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Initial Entry: CNWRA Scientific Notebook 806

Title: Southwest Research Institute (SWRI) Subcontract 499883N, Task 07 - Validation of the Finite Difference Code FLAC (Fast Lagrangian Analysis of Continua) Version 5.0

Personnel Responsible: Numerical simulations performed by Dr. Rodney Stewart Read (R. S. Read), President and Principal Consultant, RSRead Consulting Inc., Okotoks, Alberta, Canada T1S 1R3. SWRI staff oversight provided by Dr. Goodluck Ofoegbu, Principal Engineer, Geosciences and Engineering Division, Southwest Research Institute, 6220 Culebra Road, San Antonio, TX 78228-5166. Entries are signed by R.S. Read using the initials RR.

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Required Qualifications: The required expertise to conduct the numerical simulations include a sound working knowledge of FLAC and experience in its application to thermal-mechanical stability issues associated with underground openings for a potential nuclear waste repository. A Ph.D. in rock mechanics and relevant experience in the area of geotechnical engineering are also considered necessary.

Objectives and Approach: In conducting a regulatory review of a potential license application for geologic disposal of high-level waste, computer codes will be used to assess short-term stability and long-term performance of underground openings associated with a high-level waste repository. These excavations will be subjected to thermal-mechanical loading, including possible dynamic loading from earthquakes, over the service life of a repository. The stability of underground openings prior to permanent closure of the repository, and the potential for rockfall from long-term degradation of the rock mass and earthquake shaking after permanent closure are some of the key technical concerns for license application review.

The program FLAC (Fast Lagrangian Analysis of Continua) Version 5.0 is one of the computer codes that is likely to be used for geomechanical analysis of underground structures in a rock mass. It is acquired software that is not to be modified and is under configuration control at the Center for Nuclear Waste Regulatory Analyses. FLAC is a two-dimensional explicit finite difference program. It is capable of simulating the behavior of structures in rock or other materials that may undergo plastic flow when a yield limit is reached. Materials behavior is prescribed through linear or nonlinear stress/strain laws. Constitutive models can be selected to simulate highly nonlinear, irreversible responses representative of geologic materials. In addition, FLAC contains other features that are useful in the analysis of underground openings, including thermal and dynamic modelling capabilities, viscoelastic and viscoplastic (creep) models, interfaces to simulate distinct planes along which displacement may occur, and structural element models to simulate structural support (e.g., tunnel liners and rock bolts).

Relevant aspects of the FLAC Version 5.0 computer code are to be validated so it can be used to assist with license application review. Validation tests on FLAC Version 5.0 will be limited to examining the capabilities of the code in analyzing the stability of underground openings under heated and dynamic conditions.

The objective of Task 07 is to validate the finite difference code FLAC Version 5.0 against a suite of validation cases covering:

- thermal response of the rock mass
- mechanical response of the rock mass
- thermal-mechanical response of the rock mass
- mechanical response of supported tunnels
- ground-support interaction
- dynamic response of the rock mass

The specific validation cases agreed to be conducted are summarized in a letter from RSRead Consulting Inc. to Dr. Goodluck Ofoegbu of CNWRA entitled "Scope of Task 07 under CNWRA Subcontract 499883N" dated March 20, 2006. Table 1 lists these cases, which are a subset of those described in the document entitled "Software Validation Plan for the Finite Difference Code FLAC (Fast Lagrangian Analysis of Continua) Version 5.0" submitted to the Center for Nuclear Waste Regulatory Analyses by RSRead Consulting Inc. on October 19, 2005. The Validation Plan provides details on each proposed case, including an overview, test input, test procedure, relevant parameters, and means of comparing test results to other available data.

In addition to those cases listed in Table 1, three additional cases to validate the dynamic analysis capabilities of FLAC were approved March 20, 2006. These additional cases are described as follows:

1. Comparison of FLAC to SHAKE – The program SHAKE is widely used in earthquake engineering for computing the seismic response of horizontally layered soil deposits. This example compares the output of FLAC to that of SHAKE for the case of a one-dimensional layered elastic soil deposit, driven at its base by a horizontal acceleration given by a closed-form equation. The version of SHAKE used for the comparison is

SHAKE91 (Idriss and Sun 1992), which computes the response of a semi-infinite horizontally layered soil deposit overlying a uniform half-space subjected to vertically propagating shear waves. Histories of horizontal acceleration at the top of the model, shear strain at depth, and shear stress at depth are compared for the two codes along with shear stress versus shear strain in the two materials used in the model.

2. Vertical Vibration of a Machine Foundation – This case considers the vertical response of a machine foundation consisting of a rigid, massive, strip foundation resting on a soil excited by an oscillating machine force. FLAC is used to compute the response of the system, and results are compared to an analytical solution (Gazetas and Roesset 1979).

3. Comparison of Hysteretic Damping with SHAKE91 – This case considers the response of a horizontally-layered soil system comprising ten different types of soil treated as nonlinear elastic materials. Non-linearity is modeled using two sets of modulus reduction factor and damping ratio curves. The base acceleration input is a set of seismic data recorded in the Loma Prieta Earthquake. The acceleration history, response spectra, and acceleration amplification at the top of the model are compared for FLAC and SHAKE91.

Each of these three cases has associated input files that are documented in the FLAC user manual.

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Relevant information contained in the validation plan is included in the Scientific Notebook as appropriate for each validation case undertaken. Information for each case includes assumptions, initial/boundary conditions, solution algorithm, references, and primary data sources to be used in the analysis. Aspects potentially affecting computational reliability are identified for each case and evaluated as appropriate.

Software: FLAC Version 5.0 from Itasca Consulting Group, Inc. and available to the Center for Nuclear Waste Regulatory Analyses, is designed for a desktop personal computer environment. The FLAC executable file is flacv_dp.exe . The validation tests for FLAC Version 5.0 will be performed using the Microsoft Windows NT operating system Version 4.0 (Build 1381: Service Pack 6) or Microsoft Windows XP Professional (Version 5.1.2600, Service Pack 2 Build 2600). The data input files will be developed for each test case as appropriate.

To validate FLAC Version 5.0, analytical solutions, field measurements, and published results from other numerical methods will be compared to the FLAC modeling results. Output from the model simulations will be stored as electronic text files and enhanced metafile (.emf) graphic files. Post-processing of output data from FLAC will be conducted using Microsoft Excel 2003 (Version

11.8105.8107) SP2. In addition, Microsoft Word 2003 (Version 11.8106.8107) SP2 will used to create collections of graphic plots for the various simulation cases. Reports will be written using Corel WordPerfect (Version 11.0.0.233) or Microsoft Word as appropriate.

Hardware: The hardware required to conduct this validation plan includes an IBM-compatible personal computer. A hardware identification key from Itasca Consulting Group, Inc. is needed to execute the program. The test results will be presented as text outputs or graphics. A QMS 3825 or equivalent printer (e.g., Hewlett-Packard LaserJet 1200 series laser printer) will be used to process text outputs, and graphics will be printed using an HP Deskjet 9800 printer. No other hardware peripherals are needed for conducting the validation tests.

Data Management: Input files and results for each validation case will be stored to CD or DVD under a subdirectory reflecting the case number in Table 1. The filenames will be identified in the Scientific Notebook under each validation case.

Timeline: Following acceptance of the proposed validation cases outlined in the letter from RSRead Consulting Inc. of March 20, 2006, the start date for Task 07 was post-poned by SWRI until Q4 2006 at the earliest. The scope of the task was reviewed at a meeting at SWRI February 21, 2007, and the actual start date for the task was March 9, 2007.

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Table 1: Summary of Validation Cases

Case	Description	Objective	Reference
1	**Thermal Response of the Rock Mass**		
1.1	Verification of FLAC against closed-form solution for heat conduction through a composite wall [20 hours]	Validate 1D thermal conduction response of the rock mass	Itasca Consulting Group, Inc. 2005. FLAC Fast Lagrangian Analysis of Continua Optional Features, Third Edition (FLAC Version 5.0.. April 2005, Thermal Option, Section 1.7.1.1, pp 1-39 – 1-45. [Analytical solution given in manual]
1.2	Verification of FLAC against closed-form solution for conductive heating of a spherical cavity with applied heat flux [20 hours]	Validate the 3D thermal conduction response of the rock mass	Itasca Consulting Group, Inc. 2005. FLAC Fast Lagrangian Analysis of Continua Optional Features, Third Edition (FLAC Version 5.0) April 2005, Thermal Option, Section 1.7.1.5, pp 1-66 – 1-71. [Analytical solution based on Carslaw and Jaeger 1959, p. 248]
2	**Mechanical Response of the Rock Mass**		
2.1	Verification of FLAC against closed-form solution for a cylindrical hole in an infinite elastic medium subjected to isotropic stresses [20 hours]	Validate mechanical response of an isotropic elastic rock mass	Itasca Consulting Group, Inc. 2005. FLAC Fast Lagrangian Analysis of Continua Verification Problems, Third Edition (FLAC Version 5.0) April 2005, pp 1-1 – 1-20. [Analytical solution from Kirsch as published in Jaeger and Cook 1976].
2.2	Verification of FLAC against closed-form solution for a cylindrical hole in an infinite, transversely isotropic, elastic medium subjected to an isotropic stress field [20 hours]	Validate mechanical response of a transversely isotropic elastic rock mass	Itasca Consulting Group, Inc. 2005. FLAC Fast Lagrangian Analysis of Continua Verification Problems, Third Edition (FLAC Version 5.0) April 2005, pp 2-1 – 2-18. [Analytical solution based on Amadei 1982; compare to Hefny and Lo 1999]
2.3	Verification of FLAC against closed-form solution for a cylindrical hole in an infinite Mohr-Coulomb medium subjected to an isotropic stress field [20 hours]	Validate mechanical response of an elasto-plastic Mohr-Coulomb rock mass	Itasca Consulting Group, Inc. 2005. FLAC Fast Lagrangian Analysis of Continua Verification Problems, Third Edition (FLAC Version 5.0) April 2005, pp 3-1 – 3-34. [Analytical solution based on Salencon 1969; compare to Carranza-Torres 2003]
2.4	Verification of FLAC against closed-form solution for a cylindrical hole in an infinite Hoek-Brown medium subjected to an isotropic stress field assuming non-associated plastic flow (zero dilation) [20 hours]	Validate mechanical response of an elasto-plastic Hoek-Brown rock mass	Itasca Consulting Group, Inc. 2005. FLAC Fast Lagrangian Analysis of Continua Verification Problems, Third Edition (FLAC Version 5.0) April 2005, pp 4-1 – 4-14 . [Based on analytical solution by Carranza-Torres and Fairhurst 1999]
2.5	Comparison of FLAC with analytical solution for a cylindrical hole in an infinite elasto-brittle-plastic Hoek-Brown medium subjected to an isotropic stress field [75 hours]	Validate mechanical response of an elasto-brittle-plastic (strain-softening) Hoek-Brown rock mass	Analytical solution by Sharan (2003; 2005)

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Table 1 (cont.)

Case	Description	Objective	Reference
2.6	Verification of FLAC against closed-form solution for a spherical cavity in an infinite elastic medium subjected to isotropic stresses [20 hours]	Validate mechanical response of an elastic rock mass	Itasca Consulting Group, Inc. 2005. FLAC Fast Lagrangian Analysis of Continua Verification Problems, Third Edition (FLAC Version 5.0) April 2005, pp 5-1 – 5-12. [Based on analytical solutions by Goodman 1980, p. 220; Timoshenko and Goodier 1970, p. 395]
2.7	Verification of FLAC against closed-form solution for a hollow sphere subjected to an internal blast [20 hours]	Validate mechanical response of an elastic rock mass subjected to dynamic loading	Itasca Consulting Group, Inc. 2005. FLAC Fast Lagrangian Analysis of Continua Optional Features, Third Edition (FLAC Version 5.0) April 2005, Section 3.6.3, pp 3-112 – 3-120. [Based on analytical solution by Blake 1952].
2.8	Comparison of FLAC with analytical solution for stresses and displacements around non-circular tunnels excavated in an elastic rock mass [75 hours]	Validate mechanical response of an elastic rock mass	Analytical solutions used by Critescu and Paraschiv (1995; 1996); Massier (1994); Greenspan (1944); Exadaktylos and. Stavropoulou (2002)
2.9	Comparison of FLAC with analytical solution for stresses and displacements around parallel circular tunnels excavated in an elastic rock mass [75 hours]	Validate mechanical response of an elastic rock mass	Analytical solutions by Kooi and Verruijt (2001)
2.10	Comparison of FLAC with analytical solution for stress and displacement around a circular opening in an infinite non-linear elastic medium. [Young's modulus a function of confining stress] [75 hours]	Validate mechanical response of a non-linear elastic rock mass	Analytical solutions by Lionço and Assis (2000)
3	**Thermal-Mechanical Response of the Rock Mass**		
3.1	Verification of FLAC against closed-form solution for thermally-induced stress and temperature distribution in a semi-infinite elastic mass subjected to a sudden constant heat flux at surface [20 hours]	Validate thermal-mechanical response of an elastic rock mass	Itasca Consulting Group, Inc. 2005. FLAC Fast Lagrangian Analysis of Continua Optional Features, Third Edition (FLAC Version 5.0) April 2005, Thermal Option, Section 1.7.2.1, pp 1-72 – 1-79. [Analytical solutions based on Carslaw and Jaeger 1959, p. 75; Timoshenko and Goodier 1970, p. 435].

Table 1 (cont.)

Case	Description	Objective	Reference
3.2	Verification of FLAC against closed-form solution for thermally-induced stresses and radial displacement from an infinite line heat source with a constant heat-generating rate in an infinite elastic medium with constant thermal properties. [20 hours]	Validate thermal-mechanical response of an elastic rock mass	Itasca Consulting Group, Inc. 2005. FLAC Fast Lagrangian Analysis of Continua Optional Features, Third Edition (FLAC Version 5.0) April 2005, Thermal Option, Section 1.7.2.2, pp 1-80 – 1-91. [Analytical solution by Nowacki 1962].
3.3	Comparison of FLAC with approximate solutions describing the boundary stress and displacement around unlined and lined drifts subjected to thermal loading under conditions representative of Yucca Mountain [75 hours]	Validate thermal-mechanical response of an elastic rock mass containing parallel lined and unlined tunnels	Analytical solutions by Elsworth (2001)
3.4	Comparison of FLAC with closed form solution for thermoplastic response of a thick-walled tube governed by the Tresca failure criterion subjected to an internal pressure and an axisymmetric time-dependent temperature field. [75 hours]	Validate thermal-mechanical response of an elasto-plastic rock mass	Analytical solutions by Wong and Simionescu (1996). Results are compared to those from the GEOMEC numerical model using a Von Mises failure criterion.
3.5	Comparison of FLAC with closed form solution for thermoplastic response of a deep tunnel in a thermal-softening (temperature-dependent cohesion) material governed by the Tresca failure criterion subjected to an internal pressure and an axisymmetric time-dependent temperature field. [75 hours]	Validate thermal-mechanical response of an elasto-plastic rock mass with temperature-dependent cohesion	Analytical solutions by Wong and Simionescu (1997). Results are compared to those from the finite element code THYME.
4	**Mechanical Response of Supported Tunnels**		
4.1	Verification of FLAC against closed-form solution for a lined circular tunnel in an elastic medium subjected to anisotropic stresses [20 hours]	Validate mechanical response of a lined tunnel in an elastic rock mass	Itasca Consulting Group, Inc. 2005. FLAC Fast Lagrangian Analysis of Continua Verification Problems, Third Edition (FLAC Version 5.0) April 2005, pp 8-1 – 8-12. [Based on analytical solution by Einstein and Schwartz 1979]
4.2	Comparison of FLAC with closed-form solution for shaft closure of an unsupported shaft in an isotropic stress field as a function of the distance to the shaft face. [20 hours]	Validate mechanical response of a lined tunnel in an elastic rock mass	Itasca Consulting Group, Inc. 2005. FLAC Fast Lagrangian Analysis of Continua Example Applications, Third Edition (FLAC Version 5.0) April 2005, pp 8-1 – 8-12. [Based on analytical solution by Panet 1979]

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Table 1 (concluded)

Case	Description	Objective	Reference
4.3	Comparison of FLAC with closed form solutions for maximum bending moment, maximum thrust, and maximum shear force in tunnel linings subjected to a maximum applied shear strain associated with dynamic loading. [75 hours]	Validate mechanical response of a lined tunnel in an elastic rock mass subjected to dynamic loading	Analytical solutions given by Hashash et al. (2005) Pakbaz and Yareevand (2005)
4.4	Comparison of FLAC with closed form solution for wall displacements and ground pressure acting on the lining of a circular tunnel driven in a homogeneous and isotropic medium with time-dependent behavior. [75 hours]	Validate mechanical response of an isotropic rock mass with time-dependent behavior	Analytical solutions by Sulem et al. (1987)
5	**Ground Support Interaction**		
5.1	Comparison of FLAC with closed form solution for coupling-decoupling behavior of rock bolts under uniform deformation of the rock mass [75 hours]	Validate ground support interaction and performance of rockbolts	Analytical solution by Cai et al (2004a,b). Other relevant analytical solutions and examples by Brady and Lorig (1988); Indraratna and Kaiser (1990); Hyett et al. (1992); Kaiser et al. (1992); Hyett et al. (1996); Li and Stillborg (1999); Bobet (2005); Fahimifar and Soroush (2005); Grasselli (2005)
5.2	Comparison of FLAC with closed form solution for coupling-decoupling behavior of a rock bolt in a pull-test [75 hours]	Validate ground support interaction and performance of rockbolts	Analytical solution by Cai et al (2004a,b). Example application given by Itasca Consulting Group, Inc. 2005. FLAC Fast Lagrangian Analysis of Continua Example Applications, Third Edition (FLAC Version 5.0) April 2005, pp 9-1 – 9-16 [based on analytical solutions by Hyett et al 1992; Kaiser et al. 1992]
5.3	Comparison of FLAC with closed form solution for coupling-decoupling behavior of a rock bolt intersecting a joint [75 hours]	Validate ground support interaction and performance of rockbolts	Analytical solution by Cai et al (2004a,b). Other relevant analytical solutions and examples by Brady and Lorig (1988); Indraratna and Kaiser (1990); Hyett et al. (1992); Kaiser et al. (1992); Hyett et al. (1996); Li and Stillborg (1999); Bobet (2005); Fahimifar and Soroush (2005); Grasselli (2005)

[redacted]

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March 27/2007 - Initial test cases to develop procedures.

- Latest updates to FLAC 5.0 downloaded from www.itascacg.com website and installed (5.00.371 DP)

Case 1.1

Initial Entry

- Input file for Case 1.1 located and run using GIIC (graphical interface) and manually using FLAC commands. See Table 1 (pg 5) for file location details.
- File output consistent with example in FLAC manual. * Refer to FLAC manual for problem definition.
- Case to be used to finalize a process for comparing closed-form and FLAC results.
- Compare temperature distribution in model.

Base Case

- Modified FLAC input file and renamed "Case0101.dat"
- File run in FLAC to produce LOG file "case0101.log"
- Import log file into EXCEL and save as "Case0101.XLS"
- Sheet 1 is the imported LOG File with FLAC and analytical results in x, y tables. Numbers are rounded to 4 significant figures.
- Create Sheet 2 "Comparison" to construct a summary table of output to build a chart plotting Temperature vs. distance.
- Develop a set of calculations in EXCEL to calculate temperature distribution based on the analytical solution as a cross check on coding in FLAC input file. (referred to as "EXCEL" in table)
- Difference calculated as $\frac{(FLAC - EXCEL)}{(EXCEL)} \times 100\%$
- Plot shows excellent comparison between FLAC, ANALYTICAL and EXCEL data sets for base case parameters and grid set up in original input file.
- maximum difference 0.06%

* Results contained in file "Case0101.xls".

Sensitivities

- Additional cases to be run to consider different grid density and initial conditions / properties.
- Each case is named as follows "Case0101x.xls" where x is a, b, c, etc for consecutive cases.

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Grid Sensitivity - Input file modified to increase grid density by factor of 10. Saved as "Case0101a.dat"
- Case run to produce "Case0101a.log" and "Case0101a.xls".
- Results compare favourably. Max difference is 0.16%
* See file "Case0101a.xls" for results.

Note: Part of difference related to rounding errors. Consider other ways to download FLAC results to ASCII file. Explore HISTORY command if rounding errors are an issue.

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Property Sensitivity - Input file modified to change thermal conductivity in two parts of composite wall. Change K_1 from 1.6 to 0.2; change K_2 from 0.2 to 2.0.
- saved as "Case0101b.dat"
- Case run to produce "Case0101b.log" and "Case0101b.xls".
- modified three EXCEL sheets to reference page 1 log details and added EXCEL results to charts.
- added columns to calculate difference between FLAC and Analytical, between FLAC and EXCEL, and between Analytical and EXCEL (rounding error).
* Results from all three data sets compare favourably
- max. difference between FLAC and EXCEL 0.07%.
- rounding error on order of 0.03% max.

Temp. Sensitivity - Input file modified to change inner temperature at wall from 300°C to 250°C.
- saved as "Case0101c.dat".
- Case run to produce "Case0101c.log" and "Case0101c.xls"
* Results from all three data sets compare favourably.
- max. difference 0.04% between FLAC and EXCEL

* Summary: Case 1.1 - Heat Conduction through a Composite wall

- Case 1.1 completed as per "Software Validation Test Plan for the Finite Difference Code FLAC (Fast Lagrangian Analysis of Continua) Version 5.0."
- Base case and three sensitivity cases run to compare FLAC, Analytical, and EXCEL data sets. Associated files are as follows:

    Input files: Case0101.dat - Base case
    Case0101a.dat - Grid sensitivity
    Case0101b.dat - Thermal conductivity sensitivity
    Case0101c.dat - Boundary Temp. Sensitivity.

    FLAC Output Files: Case0101.log, Case0101a.log, Case0101b.log, Case0101c.log } as above

    EXCEL Files: Case0101.xls, Case0101a.xls, Case0101b.xls, Case0101c.xls } as above

- Results from FLAC and other datasets compare favourably. Difference between FLAC and EXCEL less than 0.1% in each case, well below 1% difference considered acceptable.

- Representative plots are shown on the following pages. Plots are stored in WORD file "Case0101 Plots.doc".

- Intermediate FLAC save ".SAV" files for each case also preserved. All files to be included on CD with final report.

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Same: "Case 0101 Plots.doc".

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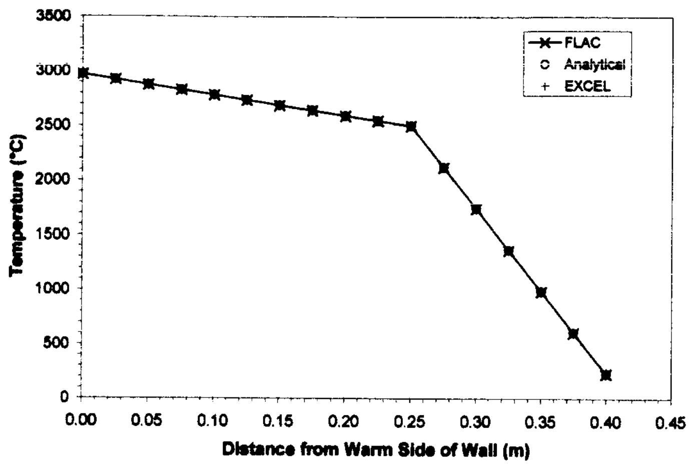
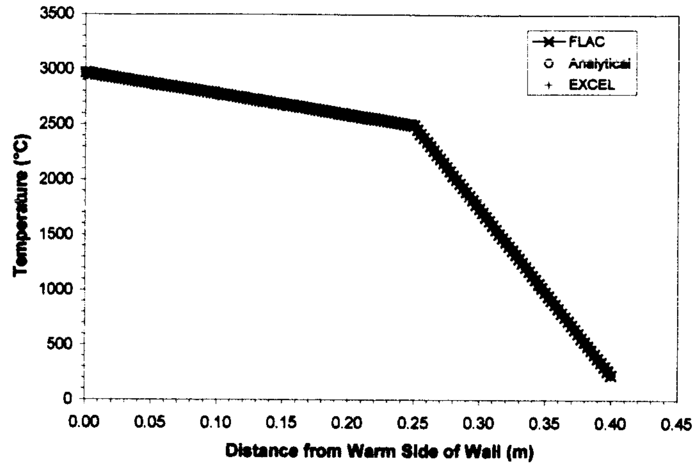
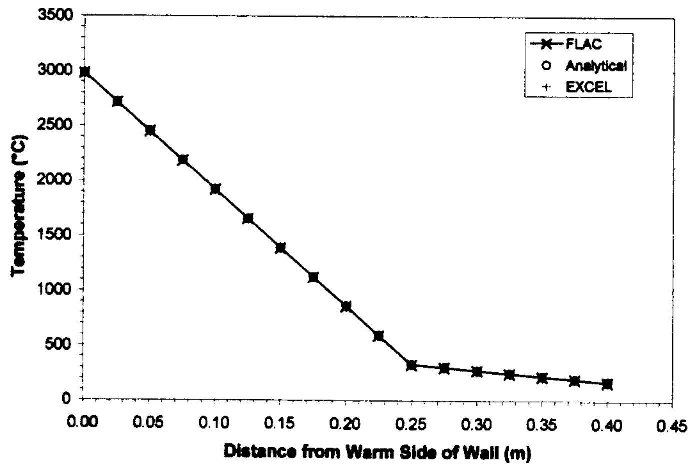
Case 1.1 - Conduction through a Composite Wall
Base Case



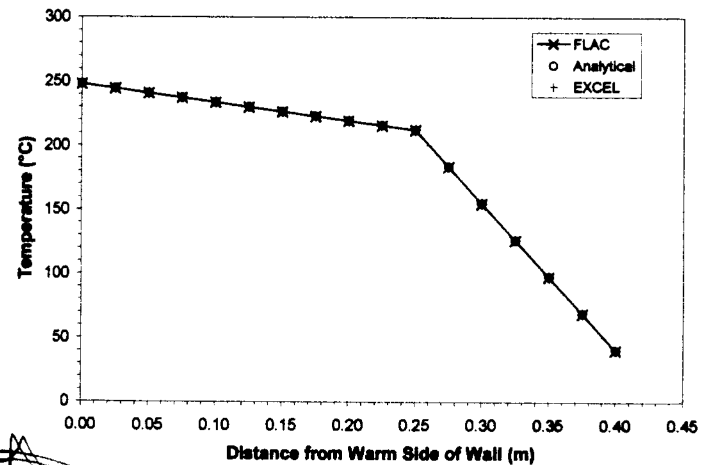
Case 1.1a - Conduction through a Composite Wall
Sensitivity to Grid Density



Case 1.1b - Conduction through a Composite Wall
Sensitivity to Thermal Conductivity



Case 1.1c - Conduction through a Composite Wall
Sensitivity to Boundary Temperature



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Base Case

Init. Ent.

*

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** Case 1.2 - Heat Conduction from a Spherical Cavity with Applied Heat Flux.

Initial Entry
- Refer to FLAC manual for problem definition (including model).
- see Table 1 on page 5 for details of case, including location in manual
- Example problem 1.5 in FLAC manual (Optional features)
- File "op_01_05.dat" contains original example input for FLAC.
- modified input file to include creation of LOG file for use in EXCEL comparison. New input file for base case named "Case0102.dat". FLAC output to "Case0102.log" used to create EXCEL work book "Case0102.xls".
- Workbook contains three sheets: Log File → original output from FLAC; Comparison → tabular and graphical summary of output from FLAC (FLAC and Analytical) and calculation of analytical solution using EXCEL.
- Plot of temperature vs time at radial distances of 0.025, 0.038 and 0.055 m from centre of sphere created to compare data sets.

Base Case
* - Results for base case show excellent agreement between all three datasets. Max difference of 0.32% between FLAC and EXCEL results at r = 0.025 m. Very minor difference between coded analytical solution and EXCEL calculation. Max difference = 0.05%.
- Sensitivity to be run on grid density, thermal properties, and initial temperature boundary conditions.

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- continue Case 1.2 analysis
- Work conducted March 28/2007 provides basis for

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comparing FLAC results, analytical result output from FLAC, and analytical results calculated in EXCEL

Initial Entry - Procedure for Analyses

- Based on experience with cases 1.1 and 1.2, the following procedure will be used to validate FLAC cases listed in Table 1 (with possible exception of dynamic cases).
   1. Locate existing FLAC input file (if documented in FLAC manual) or create FLAC input file. File saved with name "Case<u>XX</u><u>YY</u>.dat" where <u>XX</u> and <u>YY</u> are case and subcase descriptors. Additional sensitivity cases will have input files with a modifier "a", "b" etc following subcase identifier. FLAC input files are modified to produce LOG files of table values generated by FLAC. Tables include FLAC results and calculated analytical results based on closed-form solution.
   2. LOG file for each case is imported into EXCEL as worksheet 1 labelled "LOG FILE". Worksheet 2 labelled "Comparison" is constructed to reference the LOG FILE sheet to put X, Y values in columns. Format is as follows in terms of column headings:
      [Point, X Value, FLAC value, Analytical Value, EXCEL value, Difference (FLAC - Analytical), Difference (FLAC - EXCEL), Difference (Analytical - EXCEL)]

      If more than one response is plotted, additional columns are added for each new X, Y pair along with calculated differences.
   3. EXCEL columns are populated by creating an EXCEL version of the closed-form solution and adding Y-values for each X-value for comparison on the "Comparison" worksheet. Initial values used in the analyses are

[redacted]

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7 (cont.) those specified in examples documented in the FLAC manual. Workbooks for sensitivities document what changes are made relative to the base case. Responses are plotted on a standard EXCEL X-Y chart to provide a visual comparison of responses. The calculated differences are computed as follows:

a) $\text{Difference (FLAC - Analytical)} = \dfrac{(\text{FLAC} - \text{Analytical})}{\text{Analytical}} \times 100\%$

b) $\text{Difference (FLAC - EXCEL)} = \dfrac{(\text{FLAC} - \text{EXCEL})}{\text{EXCEL}} \times 100\%$

c) $\text{Difference (Analytical - EXCEL)} = \dfrac{(\text{Analytical} - \text{EXCEL})}{\text{EXCEL}} \times 100\%$

ing
d
d

The values in each of the difference columns are scanned to identify the maximum value calculated as follows:

```
Max. Difference = if(max(range)>abs(min(range)))
                  then max(range)
                  else abs(min(range))
```

i.e. reported max difference is the largest absolute value in the difference column of interest. The various difference columns provide insight into a) the difference between FLAC and analytical result calculated using FLAC and the FISH programming language in FLAC; b) the difference between FLAC results and results calculated independently in EXCEL; and c) the difference between the analytical solution coded in FLAC using FISH and results from EXCEL (including possible rounding errors in the FLAC output).

EXCEL)
g

4. Output to be reported under each section of the FLAC validation plan include a plot of pertinent

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responses, and a summary of the comparison between the various responses including max. differences calculated in the EXCEL workbook for each case and sensitivity subcase.

5. All electronic files will be stored in subdirectories by case reference. Charts may be copied into a WORD document for printing and presentation purposes. The WORD filename is the same as the identifying case eg. "Case0101Plots.doc" with Plots appended to the name.
6. Additional procedures may be required as cases are analyzed to deal with more complex datasets eg. dynamic input.
7. General sensitivities may include
   - grid density
   - initial/boundary conditions
   - properties

   as considered appropriate.
8. Added a third page to each EXCEL workbook containing background information copied from FLAC manual or from other source. This provides a synopsis of the base case; model geometry, parameters and boundary conditions.
9. In some cases, a duplicate "Comparison" worksheet is used to reduce density of points on chart. - worksheet labelled "Comparison (2)".

In-process entry.

- Reviewed workbooks generated for Case 1.1 and 1.2 and updated format to match procedure above.
- Background pages in EXCEL sheets are screen captures of pertinent sections of FLAC manual for these two cases (and subcases) and may need to be redacted if EXCEL workbooks are printed.

[redacted]

March 29/07 (cont.)

Sensitivity - Grid Density

- Created FLAC input file with double grid density (40×40) instead of 20×20 to assess effect of grid density on results. "Case0102a.dat".
- Need to modify history commands to monitor at same locations as base case. Locations i = 14 → x = 0.0375 m, i = 22 → x = 0.0575 m selected.
- Input file run with FLAC to produce LOG file "Case0102a.log" which was imported into EXCEL file "Case0102a.xls" on sheet 1 "LOG FILE".
- Data set increased from 335 rows to 3792 rows due to larger grid size and smaller timestep.
- "Comparison(2)" sheet created to reduce number of plotting points.

* Results: FLAC, Analytical and EXCEL datasets compare very favourably. Max differences as follows:

	FLAC - Analytical	FLAC - EXCEL	Analytical - EXCEL
r = 0.025 m	0.03% (0.30%)	0.04% (0.32%)	0.02% (0.02%)
r = 0.0375 m	0.03% (0.07%)	0.03% (0.08%)	0.03% (0.02%)
r = 0.0575 m	0.03% (~~0.03%~~ 0.07%)	0.04% (~~0.08%~~ 0.09%)	0.02% (~~0.05%~~ 0.06%)

- General improvement compared to base case (shown in brackets above), but original difference still very small and within acceptable limits. Mar 29/07

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Sensitivity - Thermal Properties

- Prepare sensitivity cases "b" and "c" by changing thermal properties and temperature boundary conditions
- Created FLAC input file "Case0102b.dat" from Base Case file by changing thermal conductivity from 2.51 to 10 W/m·°C

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March 30/2007 (cont.) RP

- Also changed specific heat from 911.3 to 500 J/kg°C.
- Input file run in FLAC to create output file "Case0102b.~~dat~~ log RP" which was imported to create EXCEL workbook "case0102b.xls".
- Data set increased to 2437 from 335 → adjust parameter "ntab" to 2437 to produce consistent output for Analytical results.

* Results: FLAC, Analytical and EXCEL datasets compare favourably. Max differences as follows:

	FLAC-Analytical	FLAC-EXCEL	Analytical-EXCEL
r: 0.025m	0.07%	0.07%	0.03%
r: 0.038m	0.03%	0.03%	0.04%
r: 0.055m	0.03%	0.04%	0.04%

General improvement relative to Base Case. Differences considered acceptable.

Sensitivity - Thermal Flux Boundary Condition.

- Created FLAC Input file "Case0102c.dat" from Base Case file by changing thermal flux from 5138.65 to 10000 w/m²
- Input file run in FLAC to produce output file "Case0102c.log" which was imported into EXCEL workbook "Case0102c.xls".
- Data set same size as original base case

* Results: FLAC, Analytical and EXCEL datasets ~~compare favourably~~. Max difference as follows:
RP

	FLAC-Analytical	FLAC-EXCEL	Analytical-EXCEL
r: 0.025m	0.62%	0.61%	0.02%
r: 0.038m	0.13%	0.13%	0.02%
r: 0.055m	0.10%	0.16%	0.09%

- Differences generally larger than base case, particularly at

[redacted]

March 30/2007 (cont.)

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early time. However, values still within acceptable range.

* Summary: Case 1.2 - Heat Conduction from a Spherical Cavity with Applied Heat Flux.

- Case 1.2 completed as per "Software Validation Test Plan for the Finite Difference Code FLAC (Fast Lagrangian Analysis of Continua) Version 5.0".
- Base case and three sensitivity cases run to compare FLAC, Analytical and EXCEL data sets. Associated files are as follows:

Input files: Case0102.dat - Base Case
Case0102a.dat - Grid sensitivity case
Case0102b.dat - Thermal property sensitivity case
Case0102c.dat - Thermal boundary condition sensitivity case.

FLAC Output files: Case0102.log
Case 0102a.log
Case 0102b.log
Case 0102c.log
} as above

/m²

EXCEL files: Case 0102.xls
Case 0102a.xls
Case 0102b.xls
Case 0102c.xls
} as above

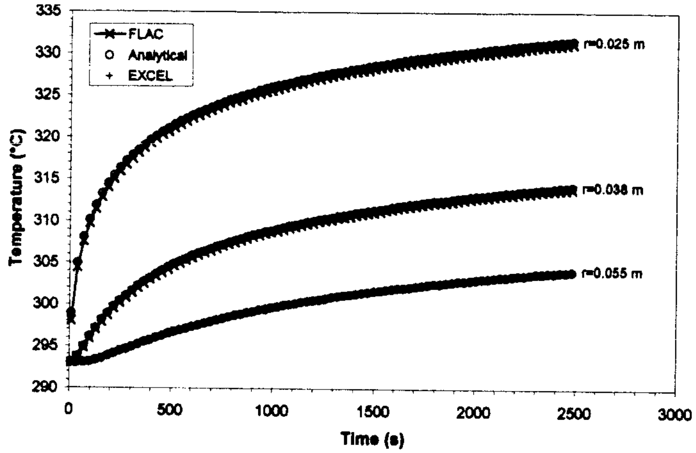
Other files: Intermediate FLAC ".SAV" files for various cases
Plot file in WORD "Case0102Plots.doc"

2

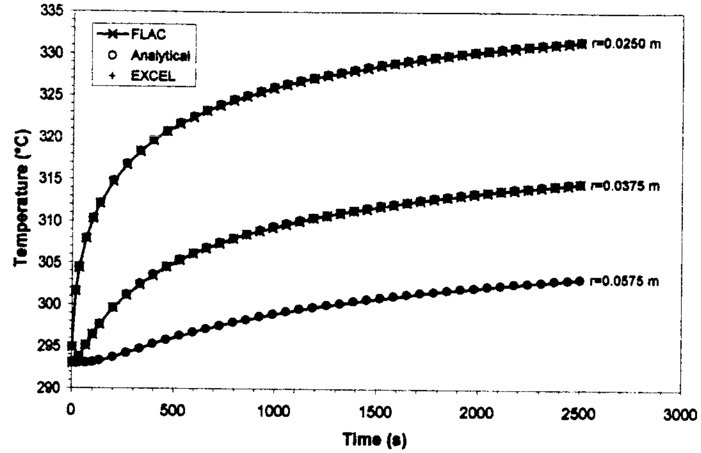
- Results from FLAC compare favourably to other datasets in each case, with maximum difference 0.62% or less in each case, well below 1% difference considered acceptable

- Representative plots shown on following page.

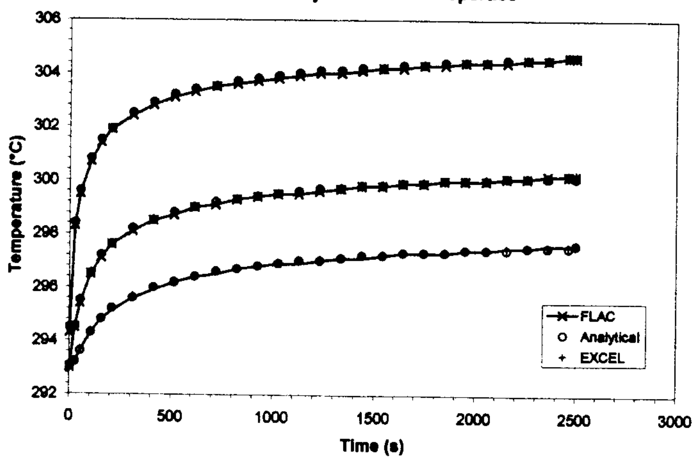
Case 1.2 - Heat Conduction from a Spherical Cavity
Base Case



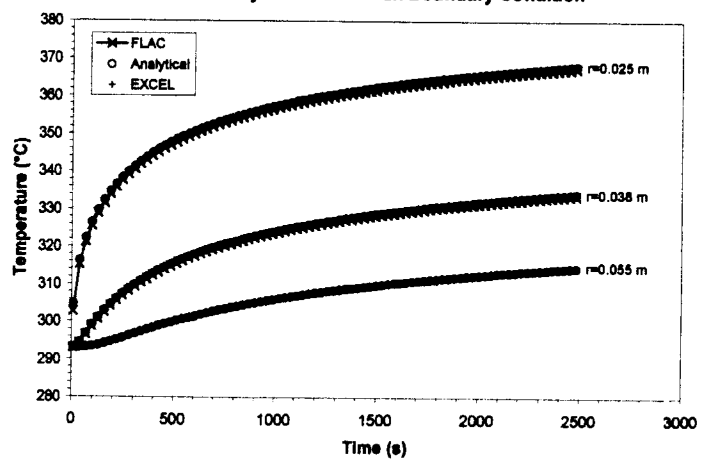
Case 1.2a - Heat Conduction from a Spherical Cavity
Sensitivity to Grid Density



Case 1.2b - Heat Conduction from a Spherical Cavity
Sensitivity to Thermal Properties



Case 1.2c - Heat Conduction from a Spherical Cavity
Sensitivity to Thermal Flux Boundary Condition



[redacted]

April 1, 2007

- administrative activities

April 3/2007

- planning activities for next cases

April 4, 2007

- planning activities, and scheduling

April 5/2007

- planning activities.

April 9/2007

Case 2.1 Initial Entry

- start Case 2.1 - Cylindrical hole in an infinite elastic medium subjected to isotropic stresses. Associated FLAC input files copied into FLAC EXE directory.
- Problem description given in FLAC Version 5.0 Verification Problems, Problem 1 (pp 1-1 to 1-20)
  - files used include "hole.dat", "Tabm1.fis", "VerProb_01.prj", and "hole.fis".

In process entry

- Modify "hole.dat" to "Case0201.dat". Current file set up to calculate stresses and displacements using three different grids, including an ~~axisym~~ axisymmetric grid and an infinite elastic boundary.
- Original file "hole.dat" printed and modifications to be defined.
  - update FISH subroutines to calculate radial and tangential stresses in non-isotropic stress field.
  - update FISH subroutine to calculate radial and tangential displacements under non-isotropic stresses.
  - use quarter symmetry grid to assess influence of stress state (isotropic vs anisotropic)
  - use axisymmetric and IEB grids to

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compare results for isotropic stress state
- use IEB grid to assess effects of boundary conditions.
- incorporate ARRAY algorithm to store calculated values and to create output. Improves accuracy of numbers versus the PRINT command in FLAC.

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In process entry

April 11/2007

- review information on ARRAY command in FISH language to develop output routine.
- plan modifications to CASE0201.DAT file to cover general case of stress boundary conditions

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- continue to develop input file for general case of a hole in an infinite elastic medium
- points of comparison to be σ_r, σ_θ, $\tau_{r\theta}$ vs radial distance at $\theta = 0, 45$ and $90°$.
- basis for calculating error plots (contoured error) in FLAC manual not clear - appears to use initial far-field stress (or mean stress) as denominator. Plots not to be used as comparison tools → rely on line plots.

April 25th/07.

April 28/07

- modify FLAC input file for general case
- test run to ensure coding correct.
- Base case input file Case0201.dat. modified to produce Log files of specific stress and displacement components.
- Create Case0201.XLS - import all LOG files as separate pages
- Input analytical solution into EXCEL

* Note: sign convention on radial displacement incorrect in FLAC manual pg. 1-2

In p… en… Case… Cas…

[redacted]

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* Likewise for tangential displacement. Related to tensile positive stress convention in FLAC.
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In process entry Case0201a.dat, Case 2.1a

- Modify axisymmetric routine using Case0201.dat to create FLAC input file Case0201a.dat.
- modify calculation of radial and tangential stress and displacement to account for axisymmetric geometry.
- Produced the following LOG files of output.

Case0201.dat	Case0201a.dat	
theta_s0201.out	same but with 0201a in filename	Rotation angle (stress)
theta_d0201.out		Rotation angle (disp.)
sigt_t0201.out		Tangential stress (theoretical)
sigt_f0201.out		Tangential stress (FLAC)
sigs_t0201.out		Shear stress (theor.)
sigs_f0201.out		Shear stress (FLAC)
sigr_t0201.out		Radial stress (theor).
sigr_f0201.out		Radial stress (FLAC)
dist_t0201.out		Tang. disp. (theor.)
dist_f0201.out		Tang. disp. (FLAC)
disr_t0201.out		Radial disp. (theor)
disr_f0201.out		Radial disp. (FLAC)
dism_f0201.out		Total disp. (FLAC)
dism_t0201.out		Total disp. (theor.)

- all LOG files input into EXCEL spreadsheets Case0201.xls and Case0201a.xls. to produce comparative plots of stresses and displacements under isotropic stress conditions.
- stresses compare favourably (FLAC, theoretical, EXCEL) with less than 5% max. difference between FLAC and EXCEL solutions in CASE0201.XLS, and about 1% difference in CASE0201a.XLS.

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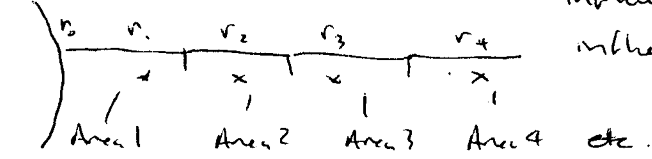
- difference in displacement between FLAC and EXCEL solutions increases from about 4% near opening to almost 50% within 1.25m of outer boundary for Case0201a.xcs.
  - difference due largely to fixed ~~displacement~~ stress boundary at 10m. RK 4/29/07
- for Case0201.xcs max difference is almost 60% near outer boundary, albeit the displacement values are small in this location.

* Need to develop measure of mean error to overcome problem with small denominator → large % error.
  - for line plots, use weighted average based on influence area for each data point to calculate weighted total EXCEL value (area under response curve), and weighted difference value between FLAC and EXCEL
- calculation as follows



influence area$_1$ = $\frac{r_1 - r_0}{1} + \frac{r_2 - r_1}{2}$ * R
influence area$_2$ = $\frac{r_2 - r_1}{2} + \frac{r_3 - r_2}{2}$
etc.

· influence area → w, value of variable → V, value of difference → D

$$\text{total error} = \frac{\sum w_i D_i}{\sum w_i V_i} \times 100\%$$

- modify excel sheets to calculate total error. April 29/2007

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- modify EXCEL sheets to include calculation of total error. Correct formulae in EXCEL displacement comparison to reference displacement r, θ values.
- check axisymmetric theoretical FISH routine to account for difference between EXCEL and theoretical values

[redacted]

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Corrections - identified source of error between EXCEL and axisymmetric theoretical displacement values → caused by incorrect reference to "LOG Theta_s" worksheet instead of "LOG Theta_d" worksheet.
- corrected both Case0201.XLS and Case0201a.xls.

Results Case 2.1 and 2.1a - Using total error calculation, results for the two cases are as follows.

	Case0201.XLS	Case0201a.xls
· Radial stress	1.09%	1.00%
· Tangential stress	0.97%	1.02%
· Shear stress	undefined*	undefined*
· Radial displacement	13.35%	13.55%
· Tangential displacement	undefined*	undefined*
· Total displacement	13.35%	13.55%

* denominator is zero.

- error in displacement due to applied stress boundary at 10 m. Use Infinite Elastic Boundary (FEB) FLAC option to check this effect.

Case 2.1b In process entry - created FLAC input file "Case0201b.dat" to simulate a cylindrical hole in an infinite elastic medium subjected to an infinite elastic boundary with specified bulk and shear modulus values.
- requires circular outer grid boundary; achieved by creating a square grid then imposing a circle using FLAC function. Null grid outside outer circle. Create central hole in same manner.
- same output files as listed on page 23 of this notebook, but with 0201b in names.
- created EXCEL workbook Case0201b.XLS and imported LOG files into separate worksheets. Only left half of grid considered in plots due to symmetric nature of problem.

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Case 2.1b Results - Use of infinite elastic boundary improves fit between theoretical and FLAC results. Errors are as follows:

FLAC-EXCEL Max difference	FLAC-EXCEL Total Error.	
21.35%	0.54%	Radial Stress
1.09%	-0.23%	Tangential Stress
Undefined*	Undefined*	Shear stress
5.14%	-3.87%	Radial Displacement
Undefined*	Undefined*	Tangential Displacement
5.14%	-3.87%	Total Displacement

* Denominator = 0.

- Largest error in stress and displacement at boundary of cylindrical opening due to irregular and relatively coarse nature of FLAC grid. Error in radial stress drops to less than 2% within 1m of opening.

Case 2.1c In Process Entry
- Created FLAC input file Case0201c.dat to assess stress and displacement response along a line at 45° to x-axis. Same output files as shown on page 23, but with 0201c in name.
- Created EXCEL workbook Case0201c.xls

Case 2.1c Results

	FLAC-EXCEL Max. Diff.	FLAC-EXCEL Total Error
Radial stress	107.64%	0.81%
Tangential stress	6.13%	0.11%
Shear stress	Undefined*	Undefined*
Radial displacement	4.95%	-3.96%
Tangential displacement	Undefined*	Undefined*
Total displacement	4.95%	-3.96%

* Denominator = 0

[redacted]

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- modified JEB model has one point at boundary zone where stresses do not compare well, Aside from this zone, stresses and displacements from FLAC compare well to analytical solution coded in EXCEL. Finer grid near opening would help resolve some of the differences.

April 30/07.

Note: Work on this task pre-empted by Task 09 - Research on bulking factor. Work to resume once Task 09 complete.

May 15/07.

March 10/2008

CNWRA requested no further work to be done on FLAC validation. Scientific Notebook SN806 (Vol 1) to be returned to CNWRA by March 31/2008. CD containing associated files to be included.

March 10/2008.

Last Page - no more entry in The subsequent pages.

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