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Multiscale Analysis of Ceramic Matrix Composites under Extreme Temperatures

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Final Technical Report

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14. ABSTRACT
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FINAL REPORT

To: http://afosr.reports.sgizmo.com/s3/>

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Reporting Period: January 15, 2019 – January 14, 2020

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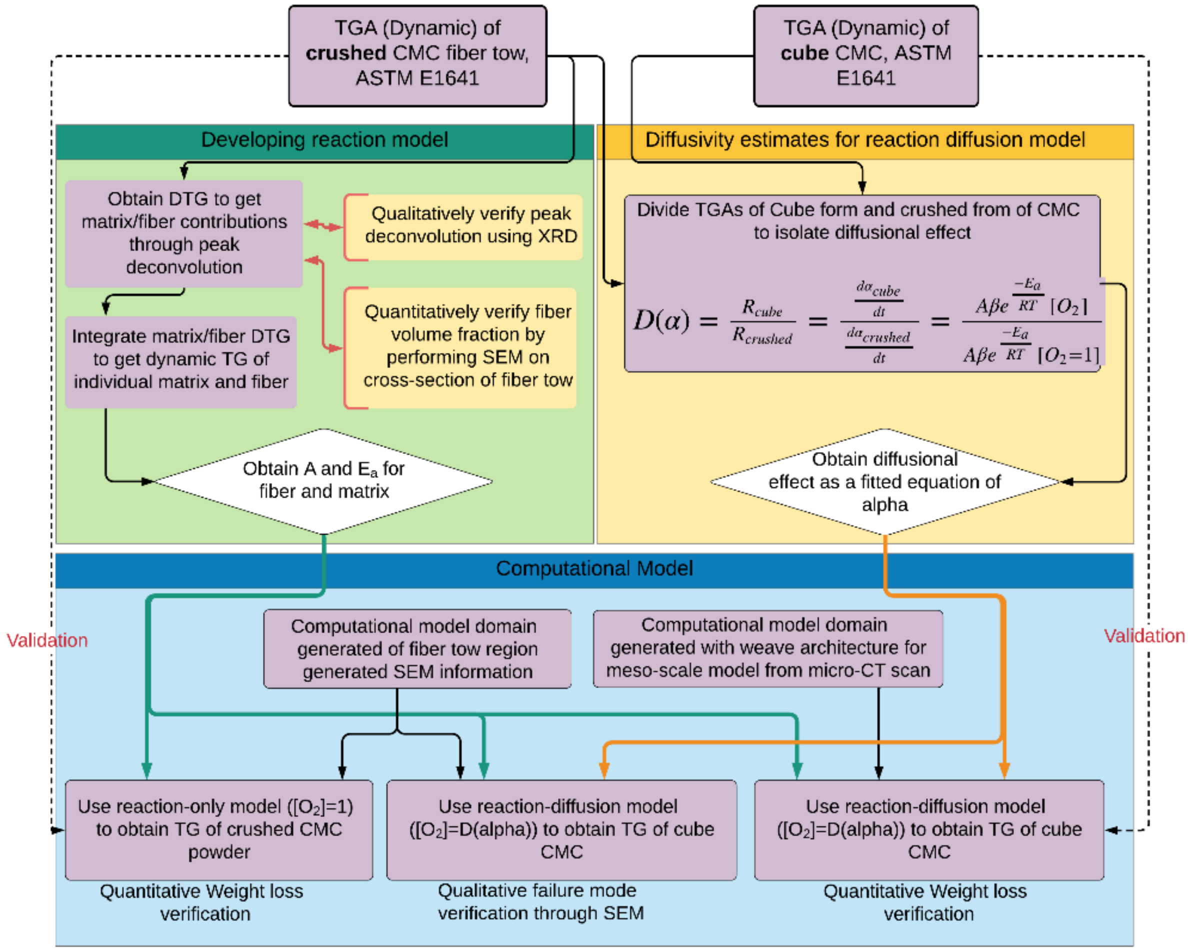

Figure 1. Overview of the integrated computational and experimental framework

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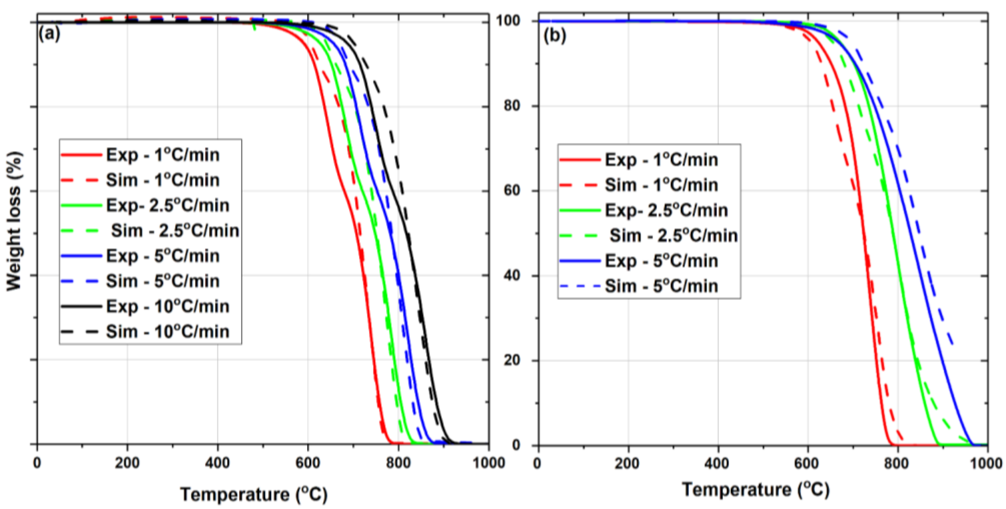

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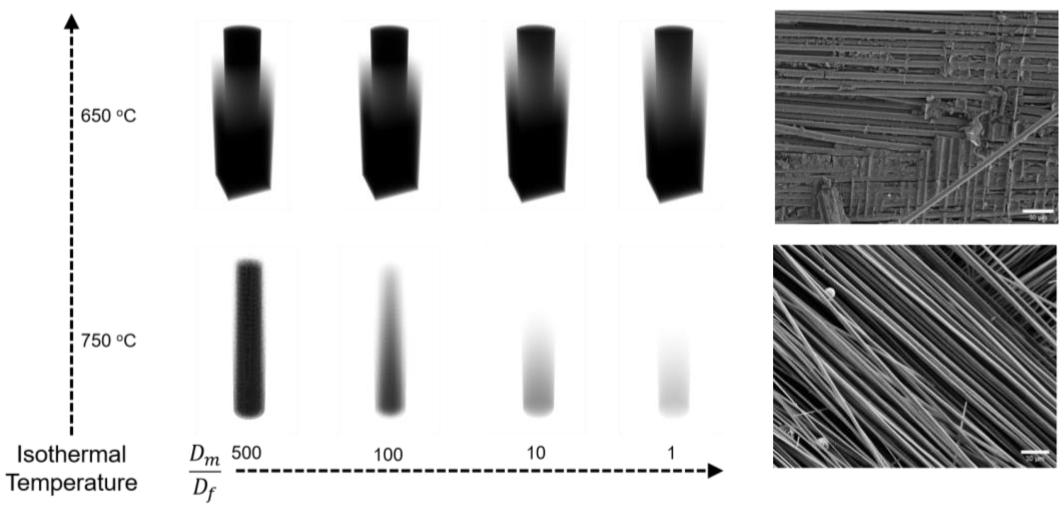

Figure 3. Microscale reaction-diffusion FEA prediction (Task I) was used to observe the qualitative degradation characteristics. In isothermal conditions at 650 $_{o}$C for 60 minutes, the matrix has not completely degraded in the computational model as also observed in SEM images. In isothermal conditions at 750 $_{o}$C for 60 minutes, complete degradation of the matrix is observed. (Task II).

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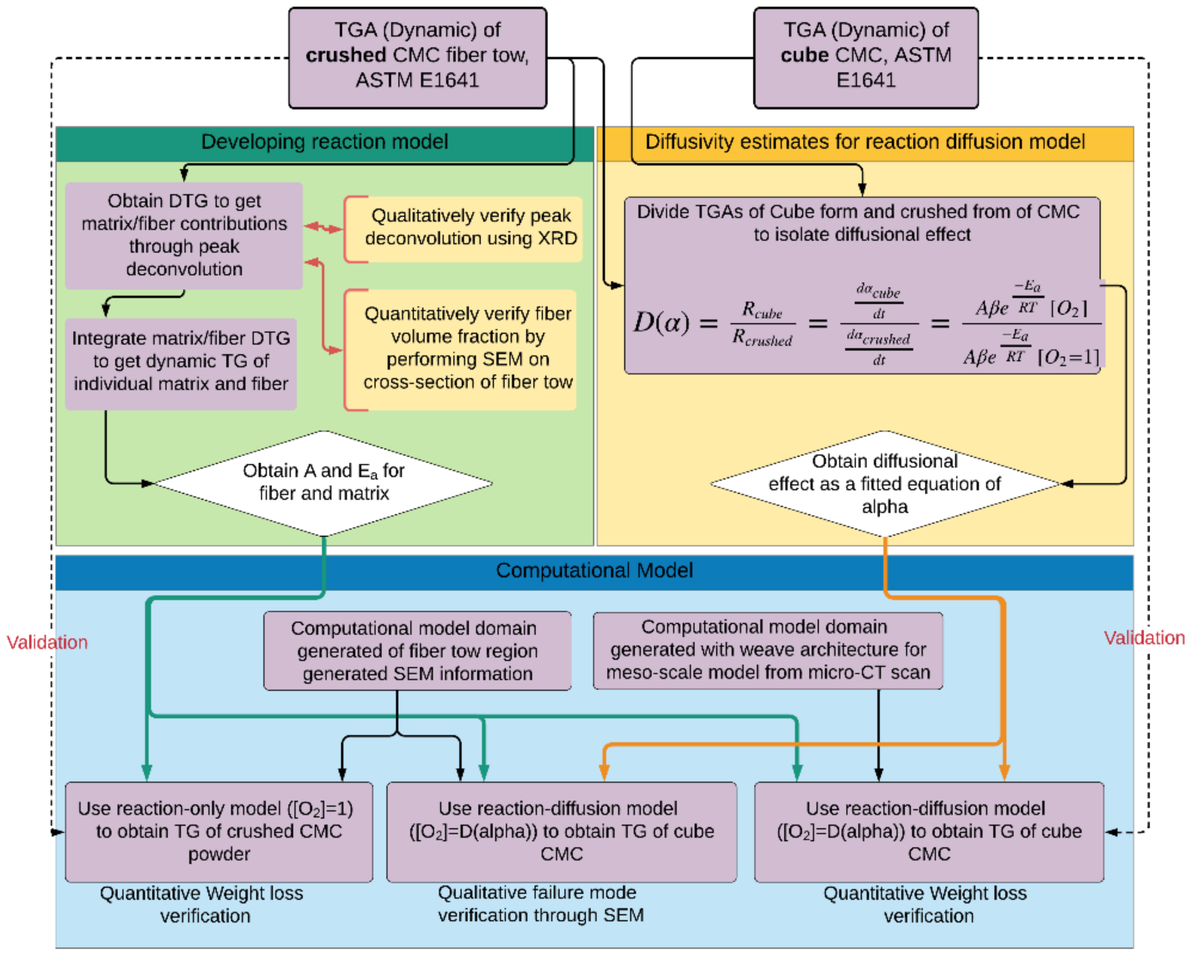

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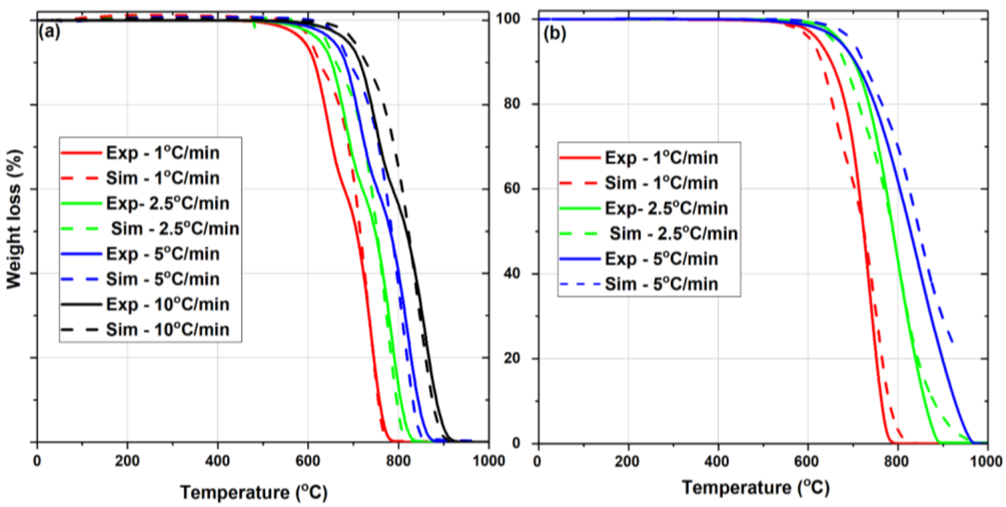

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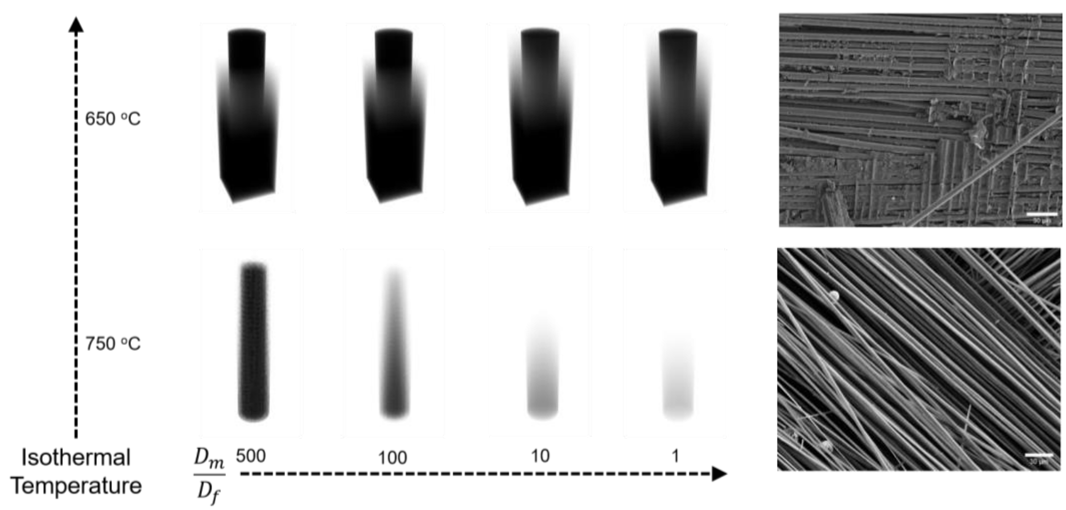

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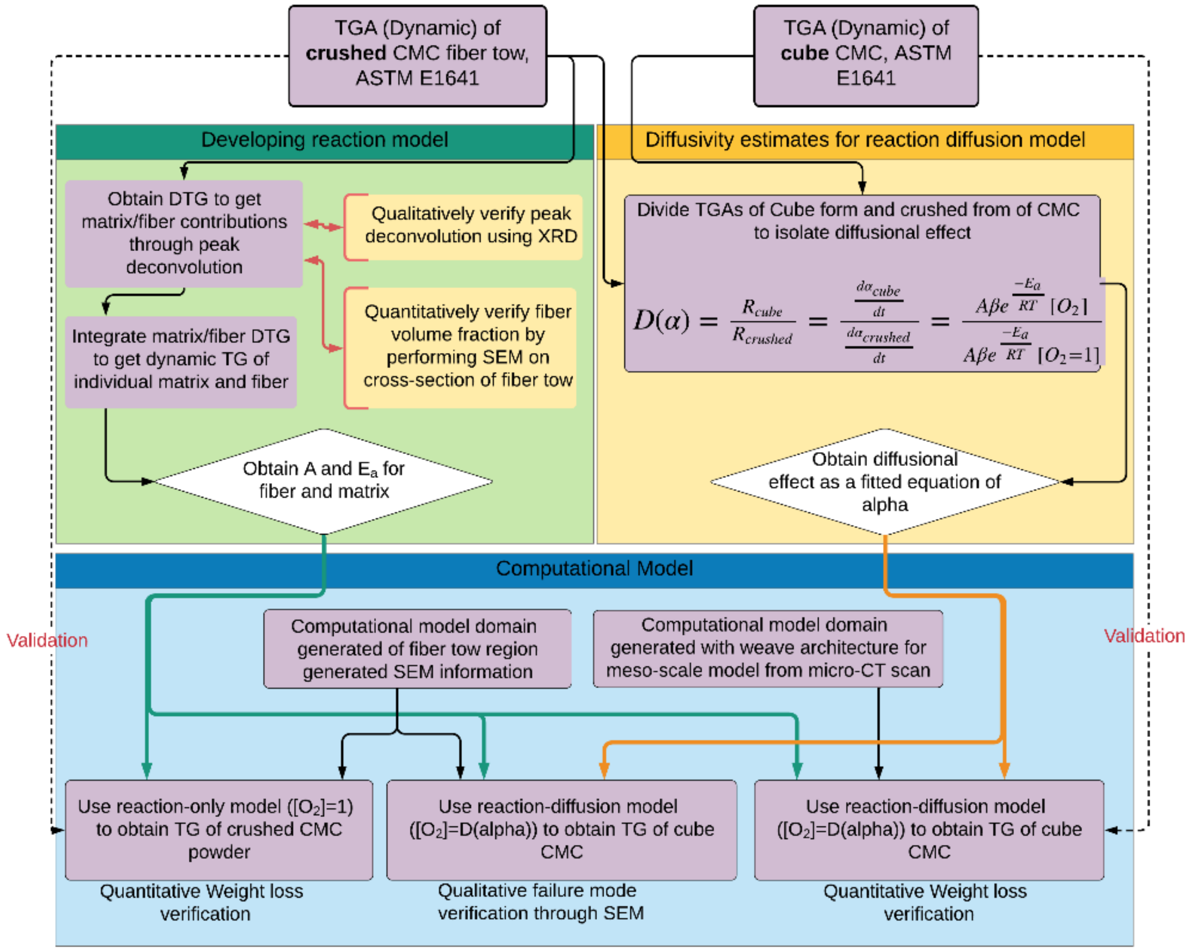

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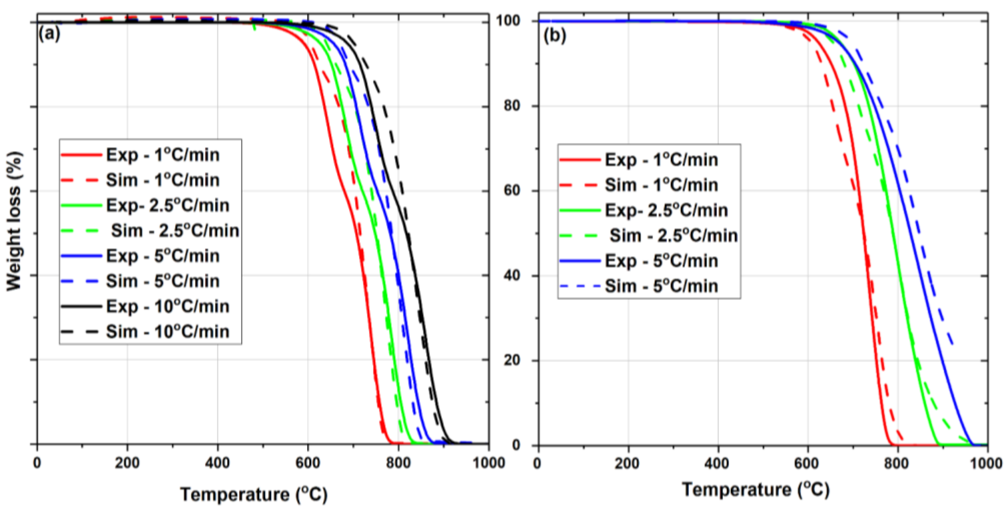

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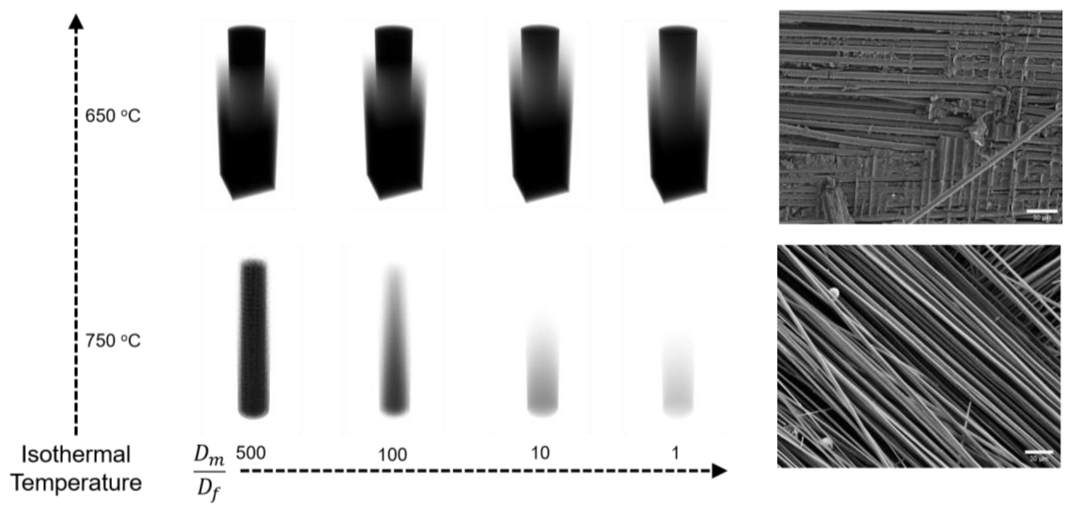

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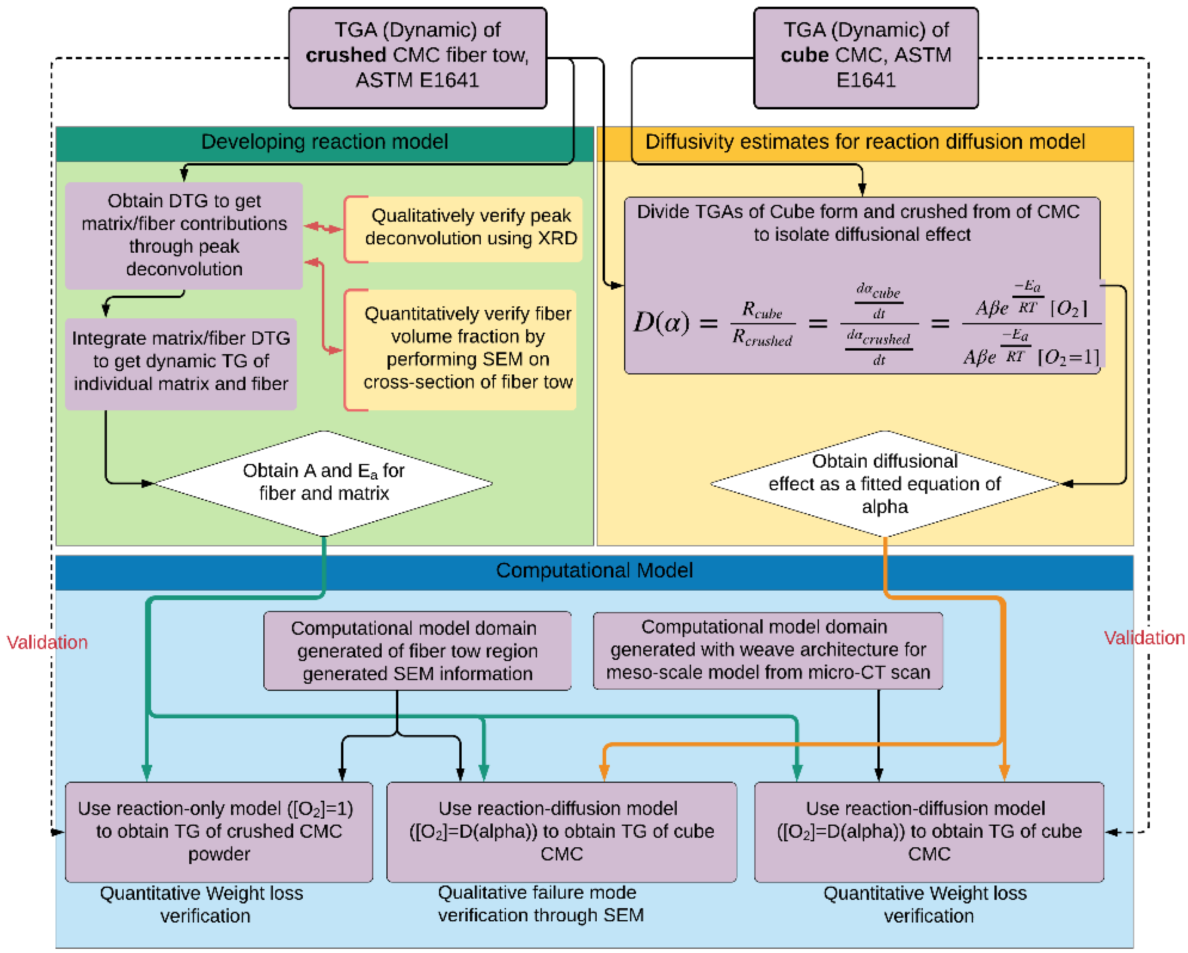

Figure 1. Overview of the integrated computational and experimental framework

Our integrated experimental and computational methodology is as follows _

1. Extract the matrix and fiber reaction constants from the weight loss curves of C/C composite (**Task II**)
2. Develop a coupled diffusion-reaction-thermal model (**Task I**)

3. Isolate the diffusion behavior to serve as input to the model (**Task II**)
4. Validate the model inputs and outputs through experiments (**Task I**)

This experimentally validated computational model was successfully developed to determine weight loss curves at the micro (fiber/matrix) and meso (tow/matrix) scale, and was experimentally validated at the micro and the macro scales. Also, this framework is capable of modeling degradation mechanisms at multiple length scales.

This research project generated one published paper and several presentations in different scientific conferences. The first paper, "***Multiscale and Multi-Physics Finite Element Modeling of Oxidation Degradation in C/C Ceramic Matrix Composites***," confirmed the good prediction between experimental and FEA simulation. TGA was performed under a specific environment, such as in the presence of oxygen and nitrogen mixture to simulate an oxidative environment, to establish the kinetics and diffusion parameters of C/C composites. This analysis was also used to determine the degradation mechanisms of C/C composite when exposed to this environment. The kinetic parameters involved with the degradation in C/C composites were measured using the Arrhenius equation, assuming the degradation behavior follows the Arrhenius type.

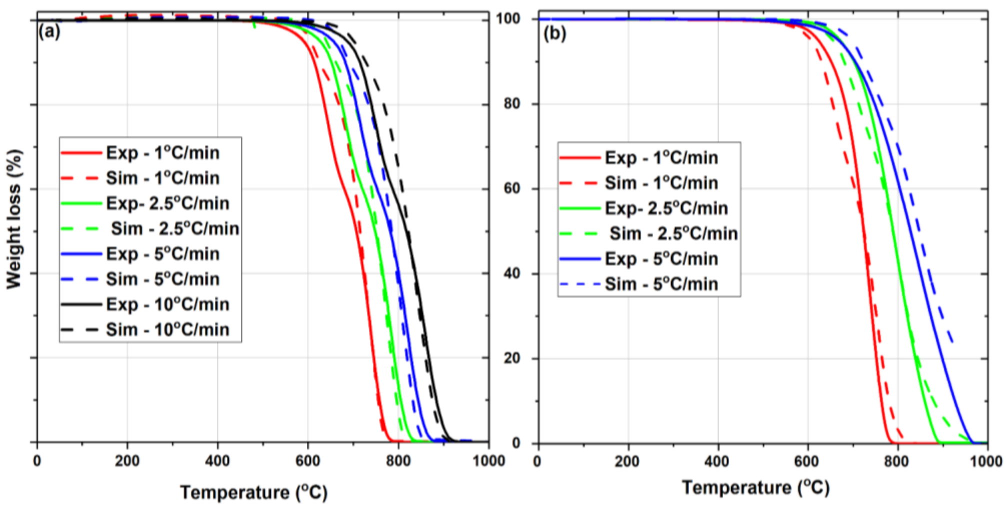

Figure 2. Thermogravimetric analysis (TGA) of (a) crushed C/C composite compared with FEA simulation based on reaction model for different heating rate (β) of 1oC/min,2.5oC/min, 5oC/min and 10oC/min, and (b) cube C/C composites compared with the reaction-diffusion model for different heating rate (β) of 1oC/min,2.5oC/min and 5oC/min.

In Figure 2, the summary of the experimental weight loss (**Task II**) percentage of crushed (Figure 2(a)) and cube (Figure 2(b)) C/C CMC obtained from TGA is presented in comparison with the FEA prediction (**Task I**). As seen from Figure 2(a), the prediction from the FEA based on the reaction model matched well with the experimental weight loss percentage with temperature. Additionally, the FEA predictions based on the reaction-diffusion model also matched well with the experimental weight-loss percentage with temperature as depicted in Figure 2 (b).

A second manuscript titled "***Oxidation degradation of C/C composites – A Multi-scale & Multi-physics finite element modeling framework***" is in prep (draft here), where the

FEA computational model uses the experimentally determined Arrhenius reactions kinetic parameters (activation energy, E, and pre-exponential factor, A) to predict weight loss curves. This will enable a designer to predict weight loss percentage using known temperature and exposure conditions. In addition to weight loss predictions, the degradation mechanism was also determined using microscale/mesoscale reaction-diffusion computational model. Unlike reaction parameters, estimating the diffusivity parameters of the matrix and fiber regions separately is not practical. Hence, a parametric study of ratio diffusivity of reactant gas (oxygen) into the matrix vs diffusivity into fiber was used to observe the degradation modes qualitatively. From this, it can be seen that at lower temperatures, such as at 650 $_{o}$C, when the matrix has not entirely vaporized, the ratio of matrix-to-fiber diffusivity is not as relevant in predicting degradation modes. However, at higher temperatures, like 750 $_{o}$C, the outcome is very sensitive to this ratio and becomes crucial in predicting the degradation mode. However, using this model, degradation modes such as fiber thinning and needle-like structure formation are obtained, as also confirmed by comparing with scanning electron microscope (SEM) images, as shown in Figure 3. Future work will involve stress induced crack formation and propagation under these oxidative environments.

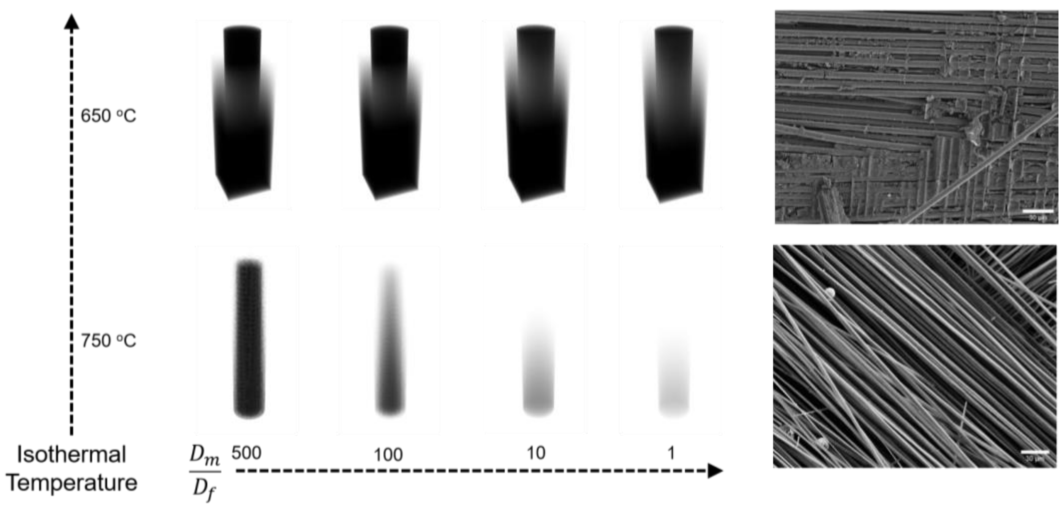

Figure 3. Microscale reaction-diffusion FEA prediction (Task I) was used to observe the qualitative degradation characteristics. In isothermal conditions at 650 $_{o}$C for 60 minutes, the matrix has not completely degraded in the computational model as also observed in SEM images. In isothermal conditions at 750 $_{o}$C for 60 minutes, complete degradation of the matrix is observed. (Task II).

FINAL REPORT

To: http://afosr.reports.sgizmo.com/s3/>

Subject: Final Report to Dr. Jaimie Tiley

Contract/Grant Title: **Multiscale Analysis of Ceramic Matrix Composites under Extreme Temperatures**

Contract/Grant #: FA9550-19-1-0003

Reporting Period: January 15, 2019 – January 14, 2020

Annual accomplishments (200 words max):

Carbon fiber reinforced Carbon matrix (C/C) composites have been shown to retain excellent thermal and mechanical properties at high temperatures in an inert atmosphere. However, these composites degrade rapidly at temperatures as low as 450◦C in oxidizing environments due to the conversion of solid carbon to gaseous oxides. An integrated experimental and computational approach was developed and implemented within this project to identify the thermo-chemical degradation of C/C composites. Here are some key accomplishments from this study:

1. A reaction-diffusion finite element model at multiple length scales was developed to determine degradation modes due to the oxidation of carbon-carbon ceramic matrix composites.
2. Fundamental kinetics and diffusion parameters were determined for carbon fibers and matrix by performing Thermogravimetric analysis (TGA) of crushed and cube C/C composites, which are used in the computational model as inputs.
3. The decomposition kinetics of individual constituents of a composite were determined by splitting that of a composite to obtain Arrhenius reaction rate constants.
4. The dependence of diffusion constants on the reaction state and the mode of degradation was established by employing the reaction-diffusion finite element model at the microscale.

Archival publications (published) during reporting period:

1. Vinay Damodaran, Pavana Prabhakar. "Multi-Physics Computational Modeling of High-Temperature Oxidation Damage in Ceramic Matrix Composites" presented at International Conference and Exposition on Advanced Ceramics and Composites (ICACC), Daytona Beach, Florida, 2019.
2. Vinay Damodaran, Muhammad Ali Imam, and Pavana Prabhakar. "Multiscale and Multi-Physics Finite Element Modeling of Oxidation Degradation in C/C Ceramic Matrix Composites." In Proceedings of the American Society for Composites—Thirty-fourth Technical Conference, Atlanta, 2019.

3. Muhammad Ali Imam, Vinay Damodaran, and Pavana Prabhakar. "Oxidation Kinetics of C/C Ceramic Matrix Composites Using Thermoravimetric Analysis" presented at Materials Science & Technology, Portland, Oregon, 2019.
4. Vinay Damodaran, Muhammad Ali Imam, and Pavana Prabhakar. Oxidation degradation modes of C/C composites – A Multi-scale & Multi-physics finite element modeling framework, (manuscript - *in prep*).

Changes in research objectives, if any: None

Changes in AFOSR program manager, if any: None

Extensions granted or milestones slipped, if any: None

Include any new discoveries, inventions or patent disclosures during this reporting period (if none, report none): None

Final Report for "Multiscale Analysis of Ceramic Matrix Composites under Extreme Temperatures"

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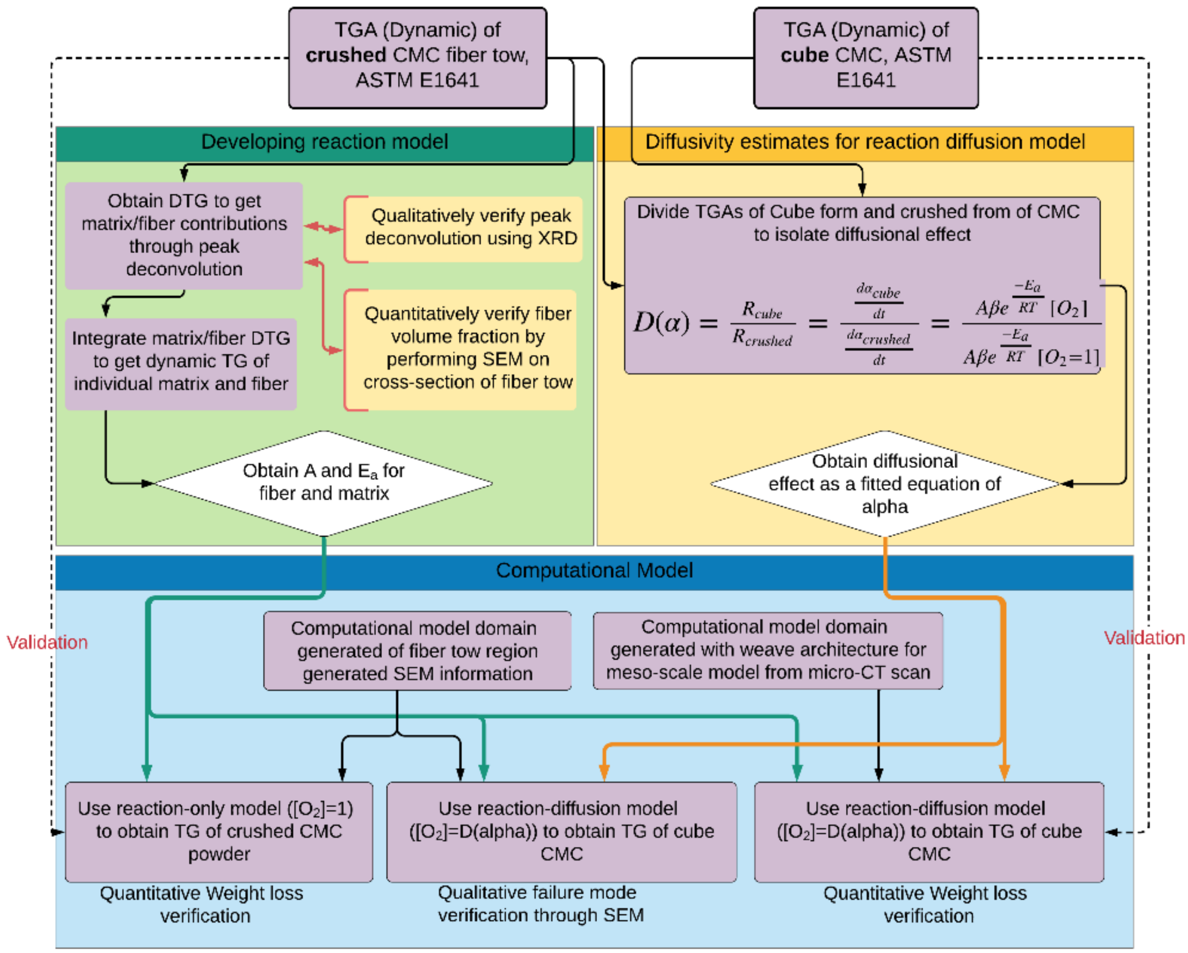

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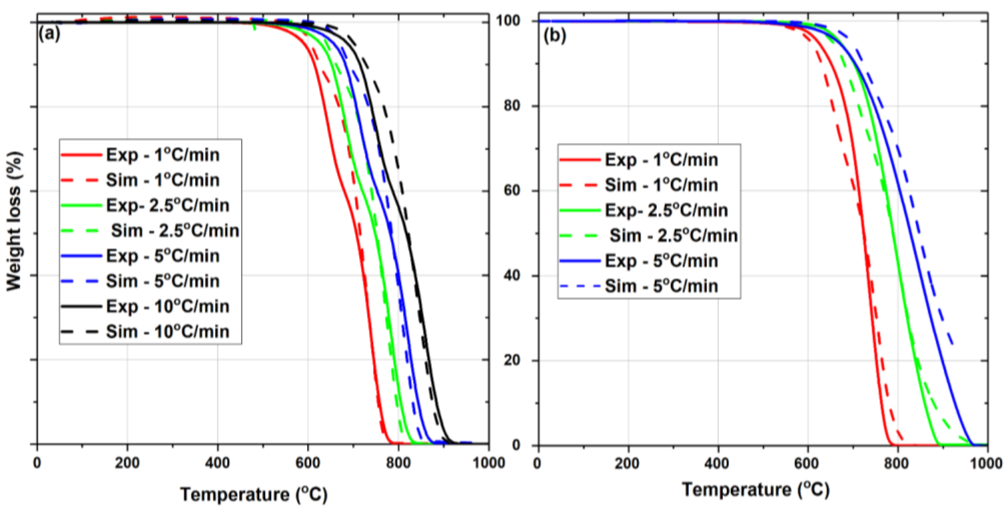

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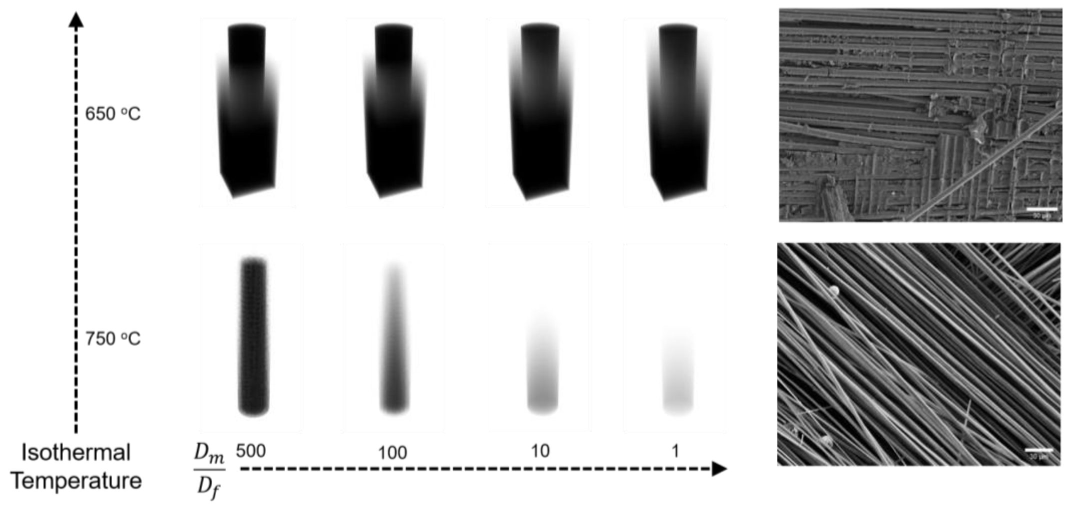

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