Verification and Validation Process of a Fire Model

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Abstract: Fire simulation tools are used frequently in the fire safety assessment of nuclear and other industrial installations. They are also used in the context of probabilistic fire risk assessment as deterministic models providing the relation between the random conditions and the consequence of an accidental fire. Fire Dynamics Simulator (FDS) is a computational fluid dynamics code developed specifically for the simulation of fire driven flows and heat transfer processes. FDS is currently the most commonly used fire model globally, and a subject of continuous validation studies by the code developers and users. The purpose of this paper is to provide an overview of methodology that is used for the estimation of model uncertainty, and to describe the implementation of the systematic and transparent quality assurance procedures for an open-source computer code.

Keywords: Fire Model, Model Uncertainty, Validation

1. INTRODUCTION

Risk-informed and performance-based analyses are being introduced into fire protection engineering practice, and the commercial nuclear power industry is no exception. In the last 15 years, the U.S. Nuclear Regulatory Commission (NRC) has directed a change in its policy to use risk-informed methods, where practical, to make regulatory decisions. As a result of this change, in the area of fire protection, the National Fire Protection Association (NFPA) completed development of the 2001 edition of NFPA 805, "Performance-Based Standard for Fire Protection for Light-Water Reactor Electric Generating Plants" (NFPA, 2001). The NRC amended its fire protection requirements in July, 2004, to allow existing reactor licensees to voluntarily adopt the fire protection requirements contained in NFPA 805 as an alternative to the existing prescriptive fire protection requirements. This allows plant operators and the NRC to use fire modeling and fire risk information, along with prescriptive requirements, to ensure that nuclear power plants can safely shut down in the event of a fire. They also use these tools to determine compliance with, or exemptions from, existing fire protection regulatory requirements. To provide the regulator and the plant operators with confidence in the calculation results, NFPA 805 requires fire models to be *verified* and *validated*. To this end, the NRC's Office of Nuclear Regulatory Research, along with the Electric Power Research Institute (EPRI) and the National Institute of Standards and Technology (NIST), conducted an extensive verification and validation (V&V) study of fire models that support the use of NFPA 805 as a risk-informed/performance-based (RI/PB) alternative within the NRC's regulatory system. This study was published in 2007 (NUREG-1824, 2007), and since that time, NIST and VTT Technical Research Centre of Finland have continued the process of verifying and validating one of the models of the NRC/EPRI study, the Fire Dynamics Simulator (FDS).

The primary components of the FDS quality assurance process are the verification and validation (ASTM E 1355). In short, verification means checking that the source code contains no errors and corresponds exactly to what is described in the code documentation. Validation, in turn, is the assessment of the code accuracy in its intended use. The results of the validation simulations are used to guide the future development work by revealing the physical quantities and parts of the model having highest uncertainties, and to estimate model uncertainty in a way that is useful for the end users. The validation results are summarized in terms of two uncertainty metrics: systematic bias and the width of the random error distribution for each output quantity. In the presentation, the mathematical derivation of the error measures is given and the underlying assumptions are discussed. The most important assumption concerns the Gaussian shape of the error distributions, justified by the complexity of both the experimental and computational procedures, meaning that the observed errors consist of many additive components. Finally, examples of validation results and how they can be used are also given.

2. QUALITY ASSURACE OF AN OPEN-SOURCE SIMULATION SOFTWARE

The need for a formal quality assurance process of open-source fire simulation software comes from the needs and requirements of the users carrying out computational analyses for performance based fire safety design. To meet the requirements set forth in codes and standards, such as the NFPA 850, or to restrict the liability of accidental losses, the designers need to show that the tools they use are developed and maintained under a credible system of quality control. In case of commercial simulation packages, this is the responsibility of the developing company. In case of open-source software with several developers from different organizations around the world, special care must be taken to ensure that the roles and responsibilities of the developers are clearly stated. The open-source nature of the code provides an obvious benefit by enabling fully transparent development and maintenance process.

In case of Fire Dynamics Simulator, the development and maintenance processes are described in a specific document called a Configuration Management Plan (McGrattan 2007). This document describes how the source code and documentation are identified and their versions controlled. The procedures for feature requests, program issues, decisions and responsibilities are explained. The procedures for testing new versions and the peer review process are also explained.

The primary components of the FDS quality assurance process are the verification and validation (ASTM E 1355). Verification deals with the mathematical and numerical solution of the underlying physical problems. In practice, it means checking that the source code contains no errors and corresponds exactly to what is described in the code documentation. The "verification suite" is a collection of simple calculations that typically test some specific feature of the model. These cases are run on a daily basis by the code developers during the development work. Validation, in turn, is the assessment of the code accuracy in its intended use. The validation suite consists of hundreds of simulated fire experiments – tests that have been carried out in some of the fire laboratories around the world. Considering the facts that the tests are all documented and experimental data provided, the FDS's validation suite is by far the largest collection of fire test data available at the moment. The validation tests are simulated before every time a new version of the model is released, taking few weeks on a relatively large cluster of computing servers.

The results of the validation simulations are used for two purposes: First, they are used to guide the future development work by revealing the physical quantities and parts of the model having highest uncertainties. However, the picture given by the validation suite in this respect is rather limited because the fires of the collection were chosen as "appropriate" in the first place. Fire tests dealing with phenomena clearly beyond the model capabilities would not have been included as they would not provide any meaningful measures of the model uncertainty. The second and more important use of the validation simulations is the estimation of model uncertainty in a way that is useful for the end users. A practical example from the field of nuclear power plant safety engineering is a case where the fire model predicts that for a specified fire scenario, the peak gas temperature in a certain location is 300 °C. If a safety relevant device placed in that location has a critical temperature of 320 °C, the quantitative estimate of the uncertainty associated with the model prediction would be needed to calculate the probability that the device will actually fail. Naturally, the critical temperature is also associated with statistical uncertainty, which can be investigated using the tools of probabilistic simulations.

3. CALCULATION OF MODEL UNCERTAINTY STATISTICS FROM VALIDATION DATA

The first step of the validation process is the choice of output quantities. In fire safety analysis, typical output quantities are gas or target temperatures, height of the smoke layer within a compartment or the concentration of toxic species. The importance of the heat transfer calculations makes also the flow velocities and heat fluxes interesting quantities for validation. In some cases, the accurate prediction of pressure may be needed. In practical applications, many of the quantities are compared against some critical value monitoring the time to reach this value. Therefore, it may be necessary to validate the capability to predict the time-to-threshold, but usually this is not made because the time-to-threshold has no defined value if the threshold is never met.

The second step is to choose the metric for comparison. In most cases, the peak value (positive or negative) is a relevant and well-defined quantity. Some exceptions could be the heating of thermally thick targets or doses of low-concentration toxics, in which case the accuracy of long-time averages would be more important than the peak values (Audouin *et al.* 2011). In any case, the computation of meaningful statistics requires that a single experimental measurement be compared against a single model prediction for each measurement point.

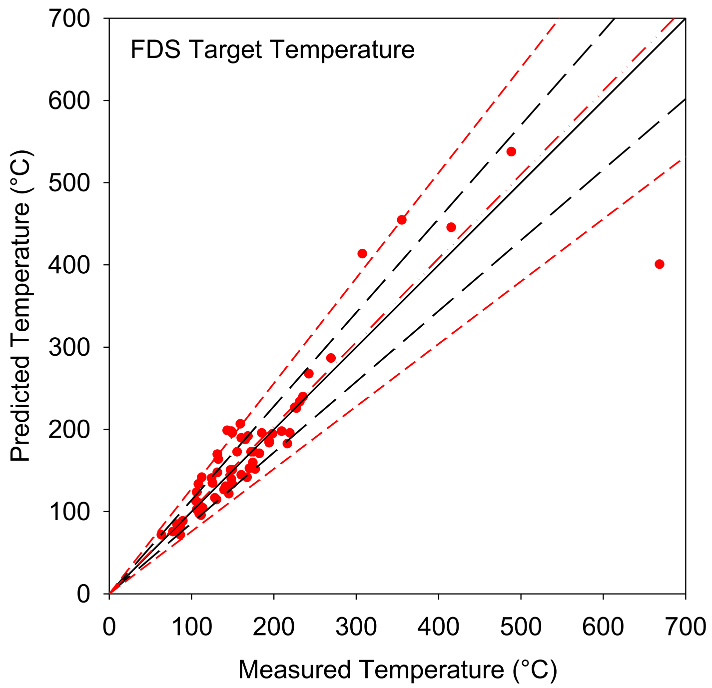

Figure 1. Sample result from validation study.

For each output quantity, a summary plot of the results is constructed. For example, Figure 1 compares the measured and predicted target temperatures (A "target" could be anything in the compartment that might heat up due to the fire). If a particular prediction and measurement are the same, the resulting point falls on the solid diagonal line. The longer-dashed off-diagonal lines indicate the experimental uncertainty. Roughly speaking, points within the longer dashed lines are said to be "within experimental uncertainty," and in such cases it is not possible to further quantify the accuracy of the prediction. Points falling outside the experimental uncertainty bounds cannot be said to be free of model uncertainty. To better make use of results such as these, two statistical parameters are calculated for each model and each predicted quantity. The first parameter, δ, is the *bias factor*. It indicates the extent to which the model, on average, under or over-predicts the measurements of a given quantity. For example, the bias factor for the data shown in Figure 1 is 1.02. This means that the model has been shown to slightly over-estimate target temperatures by 2 %, on average, and this is shown graphically by the red dash-dot line just above the diagonal. The second statistic is the relative standard deviation of the model, $\tilde{\sigma}_M$, and the experiments, $\tilde{\sigma}_E$. These indicate the uncertainty or degree of "scatter" of the model and the experiments, respectively. Referring again to Figure 1, there are two sets of off-diagonal lines. The first set, shown as long-dashed black lines, indicate the experimental uncertainty. The slopes of these lines are $1 \pm 2\tilde{\sigma}_E$ i.e. the 95% confidence intervals. The second set of off-diagonal lines, shown as short-dashed red lines, indicates the model uncertainty. The slopes of these lines are $\delta \pm 2\tilde{\sigma}_M$. If the model is as accurate as the measurements against which it is compared, the two sets of off-diagonal lines would merge. The extent to which the data scatters outside of the experimental bounds is an indication of the degree of model uncertainty.

The derivation of the relevant uncertainty statistics has previously been presented by McGrattan and Toman (2011), and it is summarized here. The calculation of δ and $\tilde{\sigma}_M$ uses this set of measured and predicted values, along with an estimate of the experimental uncertainty. The purpose of the calculation is to "subtract off," in a statistical sense, the experimental uncertainty so that the model uncertainty can be estimated. Before describing the calculation, a few assumptions must be made:

1. The experimental measurements are assumed to be unbiased, and their uncertainty is assumed to be normally distributed with a constant relative standard deviation, $\tilde{\sigma}_E$ (that is, the standard deviation as a fraction of the measured value). Table 1 provides estimates of relative experimental uncertainties for the quantities of interest, determined in NUREG-1824 (EPRI 1011999).

2. The model error is assumed to be normally distributed about the predicted value divided by a bias factor, δ. The relative standard deviation of the distribution is denoted as $\tilde{\sigma}_M$.

The computation of the estimated bias and scatter associated with model error proceeds as follows. Given a set of n experimental measurements, E_i, and a corresponding set of model predictions, M_i, compute the following:

$$\overline{\ln(M/E)} = \frac{1}{n}\sum_{i=1}^{n} \ln(M_i/E_i) \quad (1)$$

The standard deviation of the model error, $\tilde{\sigma}_M$, can be computed from the following equation:

$$\sqrt{\tilde{\sigma}_M^2 + \tilde{\sigma}_E^2} \cong \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}\left[\ln(M_i/E_i) - \overline{\ln(M/E)}\right]^2} \quad (2)$$

The bias factor is:

$$\delta = \exp\left(\overline{\ln(M/E)} + \frac{\tilde{\sigma}_M^2 - \tilde{\sigma}_E^2}{2}\right) \quad (3)$$

For a given model prediction, M, the "true" value of the quantity of interest is assumed to be a normally distributed random variable with a mean $\mu = M/\delta$ and a standard deviation of $\sigma = \tilde{\sigma}_M(M/\delta)$.

Using these values, the probability of exceeding a critical value, x_c, is:

$$P(x > x_c) = \frac{1}{2}\operatorname{erfc}\left(\frac{x_c - \mu}{\sigma\sqrt{2}}\right) \quad (4)$$

Note that the *complimentary error function* is defined as follows:

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^{\infty} e^{-t^2}\, dt \quad (5)$$

It is a standard function in mathematical or spread sheet programs like Microsoft Excel[1].

There are a few issues to consider when using this procedure:

1. All values need to be positive, and each value needs to be expressed as an increase over its ambient value. For example, the oxygen concentration should be expressed as a positive number (i.e., the decrease in concentration below its ambient value).

2. If the measurement uncertainty is over-estimated, the model error will be under-estimated. If the model error is less than the experimental uncertainty, the latter should be reevaluated. The model cannot be shown to have less error than the uncertainty of the experiment with which it is compared.

3. The procedure assumes that the quantity $\ln(M/E)$ is normally distributed. This is not necessarily true, especially in cases where there are an insufficient number of points in the sample. Figure 2 provides two examples in which the normality of the validation data is tested[2]. In cases where the data is not normally distributed, only the bias is reported.

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[1] Excel 2007 does not evaluate $\operatorname{erfc}(x)$ for negative values of x, even though the function is defined for all real x. In such cases, use the identity $\operatorname{erfc}(-x) = 2 - \operatorname{erfc}(x)$.

[2] The Kolmogorov-Smirnov test for normality has been applied using the software package SigmaPlot®10, Systat Software, Inc. The default P value of 0.05 was used.

Table 1. Experimental uncertainty of the experiments performed as part of the validation study in NUREG-1824(EPRI 1011999)

Quantity	$2\tilde{\sigma}_E$
HGL Temperature Rise	0.14
HGL Depth	0.13
Ceiling Jet Temperature Rise	0.16
Plume Temperature Rise	0.14
Gas Concentration	0.09
Smoke Concentration	0.33
Pressure (no forced ventilation)	0.40
Pressure (with forced ventilation)	0.80
Heat Flux	0.20
Surface or Target Temperature	0.14

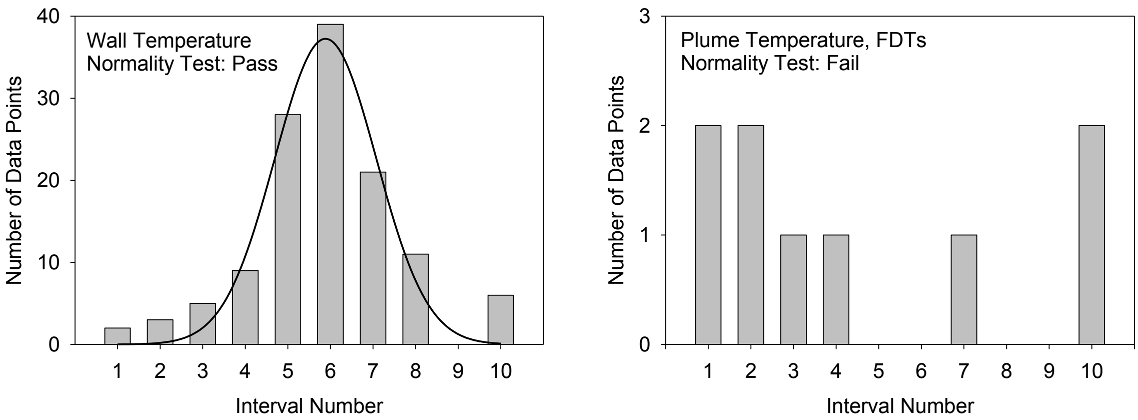

Figure 2. Two examples demonstrating how the validation data is tested for normality.

4. VALIDATION RESULTS

4.1 Applicability

The use of fire models to support fire protection decision making requires a good understanding of their limitations and predictive capabilities. NFPA 805 (NFPA, 2001) states that fire models shall only be applied within the limitations of the given model and shall be verified and validated. To support risk-informed/performance-based fire protection and implementation of the voluntary rule that adopts NFPA 805 as an RI/PB alternative, the NRC RES and EPRI conducted a collaborative project for the V&V of the five selected fire models. The results of this project were documented in NUREG-1824 (EPRI 1011999), *Verification and Validation of Selected Fire Models for Nuclear Power Plant Applications*.

Twenty-six full-scale fire experiments from six different test series were used to evaluate the models' ability to estimate thirteen quantities of interest for fire scenarios that were judged to be typical of those that might occur in a nuclear power plant. Each series represented a typical fire scenario (for example, a fire in a switchgear room or turbine hall); however, the test parameters could not encompass every possible NPP fire scenario. Five fire models were selected for the study, based on the fact that they are commonly used in fire analyses of nuclear plants in the U.S. Two of the models consist of simplified engineering correlations, two are "zone" models, and one is a CFD model (FDS).

To better understand the range of applicability of the validation study, Table 2 lists various normalized parameters that may be used to compare NPP fire scenarios with the validation experiments. These parameters express, for instance, the size of the fire relative to the size of the room, or the relative distance from the fire to critical equipment. This information is important because typical fire models are not designed for fires that are very small or very large in relation to the volume of the compartment or the ceiling height. For a given set of experiments and NPP fire scenarios, the user can calculate the relevant normalized parameters. These parameters will either be inside, outside, or on the margin of the validation parameter space. Consider each case in turn:

- If the parameters fall within the ranges that were evaluated in the validation study, then the results of the study can be referenced directly.
- If only some of the parameters fall within the range of the study, additional justification is necessary. This is a common occurrence because realistic fire scenarios involve a variety of fire phenomena, some of which are easier to estimate than others. A case in point is the burning of electrical cabinets and cables. NUREG-1824 (EPRI 1011999) does not address these fires directly, even though some of the experiments used in the study were intended as mock-ups of control or switchgear room fires. For scenarios involving these kinds of fires, the heat release rates are often taken from experiments rather than predicted by a model. It has been shown, in NUREG-1824 (EPRI 1011999) and other validation studies, that the models can estimate the transport of smoke and heat with varying degrees of accuracy, but they have not been shown (at least not in NUREG-1824 (EPRI 1011999)) to estimate the details of the fire's ignition and growth. While this does not eliminate the models from the analysis, it still restricts their applicability to only some of the phenomena.
- If the parameters fall outside the range of the study, then a validation determination cannot be made based on the results from the study. The modeler needs to provide independent justification for using the particular model. For example, none of the experiments considered in NUREG-1824 (EPRI 1011999) were under-ventilated. However, several of the models have been independently compared to under-ventilated test data, and the results have been documented either in the literature or in the model documentation. As another example, suppose that the selected model uses a plume, ceiling jet, or flame height correlation outside the parameter space of NUREG-1824 (EPRI 1011999) but still within the parameter space for which the correlation was originally developed. In such cases, appropriate references are needed to demonstrate that the correlation is still appropriate even if not explicitly validated in NUREG-1824 (EPRI 1011999).

4.2 Validation example

One example of the validation results is given to illustrate the calculation of uncertainty metrics. However, as these results depend on the exact code version used, these results shown in this presentation should not be used as reference for FDS validity.

Probably the most commonly used output quantity of a fire simulation is the temperature of the hot gas layer inside the compartment. The FDS Version 5 validation document (McGrattan *et al.* 2007) presents predictions for several test series. A summary of the predicted hot gas layer temperatures for five test series is given in Figure 3. The bias of the predictions is 0.98 and relative standard deviation is 0.05. Using the above-mentioned example, we want to know the probability that a critical temperature of 320 °C is actually reached if the predicted upper layer temperature is 300 °C and ambient temperature is 20 °C. Using equation (4)

$$P(T > 320) = \frac{1}{2}\mathrm{erfc}\left(\frac{320 - \left(20 + \frac{280}{0.98}\right)}{\left(0.05\,\frac{280}{0.98}\right)\sqrt{2}}\right) \approx 0.08 \tag{6}$$

This means that there is a 8 % probability for reaching the critical temperature, assuming the model input parameters are not subject to uncertainty.

Table 2. Summary of Selected Normalized Parameters for Application of the Validation Results to NPP Fire Scenarios (NUREG-1824/EPRI 1011999, 2007)

Quantity	**Normalized Parameter**	**General Guidance**	**Validation Range**
Fire Froude Number	$\dot{Q}^* = \frac{\dot{Q}}{\rho_\infty c_p T_\infty D^2 \sqrt{gD}}$	Ratio of characteristic velocities. A typical accidental fire has a Froude number of order 1. Momentum-driven fire plumes, like jet flares, have relatively high values. Buoyancy-driven fire plumes have relatively low values.	0.4 – 2.4
Flame Length Ratio	$\frac{H_f + L_f}{H_c}$ $\frac{L_f}{D} = 3.7\,\dot{Q}^{*2/5} - 1.02$	A convenient parameter for expressing the "size" of the fire relative to the height of the compartment. A value of 1 means that the flames reach the ceiling.	0.2 – 1.0
Ceiling Jet Distance Ratio	$\frac{r_{\mathrm{cj}}}{H}$	Ceiling jet temperature and velocity correlations use this ratio to express the horizontal distance from target to plume.	1.2 – 1.7
Equivalence Ratio	$\varphi = \frac{\dot{Q}}{\Delta H_{O_2} \dot{m}_{O_2}}$ $\dot{m}_{O_2} = \begin{cases} 0.23 \times \frac{1}{2} A_0 \sqrt{H_0} & \text{(Natural)} \\ 0.23\,\rho_\infty \dot{V} & \text{(Mechanical)} \end{cases}$	The equivalence ratio relates the energy release rate of the fire to the energy release that can be supported by the mass flow rate of oxygen into the compartment, $\dot{m}_{O_2}$. The fire is considered over or under-ventilated based on whether φ is less than or greater than 1, respectively.	0.04 – 0.6
Compartment Aspect Ratio	L/H or W/H	This parameter indicates the general shape of the compartment.	0.6 – 5.7
Radial Distance Ratio	$\frac{r}{D}$	This ratio is the relative distance from a target to the fire. It is important when calculating the radiative heat flux.	2.2 – 5.7

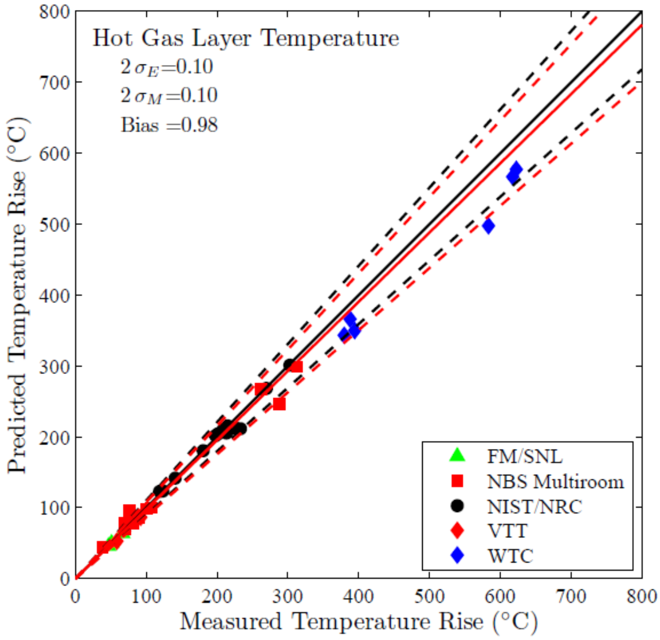

Figure 3.Summary of hot gas layer temperature predictions for five test series.

5. CONCLUSION

The presentation summarizes a procedure for developing and maintaining an open-source fire model that is used as part of a performance-based, risk-informed regulatory framework. Many of the techniques have traditionally been used within the fire protection engineering community, but to date have not been documented in a way that is necessary to maintain confidence in the models. A benefit of the procedure is that it places a relatively small burden on the end user in presenting the uncertainty of the model calculations. There is no need for an extensive statistical analysis of the model results, and because of this, it is hoped that these procedures will become widely adopted. The procedure also helps the regulator better define for what scenarios the model validation is applicable. Also, the fact that the model results are presented as probabilitues rather than single values promotes their use in the overall fire PRA.

Nomenclature

A	area
A_o	opening area
A_T	surface area of enclosure boundary
c_p	specific heat, gas, constant pressure
D	fire diameter
g	acceleration of gravity
h_k	heat transfer coefficient
H, H_c	ceiling height
H_f	height of base of fire above floor
H_o	opening height
L	compartment length
L_f	flame height
$\dot{m}$	mass flow rate
P	probability
$\dot{Q}$	heat release rate
$\dot{Q}^*$	fire Froude number
r	radial distance
r_{cj}	ceiling jet distance
t	time
T	temperature

$\dot{V}$	volume flow rate
W	compartment width

Greek:

δ	model bias factor
ΔH	heat of combustion
φ	equivalence ratio
ρ	density
$\tilde{\sigma}_E$	relative standard deviation, experiment
$\tilde{\sigma}_M$	relative standard deviation, model

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