

# 탄소-탄소 복합재료의 제조 과정 중 탄화과정의 수치 해석에 관한 연구

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## NUMERICAL SIMULATION OF THE CARBONIZATION PROCESS IN THE MANUFACTURING OF CARBON-CARBON COMPOSITES

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**KEY WORDS :** Carbon-carbon composites, Carbonization, FEM (Finite Element Method), Structural Analysis

### ABSTRACT

A method for numerical simulation of the carbonization process in manufacturing of a carbon-carbon composite is developed. A general theory, which consists of analyses of heat and mass transfer together with stress and displacement predictions, is constructed. A homogeneous, single phase, isotropic material is selected and a computer program is developed for an arbitrary 2-dimensional geometry using FEM. Material properties are obtained through experiments and references, and are modeled effectively to serve the simulation purpose. The validity of the simulation is verified through several comparisons with experimental data, where close agreements are observed. Finally, examples of actual applications are considered to exhibit the capability and utilization of the code in process optimization.

### 1. Introduction

This study focuses on development of a method for numerical simulation of the carbonization for an arbitrary 2-dimensional geometry. To illustrate the methodology, simplification to a homogeneous, single phase, isotropic material is adapted as a beginning. Phenolic foam is adapted as the sample material to serve the purpose. Material characterization is introduced, followed by detail numerical analysis and discussion.

Modeling of carbonization is performed regarding heat and mass transfer and structural analysis. A computer code is developed to simulate carbonization for an arbitrary 2-dimensional geometry. Some practical cases are considered to illustrate effectiveness of simulation.

### 2. Material Characterization

#### Weight Loss Characteristics

TGA experiments were performed with Universal TA Instruments at CytecFiberite. The typical weight loss curve is plotted in Fig.1. Degree of conversion ( $\alpha$ ) was modeled with two different mechanisms, using methodology proposed by Nam and Seferis [1].

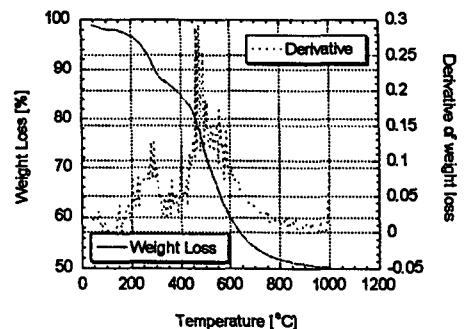


Fig. 1. Weight loss curve of phenolic foam from TGA

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### Gas Permeability

An experimental apparatus was built to measure the gas permeability of the foam. The permeability values are plotted versus sample porosity in Fig.2. Since the classic Kozeny-Carman equation is not valid in this case due to high porosity, a linear relation was assumed between porosity and permeability.

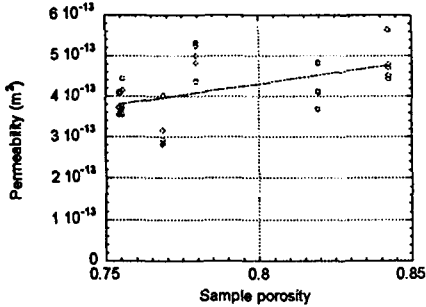


Fig.2. Results of permeability measurements

### Density and Porosity

The density and porosity of the foam was measured using a pycnometer for several samples with different degrees of carbonization. The results are given in Fig.3, and are assumed as functions of  $\alpha$ .

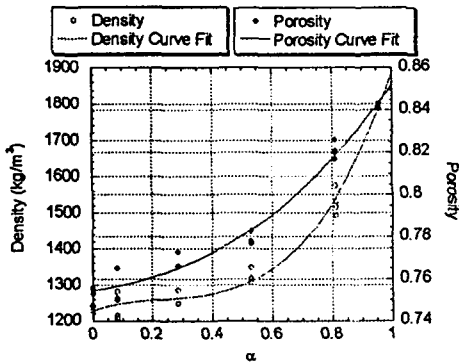


Fig.3. Density and porosity plotted versus  $\alpha$

### Shrinkage Modeling

Shrinkage is assumed as a function of  $\alpha$ , and the shrinkage of fresh foam and the sample carbonized to 400 °C are plotted against  $\alpha$  in Fig.4 (a). The coefficient of shrinkage shows the same trend with  $\alpha$  for both cases, as can be seen in Fig.4 (b). The curve fit model for the coefficient of shrinkage is used to evaluate actual shrinkage, as plotted in Fig.4 (a), which shows close agreements with experimental data.

### Thermal Expansion

Thermal expansion of carbonized foam was measured. Expansion coefficient of phenolic foam was substituted with the data given by Mottram et al [2].

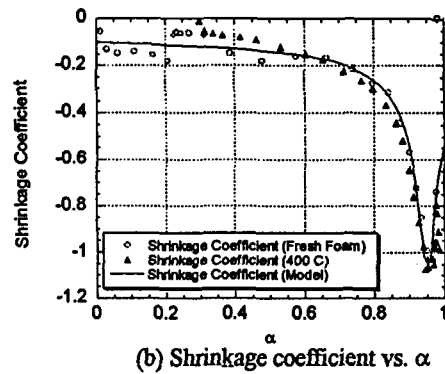
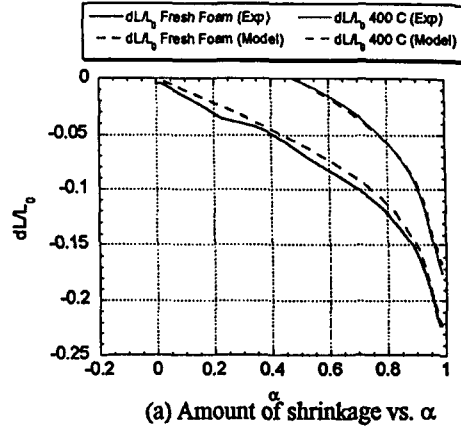


Fig.4. Shrinkage characteristics plotted versus  $\alpha$

### Heat capacity

DSC was performed at CytecFiberite to measure the heat capacity of carbonized foam for the temperature range from 30 to 400 °C. The data showed an asymptotic behavior to a linear function of temperature with slight deviations at lower temperatures. The data by Mottram et al. were used as fresh foam properties [3].

### Thermal conductivity

The thermal diffusivity of carbonized foam was measured using Flash Diffusivity Technique. The measurement was performed for the temperature range of 12 to 427 °C since errors were magnified at higher temperatures. Measurements for phenolic resin given by Mottram et al. [3] were used as the thermal conductivity of fresh foam.

### Elastic Modulus

Tensile tests using an Instron machine were performed on fresh and carbonized foam. An equation by Gibson et al was used to predict the solid modulus and to relate modulus and porosity [4].

### Properties of Volatile Gases during Carbonization

The ratio of gas components in the volatile gas was modeled as a function of  $\alpha$  using data given by Serio et al [5]. The properties of each gas components are gathered from various references and are mixed using the weight ratio and molecular weight.

## 3. Numerical Analysis

### Governing Equations and Numerical Scheme

Heat transfer during carbonization can be modeled as follows for a 2-dimensional geometry.

$$\left\{ (1-\varepsilon)\rho_s C_s + \varepsilon\rho_g C_g \right\} \left( \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = \left\{ (1-\varepsilon)k_s + \varepsilon k_g \right\} \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) \quad (1)$$

Continuity of volatile gas can be expressed as

$$\frac{\partial(\varepsilon\rho_g)}{\partial t} + \frac{\partial(\rho_g u)}{\partial x} + \frac{\partial(\rho_g v)}{\partial y} = -\frac{\partial}{\partial t} \left\{ (1-\varepsilon)\rho_s \right\} \quad (2)$$

The volatile gas can be assumed as ideal gas. The momentum equation can be substituted with Darcy's Law describing porous media flow as [6]

$$\vec{u} = -\frac{K_p}{\mu_g} \nabla P \quad (3)$$

Combining eqs (1)-(3), the temperature and pressure distribution within the composite can be evaluated. The stress distribution can be predicted using [7]

$$\mathbf{D}^T \mathbf{E}(\mathbf{D}\mathbf{u} - \varepsilon_0) = 0 \quad (4)$$

$$\boldsymbol{\sigma} = \mathbf{E}(\varepsilon - \varepsilon_0) \quad (5)$$

$$\varepsilon = \mathbf{D}\mathbf{u} \quad (6)$$

where initial strain vector  $\varepsilon_0$  is the difference between thermal expansion and shrinkage.

FEM (Finite Element Method) is adapted to solve the spatial distributions of temperature, pressure, and stress. FDM (Finite Difference Method) is used to treat the transient term.

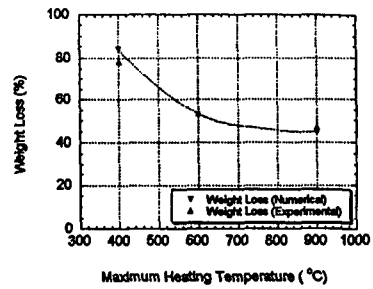
### Verifications

The validity of the simulation is verified through comparisons with experimental data for temperature profiles, weight loss and shrinkage. Examples of results are given in Fig.1. Agreements were also satisfactory in all other comparisons.

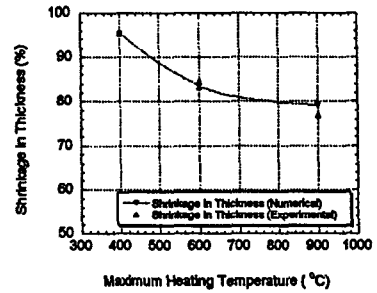
### Application Runs

#### Furnace Simulation

A typical uneven heating inside a furnace is simulated. Temperature and stress distributions are plotted in Fig.2. Photograph of the actual sample after carbonization is given in Fig.3. Stress directions imply crack orientations.

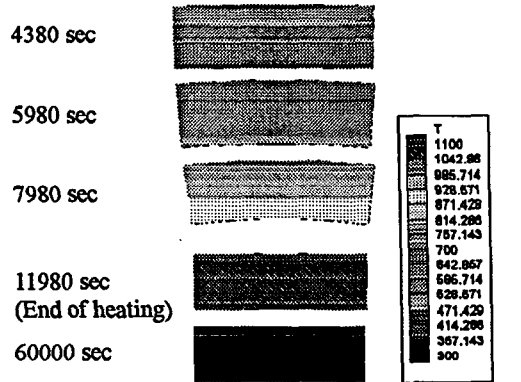


(a) Weight loss comparison

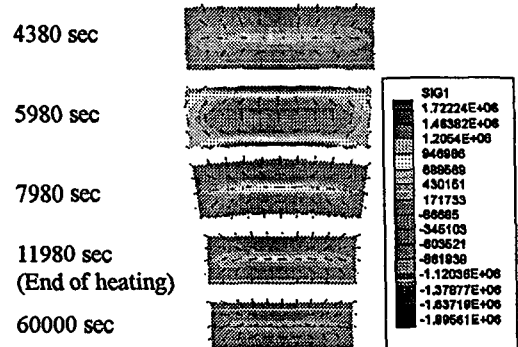


(b) Shrinkage comparison

Fig.1. Results of verification. (heating rate 1 °C/min)



(a) Temperature distribution (K)



(b) 1<sup>st</sup> principal stress (Pa)

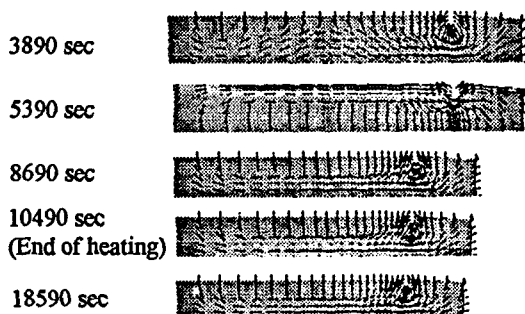
Fig.2. Numerical results of furnace simulation



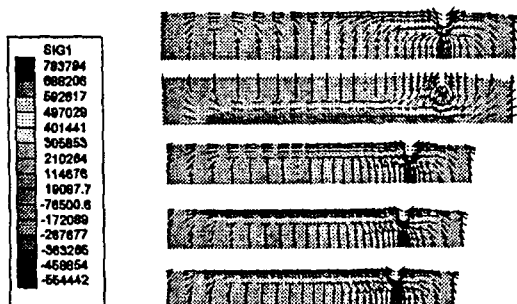
Fig.3. Actual sample after carbonization

#### Aircraft Brake Pad

Geometry of an actual aircraft brake pad is considered as a second example. Stress distributions are plotted in Fig.4. The effect of geometry on stress orientation as well as stress concentration at the groove should be noticed.



(a) 1<sup>st</sup> principal stress (Pa)



(b) 2<sup>nd</sup> principal stress (Pa)

Fig.4. Numerical results for brake pad simulation

#### 4. Conclusion

Phenolic foam is introduced as an ideal isotropic, homogeneous material and material properties are modeled in appropriate functional forms to serve the purpose of numerical simulation. Results of numerical simulation of carbonization process were verified through experiments.

#### Acknowledgements

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