MASTER

STRUCTURAL ANALYSIS OF REACTOR FUEL ELEMENTS

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CONF-770807-42

Prepared for
4th SMIRT Conference
San Francisco, CA
August 15-19, 1977

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STRUCTURAL ANALYSIS OF REACTOR FUEL ELEMENTS*

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Summary

An overview of fuel-element modeling is presented that traces the development of codes for the prediction of light-water-reactor and fast-breeder-reactor fuel-element performance. It is concluded that although the mathematical analysis is now far advanced, the development and incorporation of mechanistic constitutive equations has not kept pace. The resultant reliance on empirical correlations severely limits the physical insight that can be gained from code extrapolations.

Current efforts include modeling of alternate fuel systems, analysis of local fuel-cladding interactions, and development of a predictive capability for off-normal behavior. Future work should help remedy the current constitutive deficiencies and should include the development of deterministic failure criteria for use in design.

*Work supported by the U. S. Energy Research and Development Administration.

1. Introduction

The prediction of in-reactor fuel-element behavior has progressed significantly in the past several years primarily as a result of continued improvements in the mathematical analyses. In the present paper, an attempt will be made to put the development of these codes into perspective by reviewing where we have been, where we are now, and where we may be heading in fuel-element modeling. The review is limited to models of cylindrical fuel elements for light-water reactors (LWRs) and fast-breeder reactors (FBRs).

2. Historical Perspective

2.1. Empirical Correlations versus Physical Models

Fuel-element modeling has received serious attention for approximately the past ten years. Prior to that time fuel-element design was, for the most part, a purely empirical effort. However, the inability to reliably extrapolate the limited and highly costly fuel-element irradiation experience posed serious operational and safety questions that stalled the drive to achieve improved fuel performance. The necessity to predict fuels behavior and possible fuel-cladding interactions became apparent, and, for fast reactors, the need for a predictive capability was further intensified by the concern over stainless steel swelling.

The development of an analytical predictive capability proceeded along two reasonably distinct lines. The first attempted to use a straightforward thermal analysis coupled with an elementary mechanical analysis to string together assumed or semiempirical representations of the major driving forces, i.e., differential fuel and cladding swelling and plenum pressure loading.

Nonproprietary codes in this category developed in the USA by the AEC included SWELL [1] and BEMOD [2] from Argonne, for oxide and metal fuels, respectively, NUKER [3] from KAPL, DEFORM [4] from Battelle, and OLYMPUS [5] from Westinghouse, all for oxide fuels. These codes were inexpensive to run, produced "predictions" quickly, and through gross parametric studies they contributed considerable motivation to the need for a better understanding of fuel-element behavior.

The second type of fuel-element analysis was pioneered by Bettis Atomic Power Laboratory with the CYGRO [6,7,8] code, which attempted to establish a rigorous thermal and mechanical analysis based on finite-element techniques that could accommodate physical models of materials behavior in LWR fuel elements. But the CYGRO achievement was not widely adopted for use by the nuclear industry, primarily as a result of institutional obstacles. The code was difficult to obtain and even more difficult to operate since no user's manual was available; furthermore, it had not been adapted for use on alternate computing systems or for fast-reactor use. As a result, other "first-principles" codes were developed, both in the USA and abroad. These included LIFE [9,10,11] from Argonne, F-MODEL [12] from ORNL, CYGRO-F [13] from Westinghouse, and BEHAVE [14] from GE in the USA, COMETHE [15] from Belgian-Nucleaire, SATURN [16] from Karlsruhe, URANUS [17] from Darmstadt, and IAMBUS [18] from INTERATOM.

2.2. Thermal Analysis

The first-principles codes used different approaches in their attempt to overcome several common obstacles, but the aim was always to use physical models to the extent possible. In the thermal analysis, the calculational techniques were straightforward, and the conductivities of fuel and cladding were reasonably well known. However, the fuel-cladding gap conductance was unknown, and it

obviously varied during irradiation history as a result of fission-product accumulation, changes in gap size, and fuel-cladding mechanical interactions. Various approaches were tried, from simply specifying a constant to developing highly sophisticated models such as GAPCON [19], a version of which is currently used in the LIFE-III analysis. A series of irradiation experiments were finally performed to determine the threshold power required to melt fuel during reactor startup [20]. These irradiations yielded important benchmark data for calibrating the fuel-element gap conductance early in life. The final conductance after irradiation could be more easily deduced [21] for elements with intimate fuel-cladding contact. With this data, the thermal analysis of fuel elements, excluding local hot-spot effects, was straightforward. The only remaining difficulty was in coupling the thermal analysis to the mechanical analysis since they are obviously interdependent, but a complete iterative procedure for each deformation increment is very costly.

2.3. Nuclear Analysis

The nuclear analysis in the first-principles codes is extremely important, since fuel swelling due to accumulation of fission products and cladding swelling due to fast-neutron damage are the two main driving forces for fuel-element deformations. In addition, irradiation effects enhance fuel and cladding creep, which were not, and are still not, well understood. The approaches to fuel and cladding swelling differed widely, from the simple use of assumed incompressible swelling functions, as in the empirical codes, to detailed treatments of fission-gas behavior in the fuel and radiation damage in the cladding. The first alternative simplified the mechanics but severely reduced the value of the code predictions; the second alternative, however, was quite difficult to model and implement on a first-principles basis [22]. Major attempts to model fuel swelling on a

detailed fundamental basis include the Bettis BUBL [23,24] and Argonne GRASS [25] codes. However, these codes were never fully integrated into either CYGRO or LIFE. These fuels codes model fission-gas-bubble evolution, migration, coalescence, interactions with structural defects, and gas-release mechanisms, including bubble link-up along grain boundaries, and in the case of GRASS, the effects of fuel cracking. Although simpler fuel-swelling models were implemented in the major fuel-element codes, they did not include the compressibility of fission gas, as well as gas generation, migration, and solid fission-product swelling [26]. The compressibility of the gas poses significant numerical convergence problems in the treatment of fuel mechanics, but the stress and temperature dependence must be included in any physically realistic approach as well as fuel cracking and hot pressing (i.e., volumetric compression due to closure of fabricated porosity). The approach to modeling in-reactor enhancement of fuel creep was largely empirical, but key experiments were run [27] that made possible mapping of the expected gross effects [28].

Cladding swelling, equally as important as fuel swelling for fast-reactor irradiations, received considerable modeling attention, but the phenomenon is quite complex, the early models were by necessity crude, and, in general, were not incorporated into fuel-element codes. An early attempt at modeling the void nucleation and growth phenomenon in stainless steel was implemented into the LIFE code as an option [29], but the majority of code-swelling representations for stainless steel have been only empirical correlations that must be replaced as each new in-reactor datum point is produced. Although the "first-principles" codes can easily accommodate these empirical formulas and they are reasonably good for interpolating cladding behavior, they severely limit the

value and physical insight to be gained from code extrapolations. The situation for predicting irradiation creep in cladding was no better; few attempts were made at modeling [30] and empirical curve-fitting was the rule.

In addition to reservations about the use of empirical representations for extrapolations, they are open to another serious, fundamental challenge. The costly postirradiation data that forms the basis for these correlations are usually treated as if they were obtained under steady-state conditions of flux, temperature, and stress. This assumption is clearly not true. To properly interpret the postirradiation data, an iterative analysis of the actual thermal and stress history of the specimens is required, accounting for the relative contributions of different swelling and creep mechanisms [31] as a function of this history. A few years ago it could be argued that the analytical tools for rigorously carrying out this analysis did not exist. Today it can be performed within the analytical machinery of the fuel-element codes, with only minor modifications.

This concern for irradiation history is fundamental and remains important today, since the "first-principles" codes for fast reactors are being calibrated by following actual fuel-element irradiation histories, yet their empirical equations for cladding swelling and irradiation creep have normally been derived neglecting most history effects. The predictive advantages of the mechanistic analysis of fuels are being lost through the use of nonmechanistic, empirical relations for cladding behavior, which, to make matters worse, have usually been derived on a steady-state basis. Until this situation is improved, the deformation extrapolations of the "first-principles" codes will only be of marginally greater value than those of the purely empirical codes.

The seriousness of the stainless steel swelling problem and the consequences of our inability to accurately model the phenomenon have been particularly evident in the problem of subassembly bowing. Because of the large uncertainties in the relative magnitudes of swelling and radiation creep in stainless steel, even the direction of subassembly bowing could not be conclusively determined [32] a few years ago.

2.4. Mechanical Analysis

The mechanical analysis developed for the first-principles codes has been particularly innovative, which was forced by the complexity of the problem and accommodated by the simple cylindrical geometry. The constitutive phenomena considered for the fuel include thermoelasticity, thermal and fission-enhanced creep, swelling due to accumulation of solid and gaseous fission products, fission-gas re-solution, gas release, hot pressing, the migration of fabricated porosity that results in fuel restructuring, and fuel cracking and healing. The cladding phenomena include thermoelasticity, thermal and radiation-enhanced creep, swelling due to fast-neutron damage, and in some cases, time-dependent corrosion. Fast reactor cladding mechanics are further complicated by the interrelationship between swelling and radiation creep so that deviatoric and hydrostatic deformations are coupled [33].

The usual approach to the mechanical analysis is a generalized plane-strain analysis by finite-element or finite-difference methods and history-following by rate extrapolations or by generalizations of the method of successive elastic solutions [34]. The deformations are predicted as a function of reactor operating history in an incremental approach, modeling the element as a series of concentric cylinders subjected to thermal and mechanical boundary conditions derived from the irradiation history. The attempt to follow the

full reactor operating history was a particularly important development [35]. The need is imperative for the development and use of mechanistic models, physically meaningful interpretation of postirradiation results, and the rational prediction of the future behavior of elements at any time during their irradiation history.

Incremental approaches in modeling reactor history are, of course, required. But the choice of an intelligent increment and the iterative scheme employed can make the difference between an accurate fast solution and large computational errors and long running times. A major key to the success or failure of history-following codes has, in fact, been the development of highly efficient convergence schemes [36]. By the adoption and refinement of a sophisticated tensor approach to the prediction of total strain increments, Jankus and Roth [37] decreased the running time of the LIFE code by an order of magnitude. Their approach uses the information contained in the last n increments/iterations to determine the best prediction for the next increment/iteration. These mathematical improvements, which greatly reduce the cost of running the codes, are critical in gaining acceptance of the codes as practical tools by designers and safety analysts. In an attempt to make an additional decrease in running time, studies have been made to determine the sensitivity of code predictions to the detail included in the reactor operating history [37]. These studies have primarily shown, however, that history-following strongly influences the code predictions, and any filtering must be done with great care, if at all.

When attempting to model phenomena as complex as reactor fuel-element behavior, mathematical errors are easily compounded unless careful checks are constantly made. Benchmarking the code mechanics, therefore, against known exact solutions is critically important. It is an all too common occurrence

to find that a simple known solution cannot be recovered from a complex "production" computer code. A description of such a benchmarking exercise for the LIFE code is given in Ref. 38. In addition to mathematical benchmarks, however, the codes need irradiations tailored to prove out models. Short-term irradiations, for instance, were required to verify thermal and restructuring models, as well as longer-term irradiations with specified operating histories to verify deformation predictions.

2.5. Institutional Considerations

To focus and further coordinate fast-reactor fuel-element modeling efforts in the USA, the Atomic Energy Commission (now ERDA) in 1971 decided to pursue the development of the LIFE code on a National basis. A working group was established, consisting of representatives from General Electric, Westinghouse, Atomics International, General Atomic, Hanford Engineering Development Laboratory, and Argonne National Laboratory. Through the efforts of this group, chaired by General Electric, the LIFE code has been extensively revised and improved, has been made operational on a wide variety of computers, and has achieved a welcome degree of acceptance by the USA reactor community. The documentation for this "revised standard version" of LIFE-III, including a detailed user's manual, has recently become available through ERDA [11]. This version of LIFE-III incorporates a finite-strain analysis [39].

At least partially as a result of the limited availability of alternate codes for the past few years, the U. S. Nuclear Regulatory Commission decided to develop its own fuel-element codes, with emphasis on LWR safety analyses. Development of the FRAP codes [40,41,42] has resulted.

More recently, for LWR applications, the Electric Power Research Institute sponsored a fuel-element-code comparison study [43], which included three versions of the COMETHE code [15], CYGRO-3 [7], BEHAVE-4 [14], two versions

of GAPCON-THERMAL [19], FMODEL [12], and LIFE-THERMAL-1, a converted version of the LIFE [10] code. Based on performance in predicting LWR fuel-element behavior, ease of use, computer cost, and availability of code documentation at the time of the study, the COMETHE-III-J code was chosen for further LWR utilization by EPRI.

In the USA then, fuel-element modeling is currently based on the LIFE code for fast-breeder-reactor development, the CYGRO code for light-water breeder development, the COMETHE code for potential utility LWR use, and the FRAP codes for LWR regulatory investigations.

2.6. Local Effects and Failure Criteria

As previously noted, the first-principles codes for cylindrical fuel elements usually assume axial symmetry and generalized plane strain. This makes it difficult to account for localized effects such as fuel cracking and hot spots except in an "average" sense or through separate auxiliary analyses. Attempts to investigate local effects include Gittus' work on the interactions of cracked fuel with cladding [44], the work of Rashid [45] and others [46,47,48] on pellet-cladding interactions, and the analysis of end effects [49] and non-uniform heating [50]. A rigorous two-dimensional analysis of a cracked fuel pellet was also developed by Bettis in the PELLEN code [51]. The analyses of local effects, however, were usually not integrated into comprehensive fuel-element codes.

Although prediction of fuel-element failure on a deterministic or statistical basis has always been a major goal of fuel-element modeling, the complexity of the problem, as well as the pressing need to describe the integral behavior first, has allowed only limited analytical progress [52]. The data base for developing a failure criterion, however, has been accumulating, out-of-reactor

and in-reactor, including both specimen testing [53,54] and all-important in-reactor fuel-element failure experience [55,56,57].

3. Current Trends

3.1. Analytical Developments

The mathematical machinery for describing oxide fuel-element behavior under normal reactor operating conditions (excluding failure) is well in hand today. The constitutive relations used in the codes leave much to be desired, but the mathematical analysis is sound and efficient. As a result, while awaiting better constitutive models, the codes are being extended toward the analysis of alternate fuel systems and safety problems. Incorporation of a transient heat-transfer analysis, finite-strain calculations, and fuel-melting mechanics are examples of extensions into safety concerns, whereas the move toward a better breeding ratio and/or a proliferation-resistant fuel cycle requires models for carbide, nitride, and thorium-uranium fuels. The UNCLE code [58], an offshoot of the LIFE effort but directed toward carbide and nitride fuels, is an example of the latter, and the development of GRASS-T [59] is an example of the move toward a more detailed safety analyses of oxide fuels.

While the "normal behavior" codes are being extended, codes written expressly for safety analyses [41,60,61] are beginning to make use of much more detailed constitutive data as it becomes available. For example, the FRAP-T code [41,42], which was designed for the analysis of LWR fuel elements under accident conditions, is making use of extensive constitutive data being generated on oxidized Zircaloy cladding [62,63] in an attempt to predict behavior during and following a loss-of-coolant accident. The prediction of failure by ballooning of the cladding [64] is also included as part of these efforts.

For the analysis of subassemblies, three-dimensional codes are now available [65,66,67]. Unfortunately, however, they use constitutive correlations that limit their range of predictive validity.

3.2. Constitutive Relations

Although constitutive relations currently used in the codes are, in general, crude, many hopeful signs are evident that a more mechanistic approach will soon emerge. For LWR cladding, Nichols has made a careful analysis of the mechanics of irradiation creep [68], and extensive Zircaloy properties studies are underway at laboratories in several countries [62,69,70,71]. The development of the MATPRO program [72] for Zircaloy properties is a compilation of such efforts. In addition, the Argonne work on the properties of oxidized Zircaloy [62,63] promises to extend the data base through extreme failure conditions. Importantly, these data are being analyzed on a mechanistic basis.

For fast-reactor cladding, the drive for understanding is proceeding along several fronts. First, extensive, carefully planned in-reactor experiments are being carried out by investigators from the USA, England, France, Germany, Canada and Japan on stainless steel cladding to understand, for example, the effects of prior strain on subsequent in-reactor behavior, to determine the influence of applied stress and stress state on swelling and creep, and to quantify the overall interrelationship between swelling and creep [73]. The results of these studies are beginning to be published [74,75,76] along with more advanced mechanistic models of swelling and radiation creep [33,73,76]. Hopefully, these models will soon find their way into fuel element codes and replace the current reliance on empirical correlations. Other related efforts include continuing fundamental studies on a variety of materials [77], attempts to develop and quantify neutron simulation techniques [78], and major efforts

directed toward the development of nonswelling, high-temperature structural alloys [76]. These combined efforts are producing substantial advances in our understanding of irradiation creep and swelling, but these advances have not been incorporated, for the most part, in current design and safety analyses.

Another promising development in the representation of cladding behavior is the equation-of-state work by Hart and Li [79-82]. This will be discussed in an invited paper at SMIRT-4 [83], but basically they have shown that an equation-of-state phenomenological approach, coupled with careful stress-relaxation measurements, has excellent predictive capability over a wide range of strain rates for many materials under monotonic loading conditions. If they are successful in current attempts to predict the behavior of complex polycrystalline alloys involving both grain-matrix and grain-boundary deformation, the equation-of-state approach could form the basis for an improved representation of cladding deformation.

Unfortunately, the current outlook for improved constitutive relations for fuels is much less promising. Fundamental properties work on oxide fuels has been limited in the past two years, except for studies of fuel cracking [84] and fission-gas release during transients [85,86], which have been carried on out-of-reactor by the direct-electrical-heating technique [87]. These studies have been directed toward understanding fuel cracking during power ramps and the behavior of fuels under postulated accident conditions. They have not contributed to an understanding of the more basic phenomena of fuel swelling and creep. Extensions of the BUBL and GRASS analytical work have also been made, but only on a limited basis [59,88]. Some work has begun on carbide and nitride properties [89] in the search for a fuel cycle with a better breeding gain,

but the current concern over proliferation-resistant fuel cycles will likely result in redirection of effort toward thorium fuels properties, which are relatively poorly known [92].

3.3. Local Effects and Failure Criteria

The analysis of fuel and cladding local effects has continued and the understanding of their importance has improved. This is reflected in several recent papers [45,91-94]. In particular, the fuel-cladding mechanical interaction problem in LWR elements has continued to receive the most attention, although complicated by the anisotropy of the Zircaloy. Related experimental work has been performed to determine the possibility of fission-product-induced stress-corrosion cracking of Zircaloy cladding [95,96].

For fast-reactor elements, the volatile fission-product corrosion problem for stainless steel was treated experimentally and analytically by Maiya and co-workers [97,98], who showed that a wall-thickness allowance was a reasonable mechanical model but wall-thinning kinetics must be included rather than the simple a priori wall-thickness accounting procedure which is popular for its simplicity. However, such an approximation is not necessary, since a rigorous analysis is available that could be easily handled by the present fuel-element codes.

The thermodynamics and kinetics of carbon and nitrogen mass transport in the primary sodium circuit of LMFBRs has also been studied, and the resultant effects on cladding strength and ductility have been evaluated [99]. These results are sufficiently understood so that a detailed computer model has been developed [100], which could be readily incorporated into fuel-element codes. This again, would allow a more rational analysis of cladding degradation than a single a priori corrosion allowance.

Considerable data exist on the creep-rupture properties of unirradiated and irradiated fuel-element cladding [52,53], but little data are found on in-reactor creep-rupture and creep/fatigue of cladding [54], especially under biaxial conditions, which is more realistic for cladding loading than simple creep-rupture. The usual problem in creep/fatigue is in knowing how to take into account the cumulative damage in predicting failure [101]. Recent analytical work by Majumdar and Maiya [102,103] on a history-dependent integral damage formulation appears promising and is readily adaptable for use with a history-following code. The fundamental problem, that "creep/fatigue" is actually a creep/fatigue/corrosion problem [104], remains, however, and none of the cumulative damage formulations account for corrosion explicitly. Although some data are now being generated in sodium [105], failure criteria are normally calibrated and compared with data generated in air and then used to predict failure in other environments. The Majumdar-Maiya formulation, however, holds promise for generalization that will include environmental as well as purely mechanical damage.

The elusive goal of fuel-element failure prediction is thus very close to being within our capability. The contributing elements are identified and, in many cases, modeled. But they have yet to be integrated coherently in a first-principles approach directed toward predicting failure of fuel-element cladding. Of course, it can be argued that actual failures will be of a probabilistic and basically unpredictable nature [106,107] caused, for example, by a poor weld, a hot spot, or wire-wrap fretting. Despite this, our purpose is to design reliable fuel elements, to compare one design with another, and to predict performance through rational extrapolation. Therefore, a deterministic failure criteria would be quite useful.

4. Future Efforts

4.1. Improved Constitutive Relations

As already noted, the mathematical problems in fuel-element modeling have been largely overcome and the analytical machinery is in good shape. The next major steps must be taken to improve the constitutive relations installed in these codes. This is not only a matter of more data, but rather a matter of painstaking and careful analysis to understand what the data really represent so that it can be used intelligently. Advantage must be taken of the improvements in the mechanistic modeling of materials behavior to end the crude reliance on empirical curve fitting. Only in this way will physical insight and validity be gained in code extrapolations.

The broadening of modeling efforts into alternate and advanced fuels and for safety analyses is a necessary trend in order to use these tools effectively for today's design problems. Much progress has been made in this direction, and it will undoubtedly continue. The detailed analysis of expensive in-reactor safety tests, for example, is critical in the development of a capability that can be used for extrapolation to other test conditions.

4.2. Rational Failure Criteria

As previously discussed, the formulation of rational fuel-element failure criteria is almost within our grasp. As these criteria are formulated, they should be validated through out-of-reactor tests of simple extreme cases, such as creep-rupture, as well as through complex loading histories. The equipment to run such tests on cladding, with computer-controlled load/strain history is available. The failure criteria should also be compared, of course, with known in-reactor failures, to the extent these failures appear prototypical.

The normal behavior codes are being extended to analyze off-normal design-basis transients and must be interfaced with the safety codes. If this proves impossible, extensions in both directions should be explored. The accident codes, of course, need the normal codes to define realistic initial conditions in describing fuel elements prior to accident initiation. The importance of the knowledge of the fission-gas inventory, for instance, is critical in predicting subsequent fuel behavior and gas release during an accident transient [86].

4.3. Design Use

For all the effort devoted to fuel-element modeling, comparatively little use of the codes has been made by core designers. This is, in part, due to large delays in releasing the codes for design use, poor documentation upon release, and other institutional problems such as the use of proprietary data or gross lack of communication between designers and modelers, who are often in separate organizations. Unless designers can be shown the value of the codes, they will not use them. The significant improvements in code machinery and reliability that have been made, however, should enable parametric studies of obvious value to designers to be performed. In addition, the study of new fuel cycles should provide an opportunity to demonstrate the value of the codes in planning critical time-consuming and costly irradiations.

5. Conclusions

The current state of the art in fuel-element modeling represents a significant advancement in the mathematical treatment of the problem. But the mathematical reliability of the codes has progressed beyond the incorporation of physical models for fuel and cladding behavior. This deficiency must be corrected to improve the value of code extrapolations. Furthermore, development

of a comprehensive rational failure criterion is almost within our capability, and pursuit of this goal should yield great benefits as a comparative performance criterion for fuel-element design.

The immediate concern for the development of a proliferation-resistant fuel cycle should provide an excellent opportunity for fuel-element modelers to demonstrate the advanced state of their art and the value of their codes for fuel-element design.

Acknowledgement

The author would like to thank Dr. M. C. Billone of ANL for a technical review of the manuscript, and M. F. Adams for editorial assistance.

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