PACKAGE ID - 000387CY0MP00 CHAINT

KWIC TITLE - Contaminant Transport in Fractured Media

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

COMPLETION DATE - 03/01/1989 **PUBLICATION DATE -** 12/01/1985

DESCRIPTION - CHAINT was developed to simulate two-dimensional contaminant transport within thermally driven flow fields in the deep basalts in the Paco Basin at the Westinghouse Hanford Site. The program is designed to compute the transient, spatial distribution of contaminant concentrations subsequent to their release into the geosphere. CHAINT simulates radionuclide transport through a saturated, porous medium considering the effects of contaminant diffusion, advective transport, dispersion, radionuclide chain decay coupling, retardation, and volumetric mass injection. Boundary conditions may be fixed or set to a 'zero normal flux' value. Zoning can be used to reduce the problem size. Output includes a printed report of contaminant concentrations together with graphics files for postprocessing. CHAINT input is prepared automatically via several preprocessors and the output can be displayed in various forms using graphics postprocessors. The Q2DGEOM preprocessor was developed to generate, modify, plot and verify quadratic two-dimensional finite-element geometries. The BXGEN preprocessor generates the boundary conditions for head and temperature and ICGEN generates the initial conditions. The GRIDDER postprocessor interpolates nonregularly spaced nodal contaminant concentration data onto a regular rectangular grid. The GRIDDER output is then read by CONTOUR and PARAM. CONTOUR plots and labels contour lines for a function of two variables and PARAM plots cross sections and time histories for a function of time and one or two spatial variables. CHTFLX differentiates the concentration and hydraulic head data from the mass flux file and computes and plots mass flux and total flux of a contaminant through a surface of finite elements. NPRINT generates data tables that display the data along horizontal or vertical cross sections.

PACKAGE CONTENTS - NESC Note; Software Abstract; RHO-BW-CR-144P;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 CD Rom

METHOD OF SOLUTION - CHAINT is a two-dimensional finite-element numerical model designed to simulate transient migration of dissolved radionuclide mass in a saturated, fractured, porous

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METHOD OF SOLUTION -(CONT) medium. The steady-state process can be simulated as the asymptotic limit of the transient process. The finite-element approach permits the use of a graded mesh to accurately represent the spatial domain and its boundaries. This minimizes the space truncation error and optimizes the computational problem. The governing mass balance equation is solved using a Galerkin finite element method and a block diagonal frontal solution technique. This method allows substantial flexibility in discretization of the spatial domain. The computational network consists of both quadrilateral and triangular elements to define the continuum regions of the simulation domain, and line elements to represent the discrete fractures within the domain. Continuum portions of the medium are simulated using two-dimensional isoparametric elements, and discrete features are modeled with one-dimensional elements that are embedded along the sides of the continuum elements. The Hood frontal solution algorithm is used to solve unsymmetric finite-element matrix equations. CHAINT is numerically stable for flow/diffusion problems with a Peclet number of less than 0.5. Within line elements with larger peclet numbers, an upwinding scheme is used to improve the accuracy and stability of the solution. The simulation domain may be modeled in two cartesian dimensions or in a three-dimensional axisymmetric radial coordinate system.

COMPUTER - CRAY X-MP

OPERATING SYSTEMS - UNICOS 3.0

PROGRAMMING LANGUAGES - FORTRAN 77

SOFTWARE LIMITATIONS - Maxima of 10,000 nodes, 5,000 finite elements, 310 nodes along flux surfaces, 140 solution matrix front width, 50 elements flux surface, 50 source loading times, 25 material types, 25 time intervals, 15 traceback files, 10 flux surfaces, 6 contaminants, 5 binary input files, and 3 parents nuclide. The number of nodes define the element: 8 nodes specify a quadratic shape, 6 nodes specify a triangular shape, and 3 nodes specify a linear element. The element aspect ratio affects the accuracy of the results and should be kept to a value below 100.

SOURCE CODE AVAILABLE (Y/N) - Y

RELATED SOFTWARE - CHAINT uses the fluid flow fields generated by MAGNUM-2D to calculate the advective component of the mass transport process.

OTHER PROG/OPER SYS INFO - CHAINT requires the proprietary CA-DISSPLA graphics library to utilize the graphics post processor. This program is not included.

REFERENCES - Niell W. Kline, Richard L. England and Robert G. Baca, CHAINT Computer Code: Users Guide, RHO-BW-CR-144P, December 1985;

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REFERENCES -(CONT) CHAINT Cray Version Tape Description and Implementation Information, National Energy Software Center Note.

ABSTRACT STATUS - Abstract first distributed August 1989. CRAY X-MP version submitted October 1988, replaced March 1989.

SUBJECT CLASS CODE - R

KEYWORDS -
C CODES
RADIOACTIVITY TRANSPORT
NEWTON METHOD
ENVIRONMENTAL TRANSPORT
POROUS MATERIALS
RADIONUCLIDE MIGRATION
RADIOACTIVE WASTE MANAGEMENT
MASS BALANCE
RADIOACTIVE WASTE FACILITIES
RADIOACTIVE WASTE STORAGE
RADIOACTIVE WASTE DISPOSAL
ADVECTION
DISPERSIONS
MASS TRANSFER
FINITE ELEMENT METHOD
WASTE-ROCK INTERACTIONS
COMPUTER PROGRAM DOCUMENTATION

EDB SUBJECT CATEGORIES -
990200 540230

SPONSOR - DOE/RW

PACKAGE TYPE - SCREENED