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A Compendium of Fracture Flow Models — 1994

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A Compendium of Fracture Flow Models — 1994

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Abstract

The report is designed to be used as a decision-making aid for individuals who need to simulate fluid flow in fractured porous media. Fracture flow codes of varying capability in the public and private domain were identified in a survey of government, academia, and industry. The selection and use of an appropriate code requires conceptualization of the geology, physics, and chemistry (for transport) of the fracture flow problem to be solved. Conceptual models that have been invoked to describe fluid flow in fractured porous media include explicit discrete fracture, dual continuum (porosity and/or permeability), discrete fracture network, multiple interacting continua, multipermeability/multiporosity, and single equivalent continuum. The explicit discrete-fracture model is a "near-field" representation, the single equivalent continuum model is a "far-field" representation, and the dual-continuum model is intermediate to those end members. Of these, the dual-continuum model is the most widely employed. The concept of multiple interacting continua has been applied in a limited number of examples. Multipermeability/multiporosity provides a unified conceptual model. The ability to accurately describe fracture flow phenomena will continue to improve as a result of advances in fracture flow research and computing technology. This improvement will result in enhanced capability to protect the public environment, safety, and health.

1 Introduction

1.1 Background

This report contains summaries of numerical models describing fluid flow in fractured porous media. In addition, a brief overview of the pertinent concepts relating to fracture flow modeling is provided. The emphasis is on applications that support field-scale problem solving. The intent is to provide a stand-alone document as an aid to the individual confronted with a problem that requires fracture flow modeling. Identifying pertinent physical and chemical processes, developing a conceptual hydrogeologic model, and recognizing appropriate field data requirements are critical to successful modeling. Having accomplished those fundamental tasks, the investigator will be able to identify which of the codes herein most nearly satisfies the required simulation criteria.

Government, academia, and industry were surveyed to identify all available fracture flow codes. The capabilities, assumptions, limitations, and availability of fracture flow codes from these entities are outlined in Table 1 (pages 10–13) and summarized in Appendix A. Appendix B lists codes sorted by custodian. Appendix C describes code custodians, their support policies, and pricing structures (where variable). Appendix D lists select references sorted by code. Appendix E lists codes that were identified but unavailable.

1.2 How to Use This Document

Follow the procedure outlined below to identify fracture flow codes that will satisfy your required simulation criteria.

1. After completing hydrogeologic data acquisition and site characterization and identifying all physical and chemical processes of interest, identify an appropriate conceptual model of fracture flow.
2. Read this document.
3. Identify potentially suitable codes from Table 1.
4. Consult Appendix A for expanded descriptions of the codes identified in step 3.
5. Of the codes that remain suitable, consult the code custodian to verify that the code satisfies the required simulation criteria. Because the availability, capabilities, and limitations of many of these codes may change, this final check is important.

2 Overview of Fracture Flow Models

Research into the nature of fluid flow in fractures and multiphase fluid flow has been conducted by petroleum engineers, mining engineers, and hydrogeologists. In the past, economic resource evaluation and production were the motivation for these studies. Today, that motivation is fueled by worldwide concerns about radioactive waste isolation and migration.

Research on fluid flow in fractures and in fractured porous media has a history that spans nearly four decades (Barenblatt et al. 1960; Warren and Root 1963). This research has focused on four principal aspects of fracture flow: (1) development of conceptual models, (2) development of analytical and numerical solution schemes, (3) description of fracture hydraulic characteristics in static and deforming media, and (4) development of stochastic techniques to describe fracture flow and hydrogeologic parameter distributions. Bear et al. (1993) extensively review the research on fracture flow phenomena.

2.1 Conceptual Models of Fracture Flow

Researchers have developed several conceptual models describing fluid flow in fractured porous media. Fundamentally, each method can be distinguished on the basis of the storage and flow capabilities of the porous medium and the fracture. The storage characteristics are associated with porosity, and the flow characteristics are associated with permeability. Four conceptual models have dominated the research: (1) *explicit discrete fracture*, (2) *dual continuum*, (3) *discrete fracture network*, and (4) *single equivalent continuum*. In addition, multiple-interacting continua and multiporosity/multipermeability conceptual models have been recently introduced in the literature.

Further distinctions can be drawn on the basis of the spatial and temporal scales of integration or averaging of the flow regime. Bear and Berkowitz (1987) describe four scales of concern in fracture flow: (1) the *very near field*, where flow occurs in a single fracture and porous medium exchange is possible; (2) the *near field*, where flow occurs in a fractured porous medium and each fracture is described in detail; (3) the *far field*, where flow occurs in two overlapping continua with mass exchanged through coupling parameters; and (4) the *very far field*, where fracture flow occurs, on average, in an equivalent porous medium.

2.1.1 Explicit Discrete Fracture Formulation

Several investigators have published numerical models incorporating explicit discrete representations of fractures. TRACR3D (Travis 1984) incorporates fractures explicitly, but this model is restricted to fractures with vertical or horizontal orientation. The most recent version of the Sandia Waste Isolation Flow and Transport (SWIFT) model incorporates options for discrete fractures or dual porosity (Intercomp 1976; Ward et al. 1993). The advantage of explicit

discrete-fracture models is that they allow for explicit representation of fluid potential gradients and fluxes between fractures and porous media with minimal non-physical parameterization. However, data acquisition can become onerous where large numbers of fractures occur. Also, as the complexity of the model domain increases with increasing numbers of fractures, the computational burden increases significantly.

2.1.2 Dual-Continuum Formulation

Dual-continuum approaches were introduced by Barenblatt et al. (1960) and later extended by Warren and Root (1963). Dual-continuum models are based on an idealized flow medium consisting of a primary porosity created by deposition and lithification and a secondary porosity created by fracturing, jointing, or dissolution (Warren and Root 1963). The basis of these models is the observation that unfractured rock masses account for much of the porosity (storage) of the medium, but little of the permeability (flow). Conversely, fractures may have negligible storage, but high permeability. The porous medium and the fractures are envisioned as two separate but overlapping continua. Fluid mass transfer between porous media and fractures occur at the fracture-porous medium interface. In some numerical approaches, the mass transfer is lumped at the nodes common to the fracture and porous medium grids. The transfer occurs according to a fluid-potential-dependent coupling parameter. This approach averages or "smears" the transient response between fracture and porous medium (Elsworth, D., pers. comm.). Huyakorn et al. (1983) describe a number of different formulations of the coupling parameter.

2.1.3 Discrete-Fracture Network

Discrete-fracture-network models describe a class of dual-continuum models in which the porous medium is not represented. Instead, all flow is restricted to the fractures. This idealization reduces computational resource requirements. Fracture "legs" are often represented as lines or planes in two or three dimensions. Some codes allow for variable coupling at the fracture-leg intersections and for multiple legs to connect at a single location. For contaminant transport, some network models allow for diffusion between the fracture and porous medium.

2.1.4 Single Equivalent Continuum Formulation

The volume of interest is considered to be large enough that, on average, permeability is a sum of fracture and porous media permeability. This approximation substantially simplifies the flow problem. Pruess et al. (1986) presented a model for a single equivalent continuum in unsaturated fractured rock in which hydraulic conductivity was taken as a sum of hydraulic conductivity from the porous medium and the fracture. Pruess et al. (1990a,b) found that this approach was unacceptable in the presence of rapid flow transients, large fracture spacings, or with a very low permeability rock matrix. In broad terms, where the scales of integration are sufficiently large, the single equivalent continuum approximation will do a fair job of conserving

fluid mass. It may, however, be a poor predictor of spatial and temporal distributions of contaminant fluxes.

2.1.5 Alternative Conceptual Models

Recently, Bai et al. (1993) introduced a unified multiporosity/multipermeability approach to modeling flow in fractured porous media. They illustrate that single porosity/single permeability, dual porosity/single permeability, dual porosity/dual permeability, dual porosity/triple permeability, and triple porosity/triple permeability are all just special cases of a generalized multiporosity/multipermeability description. Consistent with Bai et al. (1993), Bear (1993) pointed out that different geologic and environmental processes can produce multiple distinct fracture subsystems in a common domain. In that case, each distinct subsystem might be modeled as a separate continuum within a single numerical model, provided a common representative elementary volume (REV) exists. A multiple-interacting continua approach has been proposed and implemented by Pruess and Narasimhan (1982, 1985) and Pruess (1991). In their approach, matrix grid blocks are divided into nested subdomains to accommodate slow changes in fluid pressures, temperatures, and phase compositions, which are strongly a function of distance from the fracture. One-dimensional calculations are then used to determine the solution within the porous block domain.

2.2 Fracture Flow in Deforming Media

Iwai (1976), Witherspoon, et al. (1980), Elsworth (1989), and Bai et al. (1993) have developed models describing fluid flow in fractured media undergoing deformation. SANGRE (Anderson 1986) simulates fluid flow and heat transport in a grid that can rotate, translate, and deform over time. The ductile and brittle deformation processes are simulated where faulting can occur on pre-defined slip-planes. SANGRE was designed to simulate the formation of petroleum reservoir traps over tens of millions of years. At high rates of media deformation, or over long periods, changing material properties can significantly impact fluid potential fields and fluxes.

2.3 Unsaturated and Multiphase Flow

Several of the codes in this review can simulate unsaturated flow. In this report, *unsaturated or variably saturated* is used to mean flow of a single phase (usually water) where that phase does not fully saturate the fractured porous media. Often, the mathematical equation solved takes the form of the well-known Richards equation. *Multiphase* is used to mean miscible or immiscible coupled flow of two or more phases.

The TOUGH family of codes (Pruess 1987, 1991) simulates nonisothermal multiphase flow in fractured porous media by using one of five equations of state, depending upon the

phases present. TRACER3D (Travis and Birdsell 1991) supports saturated, unsaturated, and multiphase flow. PORFLOW (Runchal 1994) also supports saturated, unsaturated, and multiphase flow. Huyakorn and Pinder (1978) and Kaluarachi and Parker (1989) evaluated how effectively several numerical approaches solve porous media multiphase flow equations by using finite elements. Diodato and Filley (1989), Filley et al. (1991), and Filley and Diodato (1993) employed the Implicit Pressure-Explicit Saturation (IMPES) finite-difference numerical technique (Aziz and Settari 1979) and analytical equations of state (van Genuchten 1980) to investigate multiphase fluid flow and contaminant transport in two-dimensional, anisotropic, heterogeneous porous media.

Diodato (1994) proposed a simulator for multiphase flow in fractured porous media on the basis of an explicit discrete fracture conceptual model. The code allows for fractures and geologic units at any orientation and provides built-in grid visualization capabilities. Reitsma and Kueper (1994) quantified capillary pressure as a function of saturation in a fracture in the laboratory. They found the Brooks-Corey (Brooks and Corey 1964, 1966) porous-media capillary pressure-saturation relationship to be suitable for describing this phenomenon in a fracture. Glass (1993) and Nicholl and Glass (1993) investigated in-fracture unsaturated flow instabilities by using physical and numerical models. They observed viscous fingering and zones of persistent entrapped air in a series of vertical and horizontal imbibition and drainage experiments.

2.4 Stochastic Methods

As an alternative to deterministic models, some investigators have used stochastic methods of characterizing fracture occurrence and flow in fractures. For example, de Marsily (1986) describes stochastic partial differential equations in which one or more of the parameters is a random variable. In addition, he gives several approaches to solutions. Given a sufficient data set and an appropriate distribution, the statistical moments of fracture occurrence, orientation, spacing, and aperture can be described. From these values, equivalent statistical models of fracture fields can be generated. Shimo and Long (1987) and Long (1989) have generated stochastic fracture fields by working from several different conceptual models. Neuman (1982) summarizes statistical approaches to aquifer characterization. Rouleau (1988) used the codes NETFLO/NETTRANS to simulate flow and transport in a stochastically generated discrete-fracture network. The FracMan/MAFIC code package includes stochastic fracture-network generators.

3 Numerical Methods

Research on solving fracture flow problems has included both analytical and numerical solution schemes. Because this document is not a mathematical reference, equations and solution schemes employed are not listed. Streltsova-Adams (1978) describes several analytical solutions for flow in fractured rock. Elsworth (1984) describes several analytic solutions to particular flow geometries and laminar or turbulent flow. A summary of some of the numerical approaches used can be found in Ababou (1991). Amadei and Illangasekare (1992) employed integral transforms to generate continuous expressions for fluid potential in rectangular joints. Their approach allowed for anisotropy and heterogeneity in fracture aperture and roughness and provided an analytical vehicle for the study of the cubic law. Because of the integral transform, the fracture volume did not have to be discretized. The volume itself, however, was restricted to simple geometries. More recently, Amadei and Illangasekare (1994) have expanded the method to investigate solute transport phenomena. Pinder et al. (1993) provide several analytical and numerical formulations describing fracture flow.

Differential and integral numerical methods for solving the material balance equations describing mass flow and transport in fractured porous media have been employed. For the spatial derivatives, integral methods have enjoyed more widespread use than the differential approach of the finite difference method (FDM), partly because they are amenable to irregular domain geometries. Integral methods used in fracture flow modeling include the finite-element (FEM) method and the boundary-element method (BEM). Elsworth (1984, 1987) presented a hybrid BEM-FEM procedure for simulating fracture flow problems. Rasmussen (1987) used BEM to simulate unsaturated flow in discrete fracture networks. Additionally, integrated finite-difference methods (IFDM) have been presented and applied (Edwards 1972; Narasimhan and Witherspoon 1976; Pruess 1987, 1991). Temporal derivatives are commonly treated implicitly by using a Crank-Nicholson approximation. To eliminate problems of instability at high Peclet numbers, Sudicky and McLaren (1992) used a Laplace transform technique to explicitly solve for any desired time.

4 Review Criteria

Fracture flow codes were reviewed with respect to their availability, capabilities, and limitations. Because many of the codes have the capability of modeling contaminant transport, categories describing those capabilities are included in the review. Fundamental capabilities with respect to flow and transport are summarized in Table 1. Detailed descriptions of the flow and transport capabilities and other information are included in Appendix A. The meaning of the categories and responses in Table 1 is described below.

<i>Availability</i>	Cost in U.S. or Canadian (where indicated) dollars. The Energy Science and Technology Software Center (ESTSC) pricing varies by customer and is indicated with an "E." Some of their codes may not be available to non-U.S. citizens. "Yes" means that the code is available for a nominal charge, in some cases at no cost. Consult the custodian descriptions in Appendix C for more information about individual pricing policies.
<i>Flow Model</i>	
<i>Dimensionality</i>	The number of spatial dimensions modeled.
<i>Conceptual Model</i>	"EX" explicit discrete fracture, "DU" dual continuum, "NE" discrete fracture network, and "EQ" equivalent porous medium.
<i>Steady-State</i>	"Yes" means that steady-state flow can be simulated.
<i>Transient</i>	"Yes" means that transient flow can be simulated.
<i>Heterogeneous</i>	"Yes" means that the conductive medium can be heterogeneous.
<i>Anisotropic</i>	"Yes" means that the conductive medium can be anisotropic.
<i>Unsaturated</i>	"Yes" means that the model can simulate unsaturated flow.
<i>Multiphase</i>	"Yes" means that the model can simulate multiphase flow.

Transport Model

Types "S" Solute

"H" Heat

"R" Radionuclides

Advection "Yes" means that the model can simulate advection.

Dispersion "Yes" means that the model can simulate dispersion.

Diffusion "Yes" means that the model can simulate diffusion.

Retardation "Yes" means that the model can simulate retardation.

Sorption "Yes" means that the model can simulate sorption.

Decay "Yes" means that the model can simulate decay.

If a "?" appears in any category, the code vendor did not supply the information.

TABLE 1 Capabilities of the Fracture Flow Codes (see page 8 for explanation of categories)

Model Category	Parameter	Model Name			
		3-D FE DUAL POROSITY FLOW AND TRANSPORT MODEL	BIM/BIM2D BIM3D/FRACGEN	DCM3D	FRAC3DVS
Flow Model	Availability (\$)	40	Yes	Yes	5000CAN
	Dimensionality	3	2, 3	3	3
	Conceptual Model	DU	DU	DU	EX
	Steady-State	No	Yes	No	Yes
	Transient	Yes	No	Yes	Yes
	Heterogeneous	Yes	No	Yes	Yes
	Anisotropic	Yes	No	Yes	Yes
	Unsaturated	No	Yes	Yes	Yes
Transport Model	Multiphase	No	Yes	No	No
	Types	S	S		S, R
	Advection	Yes	Yes		Yes
	Dispersion	Yes	No		Yes
	Diffusion	Yes	Yes		Yes
	Retardation	No	No		Yes
	Sorption	No	Yes		Yes
	Decay	No	No		Yes

Model Category	Parameter	Model Name			
		FRACFLO	FRACFLOW	FracMan/ MAFIC	FRACTRAN
Flow Model	Availability (\$)	E	400	1000	2500CAN
	Dimensionality	2	2	3	2
	Conceptual Model	NE	DU	DU	EX
	Steady-State	Yes	No	Yes	Yes
	Transient	No	Yes	Yes	No
	Heterogeneous	?	Yes	Yes	Yes
	Anisotropic	?	No	No	Yes
	Unsaturated	No	No	Yes	No
Transport Model	Multiphase	No	No	No	No
	Types	R		S, H, R	S, R
	Advection	Yes		Yes	Yes
	Dispersion	Yes		Yes	Yes
	Diffusion	No		Yes	Yes
	Retardation	No		Yes	Yes
	Sorption	No		No	No
	Decay	No		Yes	Yes

TABLE 1 (Cont.)

Model Category	Parameter	Model Name			
		FRANET	FTRANS	MAGNUM-2D	MOTIF
Flow Model	Availability (\$)	Yes	E	E	20000CAN
	Dimensionality	1	2	2	1, 2, 3
	Conceptual Model	NE	DU	EX, DU, EQ	EX
	Steady-State	Yes	No	Yes	Yes
	Transient	Yes	Yes	Yes	Yes
	Heterogeneous	No	Yes	Yes	Yes
	Anisotropic	No	Yes	Yes	Yes
	Unsaturated	No	No	No	Yes
Transport Model	Multiphase	No	No	No	No
	Types		S, H, R	S, H	S, H, R
	Advection		Yes	Yes	Yes
	Dispersion		Yes	Yes	Yes
	Diffusion		Yes	Yes	Yes
	Retardation		Yes	No	No
	Sorption		Yes	Yes	Yes
	Decay		Yes	Yes	Yes
<hr style="border-top: 1px dashed black;"/>					
Model Category	Parameter	Model Name			
		NEFTRAN II	NETFLO/ NETTRANS	PORFLO-3	PORFLOW
Flow Model	Availability (\$)	Yes	30CAN	Yes	995-14995
	Dimensionality	1	2	3	2, 3
	Conceptual Model	NE	NE	EX, EQ	EX, EQ
	Steady-State	Yes	Yes	Yes	Yes
	Transient	Yes	No	Yes	Yes
	Heterogeneous	Yes	No	Yes	Yes
	Anisotropic	No	No	No	Yes
	Unsaturated	Yes	No	Yes	Yes
Transport Model	Multiphase	No	No	No	Yes
	Types	R	S	S, H, R	S, H, R
	Advection	Yes	Yes	Yes	Yes
	Dispersion	No	No	Yes	Yes
	Diffusion	Yes	No	Yes	Yes
	Retardation	No	No	Yes	Yes
	Sorption	No	No	Yes	Yes
	Decay	Yes	N	Yes	Yes

TABLE 1 (Cont.)

Model Category	Parameter	Model Name			
		SANGRE	SEFTRAN	STAFF2D	STAFF3D
Flow Model	Availability (\$)	Yes	800	3000	4000
	Dimensionality	2	2	2	2, 3
	Conceptual Model	EX	EX	EX, DU	EX, DU
	Steady-State	No	Yes	Yes	Yes
	Transient	Yes	Yes	Yes	Yes
	Heterogeneous	Yes	Yes	Yes	Yes
	Anisotropic	?	Yes	Yes	Yes
	Unsaturated	No	No	No	No
Transport Model	Multiphase	No	No	No	No
	Types	H	S, R	S, R	S, R
	Advection	Yes	Yes	Yes	Yes
	Dispersion	No	Yes	Yes	Yes
	Diffusion	No	No	No	No
	Retardation	No	No	No	Yes
	Sorption	No	Yes	Yes	Yes
	Decay	No	Yes	Yes	Yes

Model Category	Parameter	Model Name			
		SWIFT II	SWIFT/486	TOUGH2	TRACR3D
Flow Model	Availability (\$)	Yes	800	E	Yes
	Dimensionality	3	3	1, 2, 3	1, 2, 3
	Conceptual Model	EX, DU	EX, DU	DU	EX, EQ
	Steady-State	Yes	Yes	No	Yes
	Transient	Yes	Yes	Yes	Yes
	Heterogeneous	Yes	Yes	Yes	Yes
	Anisotropic	Yes	Yes	Yes	Yes
	Unsaturated	No	No	No	No
Transport Model	Multiphase	No	No	Yes	Yes
	Types	S, H, R	S, H, R	S, H	S, H, R
	Advection	Yes	Yes	Yes	Yes
	Dispersion	Yes	Yes	No	Yes
	Diffusion	Yes	Yes	No	Yes
	Retardation	No	No	No	No
	Sorption	Yes	Yes	No	Yes
	Decay	Yes	Yes	No	Yes

TABLE 1 (Cont.)

Model Category	Parameter	Model Name			
		TRAFRAP-WT PC-EXT	TRINET	TRUMP	TRUST84
Flow Model	Availability (\$)	100	Yes	E	E
	Dimensionality	2	3	1, 2, 3	1, 2, 3
	Conceptual Model	EX, DU	NE	?	?
	Steady-State	No	No	Yes	Yes
	Transient	Yes	Yes	Yes	Yes
	Heterogeneous	Yes	No	Yes	Yes
	Anisotropic	Yes	No	?	Yes
	Unsaturated	No	No	No	Yes
	Multiphase	No	No	No	No
Transport Model	Types	S, R	S	S, H	
	Advection	Yes	Yes	Yes	
	Dispersion	Yes	Yes	Yes	
	Diffusion	Yes	No	Yes	
	Retardation	No	No	No	
	Sorption	Yes	No	No	
	Decay	Yes	No	No	

5 Conclusions

To select an appropriate flow code, one should carefully consider the geology, physics, and, if appropriate, chemistry of the problem to be solved. Careful consideration of the conceptual model of fluid flow in a fractured rock setting is critical to successful fracture flow modeling. Inherent in this conceptualization is the determination of spatial and temporal scales relevant to the problem. Near-field problems may require explicit discrete fracture flow models, while far-field problems may appropriately employ a single continuum model. For the large number of intermediate situations, dual-continuum models may be used. For cases of chemical or radioisotope transport, pertinent physical and chemical processes must be identified and considered as to their relative importance in describing mass transport of the constituents of concern. These processes may include advection, dispersion, adsorption/desorption, diffusion, retardation, chemical reactions, phase partitioning, decay, and radioactive decay product series.

The custodianship and the availability of all of the codes identified in this survey were confirmed. Of the 35 codes identified in an initial screening, 7 are no longer available.

Research into improved representations of fluid flow and contaminant transport in fractured rock continues at an exciting pace. Driving much of this research is interest in fractured low-permeability geologic media as repositories of high-level radioactive waste in the United States and abroad. With advances in fracture flow and contaminant transport research, as well as in computing technology, the ability to accurately model the geology, physics, and chemistry of the natural settings and processes will continue to improve. Enhanced modeling capabilities will aid groundwater protection and remediation, thereby improving the capability to protect the safety and health of the populace.

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Appendix A:

Detailed Descriptions of the Fracture Flow Codes

Appendix A: Detailed Descriptions of the Fracture Flow Codes

This appendix contains detailed descriptions of fracture flow codes identified in this survey. The categories are described below.

Code Name: Name of the fracture flow code.

Author(s): Author(s) of the code.

Year: Year the version of the code was created.

Revision: Revision level of the code.

A.1 Capabilities, Limitations, and Assumptions

Capabilities, limitations, and assumptions in the categories of flow modeling, transport modeling, and numerical methods are described. Note that the absence of a feature implies a limitation with respect to that feature. Assumptions are inherent in the different conceptual models for fracture flow and in the processes that are and are not simulated.

Flow Model: Fluid-flow-simulation capabilities including, but not limited to, dimensionality, fractured/unfractured porous media, single phase/multiphase flow, saturated/unsaturated flow, isothermal/nonisothermal flow, state-variable dependencies.

Transport Model: Radionuclide, energy, and/or solute transport processes simulated including, but not limited to, single/multiple decay chains, convection, diffusion, advection, dispersion, sorption, adsorption, reaction series, stochastic representations.

Numerical Model: Fracture flow conceptual model: explicit discrete fracture, dual continuum, discrete fracture network, single equivalent continuum, multiple interacting continua. Spatial discretization: finite difference, finite element, integral finite difference, boundary integral. Solution procedures, especially where unique. Abbreviations include Incomplete Cholesky Conjugate Gradient (ICCG) and Generalized Minimal Residual (GMRES) matrix solvers.

A.2 Quality Assurance/Quality Control

A number of categories have been identified that pertain to quality assurance and quality control with respect to the accuracy, reliability, and dependability of supplied codes.

Peer Review: "Yes" means that theory and application of theory has been subject to peer review either through professional journal publication or outside agency review.

Benchmarking: "Yes" means that the code has been benchmarked against analytical solutions of test problems.

Field Testing: "Yes" means that the code has been field tested and been shown to successfully simulate the processes encountered at field test sites.

Code Documentation: "Yes" means that the code algorithms are documented on paper and that the code is commented.

User Documentation: "Yes" means that documentation describing the use of the code exists.

I/O Check files: "Yes" means that example input files are provided. It is recommended that electronic copies of output files also be provided. A new installation test run with a supplied input file should generate an output file identical in size and content to the one supplied.

A.3 Support and Enhancements

Code Support: "Yes," if available; amount in dollars per annum if not included.

Pre-Processor: "Yes" if a pre-processor is available.

Post-Processor: "Yes" if a post-processor is available.

A.4 Other

Availability: Cost of proprietary or public domain codes. In some cases, code prices vary or codes are available for free by written request.

Custodianship: Current code custodian.

Hardware Requirements: Platform(s) on which code runs.

Source Availability: "Yes" if source code is supplied.

Source Language: Language of source code, if supplied.

References: Number of references to the code listed in Appendix D. The number is followed by a plus (+) where more references have been identified than are listed in Appendix D.

Blank entries indicate that the information is not available or that the category is not applicable. For example, the transport category is blank for a code that does not have that capability.

A.5 The Codes

3-D FE DUAL-POROSITY FLOW & TRANSPORT MODEL

Author(s)	Glover, K.C.
Year	1987
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	Three-dimensional fluid flow in low-permeability high-porosity media with parallel fracture system.
Transport Model	Solute transport by advection, dispersion, diffusion.
Numerical Methods	Dual-continuum flow model. Finite-element spatial discretization. Transport simulation solved by Gaussian elimination.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	
Field Testing	
Code Documentation	
User Documentation	Yes
I/O Check Files	

Support and Enhancements

User Support	
Pre-processor	
Post-processor	

Other

Availability	\$40
Custodianship	U.S. Geological Survey
Hardware Requirements	CPU with FORTRAN77 compiler
Source Included	Yes
Source Language	FORTRAN77
References	1

BIM/BIM2D/BIM3D/FRACGEN

Author(s)	Rasmussen, T.C., and D.D. Evans
Year	1989
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	Two- or three-dimensional steady-state saturated, unsaturated, or multiphase flow in fractured, porous or non-porous media.
Transport Model	Solute transport by advection, and diffusion.
Numerical Methods	Dual-continuum (multiporosity) conceptual model. Boundary Integral Method. Includes synthetic fracture network generator, FRACGEN.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	Laboratory testing only.
Code Documentation	Limited
User Documentation	Yes
I/O Check Files	No

Support and Enhancements

User Support	No
Pre-processor	No
Post-processor	No

Other

Availability	Research code available free upon request.
Custodianship	T.C. Rasmussen
Hardware Requirements	Any platform with a FORTRAN compiler.
Source Included	Yes
Source Language	FORTRAN
References	3

DCM3D

Author(s)	Updegraff, C.D., C.E. Lee, and D.P. Gallegos
Year	1991
Revision	1.02

Capabilities, Limitations, and Assumptions

Flow Model	Three-dimensional, transient, variably saturated flow in fractured, heterogeneous, anisotropic porous media.
Transport Model	None
Numerical Methods	Dual-continuum conceptual model. Integrated finite-difference method. Block-centered orthogonal grid. Temporally variable boundary conditions.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	No
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	Limited support provided by custodian. See custodian description.
Pre-processor	No
Post-processor	Yes, of limited capability.

Other

Availability	Yes
Custodianship	U.S. Nuclear Regulatory Commission
Hardware Requirements	Double-precision version available for 32-bit machines (INTEL-based, DEC VAX, etc.) Single-precision version available for 64-bit machines (Cray) Modifications to Cray system time/date/cpu time calls may be required.
Source Included	Yes
Source Language	FORTTRAN
References	2

FRAC3DVS

Author(s)	Sudicky, E.A., and R.G. McLaren
Year	1993
Revision	1.0

Capabilities, Limitations, and Assumptions

Flow Model	Three-dimensional, steady-state or transient, saturated or unsaturated flow in fractured or unfractured porous media.
Transport Model	Solute or radionuclide transport by advection, dispersion, diffusion, retardation, multi-species transport, straight/branching first-order decay chains, linear adsorption/desorption.
Numerical Methods	Explicit discrete-fracture conceptual model. Control volume finite element (FE) (also known as IFDM), Galerkin FE finite difference (FD). Spatial discretization as 8- or 6-point FE or 7-point FD. Richard's equation used for unsaturated flow. Optional NAPL source term. Adaptive time-stepping. ORTHOMIN solver.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	No
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	Yes
Pre-processor	Yes
Post-processor	Yes

Other

Availability	\$5000 (Canadian)
Custodianship	R. McLaren
Hardware Requirements	80386 or better, or IBM RS/6000 (AIX OS w/X)
Source Included	Yes
Source Language	FORTRAN77
References	In submission.

FRACFLO

Author(s)	Gureghian, A.B.
Year	1990
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	Two-dimensional steady-state flow in fracture network.
Transport Model	Radionuclide transport by advection, dispersion, diffusion into rock matrix, decay. Source configurations variable in space and time.
Numerical Methods	Discrete-fracture network conceptual model. Analytical solution by Fourier transform and Gauss-Legendre integration.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	
Field Testing	
Code Documentation	
User Documentation	Yes
I/O Check Files	

Support and Enhancements

User Support	Limited; see custodian description.
Pre-processor	
Post-processor	FRACGRF, FRACGRF2D, require CA-DISSPLA 10.5

Other

Availability	Yes. See custodian description for pricing scheme.
Custodianship	Energy Science and Technology Software Center (ESTSC)
Hardware Requirements	DEC VAX8700 (VMS 5.0)
Source Included	Yes
Source Language	VMS FORTRAN
References	2

FRACFLOW

Author(s)	GeoTrans, Inc.
Year	1988
Revision	1.15

Capabilities, Limitations, and Assumptions

Flow Model	Two-dimensional transient fluid flow in heterogeneous fractured porous media.
Transport Model	
Numerical Methods	Dual-continuum conceptual model. Finite-element discretization.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	Yes
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	Yes
Pre-processor	
Post-processor	

Other

Availability	
Custodianship	GeoTrans, Inc.
Hardware Requirements	80486
Source Included	Yes
Source Language	FORTRAN
References	1

FracMan/MAFIC

Author(s)	Golder Associates, Inc.
Year	1994
Revision	2.306/1.3

Capabilities, Limitations, and Assumptions

Flow Model	Three-dimensional steady-state or transient, variably saturated, density- and temperature-dependent flow in fractured porous media.
Transport Model	Transport of solutes, heat, and radionuclides by particle tracking; advection, dispersion, matrix diffusion, retardation, radionuclide decay.
Numerical Methods	Dual-porosity/single-permeability conceptual model. All flow occurs in fracture network. Finite-element spatial discretization. Conjugate gradient solver.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	Yes
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	On a consulting basis. Annual maintenance for consultation, \$10,000.
Pre-processor	Fractures can be generated on the basis of a variety of geostatistical models, including box fractal and Poisson, or by conditioning and projection onto convex sets. Interface to TOUGH available.
Post-processor	Yes

Other

Availability	\$1,000 per annum. Generally no license fee for U.S. government and academia.
Custodianship	Golder Associates, Inc.
Hardware Requirements	MAFIC: SUN, HP9000, Silicon Graphics, IBM RS/6000
Source Included	No
Source Language	C, FORTRAN
References	8+

FRACTRAN

Author(s)	Sudicky, E.A., and R.G. McLaren
Year	1992
Revision	3.07

Capabilities, Limitations, and Assumptions

Flow Model	Two-dimensional steady-state flow in fractured or unfractured porous media.
Transport Model	Solute and radionuclide transport by advection, dispersion, diffusion, retardation, and first-order decay.
Numerical Methods	Explicit discrete-fracture conceptual model. Finite-element spatial discretization. Porous media represented by quadrilateral elements, fractures represented as line elements. Laplace Transform Galerkin transport solver eliminates time directly.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	No
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	Yes
Pre-processor	Yes
Post-processor	Yes

Other

Availability	\$2,500 (Canadian)
Custodianship	R. McLaren
Hardware Requirements	80386 or better
Source Included	Yes
Source Language	FORTRAN77
References	2

FRANET

Author(s)	Kanehiro, B.Y., and C.H. Lai
Year	1987
Revision	2.0

Capabilities, Limitations, and Assumptions

Flow Model	Steady-state or transient, slightly compressible flow in a fracture network of arbitrary orientation.
Transport Model	None
Numerical Methods	Discrete-fracture-network conceptual model. Finite-element spatial discretization.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	No
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	No

Support and Enhancements

User Support	Limited
Pre-processor	No
Post-processor	No

Other

Availability	Small charge
Custodianship	Berkeley Hydrotechnique, Inc.
Hardware Requirements	Any platform with FORTRAN77
Source Included	Yes
Source Language	FORTRAN
References	1

FTRANS

Author(s)	Huyakorn, P.S.
Year	1982
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	Two-dimensional, transient, density-dependent flow in fractured or unfractured anisotropic, heterogeneous, porous media.
Transport Model	Solute, heat, and radionuclide transport by advection, conduction, dispersion, diffusion, sorption, and first-order decay with decay chains.
Numerical Methods	Dual-continuum conceptual model. Finite-element spatial discretization.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	
Code Documentation	
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	
Pre-processor	
Post-processor	

Other

Availability	Yes. See custodian description for pricing scheme.
Custodianship	Energy Science and Technology Software Center (ESTSC)
Hardware Requirements	
Source Included	
Source Language	
References	1

MAGNUM2D

Author(s)	England, R.L., N.W. Kline, K.J. Ekblad, and R.G. Baca
Year	1985
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	Two-dimensional, transient or steady-state, flow in fractured anisotropic, heterogeneous, porous media.
Transport Model	Solute and heat transport by advection, dispersion, diffusion, sorption, and multi-species decay. Can be linked with the radionuclide transport code CHAINT.
Numerical Methods	Explicit discrete-fracture, dual-continuum, or equivalent porous-medium conceptual models. Finite-element spatial discretization.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	Yes
Code Documentation	
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	Limited, see custodian description.
Pre-processor	Yes
Post-processor	Requires CA-DISSPLA

Other

Availability	Yes. See custodian description for pricing scheme.
Custodianship	Energy Science and Technology Software Center (ESTSC)
Hardware Requirements	
Source Included	
Source Language	
References	4

MOTIF

Author(s)	Guvanasen, V., and T. Chan
Year	1991
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	One-, two-, or three-dimensional, variably saturated flow in fractured, deformable, porous media.
Transport Model	Solute, heat, and single-species radionuclide transport by convection, advection, dispersion, diffusion, adsorption, decay.
Numerical Methods	User's choice between explicit discrete-fracture conceptual model and unfractured porous-media model. Finite-element spatial discretization.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	Yes
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	Yes
Pre-processor	Third party only
Post-processor	Third party only

Other

Availability	\$20,000 (Canadian)
Custodianship	Atomic Energy Canada, Ltd.
Hardware Requirements	Wide variety of UNIX (including AIX and UNICOS), VMS, and CMS platforms.
Source Included	By special arrangement.
Source Language	FORTRAN77
References	4

NEFTRAN II

Author(s)	Olague, N.E., and D.E. Longsine
Year	1991
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	One-dimensional saturated or unsaturated flow along discrete fractures of arbitrary orientation. Fractures are treated as discrete "legs" of uniform hydrogeologic properties in a network. Components of the fluid velocity field may be supplied as user input. For transient flow simulations, multiple velocity fields must be input.
Transport Model	Radionuclide transport along flow paths with matrix diffusion, dispersion, sorption, and multiple decay chains.
Numerical Methods	Discrete-fracture-network conceptual model. Finite-difference spatial discretization. Particle tracking for transport.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	Yes
Code Documentation	Minimal
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	Limited
Pre-processor	No
Post-processor	No

Other

Availability	Yes
Custodianship	U.S. Nuclear Regulatory Commission
Hardware Requirements	CPU with FORTRAN compiler
Source Included	Yes
Source Language	Microsoft FORTRAN77
References	1

NETFLO/NETTRANS

Author(s)	Rouleau, A.
Year	1988
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	Two-dimensional steady-state flow in fracture network in impermeable non-porous media.
Transport Model	Transport by advection simulated by stochastic particle tracking in virtual network based on selected directional parameters: relative flow rate, mean flow velocity, and mean length of fracture segment.
Numerical Methods	Discrete-fracture-network conceptual model. Solution to conductance network flow in domain of fractures generated stochastically by using the results of Monte Carlo realizations of fields based on statistics from field data.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Not applicable (analytical model)
Field Testing	Yes
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	None
Pre-processor	NETWORK code
Post-processor	

Other

Availability	\$30 Canadian
Custodianship	A. Rouleau
Hardware Requirements	SUN workstation, FORTRAN Compiler, IMSL Subroutines
Source Included	Yes
Source Language	FORTRAN
References	4

PORFLO-3

Author(s)	Runchal, A.K., B. Sagar, and N.W. Kline
Year	1992
Revision	1.2

Capabilities, Limitations, and Assumptions

Flow Model	Three-dimensional, Cartesian or radial, steady-state or transient, nonisothermal, variably saturated flow in fractured porous media.
Transport Model	Single dissolved species transport by advection, dispersion, diffusion, sorption, retardation, decay. Energy transport by convection, conduction, dispersion.
Numerical Methods	Equivalent porous media or lower dimensional explicit discrete fracture conceptual models. Integrated finite-difference method. PSOR, ADI, Cholesky, conjugate gradient, and other solvers.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	Yes
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	Kline, N.W.
Pre-processor	
Post-processor	Yes

Other

Availability	Yes
Custodianship	Akshai K. Runchal. Technical Contact: N.W. Kline
Hardware Requirements	80386, 80486, SUN, Silicon Graphics, IBM RS/6000, Cray, Application Dependent
Source Included	Yes
Source Language	FORTRAN77
References	4+

PORFLOW

Author(s)	Runchal, A.K.
Year	1994
Revision	2.50

Capabilities, Limitations, and Assumptions

Flow Model	Two- or three-dimensional, cartesian or radial, steady-state or transient, variably saturated or multiphase flow in fractured or unfractured, anisotropic, heterogeneous porous media. Supports freezing/thawing and evaporation/condensation.
Transport Model	Solute, heat, or radionuclide transport by advection, dispersion, diffusion, sorption, retardation, convection, conduction, dispersion, decay. Highly variable source configuration.
Numerical Methods	Equivalent porous media or lower dimensional explicit discrete-fracture conceptual models. Integrated finite-difference spatial discretization. PSOR, ADI, Cholesky, conjugate gradient, and other solvers.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	Yes
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	\$1,000–5,000
Pre-processor	Yes
Post-processor	\$495–7,495 (platform-dependent)

Other

Availability	\$995–14,995 without source (platform-dependent)
Custodianship	Akshai K. Runchal
Hardware Requirements	Any system with a FORTRAN77 compiler.
Source Included	\$995–14,995 with source (see vendor description)
Source Language	FORTAN77
References	6+ (>100)

SANGRE

Author(s)	Anderson, C.A.
Year	1986
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	Two-dimensional flow in deformable and translatable geologic media. Accommodates fractures and the simulation of ductile-brittle discontinuity-developing deformation processes, such as faulting.
Transport Model	Convective energy transport
Numerical Methods	Finite-element spatial discretization. Lagrangian grid.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	No
Pre-processor	No
Post-processor	Yes (SANGPL)

Other

Availability	Yes
Custodianship	C.A. Anderson
Hardware Requirements	CPU with FORTRAN Compiler
Source Included	Yes
Source Language	FORTRAN
References	1

SEFTRAN

Author(s)	Huyakorn, P.S., D.S. Ward, J.O. Rumbaugh, and R.W. Broome
Year	1986
Revision	2.0

Capabilities, Limitations, and Assumptions

Flow Model	Two-dimensional transient flow in fractured or unfractured, anisotropic, heterogeneous porous media.
Transport Model	Solute transport by advection, dispersion, equilibrium adsorption, and first-order decay.
Numerical Methods	Explicit discrete-fracture conceptual model. Finite-element spatial discretization. Line elements used to represent either discrete fractures or rivers.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	Yes
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	Yes
Pre-processor	Yes
Post-processor	Yes

Other

Availability	\$800
Custodianship	GeoTrans, Inc.
Hardware Requirements	80286 or better
Source Included	Yes
Source Language	FORTRAN
References	3

STAFF2D

Author(s)	Huyakorn, P.S.
Year	1988
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	Two-dimensional, steady-state or transient, flow in fractured or unfractured porous media. Real, cross-sectional, or radial-grid orientations.
Transport Model	Solute and radionuclide transport by advection, dispersion, sorption, and first-order degradation, including chain decay of multiple species.
Numerical Methods	Explicit discrete-fracture and dual-continuum (or a combination of the two) conceptual models. Finite-element spatial discretization with porous media represented as quadrilaterals and fractures as line elements. Galerkin solution technique.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	Yes
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	Yes (~\$60/h)
Pre-processor	Yes
Post-processor	Yes

Other

Availability	\$3,000
Custodianship	HydroGeoLogic Software Sales
Hardware Requirements	Many platforms; PCs, workstations, mainframes
Source Included	Yes
Source Language	FORTRAN77
References	3

STAFF3D

Author(s)	HydroGeoLogic, Inc.
Year	
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	Two- or three-dimensional, cartesian or radial, steady-state or transient, flow in fractured or unfractured, anisotropic, heterogeneous porous media.
Transport Model	Single species or decay-chain transport by advection, dispersion, linear equilibrium sorption, and first-order degradation.
Numerical Methods	Explicit discrete-fracture and dual-continuum (or a combination of the two) conceptual models. Finite-element spatial discretization. Fractures represented by one-dimensional elements in discrete fracture model. Porous matrix represented by one-dimensional elements in dual-continuum model. PCG and ORTHOMIN solvers.

Quality Assurance/Quality Control

Peer Review	
Benchmarking	Yes
Field Testing	
Code Documentation	
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	Yes (~\$60/h)
Pre-processor	Yes
Post-processor	

Other

Availability	\$4,000 first year, \$2,000 subsequent years.
Custodianship	HydroGeoLogic Software Sales
Hardware Requirements	Personal computers, workstations, minicomputers
Source Included	No
Source Language	
References	Same as Staff2D

SWIFT II

Author(s)	Intercomp, Intera
Year	1990
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	Three-dimensional transient flow in fractured or unfractured, anisotropic, heterogeneous porous media. Viscosity dependency as a function of temperature and brine concentrations.
Transport Model	Solute, heat, and radionuclide transport by advection, dispersion, diffusion.
Numerical Methods	Explicit discrete-fracture or dual-continuum conceptual models. Finite-difference spatial discretization.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	Yes
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	See custodian description.
Pre-processor	
Post-processor	

Other

Availability	Yes. See custodian description for pricing scheme.
Custodianship	Energy Science and Technology Software Center (ESTSC)
Hardware Requirements	
Source Included	No
Source Language	FORTRAN
References	3+

SWIFT/486

Author(s)	Intercomp, GeoTrans
Year	1994
Revision	2.54

Capabilities, Limitations, and Assumptions

Flow Model	Three-dimensional transient flow in fractured or unfractured, anisotropic, heterogeneous porous media. Viscosity dependency as a function of temperature and brine concentrations.
Transport Model	Solute, heat, and radionuclide transport by advection, dispersion, diffusion. Freundlich and linear adsorption isotherms.
Numerical Methods	Explicit discrete-fracture or dual-continuum conceptual models. Finite-difference spatial discretization.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	Yes
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	\$1,000 per annum
Pre-processor	
Post-processor	Two

Other

Availability	\$800
Custodianship	GeoTrans, Inc.
Hardware Requirements	80386 or better with 4 megabytes of extended memory
Source Included	Yes
Source Language	FORTTRAN
References	7+

TOUGH2

Author(s)	Pruess, K.
Year	1991
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	One-, two-, or three-dimensional, transient, nonisothermal multiphase, multicomponent fluid and coupled heat flow in fractured, anisotropic, heterogeneous porous media. Five different equations of state available, depending on phases present.
Transport Model	Multicomponent advection and heat conduction.
Numerical Methods	Dual-continuum conceptual model with multiple interacting continua (MINC) option. Integral finite-difference method. Solution is achieved through Newton-Raphson iteration on the residual by using the Harwell MA-28 solver. Requires 64-bit arithmetic for successful execution.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	Yes
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	K. Pruess, Lawrence Berkeley Laboratory; ESTSC
Pre-processor	Mesh generator
Post-processor	

Other

Availability	Yes. See custodian description for pricing scheme.
Custodianship	Energy Science and Technology Software Center (ESTSC)
Hardware Requirements	Cray X-MP, IBM RS/6000 workstation, PCs
Source Included	Yes
Source Language	FORTRAN
References	8

TRACR3D

Author(s)	Travis, B.J.
Year	1984
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	One-, two-, or three-dimensional, steady-state or transient, flow in fractured or unfractured, deformable, anisotropic, heterogeneous porous media. Flow options include single-phase saturated, single-phase unsaturated, two-phase immiscible, and others.
Transport Model	Multicomponent transport in air and/or water phases by advection, dispersion, diffusion, equilibrium or kinetic adsorption/desorption, up to n chains of radioactive decay, and biological transformation.
Numerical Methods	Orthogonal, explicit, discrete fractures occurring at edges of grid blocks or equivalent continuum-conceptual models. Integrated finite-difference method. Newton-Raphson iteration with ICCG and GMRES matrix solvers.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	Yes
Code Documentation	Yes
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	Yes
Pre-processor	
Post-processor	

Other

Availability	Yes
Custodianship	B. Travis
Hardware Requirements	Apple, IBM, SUN, HP, Vax, Cray
Source Included	Does not include biological transformation capabilities.
Source Language	FORTRAN
References	2

TRAFRAP-WT PC/EXT

Author(s)	Huyakorn, P.S., H.O. White, and T.D. Wadsworth
Year	1991
Revision	1.3

Capabilities, Limitations, and Assumptions

Flow Model	Two-dimensional, transient, fractured or unfractured, anisotropic, heterogeneous porous media.
Transport Model	Solute or radionuclide transport by convection, dispersion, diffusion, sorption, radionuclide decay.
Numerical Methods	Explicit discrete-fracture or dual-continuum conceptual models. Finite-element spatial discretization.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	Yes
Code Documentation	
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	Yes
Pre-processor	
Post-processor	

Other

Availability	\$100
Custodianship	IGWMC
Hardware Requirements	80386 or better with extended memory.
Source Included	
Source Language	
References	1

TRINET

Author(s)	Karasaki, K.
Year	1986
Revision	0.1

Capabilities, Limitations, and Assumptions

Flow Model	Three-dimensional transient flow in fracture network or porous media. Designed for well-test analysis in fractured hydrogeologic systems.
Transport Model	Solute transport by advection, dispersion.
Numerical Methods	Discrete-fracture-network conceptual model. Eulerian finite-element grid for fracture flow. Adaptive Eulerian-Lagrangian gridding for solute transport.

Quality Assurance/Quality Control

Peer Review	
Benchmarking	Yes
Field Testing	Yes
Code Documentation	
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	Limited
Pre-processor	Yes
Post-processor	Yes

Other

Availability	Limited
Custodianship	K. Karasaki
Hardware Requirements	Requires f77 compiler, SUN, DEC, CRAY. Parallel processing capable.
Source Included	Yes
Source Language	FORTTRAN77
References	5

TRUMP

Author(s)	Edwards, A.L., A. Rasmuson, I. Neretneiks, and T.N. Narasimhan
Year	1980
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	One-, two-, or three-dimensional, steady-state or transient, flow in fractured heterogeneous porous media.
Transport Model	Solute or heat transport by advection, dispersion, diffusion, conduction.
Numerical Methods	Integral finite-difference method.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	Yes
Field Testing	
Code Documentation	
User Documentation	Yes
I/O Check Files	Yes

Support and Enhancements

User Support	
Pre-processor	Yes. FED (see TRUMP references).
Post-processor	

Other

Availability	Yes. See custodian description for pricing scheme.
Custodianship	Energy Science and Technology Software Center (ESTSC)
Hardware Requirements	IBM 360 or IBM 370
Source Included	Yes
Source Language	FORTRANIV (95%), BAL (5%)
References	3

TRUST84

Author(s)	Narasimhan, T.N.
Year	1984
Revision	

Capabilities, Limitations, and Assumptions

Flow Model	One-, two-, or three-dimensional, steady-state or transient, variably saturated flow in fractured or unfractured, anisotropic, heterogeneous deformable porous media.
Transport Model	
Numerical Methods	Integral finite-difference method.

Quality Assurance/Quality Control

Peer Review	Yes
Benchmarking	
Field Testing	
Code Documentation	
User Documentation	
I/O Check Files	

Support and Enhancements

User Support	Limited, see custodian description.
Pre-processor	
Post-processor	

Other

Availability	Yes. See custodian description for pricing scheme.
Custodianship	Energy Science and Technology Software Center (ESTSC)
Hardware Requirements	DEC Vax
Source Included	Yes
Source Language	FORTRAN 77
References	5

Appendix B:
Custodians of Fracture Flow Codes

Appendix B: Custodians of Fracture Flow Codes

Custodian	Code(s)
C.A. Anderson ESA-13, MS-J576 Los Alamos National Laboratory Los Alamos, NM 87545 (505) 667-5150 canderson@lanl.gov	SANGRE
Atomic Energy Canada, Ltd. Whiteshell Nuclear Research Establishment Pinawa, Manitoba, ROE 1L0 Canada Attn: Sales & Marketing (416) 592-5296 (416) 592-4485 (FAX)	MOTIF
Berkeley Hydrotechnique, Inc. 2039 Shattuck Ave., Suite 401 Berkeley, CA 94704 Attn: B.Y. Kanehiro (510) 549-9570 (510) 549-1713 (FAX)	FRANET
Energy Science and Technology Software Center P.O. Box 1020 Oak Ridge, TN 37831 (615) 576-2606 estsc@adonis.osti.gov	FRACFLO FTRANS MAGNUM-2D SWIFT/SWIFT II TOUGH/TOUGH2 TRUMP TRUST84
GeoTrans, Inc. 46050 Manekin Plaza, Suite 100 Sterling, VA 20166 Attn: D. Ward (703) 444-7000 geotranl@access.digex.net	FRACFLOW SEFTRAN SWIFT/486

Custodian**Code(s)**

Golder Associates, Inc.
 4104 148th Ave NE
 Redmond, WA 98052
 (206) 883-0777
 fracman@golder.com

FracMan/MAFIC

HydroGeoLogic, Inc.
 1165 Herndon Parkway, Suite 900
 Herndon, VA 22070
 (703) 478-5186

STAFF2D
 STAFF3D

IGWMC
 Colorado School of Mines
 Golden, CO 80401-1887
 (303) 273-3103
 igwmc@mines.colorado.edu

TRAFRAP-WT PC/EXT

K. Karasaki
 MS 50E
 Earth Sciences Division
 Lawrence Berkeley Laboratory
 Berkeley, CA 94720
 (510) 527-6759

TRINET

N.W. Kline
 Westinghouse Hanford Co.
 P.O. Box 1970, MS HO-36
 Richland, WA 99352
 (509) 376-8080

PORFLO-3

R. McLaren
 U. of Waterloo
 Waterloo, Ontario, N2L 3G1 Canada
 mclaren@sciborg.uwaterloo.ca

FRAC3DVS
 FRACTRAN

Custodian**Code(s)**

T.C. Rasmussen
 School of Forest Resources
 University of Georgia
 Athens, GA 30602-2152
 (706) 542-4300
 trasmuss@uga.cc.uga.edu

BIM/BIM2D/BIM3D/FRACGEN

A. Rouleau
 Dept. de Science Appliquees
 University du Quebec a Chitoutimi
 Chicoutimi, Quebec G7H 2B1 Canada

NETFLO/NETRANS

A.K. Runchal
 Analytical and Computational Research, Inc.
 1931 Stradella Rd.
 Bel Air, CA 90077
 runchal@netcom.com

PORFLOW

B. Travis
 EES-5, MS-F665
 Los Alamos National Laboratory
 Los Alamos, NM 87545
 (505) 667-1254
 bjt@vega.lanl.gov

TRACR3D

U.S. Geological Survey, WRD
 437 National Center
 12201 Sunrise Valley Drive
 Reston, VA 22092
 Attn: O.A. Holloway
 (703) 648-5695 (Program Information Line)
 (703) 648-5295 (FAX)

3-D FE DUAL-POROSITY FLOW
 & TRANSPORT MODEL

U.S. Nuclear Regulatory Commission
 Office of Research, Waste Management Branch
 Washington, D.C. 20555
 Attn: T.J. McCarten
 (301) 492-3847 or 492-7000
 tjm3@nrc.gov

DCM3D
 NEFTRAN II

Appendix C:

Annotated List of Custodians of Fracture Flow Codes

Appendix C: Annotated List of Custodians of Fracture Flow Codes

Charles A. Anderson, ESA-13, MS-J576, Los Alamos National Laboratory, Los Alamos, NM 87545, *telephone*: (505) 667-5150, *internet*: canderson@lanl.gov

Charles Anderson is a staff scientist at the Los Alamos National Laboratory. He will supply a copy of SANGRE upon request. SANGRE is available in a wide variety of media formats, or by e-mail.

Atomic Energy Canada, Ltd., Whiteshell Nuclear Research Establishment, Pinawa, Manitoba, R0E1I0 Canada, att: Sales & Marketing, *fax*: (416) 592-4485.

MOTIF is available from Atomic Energy Canada, Ltd. (AECL), for \$20,000 Canadian per year lease for the executable code only. Source code is available only through special arrangement with Sales & Marketing. Limited technical support may be available from Tin Chan, senior staff scientist at AECL Research. He can be reached at (416) 592-5296 or chant@wl.aecl.ca

Berkeley Hydrotechnique, Inc., 2039 Shattuck Ave., Suite 401, Berkeley, CA 94704

Att: B.Y. Kanehiro, *telephone*: (510) 549-9570, *fax*: (510) 549-1713.

Brian Kanehiro will supply FRANET with limited support for a nominal charge.

Energy Science and Technology Software Center (ESTSC), P.O. Box 1020, Oak Ridge, TN 37831, *telephone*: (615) 576-2606, *internet*: estsc@adonis.osti.gov

The ESTSC is the repository for much of the software produced by U.S. government laboratories. It replaces the National Energy Software Center, which no longer exists. The ESTSC provides limited support for code installation only. The ESTSC provides a responsive staff to assist with software searches and acquisition. Not all of the codes that the ESTSC provides are available to non-U.S. citizens.

The ESTSC has variable pricing scale (Table C.1). Prices are in U.S. dollars for products in ESTC's "AS IS" and "SCREENED" categories. Add 20% for products categorized as "TESTED."

In addition to being a repository of largely historical codes, ESTSC has a suite of analytical solutions for verifying fracture flow and other codes called VERTPAK1. M.J. Golis of Battelle Columbus Division authored the package, which includes solutions for flow and

TABLE C.1 Cost of ESTSC Products by Platform and Customer

Customer	Cost (\$) by Platform			
	Personal Computer	Workstation	Mainframe	Supercomputer
DOE	250	400	500	1,200
Public	510	1,305	1,835	4,560
Foreign	940	2,000	2,715	6,700

transport in many different geometries. Software from a number of pertinent U.S. government agencies, such as the Geological Survey and the Environmental Protection Agency, is not archived at the ESTSC.

GeoTrans, Inc., 46050 Manekin Plaza, Suite 100, Sterling, VA 20166, att: David Ward, *telephone: (703) 444-7000, internet: geotran1@access.digex.net*

GeoTrans, Inc., is a consulting firm that specializes in groundwater analysis. GeoTrans has extensive experience in computer code research, development, and end-user training. The research of GeoTrans staff often appears in well-respected refereed journals. In addition to code sales and training courses, GeoTrans offers extensive client-support services.

Golder Associates, Inc., 4104 148th Ave. NE, Redmond, WA 98052, *telephone: (206) 883-0777, internet: fracman@golder.com*

Golder Associates is an international group of consulting companies. Since 1960, Golder Associates has provided services in soil mechanics, rock mechanics, engineering geology, and fluid flow. The FracMan/Mafic package is distributed on the basis of licensing agreements for U.S. government, academic users, and private companies. There is generally no cost for U.S. government and academic licenses.

HydroGeoLogic Software Sales, 1165 Herndon Parkway, Suite 900, Herndon, VA 22070, *telephone: (703) 478-5186.*

HydroGeoLogic is a groundwater consulting firm with many years of experience in modeling groundwater flow and transport processes. In addition to software sales, it provides modeling support for approximately \$60 per hour or on a contractual consulting basis.

International Ground Water Modeling Center (IGWMC), Colorado School of Mines, Golden, CO 80401-1887, *telephone*: (303) 273-3103, *internet*: igwmc@mines.colorado.edu

The IGWMC is a repository and distribution center for a large number of ground-water-related computer programs. The IGWMC sells software that runs on IBM PC-compatible machines under the MS-DOS operating system. Support of individual codes varies. In some cases, support for non-current versions of codes does not exist (the user is required to upgrade to receive support). In addition to software distribution, the IGWMC organizes many short courses, workshops, seminars, conferences. The IGWMC also has an extensive library of ground-water-related publications available for purchase.

K. Karasaki, MS 50E, Earth Sciences Division, Lawrence Berkeley Laboratory, Berkeley, CA 94720, *telephone*: (510) 527-6759.

K. Karasaki is a staff scientist at the Lawrence Berkeley Laboratory. He will supply a copy of TRINET upon request, with some conditions.

Niall W. Kline, Westinghouse Hanford Co., PO Box 1970, MS HO-36, Richland, WA 99352, *telephone*: (509) 376-8080.

Niall W. Kline is a staff scientist for the Westinghouse Hanford Company and serves as a technical contact for PORFLO-3. By the agreement between the U.S. Department of Energy (DOE) and ACRI, Inc., copyright of PORFLO-3 has been waived by DOE, so that ACRI may claim that right. However, the U.S. Government retains a paid-up, nonexclusive, irrevocable worldwide license for use of PORFLO-3 by the government.

Rob McLaren, U. of Waterloo, Waterloo, Ontario, N2L 3G1 Canada, *telephone*: (519) 885-1211, ext. 2257, *internet*: mclaren@sciborg.uwaterloo.ca

Rob McLaren is a Research Technologist at the Waterloo Centre for Groundwater Research. Free limited support of FRACTRAN and FRAC3DVS is available. More extensive support, if required, may be arranged on a contractual basis.

Todd C. Rasmussen, School of Forest Resources, University of Georgia, Athens, GA 30602-2152, *telephone*: (706) 542-4300, *internet*: trasmuss@uga.cc.uga.edu

Todd Rasmussen is a faculty member at the University of Georgia. He will supply copies of the research codes BIM/BIM2D/BIM3D upon request.

Alain Rouleau, Dept. de Science Appliquees, University du Quebec a Chicoutimi Chicoutimi, Quebec G7H 2B1 Canada

Alain Rouleau is a professor at the University du Quebec a Chitoutimi. NETFLO/NETTRANS is in the public domain and is provided as is for a nominal fee.

Akshai K. Runchal, Analytical and Computational Research, Inc., 1931 Stradella Rd., Bel Air, CA 90077, *telephone*: (310) 471-3023, *internet*: runchal@netcom.com

ACRi is an international consulting organization providing mathematical modeling and computer analysis of environmental pollution and engineering processes involving fluid dynamics, heat and mass transfer, turbulence, and combustion. The prices of the software distributed by this vendor vary according to the memory capabilities, single user and multiuser, source supplied or not supplied, and annual lease or "paid-up license." These prices are applicable to both the PORFLOW code and the arcPLOT post-processor. For example, a single-user, 16-MB version of the executable code can be purchased for \$2,995. The same code, with source code, can be leased annually for the same amount, or purchased for \$8,995. Installation fees are applied to all but IBM PC licenses. Educational discounts of 40% are available. Training is available for \$1,250 per day, with 3–5-day workshops recommended. Unlimited telephone support is provided at a cost of \$1,000 per year. The cost of unlimited telephone support, problem solving, and enhancement consultations is \$5,000 per year and includes product upgrades. Additional consulting is charged on the basis of time and materials.

Technical support for PORFLO 1.3, a precursor to PORFLOW, is available from N.W. Kline (see earlier entry).

Bryan Travis, EES-5, MS-F665, Los Alamos National Laboratory, Los Alamos, NM 87545, *telephone*: (505) 667-1254, *internet*: bjt@vega.lanl.gov

Bryan Travis is a staff scientist at the Los Alamos National Laboratory. He will provide a copy of TRACR3D upon receipt of a written request describing the proposed application and platform. Source code is unavailable for the most recent version of TRACR3D, which incorporates biological degradation capabilities.

U.S. Nuclear Regulatory Commission, Office of Research, Waste Management Branch, Washington, DC 20555, Att: Tim McCarten, *telephone*: (301) 492-3847 or 492-7000, *internet*: tjm3@nrc.gov

Tim McCarten is the U.S. Nuclear Regulatory Commission (NRC) sponsor and contact for DCM3D and NEFTRAN2. He will provide copies of those codes, with sample input data sets, upon request. Generally, the codes are provided as source only on diskettes formatted for DOS machines. Technical support for installation is available, at the discretion of the U.S. NRC. Distribution of these codes is limited to U.S. citizens. Eventually, the codes will be available from the ESTSC.

U.S. Geological Survey, WRD, 437 National Center, 12201 Sunrise Valley Drive, Reston, VA 22092, *telephone:* (703) 648-5695 (Program Information Line), *fax:* (703) 648-5295.

Write to this office to obtain 3D FE Dual-Porosity Flow & Transport Model. The code is supplied on 3.5-in. or 5 1/4-in. diskettes as source code. Code cost includes documentation, in this case the Water Resources Investigation Report. The code is supplied "as is" and no support is available. All requests must be provided in writing, either by mail or fax. The USGS accepts money orders or checks as prepayment. Alternatively, the USGS will ship a product with a bill in response to a purchase request.

This is also the distribution office for all USGS Water Resource Division (WRD) codes. All USGS WRD codes cost \$40.

Appendix D:

Selected References by Fracture Flow Code

Appendix D: Selected References by Fracture Flow Code

3-D FE DUAL-POROSITY FLOW & TRANSPORT

Glover, K.C., 1987, *A Dual-Porosity Model for Simulating Solute Transport in Oil Shale*, U.S. Geological Survey Water Resources Investigations Report WRI 86-4047, 88 pp.

BIM/BIM2D/BIM3D/FRACGEN

Haldeman, W.R., Y. Chuang, T.C. Rasmussen, and D.D. Evans, 1991, *Laboratory Analysis Of Fluid Flow and Solute Transport through a Fracture Embedded in Porous Tuff*, Water Resources Research 27(1):53-65.

Rasmussen, T.C., 1987, *Computer Simulation Model of Steady Fluid Flow and Solute Transport through Three-Dimensional Networks of Variably Saturated, Discrete Fractures*, in Flow and Transport through Unsaturated Fractured Rock, D.D. Evans and T.J. Nicholson, Editors, American Geophysical Union Geophysical Monograph 42.

Rasmussen, T.C., 1991, *Steady Fluid-Flow and Travel Times in Partially Saturated Fractures Using a Discrete Air-Water Interface*, Water Resources Research 27(1):67-76.

DCM3D

Updegraf, C.D. (GRAM), C.E. Lee (API), and D.P. Gallegos (SNL), 1991, *DCM3D: A Dual-Continuum, Three-Dimensional, Ground-Water Flow Code for Unsaturated, Fractured, Porous Media*, prepared by GRAM, Inc.; Applied Physics, Inc.; and Sandia National Laboratories, Albuquerque, NM (SAND90-7015) for the U.S. Nuclear Regulatory Commission, NUREG/CR-5536, February.

Gallegos, D.P., P.I. Pohl, and C.D. Updegraf, 1992, *An Investigation of the Impact of Conceptual Model Uncertainty on the Estimated Performance of a High-Level Nuclear Waste Repository in Unsaturated, Fractured Tuff*, Sandia National Laboratories report SAND90-2882, Albuquerque, NM 87185.

FRACFLO

Gureghian, A.B., 1990, *FRACFLO: Analytical Solutions for Two-Dimensional Transport of a Decaying Species in a Discrete Planar Fracture and Equidistant Multiple Parallel Fractures with Rock Matrix Diffusion*, Battelle Memorial Institute report BMI/OWTD-5, Richland, WA, July.

Gureghian, A.B., 1990, *FRACFLO User's Guide: Version 1.1 for FRACFLO, Analytical Solutions for Two-Dimensional Transport of a Decaying Species in a Discrete Planar Fracture and Equidistant Multiple Parallel Fractures with Rock Matrix Diffusion*, Battelle Memorial Institute report BMI/OWTD-6, Richland, WA, July.

FRACFLOW

Ward, D.S., D.C. Skipp, D. Giffin, and M.D. Barcelo, 1989, *Dual-Porosity and Discrete Fracture Simulation of Groundwater Flow in West Central Florida*, Proceedings, Fourth International Conference, Solving Ground Water Problems with Models, Indianapolis, Indiana, International Ground Water Modeling Center, February 7-9.

FracMan/MAFIC

Dershowitz, W., G. Lee, S. Hitchcock, and P. LaPointe, 1993, *FracMan Version 2.306 Interactive Discrete Feature Data Analysis, Geometric Modeling, and Exploration Simulation: User Documentation*, Golder Associates, Inc., Seattle, WA.

Dershowitz, W., and P. Wallmann, 1992, *Discrete Fracture Modeling for the Stripa Tracer Validation Experiment Predictions*, SKB Stripa Project Technical Report TR 92-15, SKB, Stockholm, Sweden.

Dershowitz, W., P. Wallmann, and S. Kindred, 1991, *Discrete Fracture Modeling for the Stripa Site Characterization and Validation Drift Inflow Predictions*, SKB Stripa Project Technical Report TR 91-16, SKB, Stockholm, Sweden.

Dershowitz, W., A. Herbert, and J. Long, 1989, *Fracture Flow Code Cross Verification Plan*, SKB Stripa Project Technical Report TR 89-02, SKB, Stockholm, Sweden.

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Appendix E:
Codes That Are Unavailable

Appendix E: Codes That Are Unavailable

This appendix lists codes that are either superseded by codes listed in Appendix A or are no longer available.

3D FRACTURE GENERATOR

Author(s)	Huang, C., D.D. Evans
Year	1984

FLASH

Author(s)	Baca, R.G., S.O. Magnuson
Year	

FRACT

Author(s)	Pickens, J.F.
Year	1981

FRACTEST

Author(s)	Karasaki, K.
Year	1986

GREASE/GREASE2

Author(s)	Huyakorn, P.S.
Year	1982

MULKOM

Author(s)	Pruess, K.
Year	1985

NETFLOW

Author(s)	Pahwa, S.B., B.S. Rama Rao
Year	1982

SHALT

Author(s)	Pickens, J.F., G.E. Grisak
Year	1979

STAFAN/STAFAN2

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Year	1982

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Appendix F: Distribution List

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