

A CALCULATION STRATEGY FOR THE DETERMINATION OF THE TEMPERATURE DISTRIBUTION IN RADIOACTIVE WASTE REPOSITORIES

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ABSTRACT

In the past many calculation tools have been developed for the determination of instationary temperature distributions in radioactive waste repositories (single source model / large scale model / unit cell model using analytical or numerical methods; overall model using analytical or numerical methods). In practice all these calculation tools have to be associated sensibly in a special calculation strategy making use of their actual advantages.

PROBLEM ANALYSIS

The scheme of a fictive repository for heat generating radioactive waste in rock salt formations is outlined in Fig. 1 (finite geometric extension: 60 boreholes, length 300 m, diameter 0.4 m, distance 57 m, square pattern; step-by-step disposal of the waste canisters, their heat generation following the specification of the proposed Gorleben repository (1)). This repository is taken as the basis for the following considerations.

The results of a calculation of the temperature distribution in such a repository will be influenced by two sources of error: firstly the inaccuracy of the input data - heat generation of the waste, material properties - and secondly the inaccuracy of the calculation itself - modeling, mathematical methods -. A rock salt formation, in which the disposal area will be situated, is composed of many different types of salt each having different material properties. In the calculation only a homogenous material zone with temperature dependent properties can be taken into consideration. So, for future discussions of temperature calculations a deviation in the material properties of up to $\pm 15\%$ compared to those of the homogenous material should be considered. Calculations of *in situ* experiments (2) pointed out, that the proposed thermal properties of salt (3) according to the average value of many laboratory and *in situ* measurements of different salt probes (4) is a sufficient approximation for the *in situ* value of rock salt. But for the exact calculation of measured temperature data the material properties of that specific area, where the measurements have been taken, must be determined.

CALCULATION TOOLS

In opposite to the final inaccuracies in determining the *in situ* values of the thermal properties of rock salt the inaccuracy being due to the calculation procedure itself can be reduced using more detailed models and improved mathematical methods. A quantitative analysis of the different calculation tools applying them for the calculation of

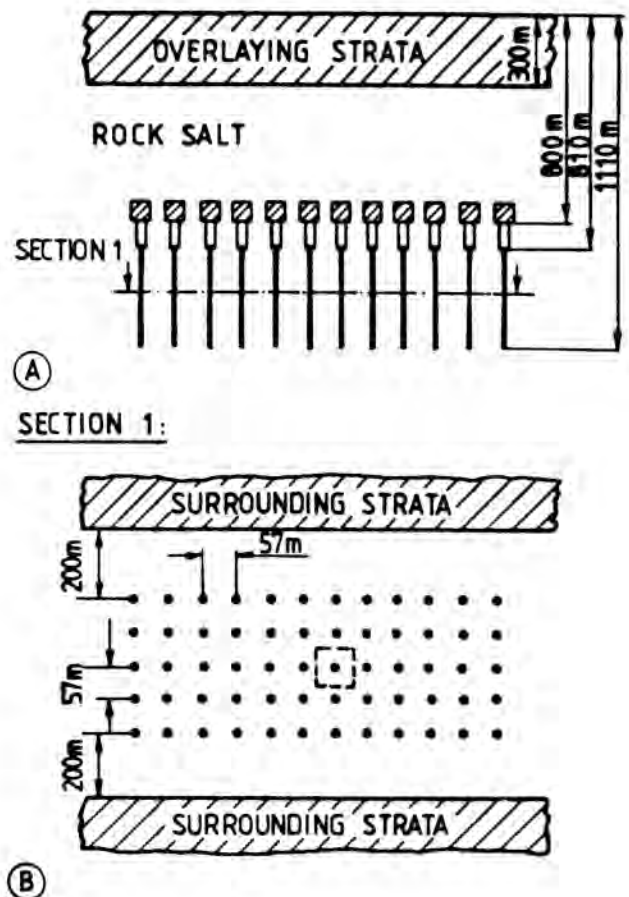


Fig. 1. Vertical (A) and Horizontal (B) Section of a Fictive Repository.

the temperature distribution in the fictive repository (see Fig. 1) obtains the following result:

1. The assumption of temperature independent (constant) material properties enables the use of analytical methods leading to the superposition principle; the time dependent temperature distribution of any disposal configuration - finite extension of the disposal area, step-by-step disposal of the waste - can be established (no model induced inaccuracy). But the use of a single constant value for the material properties do not lead to accurate results for the temperature distribution in the whole repository with its great temperature range (method induced inaccuracy up to 10%). Figure 2 illustrates the results of an appropriate calculation of the unit cell model.

So as a consequence temperature calculations have to be performed by using numerical methods taking the temperature dependent material properties into account.

2. The results of a unit cell and a single source model calculation using numerical methods (no method induced inaccuracy), shown in Fig. 3, appear to be the upper and lower bounds respectively, of the temperature distribution which can be expected for this repository (model induced inaccuracy). The accurate temperature distribution can only be calculated with an overall model.

OVERALL MODEL USING NUMERICAL METHODS

General Description of the Method

The basic idea of the new three-dimensional numerical method is the coupling of far field and near field numerical calculations merged into a single calculation procedure (5). As an example for such a calculation procedure the application of this model to the fictive repository (see Fig. 1) is shown in Fig. 4. In the first step - far field calculation - the disposal field and the entire host rock, surrounding and overlaying strata are modelled. It is possible, if necessary, to make use of given symmetries in the repository to reduce the calculation effort (CPU-time and storage). It is assumed, that the heat generation of the waste is homogeneously distributed to the whole host rock area of the disposal field. In the following steps just a limited section of the calculation cell of the preceding step is used to build the new calculation cell thus enabling a far more detailed modelling of the heat generating area. The boundaries for each calculation cell have to be situated in zones far enough away from the heat generating areas in the preceding step, so that the influence of the assumed homogenous heat generation on the temperature distribution in these zones is negligible. In the single modules of the entire calculation procedure the heat generating areas are modelled in more and more detail (disposal fields, disposal galleries, enlarged boreholes, borehole, single waste canister). The connection of each module to the subsequent one is done by using the

actual time and space dependent temperatures as the boundary condition in the new calculation step.

The last calculation step then yields the temperature distribution around a single borehole, which is now modeled in its real dimensions, taking into consideration the finite geometric extension of the disposal area and the temporal step-by-step disposal of the waste using time and space dependent boundary conditions.

Program System MODUL-STEP

The three-dimensional numerical model mentioned above has been realized in the program system MODUL-STEP. The implementation of the general calculation sequence with this program system is illustrated in Fig. 5.

At the beginning a list of all data sets to be used in the whole calculation sequence for the different programs must be available. The correct combination of these data sets is controlled by the program DISKON. Now the actual calculation starts with an iterative procedure using the different programs automatically one after the other. The procedure starts with the temperature calculation for modul (i) in MOTEMP. MOTEMP is based on a standard program (6) using the coarse-mesh method which is especially suitable for the three-dimensional calculation of large geometry structures. Peculiarities of this special finite element program are:

- the solution of the nonlinear equation system, induced by the consideration of temperature dependent material properties, using the NEWTON-RAPHSON method
- an implicit time integration with the CRANK-NICOLSON method
- an iterative solution of the linearized equation system by the successive overrelaxation method

The results of the temperature calculation of modul (i) are then prepared in the program MO3D2D, MO2D1D for further utilization. If another module in the calculation sequence has to be considered, the whole temperature field resulting from modul (i) has to be interpolated onto the new space and time discretization of modul (i+1) using the program MOINT.

MODUL-STEP has been verified (5) comparing its results of calculations of the fictive repository (see Fig. 1) for temperature independent material properties to those of an analytical calculation, which can be considered as the reference curve in this case. This comparison clearly shows the accuracy of operation of the program system. In summary, the inaccuracy of the MODUL-STEP calculation can be limited with an acceptable computational effort to less than 5% compared to the analytical solution.

CONCLUSIONS

In practice all calculation tools for the determination of instationary temperature distributions in radioactive waste repositories developed up to now (single source model / large scale model / unit cell model using analytical or numerical methods; overall model using analytical or numerical methods) have to be associated sensibly in a

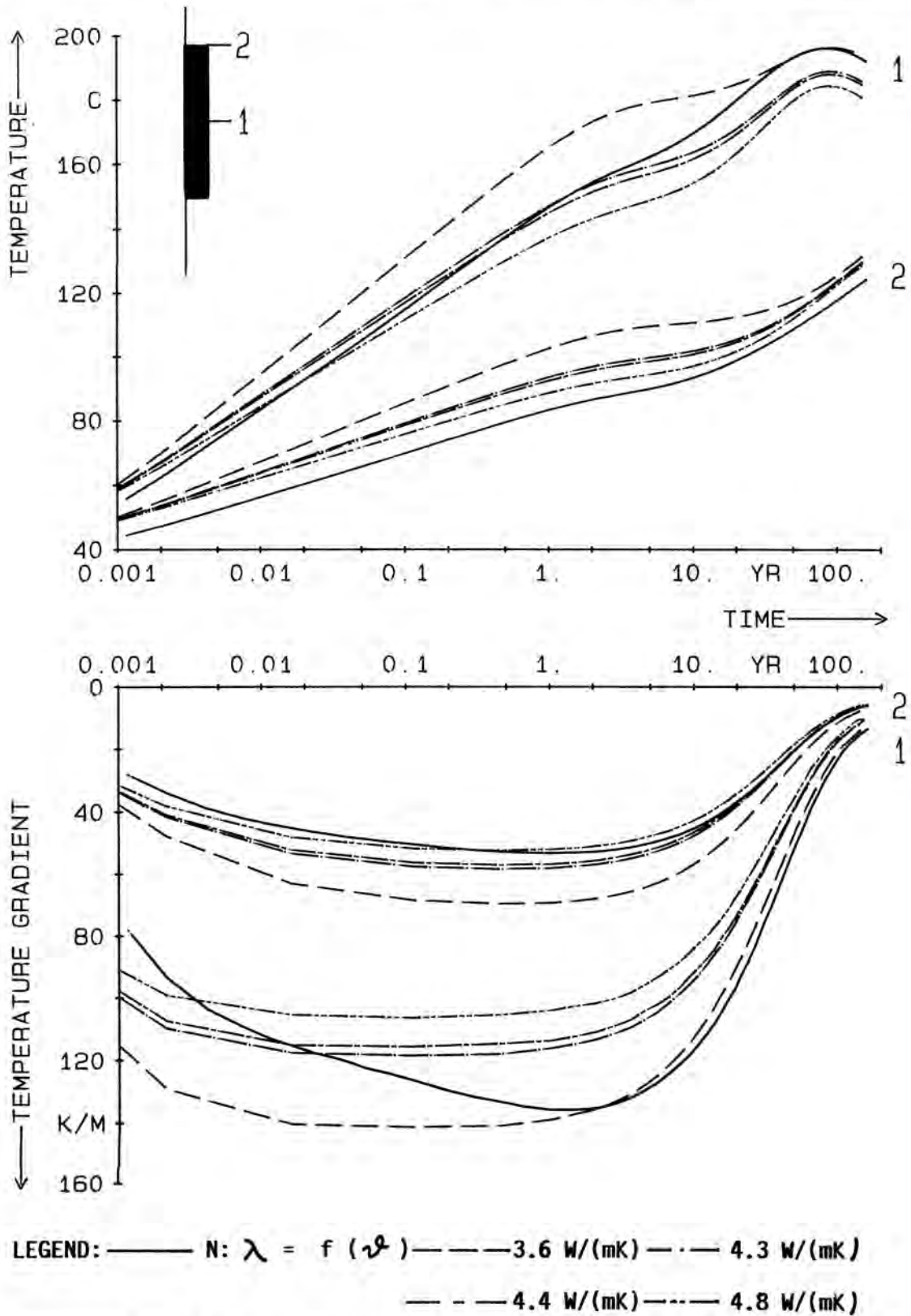


Fig. 2. Comparison Between Numerical (Temperature Dependent Material Properties) and Analytical (Temperature Independent Material Properties) Calculations of the Unit Cell Model.

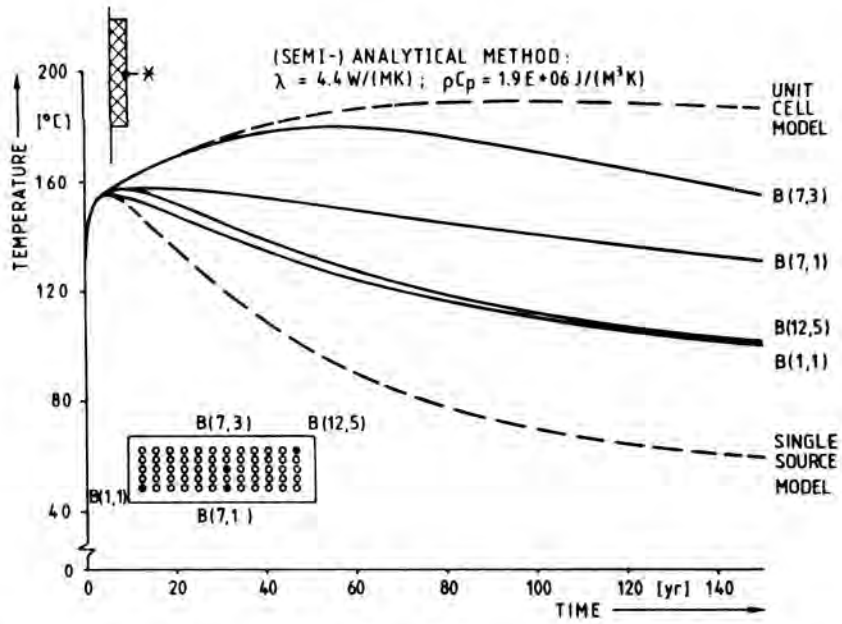


Fig. 3. Maximum Temperature vs. Time Obtained From the Analytical Calculation of the Overall Model Compared to the Results of the Unit Cell and Single Source Model Calculation.

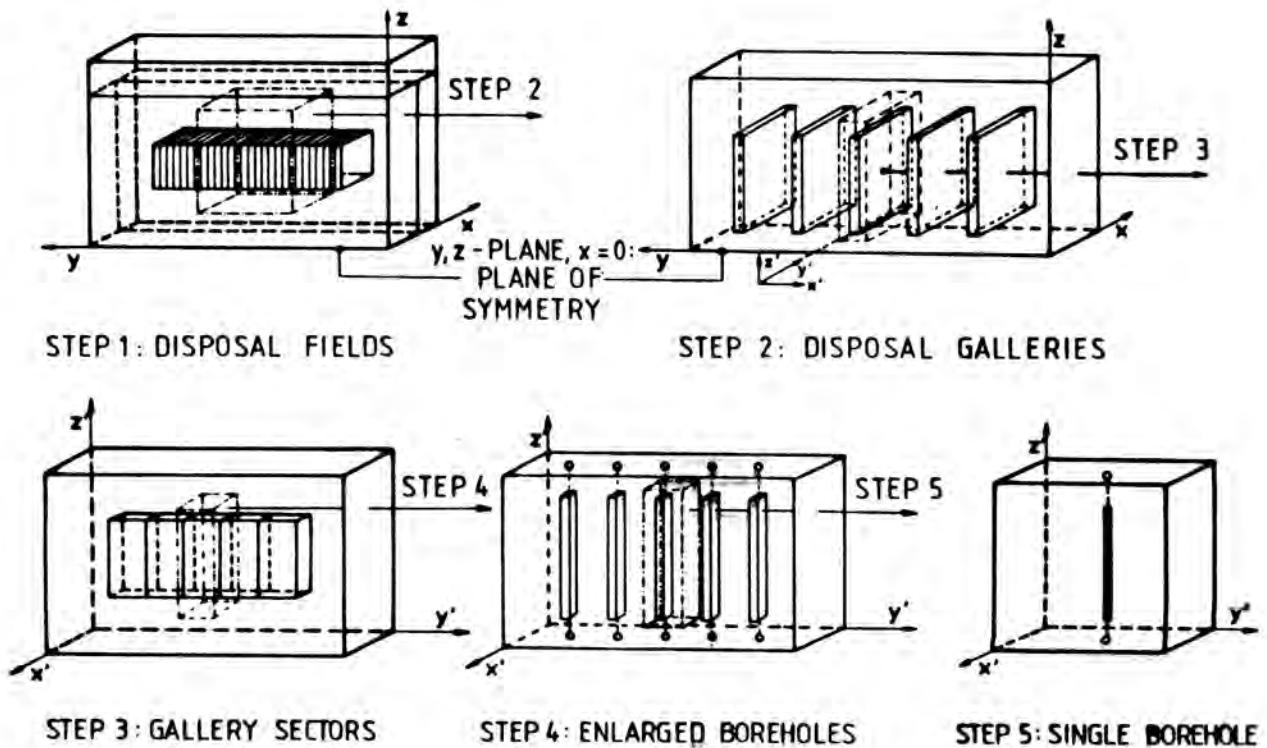


Fig. 4. Overall Model for the Three-Dimensional Numerical Calculation of Time Dependent Temperature Distributions in Repositories.

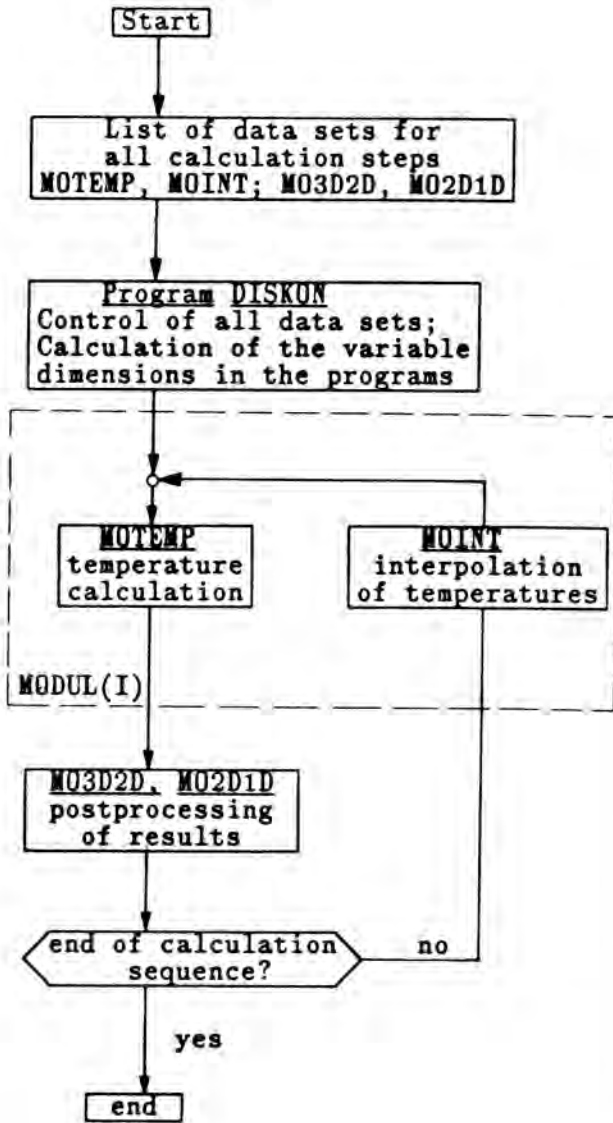


Fig. 5. General Description of the Calculation Procedure Using the Program System MODUL-STEP.

special calculation strategy making use of their actual advantages:

- the single source model should be used for modeling in situ experiments or extensive disposal structures, if the calculation time is limited to those periods of time,

in which the different heat sources do not exert any influence on each other.

- the large scale model should be used in those cases, in which just the far field temperature distribution is required.
- the unit cell model should be used for parameter studies taking the temperature dependent material properties into account.
- analytical methods in general should be used for the verification of complex numerical codes, for a first assessment of a given repository configuration as well as for system studies considering several different and complex repository configurations.
- the overall model using numerical methods - as for example the program system MODUL-STEP - should be chosen for the accurate three-dimensional calculation of the time and space dependent temperature distribution in repositories taking site-specific conditions into consideration.

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