Analytical Solution in Transient Thermoelasticity of Functionally Graded Thick Hollow Cylinders (Pseudo-Dynamic Analysis)

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Abstract:
This work studies transient thermal stresses in a thick hollow cylinder made of Functionally Graded Material (FGM). The material properties are considered to be nonlinear with a power law distribution through the thickness. The cylinder is assumed to be in plane-strain condition and has infinite length. The displacement and stresses distributions are obtained by analytical solution of the Navier governing differential equations. The transient dynamic behavior of thermal stresses are specified and discussed for various power law exponent in mechanical properties function.

Keywords: Functionally Graded Material, Thermal Stress, Pseudo-Dynamic, Thick Hollow Cylinders.

1. Introduction

Functionally graded materials (FGMs) are new kind of materials. FGMs have been shown to posses superior advantages when employed in high temperature environment. In FGMs, material properties vary continuously from one surface to the other, especially from metal to ceramic. These materials are adaptable for super- high temperature environments. Analytical and computational studies of appointing stresses and displacements in cylindrical shell made of FGM have been carried out by some of researchers as following.

Zimmerman et al. [1] considered the nonhomogeneous material properties as linear functions of radius and presented the analytical solution in one-dimensional case for cylinders of FGMs. El-abbasi et al. [2] used a new thick shell element to study the thermoelastic behavior of functionally graded shells and plates structures. They used Rayleigh-Ritz method for determining the temperature distribution across the thickness.

Temperature and stress distributions were determined in a stress-relief-type plate of FGMs with steady state and transient temperature distributions by Awaji [3]. A general analysis of one dimensional steady state thermal stresses in a thick hollow cylinder under axisymmetry and nonaxisymmetry loads was developed by Jabbari et al. [4, 5]. Liew et al. [6] presented an analysis of the thermo-mechanical behavior of thick cylinder made from FGM. They assumed that the cylinder includes many homogeneous sub-cylinders.

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Transient temperature field and associated thermal stresses in functionally graded materials have been determined by using a Finite Element-Finite Difference Method (FEM/FDM) by Wang B-L et al. [7]. Thermal shock fracture of a FGM plate and the thermal shock resistance of FGMs were analyzed by them. A general solution for the one-dimensional steady state thermal and mechanical stresses in a hollow thick sphere made of functionally graded material was presented by Eslami et al [8]. The theoretical treatment of the steady-state thermoelastic problem of a functionally graded cylindrical panel due to nonuniform heat supply in the circumferential direction was carried out by Ootao et al [9]. They obtain the exact solution for the two-dimensional temperature change in a steady state, and thermal stresses of a simple supported cylindrical panel under the state of plane strain. Analytical solutions of the three-dimensional temperature and thermo-elastic stress field in the functionally graded cylindrical panel with finite length were derived by Shao et al [10]. In their work, analytical solutions for the temperature and stress fields expressed in terms of trigonometric. The stresses and displacement were analyzed in the infinite functionally graded thick hollow cylinder under mechanical shock using multilayer method by authors in the prior work [11]. We obtained the dynamic behavior of cylinder, natural frequencies and the mean velocity of radial stress wave propagation.

This paper presents an analytical solution for transient thermo-mechanical behavior of thick hollow cylinder made of functionally graded materials under thermal and mechanical radial loads in plane strain condition. The radial and hoop stresses and the radial displacement are analytically determined by using Bessel functions. The comparisons in thermal stresses are presented for various kind of functionally graded material in different times.

2. Temperature field

To determine the thermal stresses, the temperature distribution across the thickness of cylinder should be obtained. The inner surface of cylinder is assumed to be made of ceramic and outer surface to be made of metal. The temperature distribution in the functionally graded thick hollow cylinder across the thickness was analytically determined in the prior experience of authors [12]. To obtain the temperature distribution, the following boundaries and initial conditions are considered.

$$\frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}\left(\bar{k}.\bar{r}.\frac{\partial \bar{T}}{\partial \bar{r}}\right)=\bar{\rho}\bar{c}\frac{\partial \bar{T}}{\partial \bar{t}} \tag{1}$$

$$\bar{k}\frac{\partial \bar{T}}{\partial \bar{r}}+\bar{T}=0 \qquad at \qquad \bar{r}=1 \tag{2}$$

$$\frac{\partial \bar{T}}{\partial \bar{r}}=0 \qquad at \qquad \bar{r}=b/a \tag{3}$$

$$\bar{T}(r,0)=1 \tag{4}$$

The inner and outer radii are assumed as a and b. The following nondimensional variables are used for temperature field.

$$\bar{T} = \frac{T}{T_0},\ \bar{r} = \frac{r}{a},\ \bar{t} = \frac{th}{\rho c_c.a},\ \overline{\rho c} = \frac{\rho c}{\rho c_c},\ \bar{k} = \frac{k}{ah}$$

where r, t, h, ρ ,k and c_c are radius, time, heat transfer coefficient, density, thermal conductivity and specific heat of ceramic and T_0 is a constant temperature. The temperature of body T is defined by:

$$T(r,t) = \theta(r,t) - \theta_1 \tag{5}$$

where $\theta(r,t)$ is the temperature of cylinder body and θ_1 is the temperature of fluid that flows in the cylinder. It is assumed that the thermal conductivity and ρc are the power functions of "r" as follows:

$$\bar{k} = k_0 \bar{r}^{m_1} \tag{6}$$

$$\overline{\rho c} = \rho c_0 \bar{r}^{m_2} \tag{7}$$

where $k_0, \rho c_0, m_1, m_2$ are the material constants and $\rho c_0 = 1$ is for ceramic material (inner surface). The temperature distribution is presented as follows:

$$\bar{T}(\bar{r},\bar{t}) = \sum_{i=1}^{\infty} e^{-\frac{\lambda_i^2}{\rho c_0}\bar{t}} .\bar{r}^{-\frac{m_1}{2}} \left\{ B_{1i} J_n\left(\gamma_i \bar{r}^{\frac{2-m}{2}}\right) + B_{2i} Y_n\left(\gamma_i \bar{r}^{\frac{2-m}{2}}\right) \right\} \tag{8}$$

where γ_i are the eigen-values and

$$m = m_1 - m_2 \tag{9}$$

3. Thermoelastic equations

In thick hollow cylinder with infinite length and Pseudo-Dynamic conditions, the equilibrium equation can be written as the following:

$$\frac{d\sigma_{rr}}{dr} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0 \tag{10}$$

And the constitutive equations are:

$$\sigma_{rr} = \frac{E}{(1+\nu)(1-2\nu)}\left[(1-\nu)\varepsilon_{rr} + \nu\varepsilon_{\theta\theta} - (1+\nu)\alpha\Delta T\right] \tag{11}$$

$$\sigma_{\theta\theta} = \frac{E}{(1+\nu)(1-2\nu)}\left[(1-\nu)\varepsilon_{\theta\theta} + \nu\varepsilon_{rr} - (1+\nu)\alpha\Delta T\right] \tag{12}$$

where:

$$\Delta T = T - T_0 \tag{13}$$

and $\sigma_{rr}, \sigma_{\theta\theta}, \varepsilon_{rr}, \varepsilon_{\theta\theta}, T, \alpha$ are the radial and hoop stresses, the radial and hoop strains, the temperature distribution in cylinder and the coefficient of thermal expansion. E and ν are the modulus of elasticity and Poisson's ratio. The strain –displacement relations are:

$$\varepsilon_{rr} = \frac{du}{dr} \tag{14}$$

$$\varepsilon_{\theta\theta} = \frac{u}{r} \tag{15}$$

The governing equations can be written through the following dimensionless terms:

$$\bar{\sigma}_{rr} = \frac{\sigma_{rr}(1-2\nu)}{E_c \alpha_c T_0},\ \bar{\sigma}_{\theta\theta} = \frac{\sigma_{\theta\theta}(1-2\nu)}{E_c \alpha_c T_0},\ \bar{u} = \frac{(1-\nu)u}{(1+\nu)\alpha_c a T_0},\ \bar{E} = \frac{E}{E_c},\ \bar{\alpha} = \frac{\alpha}{\alpha_c},\ \bar{r} = \frac{r}{a}$$

where E_c, α_c are the standard values (the modulus of elasticity and the thermal expansion coefficient of ceramic inner surface). In functionally graded material, $\bar{E}$ and $\bar{\alpha}$ are power function of “r” as the following:

$$\bar{E} = E_0 \bar{r}^{m_3} \tag{16}$$

$$\bar{\alpha} = \alpha_0 \bar{r}^{m_4} \tag{17}$$

where:

$$\bar{r} = 1 \rightarrow \begin{cases} \bar{E} = 1 \\ \bar{\alpha} = 1 \end{cases} \rightarrow \begin{cases} E_0 = 1 \\ \alpha_0 = 1 \end{cases}$$

thus:

$$\bar{E} = \bar{r}^{m_3} \tag{18}$$

$$\bar{\alpha} = \bar{r}^{m_4} \tag{19}$$

where m_3, m_4 are the material constants. The Navier equation in terms of the displacement for the FGM cylinder can be obtained by introducing of the above equations into the Equation (10) as the following:

$$A_0 \frac{d^2\bar{u}}{d\bar{r}^2} + B_0 \bar{r}^{-1} \frac{d\bar{u}}{d\bar{r}} + C_0 \bar{r}^{-2} \bar{u} = D_0 \bar{r}^{m_4} \frac{d\bar{T}}{d\bar{r}} + F_0 \bar{r}^{m_4 - 1}(\bar{T} - 1) \tag{20}$$

where:

$$A_0 = 1, B_0 = 1 + m_3, C_0 = \left\{ \frac{m_3 \nu + \nu - 1}{(1-\nu)} \right\}, D_0 = 1, F_0 = m_3 + m_4$$

The right side of Equation (20) can be written as follows by using Equation (8).

$$A_0 \frac{d^2\bar{u}}{d\bar{r}^2} + B_0 \frac{1}{\bar{r}} \frac{d\bar{u}}{d\bar{r}} + C_0 \frac{\bar{u}}{\bar{r}^2} = \sum_{i=1}^{\infty} e^{-\frac{\lambda_i^2}{\rho c_0}\bar{t}} \left\{ f_{1i} J_n\left(\gamma_i \bar{r}^{\frac{2-m}{2}}\right) + f_{2i} J_{n-1}\left(\gamma_i \bar{r}^{\frac{2-m}{2}}\right) + f_{3i} J_{n+1}\left(\gamma_i \bar{r}^{\frac{2-m}{2}}\right) \right\} + \sum_{i=1}^{\infty} e^{-\frac{\lambda_i^2}{\rho c_0}\bar{t}} \left\{ f_{4i} Y_n\left(\gamma_i \bar{r}^{\frac{2-m}{2}}\right) + f_{5i} Y_{n-1}\left(\gamma_i \bar{r}^{\frac{2-m}{2}}\right) + f_{6i} Y_{n+1}\left(\gamma_i \bar{r}^{\frac{2-m}{2}}\right) \right\} - F_0 \bar{r}^{m_4 - 1} \tag{21}$$

The differential of Bessel functions and coefficients f_{1i} to f_{6i} are presented in Appendix (1). By solving the Equation (21), the Bessel function composition form is assumed for the radial displacement as the following:

$$\bar{u} = \sum_{i=1}^{\infty} e^{-\frac{\lambda_i^2}{\rho c_0}\bar{t}} \left\{ z_{1i} J_n\left(\gamma_i \bar{r}^{\frac{2-m}{2}}\right) + z_{2i} J_{n-1}\left(\gamma_i \bar{r}^{\frac{2-m}{2}}\right) + z_{3i} J_{n+1}\left(\gamma_i \bar{r}^{\frac{2-m}{2}}\right) \right\} + \sum_{i=1}^{\infty} e^{-\frac{\lambda_i^2}{\rho c_0}\bar{t}} \left\{ z_{4i} Y_n\left(\gamma_i \bar{r}^{\frac{2-m}{2}}\right) + z_{5i} Y_{n-1}\left(\gamma_i \bar{r}^{\frac{2-m}{2}}\right) + z_{6i} Y_{n+1}\left(\gamma_i \bar{r}^{\frac{2-m}{2}}\right) \right\} + c_p \bar{r}^{k'} + c_1 \bar{r}^{k_1} + c_2 \bar{r}^{k_2} \tag{22}$$

The coefficients z_{1i} to z_{6i} and c_p and exponent k' should be determined by replacing Equation (22) to Equation (21). Coefficients c_1 and c_2 can be calculated by using boundary conditions. The coefficient c_p and exponent k' can be written as the following:

$$c_p = -\frac{F_0}{(A_0 m_4 + B_0)(m_4 + 1) + c_0} \tag{23}$$

$$k' = m_4 + 1 \tag{24}$$

Coefficients z_{1i} to z_{6i} would be calculated from the following equations:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & 0 & 0 & 0 \\ a_{31} & a_{32} & a_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & a_{44} & a_{45} & a_{46} \\ 0 & 0 & 0 & a_{54} & a_{55} & a_{56} \\ 0 & 0 & 0 & a_{64} & a_{65} & a_{66} \end{bmatrix} \begin{Bmatrix} z_{1i} \\ z_{2i} \\ z_{3i} \\ z_{4i} \\ z_{5i} \\ z_{6i} \end{Bmatrix} = \begin{Bmatrix} f_{1i} \\ f_{2i} \\ f_{3i} \\ f_{4i} \\ f_{5i} \\ f_{6i} \end{Bmatrix} \tag{25}$$

$$\begin{Bmatrix} z_{1i} \\ z_{2i} \\ z_{3i} \\ z_{4i} \\ z_{5i} \\ z_{6i} \end{Bmatrix} = [a]^{-1} \begin{Bmatrix} f_{1i} \\ f_{2i} \\ f_{3i} \\ f_{4i} \\ f_{5i} \\ f_{6i} \end{Bmatrix} \tag{26}$$

The components of matrix $[a]$ are given in Appendix (1). The exponents k_1 and k_2 can be determined from Equation (27).

$$A_0 k(k-1) + B_0 k + C_0 = 0 \tag{27}$$

The mechanical boundary conditions are considered as follows:

$$\sigma_{rr} = -P_1 \qquad at \quad \bar{r} = a \tag{28}$$

$$\sigma_{rr} = -P_2 \qquad at \quad \bar{r} = b \tag{29}$$

The coefficients c_1 and c_2 are calculated by using the above boundary conditions. The radial and hoop stresses can be calculated by using Equations (30) and (31).

$$\bar{\sigma}_{rr} = \bar{r}^{m_3}\left\{\frac{d\bar{u}}{d\bar{r}} + \frac{\nu}{1-\nu}\frac{\bar{u}}{\bar{r}}\right\} + \bar{r}^{m_3+m_4}\left(1-\bar{T}\right) \tag{30}$$

$$\bar{\sigma}_{\theta\theta} = \bar{r}^{m_3}\left\{\frac{\bar{u}}{\bar{r}} + \frac{\nu}{1-\nu}\frac{d\bar{u}}{d\bar{r}}\right\} + \bar{r}^{m_3+m_4}\left(1-\bar{T}\right) \tag{31}$$

4. Numerical results and discussion

The present method was verified in the prior experience of authors [12]. The functionally graded hollow cylinder with $\frac{b}{a} = 1.1$ where "*a*" and "*b*" are inner and outer radii, was considered. Suppose that the inner surface is made of graphite/epoxy with thermal conductivity $k = 0.72 \quad W/m.K$.

Table 1- The first six eigenvalues for thin hollow cylinder (b/a=1.1)[12]

m_1	γ_1		γ_2		γ_3		γ_4		γ_5		γ_6	
	present	Ref. [13]	present	Ref. [13]	present	Ref. [13]	present	Ref. [13]	present	Ref. [13]	present	Ref. [13]
0	0	0	31.4268	31.4292	62.8373	62.8385	94.2514	94.2522	125.6664	125.667	157.0818	157.0823
0.5	0	0	31.4226	31.4391	62.8352	62.8434	94.25	94.2555	125.6654	125.6695	157.081	157.0843
1	0	0	31.4308	31.4512	62.8392	62.8495	94.2527	94.2596	125.6674	125.6726	157.0825	157.0867
2	0	0	31.4699	31.4821	62.8589	62.865	94.2659	94.2699	125.6773	125.6803	157.0905	157.0928
5	0	0	31.5498	31.6271	62.8902	62.9378	94.2849	94.3185	125.6909	125.7167	157.1011	157.1221

For t = 0 and $m_1 = 0$ (homogeneous-material), the first five eigenvalues were obtained by using the boundary conditions (flux-prescribed at inner and outer surfaces) in ref. [13]. For simplicity of analysis, the power law coefficients for m_1 and m_2 were considered to be the same. These eigenvalues were compared with the results presented in ref. [13] and were in good agreement with those obtained according to ref. [13].

Consider the functionally graded thick hollow cylinder with inner radius "a" and outer radius "b". The boundary and initial conditions are defined in equation (2) to (4). Suppose that the inner surface is made of alumina (ceramic) and the inner and outer pressures are as follows:

$P_1 = 0 \quad and \quad P_2 = 0$

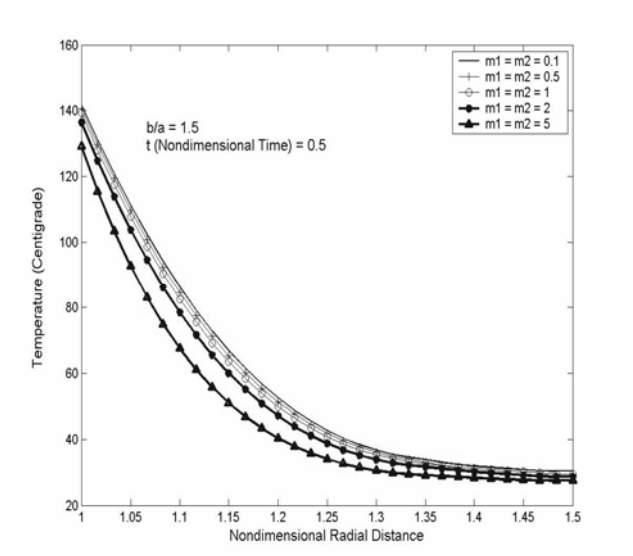

Figure 1. Radial distribution of temperature for $\bar{t}$ =0.5 and *b/a*=1.5 [12]

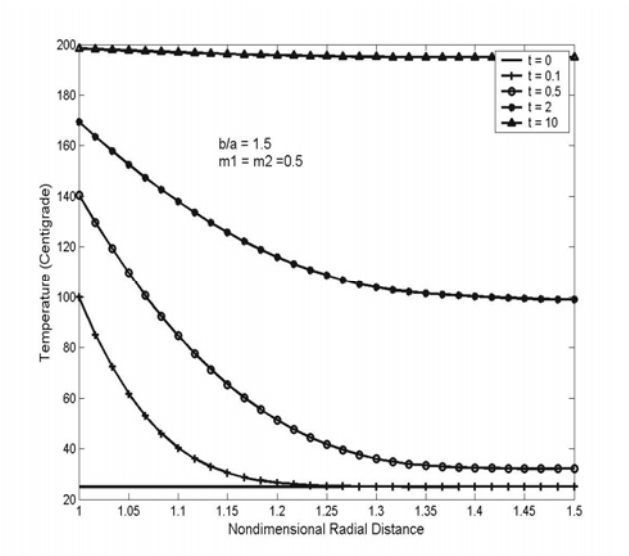

Figure 2. History of temperature radial distribution for *m1*=*m2*=0.5 and *b/a*=1.5 [12]

The alumina specifications are:

$$k_c = 46 \quad \frac{W}{m.^\circ c}\,,\ \alpha_c = 7.4*10^{-6}\big/{}^\circ c\,,\ c_c = 0.76\frac{kJ}{kg.^\circ c}\,,\ E_c = 380Gpa\,,\ \rho_c = 3800\frac{kg}{m^3}\,,\ \nu = 0.3$$

and inner radius 'a' is 0.25 m. The convection coefficient and temperature of the fluid flowing within hollow cylinder are $h = 4600\frac{W}{^\circ c}$ and $\theta_1 = 200^\circ c$. The dynamic behavior of cylinder subjected to the transient thermal load can be seen by using the proposed method. Figures 1 to 4 show the radial distribution of temperature for various time and exponents m_1 and m_2 which were obtained and discussed in our previous work [12]. These temperature distributions are considered to determine the thermal stresses.

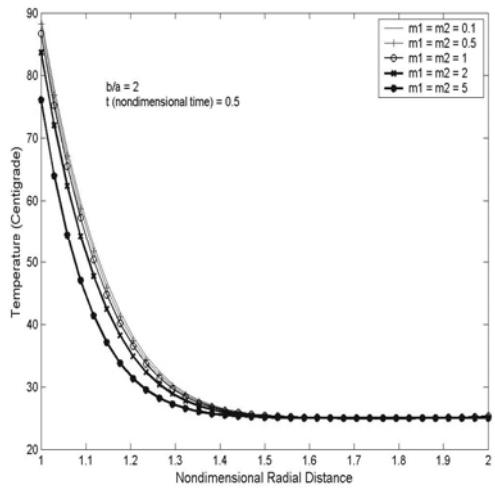

Figure 3. Radial distribution of temperature for *t*=0.5 and *b/a*=2 [12]

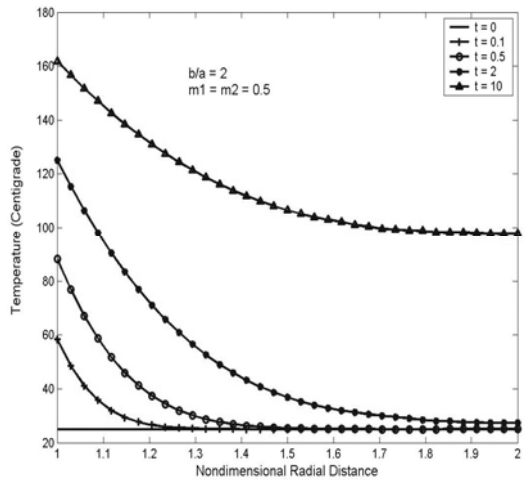

Figure 4. History of temperature radial distribution for *m1*=*m2*=0.5 and *b/a*=2 [12]

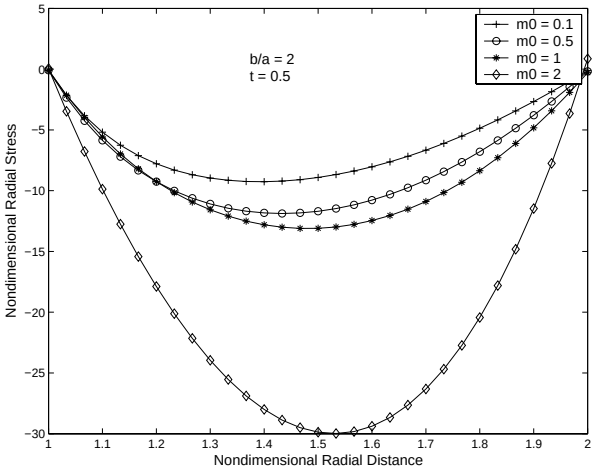

Figure 5. Nondimensional radial stress distribution across thickness for $\bar{t}$ =0.5 and *b/a*=2 and various $m_1 = m_2 = m_3 = m_4 = m_0$

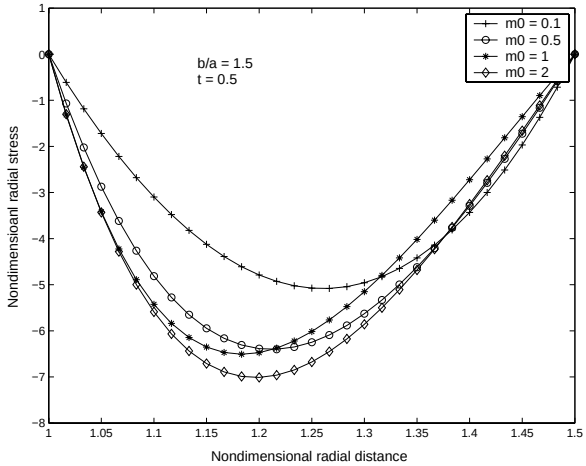

Figure 6. Nondimensional radial stress distribution across thickness for $\bar{t}$ =0.5 and *b/a*=1.5 and various $m_1 = m_2 = m_3 = m_4 = m_0$

For simplicity of analysis the power law coefficients for m_1, m_2, m_3 and m_4 are considered to be the same, $m_1 = m_2 = m_3 = m_4 = m_0$. The Figures (5) and (6) show the nondimensional radial stresses for two values of *b/a* across the thickness of shell in $\bar{t}$ *=0.5* and various values of power law index m_0. These figures show that as the power law index m_0 increase, the maximum value of radial stress is increased. The Figures (7) and (8) show the hoop stresses for two values of *b/a* in $\bar{t}$ *=0.5* across the thickness of shell. The maximum value of hoop stress is obtained in inner radius. For $m_0 < 1$, the maximum value of hoop stress is decreased as the power index m_0 is increased and these values are compression hoop stresses. For $m_0 > 1$, the maximum points of hoop stresses diagram are tension hoop stresses and these are increased as the power index m_0 is increased.

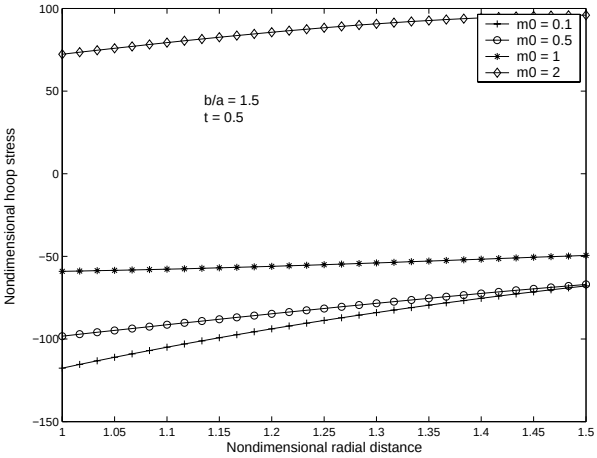

Figure 7. Nondimensional hoop stress distribution across thickness for $\bar{t}$ =0.5 and *b/a*=1.5 and various $m_1 = m_2 = m_3 = m_4 = m_0$

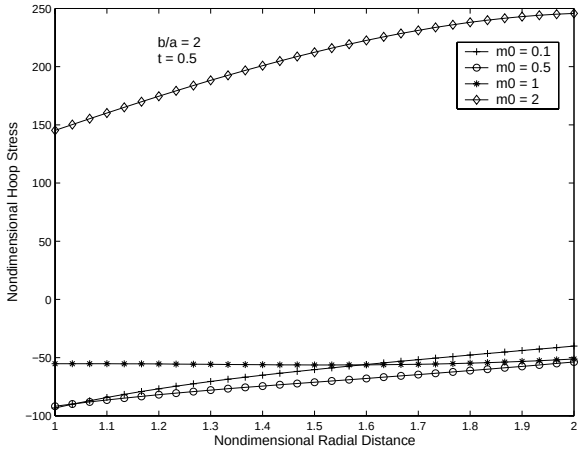

Figure 8. Nondimensional hoop stress distribution across thickness for $\bar{t}$ =0.5 and *b/a*=2 and various $m_1 = m_2 = m_3 = m_4 = m_0$

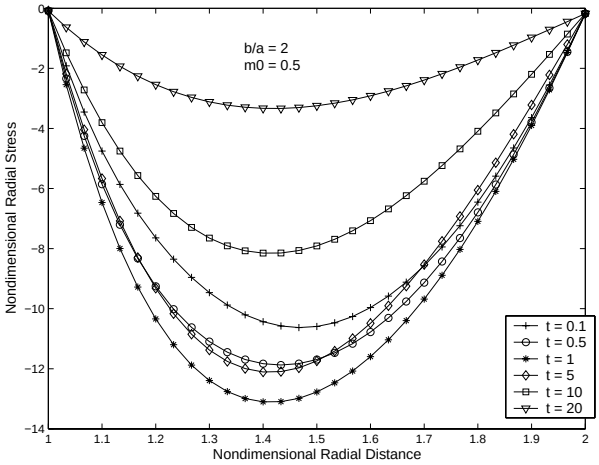

Figure 9. Nondimensional radial stress distribution across thickness for various *t* (nondimensional time) and m_0 =0.5 , *b/a*=2

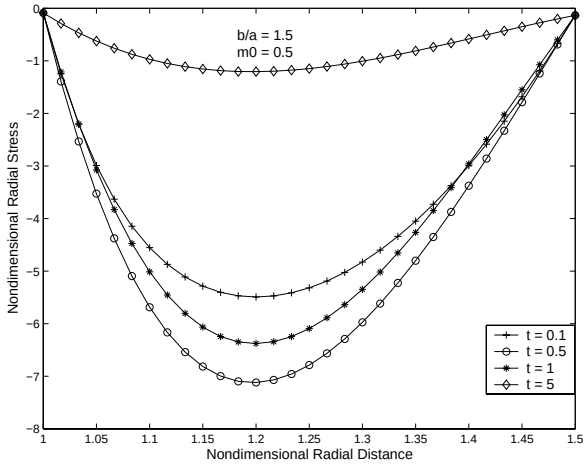

Figure 10. Nondimensional radial stress distribution across thickness for various *t* (nondimensional time) and m_0 =0.5 , *b/a*=1.5

The Figures (9) and (10) show the plot of radial stress along the radius for two values of *b/a* in m_0 *=0.5* and various values of time $\bar{t}$. The magnitude of the radial stress is increased at first and then these values are decreased and converged to zero (steady state) in all point. The hoop stresses for two values of *b/a* in m_0 *=0.5* and various values of time $\bar{t}$ across the thickness of shell are shown in Figures (11) and (12). The hoop stresses are increased with the time and these values of hoop stresses are converged to zero (steady state). The maximum value of hoop stress which is obtained in inner surface is decreased with the time.

5. Conclusion

In this paper, an analytical solution for transient thermo-mechanical behavior of functionally graded thick hollow cylinder under thermal and mechanical radial loads is presented in plane strain and axisymmetry conditions. The pseudo dynamic condition is assumed in this article.

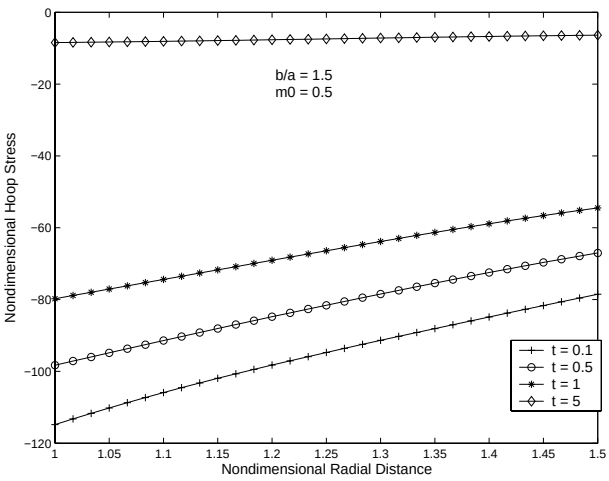

Figure 11. Nondimensional hoop stress distribution across thickness for various *t* (nondimensional time) and m_0 =0.5 , *b/a*=1.5

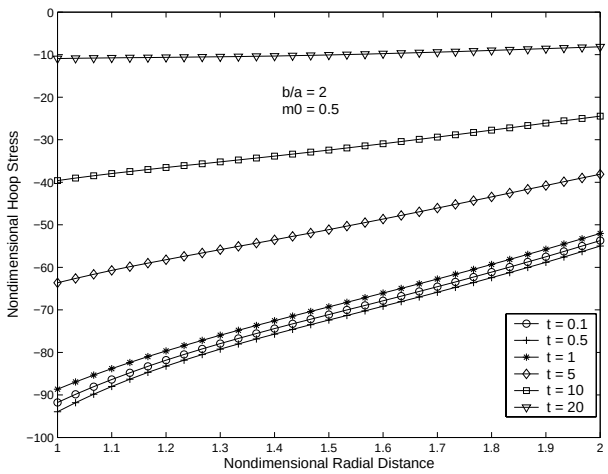

Figure 12. Nondimensional hoop stress distribution across thickness for various *t* (nondimensional time) and m_0 =0.5 , *b/a*=2

The material properties through the thickness of cylinder are assumed to be nonlinear with a power law distribution. The results of this procedure can be outlined as:

1. The transient dynamic behavior of radial and hoop thermal stresses in functionally graded thick hollow cylinder are illustrated for various power law exponents in mechanical properties function.
2. The radial and hoop stresses of functionally graded thick hollow cylinder are analytically obtained. The closed form solutions are presented for the radial and hoop stresses for FGM cylinders subjected to thermal and mechanical radial loading.

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Appendix (1):

To determine the differential of the Bessel functions, we can use the following equations a1 and a2:

$$\frac{2n}{x} J_n(x) = J_{n+1}(x) + J_{n-1}(x) \tag{a1}$$

$$\frac{dJ_n(x)}{dx} = \frac{1}{2}[J_{n-1}(x) - J_{n+1}(x)] \tag{a2}$$

The coefficients f_{1i} to f_{6i} can be obtained as follows:

$$f_{1i} = \left(F_0 - \frac{m_1}{2} D_0\right) \bar{r}^{m_4 - \frac{m_1}{2} - 1} . B_{1i} \tag{a3}$$

$$f_{2i} = 0.5 * \gamma_i * D_0 \bar{r}^{m_4 - \frac{m_1}{2}} . B_{1i} \tag{a4}$$

$$f_{3i} = -0.5 * \gamma_i * D_0 \bar{r}^{m_4 - \frac{m_1}{2}} . B_{1i} \tag{a5}$$

$$f_{4i} = \left(F_0 - \frac{m_1}{2} D_0\right) \bar{r}^{m_4 - \frac{m_1}{2} - 1} . B_{2i} \tag{a6}$$

$$f_{5i} = 0.5 * \gamma_i * D_0 \bar{r}^{m_4 - \frac{m_1}{2}} . B_{2i} \tag{a7}$$

$$f_{6i} = -0.5 * \gamma_i * D_0 \bar{r}^{m_4 - \frac{m_1}{2}} . B_{2i} \tag{a8}$$

And the components of matrix [a] are:

$$a_{44} = a_{11} = -A_0 \gamma_i^2 + C_0 \bar{r}^{-2} \tag{a9}$$

$$a_{45} = a_{12} = B_0 \gamma_i \bar{r}^{-1} - A_0 (n+1) \gamma_i \bar{r}^{-1} \tag{a10}$$

$$a_{46} = a_{13} = -B_0 \gamma_i \bar{r}^{-1} - A_0 (n-1) \gamma_i \bar{r}^{-1} \tag{a11}$$

$$a_{54} = a_{21} = A_0 \gamma_i \bar{r}^{-1} (0.5)(n+1) - 0.5 * B_0 \gamma_i \bar{r}^{-1} \tag{a12}$$

$$a_{55} = a_{22} = A_0 \bar{r}^{-2} (n+1)^2 + A_0 \bar{r}^{-2} (n+1) - B_0 \bar{r}^{-1} (n+1) + C_0 \bar{r}^{-2} - 0.5 A_0 \gamma_i^2 \tag{a13}$$

$$a_{56} = a_{23} = A_0 \gamma_i^2 (0.5) \tag{a14}$$

$$a_{64} = a_{31} = A_0 \gamma_i \bar{r}^{-1} (0.5)(n-1) + 0.5 * B_0 \gamma_i \bar{r}^{-1} \tag{a15}$$

$$a_{65} = a_{32} = A_0 \gamma_i^2 (0.5) \tag{a16}$$

$$a_{66} = a_{33} = A_0 \bar{r}^{-2} (n-1)^2 - A_0 \bar{r}^{-2} (n-1) + B_0 \bar{r}^{-1} (n-1) + C_0 \bar{r}^{-2} - 0.5 A_0 \gamma_i^2 \tag{a17}$$