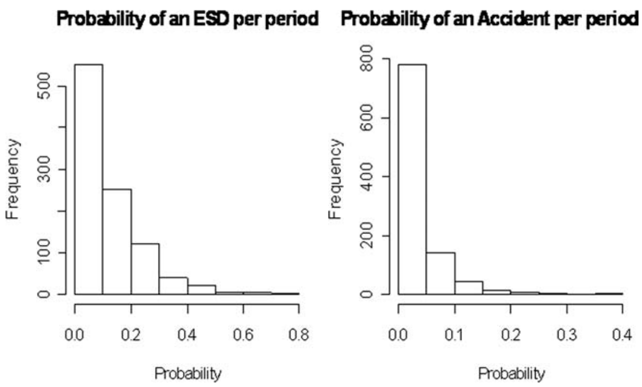

Figure 4. Probability distributions for the occurrence of an ESD and an accident per period, calculated using multivariate normal copula.

derived from the dynamic risk analysis of near-miss data from related plants. Note that similar results can be obtained for individual time periods.

Given estimates of the failure rate and probabilities of the SQOSs, incident probabilities can be estimated; that is, probabilities of the occurrence of an ESD or accident. Two types of incident probabilities are computed herein: (a) incident probabilities per period and (b) incident probabilities per abnormal event. The probability of occurrence of an ESD per period, p^{tp}_{ESD}, is obtained by multiplying the failure rate and the probabilities of $SQOS^{1-4}$ and the success probability of $SQOS^5$. And, the probability of occurrence of an accident in each period, $p^{tp}_{Accident}$, is obtained by multiplying the failure rate of $SQOS^1$ and the failure probabilities of $SQOS^{2-5}$. Similarly, the probability of the occurrence of an ESD per abnormal event, p^{AE}_{ESD}, is obtained by multiplying the failure probabilities of $SQOS^{2-4}$, and the success probability of $SQOS^5$, whereas the probability of occurrence of an accident per period, $p^{AE}_{Accident}$, is obtained by multiplying the failure probabilities of $SQOS^{2-5}$. Symbolically

$$p^{tp}_{ESD} = \theta_1\theta_2\theta_3\theta_4(1-\theta_5) \quad (23a)$$

$$p^{tp}_{Accident} = \theta_1\theta_2\theta_3\theta_4\theta_5 \quad (23b)$$

$$p^{AE}_{ESD} = \theta_2\theta_3\theta_4(1-\theta_5) \quad (23c)$$

$$p^{AE}_{Accident} = \theta_2\theta_3\theta_4\theta_5 \quad (23d)$$

To obtain the posterior distributions of the incident probabilities, random sampling from the distributions of the failure rate and probabilities of the SQOSs is used. Figure 4 presents histograms of the probabilities of occurrence of an ESD and an accident, per period. Their 95% posterior intervals and means are as follows

p^{tp}_{ESD} = [5.6e-3, 0.443], $E(p^{tp}_{ESD}) = 0.124$
$p^{tp}_{Accident}$ = [1.4e-5, 0.159], $E(p^{tp}_{Accident}) = 0.032$

Similarly, Figure 5 presents histograms of the probabilities of occurrence of an ESD and an accident, per abnormal event. Their 95% posterior intervals and means are as follows

p^{AE}_{ESD} = [3.9e-5, 3.1e-3], $E(p^{AE}_{ESD})$ = 8.7e-4
$p^{AE}_{Accident}$ = [2.4e-7, 1.1e-3], $E(p^{AE}_{Accident})$ = 2.1e-4

Thus, based on the performances of the SQOSs during the study period, on average, the probability of the occurrence of an ESD associated with pP_1 is 0.124 per period and 8.7e-4 per abnormal event. That is, an ESD is likely to occur in approximately 1 of 8 periods, or in 1 of 1150 abnormal events. Similarly, an accident is probably to occur in approximately 1 of 31 periods (1/0.032) or in 1 of 4762 abnormal events. Note that while no accidents occurred during the study period and no trips (ESDs) occurred over several periods, the Bayesian analysis estimates finite probabilities of trips and accidents for all periods—using abnormal events history data and prior information. Also, because the variance in the failure probability of $SQOS^5$ is large, the variances in the probabilities of an ESD and an accident are high. With additional data, this uncertainty can be reduced.

The probabilities of ESDs and accidents can help to assess the compliance of chemical plants with national and international safety standards. For example, the Instrumentation, Systems, and Automation Society (ISA)[50] presents safety integrity limits (SILs) to measure the level of risk-reduction provided by ESD systems. More specifically, when the probability of failure under demand (PFD) lies between 10^{-2} and 10^{-3}, the SIL is set at 2. Herein, for the FCCU, the mean

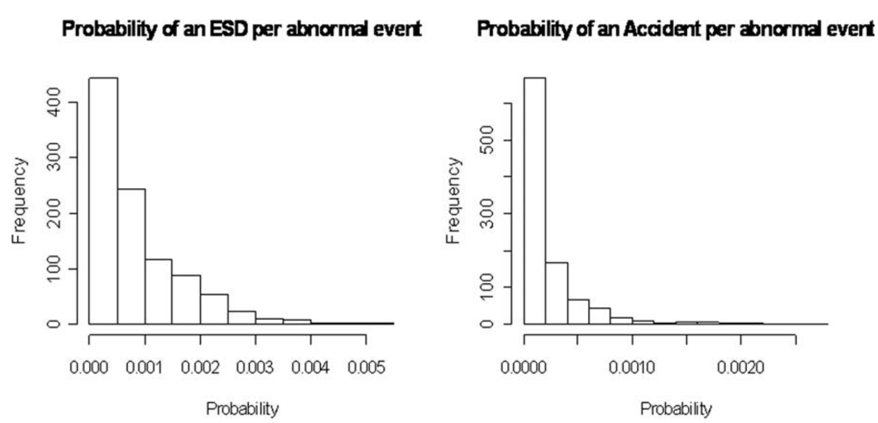

Figure 5. Probability distributions for the occurrence of an ESD and an accident per abnormal event, calculated using multivariate normal copula.

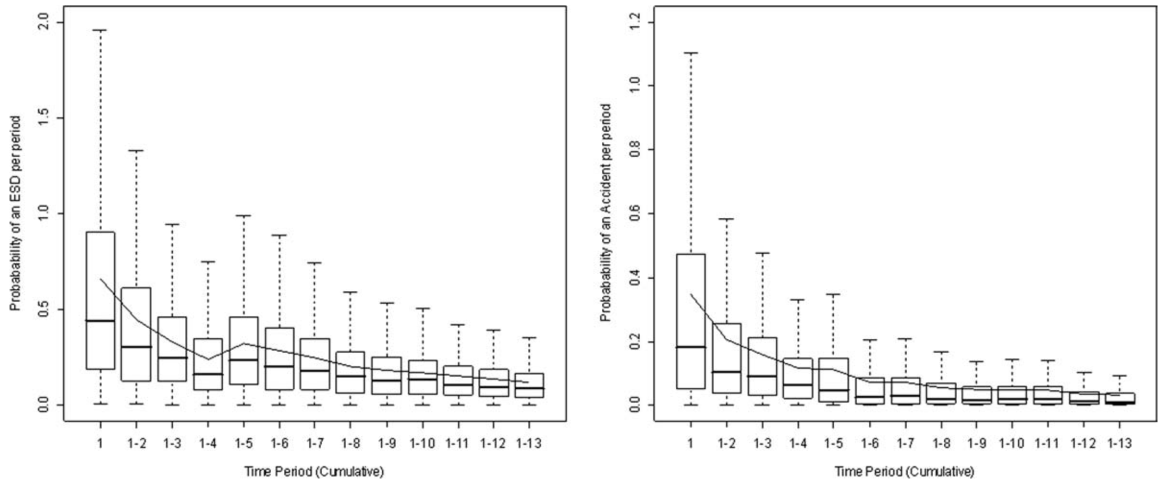

Figure 6. Box and Whisker plots for probabilities of an ESD and an accident per period, for cumulative periods (outliers are not shown).

probability of an ESD per abnormal event is on the order of 10^{-3}. Consequently, the associated SIL = 2 is compliant with the ISA safety standard.

Next, Figures 6 and 7 present box and whisker plots[41] for the probabilities of occurrence of an ESD and an accident, per period and per abnormal event, respectively, starting from the first period and cumulated through the end of each of the 13 periods. For example, the box and whisker plot for periods 1–6 (abscissa) signifies the risk estimates for the first six periods of the study period.

The figures show how the risk estimates (cumulative values) change with time periods. For the first four periods, the risk estimates experience a consistent decrease, followed by a sudden increase in the fifth period. This was due to increases in failure probabilities of levels I and II corrective actions, due to special operations in period 5. Following that, the risk estimates decrease slightly and attain a steady value. These figures provide insights on the relative performances during different time periods and can be used to compare risk levels associated with different plants and work conditions.

Also, note that beginning with the first period, with fewer data points, the variances are higher. As data are added, the variances decrease, accompanied by decreases in the influence of prior information.

Next, histograms of the posterior distributions of the elements of the Spearman rank correlation matrix, $\boldsymbol{W}$, for the overall study period, calculated using the multivariate normal copula, are presented in Figure 8. Their 95% posterior intervals and means are

$w_{12} = [-0.18, 0.92]$, $E(w_{12}) = 0.50$
$w_{13} = [-0.24, 0.87]$, $E(w_{13}) = 0.41$
$w_{14} = [-0.32, 0.79]$, $E(w_{14}) = 0.29$
$w_{15} = [-0.39, 0.75]$, $E(w_{15}) = 0.23$
$w_{23} = [-0.23, 0.88]$, $E(w_{23}) = 0.47$
$w_{24} = [-0.31, 0.84]$, $E(w_{24}) = 0.38$
$w_{25} = [-0.39, 0.78]$, $E(w_{25}) = 0.28$
$w_{34} = [-0.21, 0.90]$, $E(w_{34}) = 0.47$

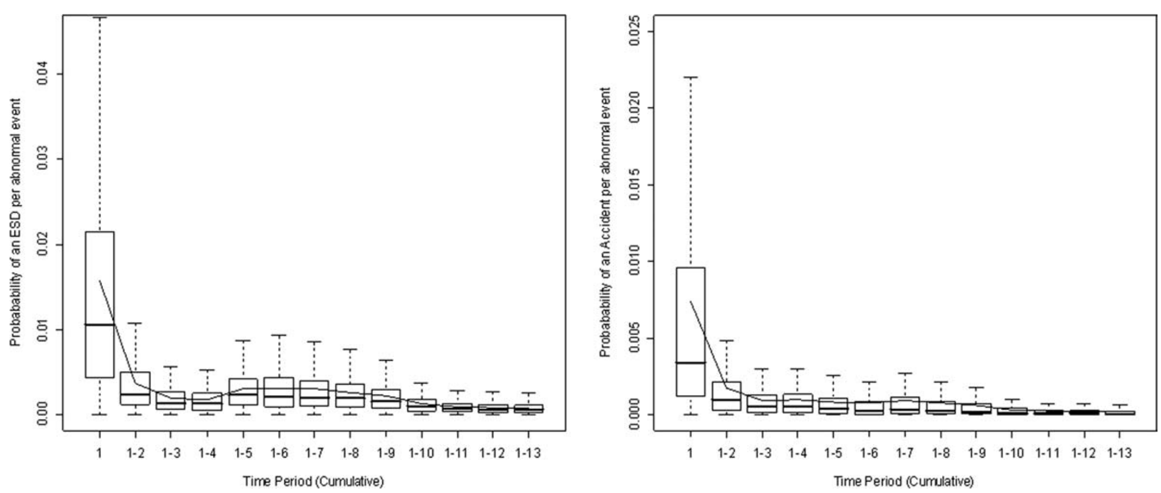

Figure 7. Box and Whisker plots for probabilities of an ESD and an accident per abnormal event, for cumulative periods (outliers are not shown).

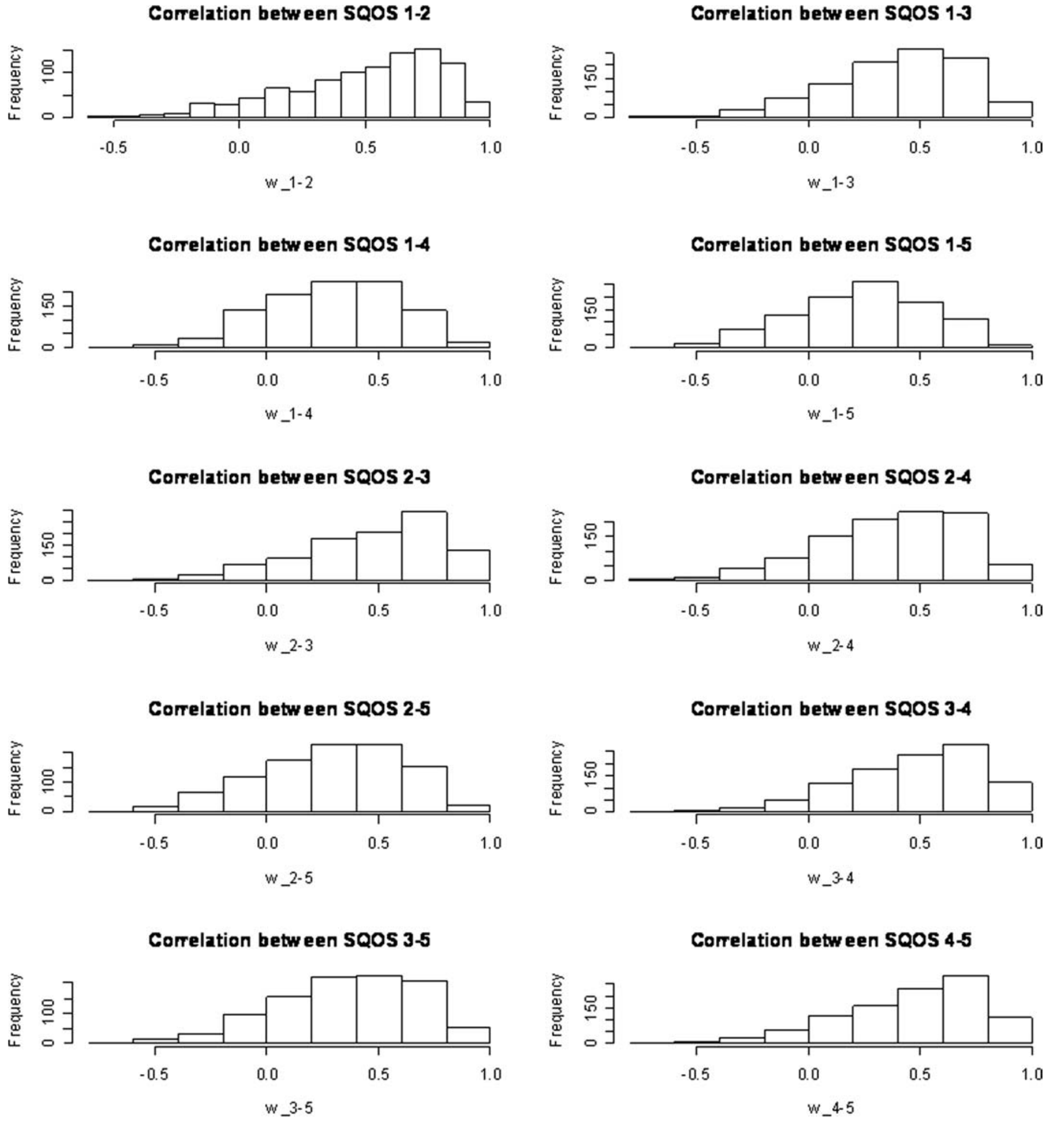

Figure 8. Marginal posterior distributions for the elements of *W* calculated using multivariate normal copula.

$w_{35} = [-0.30, 0.87], E(w_{35}) = 0.39$

$w_{45} = [-0.24, 0.89], E(w_{45}) = 0.47$

As seen, the mean values of the correlation coefficients are positive, with their distributions skewed to the left. On average, there is a significantly positive correlation of the SQOSs with their nearest neighbors, a moderately positive correlation with their next nearest neighbors, a weak positive correlation with their second nearest neighbors, and a very weak positive correlation with their third nearest neighbors, as summarized in Table 1.

In summary, this multivariate normal copula yields positive correlations between the failure rate and probabilities of the SQOSs. Next, results using the Cuadras–Augé copula are presented.

Results for pP_1 *using the Cuadras–Augé copula*

Histograms of the marginal posterior failure rate and probabilities of the SQOSs, $\boldsymbol{\theta}$, for pP_1 (over the entire study period, consisting of 13 equal periods) were also calculated using the Cuadras–Augé copula. Their 95% posterior intervals and means for $\boldsymbol{\theta}$ are

$\theta_1 = [136.32, 148.94], E(\theta_1) = 142.55$
$\theta_2 = [0.061, 0.086], E(\theta_2) = 0.072$
$\theta_3 = [0.768, 0.896], E(\theta_3) = 0.838$
$\theta_4 = [0.003, 0.066], E(\theta_4) = 0.024$
$\theta_5 = [7.78\text{e-}3, 0.709], E(\theta_5) = 0.247$

Table 1. Correlation Strengths Between SQOSs Calculated Using Multivariate Normal Copula

Distance Between SQOSs	Correlation Strength Between SQOSs
Nearest neighbor	Significant (0.47–0.50)
First nearest neighbor	Moderate (0.38–0.41)
Second nearest neighbor	Weak (0.28–0.29)
Third nearest neighbor	Very weak (0.23)

Table 2. Comparison of Mean Failure Probabilities (for the Entire Study Period)

	Mean (Cuadras–Augé Copula)	Mean (Multivariate Normal Copula)	Means (SQOSs with Zero Correlation)	MLE (Classical)
θ_1	142.5	142.6	142.7	142.8
θ_2	0.072	0.074	0.074	0.074
θ_3	0.838	0.851	0.844	0.847
θ_4	0.024	0.017	0.021	0.017
θ_5	0.247	0.215	0.250	0

Table 3. Correlation Values Using the Two Copulas

	Correlation Strength Between SQOSs	
Distance Between SQOSs	Cuadras–Augé Copula	Multivariate Normal Copula
Nearest neighbor	Moderate (0.32–0.39)	Significant (0.47–0.50)
First nearest neighbor	Weak (0.22–0.25)	Moderate (0.38–0.41)
Second nearest neighbor	Very weak (0.12–0.17)	Weak (0.28–0.29)
Third nearest neighbor	Negligible (0.11)	Very weak (0.23)

A comparison of the means using the two copulas, Bayesian analysis with independent SQOSs, and classical statistics, is presented in Table 2. The latter neither accounts for prior information nor interactions among the SQOSs—with failure probabilities based solely on the likelihood data in Part I.

Because of the availability of sufficient data for SQOS$^{1-3}$, the means of their failure rate and probability distributions, calculated using the above methods, differ slightly. Also, the impact of the shared information on their θs, obtained using the two copula models, is very weak. However, as SQOS$^{4-5}$ involve much less data, their θs depend on the method and copula, and the prior distribution parameters. For these rare events, as the data are limited, the Bayesian approach with copulas provides better failure probability estimates, accounting for the prior/expert belief about their failures as appropriate.

For the Cuadras–Augé copula, the 95% posterior intervals and means for the elements of correlation matrix are

$w_{12} = [-0.31, 0.87]$, $E(w_{12}) = 0.32$
$w_{13} = [-0.33, 0.82]$, $E(w_{13}) = 0.25$
$w_{14} = [-0.43, 0.75]$, $E(w_{14}) = 0.12$
$w_{15} = [-0.43, 0.69]$, $E(w_{15}) = 0.11$
$w_{23} = [-0.28, 0.88]$, $E(w_{23}) = 0.33$
$w_{24} = [-0.35, 0.79]$, $E(w_{24}) = 0.22$
$w_{25} = [-0.44, 0.75]$, $E(w_{25}) = 0.17$
$w_{34} = [-0.34, 0.86]$, $E(w_{34}) = 0.34$
$w_{35} = [-0.40, 0.76]$, $E(w_{35}) = 0.22$
$w_{45} = [-0.25, 0.85]$, $E(w_{45}) = 0.39$

Similarly, the distributions are skewed to the left. Although their mean values are positive, they are smaller than those using the multivariate normal copula. On average, the correlation strengths between the SQOSs are less than using the multivariate normal copula, as shown in Table 3.

Thus, the strength of the correlations between the SQOSs is contingent on the copula used for modeling. It is important to note, however, that the trends obtained from the two copulas are similar—the correlation strengths increase as the SQOSs assume closer proximity. Furthermore, the copula modeling validates the theoretical assumptions that the actions of the SQOSs are related to each other (because of nonlinear relationships between the variables and behavior-based factors). These results can persuade plant personnel to take preventive measures to avoid shutdowns and accidents. For example, when θ_2 or θ_3 increase, the onset of a special-cause(s) is likely to trigger the ESDs more often, increasing their likelihood of failure.

If sufficient data for SQOS$^{4-5}$ were available, based on the results for SQOS$^{1-3}$ in Table 2, the copulas would likely have negligible impact on their posterior failure probabilities. Here, the copulas are needed to calculate the correlation strengths—which would not differ significantly with copula choice.

Similar results were obtained for the likelihood data in Table 4, Part I, for all the primary variables—and in Table 6 for all the primary process variables.

Next, the maximum entropy principle is applied to select the best copula for the FCCU case study.

Maximum entropy principle

Copula selection can be important, especially when data are limited. For multivariate systems, copula properties like tail dependences, closed-form expressions, symmetricity, and similar, can strongly influence the selection. More recently, it is recommended that noninformative copulas be selected.[26] In one approach, an entropy function is maximized.[51–53] For the multivariate prior distribution, $f(\theta_1, \theta_2, \ldots, \theta_5)$, the differential entropy, Ent, is

$$\text{Ent}[f(\theta_1, \theta_2, \ldots, \theta_5)] = -\int \cdots \int f(\theta_1, \theta_2, \ldots, \theta_5) \times \ln[f(\theta_1, \theta_2, \ldots, \theta_5)] d\theta_1 \ldots d\theta_5 \quad (24a)$$

or

$$\text{Ent}[f(\theta_1, \theta_2, \ldots, \theta_5)] = \text{Ent}[f_1(\theta_1)] + \sum_{j=2}^{5} \text{Ent}[f_j(\theta_j)] + \text{Ent}[f_w(\boldsymbol{W})] + \text{Ent}[c(\theta_1, \theta_2, \ldots, \theta_5)] \quad (24b)$$

Table 4. Comparison of the Mean Failure Probabilities and the Probabilities of Occurrence of ESDs and Accidents (Calculated Using Multivariate Normal Copula) – With and Without Quality Data

Mean	θ_1	θ_2	θ_3	θ_4	θ_5	Prob. of an ESD per Abnormal Event	Prob. of an Accident per Abnormal Event
All primary variables	195.69	0.057	0.822	0.017	0.121	7.25e-4	1.04e-4
Primary process variables only	156.69	0.069	0.852	0.018	0.106	9.64e-3	1.17e-4

That is, the entropy of the multivariate prior distribution is the sum of the entropies of the individual marginal PDFs plus the entropy of the copula. Here, the entropy is maximized when the random variables are independent. With no information shared among the univariate marginals, the data are ''most randomly'' distributed.[54] When the random variables are dependent (given their correlation matrix), it can be shown that the differential entropy is maximized using the multivariate normal copula.[55,56] It follows that, for a given prior correlation matrix, the multivariate normal copula has a higher entropy than the Cuadras–Augé copula and thus, is less informative. Therefore, herein, the multivariate normal copula is the preferred prior.

Product-quality data in risk analysis

Referring to Part I and Pariyani et al.,[41] the safety performance of any process is characterized by its primary variables, which include both primary process and primary quality variables. When a primary process or primary quality variable moves outside its green-belt zone, a safety problem is likely to occur. However, although quality variables are causally related to process variables, abnormal events associated with primary quality variables do not necessarily imply the movement of primary process variables out of their green-belt zones, and vice versa. Hence, the abnormal events history of the primary quality variables should also influence the Bayesian risk analysis. In practice, however, quality variable data are often not estimated or recorded.

In this subsection, the impact on risk estimates of neglecting primary quality variable data is shown. Using the likelihood data in Tables 5 and 7 of Part I, Table 4 compares the mean failure probabilities and the probabilities of ESDs and accidents (calculated using Bayesian analysis with multivariate normal copula)—with and without product-quality data.

As expected, there is an increase in the mean θ_1 when all primary variables are used. However, when the product-quality data are excluded, the failure probabilities, θ_2, θ_3, and θ_4, are higher, as well as the probabilities of an ESD, and the occurrence of an accident. In particular, the latter two increase by 33% and 12%. Clearly, the quality data provide more near-miss information, yielding improved risk estimates.

Engineering and statistical perspectives

For the FCCU DCS and ESD system databases, while the correlation strengths between the failure probabilities of the SQOSs are positive, they may not be statistically significant (because of limited data, with *P*-levels close to 0.15, greater than the standard cutoff value of 0.05). With availability of more data, the statistical significance of correlations can be improved.

From an engineering perspective, the nonlinear relationships between the variables and behavior-based factors clearly establish interactions between the SQOSs. These are modeled properly using copulas. Furthermore, the correlation strengths in Table 3 are expected and corroborate the use of copula modeling. Also, the copulas share information (through correlations), providing more accurate risk estimates associated with rare events.

Conclusions

The Bayesian analysis method presented herein is capable of handling large numbers of abnormal events over extended periods of time. This use of dynamic alarm databases for risk analysis permits a more rigorous and reliable assessment of the performance of the various regulatory and protection systems, and importantly, calculation of the probabilities of shutdowns and accidents. For processing plants, the nonlinear relationships between the variables and behavior-based factors cause the SQOSs to share complex interactions with each other. To account for these interdependencies in the Bayesian model and calculate correlation coefficients between the SQOSs, copulas are needed. Although they add an additional complexity in calculations, they provide a mechanism to utilize the shared information between the SQOSs and to estimate the posterior values of elements of dependence matrix.

For the FCCU case study, several specific conclusions are drawn. Moderately critical abnormal events were very likely (85% chance) to propagate into most-critical abnormal events, primarily due to the poor controlling actions of the level II operators (i.e., $SQOS^3$). Hence, it is concluded that to prevent the occurrence of most-critical abnormal events, it is almost as important to prevent the occurrence of moderately-critical abnormal events.

Posterior correlation coefficients between the failure rate and probabilities of the SQOSs were estimated. The correlation strengths between the SQOSs are moderately to significantly positive and increase as the SQOSs gain closer proximity. Both copulas yielded positive (average) correlations (left-skewed distributions, with positive means) between the SQOSs as expected based on their physical interactions.

For rare events, like failures of the override controller, and automatic and manual ESDs, the Bayesian approach with copulas provides better failure probability estimates, accounting for the prior/expert belief about their failures as appropriate. With sufficient data, copulas permit the reliable estimation of posterior correlation coefficients. Using the maximum entropy principle, the multivariate normal copula, with a given correlation matrix, is less informative and is preferred over the Cuadras–Augé copula. It is to be noted that the maximum entropy principle provides a qualitative way to identify the ''most noninformative'' copula. Soon, we will work on developing a quantitative method to analyze the information gain (using Information theory) associated with each copula. Finally, the quality data complement the data associated with the primary process variables (safety data), and thus, provide more near-miss information for Bayesian analysis, providing better risk estimates.

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Notation

Acronyms

ASP = accident sequence precursor
BPCS = basic process control system
CCPS = Center for Chemical Process Safety (*AIChE*)
CDF = cumulative distribution function
CO = continued operation
CPIs = chemical process industries
DCS = distributed control system
ESD = emergency shutdown
FCCU = fluid catalytic cracking unit
ISA = Instrumentation, Systems, and Automation Society
MLE = maximum likelihood estimate
PDF = probability density function
PFD = probability of failure under demand
PRA = probabilistic risk analysis
rvs = random variables
SIL = safety integrity limit
SQOS = safety, quality, and operability system

English letters

a_k, b_k = parameters of Gamma prior distribution for θ_1
a_j, b_j = parameters of Beta prior distribution for θ_j (j = 2,…, 5)
A_1, B_1 = parameters of Gamma proposal distribution for θ_1
A_j, B_j = parameters of Beta proposal distribution for θ_j (j = 2,…, 5)
c = copula density
C = copula function
Data = Likelihood data; set of success and failure counts for SQOS$^{1–5}$
Ent[$f_k(\theta_k)$] = differential entropy of the prior distribution for θ_k (k = 1,…, 5)
$E(\theta_k)$ = expected value of θ_k
$f_k(\theta_k)$ = prior probability density function for θ_k (k = 1,…, 5)
$F_k(\theta_k)$ = prior CDF for θ_k (k = 1,…, 5)
$f_k(\theta_k|\text{Data})$ = marginal posterior distribution for θ_k (k = 1,…, 5)
$f_w(\boldsymbol{W})$ = prior distribution for the Spearman-rank correlation matrix
$f(\theta_1, \theta_2, \ldots, \theta_{Ns}, \boldsymbol{W})$ = joint prior distribution of failure rate and probabilities of the SQOSs and their correlation matrix
$g(\text{Data}|\boldsymbol{\theta})$ = general likelihood function in Eq. 1
$\boldsymbol{I}$ = identity matrix
J_k^t = proposal distribution for θ_k (k = 1,…, 5)
J_w^t = proposal distribution for the Spearman-rank correlation matrix
K_t^j, L_t^j = failure and success counts for SQOS j in time period t
K_T^j, L_T^j = Failure and success counts for SQOS j associated with all primary variables during the entire study period
$K_{pP_1}^j, L_{pP_1}^j$ = failure and success counts for SQOS j associated with pP_1 variable during the entire study period
K_{pP}^j, L_{pP}^j = failure and success counts for SQOS j associated with primary process variables during the entire study period
$L(\text{Data}|\boldsymbol{\theta})$ = likelihood function for SQOSs
n_t = number of abnormal events in a time period
n_T = number of abnormal events for all primary variables (see Table 5, Part I)
n_{pP_1} = number of abnormal events for pP_1 (see Table 6, Part I)
n_{pP} = number of abnormal events for all primary process variables (see Table 7, Part I).
Ns = number of SQOSs
pP_1 = primary process variable 1
$p_{\text{Accident}}^{\text{AE}}$ = probability of occurrence of an accident, per abnormal event
$p_{\text{ESD}}^{\text{AE}}$ = probability of occurrence of an ESD, per abnormal event
$p_{\text{Accident}}^{\text{tp}}$ = probability of occurrence of an accident, per time period
$p_{\text{ESD}}^{\text{tp}}$ = probability of occurrence of an ESD, per time period
r_{kq} = element (row k, column q) of product-moment correlation matrix, $\boldsymbol{R}$
$\boldsymbol{R}$ = product-moment correlation matrix
$\boldsymbol{S}$ = scale matrix
u_k = CDF of θ_k
w_{ij} = element (row i, column j) of Spearman-rank correlation matrix
$\boldsymbol{W}$ = Spearman-rank correlation matrix

Greek letters

α_{k-q} = correlation coefficient between θ_k and θ_q
v = degrees of freedom
Φ^{-1} = normal inverse transformation
θ_1 = failure rate of BPCS (SQOS^1)
θ_2 = failure probability of level I corrective actions (SQOS^2)
θ_3 = failure probability of level II corrective actions (SQOS^3)
θ_4 = failure probability of override controller (SQOS^4)
θ_5 = failure probability of ESD system (SQOS^5)
$\boldsymbol{\theta}$ = vector comprising failure rate and probabilities of SQOSs
$\boldsymbol{\Gamma}$ = unconstrained correlation matrix

Subscripts

h = counter in copula expression in Eq. 15a
j = counter for failure probabilities, j = 2,…, 5
k = counter for failure rate and probabilities, k = 1,…, 5
q = counter for failure rate and probabilities in Eqs. 15 and 16; $k \neq q$
t = a general time period
w = symbol representing association with the Spearman-rank correlation matrix

Superscripts

* = proposed value
(0) = starting value
AE = abnormal event
init = initial value
t = iteration counter
tp = time period

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