



## Modeling of Fiber Treatment Process

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### Background:

Air thermosetting (stabilization) of carbon fibers involves mass transport of oxygen to and within the fiber bundle as well as reaction of  $O_2$  with aliphatic and aromatic carbon. The forced air convection is used to first heat the fiber and then to remove the heat evolved by oxidation. The overall rate of stabilization is determined by a combined rate for the transport and reaction processes.

Figure 1 shows how a single fiber, which has a length much greater than its diameter, is in contact with heat and oxygen during the stabilization process. These fibers are bundled loosely together in the process.

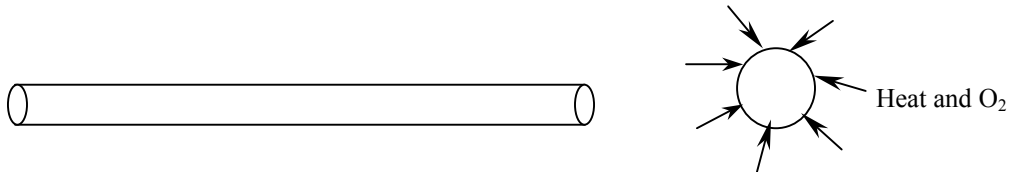


Figure 1. Illustration of Stabilization Process on a Single Fiber

A mathematical model has been set up to simulate the heat and mass balances involved in stabilization. The set of equations along with the boundary and initial conditions is solved numerically using finite difference method with either Tri-diagonal Matrix or Newton-Raphson Algorithm. The software is written in C++.

## Challenge

In order to predict the effects of various process conditions on efficiency, we need to vary parameter values within a wide range. But such change often results in oscillation in computer calculation. It should be noted that there are no programming errors in the software. We would like to optimize the software so that the computer calculation can maintain its stability over a wide range of parameter values, and we would like to accomplish this goal by developing a numerical scheme (i.e. algorithm, discretization method, step size) based on the mathematical behavior of our equations.

## Model Description

### Mass Transfer in Stabilization

	Gas Phase	Fiber
Governing equation	$\frac{\partial q}{\partial t} + u \frac{\partial q}{\partial x} = -\frac{2(1-\varepsilon)}{R\varepsilon} D \frac{\partial C_A}{\partial r} \Big _{r=R}$	$\frac{\partial C_A}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} (rD' \frac{\partial C_A}{\partial r}) - kC_A$
Initial & boundary conditions	$\frac{dq}{dx} = 0 \text{ at } x = X$ $q = q_0 \text{ at } x = 0$ $q = q_0 \text{ at } t = 0$	$\frac{dC_A}{dr} = 0 \text{ at } r = 0$ $C_A = Kq \text{ at } r = R$ $C_A = 0 \text{ at } t = 0$

### Heat Transfer in Stabilization

	Gas Phase	Fiber
Governing equation	$\tau \frac{\partial T}{\partial t} + \tau u \frac{\partial T}{\partial x} = -\beta(T - T_s)$	$\frac{\partial T_s}{\partial t} = \beta(T - T_s) + \frac{H(T_s, t)}{c_{p,\text{fiber}}} + \alpha \frac{\partial^2 T_s}{\partial x^2}$
Initial & boundary conditions	$\text{at } t=0, T = T_0 \text{ for all } x$ $\text{for } t>0, T = T_\infty(t) \text{ at } x=0$ $\text{for } t>0, \frac{dT}{dx} = 0 \text{ at } x=X$	$\text{at } t=0, T_s = T_0 \text{ for all } x$ $\text{for } t>0, \frac{dT_s}{dx} = 0 \text{ at } x=0$ $\text{for } t>0, \frac{dT_s}{dx} = 0 \text{ at } x=X$

## Notation

Symbol	Definition	Unit
$C_A$	Free O <sub>2</sub> concentration in fiber	g/cm <sup>3</sup>
$q$	O <sub>2</sub> concentration in gas phase	wt/wt
$q_0$	Initial O <sub>2</sub> concentration in gas phase	wt/wt

k	Oxidative reaction rate coefficient	1/s
u	Linear velocity of gas	cm/s
K	Equilibrium partition coefficient for O <sup>2</sup> in gas-fiber system	
ε	Percentage of void volume in fiber mat	
ρ	Gas phase density	g/cm <sup>3</sup>
T <sub>0</sub>	Temperature at which stabilization starts	K
T <sub>∞</sub>	Ambient temperature	K
T	Temperature of gas within fiber mat	K
T <sub>s</sub>	Fiber temperature	K
H(T <sub>s</sub> , t)	Oxidative reaction enthalpy	cal/g-s