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THERMAL-MECHANICAL BENCHMARK TESTING

OF FLAC

Prepared for:

U.S. Nuclear Regulatory Commission
Division of Waste Management
Contract No. NRC-02-85-002

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June 1988

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Task Order No. 005, Task 2

Task Description: to verify the FLAC code for thermal-mechanical analysis by benchmark testing. This testing is required to support use of the code for independent calculations of DOE analyses for design of high-level nuclear waste geologic repositories.

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PREFACE

This report was prepared for the U.S. Nuclear Regulatory Commission under Task Order No. 005, Task 2, Contract No. NRC-02-85-002. This report, and three companion reports, provide the documentation and verification testing of the FLAC code for application to thermomechanical analysis for studies related to high-level nuclear waste isolation in geologic media. The accompanying reports are:

(1) "Code Verification of FLAC for Thermomechanical Analysis," Itasca Consulting Group, Inc., prepared for U.S. Nuclear Regulatory Commission Contract No. NRC-02-85-002, 1987;

(2) "Implicit Thermal Logic in FLAC," Itasca Consulting Group, Inc., prepared for U.S. Nuclear Regulatory Commission, Contract No. NRC-02-85-002, March 1988; and

(3) FLAC: Fast Lagrangian Analysis of Continua (Version 2.0) User Manual, Itasca Consulting Group, Inc., 1987

This work originally was assigned to support reviews related to the Salt Repository Program. Due to policy changes in the nuclear waste isolation program, the emphasis of this work has shifted to a more generic, pro-active study for review purposes.

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THERMAL-MECHANICAL BENCHMARK TESTING OF FLAC

1.0 INTRODUCTION

FLAC (Itasca, 1987) is a computer code used for modeling thermal, mechanical and thermomechanical behavior of two-dimensional continua. The code is being used to provide independent calculations in support of the NRC reviews of DOE designs for high-level nuclear waste geologic repositories.

This report presents the results of a benchmark test study performed with FLAC. A benchmark test is a comparative analysis of a specific problem using several codes which are based on different numerical algorithms but which contain the same constitutive behavior. The approach is identified as a viable method to indicate the accuracy of the algorithms used to represent mathematically the specific material behavior. This approach is necessary for codes containing non-linear material models because closed-form, classical solutions incorporating non-linear behavior are normally not available for comparison to the numerical solution.

The exercise described as the "Second WIPP Benchmark Problem" (Morgan et al., 1981) was used to benchmark FLAC. This problem is identified as the most thorough benchmark exercise to date for thermomechanical codes performing analyses related to nuclear waste isolation studies (Hart et al., 1987). This exercise was performed specifically for the WIPP Salt Testing Program and emphasized the verification of codes containing a salt creep constitutive model. However, the exercise also covered other material behaviors not specific to salt, such as the behavior of interbedded materials, slip along discontinuities, and temperature-dependent conductivity. Thus, the WIPP exercise provides a means to verify the accuracy of several thermal-mechanical features in FLAC.

The primary material behavior model studied in the benchmark exercise was the WIPP Baseline Creep Law. This law has frequently been used to model nuclear waste isolation in salt and has been implemented in FLAC [Itasca, 1987, Supplement No. 2]. The law is a non-linear, empirical relation that cannot be verified in a code by comparison to closed-form solutions.

Interface, or slideline, logic was also verified in this exercise. Interface logic in FLAC models the presence of discontinuous features such as clay seams, joints, or bedding planes.

Additionally, the FLAC representation of the behavior of interbedded materials was evaluated by prescribing different material behaviors for different regions in the test model.

The behavior of temperature-dependent thermal conductivity can be simulated in FLAC by defining conductivity as a non-linear function of the following form:

$$k(T) = k_0 + k_1 T^{n_1} + k_2 T^{n_2} \qquad (1)$$

where T is the temperature in Kelvin, and k_0, k_1, k_2, n_1 and n_2 are fitting parameters. This algorithm in the code was verified in this test.

2.0 THE BENCHMARK EXERCISE

Morgan et al. (1981) describe a benchmarking exercise in which nine (9) codes were used to model two different problems involving hypothetical drifts for nuclear waste isolation. The nine codes (ANSALT, DAPROK, JAC, REM, SANCHO, SPECTROM, STEALTH, and two different version of MARC) did not produce identical results, but showed the differences that can arise between codes even when all input parameters and model dimensions are identical.

The first problem represented an isothermal drift; the second was heated. The two drift configurations are shown in Figs. 1 and 2. The figures also show the various materials modeled, the dimensions of the drifts, and the location of the slidelines.*

In the second (heated) problem, the heat source was taken as a long source beneath the floor. Its output was

$$s(t) = 169.5 \exp(-t/1.365e9) \text{ W/m} \qquad (2)$$

where t is time in seconds. Radiation was modeled indirectly, as a high-conductivity material in the drift.

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*For the FLAC simulation, the boundary conditions were changed slightly: the "fixed line" boundary shown in the upper right-hand corner of the models in Figs. 1 and 2 was changed to a slideline, and the lower pressure boundary was replaced by a fixed y-displacement boundary.

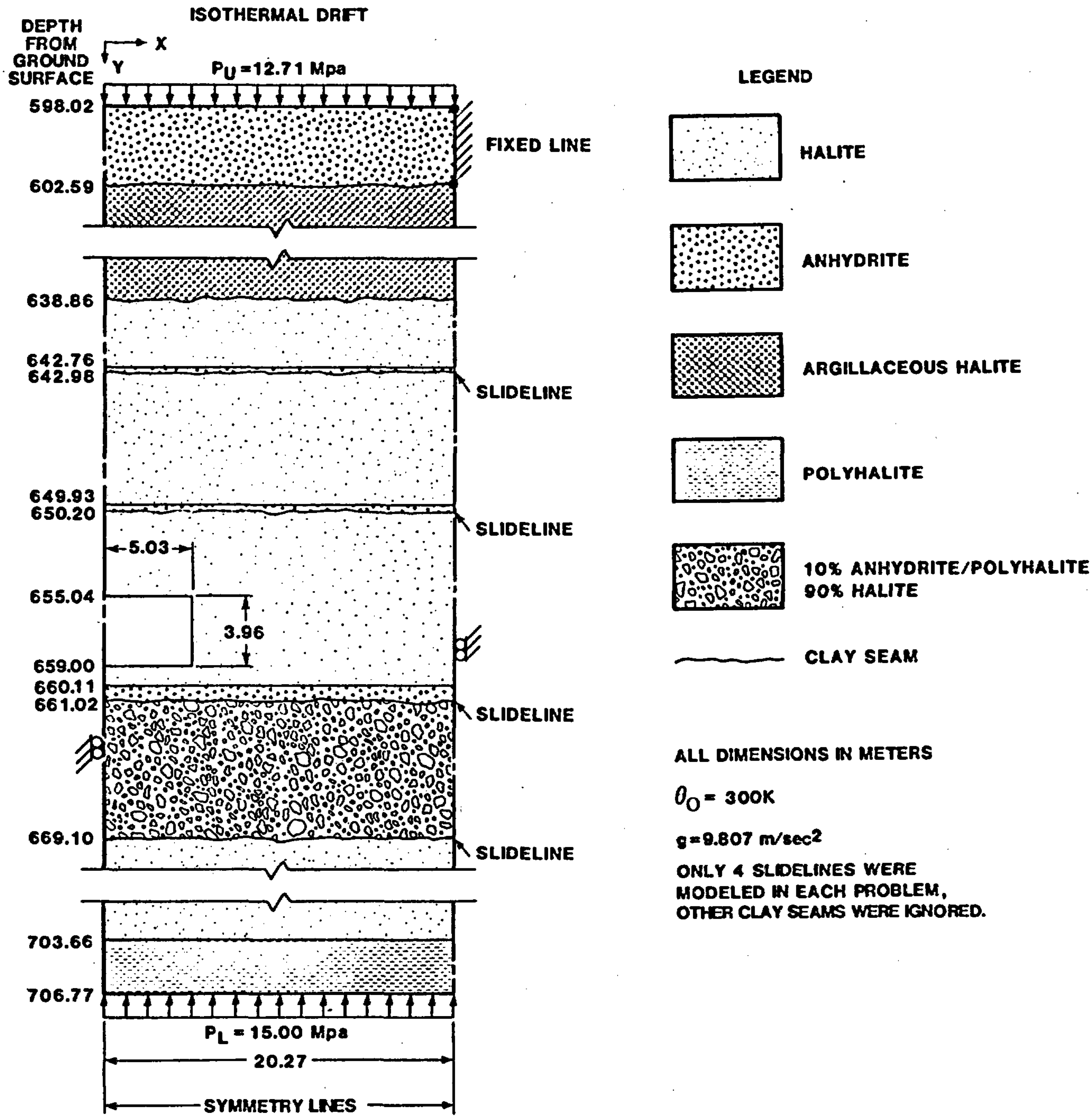


Fig. 1 Isothermal Drift Configuration [Morgan et al., 1981]

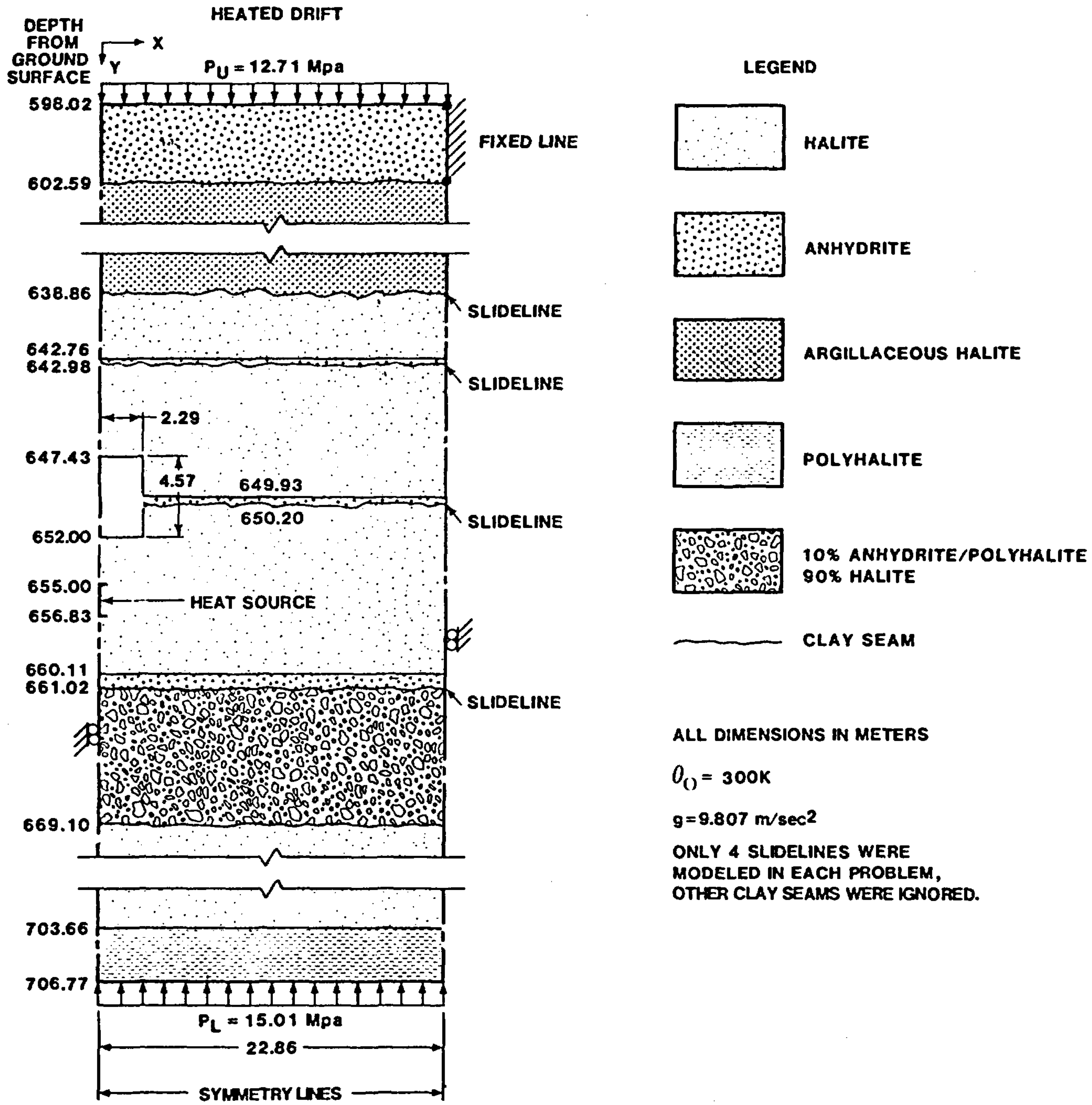


Fig. 2 Heated Drift Configuration [Morgan et al., 1981]

The material properties for the various layers are summarized in Tables 1 and 2.

Table 1

MECHANICAL PROPERTIES FOR THE SECOND BENCHMARK PROBLEM

(Repository Level, Nominal 655m)

[Morgan et al., 1981]

	Elastic Constants		Creep Constants		
			D	n	Q
Material	υ	E (Pa)	($Pa^{-4.9} \cdot s^{-1}$)		(kcal/mole)
halite	0.25	2.48E+10	5.79E-36	4.9	12.0
argillaceous salt	0.25	2.48E+10	1.74E-35	4.9	12.0
10% A-P, 90% H	0.25	2.65E+10	5.21E-36	4.9	12.0
anhydrite	0.33	7.24E+10	0.0	---	----
polyhalite	0.33	7.24E+10	0.0	---	----
clay seam	friction slip line: $\mu_{static} = \mu_{dynamic} = 0.0$				

Table 2

THERMAL PROPERTIES FOR THE SECOND BENCHMARK PROBLEM

[Morgan et al., 1981]

Material	Density (ρ) Mg/m^3	Specific Heat (C_p) J/(kg·K)	Coefficient of Linear Thermal Expansion (α) K^{-1}	Thermal Conductivity* Parameters λ_o W/(m·K)	γ
halite	2.167	860.0	45.0E-6	5.0	1.14
argillaceous salt	2.167	860.0	40.0E-6	4.0	1.14
10% A-P, 90% H	2.167	860.0	42.7E-6	5.0	1.14
anhydrite	2.167	860.0	20.0E-6	4.5	1.14
polyhalite	2.167	860.0	24.0E-6	2.0	1.00
"Equivalent Thermal Material"	1	1000.0	-------	50.0	0.0

* $k = \lambda_o(300/\theta)^\gamma$, where θ is temperature in Kelvin

According to Morgan et al. (1981, p. 20), the "conductivity k was originally . . . incorrectly prescribed as $k = \lambda_o(\theta/300)^\gamma$.

All participants in Benchmark II were instructed to use the incorrect expression because most of the calculations were near completion when the error was discovered . . . . The Benchmark II comparisons were not affected by this error, because all participants used the same expression. However, if the properties in this table are used for calculations other than the Benchmark II calculations, the correct conductivity expression should be used." For comparison purposes, the incorrect expression was used in the FLAC simulations.

The creep law used is described below in terms of the total strain rate:

$$\dot{\varepsilon}_{ij} = -\frac{\nu}{E}\dot{\sigma}_{kk}\,\delta_{ij} + \frac{1+\nu}{E}\dot{\sigma}_{ij} + \dot{\varepsilon}^{c}_{ij} \qquad (3)$$

where $\dot{\sigma}_{ij}$ = derivative with time of stress i,j ,

δ_{ij} = Kronecker's delta,

ν = Poisson's ratio,

E = Young's modulus, and

$\dot{\varepsilon}^{c}_{ij}$ = creep strain rate,

where $\dot{\varepsilon}^{c}_{ij} = (1.5)^{1/2}\,\dot{\bar{\varepsilon}}\,\dfrac{\sigma'_{ij}}{(\sigma'_{mn}\,\sigma'_{mn})^{1/2}}$

where $\dot{\bar{\varepsilon}} = D\,\bar{\sigma}^{n}\exp(-Q/R\theta)$,

σ'_{ij} = deviatoric stress i,j ,

D, Q, n = creep model parameters,

R = universal gas constant, and

θ = temperature (in K).

3.0 FLAC RESULTS

The results from FLAC were compared to the results reported by Morgan et al. (1981) for the two benchmark problems. Additionally, certain key features of the problems were varied to evaluate their effect on the results.

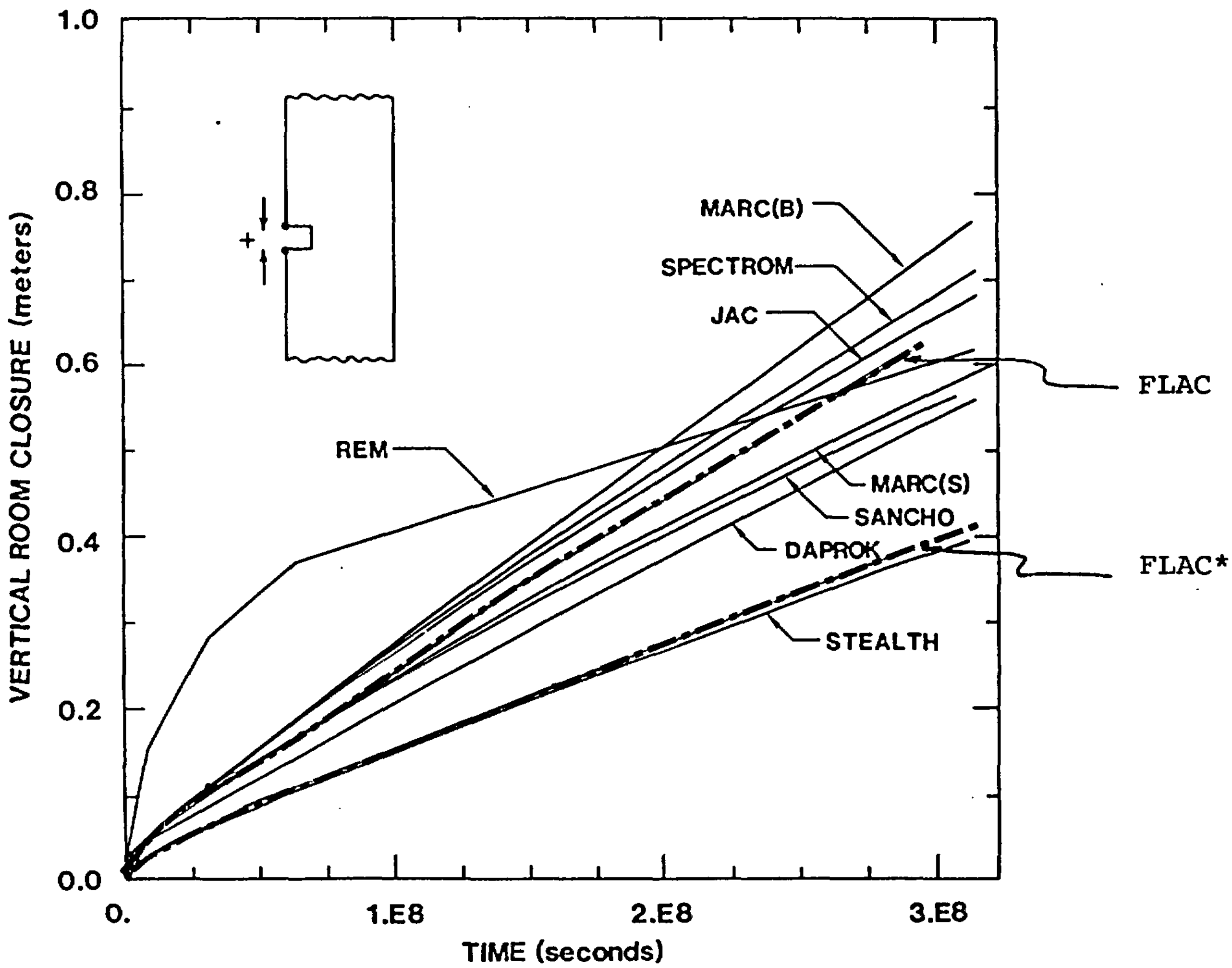
3.1 Isothermal Problem

Figures 3 to 11 show the results from FLAC, compared to the other codes. All the results agree extremely well. The closure histories in Figs. 3 and 4 show FLAC almost exactly centered between the results for the most closely clustered codes. The stress profiles in Figs. 5, 6 and 7 also show FLAC agreeing well with the other codes. In addition, the results from FLAC seem to vary more smoothly than some of the others, which is probably more realistic. The relative slip profiles shown in Figs. 8 to 11 are also in good agreement. In these figures, FLAC does not show the average behavior of the other codes, but this is not indicative of any error or problem. No one set of results should be considered as the "correct" solution. Only if the results vary distinctly from the average behavior should the assumptions of the code be checked.

For example, if the slidelines and the thin anhydrite interbeds are ignored in the FLAC analysis, the results are on the lower extreme of those reported in the benchmark study (see Figs. 3 and 4). Also, the stress profile in this instance does not exhibit the sharp spike seen from the other models (Fig. 5).

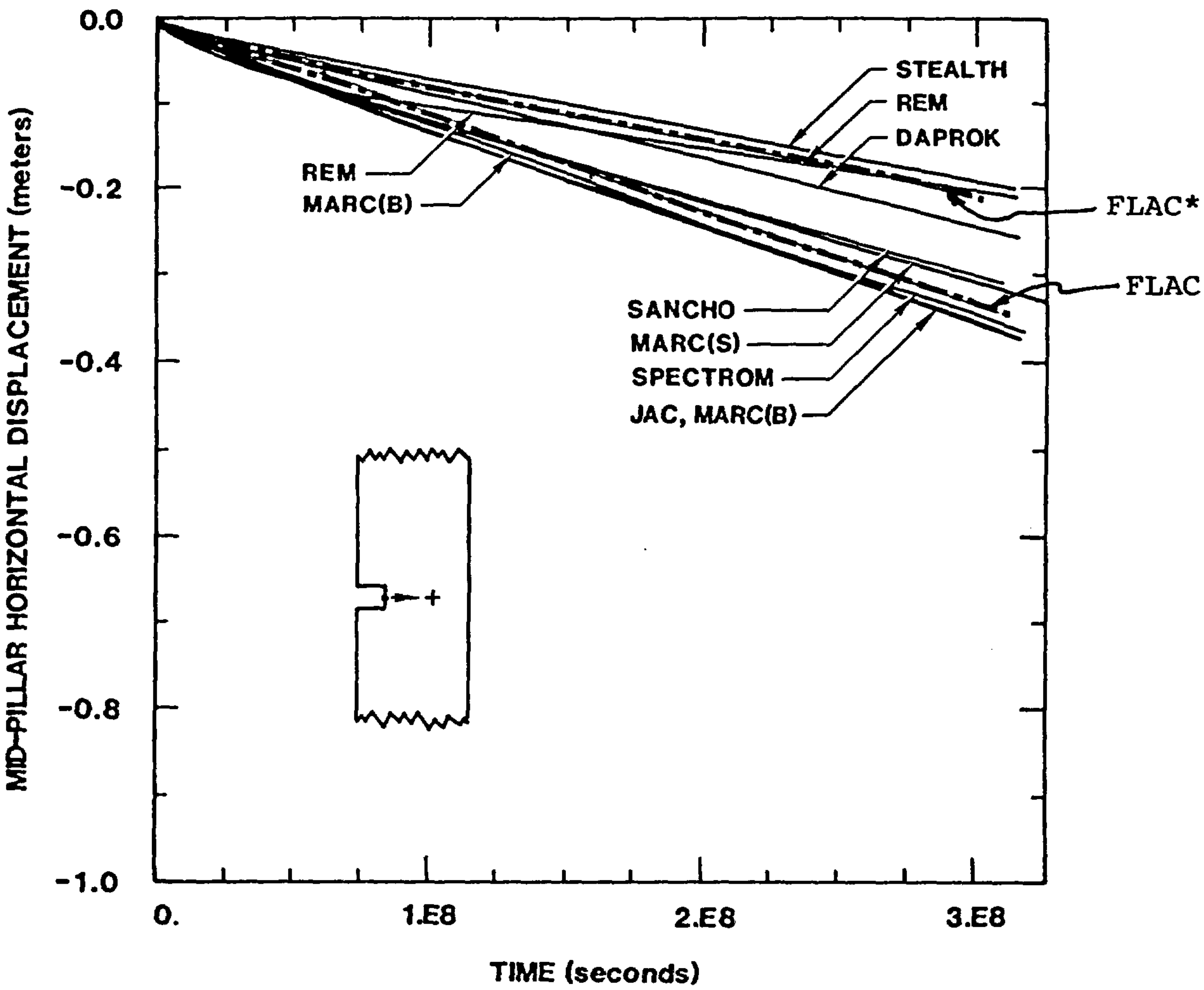
However, if only the clay seams are modeled (i.e., slidelines are used but the anhydrite interbeds are ignored), the comparison of results worsens. In this case, the vertical room closure, for example, is approximately three times greater than the maximum values shown in Fig. 3. The poor agreement is attributed to the omission of the thin, stiff anhydrite layers, especially the layer immediately beneath the floor.

These simulations indicate both the importance of modeling inhomogeneous behavior correctly in the numerical analysis and, also, the apparent significance of inhomogeneities on rock mass behavior.



*model without interface elements and anhydrite layers

Fig. 3 Vertical Closure Histories for the Isothermal Room [Morgan et al., 1981]



*model without interface elements and anhydrite layers

Fig. 4 Mid-Pillar Horizontal Displacement Histories for the Isothermal Room [Morgan et al., 1981]

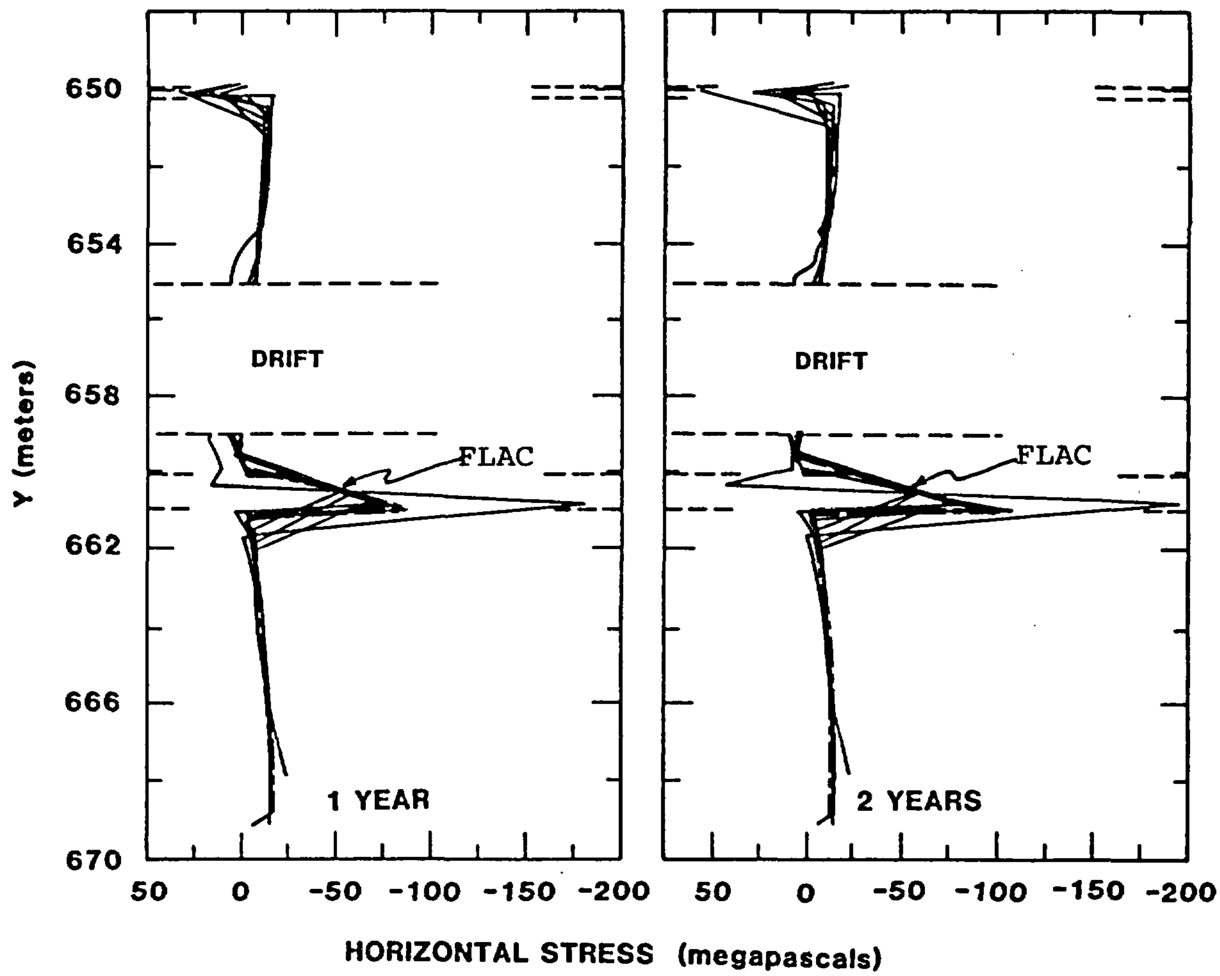


Fig. 5 Horizontal Stress Profiles Along the Vertical Centerline of the Isothermal Room at 1 and 2 Years [Morgan et al., 1981]

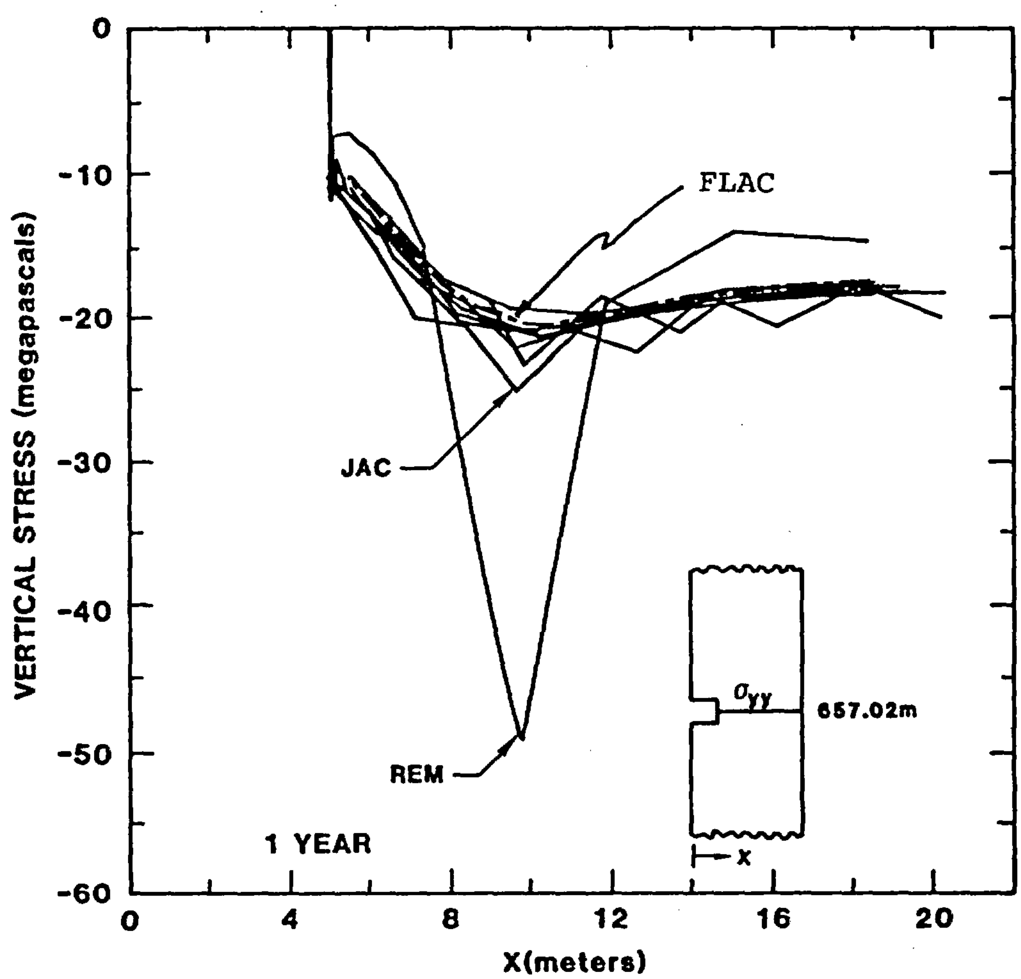


Fig. 6 Vertical Stress Profiles Through the Pillar of the Isothermal Room at 1 Year [Morgan et al., 1981]

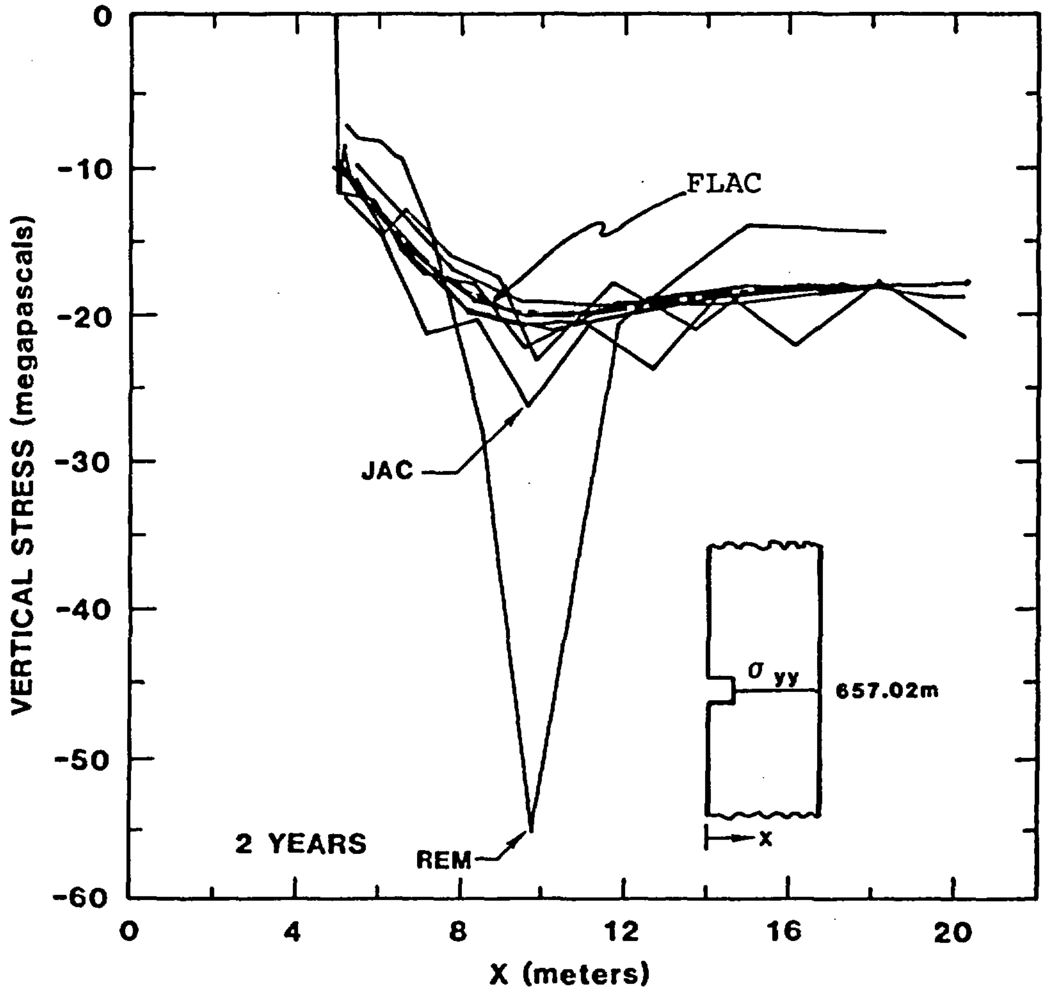


Fig. 7 Vertical Stress Profiles Through the Pillar of the Isothermal Room at 2 Years [Morgan, et al., 1981]

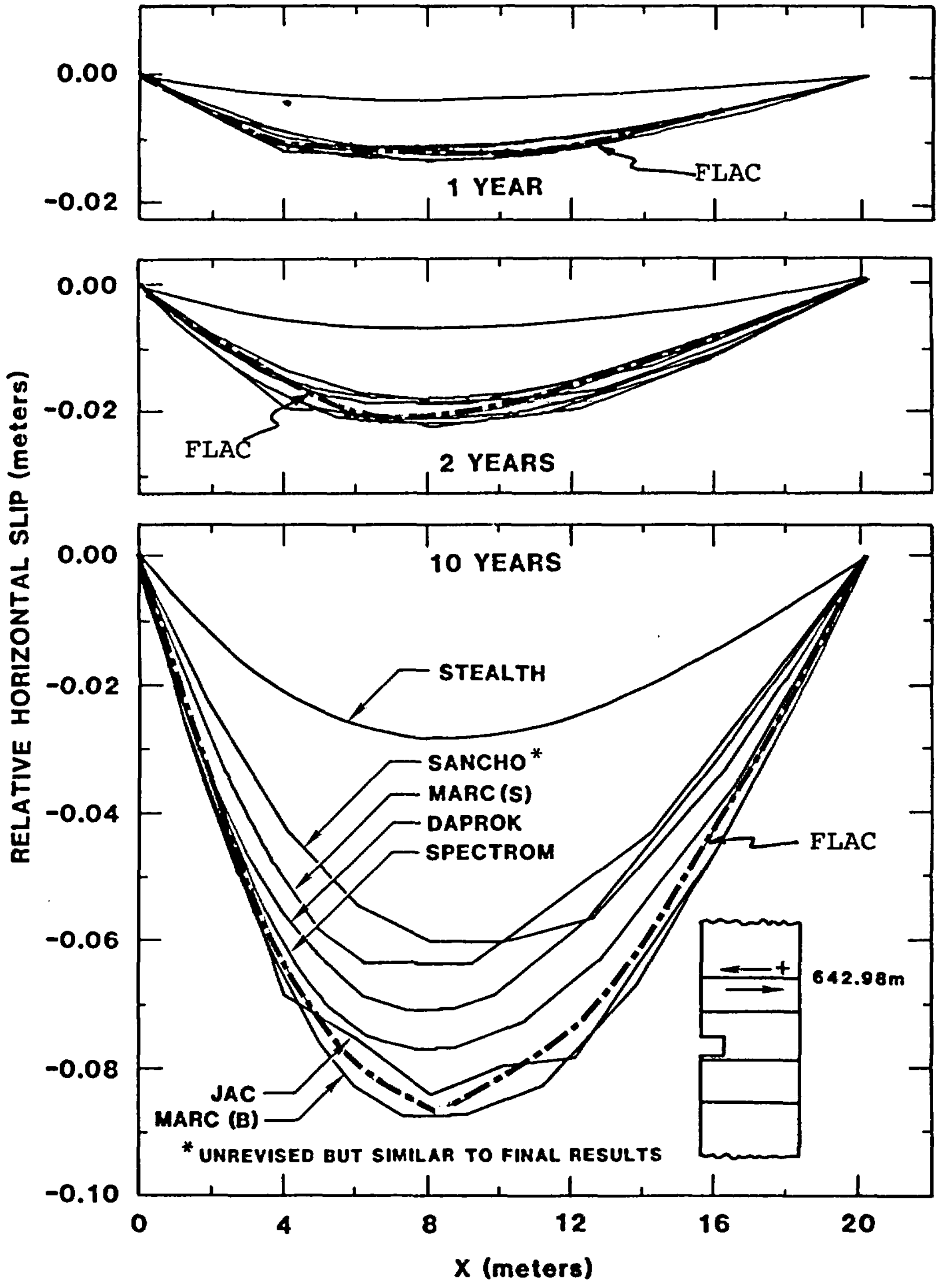


Fig. 8 Relative Slip Across the 642.98m Slide Line for the Isothermal Room at 1, 2 and 10 Years [Morgan et al., 1981]

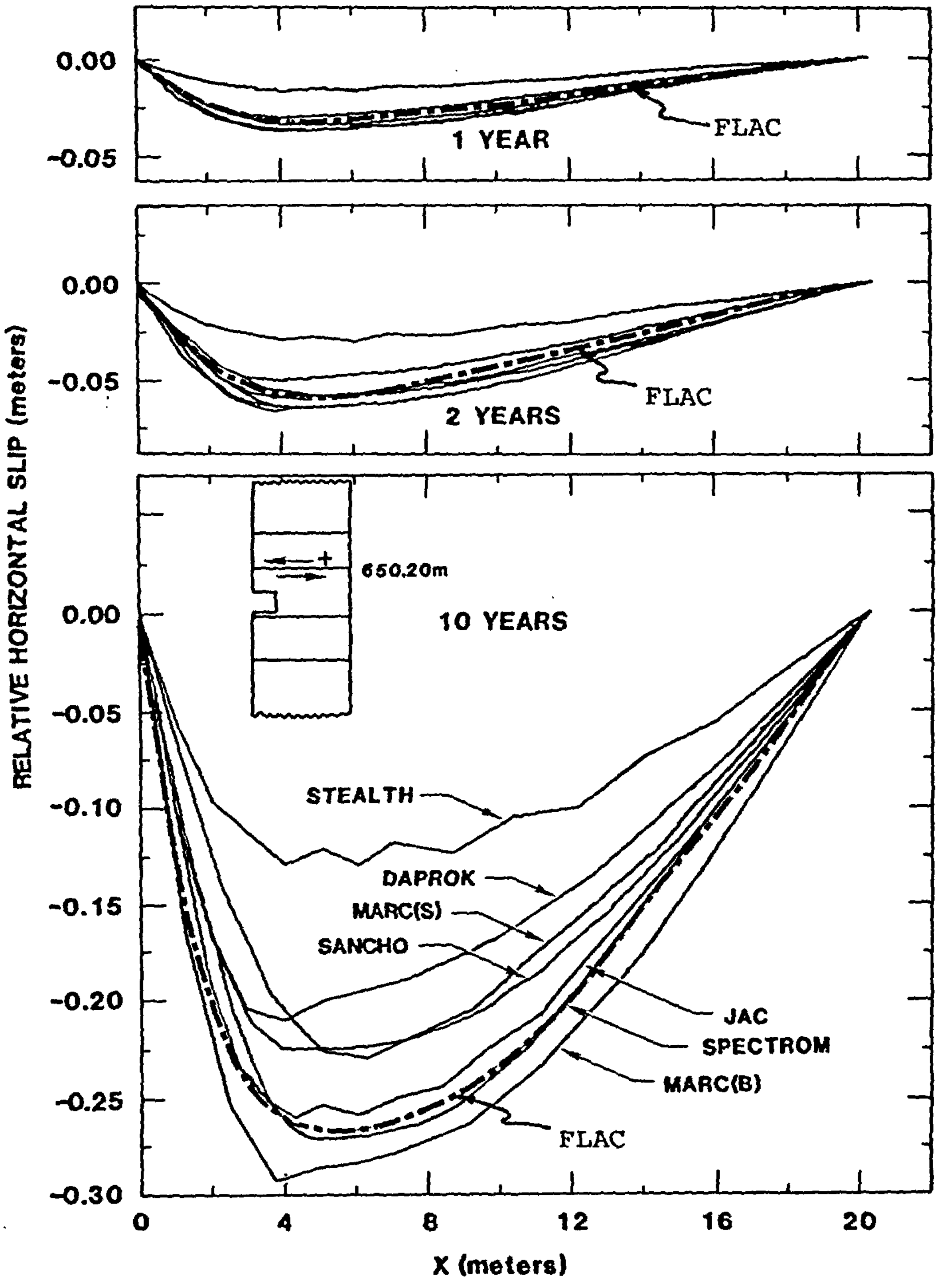


Fig. 9 Relative Slip Across the 650.20m Slide Line for the Isothermal Room at 1, 2 and 10 Years [Morgan et al., 1981]

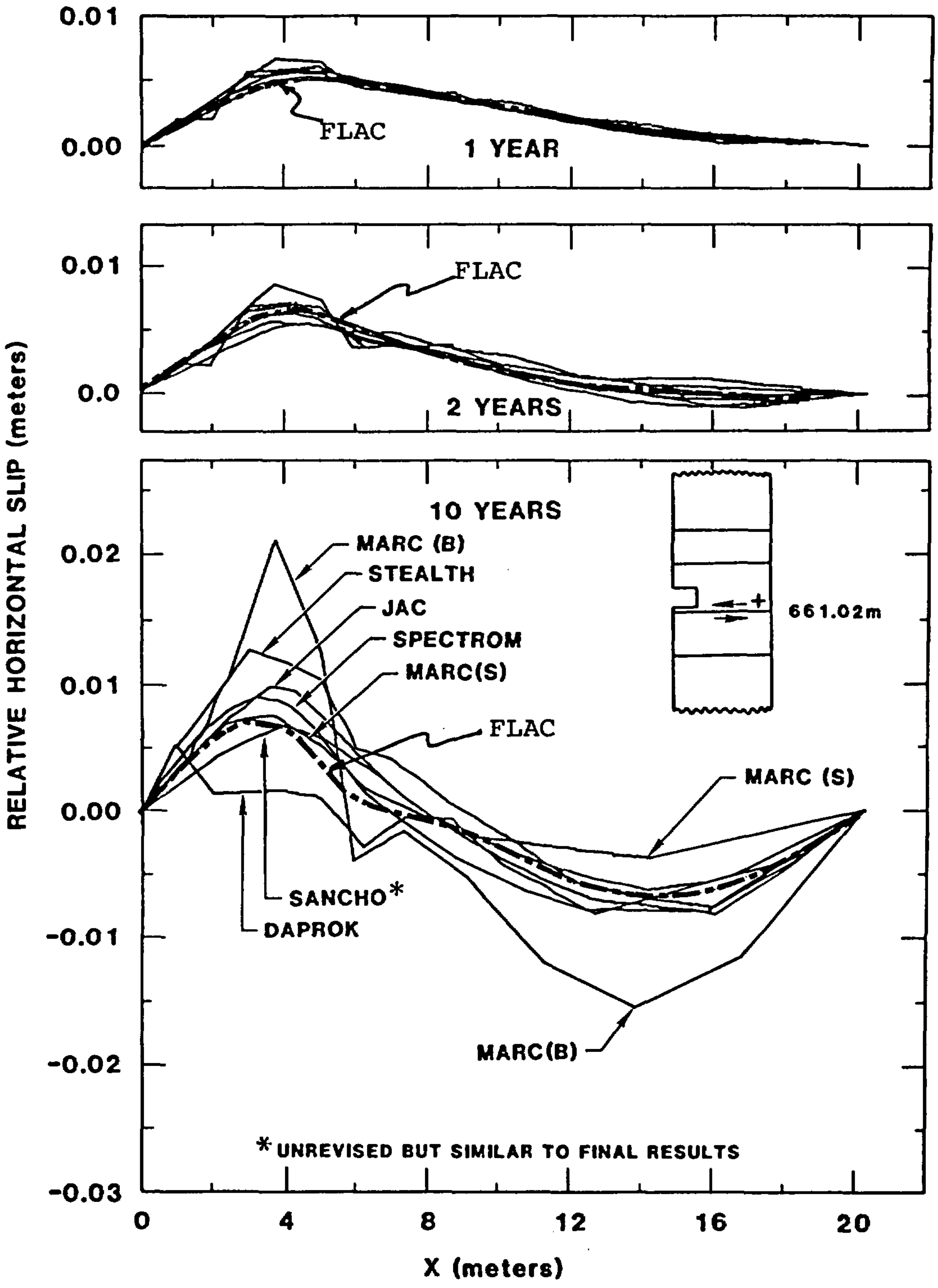


Fig. 10 Relative Slip Across the 661.02m Slide Line for the Isothermal Room at 1, 2 and 10 Years [Morgan et al., 1981]

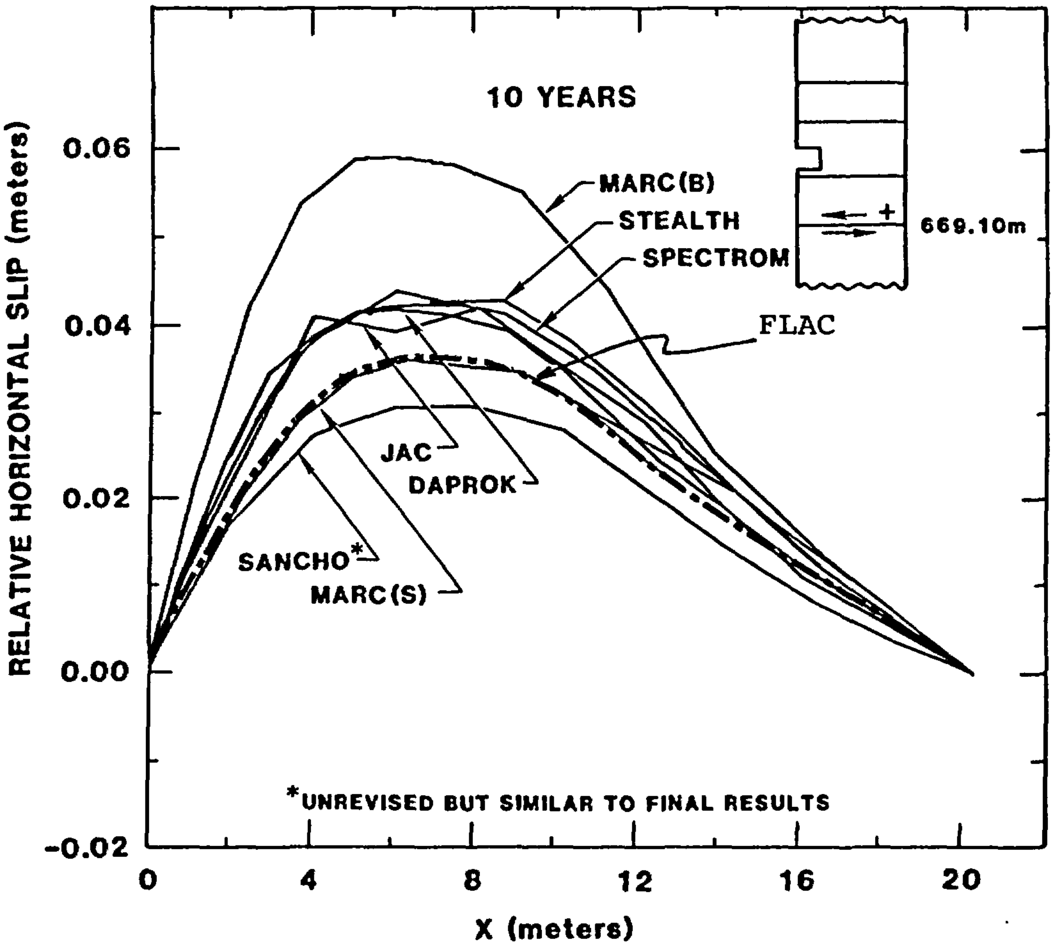


Fig. 11 Relative Slip Across the 669.10m Slide Line for the Isothermal Room at 10 Years [Morgan et al., 1981]

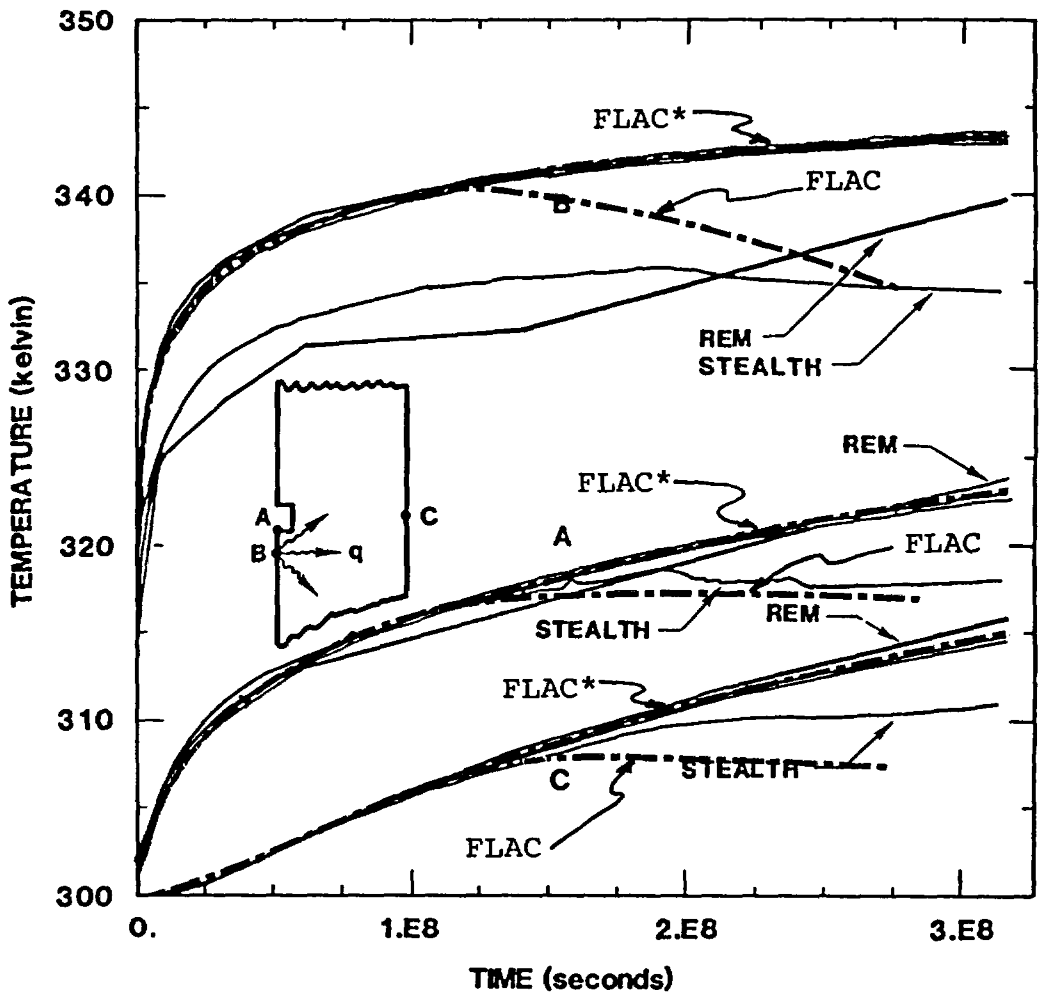
3.2 Heated Room

The comparison of FLAC results for the heated room problem to the other benchmark codes is presented in Figs. 12 through 19. The results compare well until approximately three years of heating, at which time the temperatures drop significantly compared to the other codes (see Fig. 12). This anomalous behavior is attributed to the simulation of radiation in the model. The high thermal diffusivity of the "equivalent material" (see Table 2) used to model radiation causes FLAC, which is based on an explicit time integration solution procedure, to use extremely small timesteps. This produces truncation errors in the calculation of temperature changes at late times, when temperature changes are small.

The vertical closure predicted by FLAC (Fig. 13) agrees well with the other codes until approximately the time the temperatures start deteriorating. The incorrect temperatures cause incorrect creep rates and thermal expansion effects which are believed to affect these results. The horizontal displacement (Fig. 14) does not exhibit these problems and agrees well with the other codes. However, the extremely close agreement of all the codes suggests that this displacement is not sensitive to the algorithm or temperatures anyway. The relative slip profiles on the interfaces (Figs. 15 to 17) agree extremely well after one year, and are slightly lower after two years. The stress profiles in Figs. 18 and 19 agree well with the other codes.

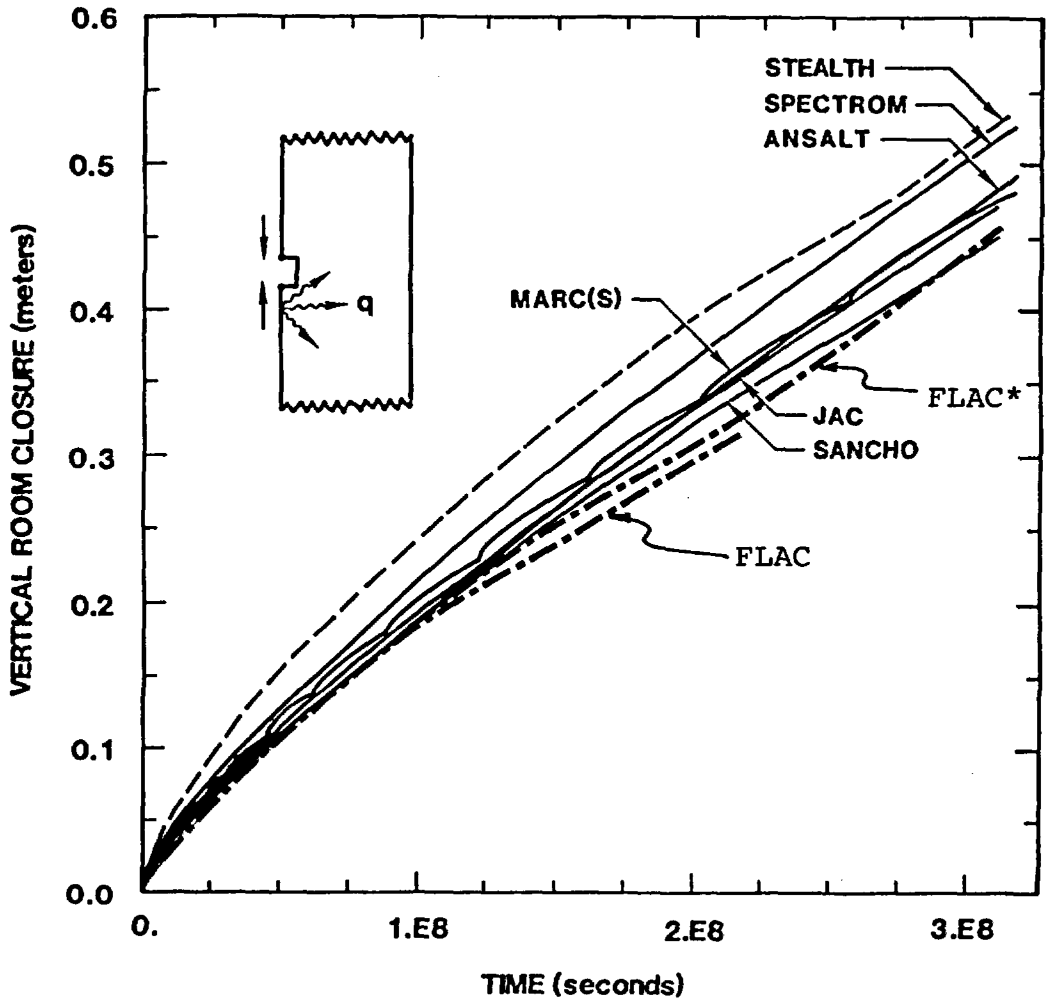
An implicit thermal solution algorithm was added to FLAC to improve the late-time temperature calculations (Mack, 1988). The implicit formulation does not have the problem with truncation errors that the explicit formulation has and is better suited for taking large timesteps at late-time, when temperature changes are small. The improvement of the results with implicit thermal logic is indicated in the plots (Figs. 12 and 13).

The heated room analysis with FLAC was also performed for the case of constant thermal conductivity rather than the temperature-dependent relation given in Table 2. This simulation produced temperatures 10% greater than the values plotted in Fig. 12.



*FLAC with implicit thermal logic

Fig. 12 Temperature Histories for the Heated Room at (A) the center of the room floor, (B) the heat source, and (C) the intersection of the pillar centerline with the horizontal centerline of the room [Morgan et al., 1981]



*FLAC with implicit thermal logic

Fig. 13 Vertical Closure Histories for the Heated Room [Morgan et al., 1981]

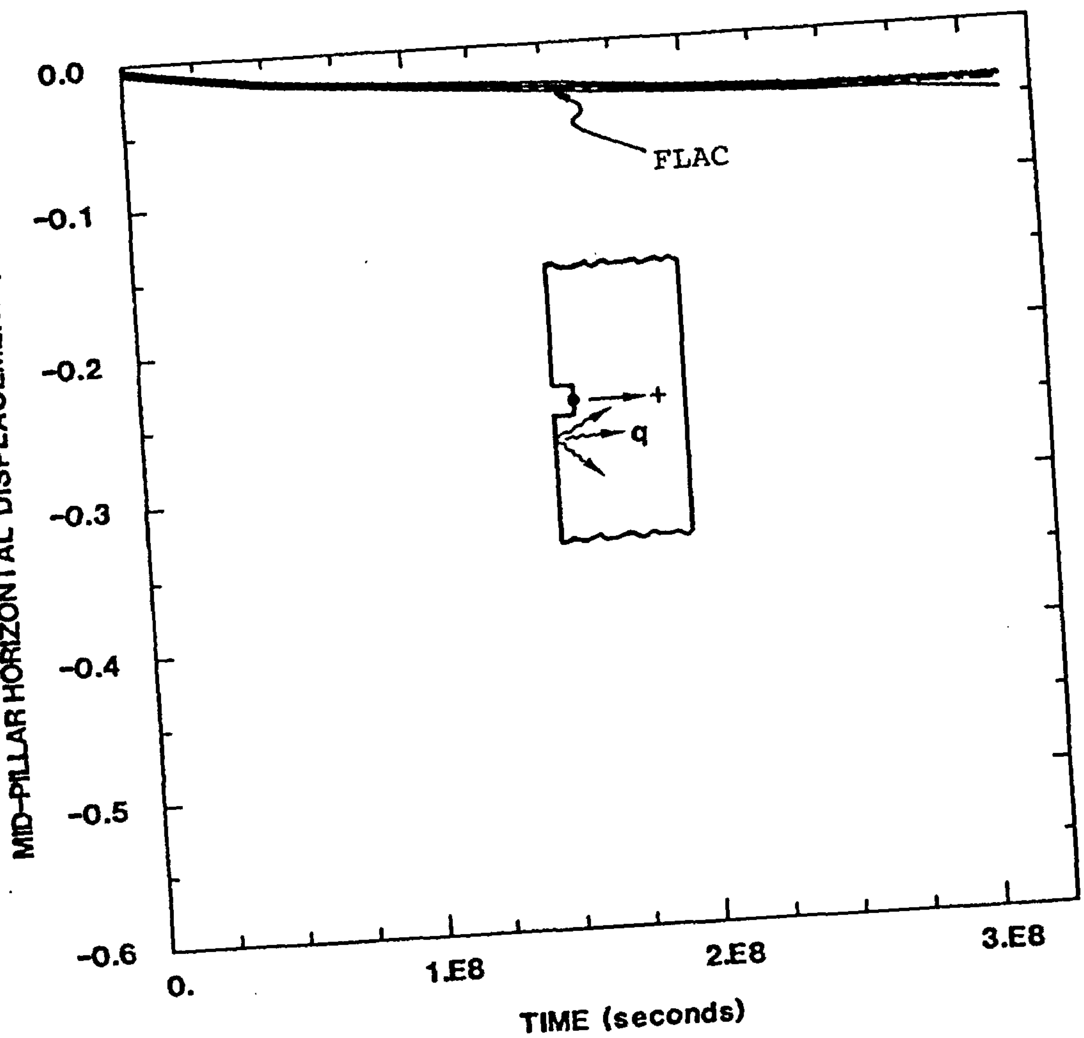


Fig. 14 Mid-Pillar Horizontal Displacement Histories for the Heated Room [Morgan et al., 1981]

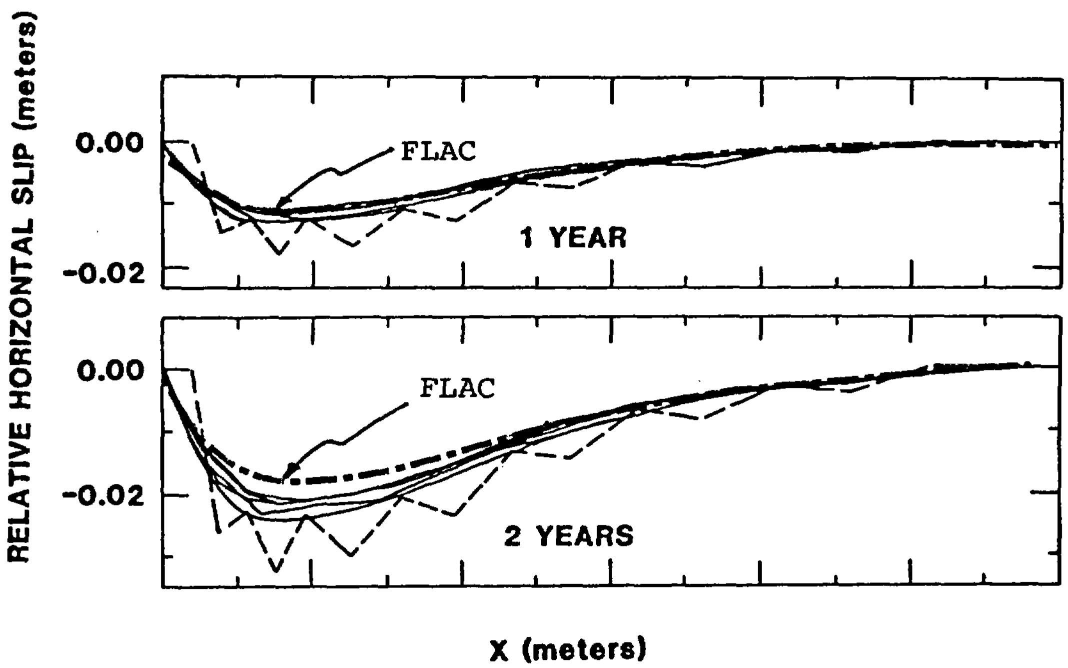


Fig. 15 Relative Slip Across the 642.98m Slide Line for the Heated Room at 1 and 2 Years [Morgan et al., 1981]

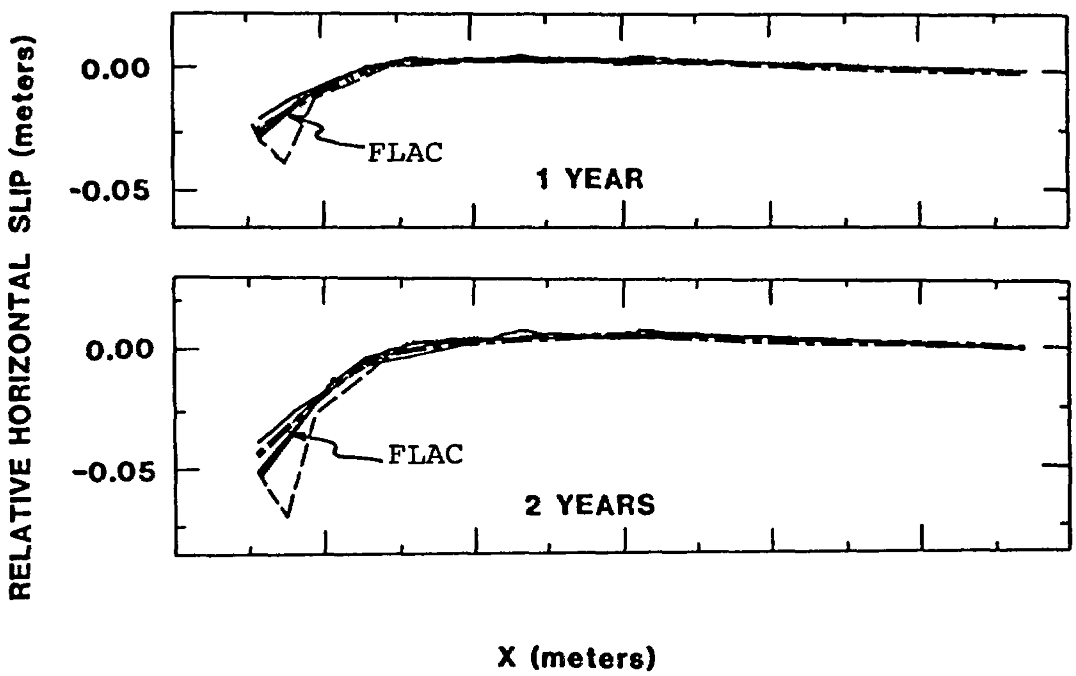


Fig. 16 Relative Slip Across the 650.20m Slide Line for the Heated Room at 1 and 2 Years [Morgan et al., 1981]

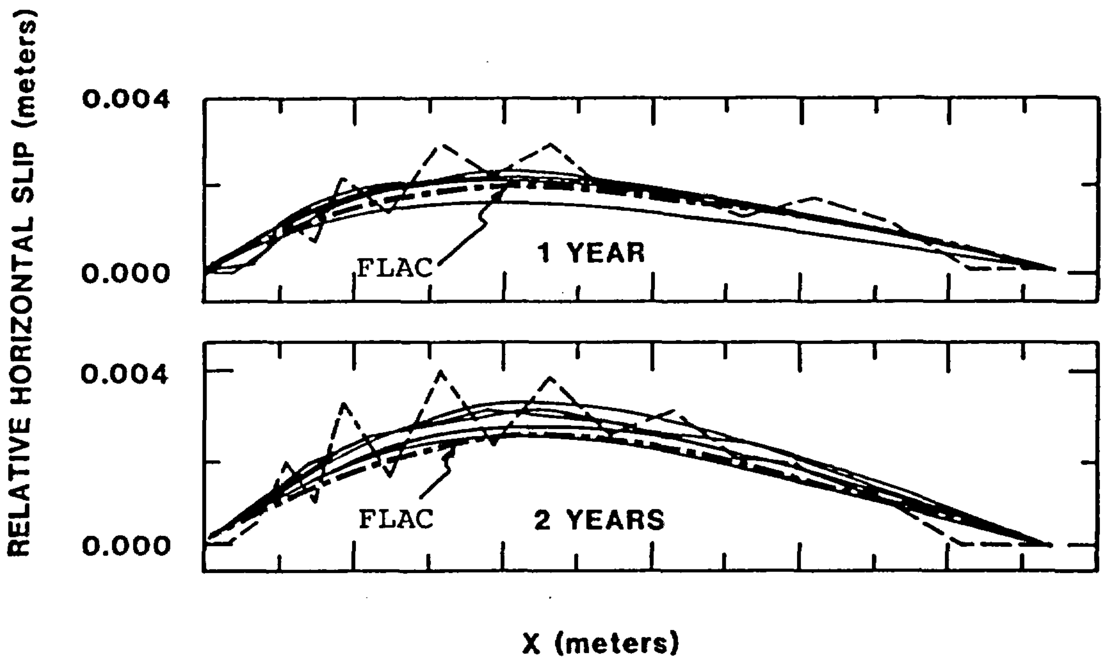


Fig. 17 Relative Slip Across the 661.02m Slide Line for the Heated Room at 1 and 2 Years [Morgan et al., 1981]

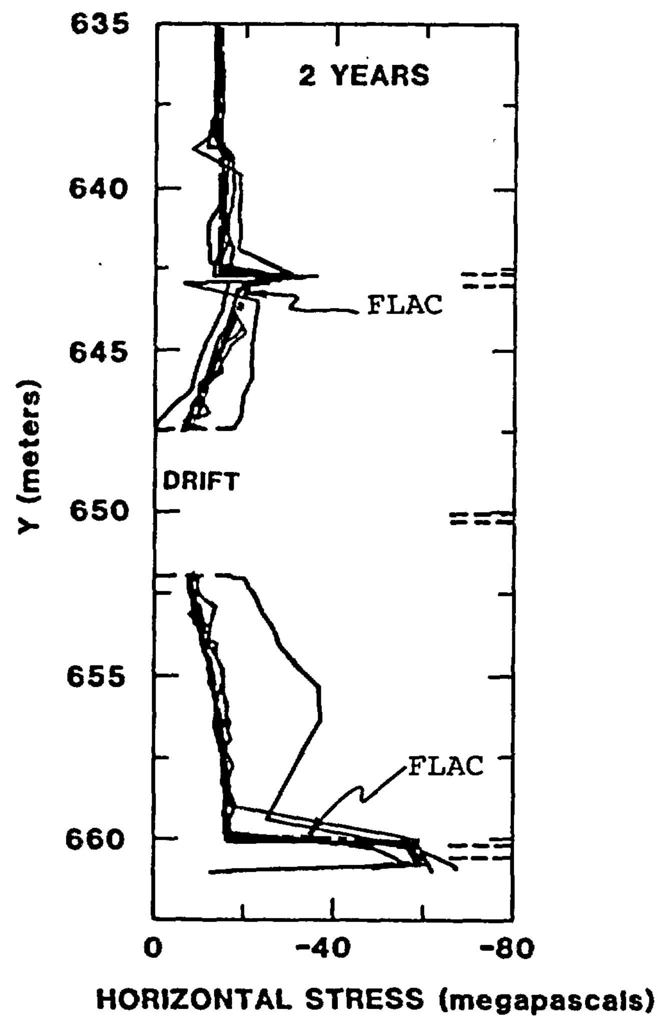


Fig. 18 Horizontal Stress Profiles Along the Vertical Centerline of the Heated Room at 2 Years [Morgan et al., 1981]

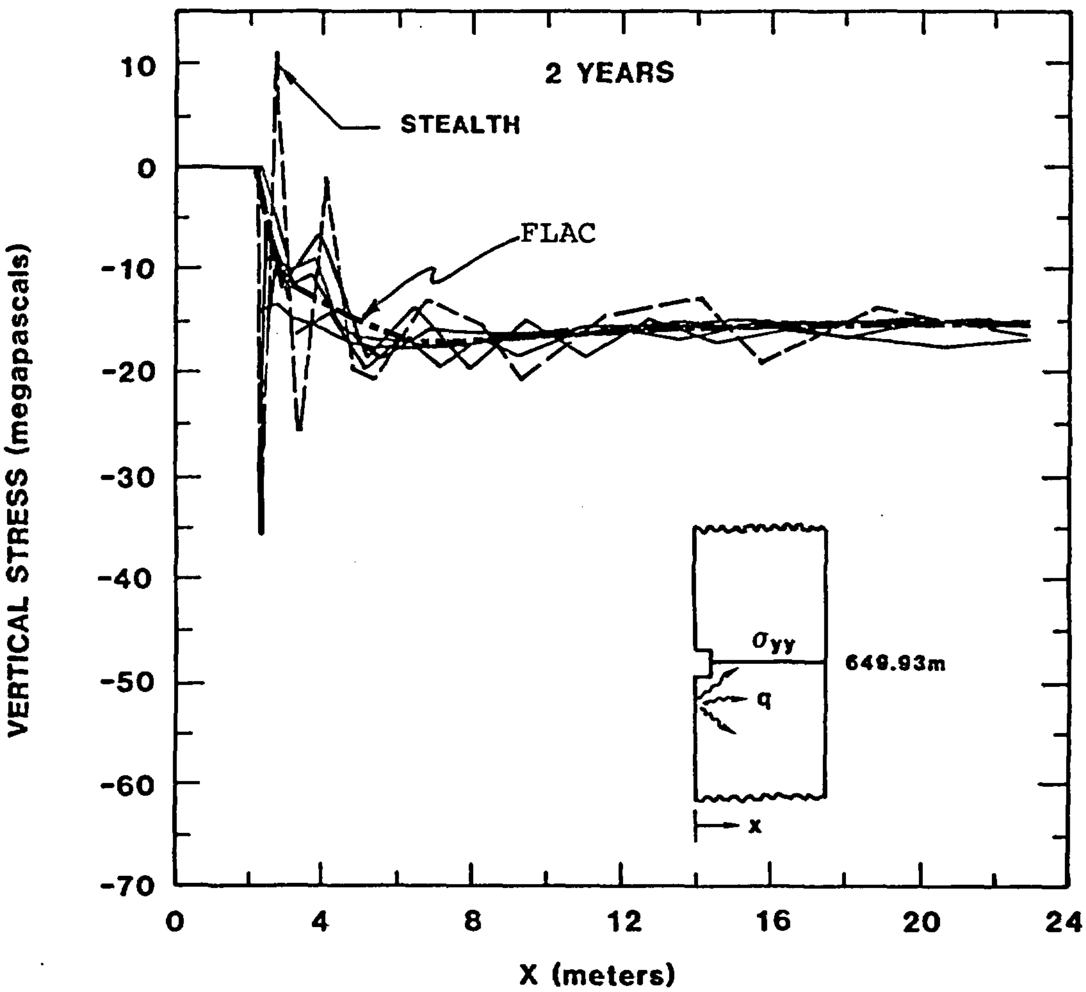


Fig. 19 Vertical Stress Profiles Through the Pillar of the Heated Room at 2 Years [Morgan et al., 1981]

4.0 DISCUSSION AND CONCLUSIONS

The results of this benchmark study indicate that FLAC compares well with other codes for performing thermal-mechanical analysis in nuclear waste isolation studies. The isothermal analysis showed good agreement for the FLAC model incorporating the WIPP creep model, interface logic, and interbedded materials.

In the thermomechanical simulation, FLAC showed good agreement to other codes for early time heating where temperature changes were great. However, at late-time heating, a discrepancy in results was observed. This was traced to the large difference between the thermal diffusivity of the "equivalent material" used to model the room radiation and that of the other materials in this model. This effect is analogous to the difficulties sometimes observed in mechanical modeling of materials with large stiffness differences. The incorporation of an implicit thermal solution scheme in FLAC was found to resolve this problem.

This study exhibits an important benefit of benchmarking. While the thermal part of FLAC has been verified against analytical solutions (Mack, 1987), inaccuracy arose in the application of the code to a realistic problem. Although a solution to the accuracy problem has been found, it is only through benchmarking against other codes that the problem was detected. It also appears (Fig. 12) that other well-established codes had deficiencies which were detected in the original study.

5.0 REFERENCES

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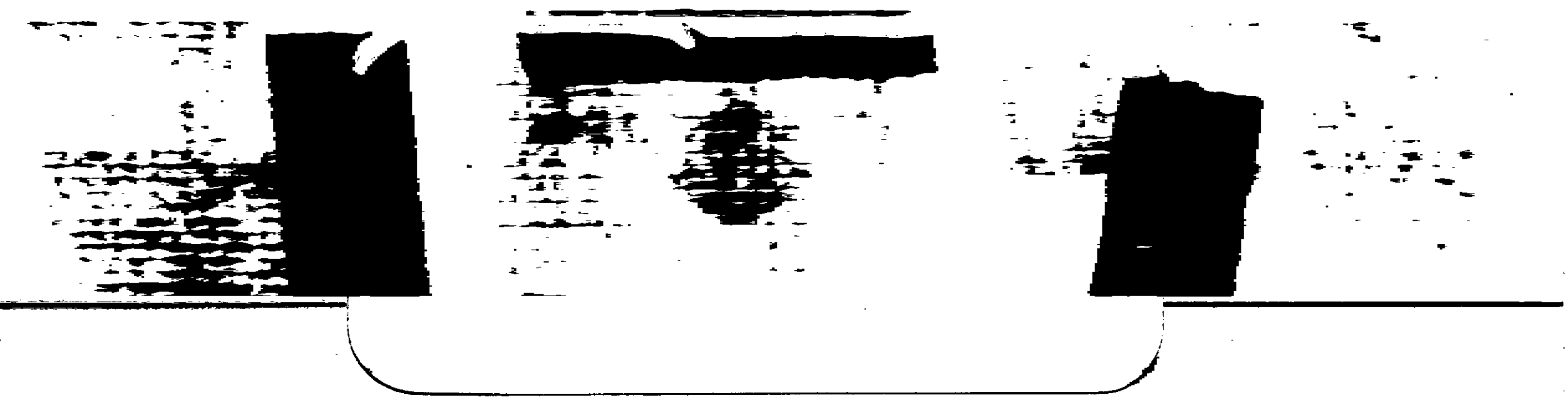

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