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Study of carbon densification growth in a cylindrical pore through chemical vapor infiltration process

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Abstract: Carbon-Carbon composites are the materials of 21st century. Among various techniques for processing of Carbon-Carbon composites, Chemical vapor infiltration (CVI) is the more economical and commonly employed one. Modeling studies on CVI process is an efficient test for optimizing the process parameters and to study the feasibility of the process. The dynamic modeling and simulation of CVI process is discussed. The process under consideration employs thermal cracking of methane gas to produce solid carbon and gaseous hydrogen. Among different CVI systems, an isothermal, 2-dimensional model is considered in this work. The carbon preform is kept at an elevated temperature, in an isothermal, isobaric reactor and when the methane gas reaches the preform and attains its temperature, thermal cracking occurs and the solid carbon produced diffuses through the porous preform to fill the pores and reduces the porosity to get a dense carbon matrix. Since the process involves diffusion, Dusty Gas Model and Fick's law of diffusion are used for modeling. Computer simulation is done to solve the resulting partial differential equations.

Deposition of Carbon from Methane cracking, at various distances from the open end of the cylindrical pore can be obtained from the model. The change in the porosity of the carbon preform due to the deposition of solid carbon, as the process progresses, is also obtained. The theoretically determined values are compared with the experimental works to check the validity of the model. The use of mathematical models can avoid time consuming and expensive trial and error practices and help in rapid evaluation of novel reactor designs and modes of operation. A computer model allows optimization of process parameters and production of uniform, dense composites. These types of mathematical models can provide insight into the physiochemical processes governing CVI as well as valuable guidelines for experimental research.

Index Terms— Chemical vapor infiltration, diffusion, Carbon-Carbon composites, Dusty Gas Model, Fick's law of diffusion

I. INTRODUCTION

Composite materials are those materials composed of two or more distinctly identifiable macro constituents that differ in form or composition and are insoluble in each other[1]. In composite materials, fibers or particles are embedded in the matrix of another material. The classes of composites vary from natural composites like timber, soil agglomerates, minerals etc. to advanced fibre reinforced plastics (FRP). Due to their high stiffness to weight ratio, composite materials are having a variety of applications as in automotive, electronic, wear, aerospace industries etc. Among all, aerospace industry is the most important. Depending upon the matrix used, composite materials are classified as metal matrix, ceramic matrix, polymer matrix, and carbon or graphite matrix. Among these, carbon matrix composites are highly superior due to their high strength and rigidity and ability to withstand high temperature up to 2300° C.

Carbon-Carbon composites rank first among composite materials with spectrum of properties and applications in various sectors. These are made of fibers in various directions and carbonaceous polymers and hydrocarbons as matrix precursors. Carbon-Carbon composites are very much useful for high temperature applications due to their excellent thermal properties. Like carbon, Carbon-Carbon composites can also be manufactured by using different solid, liquid and gaseous routes such as solid pyrolysis using thermosetting resins, or pitch route using liquid infiltration carbonization route or Chemical Vapor Infiltration (CV1) route. Among all, CV1 is the most common and most economical method[2].

Chemical vapor infiltration of carbon from pyrolysis of hydrocarbons is a technique of great interest for different applications, such as the densification of porous materials in the preparation of Carbon-Carbon composites for the aeronautics and space industries and the preparation of carbon molecular sieves by partial blocking of micropore entrance. The process includes the deposition of hydrocarbon gases on a carbon substrate. The gas containing active carbon diffuses into a fibrous substrate so as to obtain uniform deposition on the matrix. Substrate and susceptor design, source and carrier gases, temperature pressure are to be considered, while determining matrix characteristics, apart from efficiency, uniformity and rate of process.

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Design studies are typically accomplished by constructing mathematical models that simulate the process. Such models use experimental data and mass transfer fundamentals to estimate parameters for the equilibrium and mass balance equations that describe the process. Once a representation of the process is obtained, operating parameters can be obtained as a function of key process variables, and the economics of the design can be assessed. Mathematical optimization procedure can then be used to determine the optimal design for a given economic objective function. Design studies thus explore the critical process parameters on the economics. Areas of improvement can be identified, and a decision can be made whether to continue development of the process[3].

Of course, the predictions of a design study are only as good as the mathematical models that are used to describe the process. Therefore, they should not be considered as a replacement for experimentation. However, by using process simulation in conjunction with basic experimental measurements, the feasibility of a process application can be assessed early in the development, there by guiding the course of future work[3].

The modeling and simulation of a CVI process using methane cracking to produce, solid carbon is taken up in this work. Among different CVI techniques, an isothermal, isobaric two-dimensional model of CVI process is considered in this work. The model is applied as a guideline for choosing optimum conditions for producing a dense carbon matrix composite. From this model, process diagrams are constructed that can help an experimentalist to choose the best conditions for the CVI process using isothermal conditions. Mathematical models can provide insight into the physicochemical processes governing CVI as well as valuable guidelines for experimental research. The use of mathematical models can avoid time consuming and expensive trial and error practices and help in rapid evaluation of novel reactor designs and modes of operation. A computer model allows optimization of process parameters and production of uniform, dense composites. A two dimensional simulation of isothermal isobaric CVI is presented in this thesis work because this is the most widely accepted model of CVI. The model is developed based on the work of Jiefei Huang[25]. In this work, methane cracking process for producing solid carbon matrix is analyzed .We assume only two gas .species methane and hydrogen are involved in the CVI process. Therefore, a simplified gas diffusion mechanism is used in our work.

The analysis of the densification of a porous substrate by CVI requires the consideration of diffusion and reaction of gases in a porous substrate occurring simultaneously with the deposition of a solid product. The work presented here is to incorporate a scheme for the formation of carbon deposits during the pyrolysis of methane into a model, which accounts for the diffusion, reaction and porosity changes occurring during carbon infiltration. This model enables the prediction of the porosity as functions of reaction conditions and time of deposition. The porosity is defined as the ratio of void volume to the total volume of the preform. The modeling partial differential equations arc generated from reacting species mass balances on CH_4, H_2 and the deposited carbon matrix (which is directly related to porosity).

II.   LITERATURE SURVEY

2.1 MASS DIFFUSIVITY

Fick's first law relates the diffusive flux to the concentration field, by postulating that the flux goes from regions of high concentration to regions of low concentration, with a magnitude that is proportional to the concentration gradient (spatial derivative). In one (spatial) dimension, this is

$$J = -D\frac{\partial \phi}{\partial x}$$

where

- J is the diffusion flux in dimensions of [(amount of substance) length^{-2} time^{-1}], example $\left(\frac{\text{mol}}{\text{m}^2 \cdot \text{s}}\right)$. J measures the amount of substance that will flow through a small area during a small time interval.
- D is the **diffusion coefficient** or **diffusivity** in dimensions of [length^2 time^{-1}], example $\left(\frac{\text{m}^2}{\text{s}}\right)$
- ϕ (for ideal mixtures) is the concentration in dimensions of [(amount of substance) length^{-3}], example $\left(\frac{\text{mol}}{\text{m}^3}\right)$
- x is the position [length], example m

D is proportional to the squared velocity of the diffusing particles, which depends on the temperature, viscosity of the fluid and the size of the particles according to the Stokes-Einstein relation. In dilute aqueous solutions the diffusion coefficients of most ions are similar and have values that at room temperature are in the range of 0.6×10^{-9} to 2×10^{-9} m^2/s. For biological molecules the diffusion coefficients normally range from 10^{-11} to 10^{-10} m^2/s.

In two or more dimensions we must use ∇, the del or gradient operator, which generalises the first derivative, obtaining

$J = -D\nabla\phi$.

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The driving force for the one-dimensional diffusion is the quantity $-\dfrac{\partial \phi}{\partial x}$ which for ideal mixtures is the concentration gradient. In chemical systems other than ideal solutions or mixtures, the driving force for diffusion of each species is the gradient of chemical potential of this species. Then Fick's first law (one-dimensional case) can be written as:

$$J_i = -\frac{Dc_i}{RT}\frac{\partial \mu_i}{\partial x}$$

where the index i denotes the ith species, c is the concentration (mol/m^3), R is the universal gas constant (J/(K mol)), T is the absolute temperature (K), and μ is the chemical potential (J/mol).

Diffusivity or diffusion coefficient is proportionality constant between the molar flux due to molecular diffusion and the gradient in the concentration of the species (or the driving force for diffusion). Diffusivity is encountered in Fick's law and numerous other equations of physical chemistry. It is generally prescribed for a given pair of species. For a multi-component system, it is prescribed for each pair of species in the system. The higher the diffusivity (of one substance with respect to another), the faster they diffuse into each other. This coefficient has an SI unit of m²/s (length²/time).

Temperature dependence of the diffusion coefficient

Typically, a compound's diffusion coefficient is ~10,000x greater in air than in water. Carbon dioxide in air has a diffusion coefficient of 16 mm²/s, and in water its coefficient is 0.0016 mm²/s. The diffusion coefficient in solids at different temperatures is often found to be well predicted by where

- is the diffusion coefficient
- is the maximum diffusion coefficient (at infinite temperature)
- is the activation energy for diffusion in dimensions of [energy (amount of substance)$^{-1}$]
- is the temperature in units of [absolute temperature] (kelvins or degrees Rankine)
- is the gas constant in dimensions of [energy temperature^{-1} (amount of substance)$^{-1}$]

An equation of this form is known as the Arrhenius equation. An approximate dependence of the diffusion coefficient on temperature in liquids can often be found using Stokes-Einstein equation, which predicts that: where:

- T_1 and T_2 denote temperatures 1 and 2, respectively
- D is the diffusion coefficient (cm²/s)
- T is the absolute temperature (K),
- μ is the dynamic viscosity of the solvent (Pa·s)

The dependence of the diffusion coefficient on temperature for gases can be expressed using the Chapman-Enskog theory (predictions accurate on average to about 8%):
where:

- 1 and 2 index the two kinds of molecules present in the gaseous mixture
- T – temperature (K)
- M – molar mass (g/mol)
- p – pressure (atm)
- – the average collision diameter (the values are tabulated (Å)
- Ω – a temperature-dependent collision integral (the values are tabulated but usually of order 1) (dimensionless).
- D – diffusion coefficient (which is expressed in cm²/s when the other magnitudes are expressed in the units as given above)

Pressure dependence of the diffusion coefficient

For self-diffusion in gases at two different pressures (but the same temperature), the following empirical equation has been suggested:
where:

P_1 and P_2 denote pressures 1 and 2, respectively

D is the diffusion coefficient (m²/s)

ρ is the gas mass density (kg/m^3)

Effective diffusivity in porous media

The effective diffusion coefficient[4] describes diffusion through the pore space of porous media. It is macroscopic in nature, because it is not individual pores but the entire pore space that needs to be considered. The effective diffusion coefficient for transport through the pores, D_e, is estimated as follows:
where:

- D - diffusion coefficient in gas or liquid filling the pores(m^{2}s^{-1})
- ε_t - porosity available for the transport (dimensionless)
- δ - constrictivity (dimensionless)
- τ - tortuosity (dimensionless)

The transport-available porosity equals the total porosity less the pores which, due to their size, are not accessible to the diffusing particles, and less dead-end and blind pores (i.e., pores without being connected to the rest of the pore system). The constrictivity describes the slowing down of diffusion by increasing the viscosity in narrow pores as a result of greater proximity to the average pore wall. It is a function of pore diameter and the size of the diffusing particles.

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2.2 One dimensional diffusion equation

The problem statement, all variables and given/known data

Solve:

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2}, 0 < x < \pi, t > 0$$

with initial condition

$$u(x,0) = f(x) = \begin{cases} 1, & 0 \leq x < \pi/2 \\ 0, & \pi/2 \leq x < \pi \end{cases}$$

and with non-homogeneous boundary conditions

$$u(0,t) = 1, u(\pi,t) = 0$$

The attempt at a solution

Solution for the fourier series method is:

$$u(x,0) = \frac{A_0}{2} + \sum_{n=1}^{\infty} e^{-kn^2 t}(A_n \cos(nx) + B_n \sin(nx))$$

There is a standard way of handling problems with non-homogeneous boundary conditions: "homogenize" them!

The simple linear function $1 - \frac{1}{\pi}x$ satisfies the boundary conditions. Now let $v(x,t) = u(x,t) - 1 + \frac{1}{\pi}x$

It is easy to see that v(x,t) also satisfies

$$\frac{\partial v}{\partial t} = k\frac{\partial^2 v}{\partial x^2}$$

but the boundary conditions for v are v(0, t)= 0, $v(\pi,t) = 0$.

Of course, we have to change the initial condition to

$$v(x,0) = \begin{cases} \frac{1}{\pi}x, & 0 \leq x < \pi/2 \\ \frac{1}{\pi}x - 1, & \pi/2 \leq x < \pi \end{cases}$$

Now we can write v in a purely sine series:

$$v(x,t) = \sum_{n=1}^{\infty} e^{-kn^2 t} B_n \sin(nx)$$

II. Materials and Methods

The modeling studies on CVI process was carried out at Composites Entity (CMSE) of Vikram Sarabhai Space Centre. CMSE is assigned with the task of design, development, production, testing and assembly of composite products for ISRO's launch vehicles and satellites. The typical composite products in the launch vehicles are composite motor cases, pressurant tanks, igniters for motor cases, ablative nozzles and Carbon-Carbon components. Some of the composite satellite components are antenna reflectors, solar panels, payload platforms, flexible booms, support structures, yokes etc.

Composite materials play a vital role in the realization of ISRO's current and futuristic programs like reusable launch vehicle, air-breathing propulsion etc. design and development of thermo-structural products capable of withstanding the stringent flight conditions is the responsibility of composite entity. Carbon-Carbon composite products will be an important breakthrough as far as the materials are concerned. Over the years, composite entity has acquired state-of-the-art technology in the entire realm of product realization like design, analysis, process engineering, test and evaluation. The processing facility set up by the group today rank among the best of its kind in the country.

Mathematical modeling procedure

Mathematical modeling of the CVI process involves the description of the transport and reaction phenomena occurring inside the composite. The system is characterized by the time evolution of species concentration and pore structure. In general, important processes include the diffusion of gaseous species into and out of the fiber-matrix composite and the chemical reaction. The governing equations for the processes occurring are considered for obtaining the modeling equations and hence the modeling parameters.

Material for experiment

A rectangular graphite block of 70 X 24 X 22 mm size is used for analysis. On this block a blind cylindrical hole of 3 mm depth and 1.2 mm diameter is drilled centrally using precise micro machining tools.

Elevation of block with hole   Plan of block with hole
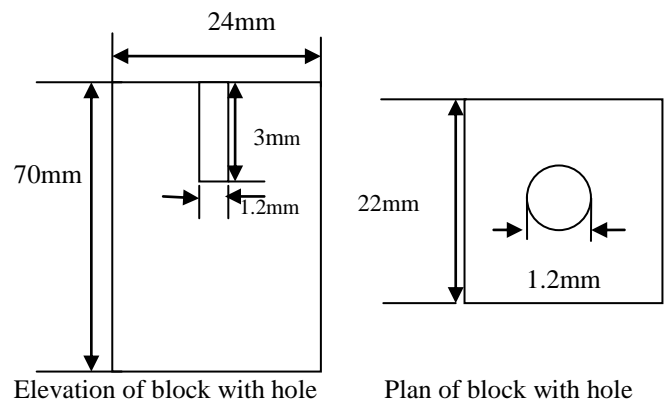
Cylindrical pore (enlarged view)
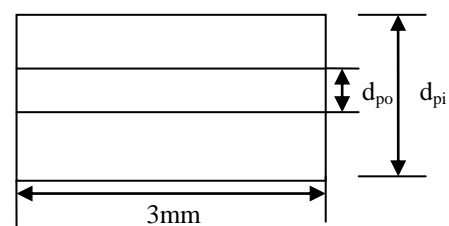
d_{po} --- diameter after deposition
d_{pi} ---- pore diameter before deposition
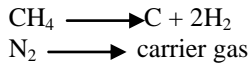
Figure1. Cylindrical Carbon perform

The two processes involved in the system are:

Chemical reaction

The rectangular graphite block is arranged between graphite fixtures and dry bonding is done in CVI furnace for 72 hours. CVI typically uses a hydro carbon

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containing gas to infiltrate a porous perform. The high temperatures so as to leave a carbon coating on the fibre structure of the preform, thereby increasing the density of the rectangular graphite block. Here, methane cracking is the process employed for producing solid carbon. The methane gas is fed to the reactor and when it reaches the preform, it undergoes thermal cracking due to high temperature of carbon perform.

Pyrolysis

$$CH_4 \longrightarrow C + 2H_2$$
$$N_2 \longrightarrow \text{carrier gas}$$

Cracking of Methane.

$$CH_4 \longrightarrow C_1 \longrightarrow C_2 \longrightarrow C \geq 6$$

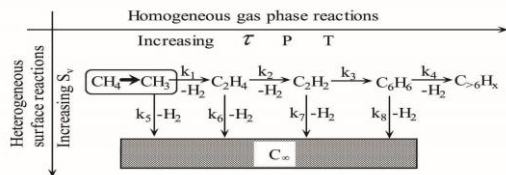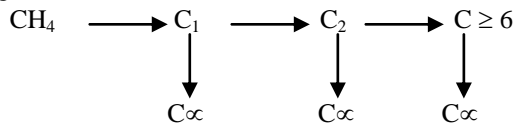$$C\infty \qquad C\infty \qquad C\infty$$

Figure. 2: The multi – step deposition model with consideration of the hydrogen inhibition.

(τ the residence time, P the pressure, T the temperature, S$_v$ volume related surface area, k- reaction constants).

Diffusion
Dusty Gas model

The dusty gas model is a theory which describes the transport of gases through porous media. It is so called because it treats the porous medium as a component of gas mixture, consisting of giant molecules like dust in a gas. Transport equation for the gas through the porous media are derived by applying the kinetic theory of gases to this 'Super Mixture' of free gas and fixed in space solid molecules.

Fick's first law relates diffuse flux to the concentration as,

$$J = - \frac{\partial C_i}{\partial x}$$

J is the diffusion flux per unit area per unit time.
C_i is concentration
x is the distance from inlet.

Fick's second law predicts how diffusion causes the concentration to change with time.

$$\frac{\partial C_i}{\partial t} = D \frac{\partial^2 C_i}{\partial x^2}$$

where C_i is the concentration
t is the time
D is diffusion coefficient
x is distance from inlet

It is derived from Fick's First law and mass balance that,

$$\frac{\partial C_i}{\partial t} = \frac{-\partial}{\partial x} J = \frac{\partial}{\partial x} \left(D_{eff} \cdot \frac{\partial}{\partial x} C_i \right) + R$$

where R is rate of reaction which is a constant

$$D_{eff} = \frac{D_{bin} \cdot D_{knu}}{D_{bin} + D_{knu}}$$

D_{bin} is binary diffusion coefficient which is a constant.
D_{knu} is Knudsen diffusion coefficient

$$D_{knu} = \frac{d_{pore}}{3} \sqrt{\frac{8 \kappa NT}{\Pi M_A}}$$

where d_{pore} is diameter before deposition
κ is Boltzmann's constant
N is Avagadro's number
T is temperature
M_A is mass of the reacting gas

Recongnize and specify Boundary conditions

A mass transfer process is fully described by the differential equations of mass transfer only if the initial boundary and initial conditions are specified. Typically, initial and boundary conditions are used to specify limits of integration or to determine integration constants associated with the mathematical solution of the differential equations for mass transfer. Since the process is done for 72 hours at the initial time zero. The concentration of methane that enters the blind hole is 1 l/min. A blind cylindrical hole of 3mm depth which is divided into 86 equal slices. Hence the initial distance from the inlet is 0.035mm. The initial pore diameter is taken as
1.2 mm.
Table 1.Boundary conditions

Ci(:,1)	1 l/min
dp (:,1)	1.2mm
dp(1, :)	1.2mm

Solution of modeling equation
Solve the differential equations to get the concentration profile and pore diameter different points of the hole

Programming in MATLAB code

MATLAB , which stands for MAT mix LABortaory, is a very powerful technical language for mathematical programming. MAT LAB has become a popular technical language to mathematicians, engineers and scientists. It can be used for data acquisition, data analysis, graphical

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visualization, numerical analysis, algorithm development, signal processing, and many other applications. Writing program in MATLAB is much easier compared to those in other programming languages like FORTRAN, C, C++ or Java. This is because when writing a program in MATLAB, we do not have to worry about the declaration of variables, their types, sizes and memory requirements, which are the main source of problems in other languages.

RESULTS
Construction of solution

The principle difficulty faced in these types of works is the evaluation of transfer coefficients like diffusivity. The identification and calculation of these constants for the particular reaction is given in the table below. Usually, the reaction temperature and pressure are optimized by a large number of trial and error calculations, considering the side reactions occurring also. However, due to time constraints, the reaction is assumed to be first order with only two gas species, viz, methane and hydrogen taking part.

Table 2. Boundary conditions

$C_i(:,1)$	1 L/min
$\partial C_i /\partial t$	0
dp (:,1)	1.2mm
dp(1, :)	1.2mm

The output is obtained in table of the order: Actual pore radius after deposition, Numerical pore radius after deposition, Variation between the two (error), Fractional error, and Fractional error percentage. The output from the program is analyzed and saved after 72 hours of reaction.

Table 3. Values of pore diameters before and after deposition

Slide No.	(x) micron	dpi micron	dpo micron	Deposition micron
10	453.44	1307.033	1307.033	0
20	802.24	1270.72	1198.113	72.607
30	1151.04	1198.113	1161.801	36.312
40	1499.84	1198.113	1161.801	36.312
50	1848.64	1198.113	1161.801	36.312
60	2197.44	1198.113	1161.801	36.312
70	2546.24	1198.113	1161.801	36.312
80	2895.04	1198.113	1161.801	36.312
x = distance from open end of the hole				
dpi = pore diameter before deposition				
dpo = pore diameter after deposition				

Slide No.10 (x=453.44 μm)

Before deposition   After deposition

Slide No. 20 (x=802.24 μm)

Before deposition   After deposition

Slide No. 30 (x=1151.04 μm)

Before deposition   After deposition

Slide No. 40 (x=1499.84 μm)

Before deposition   After deposition

Slide No. 50 (x=1848.64 μm)

Before deposition   After deposition
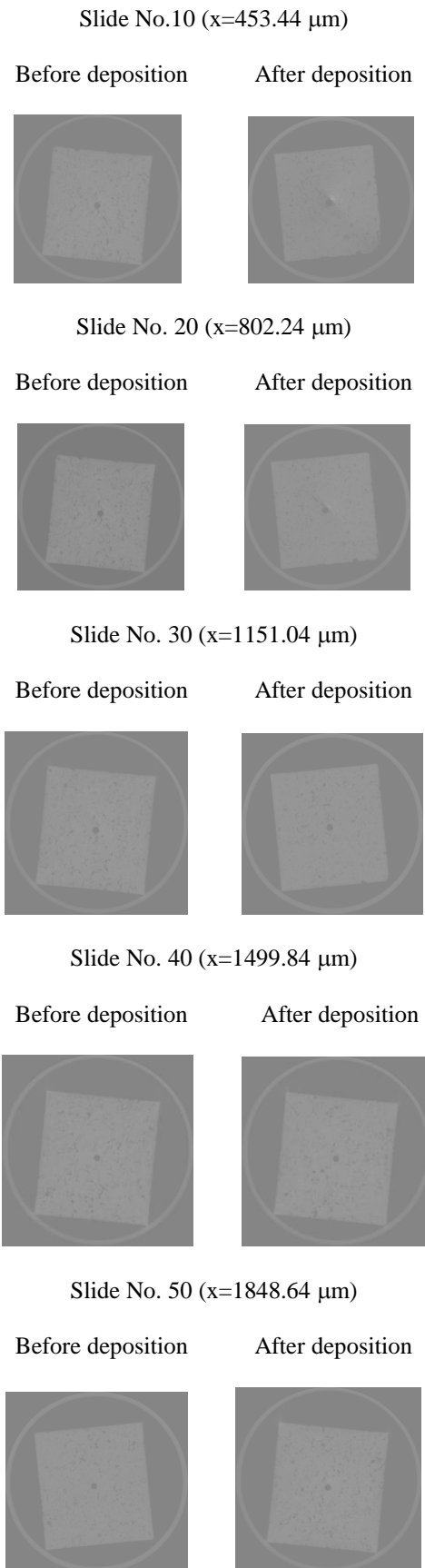
Figure .3 Sample slides of Micro CT scan showing pore diameters before and after deposition

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Table.4 Showing values of pore diameters before and after deposition along with size of hole

| Slice no	x	dpi	dpo	Size of hole
	micron	micron	micron	micron
1	139.52	1343.35	1343.35	1200
2	174.4	1379.64	1343.35	1200
3	209.28	1343.35	1234.43	1200
4	244.16	1343.35	1198.11	1200
5	279.04	1307.03	1270.72	1200
6	313.92	1307.03	1125.51	1200
7	348.8	1307.03	1233.28	1200
8	383.68	1307.03	1234.43	1200
9	418.56	1307.03	1198.11	1200
10	453.44	1307.03	1307.03	1200
11	488.32	1307.03	1270.72	1200
12	523.2	1307.03	1234.43	1200
13	558.08	1307.03	1270.72	1200
14	592.96	1307.03	1234.04	1200
15	627.84	1307.03	1234.43	1200
16	662.72	1307.03	1270.72	1200
17	697.6	1307.03	1270.72	1200
18	732.48	1307.03	1270.72	1200
19	767.36	1307.03	1198.11	1200
20	802.24	1270.72	1198.11	1200
21	837.12	1234.43	1198.11	1200
22	872	1270.72	1234.43	1200
23	906.88	1307.03	1161.8	1200
24	941.76	1198.11	1089.19	1200
25	976.64	1198.11	1161.8	1200
26	1011.52	1234.43	1161.8	1200
27	1046.4	1161.8	1125.51	1200
28	1081.28	1198.11	1161.8	1200
29	1116.16	1198.11	1125.51	1200
30	1151.04	1198.11	1161.8	1200
31	1185.92	1198.11	1161.8	1200
32	1220.8	1198.11	1161.8	1200
33	1255.68	1198.11	1125.51	1200
34	1290.56	1234.43	1161.8	1200
35	1325.44	1198.11	1161.8	1200
36	1360.32	1234.43	1198.11	1200
37	1395.2	1198.11	1161.8	1200
38	1430.08	1198.11	1125.51	1200
39	1464.96	1198.11	677.33	1200
40	1499.84	1198.11	1161.8	1200
41	1534.72	1198.11	1125.51	1200
42	1569.6	1198.11	1125.51	1200
43	1604.8	1198.11	1125.51	1200
44	1639.36	1198.11	1161.8	1200
45	1674.24	1198.11	1161.8	1200
46	1709.12	1198.11	1161.8	1200
47	1744	1198.11	1161.8	1200
48	1778.88	1270.72	1125.51	1200
49	1813.76	1198.11	1161.8	1200
50	1848.64	1198.11	1161.8	1200
	x = distance from open end of the hole			
	dpi = pore diameter before deposition			
	dpo = pore diameter after deposition			
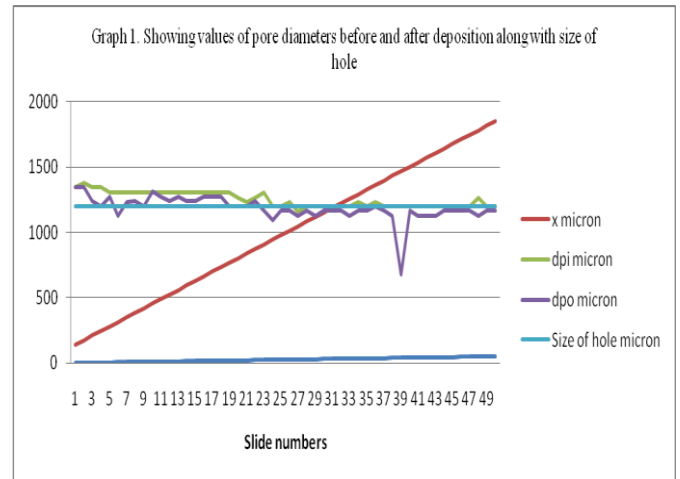
Graph 1. Values of pore diameters before and after deposition along with size of hole

Table 5.Showing values of pore diameters and deposition

| Sl no.	Slide no	x	dpi	ei	Theoretical	dpo	Deposition
		micron	micron	micron	micron	micron	Micron
1	1	139.52	1343.345	143.345	1200	1343.345	0
2	2	174.4	1379.64	179.64	1200	1343.345	36.295
3	3	209.28	1343.345	143.345	1200	1234.425	108.92
4	4	244.16	1343.345	143.345	1200	1198.113	145.232
5	5	279.04	1307.033	107.033	1200	1270.72	36.313
6	6	313.92	1307.033	107.033	1200	1125.506	181.527
7	7	348.8	1307.033	107.033	1200	1233.276	73.757
8	8	383.68	1307.033	107.033	1200	1234.425	72.608
9	9	418.56	1307.033	107.033	1200	1198.113	108.92
10	10	453.44	1307.033	107.033	1200	1307.033	0
11	11	488.32	1307.033	107.033	1200	1270.72	36.313
12	12	523.2	1307.033	107.033	1200	1234.425	72.608
13	13	558.08	1307.033	107.033	1200	1270.72	36.313
14	14	592.96	1307.033	107.033	1200	1234.043	72.9905
15	15	627.84	1307.033	107.033	1200	1234.425	72.608
16	16	662.72	1307.033	107.033	1200	1270.72	36.313
17	17	697.6	1307.033	107.033	1200	1270.72	36.313
18	18	732.48	1307.033	107.033	1200	1270.72	36.313
19	19	767.36	1307.033	107.033	1200	1198.113	108.92
20	20	802.24	1270.72	70.72	1200	1198.113	72.607
21	21	837.12	1234.425	34.425	1200	1198.113	36.312
22	22	872	1270.72	70.72	1200	1234.425	36.295
23	23	906.88	1307.033	107.033	1200	1161.801	145.232
24	24	941.76	1198.113	-1.887	1200	1089.194	108.919
25	25	976.64	1198.113	-1.887	1200	1161.801	36.312

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Sl no.	Slide no	x	dpi	ei	Theoretical dpo	dpo	Deposition
		micron	micron	micron	micron	micron	Micron
26	26	1011.52	1234.425	34.425	1200	1161.801	72.624
27	27	1046.4	1161.801	-38.199	1200	1125.506	36.295
28	28	1081.28	1198.113	-1.887	1200	1161.801	36.312
29	29	1116.16	1198.113	-1.887	1200	1125.506	72.607
30	30	1151.04	1198.113	-1.887	1200	1161.801	36.312
31	31	1185.92	1198.113	-1.887	1200	1161.801	36.312
32	32	1220.8	1198.113	-1.887	1200	1161.801	36.312
33	33	1255.68	1198.113	-1.887	1200	1125.506	72.607
34	34	1290.56	1234.425	34.425	1200	1161.801	72.624
35	35	1325.44	1198.113	-1.887	1200	1161.801	36.312
36	36	1360.32	1234.425	34.425	1200	1198.113	36.312
37	37	1395.2	1198.113	-1.887	1200	1161.801	36.312
38	38	1430.08	1198.113	-1.887	1200	1125.506	72.607
39	39	1464.96	1198.113	-1.887	1200	677.33	520.783
40	40	1499.84	1198.113	-1.887	1200	1161.801	36.312
41	41	1534.72	1198.113	-1.887	1200	1125.506	72.607
42	42	1569.6	1198.113	-1.887	1200	1125.506	72.607
43	43	1604.8	1198.113	-1.887	1200	1125.506	72.607
44	44	1639.36	1198.113	-1.887	1200	1161.801	36.312
45	45	1674.24	1198.113	-1.887	1200	1161.801	36.312
46	46	1709.12	1198.113	-1.887	1200	1161.801	36.312
47	47	1744	1198.113	-1.887	1200	1161.801	36.312
48	48	1778.88	1270.72	70.72	1200	1125.506	145.214
49	49	1813.76	1198.113	-1.887	1200	1161.801	36.312
50	50	1848.64	1198.113	-1.887	1200	1161.801	36.312
dpi = pore diameter before deposition							
dpo = pore diameter after deposition							
ei = error due to drilling							
ei = 1200 - dpi							
Deposition = dpi -dpo							
x= distance from open end of hole							
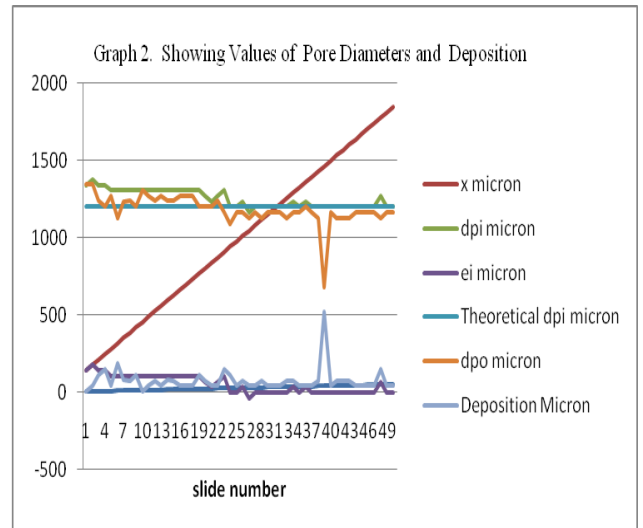
Graph 2. Showing Values of Pore Diameters and Deposition
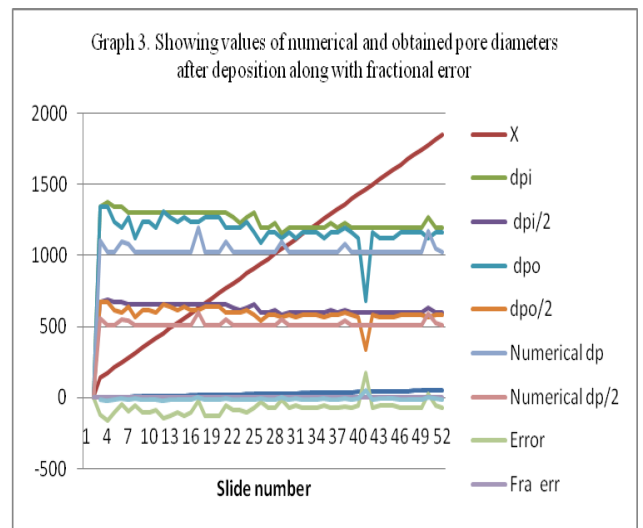
Graph 3. Showing values of numerical and obtained pore diameters after deposition along with fractional error

CONCLUSION

The work was aimed primarily on the development of computational toolbox using Numerical Solution methods for the modeling and simulation of Isothermal Two-dimensional Chemical Vapor Infiltration process used for the densification of Carbon- Carbon composites. The study was done at Composites Entity, VSSC. The process under consideration employs thermal cracking of methane gas to produce solid carbon that diffuses through the porous preform and hence produces a solid carbon matrix. An analysis of the partial differential equations that describes the Chemical Vapor Infiltration processes is presented in this paper. The mathematical model requires partial differential equation, describing the gas phase.

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Computer simulation is done to solve the resulting partial differential equation.

The basic objective of this problem is to obtain a deposition profile, which shows the rate of infiltration/deposition, with a prescribed amount of uniformity, in the shortest possible time. Dusty gas model is used for modeling this work. Experimentally a cylindrical pore in a graphite block is densified by carbon deposition. Using MATLAB code, the deposition at various positions of the hole is predicted. This value is compared with experimental work using Micro CT scanning technique. Slight variation around ten percentage is viewed which may be due to errors in drilling the hole, measuring the pore diameters etc.

The understanding of CVI process has been substantially increased by the efforts to model the various systems. The complex, interactive phenomena in CVI are difficult to represent. However, a combination of insightful modeling with key experimental efforts in delineating has been very fruitful. There can be substantial improvements in processing time and best deposition patterns can be predicted if this work is extended, considering different reaction rates. Scale up of the CVI process is generally successful, with current efforts focused on tubular components.

SCOPE OF FUTURE WORK

The aim of this thesis is primary the construction of the software tools to implement high-dimensional simulation and model reduction studies. There are many improvements that can build on this work.

8.1 Improvements in the Numerical Technique

For more number of iterations the computational steps become more time consuming. Therefore, important progress can be made by some improvements on the design and coding of the computing algorithm, which reduces the working time.

8.2 Advanced Programming Approach

Based on a Sun Sparc ultra-10 workstation, the time integration of the CVI problem can be less time consuming, if object-oriented programming frame work is implemented. Development in an Object-Oriented approach to organize the physical parameters will increase the software reuse. The goal is to create a framework that would require the least possible changes that needed to be made when the user switches from one simulation problem to a different one. Development of Object-Oriented methods for a "heterogeneous" BVP based simulation problems, where the BVPs are defined on separate physical domains; Integration of Object-Oriented based MWR techniques with MATLAB optimization,

control, and other toolboxes etc. are also some suggested methods

8.3 Extension to different geometries of Carbon Preform

The present work is done for a two-dimensional cylindrical co-ordinate perform. The same methods of simulation can be extended to more commonly used Cartesian co-ordinates and also for more complex spherical co-ordinates. The changes occur in the case of continuity equations only. The modeling theories and the codes used will be similar. With the use of highly sophisticated software tools like ANSYS, the modeling and simulation can be done for irregular geometries. Steady state considerations will be simpler than dynamic approach. The complexity of the system can be varied from two-dimensional to three-dimensional. Optimization of the process parameters as temperature and pressure will also be an important advancement in this field.

8.4 Improvements in the CVI Modeling

One of the drawbacks of the isothermal CVI process is its long reaction time. This can be overcome by using a thermal-gradient system. In a thermal gradient CVI process, the highest temperature is at the center of the preform, or at one end, depending on the heating mechanism. The reactant gas diffuses through the perform from the cold to the hot surface. This allows the reactant gases to diffuse to the hot end before reacting to deposit the matrix at the hot end. If the gradients are large enough, a moving densification front is created so that dense matrix grows from the hot end to the cool end of the preform. A higher deposition rate than for isothermal processes can be achieved without the 'canning' problem with such a process. To model a CVI process with thermal gradients, the improvement to be done is the addition of a temperature governing equation.

Also by considering the rate of reaction as a variable with respect to time (t) and distance from open end of the pore(x), the rate of deposition can be predicted numerically.

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