PACKAGE ID - 000223D078000 CFEST1.1

KWIC TITLE - Coupled Fluid Energy Solute Transport

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

COMPLETION DATE - 10/01/1988 **PUBLICATION DATE -** 10/01/1987

DESCRIPTION - CFEST is a Coupled Fluid, Energy, and Solute Transport code for the study of a multilayered, nonisothermal ground-water system. It can model discontinuous as well as continuous layers, time-dependent and constant source/sinks, and transient as well as steady-state flow. The finite element method is used for analyzing isothermal and nonisothermal events in a confined aquifer system. Only single-phase Darcian flow is considered. In the Cartesian coordinate system, flow in a horizontal plane, in a vertical plane, or in a fully three-dimensional region can be simulated. An option also exists for the axisymmetric analysis of a vertical cross section. The code employs bilinear quadrilateral elements in all two dimensional analyses and trilinear quadrilateral solid elements in three dimensional simulations. The CFEST finite element formulation can approximate discontinuities, major breaks in slope or thickness, and fault zones in individual hydrogeologic units. The code accounts for heterogeneity in aquifer permeability and porosity and accommodates anisotropy (collinear with the Cartesian coordinates). The variation in the hydraulic properties is described on a layer-by-layer basis for the different hydrogeologic units. Initial conditions can be prescribed hydraulic head or pressure, temperature, or concentration. CFEST can be used to support site, repository, and waste package subsystem assessments. Some specific applications are regional hydrologic characterization; simulation of coupled transport of fluid, heat, and salinity in the repository region; consequence assessment due to natural disruption or human intrusion scenarios in the repository region; flow paths and travel-time estimates for transport of radionuclides; and interpretation of well and tracer tests.

PACKAGE CONTENTS - NESC Note; Software Abstract; BMI/ONWI-660; Media Includes Source, Sample Problems, Machine Readable Documentation, Control Information;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 CD Rom

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METHOD OF SOLUTION - CFEST solves partial differential equations (PDEs) for pressure, temperature, and solute concentration for large, multilayered, natural hydrologic systems using the finite element method. These equations are coupled with fluid properties of density and viscosity. The relationship between porosity and pore-water pressure is also taken into account. The algorithm used to solve this coupled set of PDEs is based on linearization of the coupled equations. The scheme utilized to solve the resulting large, sparse matrices involves two matrices, one to store only nonzero coefficients and the other to identify the column associated with these coefficients. Vectors containing the first and last rows associated with each column are used to limit operations to only the required number of rows of the system matrix. For constant time steps and steady-state flow (ignoring density variation effects), the equation solver uses a back substitution scheme. When density or viscosity effects are considered, a new system matrix is developed and solved at each time step. The latest known values of pressure, temperature, and solute concentration are used to compute fluid and aquifer properties.

COMPUTER - DEC VAX11/780

OPERATING SYSTEMS - VMS 4.1; VMS 5.1

PROGRAMMING LANGUAGES - FORTRAN V

SOFTWARE LIMITATIONS - Maxima of 4000 nodes, 4000 elements, 1000 surface nodes, 1000 surface elements, 999 grid points, 100 element sources, and 100 element sinks. CFEST is primarily designed for a confined aquifer system. Unconfined steady-state and transient solutions can be obtained by iterative execution and upgrading the top elevation of the saturated zone. Variable density solutions are obtained by iterative substitution. The user must set appropriate limits for updating fluid density to avoid steady-state transport solutions that may cause oscillatory results. Multidimensional transport of a single radionuclide is supported. Radionuclide chain migrations are not simulated.

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - Data for physical quantities is accepted in any consistent system of units. The user can specify the conversion factors for coordinates, hydraulic conductivity/permeability, head, temperature, and concentration data to develop a consistent set of units for internal use. Restart capabilities allow continuation from any previously completed time step or simulation.

RELATED SOFTWARE - CFEST was originally developed in a DEC PDP11/70 version for the DOE Underground Energy Storage Program as an extension of the PDP11 version of FE3DGW.

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RELATED SOFTWARE -(CONT)
OTHER PROG/OPER SYS INFO - The auxiliary plotting programs make calls to proprietary CalComp software; this software is not included.

TIME REQUIREMENTS - NEADB executed the sample problem in less than 2 CPU minutes on a DEC VAX8810.

REFERENCES - Sumant K. Gupta, Charles R. Cole, Charles T. Kincaid, and Amy M. Monti, Coupled Fluid, Energy, and Solute Transport (CFEST) Model: Formulation and User's Manual, BMI/ONWI-660, October 1987; CFEST1.1, NESC No. 9537, CFEST1.1 Tape Description, National Energy Software Center Note 89-02, October 25, 1988.

ABSTRACT STATUS - Abstract first distributed October 1988. DEC VAX11/780 version submitted March 1988, sample problems executed by NEADB November 1990 on a DEC VAX8810.

SUBJECT CLASS CODE - R

KEYWORDS -
COMPUTER PROGRAM DOCUMENTATION
C CODES
DARCY LAW
GROUND WATER
THREE-DIMENSIONAL CALCULATIONS
RADIOACTIVE WASTE DISPOSAL
FLUID FLOW
SITE CHARACTERIZATION
AQUIFERS
FINITE ELEMENT METHOD
PARTIAL DIFFERENTIAL EQUATIONS
HYDROLOGY

EDB SUBJECT CATEGORIES -
990200 052002 540330

SPONSOR - DOE/RW

PACKAGE TYPE - SCREENED