

## CFD-FEA SIMULATION FRAMEWORK FOR COMPOSITE STRUCTURES IN FIRE

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**Keywords:** fire simulation, polymer matrix composite, computational fluid dynamics, finite element analysis

### Abstract

*Virtual fire testing could serve to improve the cost-efficiency of developing new composite materials for transport sector applications. Here, we present a simulation framework for the fire-response of polymer matrix composites, based on sequential and one-directional coupling of existing software tools. The open-source code Fire Dynamics Simulator is used to model the fire environment, including the heating and thermal decomposition of involved materials. The fire simulation is coupled with a finite element analysis, which is used to model the degradation of material properties, as well as the consequent reduction in load-bearing capacity and the actual mechanical response. The supported finite element analysis software include ABAQUS and ANSYS. Besides enabling virtual fire testing, the framework is suitable for larger scale simulations of onboard fires in e.g. aircraft, trains and ships.*

### 1. Introduction

Poor fire performance is one of the biggest factors limiting the use of lightweight polymer matrix composites in transport sector applications. Problems arise at elevated temperatures, where softening and decomposition of the polymer matrix results in the degradation of mechanical properties and the production of smoke and toxic or flammable gases. If novel composite materials are to be introduced to practical applications, their fire behaviour has to be assessed through testing. However, as fire testing tends to be expensive, significant savings could be obtained if it were possible to perform virtual fire tests as a routine part of product development. A simulation framework suitable for the virtual tests would also enable the advanced simulation of onboard fires in e.g. aircraft, trains and ships, extrapolating beyond the scope of standard tests.

Virtual fire testing requires multi-field simulation capabilities. This includes models for the heating and decomposition of combustible materials, evolution of smoke and toxic products, flame spread, degradation of load-bearing capacity and the mechanical response of structures. Presently available simulation tools are capable of describing the aforementioned physical and chemical phenomena. However, these capabilities are spread among distinct software which are, in general, not interoperable. A practical fire-structure simulation would require either the integration of the relevant sub-models into a single piece of software, or coupling of existing software developed for the specific tasks.

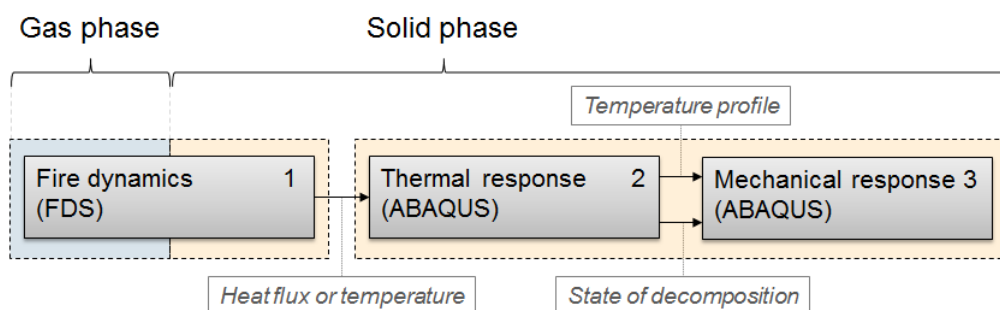
In this paper, we present a multi-field simulation framework for the fire-response of polymer matrix composites. The framework is based on coupling existing software for Computational Fluid Dynamics (CFD) and Finite Element Analysis (FEA). The open-source CFD-software Fire Dynamics Simulator (FDS) [1] is used to model the fire environment, including the heating and thermal decomposition (i.e. pyrolysis) of involved materials. The fire simulation is coupled with an FEA analysis which is used to model the degradation of material properties, as well as the consequent reduction in load-bearing capacity and the mechanical response. The commercial software ABAQUS and ANSYS can be used for the FEA-analysis. A coupling tool called FDS2FEM [2] forms an essential part of the framework in providing transfer of time-dependent thermal boundary conditions between the simulation codes.

Besides the software implementation, the framework relies on small-scale experiments to parametrize the material models used in both the CFD and FEA analyses. The employed experimental techniques include Thermogravimetric Analysis (TGA), Differential Scanning Calorimetry (DSC) and cone calorimetry for the thermal modelling, and additionally Dynamic Mechanical Thermal Analysis (DMTA) and standard tensile testing for the mechanical modelling. For the pyrolysis models, a parameter estimation technique employing Genetic Algorithms (GA) [3] is used to derive the parameter values from experimental data.

## 2. Simulation framework for fire-structure analysis

### 2.1. Overview of the software implementation

The proposed approach to fire-structure analysis is based on software co-operation. Modelling of the fire environment, which in itself is a multi-field simulation problem (see e.g. [1]), is handled by FDS—an established software tool in the field of fire safety engineering. As FDS does not have a sub-model for the thermal-mechanical response of solids, either the FEA-software ABAQUS or ANSYS is used to supplement its capabilities. This is achieved by sequential and one-directional thermal boundary condition transfer between the associated software. Being sequential and one-directional means that the fire simulation is completed before the thermal-mechanical analysis is initiated. It also means that there is no feedback from the latter to the former. A schematic diagram of the coupling approach is shown in Figure 1. An overview of the software implementation is given in the remainder of this chapter.



**Figure 1.** Schematic diagram of a sequentially coupled fire-structure analysis. Thermal exposure to surfaces is extracted from the fire dynamics simulation and used as a time-dependent boundary condition in a subsequent thermal-mechanical analysis.

## *2.2. Simulation of fire dynamics*

Running a fire-structure analysis within the proposed framework begins with the simulation of fire dynamics. This is done using the open-source software FDS. FDS is a CFD-model of fire-driven fluid flow that incorporates coupled sub-models for inter alia hydrodynamics, gas phase chemical reactions, radiation transport and solid phase heat conduction and pyrolysis. Detailed descriptions of the mathematical models and their numerical implementation can be found in the FDS Technical Reference Guide [1]. As a CFD-solver, FDS has the distinctive feature of being confined to rectilinear meshes. This imposes some restrictions on the representation of structures with curved shapes, often present in composite applications.

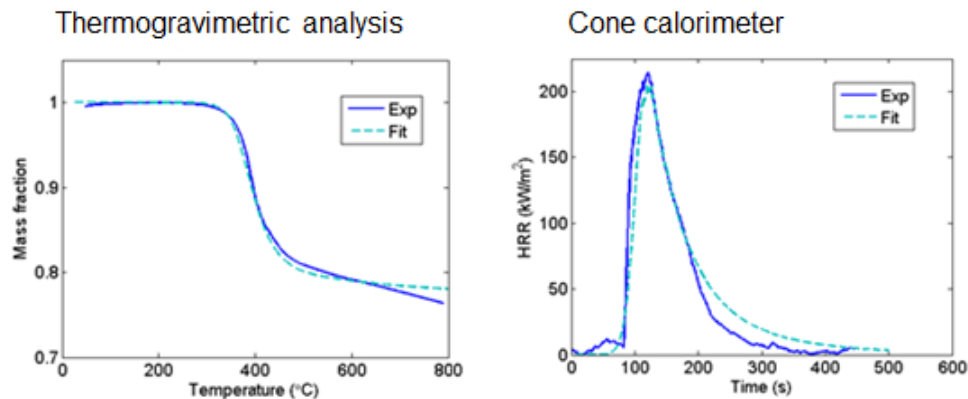
While all of the above mentioned physics and chemistry sub-models are necessary for a viable fire simulation, the solid phase heat conduction and pyrolysis models play a central role in the simulation of polymer matrix composites and their reaction to fire. Proper use and parametrization of these models is a determining factor for the reliability of the simulation framework as a whole.

In FDS, solid surfaces are described as consisting of one or more layers, which in turn are composed of one or more material components. Each material component can undergo multiple thermal degradation reactions, and each of these reactions can produce multiple gas and solid phase products. In order to predict flame spread on surfaces, pyrolysis of the involved materials must be taken into account. Pyrolysis means thermal decomposition in the absence of oxygen, but also oxidative solid phase reactions can be involved. When a polymeric material decomposes, it releases different gaseous products, of which some may burn in air. This produces heat, which accelerates the thermal degradation even further.

In the solid phase model, the mass loss and gas release of pyrolysis are coupled with the temperature of the material. As mentioned before, each material component may have several degradation reactions that occur either simultaneously or consecutively. The reaction rate depends on temperature and three reaction-specific parameters (i.e. kinetic parameters). Heat conduction inside the material is calculated in one dimension, in the direction of the surface normal. The heat conduction depends on material density, thermal conductivity and specific heat capacity, while radiation and convection from the gas phase define the thermal boundary condition on the exposed surface. A detailed treatment of the pyrolysis model can be found in the FDS Technical Reference Guide [1].

All of the parameters needed by the solid phase model cannot be measured directly. These include the kinetic parameters that are used to describe pyrolysis, and which need to be estimated from small and bench scale experiments by fitting simulated results to experimental ones. The proposed simulation framework incorporates a parameter estimation technique that employs GA to derive the kinetic parameters from a TGA experiment. TGA, a small-scale technique, measures the mass of a sample as a function of temperature. For bench scale, cone calorimeter results are used. In cone calorimetry, a sample with surface area  $10\text{ cm} \times 10\text{ cm}$  is placed under a cone-shaped heater with radiant heat fluxes typically in the range  $25\text{--}75\text{ kW/m}^2$ . The released gases are ignited with a spark igniter. During the experiment, sample

mass and heat release rate are measured, among others. The idea of the parameter estimation process is shown in Figure 2. A detailed treatment can be found in reference [3].

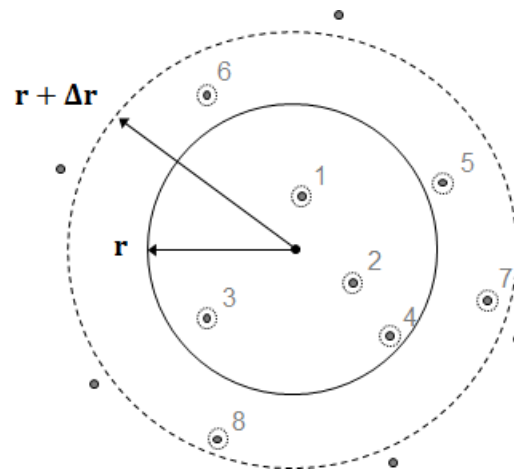


**Figure 2.** Idea of the parameter estimation process. On the left is a temperature-mass curve from a TGA experiment and a corresponding FDS simulation with relevant model parameters adjusted for a close fit. On the right is a similar treatment of a cone calorimeter experiment. The employed material is a fibre-reinforced polymer matrix composite.

### 2.3. Coupling the fire and thermal-mechanical analyses

FDS enables the output of thermal loads on surfaces using various physical quantities. For the current work, the relevant quantities are surface temperature, net heat flux and adiabatic surface temperature (see e.g. [4]). The FDS output can be used as a boundary condition in a subsequent FEA analysis. However, there are two major obstacles to this that require the involvement of an external coupling tool. Firstly, the numerical data extracted from the fire simulation is not understood by the FEA software as such. It has to be converted to a format that can be read into the thermal-mechanical analysis. Secondly, the spatial and temporal discretizations of the fire and thermal-mechanical models tend to be different. In some cases, this might also be true for the geometric details of the models. Thus, a justifiable mapping is needed between the two representations.

To address the above mentioned issues, we have developed a coupling tool called FDS2FEM. It can be used to extract thermal boundary conditions from an FDS simulation, to transform the data between the FDS and FEA representations, and to output the resulting data in a format that can be read into a thermal-mechanical analysis. The data transformation, or mesh mapping, employs a simple nearest-neighbour scheme (Figure 3). Boundary condition value at each FEA node (i.e. target node) is defined by the values at one or more FDS nodes (i.e. source nodes) in its immediate neighbourhood. The target value is calculated as a distance-weighted average of the source values. The selection of source nodes can be based on a user-defined cut-off radius, user-defined number of nearest neighbours or both of the aforementioned. A more detailed description of the mesh mapping algorithm is given in reference [2]. FDS2FEM is implemented as a command-line tool for Linux and Windows operating systems. It employs a configuration file based user interface, as do the other associated software.



**Figure 3.** Principle of the nearest-neighbour mapping scheme. The black dot in the middle represents the target node and the gray dots represent the source nodes. The user-given radius  $r$  defines the immediate neighbourhood of the target node. The radius  $r + \Delta r$  is used to find close outliers. Source nodes encircled by a dashed line are chosen for distance-weighted averaging.

### 2.3. Simulation of thermal-mechanical response

The last step in the simulation framework is the thermal-mechanical analysis. For this purpose, two alternative FEA software are supported, namely ABAQUS and ANSYS, which are commercial products of Dassault Systèmes and ANSYS Inc., respectively. Both software offer a variety of tools for analysing composite structures under simultaneous thermal and mechanical loads. The following approach, which is specific to ABAQUS, is employed in the simulation framework. A similar thermal-mechanical model for ANSYS is still under development. Otherwise, integration of ANSYS into the simulation framework is already realized (thermal boundary condition transfer, analysis of non-combustible materials).

In principle, the thermal and mechanical analyses can be run concurrently. However, this kind of analysis is typically computationally expensive for structures of practical interest. In the chosen approach, the thermal and mechanical analyses are run sequentially. Given the thermal boundary condition from the fire simulation, a combined heat transfer and thermal degradation analysis is performed to calculate the temperature profile inside the composite, the state of pyrolysis of the resin and eventually the oxidation of the fibres. The thermal degradation model employs Arrhenius kinetics with a single stage reaction process, and is realized using a user-defined subroutine (HETVAL). The approach is based on a model proposed by Henderson [5].

After the thermal analysis, the temperature and residual resin content profiles are passed as input to a subsequent mechanical analysis. The mechanical analysis employs a transversely isotropic material description and temperature and residual resin content dependent elastic constants, which are realized using a user-defined subroutine (UMAT). Failure initiation is predicted using a three-dimensional set of failure criteria, based on Hashin's theory [6]. The model is applicable to composite materials with a unidirectional or quasi unidirectional (i.e. non-crimp fabrics) structure.

To minimise the number of experiments needed to parametrize the thermal and mechanical models, the material properties are measured at the scale of the constituents, and calculated at the ply scale using micromechanics—more precisely, the Halpin-Tsai model [7]. This approach is flexible, as multiple architectures can be investigated as long as micromechanical relations are available. However, micromechanical relationships are based on perfect geometries and do not take into account effects such as residual stresses induced during manufacturing.

### **3. Practical steps for virtual fire testing**

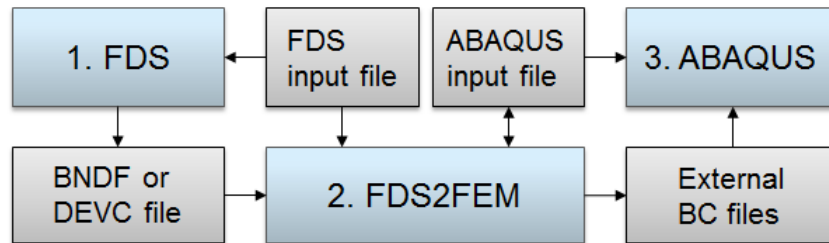
As a summary, we describe the practical steps for a fire-structure analysis within the proposed framework. The analysis can be e.g. a virtual version of a fire test, that is used to assess the time-to-failure of a composite structure under mechanical loading in a fire environment. The following description is written with this kind of application in mind.

Experimentally deduced material properties form the foundation of a viable analysis. These are used as input parameters to the material models. Depending on the level of detail used to describe the composite architecture, the parameters might refer to those of the composite as a whole, or to those of the constituent materials. Besides the geometry and architecture of the specimen, the initial density, specific heat capacity and thermal conductivity are needed for both the fire and thermal-mechanical models. Also, a description of thermal decomposition is needed in both models (kinetic parameters, heat of reaction, etc.). These parameters can be obtained from TGA, DSC and cone calorimeter experiments. Specific heat capacity can be obtained using e.g. DSC, and thermal conductivity using the transient plane source method. More information on how the thermal properties are deduced can be found in reference [3]. Parameters required by the mechanical analysis include temperature-dependent elastic modulus, coefficient of thermal expansion, Poisson's ratio and tensile strengths, among others. These can be obtained, apart from the coefficient of thermal expansion, from DMTA experiments and standard tensile testing in a climate chamber.

When the required material properties are available, the next step is the construction of the FDS and FEA models. For a typical mid-scale application, the FDS model describes a fire environment that consists of much more than just the composite specimen. Other possible components include burners, experimental frames, ventilation, measurement devices and, what is important, a sufficient gas-phase volume to capture relevant flow field phenomena. On the other hand, the FEA model typically consists of the composite specimen alone. In any case, the specimen has to be represented in both models with a similar shape and similar proportions. The coupling tool FDS2FEM imposes some further restrictions on the FDS and FEA input files. Specifically, the surfaces used for boundary condition exchange have to be marked.

In the next step, the fire simulation is run and user-requested output files are created. These are either ASCII-files that contain point measurement data (so-called DEVC files) or binary files that contain nodal data (so-called BDNF files). Thermal boundary conditions should be extracted only from relevant surfaces of the specimen. After the fire simulation, FDS2FEM is configured. The configuration file includes, among others, a set-up for the nearest-neighbour

mapping algorithm. When run, FDS2FEM generates a time-dependent boundary condition for each target node of the thermal-mechanical model. The boundary condition is written into the FEA input file and external data files using standard commands. After this, the two-step thermal-mechanical model is ready to be run. The process described above is summarized in Figure 4.



**Figure 4.** Outline of a fire-structure analysis from a software point of view. The order in which the programs are executed, is denoted. Data flow is indicated by the arrows.

#### 4. Conclusions

We have developed a simulation framework for fire-structure analysis, that is applicable for polymer matrix composites. The framework is based on sequential coupling of existing CFD and FEA software: FDS for the simulation of the fire environment and ABAQUS or ANSYS for thermal-mechanical analysis. It can be employed for the virtual testing of composite products and the fire safety assessment of their real applications. The coupling of fire and thermal-mechanical models is realized in a way that makes it relatively easy to prepare the models separately—even by different experts working for different companies. This kind of robustness is believed to promote the use of the framework for i.a. practical material development.

The most obvious limitation of the presented approach is that there is no feedback from the thermal-mechanical analysis to the fire simulation. Thus, the mechanical response of the involved structures can not affect the fire dynamics. This is not an issue as long as the deformations are minor, but if they become significant, the analysis has to be rejected for being clearly unphysical. Another inconvenience comes from the mapping algorithm. Since there is no single configuration that would work in all situations, there is a need for careful user-judgement every time a new FDS-FEA mapping is being done.

In the application of the developed framework, the estimation of the material model parameters constitutes a substantial amount of work for the user. Over the last few years, mathematical and software tools have been developed within the fire science community for the pyrolysis modelling, i.e. the thermal-chemical response of the solid materials. For the thermal-mechanical models, however, the mathematical methods are very much model dependent and general tools for determining the thermal-mechanical parameters are not available. Development of such tools would be needed to extend the use of the tools outside the research community.

Ongoing and future work on the presented simulation framework includes developing guidelines for proper use of the mesh mapping algorithm, as well as validation of the complete simulation framework against mid-scale experiments on newly developed polymer matrix composites. The experiments will consider both fire spread and mechanical failure.

## 5. Acknowledgments

Majority of this work has been carried out within the EU-project FIRE-RESIST (grant number 246037). Timo Korhonen and Merja Sippola from VTT Technical Research Centre of Finland are acknowledged for their contributions to the coupling tool FDS2FEM.

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