On Validating Finite Element Results From Commercial Software By Applying Tests Of Reasonableness

by
Lawrence Agbezuge,
Visiting Associate Professor,
Rochester Institute of Technology, Rochester, NY

Abstract

The main reason for presenting this paper is to emphasize the principle that engineers should not blindly use commercial software to solve industrial problems unless (a) the physics of the problem is understood, and (b) tests of reasonableness are utilized when interpreting results from the software. This principle is demonstrated in teaching the use of ANSYS® (a commercial Finite Element package) for solving an engineering problem.

The basic concepts taught in an applied Finite Element Analysis course were utilized to solve a transient heat transfer problem in a cylindrical duct whose thermal conductivity is temperature dependent. The problem was given to graduate students to be solved with commercial software (licensed for academic research) as a project for the final examination. A significant number of the students were engineers working for a company in the Rochester area.

The students were expected to satisfy four primary goals in solving the assigned problem. The goals were (1) to examine the governing equation in order to understand the nonlinear nature of the boundary value problem, (2) to correctly define the mixed boundary conditions for the problem, (3) to select two appropriate time steps in the numerical solution of the nonlinear problem, (4) to utilize finite difference solution of a linearized version of the problem as a test of reasonableness. Analysis of thermal stresses in the cylindrical duct, though not required for this project, was discussed with the students as an important aspect of analyzing thermal gradients and stresses in pressure vessels.

Solution of the allied tractable problem provided a feel for "orders of magnitude" and trends obtained from commercial software. In order to solve the linearized problem and to use the commercial software correctly, it was necessary that the physics and numerical methods utilized by the commercial software be understood.

1. **Introduction**

The subject of this paper is the solution of a nonlinear boundary value problem that involves thermally induced stress gradients in a cylindrical duct. The temperature dependent thermal conductivity of the duct introduces nonlinearity in the governing equation that is not readily apparent. The students were assigned this problem so that they could uncover the hidden details of the problem so that the solution of the problem with commercial software should address the nonlinearity of the problem. In order to have confidence in the results obtained from commercial software, the students were required to solve a linearized version of the problem numerically by using the finite difference method. Results from the two analyses should be compared in order to establish orders of magnitude and a "test of reasonableness". The solution of an allied problem[4] was provided to the students to help them with the assigned project.

Developments of many subsystems that comprise a complex engineering system involve the numerical solution of boundary value problems. Many commercially available finite element analysis programs such as Ansys® are available to the engineer for solving many classes of boundary value problems. In order to effectively use these commercial programs, the engineering curriculum at many accredited engineering schools train the engineer in the use of at least one commercially available finite element analysis package.

One important part of the training should enable the engineer to classify the governing equation as parabolic, elliptic or hyperbolic[1] so that the expected nature of the solution will be known. For example, parabolic partial differential equations involve the first order time derivative, while hyperbolic equations involve the second order time derivative.

Another important part of the training should enable the engineer to correctly define mathematically, the boundary conditions for the problem as of the Dirichlet, Neumann or Mixed type[2,3]. Unless the boundary conditions are correctly defined, the solution obtained will not apply to the problem that is solved.

Yet another important part of the training that is often overlooked in an academic environment is a test of reasonableness or validation of the solution obtained from commercially available software. A test of reasonableness could involve experimental data acquisition, which is time consuming and costly. An alternate test of reasonableness is to obtain the solution of a similar but simplified problem. Results from the simplified problem should provide trends and order of magnitude of results that should compare favorably with results obtained from commercially available software.

2. Problem Description

A long cylindrical duct (figure 1) is initially at temperature 300 K. Assume that at time *t=0*, the inner radius of the pipe is subjected to a temperature of $800^0 K$, and maintained at this temperature thereafter. On the outer radius of the pipe, the bottom half is insulated. The upper half is cooled by convection, with heat transfer (film) coefficient of $h=15\ W/(m^2\text{-}K)$. Ambient temperature is $300^0 K$. Thermal and structural properties of the duct are given in table 1.

Because thermal gradients along the length of the duct are small compared with radial thermal gradients, the problem will be solved as a plane thermal problem and as a plane strain problem.

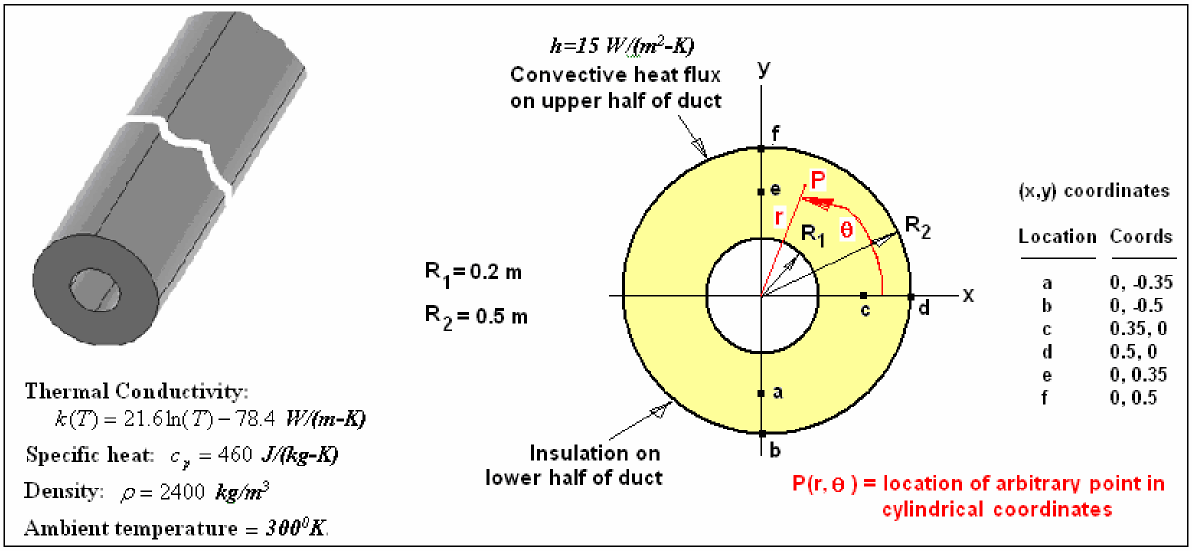

Figure 1

The goals of this project are

1. Obtain the transient solution for the problem by using the academically licensed version of the commercial finite element program Ansys®.
2. Write the governing equations in cylindrical coordinates, and show that because of temperature dependent thermal conductivity of the duct, the governing equation is nonlinear.
3. Obtain the steady state solution for the problem and record the temperatures at the six locations *a,b, …, f* of figure 1. Temperatures at these locations will be compared with those obtained from the solution of a linearized, steady state finite difference formulation of the problem. This comparison will serve as validation or a test of reasonableness.
4. Use the steady state thermal gradients obtained from the FE solution to compute thermal stress distribution in the duct.

Table 1
Thermal Conductivity, $k(T) = 21.6\ln(T) - 78.4$ *W/(m-K),*
where T=temperature in [300,800] K
Specific Heat, $c_p = 950$ *J/(kg-K)*
Density, $\rho = 2400$ *kg/m^3*
Young's Modulus, $E = 150$ *GPa*
Poisson's Ratio, $\nu = 0.25$
Coefficient of thermal expansivity, $\alpha = 20.0e-6\ K^{-1}$

3. Governing Equations and Boundary Conditions

The governing equation is

$$\nabla.(k\nabla T) = \rho c_p \frac{\partial T}{\partial t}, \tag{1}$$

where $k(T) = 21.6\ln(T) - 78.4\ W/(m-K)$; $\rho = 2400\ kg/m^3$; $c_p = 950\ J/(kg-K)$ are thermal conductivity, density and specific heat respectively (see figure 1 and table 1).

Because the problem is considered as a plane problem, variations along the z-axis will be ignored. In cylindrical coordinates, the governing equation is

$$\frac{dk}{dT}\left[\left(\frac{\partial T}{\partial r}\right)^2 + \frac{1}{r^2}\left(\frac{\partial T}{\partial \theta}\right)^2\right] + k(T)\left[\frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 T}{\partial \vartheta^2}\right] = \rho c_p \frac{\partial T}{\partial t} \tag{2}$$

The presence of the terms $\left(\frac{\partial T}{\partial r}\right)^2$ and $\left(\frac{\partial T}{\partial \theta}\right)^2$ makes the governing equation nonlinear. Because the problem is nonlinear, Ansys® needs small time steps for the early part of the solution. Iteratively, the nonlinear product terms are evaluated as a linear approximation until convergence is obtained before another time step is taken.

As an example, at a given time step, the product term $\left[\left(\frac{\partial T}{\partial r}\right)^2\right]^{(k+1)}$ at iteration level (k+1) is approximated as $\left[\left(\frac{\partial T}{\partial r}\right)\right]^{(k+1)}\left[\left(\frac{\partial T}{\partial r}\right)\right]^{(k)}$ because all quantities at the previous iteration level (k) are known. In the early stages of the solution, when gradients are rapidly changing, it is necessary to take small time steps. As the solution approaches steady state conditions, the gradients will be changing very slowly, and large time steps may be taken.

For the solution in Ansys®, the PLANE77 thermal element is selected. Thermal properties for specific heat and density are entered as constants. Thermal conductivity is calculated from the given relationship and entered in tabular form

T (K)	300	400	500	600	700	800
k(T), W/(m-K)	45	51	56	60	63	66

The boundary conditions, for the cylindrical coordinate system (figure 1) are

$$T(R_1,\theta,t) = T_{wall}\text{ , (}T_{wall}\text{=temperature at the inner radius)} \quad (3)$$

$$\frac{\partial T}{\partial r}(R_2,\theta,t) = 0\text{, for } \theta \in [-\pi,0] \quad \text{(insulation)} \quad (4)$$

$$k(T)\frac{\partial T}{\partial r}(R_2,\theta,t) + h[T(R_2,\theta,t) - T_\infty] = 0\text{, for } \theta \in [0,\pi] \quad \text{(convection)} \quad (5)$$

Nodes at (R_2,θ,t) for $\theta = 0$ or $\theta = \pi$ carry two different boundary conditions. They are singular nodes. Typically, one of the two boundary conditions is applied because the boundary conditions are Natural Boundary Conditions. The error incurred by making the approximation is negligible if the meshing is refined. Because of symmetry about the vertical axis, half of the problem, for $\theta \in [-\pi/2,\pi/2]$ could be solved.

4. Finite Element Solution

The transient solution uses two time steps. The first time step of $\Delta t = 0.1$ s is used for the initial portion of the solution where the nonlinear terms are most important. The second time step of $\Delta t = 100$ s is used for the long term solution.
Results for the transient solution (*t=[0, 5000] s*) are shown in figures 2 and 3. Notice that because the bottom half of the duct is insulated, temperatures in the bottom half of the pipe are higher than in the top half. Minimum temperature after 5000s is 753 K, which is reasonably close to the steady state value (obtained in a separate FE solution).
Contour plot for steady state temperature distribution is shown in figure 4. The solution was saved to be used in subsequent thermal stress analysis.
The thermal solution was saved into a database file, and the element type was switched from the 8-node 2-dimensional thermal PLANE77 element[5] into its equivalent 8-node structural PLANE82 element[6] with the plane strain solution[7] option. All thermal loads were removed and the outer diameter of the cylindrical duct was fixed in all degrees of freedom.
The steady state structural solution yields Maximum Von Mises stress and strain of 3.90 Gpa and 0.03 respectively. The maximum stress and strain occur at the lowest point of the inner diameter of the duct ($r = R_1$, $\theta = -\pi/2$).

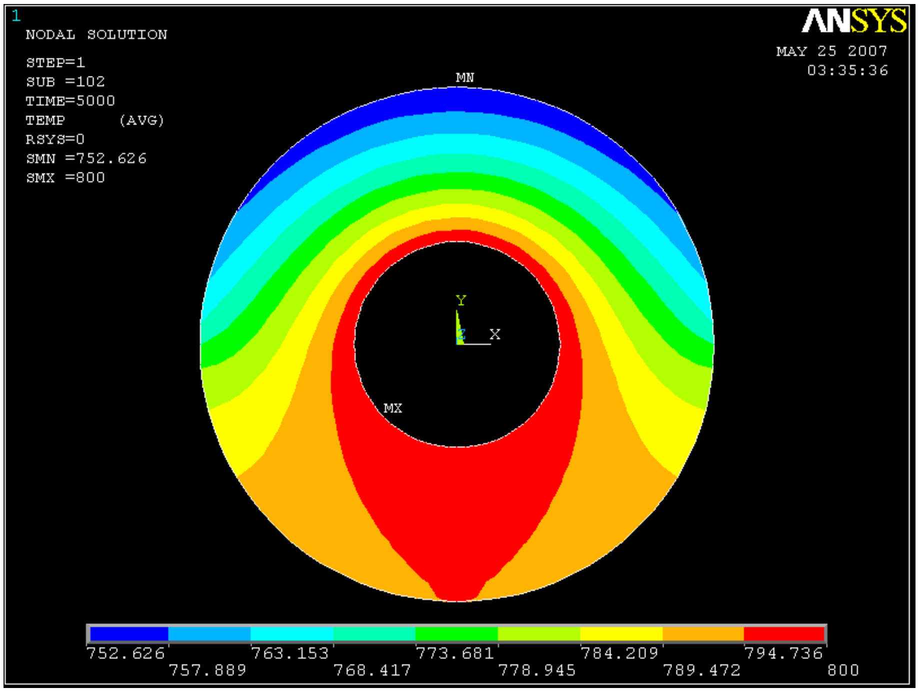

Figure 2: Contour plot for T(r,θ,t) after 5000 s

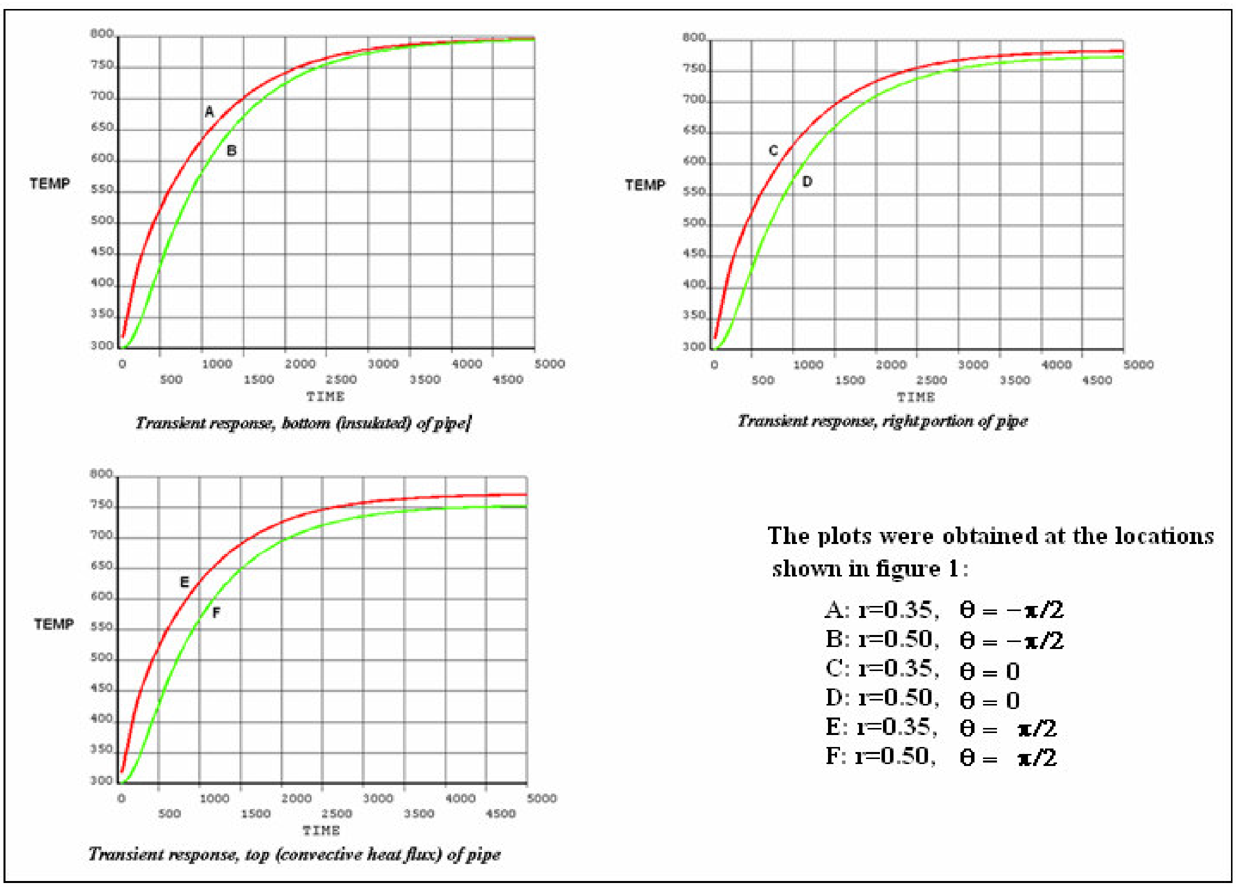

Figure 3: Transient thermal response at selected locations

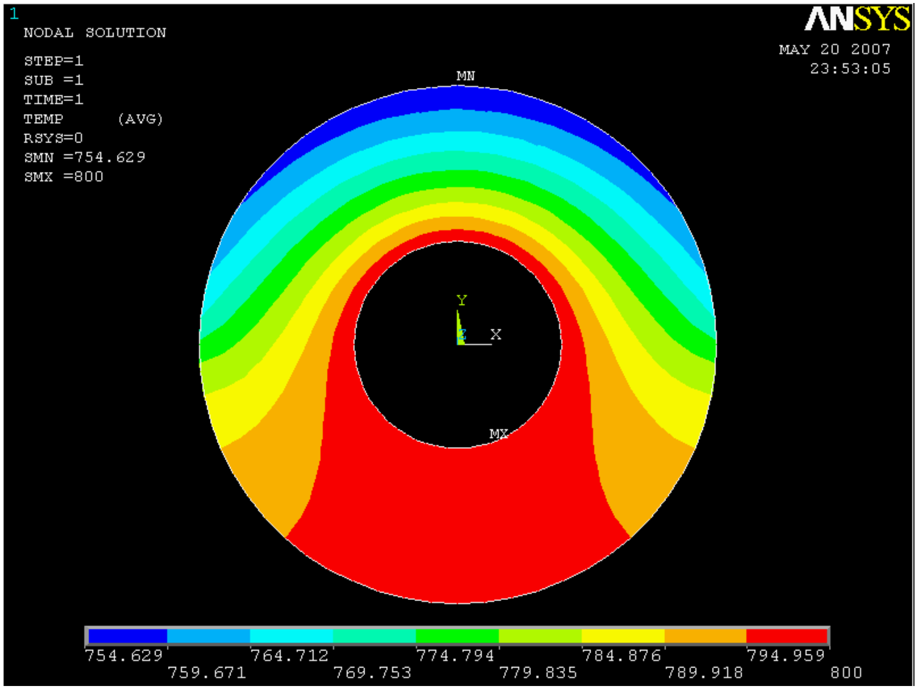

Figure 4: Contour plot for steady state temperature distribution

5. Finite Difference Solution

As a test of reasonableness, another method of solution for the problem was pursued. Experimental verification was not a desirable option because the resources that will be required will be expensive, and an exact mathematical solution was not pursued because of time constraints. A finite difference solution was the most reasonable option.

The governing equation for solving the steady state problem is

$$\frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 T}{\partial \theta^2} = 0, \text{ in the domain } \Omega \qquad (6)$$

where $\Omega \Rightarrow (r = [R_1, R_2]; \theta = [0, \pi]$, because symmetry about the plane *y-y* is used to solve half of the problem as shown in figure 5.

The thermal conductivity, considered as a constant value, is obtained as the integrated average value

$$\bar{k} = \frac{1}{(T_2 - T_1)}\int_{T_1}^{T_2} [-78.4 + 21.6\ln(T)]dT = 57.1 \qquad (7)$$

The boundary conditions are as follows:

Because the lower half of the duct is insulated at the outer radius

$$\frac{\partial T}{\partial r} = 0,\ r = R_2,\ \theta = [-\pi/2, 0] \qquad (8a)$$

Because the upper half of the duct is subjected to convective heat flux at the outer radius

$$\bar{k}\left[\frac{\partial T}{\partial r}\right]_{r=R_2} + h[T(R_2,0) - T_\infty] = 0 \qquad (8b)$$

h =heat transfer (film) coefficient and T_∞ =ambient (bulk) temperature.
Because a wall temperature, T_w, is specified on the inner radius of the duct

$$T(R_1,\theta) = T_w = 800^0 K \qquad (8c)$$

Because of symmetry

$$\frac{\partial T}{\partial \theta} = 0,\ r \in [R_1, R_2],\ \theta = [-\pi/2, \pi/2] \qquad (8d)$$

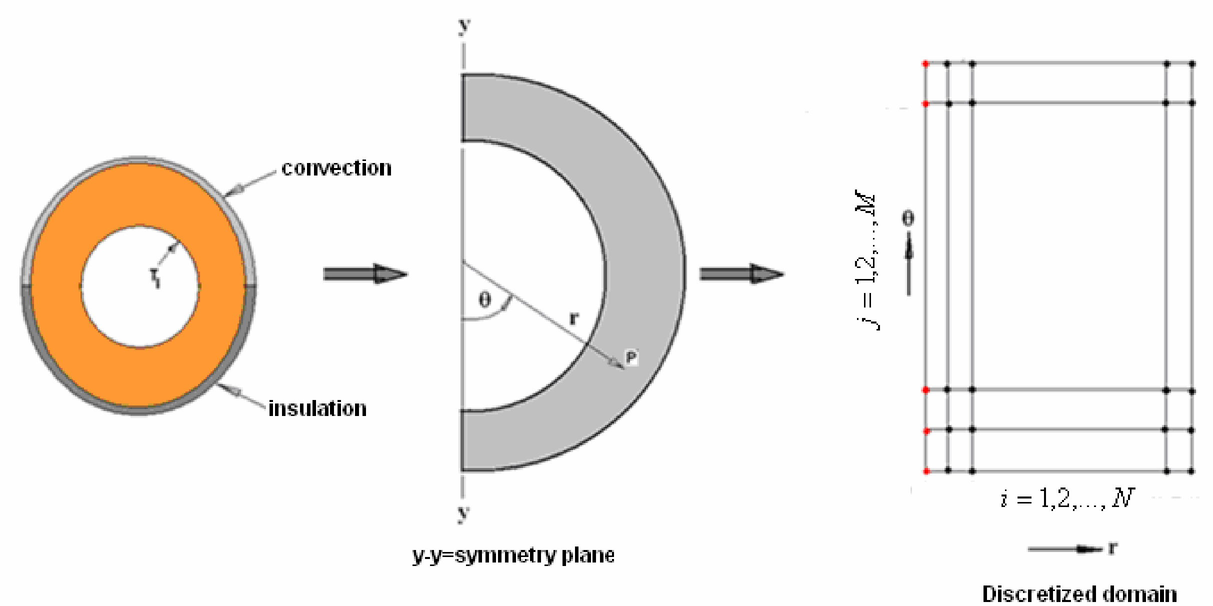

Figure 5: Discretization scheme

The problem is discretized in the (r,θ) coordinate system as

$$\frac{1}{r_i}\frac{[T_{i+1,j} - T_{i-1,j}]}{2\Delta r} + \frac{[T_{i+1,j} + T_{i-1,j} - 2T_{i,j}]}{(\Delta r)^2} + \frac{1}{r_i^2}\frac{[T_{i,j+1} + T_{i,j-1} - 2T_{i,j}]}{(\Delta\theta)^2} = 0$$

or $\alpha_i[T_{i+1,j} - T_{i-1,j}] + T_{i+1,j} + T_{i-1,j} - 2(1+\beta_i)T_{i,j} + \beta_i[T_{i,j+1} + T_{i,j-1}] = 0$ (9)

where $r_i = R_1 + (i-1)\Delta r$, $i = 1,2,...,N$

$\theta_j = -\pi/2 + (j-1)\Delta\theta$, $j = 1,2,...,M$

$\Delta r = (R_2 - R_1)/N$, $\Delta\theta = \pi/M$

N, M are the number of divisions in r and θ respectively.

In discretized form, the boundary conditions are

$$T_{N+1,j} = T_{N-1,j},\ j = 1,2,....,\frac{M}{2} \ \text{(insulation)} \qquad (10a)$$

$$T_{N+1,j} = T_{N-1,j} + \frac{2h\Delta r}{\bar{k}}[T_\infty - T_{N,j}],\ j = \frac{M}{2}+1,2,...,M \ \text{(convection)} \qquad (10b)$$

$$T_{1,j} = T_w,\quad j = 1,2,...,M \ \text{(wall temperature)} \qquad (10c)$$

$$T_{N+1,j} = T_{N-1,j} \text{ and } T_{i,0} = T_{i,2}\,,\; i = 1,2,...,N\,,\; j = 1,M \quad \text{(symmetry)} \qquad (10d)$$

The numerical solution was implemented in Matlab®. Results are given in the next section.

6. Results and Discussion

Most of the students did a reasonably good job at meeting the goals of the assigned project.

The majority of the students had little difficulty in obtaining the transient solution for the problem by using the academically licensed version of the commercial finite element program Ansys®. The reason was that many lab sessions and tutorials had provided the students with the skills necessary for performing the finite element analysis.

However, many students had difficulty writing the governing equations in cylindrical coordinates, and showing that because of temperature dependent thermal conductivity of the duct, the governing equation is nonlinear. Perhaps better preparation in engineering mathematics and heat transfer should be a prerequisite for this course.

Many students could not formulate the finite difference form of the governing equations. The instructor had to provide much help to many of the students. The students who did not have much difficulty had taken courses in advanced engineering mathematics, heat transfer and CFD (Computational Fluid Dynamics).

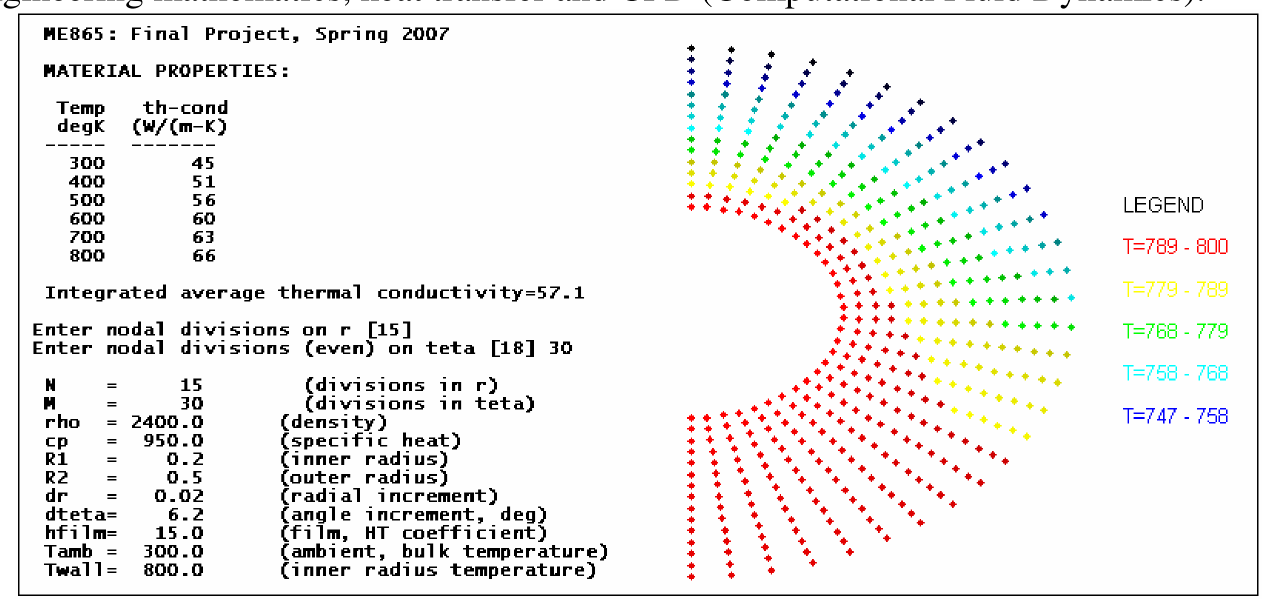

Figure 6: Solution from Matlab® code

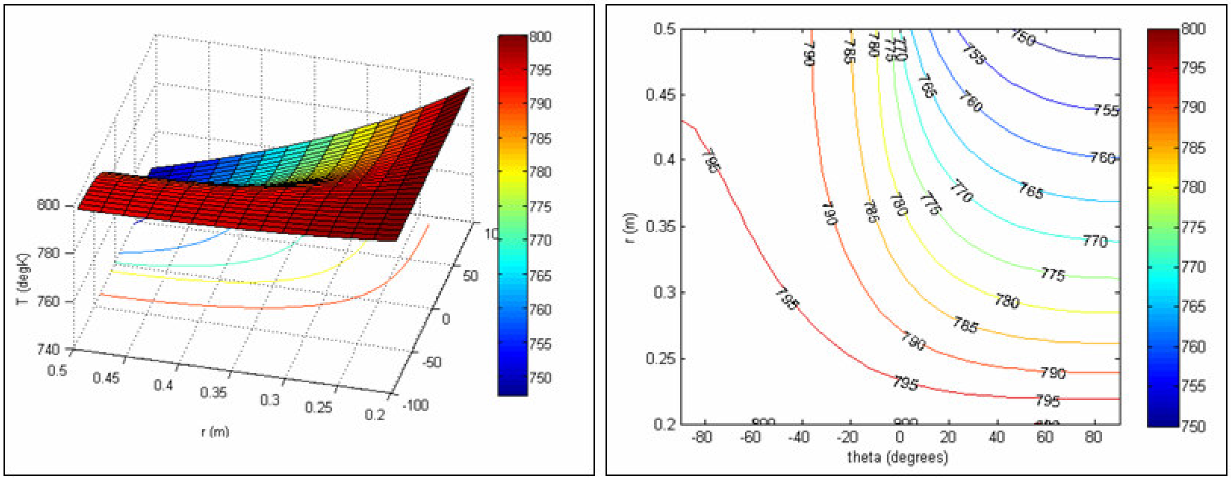

Figure 7: Contour plots from Matlab® code

Location	ANSYS(R) Solution	FD Solution	%Relative Error
A	798	795	0.4
B	797	794	0.4
C	785	782	0.4
D	776	774	0.3
E	777	771	0.8
F	755	747	1.1

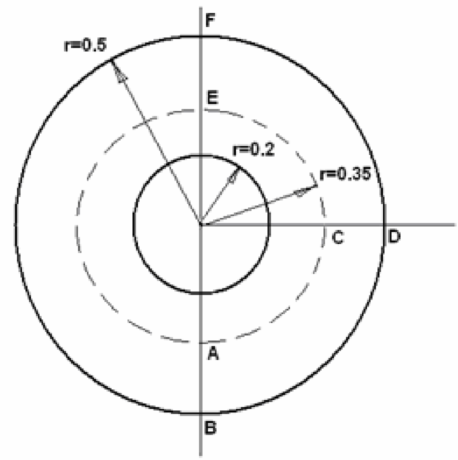

Fig 8: Comparison of FE and FD solutions

Most of the students needed help in writing the code in Matlab®. Similar code from an allied problem[4] was provided to the students to guide them in writing the Matlab® code. Furthermore, the instructor was available to consult with the students and to help them debug computer code. About 80 percent of the students had taken a course in Numerical Methods with the instructor and had been trained to write Matlab® code, therefore the coding aspect of the project was a reasonable assignment.

7. Conclusions

The results from the finite difference solution are shown in figures 6-8.
The agreement between the finite element and finite difference results is much better than was expected. Because the problem was linearized for the finite difference solution, significant differences were expected between the two solutions. The probable reason for the good agreement is that nonlinear effects

diminish as the solution approaches steady state, as was demonstrated in figures 2 and 4 of the finite element solutions. On the other hand, nonlinear effects are very significant at the beginning stages of the solution. In the solution of the transient problem, Ansys® required small time steps and performed several iterations in the early stages of solving the problem.

As a practical problem, the skills acquired from the solution of the assigned problem could be utilized in the design and analysis of pressure vessels, pipes for transporting liquids, or the design of molds for curing thermoplastic or thermoset resins.

This project is a worthwhile project for senior undergraduate and graduate students who on graduation, may be expected to provide finite element solutions to many types of engineering problems in research and development.

The students understood from this project that

- It is necessary to understand the physics and the fundamentals behind governing equations that define a boundary value problem, and the assumptions made in deriving the governing equations,
- It is necessary that boundary and initial conditions be correctly defined for boundary value problems,
- It is necessary to have reasonable knowledge about equations that are solved by a commercial finite element software package in order to input correct data into the software.
- It is necessary to validate finite element solutions obtained from commercial software by applying tests of reasonableness. The validation could mean solving an allied tractable version of the actual problem in order to have "a feel" for trends and orders of magnitude obtained from commercial software. In some cases, experimental data acquisition may be required.

8. **References**

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(b) search for *PLANE77* in a google or yahoo search box.
[6] Ansys *PLANE82* element: See for example
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8. **Bibliography**

Lawrence Agbezuge is Visiting Associate Professor in the Mechanical Engineering Department of the Rochester Institute of Technology, NY. He worked 5 years in offshore oil drilling simulations for Exxon Production Research Company, Houston, TX. He also worked 24 years in ink jet printing, color imaging and paper science for Xerox Corporation, Webster, NY. He obtained M.S.M.E. (1968) and Eng.Sc.D. (1972) from Columbia University, NY.