

**PACKAGE ID** - 001196IBMPC00 GTCVI

**KWIC TITLE** - Simulates the Forced-Flow Chemical Vapor  
Infiltration in Steady State

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**LIMITATION CODE** -UNL                   **AUDIENCE CODE** - UNL

**COMPLETION DATE** - 10/01/1996   **PUBLICATION DATE** - 10/01/1996

**DESCRIPTION** - GTCVI is a finite volume model for steady-state simulation of forced-flow chemical vapor infiltration in either Cartesian or cylindrical coordinates. The model solves energy and momentum balances simultaneously over a given domain discretized into an array of finite volume elements. The species balances and deposition rates are determined after the energy and momentum balances converge. Density-dependent preform properties are included in the model. Transient average density, backpressure, temperature gradient, and average radial deposition rates can be summarized. Optimal infiltration conditions can be found by varying temperature, flow, and reactant concentration.

**PACKAGE CONTENTS** - Media Directory: Software Abstract; User's Manual:  
Media Includes Source Code, Programmer Documentation;

**SOURCE CODE INCLUDED?** - Yes

**MEDIA QUANTITY** - 1 3.5 Diskette

**METHOD OF SOLUTION** - GTCVI solves a set of linear algebraic equations using a finite-difference method over the discretized domain specified. The energy and momentum balances are coupled. Therefore, an initial guess for the temperature is given and solution of the energy balance calculated. The momentum balance is then solved for the pressure using the calculated temperature values. The convergence criteria are then checked for both temperature and pressure. If either criterion is not reached, then the pressure values are then used in re-solving the energy balance for temperature. This iterative scheme is performed until both the temperature and pressure values meet the specified convergence criteria. Then, the species balance is then solved using the converged temperature and pressure values. A deposition rate is then calculated and assumed constant throughout a specified time interval (30 min., 2 hours, etc.)

**COMPUTER** - IBM PC

**OPERATING SYSTEMS** - Windows 95, Windows NT, or Macintosh operating  
system

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**PROGRAMMING LANGUAGES** - Fortran 77

**SOFTWARE LIMITATIONS** - Each transient file produced by GTCVI is approximately 1 MB in size. Each model simulation is about 30 MB in size. The memory needed for the source code is negligible (less than 1 MB). The Fortran compiler must recognize the Fortran 77 programming language.

**SOURCE CODE AVAILABLE (Y/N)** - Y

**UNIQUE FEATURES** - Chemical vapor infiltration can be simulated in either Cartesian or cylindrical coordinates. The discretization of the domain, material and gas parameters, deposition kinetics, and time interval lengths can be input into the model. Summaries of transient average density, backpressure, temperature gradient, and deposition rate profiles can be constructed from the model output for analysis. Also steady-state density, temperature, and reactant concentration profiles can be produced at any given time step.

**RELATED SOFTWARE** - A spreadsheet (Microsoft Excel, Corel Quatro Pro, Lotus 1-2-3, etc.) and a graphing package can be used to plot the transient and steady-state profiles.

**OTHER PROG/OPER SYS INFO** - The extension for an input file is .INP. The input file name can contain a minimum of six characters. The extension for a material file is .MAT. The extension for a gas file is .GAS. The input, material, and gas files must follow the format described in the GTCVI manual.

**HARDWARE REQS** - At least 16 MB of RAM memory and 1 GB of hard drive space are suggested. If a spreadsheet and/or graphing package is used, extra RAM will help in multitasking. A processing speed greater than 80 MHz is suggested.

**TIME REQUIREMENTS** - A typical model simulation can take anywhere from 30 minutes to 2 1/2 hours for a 266 MHz processor. Of course, the total simulation time depends on the processor speed.

**ABSTRACT STATUS** - Released AS-IS 2/25/98

**SUBJECT CLASS CODE** - HZ

**KEYWORDS** -

COMPUTER PROGRAM DOCUMENTATION  
G CODES  
CHEMICAL VAPOR DEPOSITION  
STEADY-STATE CONDITIONS  
FINITE DIFFERENCE METHOD  
CARTESIAN COORDINATES

**EDB SUBJECT CATEGORIES** -  
990200

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SOFTWARE ABSTRACT

PAGE 3

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**SPONSOR** - DOE/FE

**PACKAGE TYPE** - AS - IS