



**AUSTRALIAN ATOMIC ENERGY COMMISSION
RESEARCH ESTABLISHMENT
LUCAS HEIGHTS**

**AN EQUILIBRIUM MODEL FOR CALCULATION OF BURNUP IN
A RECIRCULATING PEBBLE BED REACTOR**

by

**A. BICEVSKIS
E.W. HESSE**

September 1966

AUSTRALIAN ATOMIC ENERGY COMMISSION
RESEARCH ESTABLISHMENT
LUCAS HEIGHTS

AN EQUILIBRIUM MODEL FOR CALCULATION OF BURNUP IN
A RECIRCULATING PEBBLE BED REACTOR

by

A. BICEVSKIS

E. W. HESSE

ABSTRACT

The general problem of burnup calculations for a pebble bed reactor is discussed. An efficient calculational scheme is developed by treating operation at equilibrium with a random distribution of pebbles. Assuming a constant flux level and spectrum, analytical solutions are obtained for time averaged nuclide concentrations. With a specified feed composition, average power density, and burnup, consistent values of average nuclide concentrations and flux spectrum are derived in an iterative manner.

It is shown by physical reasoning and numerical calculation that the assumptions are justified for the large pebble bed reactors based on $\text{PuO}_2 - \text{ThO}_2 - \text{BeO}$ fuels selected for a reactor feasibility study.

The spectrum weighted improved one-group treatment lends itself to efficient coupling of burnup and power plant optimization studies and it may also find application to other reactor systems.

CONTENTS

	Page
1. INTRODUCTION	1
2. DESCRIPTION OF PEBBLE BED REACTOR	1
3. OBJECTIVES AND PRINCIPLES OF PEBBLE BED REACTOR BURNUP CALCULATIONS	1
4. OPERATION AT EQUILIBRIUM	2
5. CORE MODEL BASED ON RANDOM DISTRIBUTION OF PEBBLES	2
6. SOLUTION OF BURNUP EQUATIONS	3
6.1 General Problem	3
6.2 Simplified Model	3
7. PRACTICABLE SCHEME OF BURNUP CALCULATIONS	4
8. COUPLING OF BURNUP AND CRITICAL SIZE CALCULATIONS	4
9. JUSTIFICATION OF ASSUMPTIONS FOR THE P.B.R. DESIGN STUDY	5
9.1 Operation at Equilibrium	5
9.2 Random Distribution of Pebbles	5
9.3 Constant Flux Level and Spectrum	6
10. COMPARISON WITH SPACE DEPENDENT CALCULATIONS	6
11. APPLICABILITY TO OTHER REACTOR SYSTEMS	7
12. ACKNOWLEDGEMENTS	7
13. REFERENCES	7

Figure 1 Iterative Scheme of Zero-Dimension Burnup Calculations for a Pebble Bed Reactor

1. INTRODUCTION

In September 1963 a feasibility study of the pebble bed reactor was commenced at the A.A.E.C. Research Establishment, Lucas Heights. It was recognized that the available methods of burnup calculation based on fixed fuel reactors would not be suitable for a pebble bed reactor. New computational methods were developed and the general principles are described in this report.

A separate report describes the detailed survey results (Bicevskis 1966a).

2. DESCRIPTION OF PEBBLE BED REACTOR

In essence, the pebble bed reactor considered in this study consists of a core, formed by randomly packed spherical beryllium oxide fuel elements, surrounded by a reflector. This core arrangement lends itself to on-load continuous charging of the fuel. It is relatively simple to add fresh fuel in the form of pebbles at any point on top of the core and withdraw partially spent fuel from the bottom.

In our study, a typical value of the BeO pebble diameter is 1 inch. The BeO matrix contains uniformly dispersed 200 micron particles consisting of a mixture of PuO₂ and ThO₂.

Several pebbles per minute are added to the core, the total inventory being in excess of one million.

3. OBJECTIVES AND PRINCIPLES OF PEBBLE BED REACTOR BURNUP CALCULATIONS

The basic objective of the study was to select a plant design which would result in the lowest overall generation cost. The fuel cost of the reactor constitutes a substantial part of the overall cost and it is therefore of great importance to assess the nuclear performance accurately and to make the results available in a form suited to the overall power plant optimization study carried out by means of the code NUROSYS (R.O. Bardwell and D.J. Mercer, unpublished). The main objective of the core investigations was to obtain the nuclear performance of various combinations of the fissile (Pu) and fertile (Th) materials in the feed fuel.

The throw-away fuel cycle was investigated. In this cycle the fuel costs are mainly affected by the achievable burnup and average core power density.

As commonly used, the term "burnup" describes the degree of fuel utilization. Typical units in use are megawatt days per tonne of fissile or heavy material originally present, fissions per initial fissile atom (F.I.F.A.), and percentage of fissile or heavy atoms destroyed. In general, burnup in a particular reactor may be limited by:

- (1) Loss of "reactivity".
- (2) Inability to control the reactor.
- (3) Materials damage.

The average core power density is also governed by materials damage considerations and it has, in turn, a bearing on reactivity lifetime.

Thus, burnup and core power density dependence cannot be separated. For a complete description of the problem, one would require both space and time dependent burnup calculations and an extremely large computational effort would be required to solve this general problem for a range of fuel compositions. Therefore for a preliminary study, an attempt must be made to reduce the number of variables involved.

The following discussion is restricted to reactivity lifetime, and the average core power density is taken as constant, to be specified by separate investigations.

In order to arrive at a simple calculational model the following main assumptions are made:

- (1) Operation at equilibrium
- (2) Random distribution of pebbles
- (3) Pebble burnup takes place in a flux field which is constant as regards both the absolute level and spectrum.

Some of the assumptions are discussed as they are introduced. In Sections 9 and 10 more specific physical arguments in conjunction with numerical calculations are produced in order to check on the validity of the calculating scheme for the study of the selected pebble bed reactor and fuel compositions.

4. OPERATION AT EQUILIBRIUM

There are two extreme modes of operating reactors; all fuel may be discharged at fixed intervals, or fuel may be added and withdrawn continuously as exemplified by the pebble bed reactor. Most reactors would operate somewhere between the two extremes.

As regards burnup, the "intensive" properties of a fuel element, such as nuclide concentrations, are always time dependent. For fixed fuel reactors the "extensive" quantities, namely leakage and effective multiplication factor, are also time dependent as the local nuclide concentrations and flux levels change during the operating period. However, for a continuously fuelled reactor with fuel movement in the core it is in principle possible to reach a steady state or equilibrium operation which is characterized, externally, by constant feed and withdrawal rates of fuel and, internally, by time independent distributions of flux and core material properties.

Our calculational model is based on operation at equilibrium, thus eliminating time dependence from the calculation of the extensive quantities.

5. CORE MODEL BASED ON RANDOM DISTRIBUTION OF PEBBLES

For the pebble bed reactor under discussion two modes of operation at equilibrium may be postulated. First, one can assume a definite pattern of fuel management. As an example, for the usual case where the pebbles make several passes through the core, all the new pebbles could be added at the centre and the used fuel in subsequent passes could be added progressively more towards the periphery. The reactivity lifetime aspect of fuel management has been considered by Bicevskis (1966b) and by Hesse (1966a) who treated both the reactivity lifetime and power density distribution.

The other possible mode of operation is to have a completely random feed to the core. As the number of pebble passes is increased (higher down-flow velocity) the vertical bias in pebble properties is reduced. In the limit, a random axial distribution is obtained and thus a random three dimensional distribution. We adopt the random distribution of the pebbles as the basis for our calculational model.

The pebble reactor cores investigated in our study contain a large number of small pebbles. By adopting the usual volumetric weighting technique we represent the random distribution of the pebbles by its average, thus obtaining a core of a uniform composition.

We assume that all pebbles are rejected from the reactor with the same degree of burnup or the same nuclide concentrations. We also make the usual assumption that the reactor space average may be represented by the pebble time average (the justification of this procedure may be discussed in terms of the ergodic hypothesis).

We now consider the burnup calculation of a pebble which will lead to a simple procedure for obtaining the time averaged properties.

6. SOLUTION OF BURNUP EQUATIONS

6.1 General Problem

In general, for any burnup problem the nuclide concentrations are governed by the usual set of ordinary linear first order differential equations.

As a typical example, the following simplified equations describe the Th₂₃₂-U₂₃₃ chain:

$$\frac{dN_{t2}}{dt} = -N_{t2} \bar{\sigma}_a \Phi$$

$$\frac{dN_{p3}}{dt} = N_{t2} \bar{\sigma}_a \Phi - N_{p3} \bar{\sigma}_a \Phi - \lambda N_{p3}$$

$$\frac{dN_{u3}}{dt} = \lambda N_{p3} - N_{u3} \bar{\sigma}_a \Phi$$

$$\frac{dN_{u4}}{dt} = N_{u3} \bar{\sigma}_c \Phi + N_{p3} \bar{\sigma}_a \Phi - N_{u4} \bar{\sigma}_a \Phi$$

The subscripts of atomic densities represent abbreviations of the nuclide symbols, and the corresponding spectrum weighted microscopic absorption and capture cross sections are denoted by $\bar{\sigma}_a$ and $\bar{\sigma}_c$ and defined as follows:

$$\bar{\sigma} = \frac{\int_0^{\infty} \phi(E) \sigma(E) dE}{\int_0^{\infty} \phi(E) dE},$$

Φ denotes the total or integrated flux:

$$\Phi = \int_0^{\infty} \phi(E) dE$$

In the general case of a fixed fuel reactor, for any position in the core the reaction rates per atom, $\bar{\sigma} \Phi$, are time dependent. This necessitates the solution of the above set of differential equations with time dependent coefficients. The time dependence of the reaction rates cannot be expressed analytically but must be obtained by periodically recalculating the neutron spectrum. Thus a step-wise solution of the problem is indicated for a fixed fuel reactor, the length of the period between spectrum calculations depending on the severity of the changes in the reaction rates.

6.2 Simplified Model

Assume that both the spectrum and the absolute value of the flux are constant. It follows that both the spectrum weighted one-group cross sections and the total flux are also constant. Thus, all the coefficients in the set of the burnup differential equations are constant and analytic solutions are available as a sum of exponentials.

Integrating the nuclide concentrations with respect to time, one again obtains analytic solutions in terms of exponentials for the time averaged concentrations.

By assuming a constant flux spectrum and absolute level it is implied that there is no space dependence within a pebble. The burnup process of a pebble is now represented by a point model.

7. PRACTICABLE SCHEME OF BURNUP CALCULATIONS

The above discussion on the average properties, in principle, leads to the following scheme of burnup calculations for a specified initial composition, average power density, and F.I.F.A.:

- (i) Guess an average composition.
- (ii) Calculate the spectrum and obtain the flux weighted one-group cross sections.
- (iii) Normalize the flux for the required power density.
- (iv) Solve burnup equations for specified compositions and conditions.
- (v) Obtain new average concentrations and repeat steps (ii) to (v) until the results converge.

The scheme shown in Figure 1 gave good convergence. The "inner iteration" takes the burnup to the specified F.I.F.A. giving good estimates of the average composition. With the adopted analytic method of solution, it was more efficient to change the burnup time than to adjust the flux level. The time taken for the solution of burnup equations was very small. It was also discovered that, with the depicted arrangement, power density was a good indicator of convergence. In principle, the exit criterion could have been the convergence of some other variable such as the average concentration of a representative nuclide.

Pollard and Robinson (1966) incorporated the above scheme in their burnup code GYMEA as one of the burnup options. The scheme has proved extremely useful and has been used in extensive burnup surveys (Bicevskis 1966a).

8. COUPLING OF BURNUP AND CRITICAL SIZE CALCULATIONS

Assuming a bare reactor of uniform composition one may write the conventional one-group diffusion equation:

$$\bar{D} \nabla^2 \Phi + \bar{\nu} \bar{\Sigma}_f \Phi - \bar{\Sigma}_a \Phi = 0$$

and

$$\nabla^2 \Phi + \bar{B}_m^2 \Phi = 0$$

where the "average material buckling" is defined as

$$\bar{B}_m^2 = \frac{\bar{\nu} \bar{\Sigma}_f - \bar{\Sigma}_a}{\bar{D}}$$

and the macroscopic cross sections are obtained as time averages from the burnup calculations.

In carrying out burnup surveys one may plot, for any initial composition, the relationship between the average material buckling and F.I.F.A.

For a bare system which is "just critical" $\bar{B}_m^2 = B_g^2$

One may say that any average material buckling defines an equivalent just-critical reactor system. Approaching the problem in a different way, for a given reactor system as represented by the geometric buckling and for a given fuel feed composition, the reactivity lifetime is defined by that fuel residence time (burnup) which gives an average material buckling equal to the specified geometric buckling.

The geometric buckling can be derived for any reactor configuration. As an example, for a cylindrical reactor:

$$B_g^2 = (2.405/R)^2 + (\pi/H)^2 ,$$

where R and H are the radius and height, respectively. Both R and H may be obtained directly for a bare system. For a reflected system they may be considered as effective dimensions and the true core size obtained by means of "reflector savings", the latter being a function of the core composition and of the composition and thickness of the reflector.

Multi-group space dependent diffusion and transport calculations may be carried out to check the criticality prediction by means of the condensed one-group treatment. The equivalent geometric buckling may be adjusted to allow for parasitic absorption or streaming obtained by separate calculations.

For the large pebble bed reactors considered, the leakage term has a negligible effect on the spectrum weighted one-group cross sections and it was neglected. For other applications (small reactors) it may be necessary to allow for the effect of leakage on the core spectrum.

In applying this method to the plant optimization the burnup information was pre-calculated in the form of an average material buckling as a function of F.I.F.A. for various fissile and fertile combinations with the average core power density as a parameter. This information was then stored in the plant optimization code NUROSYS and used with the multi-dimensional search techniques. The above approach has proved quite practicable and has found extensive application in the pebble bed reactor optimization studies.

9. JUSTIFICATION OF ASSUMPTIONS FOR THE P.B.R. DESIGN STUDY

9.1 Operation at Equilibrium

Operation at equilibrium provides a convenient basis for comparing reactor designs and fuel compositions.

It would take some time to reach equilibrium if the reactor is started up with the core full of fresh fuel. The approach time is related to the ratio of fuel residence time in core to the reactor lifetime, these latter values being for our pebble bed reactor, respectively, approximately 4 and 25 years. To shorten the approach period, the first charge could be selected to approximate the desired equilibrium core composition if the equilibrium materials (mainly U233) are available.

It has been shown (Bicevskis, Hesse and Mercer 1966) that the absolute value of the fuel costs depends on the manner in which equilibrium operation is reached. In order to check on any errors introduced by a comparison at equilibrium, the complete reactor plant lifetime should be investigated in the context of the overall development of fuel cycles and power generation.

9.2 Random Distribution of Pebbles

A random distribution of pebbles was selected as a basis for our comparative optimization studies.

For a practicable pebble bed design, it is not difficult to arrange for a random feed of the pebbles at the top of the core. For a typical design six pebble passes through the core were envisaged. This would introduce a vertical bias in the local average composition from top to bottom of approx. 1/6 of the total change taking place during the burnup. If the core is assumed to be uniform, based on the overall average, the local averages would depart at most by 1/12 from the assumed uniform composition.

We are also basing our comparative study on the assumption that all the pebbles are rejected with the same exit composition. In any practicable scheme some variation is unavoidable. The simplified model would represent an average exit composition.

9.3 Constant Flux Level and Spectrum

We have assumed a constant flux level and spectrum for the burnup calculation. In any realistic recirculating pebble bed reactor the pebbles would take different paths through the core and would experience different time histories as regards both the flux level and spectrum.

We have investigated burnup of pebbles exposed to constant flux and to realistic variations in the flux level at the same spectrum giving in all the cases the same integrated or time averaged flux. The differences in average material buckling were negligibly small for typical pebble bed compositions and burnup. This calculation was carried out with a synthetic fission product treatment which allowed for no decay except in the case of Xe135. The only other significant nuclide having both decay and absorption reactions was Pa233. If no decay reactions take place, all burnup equations may be expressed in terms of integrated flux or flux-time and the time dependent variation of flux is of no consequence.

In general, for a reflected reactor of a uniform composition the core spectrum is constant some distance away from the reflector. A typical pebble bed design had a core diameter of 15 feet and height of 10 feet. Thus, there is a large central region of constant spectrum which is based on the average core composition. With a flux distribution approaching the cosine shape the flux level is high in the central region. Therefore, a large contribution to the total neutron production and absorption will take place under conditions of a constant flux spectrum.

For a typical design there is a temperature gradient of approximately 600°K between the top and bottom of the core. To check on the effect of temperature on neutron spectrum and reactivity lifetime we have carried out burnup calculations at 600, 900, and 1200°K for the same composition and F.I.F.A. Averaging the results at 600°K and 1200°K we obtained practically the same average material buckling as at 900°K.

The above comments relate to the variations in the "macroscopic" or reactor flux encountered by a pebble moving through the core. In our context distortion in both the flux level and spectrum may take place if the pebble composition at any instant departs from the average values used in the spectrum calculation. This effect would be most pronounced in a new fuel element which contains PuO₂ (78 per cent. Pu239, 17 per cent. Pu240 and 5 per cent. Pu241) besides ThO₂ and BeO.

Multigroup transport calculations were carried out for a typical new fuel element surrounded by a medium representing the average core composition. The depression in the group fluxes and power density was less than five per cent.

For a typical burnup calculation (F.I.F.A. of 1.4) all cross sections, first, of Pu239 and, second, Pu240 were reduced by 20 per cent., which would simulate a corresponding reduction (shielding) in the effective flux level. No significant change in the average material buckling was obtained (J.P. Pollard - private communication). This result may be explained by the fact that at the burnup considered, practically all the Pu239 and Pu240 have been consumed, making a net contribution to the neutron balance which only depends on the η -value of Pu239 and on the initial atomic densities of both isotopes.

10. COMPARISON WITH SPACE DEPENDENT CALCULATIONS

In the preceding section an attempt was made to justify each assumption separately mainly in terms of the equilibrium neutron balance expressed as average material buckling. Some overlapping of the discussion is evident which is indicative of the difficulty in separating the assumptions.

The more difficult objective of providing estimates of reactivity lifetime for optimization studies can only be verified by space dependent calculations. This task was carried out by means of the fuel-management burnup code FRIZLE (Hesse 1966a).

The FRIZLE code allows for local spectrum and temperature effects and treats the space dependence in two dimensions and six neutron energy groups. A management pattern of seven passes with a random feed to the top of the core and the core split up into six axial zones having their own local flux and temperature, was compared to the uniform composition obtained from zero dimensional

burnup calculations based on the infinite recirculation model. The same reactivity lifetime was obtained in both cases for the same initial fuel composition, core size, and average power density. The case of only one fuel pass through the core with the same six axial zones also gave the same lifetime. This suggests that the zero dimensional constant flux model is acceptable for reactivity lifetime estimates of management schemes with random feed to the top of the core, irrespective of the number of axial passes.

Space dependent calculations also showed that with the spectrum condensed one-group treatment it was possible to make accurate predictions of the equivalent geometric buckling as a function of the core size, reflector thickness, and height to diameter ratio (the condensed one-group treatment gave good estimates of criticality (Hesse 1966b)).

At the outset it was stated that we were aiming at an efficient method for relative assessment of various fuel combinations. As shown by the FRIZLE comparison our method even provides a good absolute reactivity lifetime estimate for a given reactor size and should meet more than adequately the requirements for a comparative optimization study at equilibrium.

11. APPLICABILITY TO OTHER REACTOR SYSTEMS

The methods as described above have been developed specifically for pebble bed reactors at equilibrium. However, it is felt that the same methods, possibly with some modifications, would also be of some use for other reactor types.

The continuously fuelled reactor at equilibrium represents the ultimate in neutron economy and would provide an upper limit on burnups achievable on reactivity lifetime grounds. The great advantage of the method proposed is the speed and low computing costs for the automated system. Further savings may be achieved by suitably scheduling a series of runs to make use of the converged values of similar previous cases.

Zero dimensional burnup methods are in common use mainly because of their simplicity, but one may not expect a high accuracy from the results. In this work we have attempted to verify the assumptions, which are often tacitly made, and to show that, despite their disarming simplicity, the mathematical models postulated for the constant spectrum equilibrium system provide a good analogue for recirculating pebble bed reactors and, possibly, some similar continuously fuelled reactors.

12. ACKNOWLEDGEMENTS

The authors gratefully acknowledge the part played by R. O. Bardwell (at present with the Denver and Rio Grande Western Railroad Company) in the formulation of some of the basic concepts and in the development of the methods used in the evaluation of survey results and for the coupling to the plant optimization study.

13. REFERENCES

- Bicevskis, A. (1966a). - A Burnup Survey of Pu-Th-BeO Fuels and Comments on Selection of Fuel for Pebble Bed Reactors. A.A.E.C. report in preparation.
- Bicevskis, A. (1966b). - Perturbation Theory Approach to Fuel Management Study of the Pebble Bed Reactor. AAEC/E161.
- Bicevskis, A., Hesse, E.W., and Mercer, D.J. (1966). - Fuel Cycle Studies for a Beryllium Oxide Pebble Bed Reactor. Second International Thorium Fuel Cycle Symposium, Gatlinburg, Tennessee, May 3-6, 1966.
- Hesse, E.W. (1966a). - A Description of the Detailed Treatment of some Fuel Management Problems of the P.B.R. and of the Two Dimensional Fuel Management Code FRIZLE. A.A.E.C. report in preparation.

Hesse, E.W. (1966b). - Criticality Assessment of the Pebble Bed Reactor using Beryllium Oxide as well as Graphite Moderators. A.A.E.C. Report in Preparation.

Pollard, J.P., and Robinson, G.S. (1966). - GYMEA - A Nuclide Depletion, Space Independent, Multigroup Neutron Diffusion, Data Preparation Code. AAEC/E147.

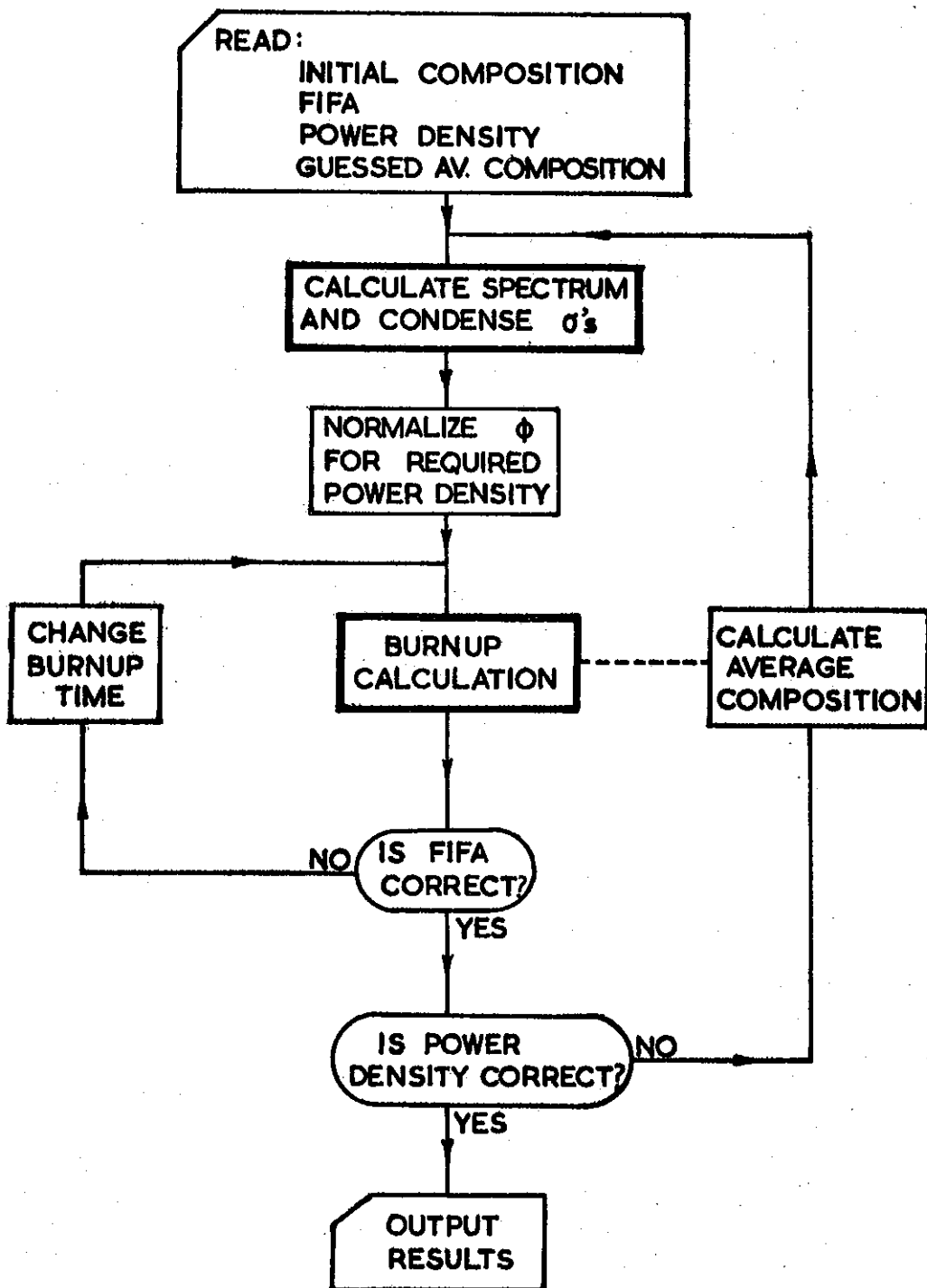


FIGURE 1. ITERATIVE SCHEME OF ZERO-DIMENSION BURNUP CALCULATIONS FOR A PEBBLE BED REACTOR

