



# Computer simulation of a pressure-volume-temperature process

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## Abstract

**Purpose** – The study of pressure-volume-temperature (PVT) process is necessary to understand the physical behaviour of materials. This paper seeks to develop a simulation procedure to predict phase behaviour.

**Design/methodology/approach** – The procedure consisted of the application of a thermo-mechanical nonlinear model that simulated the behavior of the test sample in the PVT apparatus. Software Ansys was used for modeling this case, making a subroutine in APDL language. The real time data of the experimental procedure in PVT apparatus were applied in the computer simulation, that is the real time of application of pressure and heating scaling of the sample were taken into account. A specific case was simulated and its results compared with those obtained from the real experimental test. In order to evaluate phase changes, enthalpy was considered using an approximated expression described in the paper.

**Findings** – Results obtained from the simulation were compared with the resulting isobaric graphics of the experimental test. Results show a good correlation, obtaining in addition stress-strain behavior of the sample. This simulation procedure allows one in a simple way to vary the properties and characteristics of the sample. This makes the computer simulation a useful tool together with the experimental test, in the development of novel materials.

**Research limitations/implications** – Results of the numerical simulation are based on the properties and characteristics of the sample. In this study, real data of the material were used; however, some others had to be assumed based on references on this topic.

**Practical implications** – The coupled field analysis and the subroutine built in an Ansys environment are of a general purpose applicable to many kinds of material without practical limitations but getting a priori the required data and properties needed for running the simulation test.

**Originality/value** – Computer simulation of PVT process is not a common procedure – the experimental study of the material is mainly the procedure used to define the stated equations of a material and for knowing their phase changes. Computer simulation is a procedure that provides other important features of the material that the experimental study cannot produce simultaneously.

**Keywords** Simulation, Finite element analysis, Phase transformations

**Paper type** Technical paper



## Introduction

Pressure-volume-temperature (PVT) studies are necessary to understand the physical behaviour of materials. In fact, they represent a significant part of the thermo-analytic techniques being currently used. Moreover, PVT is the only technique that involves pressure as a variable. In fact, many materials are sensitive to pressure, volume change, dependence of pressure in temperature evolution, as well as to kinetics of phase transition, are significant aspects, not only from a scientific viewpoint, but also in practical applications related to materials engineering. Results from a standard PVT test are directly applicable to equilibrium states studies, including formulation of the state equation and its theoretical modelling.

Data recorded from a PVT experiment are referred to specific volumes of a material as a function of pressure and temperature. PVT registers are presented as operating isotherms or isobars. Materials phase change evaluation is of great interest (Dantzing, 1989). Phase changes are characterized by the enthalpy, given as:

$$\text{Enth}(T) = \int_{T_1}^{T_2} \rho c(T) dT \quad (1)$$

where:  $\rho$  – material density;  $c(T)$  – specific heat;  $T_1, T_2$  – integration temperature limits.

## Simulation of a PVT process

Simulation of this process was done as a coupled thermo-mechanical analysis of a nonlinear type, because there were constitutive parameters given as functions of time, being enthalpy one of them. Thermo-mechanical model are shown below (Cook *et al.*, 1988; Incropera and DeWitt, 1981; Kays and Crawford, 1993; Ansys, 2004):

- *Thermal model*

$$[C]\{\dot{T}\} + [K]\{T\} = \{F(t)\} \quad (2)$$

where:  $T$  – temperature;  $[C]$  – specific heat matrix;  $[K]$  – conductance matrix;  $\{F(t)\}$  – equivalent force vector of temperature.

- *Mechanical model*

$$[S]\{\mathbf{u}\} - \{Fth\} = [Me]\{\ddot{\mathbf{u}}\} + \{Fe\} \quad (3)$$

being:  $\{\mathbf{u}\}$  – displacement vector;  $[S]$  – stiffness matrix;  $\{Fth\}$  – equivalent force vector of temperature;  $[Me]$  – consistent mass matrix;  $\{Fe\}$  – pressure vector on the element.

To couple these fields, we use the Ansys method named sequentially coupled physics analysis. This is an indirect method that can couple the two fields (thermal and mechanical) by applying results from the first analysis (thermal) as loads for the second analysis (mechanical). The loads transfer occurs external to the analysis, the nodal temperatures file are applied as “body force” loads in the subsequent stress analysis.

## Case study. experimental test

A PVT study was performed on a polyethylene terephthalate sample by mean of a commercial apparatus GNOMIX (Gnomix, 1990) of the constrained fluid type at the

Advanced Polymer Laboratory and Optimized Materials (LAPOM) of the University of North Texas, USA (Figure 1). Sample initial data are:

- sample weight  $W_M = 0.06$  gr;
- material specific weight  $P_E = 1.3804$  gr/cm<sup>3</sup>;
- initial temperature (environment temperature) = 18°C; and
- final temperature = 146°C.

Sample was constrained in Hg (Mercury) under a quasi-hydrostatic pressure varying from 0 a 200 MPa. Temperature was increased up to 146°C. Temperature rate increase was 4°C/min. Pressure application time for each isotherm was 10 min, while the unloading lasted 5 min. Obtained experimental results are shown in Figure 2.

**Computer simulation**

Sample initial data under which the computer modelling was done are the same from the experimental test, except that others needed parameters were supposed according some references (Colucci *et al.*, 1997; Courtney, 1990; Gere and Timoshenko, 1986). Thermal conductivity and specific heat of the material are shown in Figures 3 and 4.

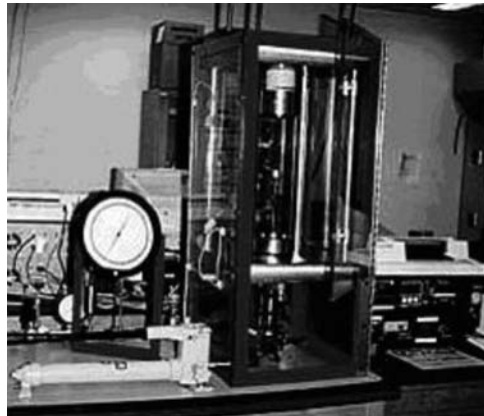
In this study, enthalpy as given in equation (1), was computed numerically. The approximate solution is given by (see Appendix):

$$Enth_{i+1} = Enth_i + \left(\frac{\Delta T}{2}\right) \left(\frac{W}{V_d}\right) \left(\frac{1}{1 + 3\alpha\Delta T}\right) (C(T_i) + C(T_{i+1})) \quad (4)$$

where:  $V_d$  – volume of the deformed sample (step  $i$ );  $W$  – sample weight;  $\alpha$  – coefficient of material volumetric expansion;  $\Delta T$  – temperature step;  $C(T)$  – specific heat (shown in Figure 4).

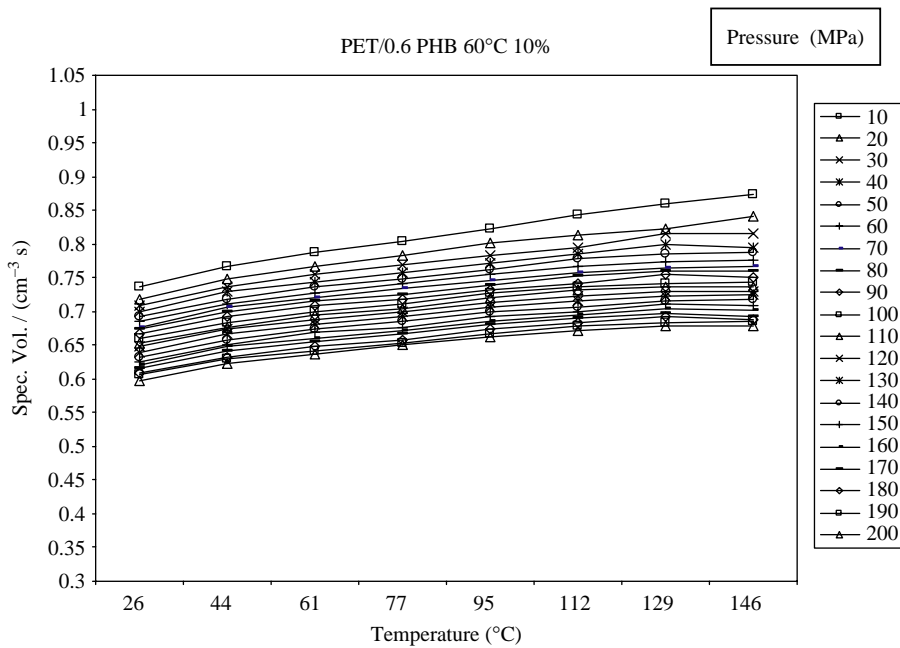
Actually, the elasticity modulus  $E$  and Poisson ratio  $\mu$ , required for structural analysis, both change with temperature. However, for our analysis,  $\mu$  was considered constant while  $E$  varying according to data shown in Figure 5.

Block scheme of the simulation procedure is shown in Figure 6. The aforementioned analysis was applied to a cubic sample of a given initial volume. However, this has no



**Figure 1.**  
Gnomix PVT Apparatus

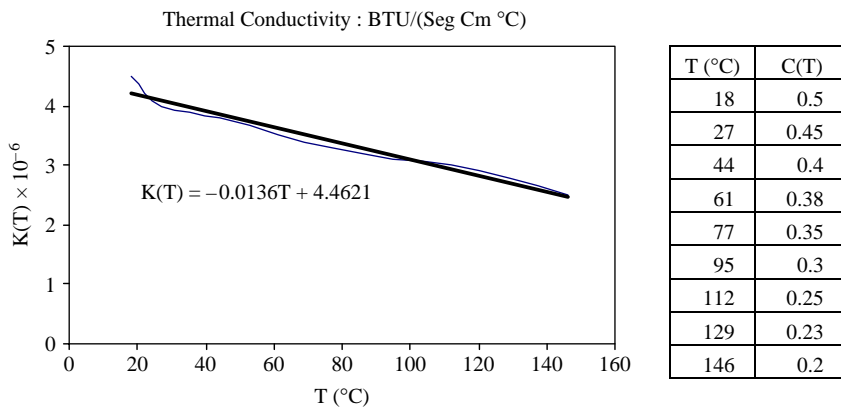
Source: LAPOM, University of North Texas



Pressure-volume-  
temperature  
process

**Figure 2.**  
Experimental PVT results  
of the sample

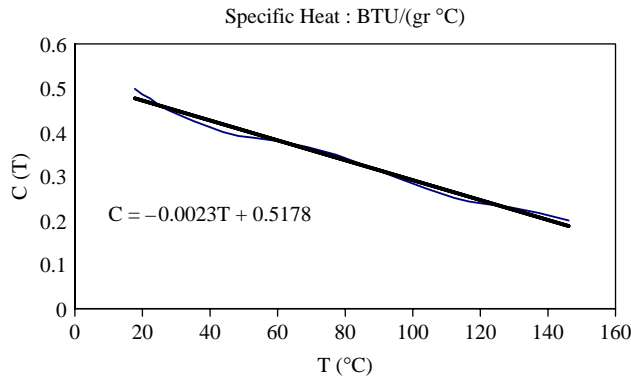
**Note:** Isobars



**Figure 3.**  
Thermal conductivity:  
 $K(T)$

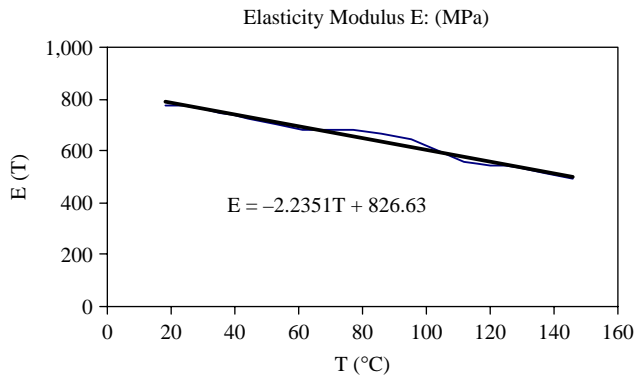
effect on the final results. Indeed, pressure and temperature effects have more influence at points inside the body, being their effect of the hydrostatic type. On the other hand, since the sample was immersed on Hg, boundary conditions were assumed on displacements, in such a way of avoiding body instability. Thus, symmetry planes were applied corresponding to the boundary conditions. It was also assumed that temperature transmitted by the Hg, which in turn is transmitted by the thermal device generates neither distortions, nor produce significant changes on the thermal forces application.

**Figure 4.**  
Specific heat



T (°C)	K(T) ×10 <sup>-6</sup>
18	4.5
27	4
44	3.8
61	3.5
77	3.3
95	3.1
112	3
129	2.8
146	2.5

**Figure 5.**  
Elasticity modulus of the sample as a temperature function



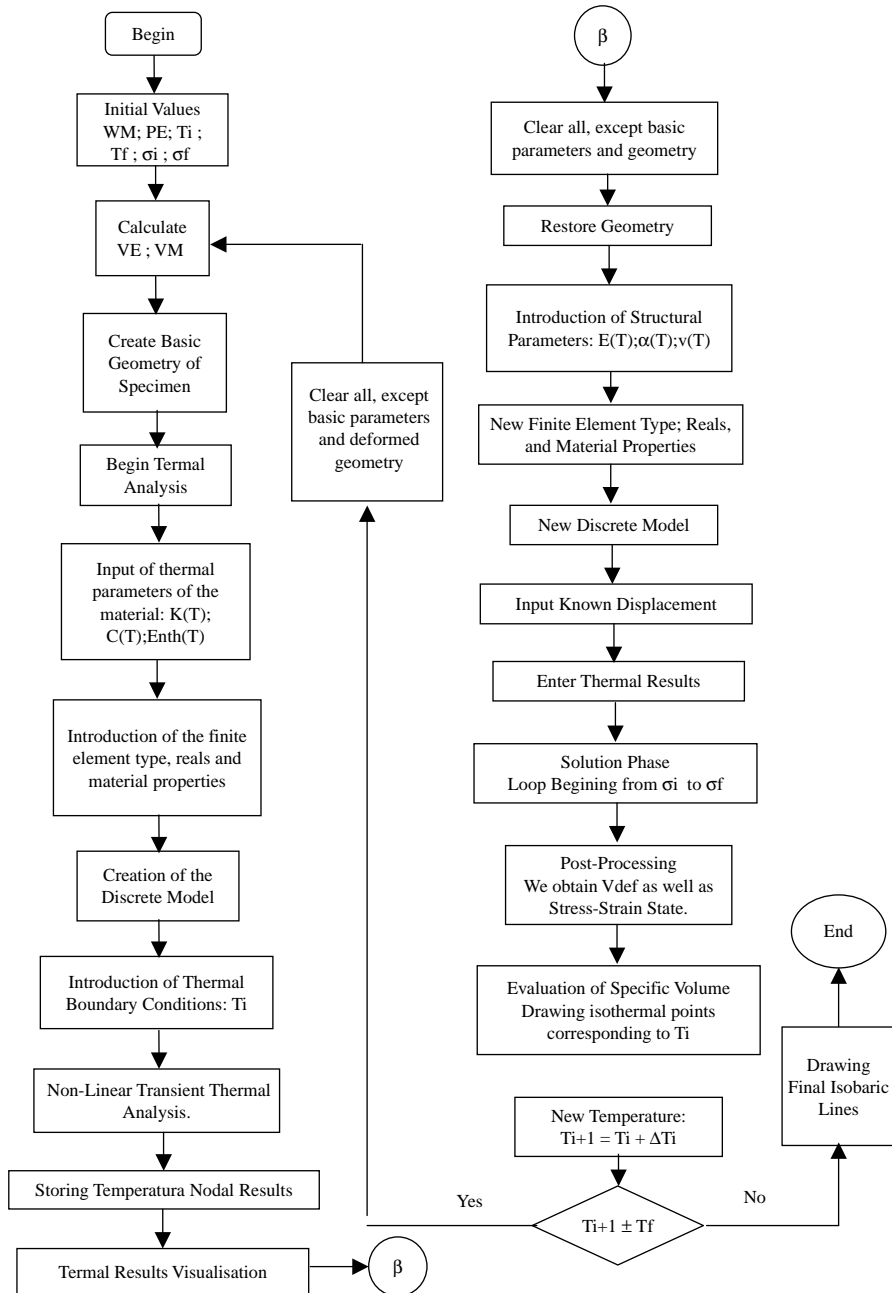
18	774.6
27	767
44	722.9
61	684
77	678
95	645.2
112	558
129	534.5
146	490.8

**Results and discussion**

Computer simulations results are shown in graphical fashion. Figure 7 corresponds to a body boundary at 26°C, and after 2.25 min hydrostatic pressure is applied (a central cut of the cube, corresponding to the body temperature distribution is shown here). Hydrostatic type pressure distribution is also shown in Figure 8.

Pressure on the sample was monotonically increased up to 200 MPa. During this loading process, temperature tends to be distributed symmetrically inside the sample. The body temperature at 7.75 min is shown in Figure 9, whereas the corresponding one at 12.25 min is shown in Figure 10. At this time, pressure was released and unloading started. During the unloading process, inside temperature continued to be distributed symmetrically. Thus, when the pressure unloading ended at 17.25 min, one had the final temperature distribution as shown in Figure 11. To this point, one stage of the PVT simulation process ended. Then, temperature was increased to 44°C and the cycle repeated. For the case in study, the maximum temperature reached was 146°C. Volume variations were recorded at different time for constructing the final plot of isobars.

A sample deformed configuration for a pressure of 200 MPa and 27°C is shown in Figure 12. The computer simulation of the PVT process allows a visualization

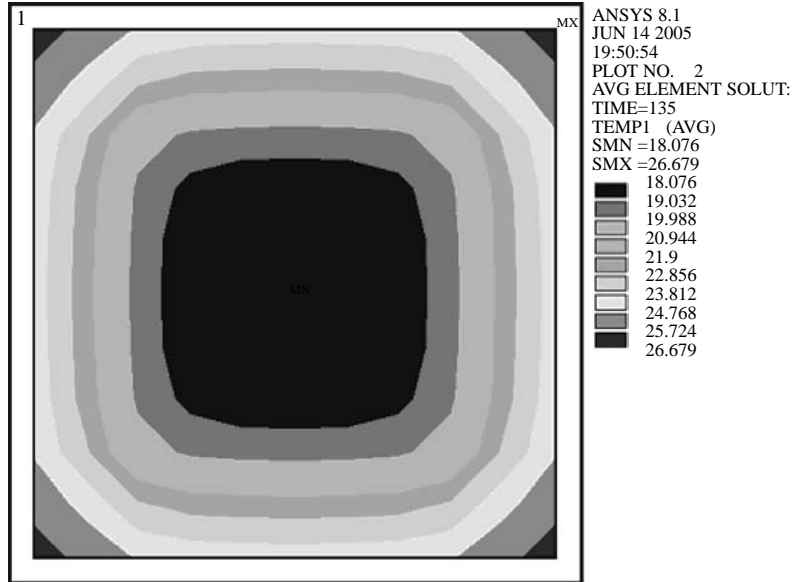


**Notes:** Here, WM is the weight of the sample; PE is the specific weight of the sample;  $T_i$  and  $T_f$  are the initial and ending temperature values;  $\sigma_i$  and  $\sigma_f$  are the hydrostatic pressure initial and ending on the sample; VE is the specific volume of the sample; VM is the volume of the sample

**Figure 6.**  
Block scheme of the  
thermo structural analysis  
of a PVT process

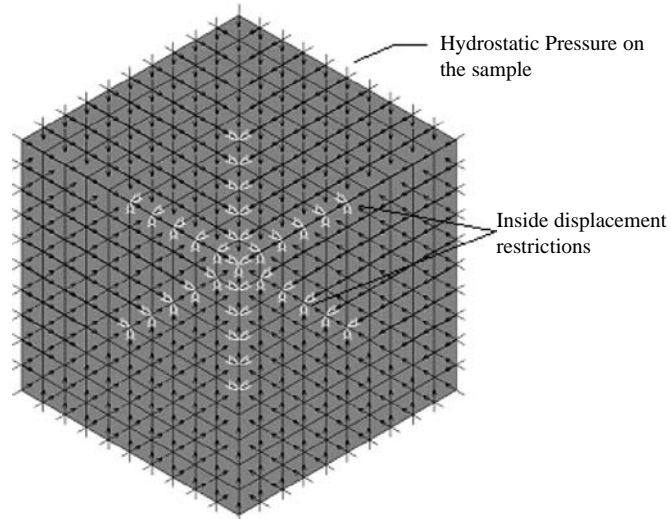
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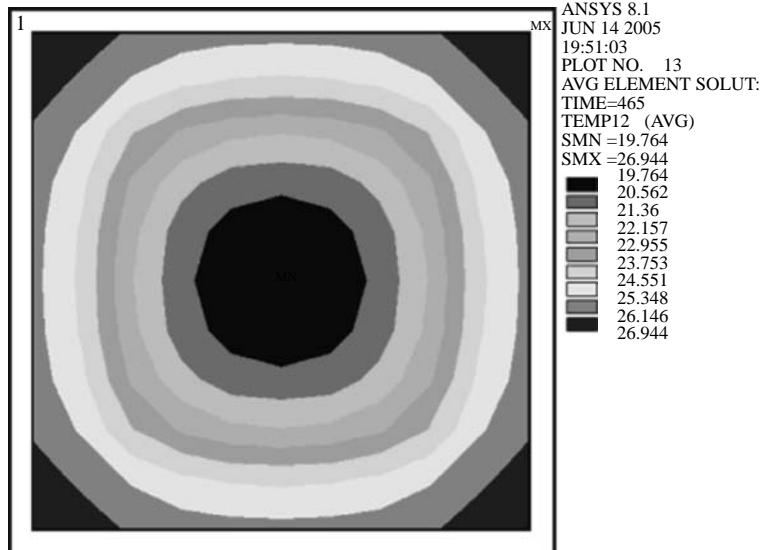
**Figure 7.**  
Temperature distribution  
inside the sample at  
2.25 min

**Note:** At this time begin the application of loads

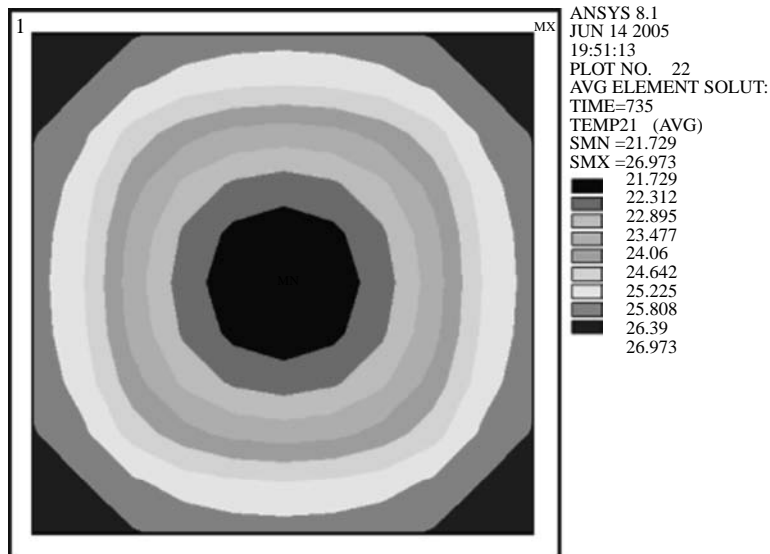


**Figure 8.**  
Hydrostatic pressure on  
the sample

of stresses and deformations at any instant. For this pressure (200 MPa), are shown for example in Figure 13 the Von-Mises stresses. After repeating the loading process and temperatures, the final plot of isobars was obtained and is shown in Figure 14.



**Figure 9.**  
Temperature distribution  
inside the sample  
at 7.75 min



**Figure 10.**  
Temperature inside the  
sample at 12.25 min

**Note:** Begin the unload phase

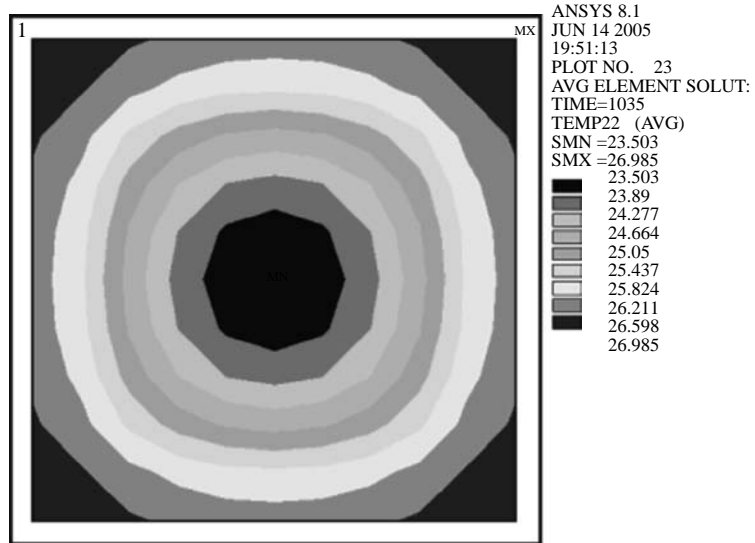
### Conclusions

The above-mentioned modelling process allows the simulation of a PVT process of a sample. Moreover, it also allows obtaining material phase changes if needed. The approach followed can be described as a nonlinear, dynamic thermo-structural coupled analysis.



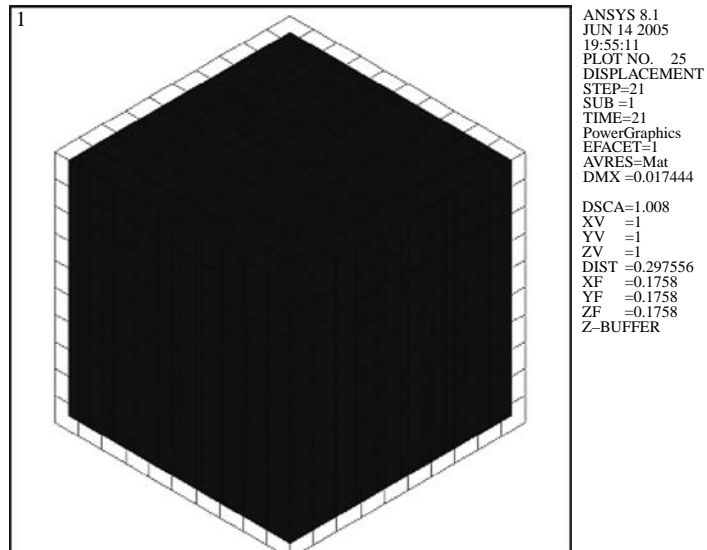
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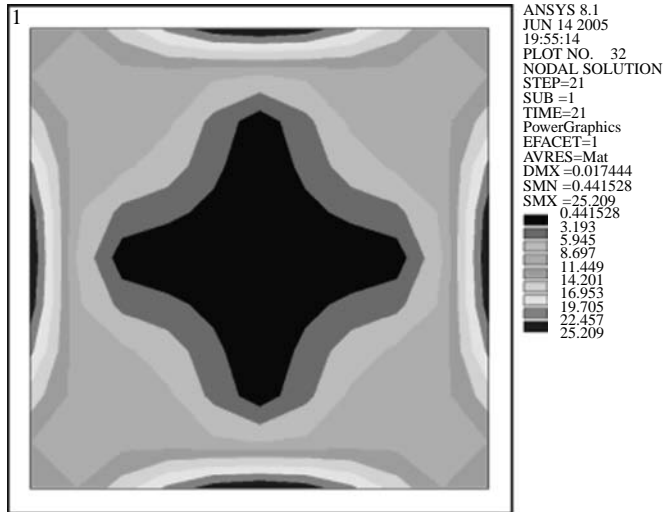
**Figure 11.**  
Temperature inside the  
sample at 17.25 min

**Notes:** Finish the unload phase. Temperature will increase now to 44°C

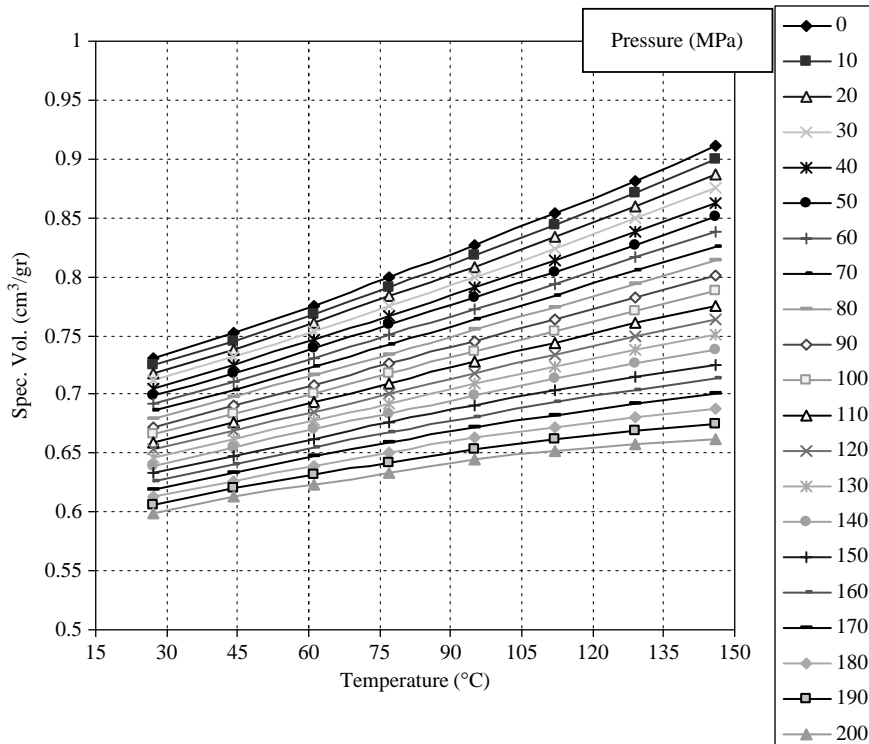


**Figure 12.**  
Deformed sample for  
a pressure 200 MPa

Thermal analysis is of the nonlinear type because involves constitutive parameters given as functions of time. One of them, enthalpy, allows to determine any possible change of phase. Thermal problem has the feature of being a time evolution problem. For this, cycle analysis was performed for a time step previously defined.



**Figure 13.**  
Von-Mises Stress on the  
sample for a pressure  
200 MPa



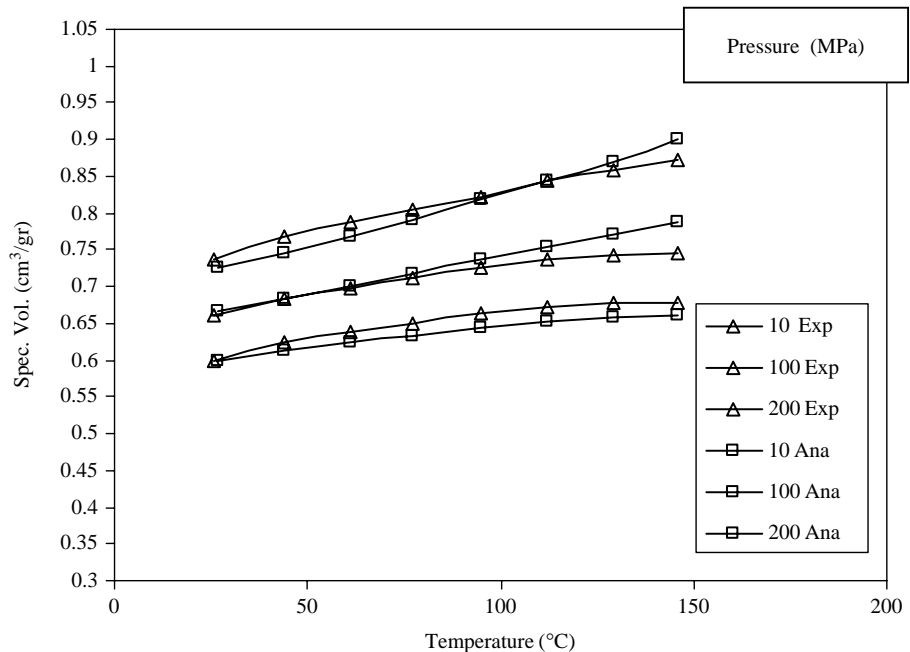
**Figure 14.**  
Obtained computer  
modeling PVT Isobars

The structural problem, in turn, associates also nonlinear constitutive parameters such as elasticity modulus, specific heat, and thermal conductivity.

The integral analysis of the sample was done through the coupling of two fields. For this, the thermal analysis was run first, and then its output entered to the structural analysis. One of the relevant aspects of this type of analysis is the rich information of the material, since one can observe its time behaviour either as temperature, inside stresses, deformations, and so forth. Clearly, these are aspects hardly being available if one makes it experimentally. The disadvantage of the present analysis, of course, is that, for its construction required constitutive parameters for material characterization and the body behaviour are thus dependent on them.

For the case study presented, it can be observed the great closeness of results obtained from both, namely, computer simulation and experimentally. Thus, one can highlight the utmost importance of this type of studies, which enrich information on basic aspects of a material. Furthermore, starting from the PVT isobars plots and using statistical procedures of multiple regression (Montgomery *et al.*, 2002) one can construct the material state equation, such as Hartman's equations (Hartmann and Haque, 1985).

To appreciate the obtained agreement between analytical and experimental results, we draw Figure 15. Here, we show only three representatives isobars, namely at 10, 100 and 200 MPa hydrostatic pressure. Difference between each pair is minimal.



**Figure 15.**  
Comparative PVT Isobars

**Note:** Experimental vs Analytical results

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## Appendix

Enthalpy is given by equation (1), here reproduced:

$$\text{Enth}(T) = \int_{T_1}^{T_2} \rho C(T) dT$$

where  $\rho = W/V_{\text{def}}$ . Also,  $V_{\text{def}} = V_1 + V_1 \theta$ . Here,  $W$  is the sample weight, and  $V_{\text{def}}$  is the deformed sample volume at Temperature  $T_2$  measured with respect to sample volume at  $T_1$ . Parameter  $\theta$  according (Gere and Timoshenko, 1986) refers the sum of deformations:

$$\theta = \varepsilon_x + \varepsilon_y + \varepsilon_z$$

External temperature on a thermal homogeneous material generates equal temperature deformation  $\varepsilon_i$  in all three principal directions, so we write  $\theta = 3 \varepsilon_i$ . Also temperature deformation,  $\varepsilon_i = \alpha \Delta T$ . Introducing in equation (1) before mentioned relationships, we arrive to the following expression:

$$\text{Enth} = \int_{T_1}^{T_2} \left( \frac{W}{V_{\text{def}}} \right) \left( \frac{C(T)}{1 + 3\alpha\Delta T} \right) dT$$

Inside this expression,  $\Delta T = T_2 - T_1$  is the temperature step.  $C(T)$  is the specific Heat of the material, and  $\alpha$  is the coefficient of volumetric expansion of the material. According to the proposed procedure (Figure 5)  $V_{\text{def}}$  is obtained each step temperature, then knowing this parameter, and using trapezium's rule integration we arrive to proposed approximate equation (4):

$$\text{Enth}_{i+1} = \text{Enth}_i + \left( \frac{\Delta T}{2} \right) \left( \frac{W}{V_d} \right) \left( \frac{1}{1 + 3\alpha\Delta T} \right) (C(T_i) + C(T_{i+1}))$$

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