Potential of surrogate modelling for probabilistic fire analysis of structures

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ABSTRACT

The interest in probabilistic methodologies to demonstrate structural fire safety has increased significantly in recent times. However, the evaluation of the structural behavior under fire loading is computationally expensive even for simple structural models. In this regard, machine learning-based surrogate modeling provides an appealing way forward. Surrogate models trained to simulate the behavior of structural fire engineering (SFE) models predict the response at negligible computational expense, thereby allowing for rapid probabilistic analyses and design iterations. Herein, a framework is proposed for the probabilistic analysis of fire exposed structures leveraging surrogate modeling. As a proof-of-concept a simple (analytical) non-linear model for the capacity of a concrete slab and an advanced (numerical) model for the capacity of a concrete column are considered. First, the procedure for training surrogate models is elaborated. Subsequently, the surrogate models are developed, followed by a probabilistic analysis to evaluate the probability density functions for the capacity. The results show that fragility curves developed based on the surrogate model agree with those obtained through direct sampling of the computationally expensive model, with the 10^{-2} capacity quantile predicted with an error of less than 5%. Moreover, the computational cost for the probabilistic studies is significantly reduced by the adoption of surrogate models.

Keywords: Structural fire safety, Probabilistic studies, Regression, Surrogate modeling, Reinforced concrete.

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1 Introduction

The fire safety design of structures is traditionally done through the application of prescriptive guidance and code-based recommendations, to meet prescribed nominal fire resistance requirements (ISO, 2019). The fire resistance requirements themselves, as well as the considered nominal fire exposures, load combinations, characteristic material properties, safety factors and limit criteria, all contribute to attaining an adequate level of safety in case the as-built structure experiences a (real) fire. The obtained safety level when applying the traditional design procedure is, however, unknown, and the attainment of an adequate safety level is fundamentally based on precedent (Van Coile et al., 2019). The above implies that the updating of traditional design approaches to adjust to innovations in the built environment or to specify requirements for exceptional designs (Hopkin et al., 2017) relies on 'lessons learned from failure' (Spinardi et al., 2017). However to avoid disaster, to allow for the safe introduction of design innovation and the specification of adequate provisions for exceptional structures, and to properly mitigate evolving risk exposure (for example due to climate change and urbanization (McNamee et al., 2019), an explicit consideration of the risk profile of the structure is necessary (Van Coile et al., 2019). In other words, the full range of possible fires, and their associated probabilities must be taken into account, as well as the uncertainties in the structural fire performance and resulting consequences. The current paper is concerned specifically with the efficient probabilistic evaluation of structural fire performance.

The probabilistic structural fire analysis can, in principle, be done through repeated evaluation of the structural model for different realizations of the stochastic variables. Such a "Monte Carlo" approach has been applied for example by Heidari et al. (2019) and Van Coile et al. (2014) for a fire-exposed concrete slab, and by Guo et al. (2013), Elhami Khorasani et al. (2015) and Hopkin et al. (2018) for an insulated steel member. A drawback of the Monte Carlo approach is the computational expense implied by the repeated sampling. More efficient

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stochastic modelling procedures have been applied to structural fire engineering (SFE), for example by Gernay et al. (2019a) and Guo et al. (2015). While both studies managed to reduce the number of simulations drastically, both require additional expert knowledge and careful error analysis. Furthermore, these efficient methodologies still do not allow for quasi-instantaneously updating the probabilistic structural fire analysis during design iterations. This limitation is especially relevant where the structural fire analysis involves a large and complex structural model.

The preceding paragraphs indicate a need for a probabilistic structural fire analysis methodology which is (i) conceptually easy to understand; and (ii) allows for fast design iterations. One promising approach is the use of fragility curves. Commonly used to represent the exceedance probability of a predefined damage state in function of an intensity measure or engineering demand parameter, fragility curves have been derived for SFE, for example, by Gernay et al. (2016, 2019b) for steel frame buildings through Monte Carlo approaches, and by Ioannou et al. (2017) for reinforced concrete buildings through expert elicitation. If reference fragility curves are listed (i.e. are precalculated), or can be efficiently evaluated, then the probabilistic approach can find application in design practice. Such an approach is well-developed in earthquake engineering and multiple SFE studies, such as Hamilton (2011), Lange et al. (2014) and Shrivastava et al. (2019), have focused on applying these earthquake procedures to structural fire design. In earthquake engineering, the computational expense is commonly limited by assuming a lognormal distribution for the fragility curve, see e.g. (Baker and Cornell, 2006). Such an assumption may allow for a more efficient evaluation, but can however be inappropriate for SFE, as illustrated in (Gernay et al., 2019b) and (Van Coile et al., 2013). Furthermore, reducing the number of computationally expensive model evaluations is helpful, but does not resolve the fundamental issue that considerable effort and expert handling is required when running computationally advanced models. The option of pre-calculated

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fragility curves being listed by industry organizations, academic institutions or standardization bodies (as is done for seismic design, see FEMA P58) has been advocated for SFE in (Van Coile et al., 2020), but is difficult to achieve without further simplification or intermediate steps, considering the infinite number of design alternatives, even when considering isolated members.

In summary, for probabilistic approaches to find application in SFE design, a computationally efficient methodology which does not rely on the direct use of advanced numerical models to evaluate design iterations is advantageous. Taking into account recent applications of Machine Learning (ML) techniques for fire safety applications, e.g. Dexters et al. (2019), Naser (2019a), and Fu (2020), the hypothesis is put forward here that ML approaches can be instrumental in achieving the above computationally efficient methodology. More specifically, if the advanced numerical models currently used in SFE can be accurately approximated by a surrogate model developed through ML, then probabilistic studies for a fire exposed structure can be achieved quasi-instantaneously with limited loss of accuracy. Furthermore, fast design iteration can then be achieved at negligible additional computational cost.

The study presented further acts as a proof-of-concept for probabilistic SFE evaluations supported by surrogate modelling. The structure of the paper is as follows. Section 2 starts with a succinct state-of-the-art discussion on ML techniques in SFE. It is concluded that regression-based surrogate modelling will be explored further in this study, being both intuitive and straightforward in its implementation. Section 2 then continues with a description of the procedures for training a regression-based surrogate model. Subsequently, Section 3 demonstrates the development and effectiveness of a surrogate model for (i) a computationally less demanding test case of a concrete slab with known temperature profile; and (ii) a concrete column taking into account geometric imperfections. Finally, in Section 4 fragility curves (cumulative density functions) are evaluated for the test cases, using both the original ("actual")

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model and the surrogate model. The comparison between the obtained distributions validates the proof-of-concept for probabilistic analysis of fire exposed structures through regression-based surrogate models.

2 Regression-based surrogate modelling

Surrogate models derived through ML techniques have been used to evaluate the response of physical systems in a wide range of fields (Forrester et al., 2008; James et al., 2013). The applied techniques include regression, genetic algorithm, and artificial neural networks (ANN). These approaches, when properly used (within the boundaries of the physical system, maintaining interpretability and avoiding the black box effect for the trained model (Rudin, 2019)), provide useful and efficient tools for engineers. While application of ML approaches in fire safety engineering is relatively new, an increasing number of studies have been published in recent years. Dexters et al. (2019), for example, applied regularized logistic (lasso) regression for the prediction of flashover in a scaled fire compartment with sandwich panel walls. Their trained model was presented as a dynamic tool for specifying new test configurations. In the area of structural fire engineering (SFE), a series of studies have been initiated by Naser. In (Seitllari and Naser, 2019) for example, multi-linear regression, genetic algorithm and ANN were adopted to predict explosive spalling phenomena for a fire exposed concrete column. The genetic algorithm was reported to achieve a spalling prediction accuracy of about 95 %. Naser further explored ML methodologies for the prediction of the fire resistance of timber elements and bridge vulnerabilities (Naser, 2019a; Naser, 2019b). Other recent applications of ML in the field of SFE can be found for example in (Fu, 2020) and (Panev et al., 2021). This recent literature suggest a wide application range for ML techniques in fire safety engineering, hardly explored.

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Regression is arguably better suited to construct interpretable surrogate models than other ML techniques such as ANN, especially when considering simple relationships such as polynomial functions, because the regression coefficients directly inform about the contribution of the respective parameters (features) in the considered model output. These features relate to the selected physical parameters, such as the concrete cover or fire load density, which are considered to govern the model output of interest, such as the fire resistance or the occurrence of flashover in a compartment. Considering the above, polynomial regression-based surrogate modeling is adopted here to approximate the response of fire exposed structural elements.

Figure 1 shows the steps for the development of a regression-based surrogate model. These steps are discussed in detail in the following paragraphs. Firstly, the basic input variables must be selected, and a sampling scheme applied to obtain the corresponding model realizations (Section 2.1). Then, a (polynomial) regression function is specified which acts as a hypothesis for the surrogate modelling (Section 2.2). This surrogate model hypothesis defines the model 'features', whose relationship determines the response of a physical system. Finally, the regression coefficients are determined through an optimization procedure, such as gradient descent, during which a 'cost function' is minimized (Section 2.3). The optimization however highlights a number of issues related to the varying magnitude and dimensionality of the features. To avoid these, the features are scaled (2.4). Furthermore, issues of overfitting and underfitting of the model may occur (2.5). Finally, the accuracy of the trained model must be determined, and the applied model (hyper-)parameters, such as the number of sampling points, must be confirmed, which is done through application of the cross-validation and test data (2.6).

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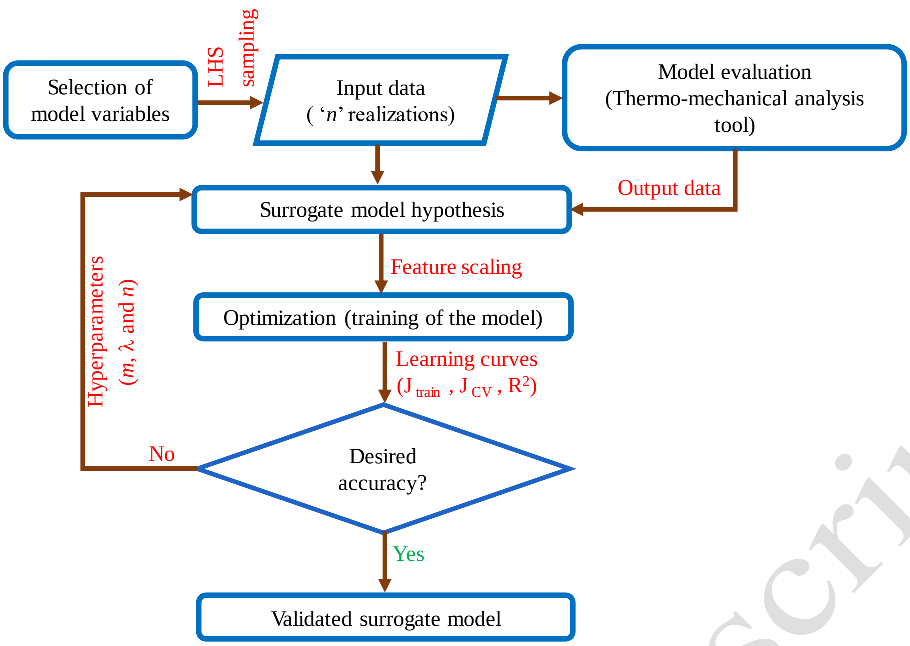

Figure 1 Methodology for regression based surrogate modeling

2.1 Selection of model variables, input data generation, and model evaluation

The first step involved in the development of a surrogate model through polynomial regression is the selection of the model variables, on which the behavior of the computationally expensive physical system depends. If $\boldsymbol{x}$=[x_1, x_2, x_3,………… $x_{r\text{-}1}$, x_r] represent a vector of variables, then the response, y of the physical system, $h(\boldsymbol{x})$ is given by:

$$y = h(\boldsymbol{x}) \tag{1}$$

The surrogate model is generally developed for a specific purpose. It is thus not necessary to consider all possible parameters of the physical system as input variables for developing a surrogate model. This implies that parameters which are considered fixed within the scope of the model are not considered explicitly for the surrogate model development. Therefore, in the current study only the (independent) variables that are considered uncertain in the probabilistic assessment are considered as input variables for the surrogate model.

Once the model variables are chosen, an appropriate sampling scheme needs to be adopted to evaluate the model realizations, y_i, to train a surrogate model. These realizations are obtained

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with a sophisticated model of the physical system (e.g. a finite element model). The sampling scheme should cover the entire parameter space of interest, while at the same time limiting the number of realizations as much as possible (Forrester et al., 2008). A Latin Hypercube Sampling (LHS) scheme will be adopted in the current study for the input data (Olsson et al., 2003). Importantly, mode~~l~~ling limitations of the finite element model will also apply to the surrogate model. If the finite element model is unable to capture shear failure, then the same limitation will apply to the surrogate model.

2.2 Surrogate model hypothesis

For polynomial regression, the hypothesis for the surrogate model is a summation of polynomial terms. A 2nd order polynomial hypothesis (m = 2) for the surrogate model, considering two independent variables x_1 and x_2 can be given by Eq.(2). Here $\hat{y} = \hat{h}(\boldsymbol{x})$ indicates the surrogate model approximation for the actual (physical) model $y = h(\boldsymbol{x})$, [θ_0, θ_1,…, θ_5] are regression coefficients, in which θ_0 refers to the bias term, x_1 and x_2 are the realizations of the independent variables, x_1^2 and x_2^2 are higher order terms, and x_1x_2 is the interaction term of the surrogate model. Together, the first order, higher order and interaction terms are the ‘features’ for the regression surrogate model. For further discussion on the regression hypothesis reference is made to (Forrester et al., 2008).

$$\hat{y} = \hat{h}(\boldsymbol{x}) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2 \tag{2}$$

2.3 Cost function and model fitting

The regression coefficients $\boldsymbol{\theta}$ in Eq. (2) are estimated through the minimization of the cost function, ‘$J(\theta)$’, which is a measure of error in prediction for a given data. The cost function for training a surrogate model (James et al., 2013) is given by Eq. (3) and can be understood as the half the mean squared error of the prediction for the training data set.

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$$J(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(\hat{h}(\boldsymbol{x}_i) - y_i\right)^2 \tag{3}$$

An optimization algorithm needs to be adopted for the determination of the coefficients θ_0, $\theta_1,\ldots,\theta_r$, which minimize the cost function in Eq.(3). In this regard, numerous optimization algorithm for cost function optimization can be found for example in the Python Scipy library (Virtanen et al., 2020). In the current study, the gradient descent algorithm is selected (Forrester et al., 2008; Du et al., 2018). The gradient descent algorithm follows a downhill approach for the minimization of the cost function, whereby regression coefficients are updated at each iteration in the opposite direction to the positive gradient of $J(\theta)$. The regression coefficients for the surrogate model adopted at each subsequent iteration are given by:

$$\theta_l = \theta_l - \alpha\frac{\partial}{\partial\theta_l}J(\theta) \tag{4}$$

where, α is the learning rate of the surrogate model for gradient descent method. The iteration is done simultaneously for all coefficients l. Convergence is achieved once the difference in cost function evaluation between iterations falls below a predefined tolerance. The estimated regression coefficients can then be used to predict the response of the physical system.

2.4 Feature scaling

The procedure outlined above with the cost function of Eq. (3) has as disadvantage that the cost evaluation is dependent on the dimension of the model output. This makes it difficult to recommend a tolerance factor denoting convergence, and results in an unequal weighting of features in the coefficient updating of Eq. (4). Consequently, the features need to be scaled so that all variables are of comparable dimensions in order to implement regression algorithms. Here, a standardization technique is implemented which normalizes the independent variables, i.e. the features are scaled to have zero mean and unit variance. The normalized independent

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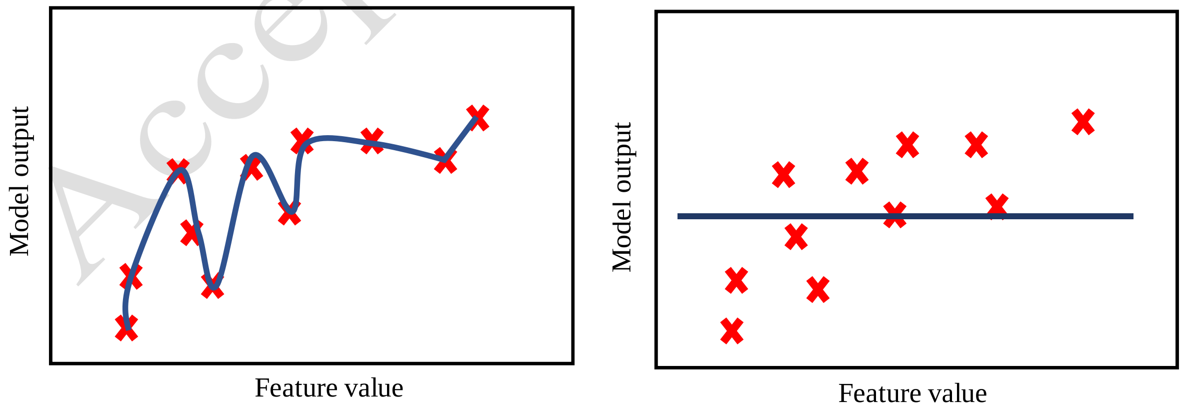
variables are given by Eq. (5), with c the original feature value, μ_c the feature mean, σ_c the feature standard deviation, and c_{norm} the normalized feature value.

$$c_{\text{norm}} = \frac{c - \mu_c}{\sigma_c} \tag{5}$$

2.5 Fitting issues

The predicted response for the surrogate model depends on how well it was trained, which relates to the adopted order of polynomial (m) and size of the sample (n). An inappropriate order of polynomial for the surrogate model might lead to underfitting or overfitting of the training data (Forrester et al., 2008). Although an overfitted surrogate model can accurately predict the response for training data, it might be incapable of predicting the results for unseen cases. In contrary, an underfitted surrogate model predicts the results for both the trained and untrained data inaccurately. Figure 2 illustrates these concepts. Likewise, if the size of the sample is not sufficient to map the entire sample space of the variables, the surrogate model might be incapable of predicting the response of the physical system precisely. Thus, an appropriate size of the LHS sample needs to be determined for training a surrogate model to predict the response accurately.



(a) Overfitting (b) Underfitting

Figure 2 Issues in developing surrogate model

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The issue of overfitting of the training data can be addressed by introducing a regularization parameter (λ) in the cost function. Eq. (6) gives an expression for a regularized cost function to train a surrogate model.

$$J_{\text{learn}}(\theta) = \frac{1}{2n}\sum_{i=1}^{n}\left(\hat{h}(\mathbf{x_i}) - y_i\right)^2 + \frac{\lambda}{2n}\sum_{l=1}^{r}\theta_l^2 \tag{6}$$

The regularization parameter penalizes the coefficients in the surrogate model. This means that, if higher order polynomials are adopted with more non-zero coefficients, the cost function is artificially increased by an additional cost term. As the value of the regularization parameter influences the result of the optimization, it needs to be chosen wisely. The same statement applies to the order of the polynomial model and the number of training samples. These parameters are known as hyperparameters and they can be determined through application of learning curves.

2.6 Hyperparameters, learning curves and performance evaluation

To evaluate and improve the performance of the machine learning algorithms (i.e. perform hyperparameter optimization), three different input data sets are considered: a training set, a cross-validation set and test data set. The training set is applied to find the optimum vector of coefficients, $\boldsymbol{\theta}$, for given hyperparameters, while the cross-validation data set is used to evaluate the optimum value of the hyperparameters, i.e. to distinguish between the different models trained on the training set. Finally, the test data set allows to evaluate the prediction accuracy of the surrogate model on an unseen set of datapoints.

A complete LHS sample is considered as a training set to ensure that the entire sample space of independent variables is assessed by the computationally expensive physical system. The cross-validation and test data set can however be generated randomly (Monte Carlo simulation). The prediction errors for the training (J_{train}) and cross-validation data sets (J_{cv}), are given by:

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$$J_{\text{train}}(\theta) = \frac{1}{2n_{\text{train}}} \sum_{i=1}^{n_{train}} \left(\hat{h}(\boldsymbol{x}_{\boldsymbol{train,i}}) - y_{train,i} \right)^2 \tag{7}$$

$$J_{cv}(\theta) = \frac{1}{2n_{\text{cv}}} \sum_{i=1}^{n_{cv}} \left(\hat{h}(\boldsymbol{x}_{\boldsymbol{cv,i}}) - y_{cv,i} \right)^2 \tag{8}$$

Learning curves refer to the plot of these estimated training and cross-validation costs, where a hyperparameter to be optimized is varied, while other parameters are assumed constant. The hyperparameters in the current study are the regularization parameter value (λ), the order of the polynomial model (m), and the size of the LHS sample (n). The optimum hyperparameters are determined as those for which the cross-validation cost function indicates that further complexity does not result in a significant reduction in cross-validation cost (estimation error), or even results in a cost increase.

After the evaluation of the hyperparameters, the performance of the developed surrogate model can be assessed based on test data set, for which the coefficient of determination, R^2 (Draper and Smith, 1998) can be determined. The R^2 value refers to the prediction efficiency of the model and is given by:

$$R^2 = 1 - R_{res} / R_{tot} \tag{9}$$

where, $R_{\text{res}} = \sum_{i=1}^{n_{test}} \left(\hat{h}(\boldsymbol{x}_{\boldsymbol{test,i}}) - y_{test,i} \right)^2$ and $R_{\text{tot}} = \sum_{i=1}^{n_{test}} \left(y_{test,i} - \bar{y}_{test} \right)^2$ are the residual and total sum of squares, respectively, in which $\bar{y}_{\text{test}}$ is the mean of the test data set. The value of the coefficient of determination ranges from 0 to 1, with ‘1’ representing a perfectly fitted surrogate model.

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3 APPLICATION: SURROGATE MODEL DEVELOPMENT

To demonstrate the application of regression-based surrogate models to SFE, a simple and an advanced non-linear model are considered as physical systems in this study. The terms 'actual models' and 'physical systems' are further used interchangeably. In the above "simple" refers to an SFE model which does not require numerical approaches. The considered simple model is presented in Section 3.1 and relates to the bending moment capacity of a simply supported concrete slab, considering known temperature for the reinforcement. The advanced model on the other hand involves significant computational cost. The considered advanced non-linear models is presented in Section 3.2 and relates to the load bearing capacity of a concrete column under fire considering second order effect.

3.1 Simple non-linear model: concrete slab bending capacity for known rebar temperature

3.1.1 Physical system: analytical equation for moment capacity of RC slab

The analytical model adopted by Van Coile et al. (2013) to estimate the resisting moment of a fire exposed RC slab for a known rebar temperature is considered here as a simple non-linear model. The governing equation is given by Eq. (12) where, A_s is the area of tensile reinforcing bars in the slab, ϕ is the diameter of the tensile reinforcing bars in the slab, h and b refer to the depth and width of the slab, c is the concrete cover to the reinforcement, $f_{c,20°C}$ refers to the 20°C compressive strength of the concrete, and $f_{y,20°C)}$ and $k_{fy(T)}$ are respectively the reinforcement yield strength at 20°C and the yield strength retention factor at T degrees Celsius.

$$M_{\mathrm{R}} = A_{\mathrm{s}} k_{f_{\mathrm{y}}(\mathrm{T})} f_{\mathrm{y,20°C}} (h - c - \frac{\phi}{2}) - 0.5 \frac{(A_{\mathrm{s}} k_{f_{\mathrm{y}}(\mathrm{T})} f_{\mathrm{y,20°C}})^2}{b f_{\mathrm{c,20°C}}} \quad (12)$$

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The RC slab is considered to be exposed to the fire at the bottom face, and to have sufficient depth for the concrete compressive zone to retain its strength (i.e. remain below approximately 200°C).

3.1.2 Development of the surrogate model

To develop the surrogate model following the procedure of Figure 1, first the model variables based on Eq. (12) are identified as $f_{c,20°C}$, $f_{y,T} = (k_{fy(T)} \cdot f_{y,20°C})$, c, h and A_s. The slab capacity is evaluated for a fixed unit width (b=1m) and the reinforcing bars are considered to be 12 mm in diameter. Next, the range of interest for the surrogate model is specified for each of the independent variables by an upper and a lower limit, as listed in Table 1. The surrogate model is intended to accurately simulate the physical system within these bounds for the variables, and therefore a uniform distribution is adopted, ensuring equal weighting in the subsequent sampling. Adopting the LHS scheme, the required input data are generated, as discussed in Section 2.1, for the cross-validation set a Monte Carlo scheme is applied. With Eq. (12) representing the physical system, the bending moment of the slab (the 'model evaluation' or output) can easily be evaluated for the considered combinations of input variables. The combinations of input variables and the corresponding bending moment capacities are then used to develop the surrogate model.

Table 1: Model variables for the fire exposed RC slab case study, with their lower and upper limits for the sampling space and dimensions

Independent variables	Lower limit	Upper limit	Unit	Distribution
Concrete strength, $f_{c,20°C}$	15	80	MPa	
Rebar strength, $f_{y,T}$	100	1000	MPa	
Concrete cover, c	20	70	mm	Uniform
Slab thickness, h	100	300	mm	
Reinforcement area, A_s	0.10	0.25	% (section area)	

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As discussed in Section 2.6, the surrogate model is dependent on the considered hyperparameters (number of training samples n, regularization parameter λ, order of the model m). The optimum values for the hyperparameters are estimated based on the cost functions (J_{train} and J_{cv}), i.e. by establishing learning curves. Figures 3 and 4 show the developed learning curves for the surrogate model to determine the hyperparameters in the test case. According to Figure 3, the 2nd order polynomial approximation has higher accuracy than the 1st order polynomial. However, there is no significant improvement for surrogate models with order 'm' > 2. The computational burden also gradually increases with the adoption of a higher order hypothesis for the surrogate model, due to the increased number of features with higher order polynomials and interaction terms, complicating the optimization. Therefore, a 2nd degree polynomial is adopted as surrogate model hypothesis for the fire exposed RC slab.

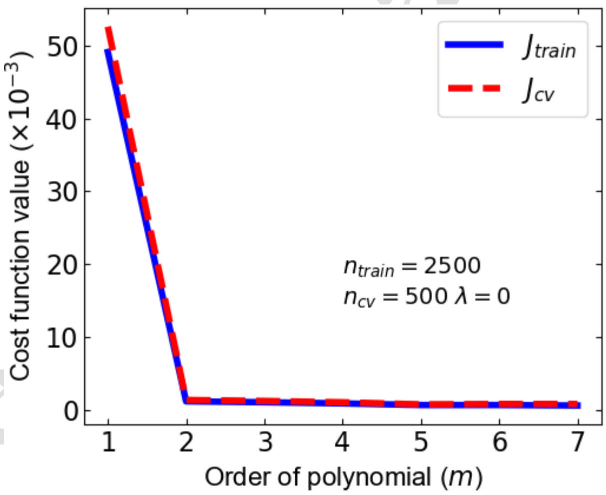

Figure 3 Cost function value for the surrogate model, in function of the order m of the regression model hypothesis

Figure 4 helps determining the hyperparameters (n and λ) for the considered surrogate model. Based on Figure 4(a), an optimum size of the LHS sample for training the surrogate model can be evaluated. In the figure, mean values for J_{train} and J_{cv} are plotted against the training sample size for a 2nd order surrogate model, considering a constant cross-validation set n_{cv} of size 500. Mean values are listed because for low sample sizes, the cost evaluation can depend on the

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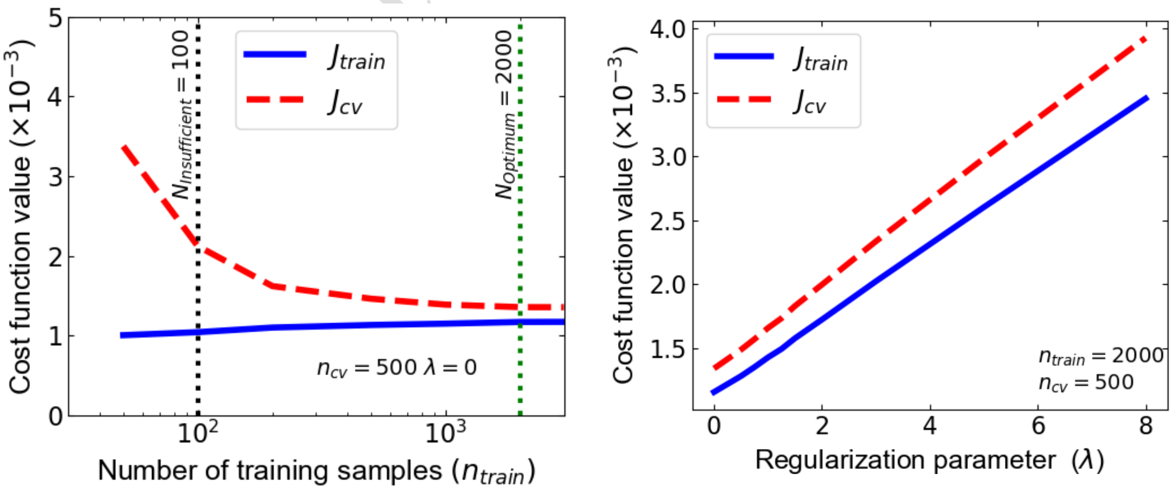
specific set of LHS realizations. Therefore, a repeated sampling approach is adopted, where 10^3 LHS samples for each of the training sets are developed. As the J_{train} and J_{cv} have converged for a training set of 2000 LHS samples, this sample size is observed to be sufficient (i.e. optimal) for the surrogate model. On the other hand, based on the learning curves 100 LHS sample points is insufficient for developing a precise surrogate model, as a further increase of n results in a significant decrease of J_{cv}. The regularization parameter has not been considered for the estimation of both the optimum order of polynomial and number of training sample size. For the considered surrogate model order and number of training samples this is reasonable, as demonstrated in Figure 4(b) where J_{train} and J_{cv} are plotted in function of the regularization parameter λ. The regularization parameter is found to have no influence over the developed surrogate model and thus can be neglected for the development of the surrogate model here. However, the regularization parameter becomes important when a larger model order is considered. These situations however do not result in a lower J_{cv} than for the hyperparameter-combination (n_{train} = 2000, m = 2 and λ = 0), while at the same time increasing computational cost significantly.



(a) (b)

Figure 4 Cost function value for the surrogate model, in function of (a) the number of training samples, n_{train} and (b) the regularization parameter, λ

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3.1.3 Evaluation of surrogate model performance and discussion

Figure 5 represents the developed surrogate model based with assessed optimum hyperparameters (n_{train} = 2000, m = 2 and λ = 0). In the Figure, the regression coefficients are shown for the normalized features of the surrogate model (2nd degree polynomial model). The values for these coefficients are also listed in the Annex.

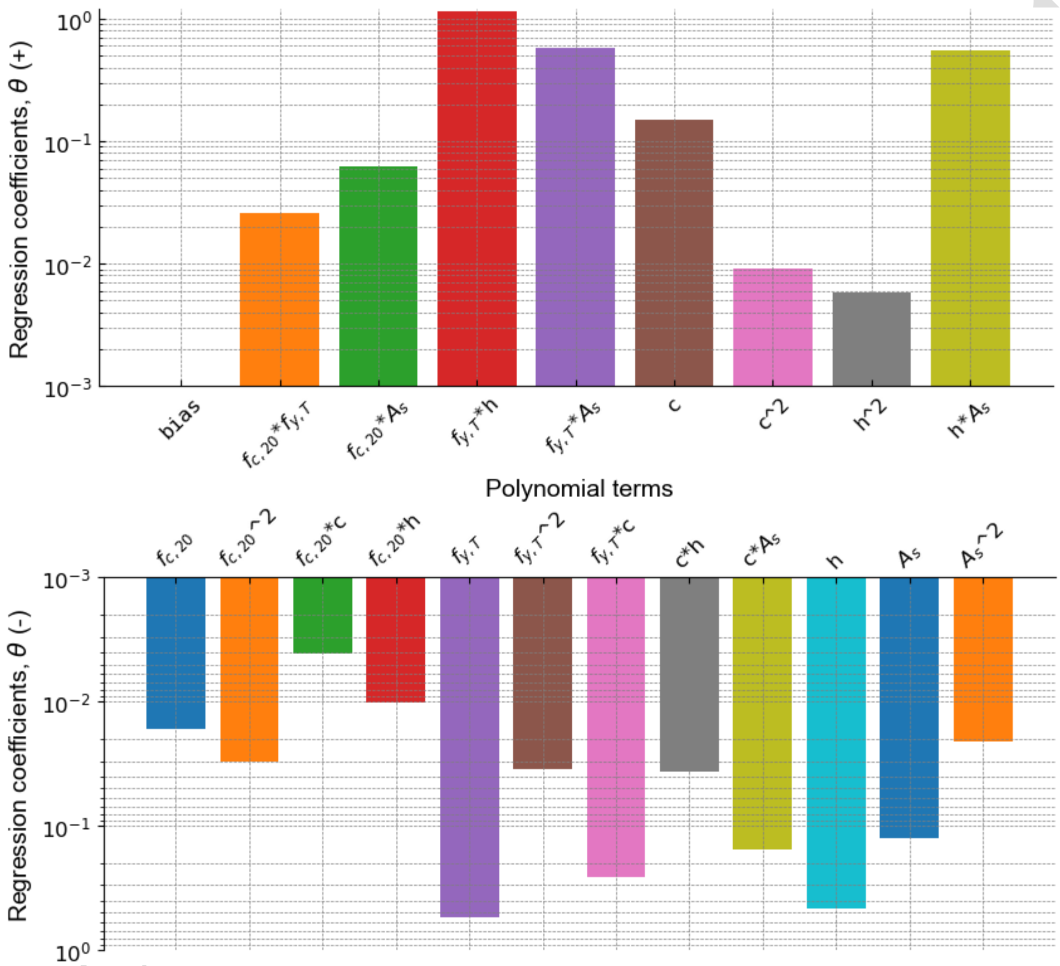

Figure 5 Obtained regression coefficients for 2nd order surrogate model with normalized features. Positive coefficients in the upper graph, negative coefficients in the lower graph.

These regression coefficients, also referred to as 'weights' of a particular feature, indicate the influence of respective features on the response of the system. For example, the polynomial term '$f_{y,T}*h$' has a higher value for its regression coefficient than the other polynomial terms, and thus has higher influence on the moment capacity of the slab. The surrogate model thus can also be helpful in assessing the influence of a particular variable or combination of variables on the response of the actual model.

The performance of the developed surrogate model is evaluated by comparing the actual and predicted response for the test data set (unseen random data), where the coefficient of determination (R^2) is estimated as stated in Section 2.6. Figure 6 shows the comparison of the moment capacity of the RC slab for the 500 realizations of the test set, as evaluated respectively by the actual model and the developed surrogate model. The R^2 value for the surrogate model of RC slab is found to be 99.75 %, indicating very good accuracy.

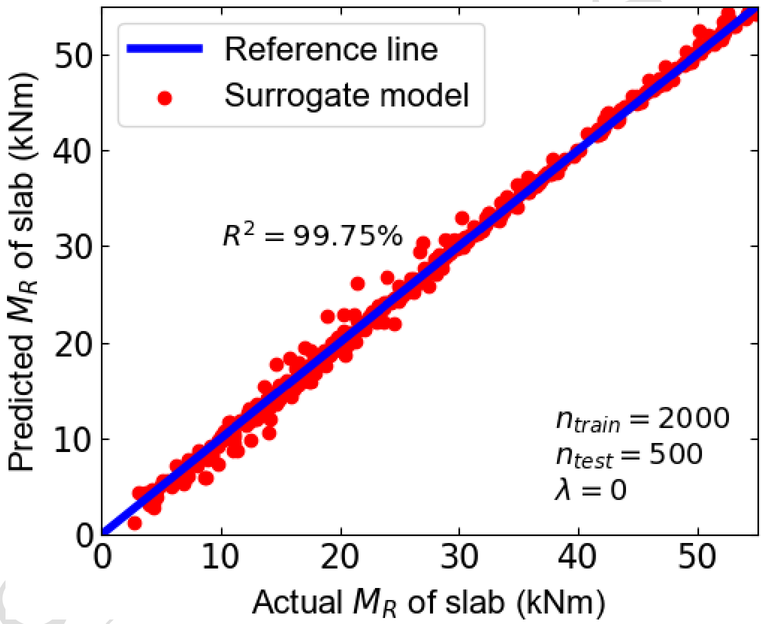

Figure 6 Performance of the developed surrogate model for the moment capacity of RC slab with known rebar temperature

3.2 Advanced non-linear model: Finite element evaluation of RC column load bearing capacity

3.2.1 Physical system

This model deals with the axial load bearing capacity of an RC column exposed to the ISO 834 standard fire on four sides. A probabilistic study for the considered column has been presented

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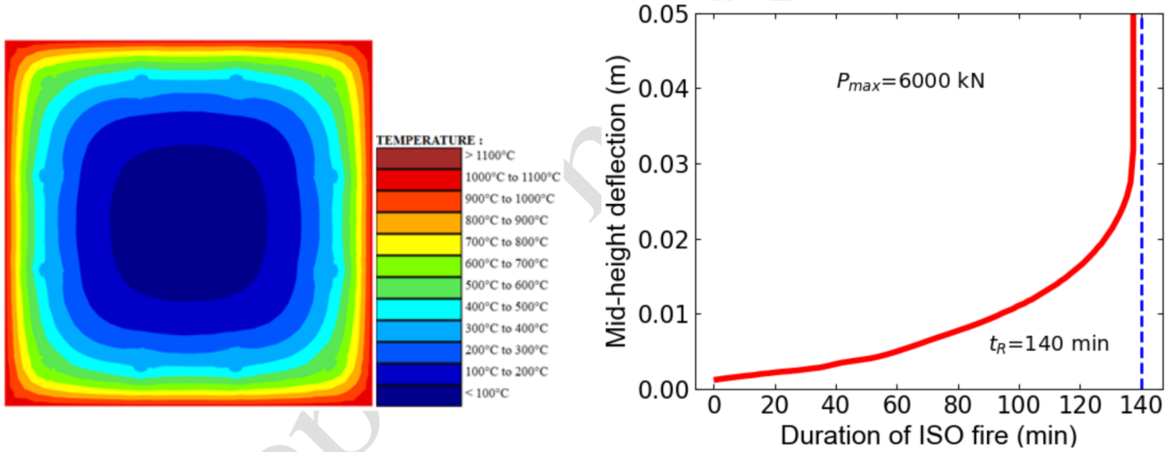
in (Van Coile et al., 2020) and has been incorporated in ISO/TR 24679-8:2020 (ISO, 2020). The column capacity assessment is done through the dedicated Finite Element (FE) software SAFIR® (Franssen and Gernay, 2017). The column cross-section is 500 mm × 500 mm with 12 reinforcing bars of 20 mm diameter. The height is 4 m and the column is pinned at the bottom and has a roller support at the top (Van Coile et al., 2020). The concrete is a C30/37 and the reinforcing steel is of grade 500. The thermal response is modeled in accordance with Eurocode EN 1992-1-2:2004. Figure 7 shows the thermal and mechanical response for the above considered RC column exposed to ISO 834 fire, with an axial load of 6000 kN at an eccentricity of 1.5 cm. In this specific evaluation, the column is found to have fire resistance of 140 min, with the temperature of the rebars reaching 598°C.



(a) Temperature distribution in the column at an ISO 834 duration of 140 min

(b) Deflection-time history at mid-height for the column

Figure 7 Thermal and mechanical response for RC column exposed to ISO 834 fire, with an axial load of 6000 kN at an eccentricity of 15 mm

3.2.2 Development of the surrogate model

Six variables are considered to govern the model response. These are the retention factor quantile parameters for the concrete compressive strength (ε_{kfc}) and reinforcement yield stress (ε_{kfy}), the concrete cover (c), average eccentricity (e), out of straightness (oos), out of plumbness (oop) and the applied load (P). The parameters ε_{kfc} and ε_{kfy} are parameters defining the quantile

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of the retention factors at elevated temperature in accordance with the strength retention models by Qureshi et al. (2020). The model variables e, oos and oop refers to the three basic eccentricities associated with the column, as considered in JCSS probabilistic model code (2013).

Next, the input data for the physical model evaluation is obtained through an LHS sample of the model variables. The considered range for the sample space is listed in Table 2. An initial training sample size of 10^4 realizations is considered, while a separate (fixed) Monte Carlo set of 1250 realizations is evaluated as a cross-validation data set.

Having evaluated the physical model for the input realizations of the model variables, the surrogate modelling hypothesis is defined. To allow for comparison with the (numerically expensive) evaluations by Van Coile et al. (2020), the surrogate model is developed to predict the maximum load bearing capacity P_{max} of the concrete column, considering a specified ISO 834 exposure duration and specific realizations for the other model variables. In other words, the evaluated fire resistance time t_E of the RC column is considered as input parameter for the surrogate model development, while the associated applied load P is to be considered as the response by the surrogate model. To elucidate the motivation for the above procedure further, note that in Van Coile et al. (2020) the maximum load P_{max} for a given ISO 834 standard fire duration t_E was determined through an iterative search algorithm for $P_{\max}$. The corresponding probabilistic analysis was very computationally expensive owing to the need to perform multiple finite element evaluations for each sample realization. The surrogate modelling procedure applied here is intended to result in a computationally much more efficient process. Note that for a given set of parameters, the SAFIR model evaluation is the same irrespective whether this set of parameters was obtained by an iterative approach to find P_{max} for given t_E.

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It is important to note that the surrogate model aims at approximating the physical system (SAFIR model) and will thus incorporate the limitations and assumptions of the numerical model. General assumptions include for example perfect bond between concrete and steel. Limitations relate for example to the inability of the beam model to consider shear or spalling. For further overview on the general SAFIR modelling assumptions and limitations, reference is made to (Franssen and Gernay, 2017). Furthermore, in the current case study, the SAFIR model takes into account Eurocode material properties. The surrogate model can thus not be interpreted more generally considering material models from other guidance documents.

Table 2. Model variable for the RC column case study, with their lower and upper limits for the sampling space and dimensions

Independent variables	Lower limit	Upper limit	Unit	Distribution
Concrete strength retention factor, ε_{kfc}	-4.00	4.00	-	
Rebar yield strength retention factor, ε_{kfy}	-4.00	4.00	-	
Concrete cover, *c*	16	96	mm	Uniform
Average eccentricity, *e*	-0.03	0.03	mm	
Out of straightness, oos	-0.03	0.03	mm	
Out of plumbness, oop	-0.01	0.01	rad	
Applied load, *P*	1000	10500	kN	

Figure 8 shows the learning curves generated as part of the surrogate model development. Based on Figure 8(a), a 4th order polynomial is found more precise compared to polynomials with $m \leq 3$. On the other hand, there is no further significant decrease in error for predictions on the cross-validation set for $m \geq 5$. Thus, a 4th order polynomial approximation is adopted for the surrogate model. Similarly, based on Figure 8(b) a training set of 10^4 LHS samples is found adequate to develop surrogate model since the prediction error on the cross validation set shows signs of convergence with limited further reduction in J_{cv} for $n_{\text{train}} \geq 6000$. In the same way,

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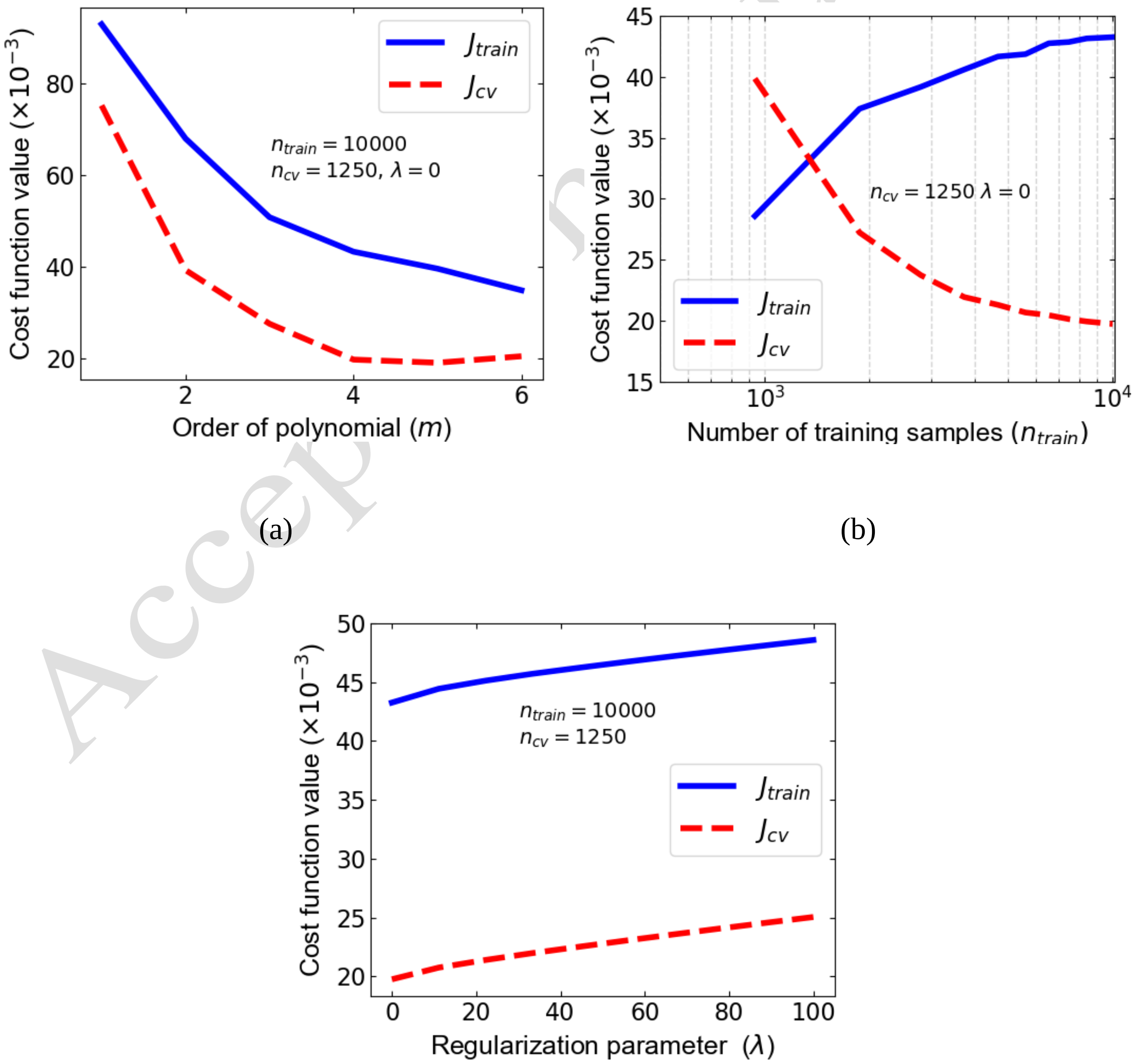
Figure 8(c) suggests that the considered surrogate model does not require a regularization parameter. It can be seen that the learning curves in Figure 8 indicate a higher prediction error for the training data as compared to the cross validation data. This is however not the case for n_{train} = 10^3, see Figure 8(b). Taking into account this observation, and noting that the LHS sampling procedure ensures that training samples are generated across the entire space of model variables, it is hypothesized that the training data sets with a larger number of samples than the 1250 cross validation samples result in a larger probability of obtaining 'extreme cases' for which the model performs less well. This hypothesis will be evaluated in detail as part of follow up research.



(a) (b)

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(c)

Figure 8 Learning curves to develop surrogate model for RC column under ISO 834 fire

3.2.3 Evaluation of surrogate model performance and discussion

Figure 9 shows the performance of the developed surrogate model for the test data set. The R^2 value for the surrogate model was found to be approximately 95 %. As the considered evaluation of load capacity of column involves complex structural fire calculations, the estimated error can be considered reasonable. Thus, the surrogate model can be considered to effectively simulate the entire thermal and mechanical calculation for FE model of RC column and estimate the load bearing capacity of the RC column for a specified fire duration t_E. It is noteworthy that the evaluation of the test set using the actual SAFIR model took about 60 core-hours on a state-of-the-art PC, while the evaluation of the same test set through the surrogate model is quasi-instantaneous.

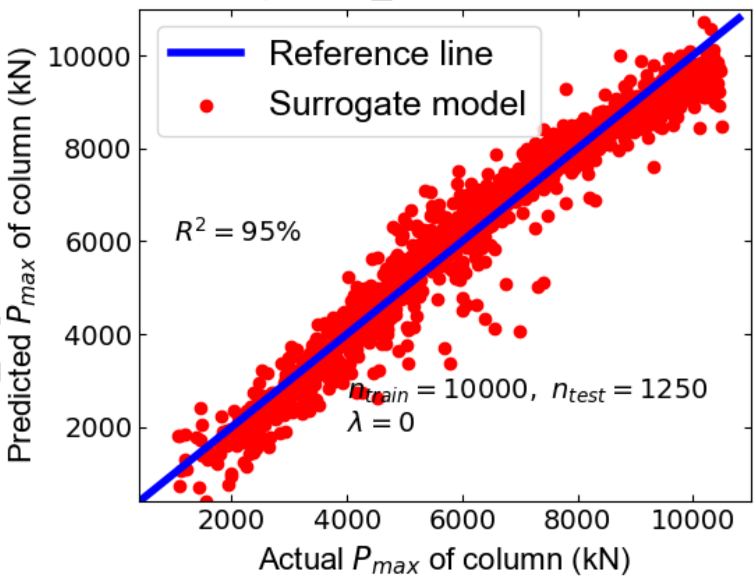

Figure 9 Performance of the developed surrogate model for RC column under ISO 834 exposure

As discussed earlier in Section 3.1, the developed surrogate model can be helpful in determining the influencing parameters of the physical system. The duration of fire exposure (t_E) has the highest absolute value for the regression coefficients (≅1.32) compared to all other polynomial terms and thus can be regarded as the most influencing parameter. The bias term is almost equal to zero and thus has negligible effect on the physical system.

4 APPLICATION OF SURROGATE MODELS FOR PROBABILISTIC STUDIES

The proposed framework for probabilistic studies of fire exposed structures through regression based surrogate models is visualized in Figure 10. The first steps correspond to the development of the surrogate model as a substitute for the physical system. Once the surrogate model is adequately trained, the probabilistic distributions for the model parameters are considered (based on literature) for the specific design. The probability distribution of the model output is then evaluated by sampling the model variables according to their probabilistic distributions (LHS is adopted herein), and evaluating the surrogate model for each realization. As the surrogate model is not computationally expensive, the probabilistic evaluation can be assessed at limited computational cost.

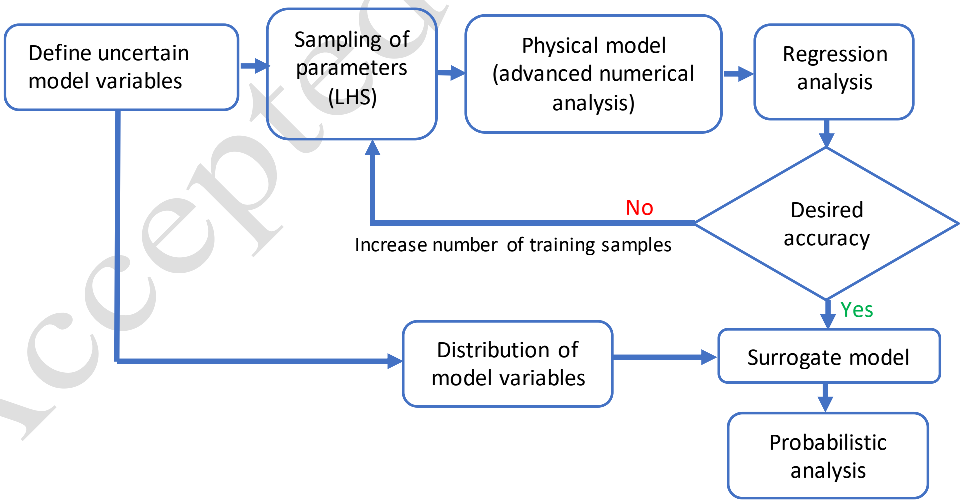

Figure 10 Framework for probabilistic studies of fire exposed structures through surrogate modeling approach

The framework of Figure 10 is applied to probabilistic studies of the cases of Section 3. The obtained probability density functions (PDF) and cumulative density functions (CDF) are

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validated against the traditional direct Monte Carlo evaluations of the numerical models (i.e. repeated sampling of the computationally expensive physical system). This is intended to demonstrate the feasibility of the proof-of-concept. Finally, the surrogate models will be employed for probabilistic studies for structural fire scenarios for which no computationally expensive validation is available, demonstrating the practical value of the proposed approach. The proposed approach however comprises

4.1 Simple non-linear model: probabilistic study of a concrete slab bending capacity for known rebar temperature

The surrogate model developed in Section 3.1 for the estimation of the moment capacity of an RC slab with known rebar temperature is applied. The temperature distribution in the slab is deterministic, and is evaluated taking into account the recommendations of EN 1992-1-2:2004, using the thermal model as presented by Thienpont et al. (2019). Table 3 shows the probability distribution of the variables, based on Thienpont et al. (2019). The steel yield strength retention factor is multiplied with the mean 20°C yield strength of 581 MPa. In this Table, μ denotes the mean value and σ denotes the standard deviation. To develop the fragility curves, an LHS scheme with 10^4 realizations is adopted.

4.1.1 Nominal ISO 834 exposure

A nominal exposure of 120 min ISO 834 at the bottom face is considered, with convection cooling applied at the top face. Figure 11(a) shows the comparison of the obtained probability density function (PDF) for the actual and surrogate model. The PDF obtained through the surrogate model (N_{train} = 2000) almost coincides with the one obtained through a direct evaluation of the actual model of Eq. (12). The PDF obtained from a surrogate model trained with 100 LHS samples ($N_{\text{insufficient}}$) also agrees, but with a slightly larger difference. The mean value for the bending moment capacity at 120 minutes of ISO 834 exposure is 32.61 kNm according to the actual model, whereas the surrogate models trained with 100 and 2000 LHS

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samples result in mean value estimates of 32.77 kNm and 32.58 kNm, deviating by 0.5 % and 0.09 % respectively from the actual model's result.

Table 3 Probabilistic distributions for the model variables for the RC slab, known rebar temperature

Stochastic variables	**Distribution**	**Mean**	**COV**
Concrete strength, $f_{c,20°C}$ ($f_{ck,20}$ = 30 MPa)	Lognormal	42.9 MPa	0.15
Retention factor for yield strength of rebars, k_{fy}	Logistic model (Qureshi et al., 2020)	Temperature-dependent	Temperature-dependent
Concrete cover, c	Beta [μ-3σ; μ+3σ]	35 mm	0.14 σ = 5 mm
Slab depth, h	Normal	200 mm	0.025 σ = 5 mm
Area of tensile reinforcement, A_s (nominal area $A_{s,nom}$ = 0.1965 % of section area)	Normal	1.02 $A_{s,nom}$	0.02

Likewise, Figure 11(b) compares the obtained cumulative density functions. Here, the difference for the surrogate model with n_{train} = 100 is more noticeable, notably for the lower quantiles of the CDF. In Figure 11(b), the 10^{-2} capacity quantile (99 % probability of a larger capacity) for the RC slab is predicted as 14.91 kNm and 15.83 kNm based on the surrogate model developed from 100 and 2000 LHS sample, which is very close to the 15.89 kNm obtained through the actual model. Table 4 lists and compares the actual and predicted moment capacity of the heated RC slab for different capacity quantiles. The Table shows that even the 10^{-4} quantile capacity of the slab is predicted with great accuracy by the surrogate model. Therefore, the direct CDF evaluation through 10^4 evaluations of the actual (physical) model can be accurately approximated by evaluations applying a surrogate model which has been trained using just 2000 (physical) model evaluations. Although the computational expense is

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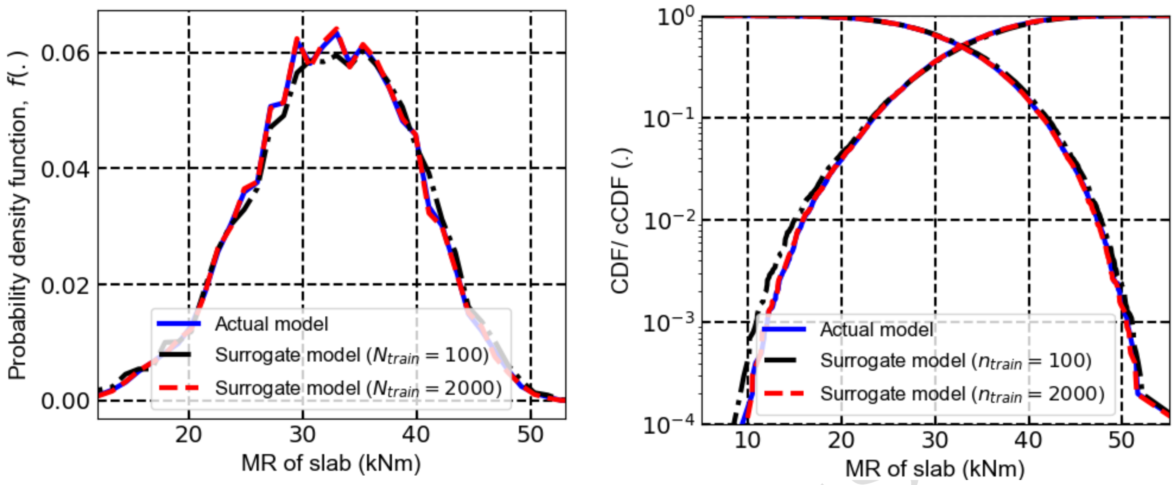
negligible for the considered case, the number of physical model evaluations is reduced significantly by adopting the surrogate modeling methodology.



(a) (b)

Figure 11 Comparison of (a) probability density function (PDF) and (b) cumulative density function (CDF) for the RC slab exposed to 120 min of ISO 834 fire

Table 4 Capacity quantiles for the RC slab exposed to ISO 834 fire

S.N	**CDF (.)**	**M_R of slab (kNm) for ISO fire**		
		n_{train}=100	n_{train}=2000	*Actual model*
1.	10^{-1}	23.21	23.39	23.40
2.	10^{-2}	14.91	15.83	15.89
3.	10^{-3}	10.86	12.08	12.04
4.	10^{-4}	8.45	9.45	9.34

4.1.2 Parametric fire exposure

The surrogate models can be applied directly for different fire exposure scenarios. Here, a Eurocode parametric fire (EN 1991-1-2:2002) with Γ = 1 and t_{max} = 120 min is considered. The temperature of the reinforcing steel bar is estimated considering a regression model proposed by Thienpont et al.(2019), which gives the reinforcement temperature for a given duration of heating phase and concrete cover.

Figure 12 shows the CDF for the RC slab based on the actual and surrogate models. The estimated mean values for the minimum resisting moment of the slab during the parametric fire

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exposure ('burnout' resistance; Gernay, 2019) based on 2000 and 100 LHS samples is approximately 27.27 kNm. Applying a direct evaluation of the 'actual model' the mean capacity of the slab is estimated as 27.28 kNm. Again, the fragility curve developed based on surrogate model agrees with that developed from the actual model, also for low capacity quantiles.

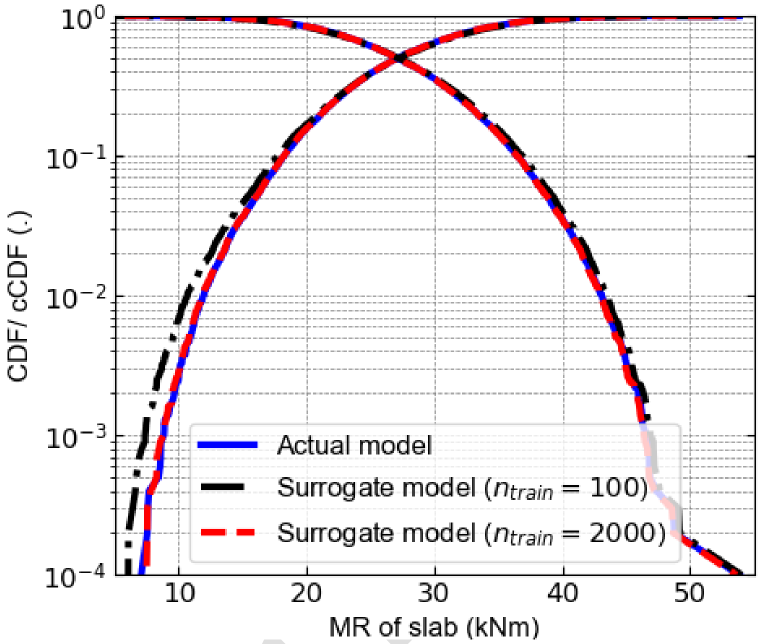

Figure 12 Comparison of cumulative density function based on actual and surrogate model for RC slab under parametric fire ($\Gamma = 1$, $t_{max} = 120$ min)

4.2 Advanced non-linear model: Finite element evaluation of RC column load bearing capacity

The surrogate model developed in Section 3.2 for the evaluation of the load bearing capacity (P_{max}) of an RC column exposed to ISO 834 standard heating is adopted. Table 5 shows the stochastic variables, adopted from Van Coile et al. (2019). The fragility curve is developed based on 10^4 LHS samples of the stochastic variables as considered in earlier sections.

Table 5 Probabilistic distributions for the model variables for the RC column exposed to ISO 834 fire

Stochastic variables	Distribution	Mean	Standard deviation
Retention factor for yield strength of rebars, k_{fy} ($f_{yk,20}$ = 500 MPa; $\mu_{fy,20}$ = 560 MPa)	Logistic model (Qureshi et al., 2020)	Temperature-dependent	Temperature-dependent
Retention factor for concrete strength, f_c ($f_{ck,20}$ = 30 MPa; $\mu_{fc,20}$ = 42.9 MPa)			
Concrete cover, *c*	Beta [μ-3σ; μ+3σ]	47 mm	5 mm
Average eccentricity, *e*	Normal	0	0.004 m
Out of straightness, oos	Normal	0	0.004 m
Out of plumbness, oop	Normal	0	0.0015 rad

4.2.1 Validation for probabilistic studies

Figure 13(a) shows the comparison of the PDF evaluated by 10^4 evaluations of the actual and surrogate models. The PDFs from the two models agree reasonably well. The mean predicted capacity of the RC column after 4 hours of ISO 834 fire exposure based on actual and surrogate model are 5038 kN and 5137 kN, respectively. Similarly, the CDF based on surrogate model for the RC column is in good agreement with the CDF from the actual model, especially for low quantiles of P_{max}, as shown in Figure 13(b). As listed in Table 6, the 10^{-2} capacity quantile for the RC column is 2931 kN, which is predicted as 3010 kN (2.5 % error) through the surrogate model. From the perspective of computational expense, the probabilistic evaluation through the surrogate model was quasi-instantaneous, while the iterative evaluation of P_{max} in the actual model required multiple core-weeks on a modern PC (evaluation done through multi-processing in approximately 7 days).

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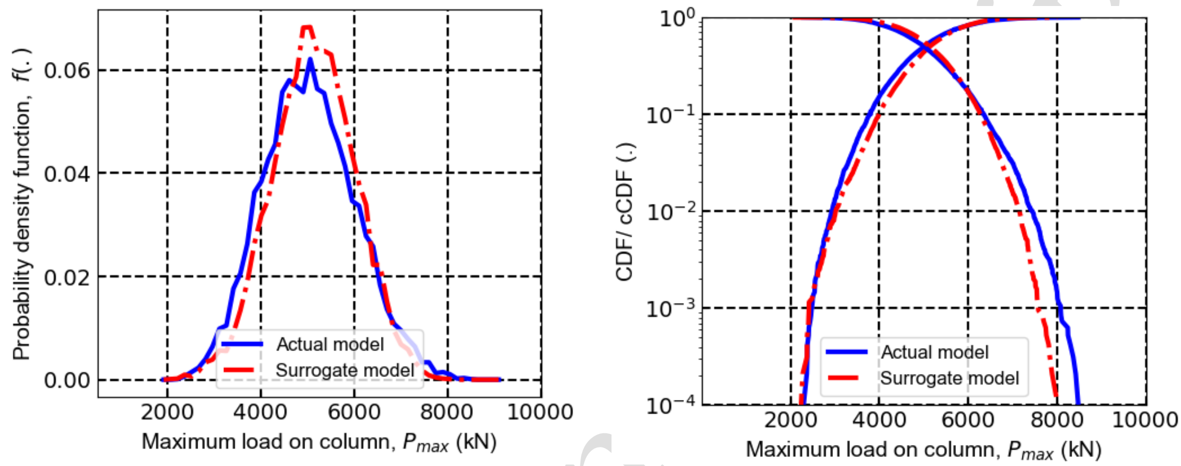
Table 6 Capacity quantiles for RC column exposed to ISO 834 fire

S.N	**CDF (.)**	**M_R of slab (kN) for RC column**		
		Surrogate model	*Actual model*	*Error* (%)
1.	10^{-1}	3987	3805	4.7
2.	10^{-2}	3010	2931	2.70
3.	10^{-3}	2475	2414	2.52
4.	10^{-4}	2240	2300	2.60



(a) (b)

Figure 13 Comparison of (a) probability density function and (b) cumulative density function for RC column under 240 min of ISO 834 fire exposure

4.2.2 Generalized probabilistic evaluation

The evaluation of P_{max} through the actual model requires a computationally expensive iterative approach, see (Van Coile et al., 2020). This makes the updating of the probabilistic evaluation for design iterations impractical. Here, the surrogate model is applied to quasi-instantaneously perform probabilistic analyses for different ISO 834 exposure durations. Figure 14 shows obtained CDFs based on the surrogate model. The mean capacity of RC column after 1, 2, 3 and 4 hr of standard fire exposure is estimated with the surrogate model as 8547 kN, 7290 kN, 6210 kN and 5137 kN, respectively. Similarly, the 10^{-2} capacity quantile are 3010 kN, 3852 kN, 4944 kN and 6513 kN. As the variable P_{max} relates to the load bearing capacity of the column, the results in Figure 14 can also be directly understood as fragility curves, where the horizontal axis relates to the 'intensity measure' of total applied load. Such efficient generation of fragility curves through surrogate modeling can be helpful in design iterations.

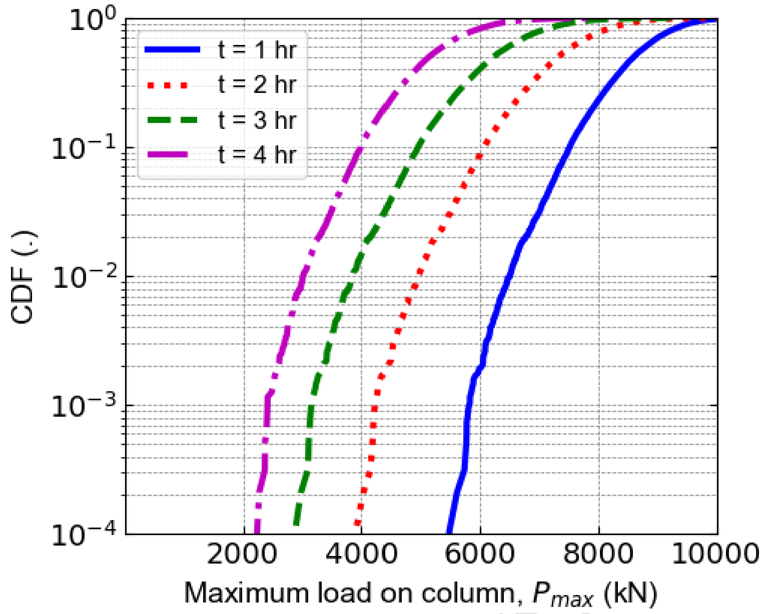


Figure 14 Cumulative density function for RC column exposed to different duration of ISO 834 fire

5 CONCLUSIONS

The potential of regression-based surrogate models for probabilistic studies of fire exposed structure has been demonstrated. As a part of the proof-of-concept, the approach has been applied to two structural fire engineering (SFE) models: (i) the bending moment capacity of a concrete slab during fire, as defined by a simple analytical equation; and (ii) the load bearing capacity of a concrete column during fire, considering an advanced numerical model. For both cases, the fragility curves obtained through the surrogate model match with those obtained through a direct application of the analytical/numerical model. The developed surrogate models could predict the 10^{-2} capacity quantiles with an error of less than 5 %. A very significant improvement in computational efficiency is observed. Furthermore, the surrogate modeling methodology for probabilistic analysis has the important advantage that it can be applied to quasi-instantaneously develop fragility curves considering modifications in the design or fire scenarios, allowing probabilistic methods to be used as part of fast design iterations. It is

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concluded that surrogate modelling approaches are particularly promising for probabilistic structural fire engineering studies. As a next step in the application of surrogate models in SFE, one suggestion is for surrogate models to be developed by interested individuals, industry organizations, academic institutions and other. The latest surrogate models to be used by practitioners can be made available in online repositories, with background to the model training and validation made publicly available (e.g. through peer-reviewed journals).

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Annex: Evaluation of concrete slab bending capacity for known rebar temperature (Simple non-linear model)

Table 1 Regression coefficients, with mean and standard deviation of polynomial terms of the surrogate model (*m*=2)

S.N	Polynomial terms, *c*	Dimension	Regression coefficients, θ	Mean, μ_c	Standard deviation, σ_c
0.	Bias	-	6.01E-15	1.00E+00	0.00E+00
1.	$f_{c,20°C}$	N/m^2	-1.66E-02	4.75E+01	1.88E+01
2.	$f_{c,20°C}$^2	N^2/m^4	-3.03E-02	2.61E+03	1.81E+03
3.	$f_{c,20°C} \times f_{y,T}$	N^2/m^4	2.62E-02	2.61E+04	1.68E+04
4	$f_{c,20°C} \times c$	N/m	-4.10E-03	2.19E+00	1.05E+00
5	$f_{c,20°C} \times h$	N/m	-1.008E-02	9.52E+00	4.81E+00
6	$f_{c,20} \times A_s$	N	6.26E-02	1.90E-02	8.06E-03
7	$f_{y,T}$	N/m^2	-5.47E-01	5.50E+02	2.60E+02
8	$f_{y,T}$^2	N^2/m^4	-3.46E-02	3.70E+05	2.92E+05
9	$f_{y,T} \times c$	N/m	-2.601E-01	2.53+01	1.39E+01
10	$f_{y,T} \times h$	N/m	1.14E+00	1.10E+02	6.24E+01
11	$f_{y,T} \times As$	N	5.83E-01	2.20E-01	1.10E-01
12	*c*	m	1.50E-01	4.60E-02	1.15E-02
13	*c*^2	m^2	9.15E-03	2.25E-03	1.07E-03
14	$c \times h$	m^2	-3.67E-02	9.20E-03	3.57E-03
15	($c \times As$)	m^3	-1.53E-01	1.84E-05	5.38E-06
16	*h*	m	-4.57E-01	2.00E-01	5.77E-02
17	*h*^2	m^2	5.76E-03	4.33E-02	2.33E-02
18	($h \times A_s$)	m^3	5.54E-01	8.00E-05	2.60E-05
19	A_s	m^2	-1.25E-01	4.00E-04	5.77E-05
20	A_s ^2	m^4	-2.08E-02	1.63E-07	4.63E-08

The surrogate model was trained for normalized model output, with μ_{MR} =330743 Nm and σ_{MR} = 21605 Nm. Based on the above Table, the moment capacity of slab can be estimated as:

$$M_R\left[Nm\right] = \left(\theta_0 + \sum_{i=1}^{20}\left(\frac{c_i - \mu_i}{\sigma_i}\right)\theta_i\right)21605 + 330743$$

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