

Mechanical Modeling of Porous Oxide Fuel Pellet – A Test Problem

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Computer Science and Mathematics Division
Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program

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PROBLEM**

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ABSTRACT

A poro-elasto-plastic material model has been developed to capture the response of oxide fuels inside the nuclear reactors under operating conditions. Behavior of the oxide fuel and variation in void volume fraction under mechanical loading as predicted by the developed model has been reported in this article. The significant effect of void volume fraction on the overall stress distribution of the fuel pellet has also been described.

1. OVERVIEW

An important oxide fuel issue that can have significant impact on the fuel performance is the mechanical response of oxide fuel pellet and clad system. Specifically, modeling the thermo-mechanical response of the fuel pellet in terms of its thermal expansion, mechanical deformation, swelling due to void formation and evolution, and the eventual contact of the fuel with the clad is of significant interest in understanding the fuel-clad mechanical interaction (FCMI). These phenomena are nonlinear and coupled since reduction in the fuel-clad gap affects thermal conductivity of the gap, which in turn affects temperature distribution within the fuel and the material properties of the fuel. Consequently, in order to accurately capture fuel-clad gap closure, we need to account for fuel swelling due to generation, retention, and evolution of fission gas in addition to the usual thermal expansion and mechanical deformation. Both fuel chemistry and microstructure also have a significant effect on the nucleation and growth of fission gas bubbles. Fuel-clad gap closure leading to eventual contact of the fuel with the clad introduces significant stresses in the clad, which makes thermo-mechanical response of the clad even more relevant.

The overall aim of this test problem is to incorporate the above features in order to accurately capture fuel-clad mechanical interaction. Because of the complex nature of the problem, a series of test problems with increasing multi-physics coupling features, modeling accuracy, and complexity are defined with the objective of accurate simulation of fuel-clad mechanical interaction subjected to a wide-range of thermo-mechanical stimuli.

1.1 KEYWORDS

Void volume fraction, elasticity, plasticity, nonlinear mechanics, and finite element method.

1.2 RELATED TEST PROBLEMS

None.

2. GEOMETRY

Initially, before the reaction starts within the reactor, the oxide fuel is in the form of cylindrical pellets, 0.3225 inches in diameter and 0.387 inches long that are stacked vertically. The inner and outer diameters of the clad are 0.3290 and 0.3930 inches respectively. This implies a clad thickness of 0.032 inches. But in this test problem we concentrate on the particular case when due to burnup the fuel have expanded and touched the clad. The clad is Zr alloy and no gap is considered between fuel and the clad (Fig: 1). The combination of pellet and clad is free to expand in the radial directions under the axial compressive loading (usually in the nuclear reactor, the cladding is restrained from free expansion in the radial direction [1,9]). Since in this problem, the fuel has already gone through some burnup resulting in release of fission gas and expansion of the fuel pellet to touch the clad, an arbitrary distribution of voids within the pellet is assumed to initialize the simulations.

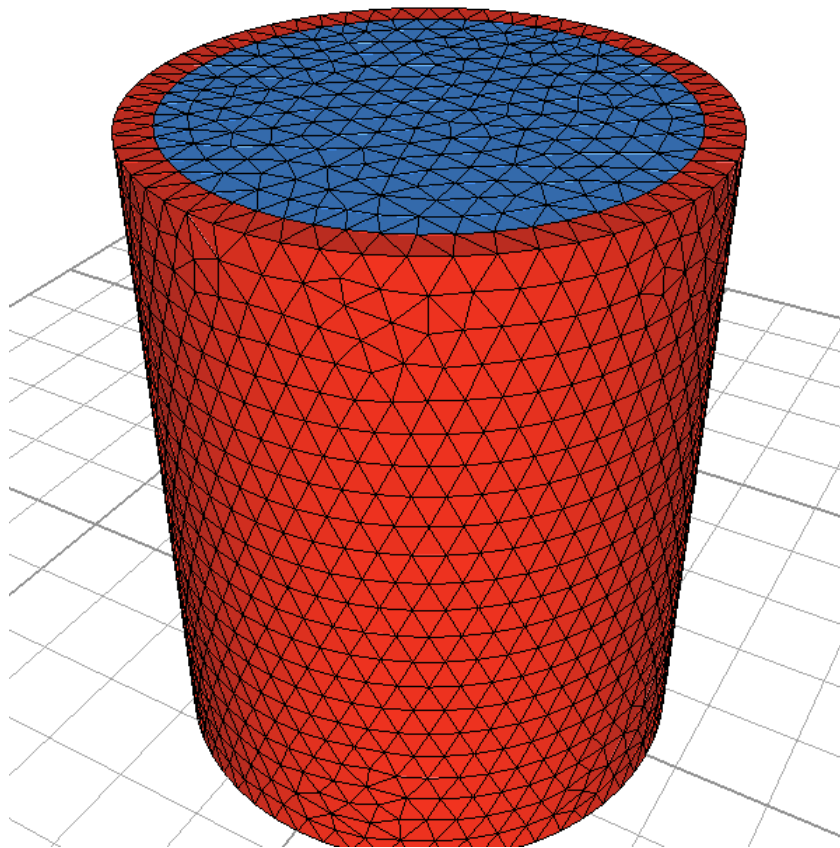


Fig. 1. Initial geometry of the combined fuel and clad. The fuel is touching the clad, so there is no gap between them.

3. PHYSICS

The preliminary test problem that we consider is a mechanical simulation of an oxide fuel pellet. The objective of the test problem is to simulate the evolution of void volume fraction within the fuel pellet under a prescribed mechanical loading. Only intra-granular voids are modeled in this problem [2,5,6]. The homogenized material model assumes that these voids are spherical in shape. The physics tested includes the effect of fuel porosity on the elasto-plastic response of the fuel-clad system under compression. Subsequent extensions of the problem would include temperature effects and inter-granular ellipsoidal voids.

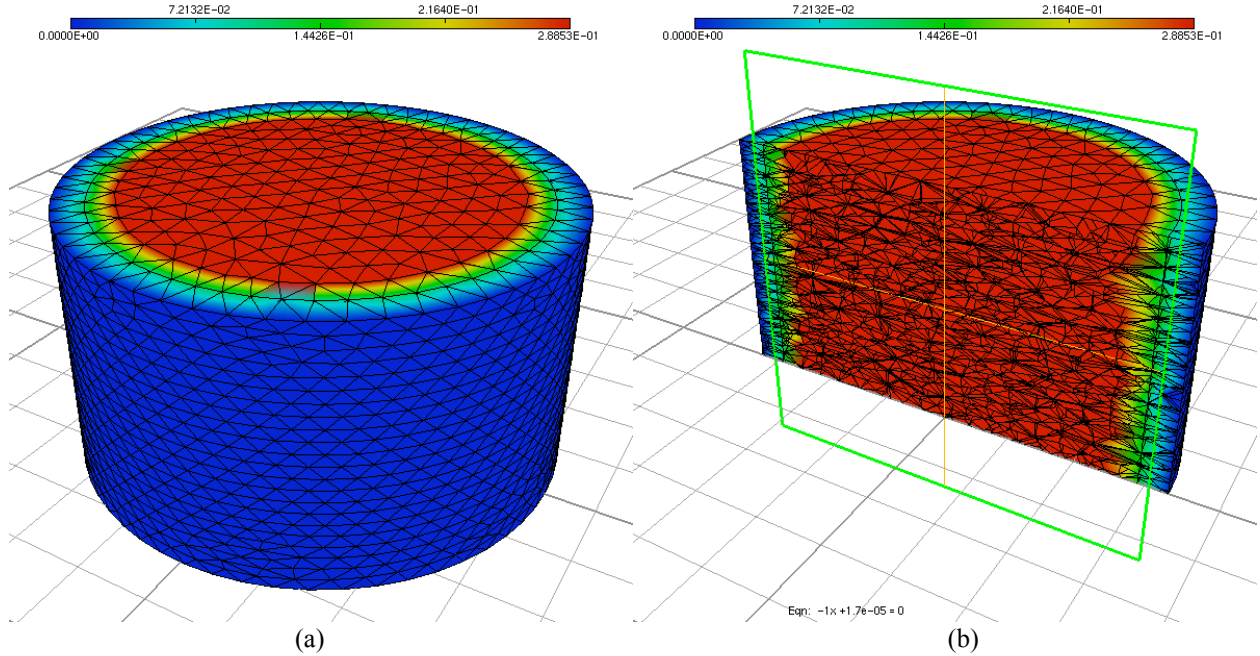


Fig. 2. Evolution of void fraction within the fuel pellet. (a) A uniform void fraction of 0.3 was imposed over the pellet in the beginning. Due to the applied compressive loading, void fraction decreases over the pellet. The reduction in the void volume fraction within the fuel is uniform throughout the pellet. At the fuel-clad interface, the apparent reduction in void volume fraction to a value of 0.15 is due to the smoothing effect of the software used to generate the contour plots. (b) A cross-sectional view of the void volume fraction within the fuel-clad system.

Two sets of simulations were generated, one with uniform initial void volume fraction (Fig. 2) and the other with random values of the initial porosity (Fig. 3) distributed over the pellet. Both the fuel and clad were assumed to be initially stress free. A prescribed displacement boundary condition (compressive) is applied to the top surface of the pellet and clad. Symmetric boundary conditions are applied at the mid-plane of the pellet. The fuel pellet is modeled as a poro-elasto-plastic material with a pressure sensitive yield function akin to standard Gurson model [2]. The voids within the fuel can be either in drained or saturated state [5,6]. Porosity evolves as a function of the hydrostatic component of plastic strain and is given by $\dot{f} = (1 - f)\dot{\epsilon}_{kk}^p$, where, f = void volume fraction, \dot{f} = rate of change of void volume fraction and $\dot{\epsilon}_{kk}^p$ is the rate of change of plastic dilatational strain [3]. A standard isotropic linear elasticity model is used for modeling the mechanical response of clad. Once this preliminary demonstration is completed, this model will be extended to couple the thermal effects with the mechanics and eventually chemistry, microstructure evolution and species redistribution will also be added.

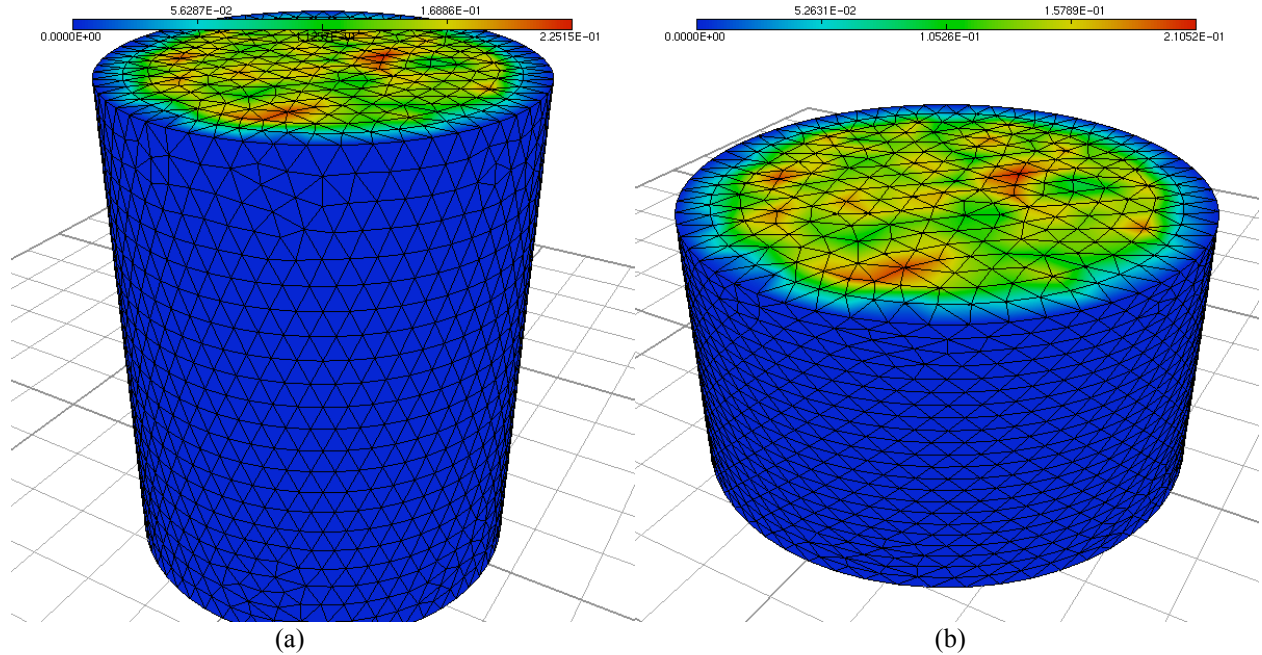


Fig. 3. Evolution of void fraction within fuel pellet. (a) A random void fraction was imposed over the pellet in the beginning. (b) Final void fraction within the fuel-clad system. Void fraction decreases over the pellet due to the applied compressive loading.

3.1 DATA REQUIREMENTS (INPUT)

Initial pellet and clad geometries, elasto-plastic properties for oxide fuel and elastic properties of Zr alloy cladding. The parameters used in these simulations are listed in Appendix A.

3.2 MESH REQUIREMENTS

Tetrahedral or hexahedral mesh for fuel pellet and clad.

4. EXPECTED RESULTS (OUTPUT)

1. Spatial stress distribution in the fuel and cladding
2. Spatial void fraction evolution within the fuel

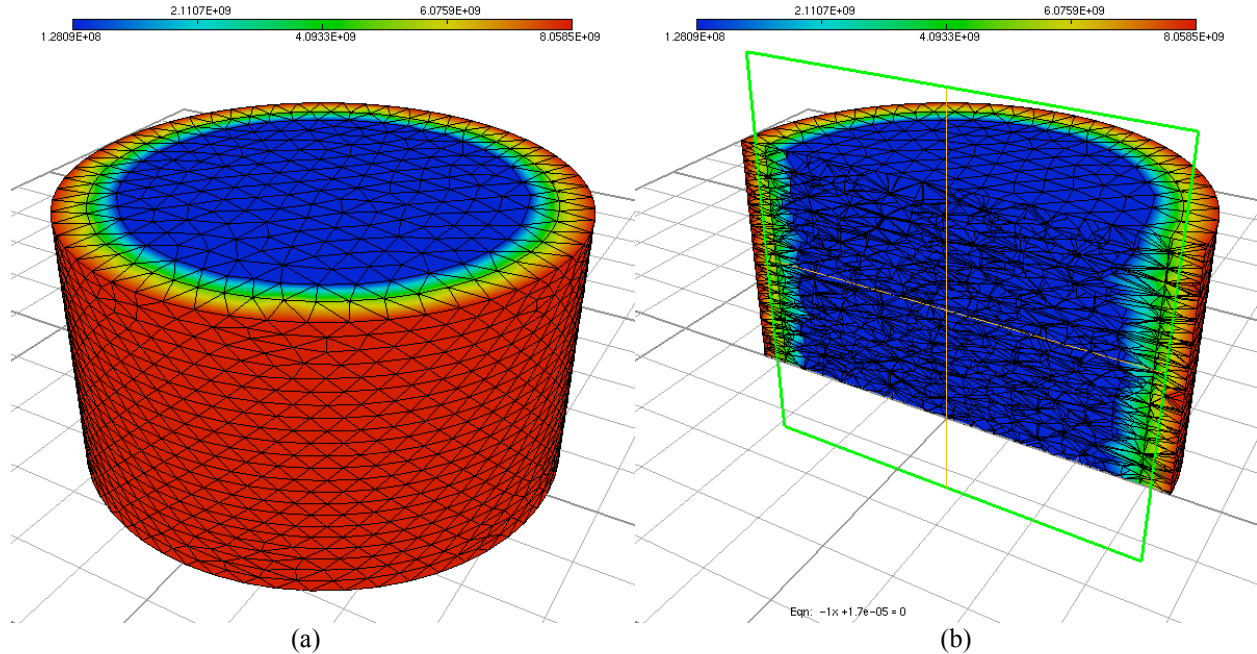


Fig. 4. Evolution of equivalent stress within the fuel pellet and clad. Initial volume fraction of 0.3 inside the fuel pellet was assumed. (a) Under compressive loading the stresses evolve within the fuel and clad. Because of high volume fraction the stress within the fuel is comparatively lower than the stress on the clad. The stress distribution is uniform on both the fuel pellet and cladding. The apparent stress gradient visible on the fuel-clad interface is due to the smoothing effect of the contour plotting software. (b) A cross section view of the same figure showing the uniform axial distribution of stress inside the fuel pellet.

Fig: 2 and fig: 3 contain the spatial void fraction evolution result and fig: 4 describe the stress distribution within the fuel and cladding.

A comparative study is conducted for the evolution of volume fraction under compressive loading within the fuel pellet for two conditions:

- (a) The radial expansion of the outer surface of the clad is constrained.
- (b) Radial expansion of the outer surface of the clad is allowed.

The initial void volume fraction within the fuel was assumed to be $f = 0.3$. The results are given in fig: 5. Under constrained deformation the fuel pellet could not deform freely which resulted in generation of higher hydrostatic stress inside the pellet. This caused the volume fraction to drop from 0.3 to 0.27. On the other hand, the free deformation of the pellet and cladding generated lesser hydrostatic stress, which resulted in decrease in void volume fraction from 0.3 to 0.29 only. Fig: 6 shows how the void volume fraction varies along any arbitrary diameter on the fuel-clad system. The diameter has been normalized between -0.5 to +0.5 to ensure the generality of the distribution. Due to compression the void volume fraction decreases and the reduction is uniform throughout the fuel system. The clad has zero void volume fractions. The apparent gradient visible in the variation of void volume fraction in fig: 5 are due to the contour plotting mechanism used by the software to generate these figures.

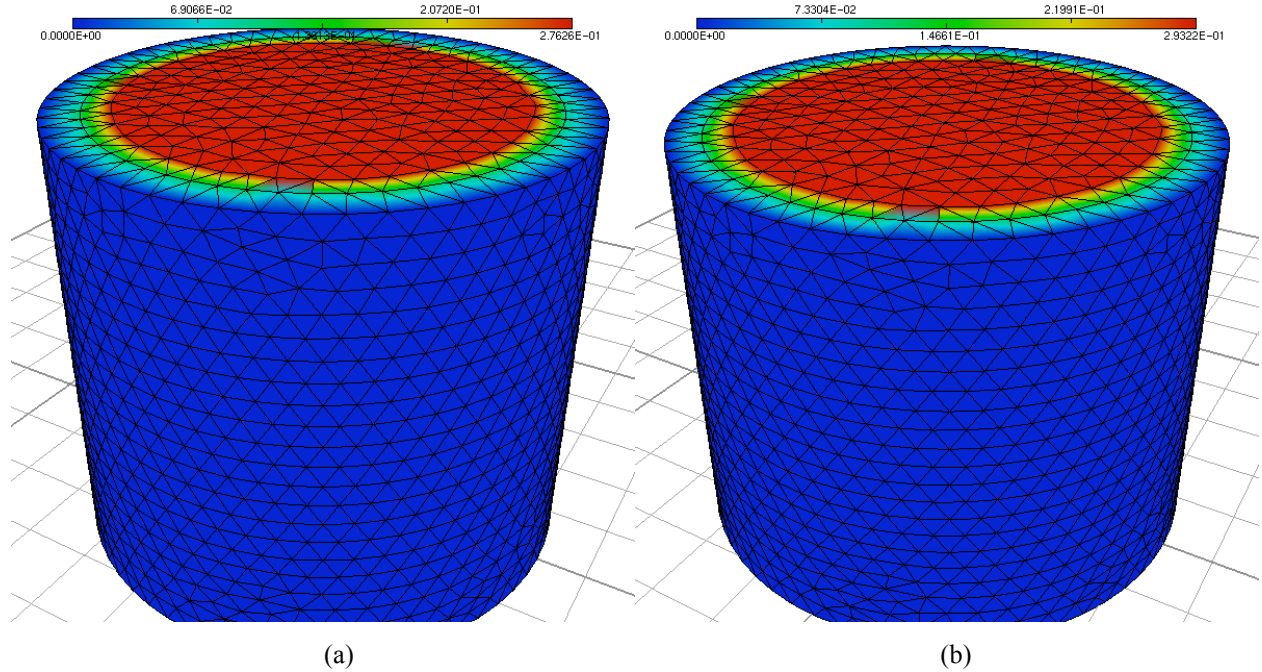


Fig. 5. A comparative study for the evolution of volume fraction within the fuel pellets under two conditions: (a) The radial expansion of the outer surface of the clad is constrained. (b) Radial expansion of the outer surface of the clad is allowed. The initial void volume fraction within the fuel was assumed to be $f = 0.3$. For the constrained case the void volume fraction reduced from 0.3 to 0.27 (approximately 10% reduction). For the second case only 3% reduction in void volume is observed. The distribution of void volume fraction along any diameter within this fuel-clad system is given in fig: 6.

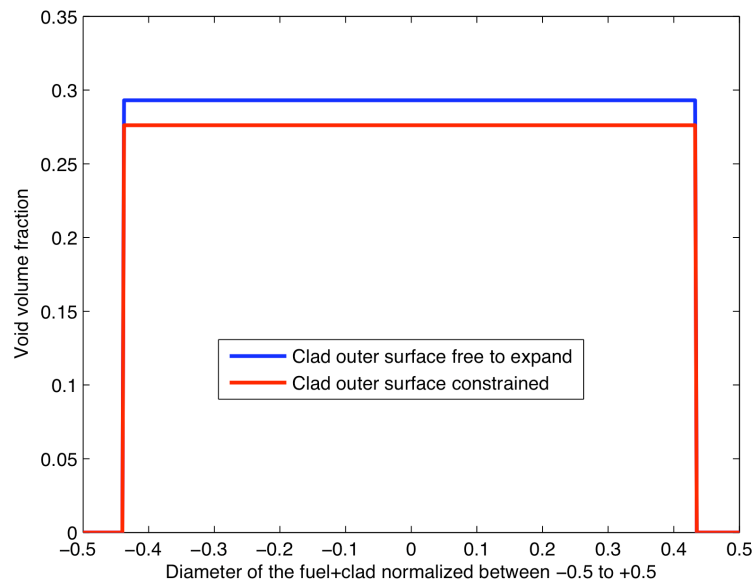


Fig. 6. Variation in the void volume fraction along any diameter (normalized between -0.5 to +0.5) inside the fuel-clad system. Initially the void volume inside the fuel was $f = 0.3$ and zero within the clad. After compression the void volume fraction decreases uniformly inside the fuel. This figure shows the distribution of f within the fuel and the clad after compression. For the case where the outer surface of the clad was restrained from radial expansion, the hydrostatic stress generation within the fuel was more resulting in more reduction of void volume fraction than the case with free radial expansion of the outer surface of the clad.

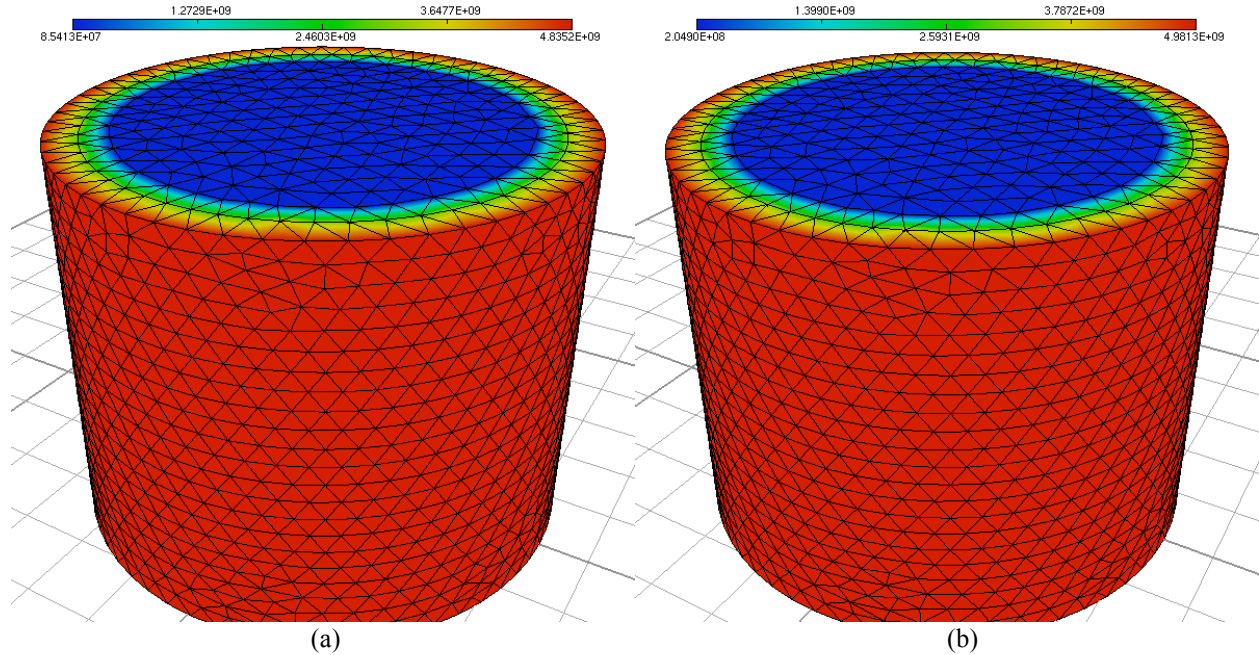


Fig. 7. A comparative study for the evolution of stress within the fuel-clad assembly is conducted for: (a) Fuel pellet containing initial porosity $f = 0.3$, (b) Fuel pellet without porosity. The fuel pellets with pores show a stress distribution of 85 MPa; whereas, the other pellet with no porosity reach stress level around 204 MPa.

Another comparative study for the evolution of stress within the fuel-clad assembly is conducted for:

- (a) Fuel pellet containing initial porosity $f = 0.3$.
- (b) Fuel pellet without porosity.

Under compressive displacement loading, the fuel pellet with pores showed a uniform equivalent stress distribution of 85 MPa at the end of deformation. Whereas, the other pellet with no porosity [4,7], displayed uniform stress distribution of 204 MPa. The simulation results are shown in fig: 7. This comparison shows the importance of including the effect of void volume fraction in the analysis of oxide fuels.

In addition to the above results, later extensions of the model would result in

1. Thermo-mechanical evolution of porosity and gap closure leading to mechanical contact
2. Chemical phases distribution within the pellet
3. Species distribution in the pellet
4. Fission gas release from fuel
5. Microstructure evolution

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APPENDIX A.
LIST OF MATERIAL PROPERTIES

APPENDIX A. LIST OF MATERIAL PROPERTIES

Table: Material Properties

| Material Property | Oxide Fuel | Clad |
|------------------------------|------------|--------|
| Young's moduli (GPa) | 174.92 | 160 |
| Poisson's Ratio | 0.316 | 0.33 |
| Yield Stress (MPa) | 145 | -- |
| Hardening Parameter (GPa) | 2.1 | -- |
| Density (kg/m ³) | 10660.0 | 7818.0 |