



Transient three-dimensional simulation of densification process of carbon fibre preforms via chemical vapour infiltration of carbon matrix from methane



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HIGHLIGHTS

- 2D woven cloth and random distributed felt were infiltrated.
- A novel pore structure evolution model was proposed.
- Simulation couples multi-step reaction model with pore structure evolution model.
- Transient 3D simulation of CVI process was successfully implemented.
- Predicted results of bulk density agree well with experimental results.

ARTICLE INFO

Article history:

Received 3 July 2017

Received in revised form 22 September 2017

Accepted 21 October 2017

Available online 23 October 2017

Keywords:

C/C composites

Chemical vapour infiltration

Transient 3D simulation

Porous structure

Numerical modelling

ABSTRACT

Chemical vapour infiltration (CVI) is widely used for fabricating carbon fibre-reinforced carbon materials for aircraft brake disks. This study aims at developing a numerical simulation method for predicting densification of the material during the CVI. Based on the multi-step reaction and deposition models, including the hydrogen inhibition model of pyrocarbon growth, transient 3D simulations of the CVI using methane as a precursor of the pyrocarbon were carried out via the finite element method coupling the mass transfer (by convection and diffusion) and the evolutive porous structure model with gas-phase and surface chemical reactions. The CVI of two different types of preforms was studied. The pore structure evolution models were derived not analytically but numerically with the aid of a computational tool for visualizing the fibre structures. An acceptable agreement was found between the predicted densification profiles and the experimental data obtained using a laboratory CVI reactor at a temperature of 1343 K, a methane pressure of 30 kPa and a total deposition time of 120 h.

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1. Introduction

Chemical vapour infiltration (CVI) for fabricating fibre-reinforced carbon matrix composites is a method that is used to infiltrate pyrolytic carbon (pyrocarbon) matrix into the porous fibre preform via hydrocarbon pyrolysis (Chand, 2000; Delhaes, 2002; Golecki, 1997; Vignoles, 2015a,b; Yan and Xu, 2010). The isothermal and isobaric CVI (ICVI) process is one of the common commercial methods for producing the carbon/carbon (C/C) composite, which is an extremely complicated process (Zhang and

Hüttinger, 2001). Generally, the gas phase reactions of the reactant gas molecules, surface reactions of precursors at active sites on the fibre surface, diffusion or convection of the gaseous species in the reactor, and pore structure evolution of the carbon preform occur simultaneously during the infiltration process (Vignoles et al., 2001, 2007). The primary objective for fabricating the C/C composite via the CVI process is to reduce the infiltration time while maintaining its high and uniform density (Vignoles, 2015a,b). Unfortunately, there is an inherent competition between the diffusion of the gaseous species and the pyrocarbon deposition during the progressive densification of the porous preform (Besmann et al., 1991, 1996; Roman and Stinton, 1995). Time-dependent structural characteristics of the carbon preform, e.g., equivalent radius of pore, tortuosity, total porosity, and surface area to volume

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Nomenclature

Symbols used

ρ [kg m ⁻³]	density
μ [Pa s]	dynamic viscosity
u [m s ⁻¹]	velocity
u_0 [m s ⁻¹]	inlet velocity
p [Pa]	pressure
c_i [mol m ⁻³]	concentration of species i
c_0 [mol m ⁻³]	initial concentration of methane
D_i [m ² s ⁻¹]	Fick diffusion coefficient of species i
R_i [mol m ⁻³ s ⁻¹]	chemical reaction term of species i in the free flow channel
$R_{i(sv)}$ [mol m ⁻³ s ⁻¹]	chemical reaction term of species i in preform
D_i^{eff} [m ² s ⁻¹]	effective diffusion coefficient of species i
M_C [g mol ⁻¹]	molar mass of carbon

ξ [-]	porosity
ξ_0 [-]	initial porosity
ρ_0 [g cm ⁻³]	initial density of the preform
ρ_C [g cm ⁻³]	pyrocarbon density
$R_{C(sv)}$ [mol m ⁻³ s ⁻¹]	chemical reaction term of pyrolytic carbon in preform
k_i [s ⁻¹] or [m s ⁻¹]	reaction rate constant for reaction i
T [K]	temperature
V_i [cm ³ mol ⁻¹]	volume increment for species i
M_i [g mol ⁻¹]	molar mass of species i
δ [Å]	collision diameter
T^* [-]	reduced temperature
$\Omega(T^*)$ [-]	collision integral
ε/κ [K]	maximum energy of attraction divided by Boltzmann constant

ratio constantly change, which dramatically prevents the gaseous species from diffusing into the inner part of the preform. Accordingly, the early surface pore closure is inevitably formed during the industrial production process, and the intermediate machining steps are recommended to open the closed surface pores of the preform (Ibrahim and Paolucci, 2011). The numerical simulation of the CVI process based on detailed models for the chemical reactions and mass transport are expected to shed light on the underlying laws of the infiltration process, which further support the development and optimization of the production process of C/C composites (Li et al., 2008; Norinaga and Deutschmann, 2007; Tang et al., 2014).

Complex pore networks normally exist in the carbon preform, as observed using X-ray computed tomography (Kastner et al., 2012; Kinney et al., 1993; Panerai et al., 2015), which is also applied to assess the geometrical and transport properties of the preform at various stages of infiltration (Coindreau et al., 2011). As an alternative method to the computed tomography, many idealized pore models have been developed to analyse pore filling during the CVI process, such as the cylindrical pore model (Birakayala and Evans, 2002), random overlap model (Currier, 1991; Guan et al., 2013) and the node-percolation model (Starr, 1995). However, these models fail to give a sufficiently appropriate description to the evolution of various pore structural parameters among different fibre architectures during the progress of CVI. In contrast to the drawbacks, the pore structure evolution model, as in this study, is the real-time simulation with a three-dimensional visualization of the pore topology evolution during the densification process based on the approximation of the growing solid phase (Pfrang et al., 2007). The structural characteristics of the preform in three dimensions (3D) during the CVI process are then accurately computed via this model. This numerical method allows researchers to build complex architectures of the carbon preform and obtain the related structural characteristics and gas transport properties.

The properties of C/C composites are controlled by the fibre preform, the deposited matrix and the interaction between the preform and matrix (Wu et al., 2017). The preform itself, as the backbone of the C/C composite, plays the key role for the strength and stiffness of the composite (Fitzer, 1987). Consequently, for the first time, the two-dimensional (2D) woven cloth and randomly distributed felt are used as research subjects to analyse and compare the pore structure evolution and densification process between these two types of preforms. The present study aims at developing a general and efficient method for simulating the CVI process for various carbon fibre preforms. The pore structure evo-

lution and related structural characteristics of these two preforms were first numerically visualized by the approximation of the growing solid phase in the CVI process. Second, based on the above-proposed pore structure evolution model with the multi-step chemical reaction model from our previous study (Li et al., 2008), the CVI simulation of the preforms was realized by coupling the convection-diffusion equations, the Navier-Stokes equation of the laminar flow. Finally, as for the ICVI process to fabricate C/C composite using methane, the experimental results from a laboratory CVI reactor were compared with the predictions for evaluating the developed numerical simulation critically.

2. Experimental setup

Fig. 1 sketches the laboratory scale CVI reactor for the fabrication of C/C composite. Rectangular-shaped pitch-based 2D woven cloth or carbon fibre felt with a dimension of 36 mm (length) \times 16 mm (width) \times 58 mm (height) was fitted in a sample holder made of graphite. The narrow zone between the graphite tube and the sample holder was treated as the gas flow channel. The carbon fibre preforms were densified from methane (99.99%), which was supplied from the bottom of the reactor. The initial bulk density, fibre diameter and porosity of the cloth preform were 0.65 g/cm³, 7 μ m and 63%, respectively; for the felt preform, they were 0.12 g/cm³, 13 μ m and 93%, respectively. The CVI experiments were performed at 1343 K, 30 kPa, for 0–120 h of densification. The residence time of methane through the narrow channel was 0.4 s (cloth) or 0.5 s (felt). The experiments were conducted by changing the infiltration time, and then the time-dependent change in weight gain due to the CVI was measured. The simplified 3D geometry of the CVI reactor for the simulation of the infiltration process is shown on the top right-hand side of Fig. 1. To save the computation time, the geometry of the 3D CVI reactor was simplified into one-quarter of the original with consideration of symmetry.

3. Methodology

3.1. Reaction model

Due to the time-consumption and convergence problem using the detailed reaction mechanism, a simplified chemical reaction model (Becker and Hüttinger, 1998) was applied to simulate both the methane pyrolysis and carbon deposition in the reactor, as shown in Fig. 2. Methane (c_1), ethylene (c_2), acetylene (c_3), benzene (c_4) and hydrogen (c_5) were considered in the reaction model.

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