DEVELOPMENT OF AN INTERACTIVE COMPUTATIONAL TOOL FOR TRANSPORT PHENOMENA EDUCATION IN THE FOOD ENGINEERING UNDERGRADUATE PROGRAM AT FZEA-USP

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Abstract. *By means of its Undergraduate Pro-Rector, the University of São Paulo (USP) has put forward the so-called "Education with Research" plan in order to support research projects dedicated to education challenges in USP's undergraduate programs and courses. Accordingly, the present project has proposed the development of an interactive computational tool (i.e., an academic simulator) to assist and complement Transport Phenomena education in the Food Engineering undergraduate program offered at the Faculty of Animal Science and Food Engineering (FZEA-USP). As a pilot approach, heat transfer was first chosen since such transport phenomenon is inherent to any thermal processing of foodstuff. In view of that, a graphical user interface was elaborated in Visual Basic for the proposed simulator while numerical solution of the governing differential equation was implemented in a computational code written in FORTRAN based on the subroutine MOLCH ("method of lines with cubic Hermite polynomials") from IMSL (International Mathematical and Statistical Library). Conceived as Windows © compatible and to be employed by undergraduate students beginning their studies in heat transfer, such software is intended to be simple and friendly.*

Keywords: *engineering education, transport phenomena, heat transfer, numerical simulation.*

1. INTRODUCTION

1.1. Transport Phenomena education: some challenges

By means of resolution CNE/CES 11/2002 (Brazil, 2002), since 2002 Brazil's High Education Committee via its National Education Council has included Transport Phenomena among basic courses in all Engineering undergraduate programs. This is justified as Engineers are very much likely to deal with fluid flow, energy conversion, and/or species (mass) transfer (Brunello, 1978). Despite transfer processes occur simultaneously, they are separately presented for the sake of understanding, formulation and solution, for that reason being grouped into distinct courses on transport of momentum, energy and mass. Such rationale is adopted by the Food Engineering undergraduate program offered at the Faculty of Animal Science and Food Engineering, University of São Paulo (FZEA-USP) so that ZEA0563 (Transport Phenomena I), ZEA0662 (Transport Phenomena II) and ZEA0764 (Transport Phenomena III) are courses scheduled to be offered at the 5th, 6th and 7th semesters of the program.

Transport phenomena modeling leads to relatively complex equations whose solution usually evokes simplifying assumptions and/or regular geometries, which tends to push problems away from reality. A discussion on the fact that, for example, Fluid Mechanics is a science based on several considerations and hypotheses can be found in Silva *et al.* (2005) and such thoughtful issue should be debated in classrooms so that students do not render themselves to think that practice and theory are wide ways apart and, hence, correction factors (coefficients) should be always introduced to bring (ideal) solutions back to real world. According to Gad-El-Hak (1997), the ability to properly introduce and use simplifying assumptions requires a scientific maturity not usually developed in typical undergraduate students and, as a result, didactic challenges arise regarding the familiarity to the interplay between physical phenomena and calculus.

Efforts to help developing the aforesaid ability are welcome and students' ability to deal with model frameworks is an aspect to be studied. Besides conservation principles, transport phenomena modeling evokes additional constitutive equations when the number of unknowns exceeds that of governing equations. Although relying on simplifications, integral modeling of conservation principles allow one to accurately solve several problems when one is conveniently interest on overall behavior. However, such approach prevents one from obtaining detailed information about properties that could be vital to optimization whereas point-to-point description is also useful to properly assess mean (average) values used in integral formulations. Relying on differential control volumes, conservation principles are expressed in terms of differential equations whose solution allows one to achieve detailed knowledge of those properties.

1.2. Transport Phenomena education: use of numerical simulation

Initially used for academic purposes, numerical simulation has experienced a notable evolution and has become an important engineering tool. Together with the development of powerful methods, the availability of relatively cheap high-performance computers has induced and spread out the application of numerical modeling to several engineering branches (Maliska, 1995), including Food Engineering (Sablani *et al.*, 2007; Sun, 2007). In principle, one may properly tackle relatively transport phenomena using numerical simulation, evoking as few simplifying assumptions as possible, accounting for effects sometimes relaxed (if not ignored). Such is the case of foodstuff or biotechnological products of interest presenting non-linear and/or anisotropic properties as well as irregular shape (Wang & Sun, 2003).

Relying on comprehensive models, numerical simulation may benefit the food sector with respect to, for instance (but not restricted to), production control, final product quality and process optimization (Romano, 2005). In the food industry, common discretization techniques include finite-difference methods (FDM), finite-element methods (FEM), an finite-volume methods (FVM) (Wang & Sun, 2003) while computational fluid dynamics (CFD) has been largely applied to many processes of interest (Sun, 2007).

By enabling one to solve full Navier-Stokes equations, the remarkable development of CFD may broaden as well as modify Transport Phenomena education at Engineering programs (Gad-El-Hak, 1998) as CFD may help solving and then visualizing velocity (flow), pressure and temperature fields if suitably used with graphical tools (post-processors). From the didactic viewpoint, this becomes interesting since Food Engineers should bear in mind what happens to raw material (in terms of reactions and transformations) when designing a process or equipment.

1.3. Transport Phenomena education: "Education with Research"

Introduced by USP Undergraduate Pro-Rector and aiming at contributing to education understanding, "Education with Research" is a plan supporting research projects related to education challenges concerning USP undergraduate programs. Submitted projects fell into two non-excluding (i.e., potentially complimentary or combined) research lines:

- *Education with research*: aiming at using research along with education, projects within this line were concerned with undergraduate students' knowledge maturity, including research skills and reasoning, so that they become able to permanently incorporate scientific and technological development into professional practice, eventually taking them as research focus.
- *Researching education*: aiming at research activities directly related to education, projects in this line dealt with undergraduate education as practiced at USP, including their multiple possibilities and aspects (e.g.: classrooms, syllabus, education strategies and technologies, professional training, students insertion into the professional market, etc.), besides investigating the professional development of faculty members (affiliated to undergraduate programs) as well as broadening expertise on university education.

Within the context of the first research line above, this project aimed at developing an academic (non-commercial) interactive numerical simulator to assist as well complement Transport Phenomena education in the Food Engineering undergraduate program at FZEA-USP, stimulating and developing students' ability to research, formalize, compare and discuss model frameworks of interest. Although there are several text-books available for Transport Phenomena, it is worth citing that there is very little academic software dedicated to such area, as far as Food Engineering is particularly concerned. Based on the potential for numerical simulation to become a didactic tool (under the "learning by doing" rationale), the idea of this work was to enhance students' capacity to identify conditions at which model frameworks are conceived so that they can be properly used within their scope and limitations as well as to recognize common inherent analogies among distinct transport phenomena (and mechanisms) in several applications of interest.

2. THEORY

Despite the broad variety of existing food and biotechnological products, model frameworks to simulate transport phenomena interesting to Food Engineering have common features that allow a rather general formalization, which can be adapted depending on process conditions. Particular aspects of distinct processes can be expressed through specific boundary and/or initial conditions as well with help of specific properties and/or closures. Bearing in mind a intensive property ϕ and a Cartesian coordinate system (x, y, z) so that corresponding velocity components are u, v e w, the so-called general transport equation (GTE) reads:

$$\frac{\partial(\rho\phi)}{\partial t}+\frac{\partial(\rho u\phi)}{\partial x}+\frac{\partial(\rho v\phi)}{\partial y}+\frac{\partial(\rho w\phi)}{\partial z}=\frac{\partial}{\partial x}\left(\Gamma_\phi\frac{\partial\phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\Gamma_\phi\frac{\partial\phi}{\partial y}\right)+\frac{\partial}{\partial z}\left(\Gamma_\phi\frac{\partial\phi}{\partial z}\right)+S_\phi \tag{1}$$

where t is time and ρ is density while the diffusion coefficient Γ_ϕ and the source (sink) term S_ϕ are identified in line with the transported property ϕ. Differential formulation of conservation principles are obtained after proper substitution of all necessary terms into GTE, Eq. (1).

In this project, Eq. (1) was applied to heat transfer with $S_\phi = S_T$ regarding solely to eventual heat sources or sinks. Evoking the continuity equation and assuming fixed values for density ρ, constant-pressure specific heat c_P and thermal conductivity k, Eq. (1) leads to the following partial differential equation (PDE) for temperature T (Bird *et al.*, 1960):

$$\rho c_P\left(\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}+w\frac{\partial T}{\partial z}\right)=k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right)+S_T \tag{2}$$

For one-dimensional (1-D) problems $T = T(x,t)$ and $v = w = 0$. Indicating $\alpha = k/(\rho c_P)$ as thermal diffusivity, Eq. (2) then simplifies to the following PDE (Incropera & DeWitt, 1998):

$$\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}=\alpha\frac{\partial^2 T}{\partial x^2}+S'_T \quad , \quad S'_T=\frac{S_T}{\rho} \tag{3}$$

3. MATERIALS AND METHODS

The basic idea was to conceive and implement computational modules to accomplish the following task list:

- Data acquisition from via a graphical user interface (GUI);
- Data processing (namely, numerical solution of the heat transfer problem established by the user);
- Presentation (i.e., post-processing) of numerical results.

In view of that, the following development steps were conceived:

- Search for available / existing numerical simulators for Transport Phenomena undergraduate education (possibly with particular emphasis on Food Engineering undergraduate programs);
- Search and selection of case-studies involving momentum, energy or mass transport, related to Food Engineering;
- Conception and elaboration of a graphical user interface using Visual Basic for the proposed academic simulator;
- Preliminary implementation of the academic simulator in order to numerically solve user-selected cases;
- Tests and initial validation of the simulator implemented.

With respect to case selection, attention was devoted to problems involving transport phenomena applied to Food Engineering. Heat transfer was chosen as a pilot development since it is a transport phenomenon inherent to any food thermal processing. It is worth mentioning that chilling and cooking directly influence end product quality. Subsequent development steps evoked computational resources as programming environments and numerical routines. GUI was built using Visual Basic while data processing modules were implemented using FORTRAN 90/95, relying on Math / Library routines from IMSL ("International Mathematical and Statistical Library"). Option for such routines are due to the fact they operate as "black-boxes", dismissing detailed knowledge of their logic from programmers.

4. RESULTS AND DISCUSSION

4.1. Search for academic simulators for Transport Phenomena education and for problems of interest

Prior to elaborating the computational program, existing academic simulators similar to the one here proposed were searched. Accordingly, the didactic simulator "1D Heat Transfer" (Silva *et al.*, 2005) for steady-state 1-D diffusive-convective heat transfer was particularly conceived for undergraduate education in Mechanical Engineering. Such software was then taken for reference inasmuch as it presented similar features as those intended. In addition, it is able to carry on either transient or steady-state simulations while allowing users to freely set boundary conditions at both (i.e., east and west) 1-D solution domain ends (e.g.: infinite walls, infinite cylinders, and symmetric spheres).

It is worth citing that the model adopted in "1D Heat Transfer" is based on Eq. (3) so that users should properly describe the 1-D (steady-state or transient) problem by providing values for control parameters such as k, ρ, c_p and S_T. Moreover, it is assumed that velocity u is known and provided as well. Finally, it is equally up to users to prescribe the necessary initial (for transient problems) and boundary conditions for proper problem definition. In such simulator, Eq. (3) is discretized via finite-volumes method and numerically solved following a fully implicit formulation.

Bearing in mind prospective comparisons to results from "1D Heat Transfer" simulator, case-studies focusing on Transport Phenomena applied to Food Engineering were sought. Accordingly, problems involving foodstuff chilling and cooking is of major importance as they are directly related end-product quality as well as because heat transfer is transport phenomenon inherent to any food thermal processing.

4.2. Implementation of the graphical user interface for the simulator under development

A graphical user interface (GUI) was elaborated using Visual Basic based on a single dialog box so that users could follow all necessary simulation parameters at the same time. Figure 1 shows the layout proposed for such dialog box (in Portuguese). In addition, some menus were created in order to help users with respect to running the simulator itself.

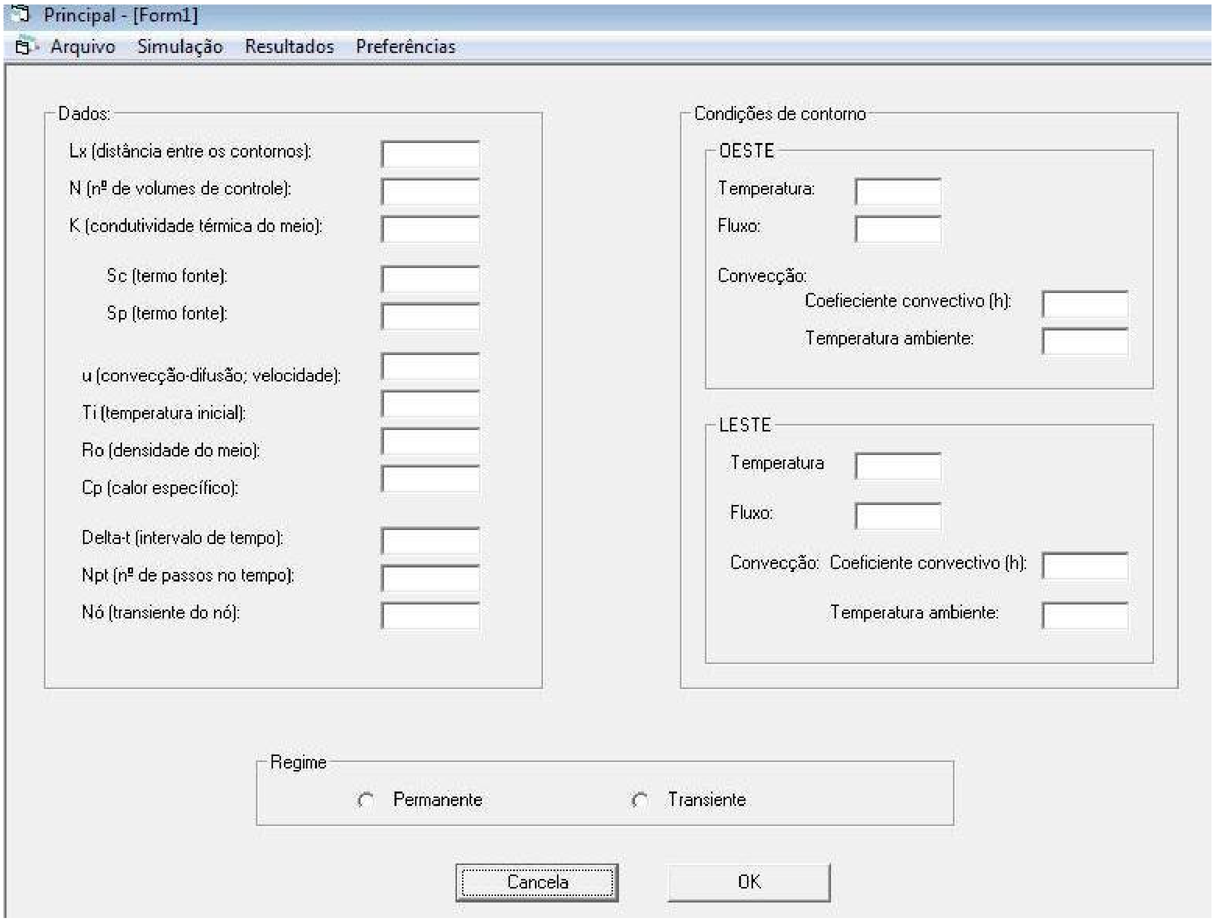

Figure 1. Initial dialog box of the proposed GUI.

Menu "Arquivo" (File) is utilized to create and define new data files, to open previously defined files, and to close (exit) the software, as depicted in Fig. 2. After simulating a given problem, the formerly disabled menu "Resultados" (Results) assumes the appearance shown in Fig. 3. As suggested in Fig. 4, via menu "Preferências" (Customize) users may set colors for plots to be drawn during simulations. Finally, after all necessary information has been provided by the user, menu "Simulação" (Simulation) starts the numerical solution procedure (Fig. 5).

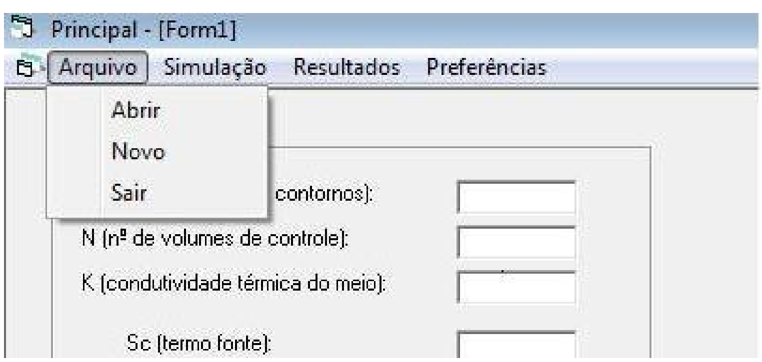

Figure 2. Actions within menu "Arquivo" (File) available to users.

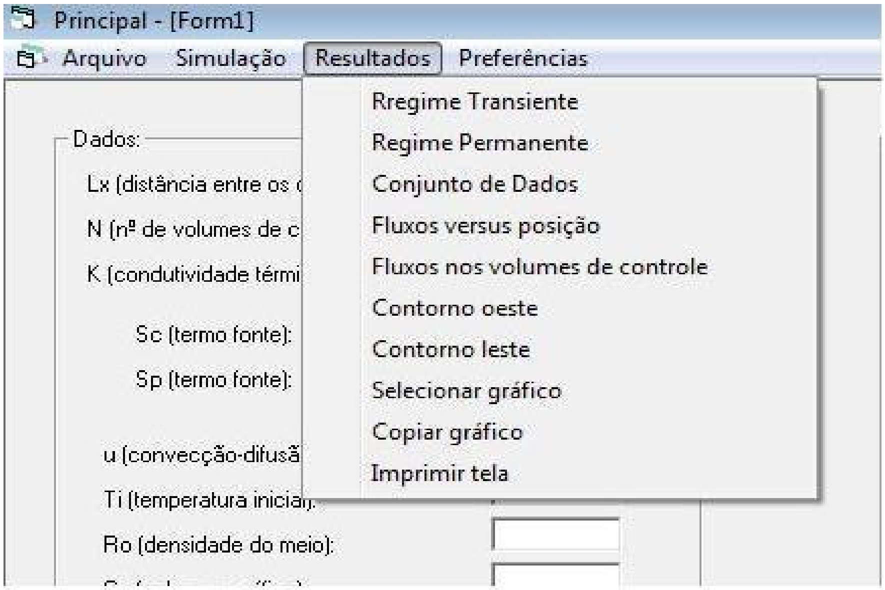

Figure 3. Actions within menu “Resultados” (Results) available to users.

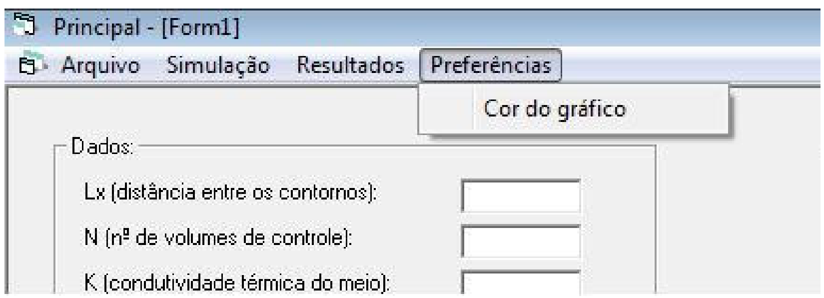

Figure 4. Actions within menu “Preferências” (Customize) available to users.

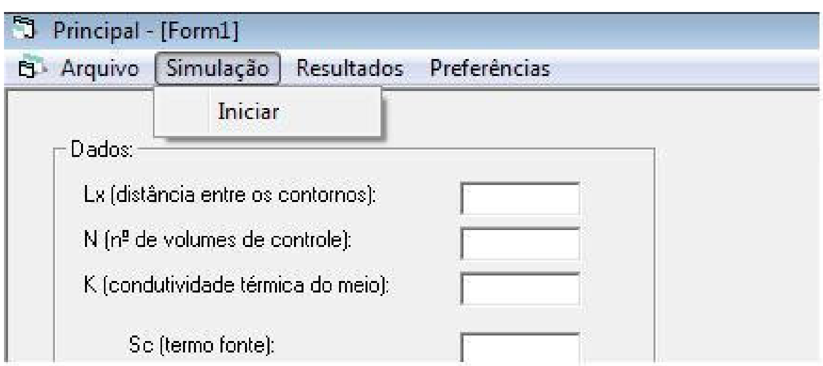

Figure 5. Running the numerical solution procedure via menu “Simulação” (Simulation).

4.3. Implementation of the numerical solution for the governing differential equation

In order to implement the computational to code to numerically solve Eq. (3), routine MOLCH (“method of lines with cubic Hermite polynomials”) from IMSL Math / Library was employed. Suitably adapted to simulate Transport Phenomena of interest, MOLCH belongs to a “family” of computational routines for numerical solution of ordinary or partial differential equations (ODEs or PDEs). Among other routines in the “family” it is worth citing IVPAG (“initial value problem with Adams-Moulton-Gear method”) and IVPRK (“initial value problem with Runge-Kutta method”) to solve initial-value 1st-order ODEs, as well as BVPFD (“boundary value problem with finite difference”) for boundary-value problems involving differential equation systems.

On general basis, routine MOLCH solves PDEs related to 1-D (transient or steady-state) problems that can be formalized in the form:

$$\phi_t = f(x, t, \phi, \phi_x, \phi_{xx}) \quad , \quad \text{where} \quad \phi_t = \frac{\partial \phi}{\partial t} \quad , \quad \phi_x = \frac{\partial \phi}{\partial x} \quad , \quad \phi_{xx} = \frac{\partial^2 \phi}{\partial x^2} \tag{4}$$

Function $\phi = \phi(x, t)$ can be identified to the property of interest (in the present case, to the temperature). In order to properly call routine MOLCH, a program in FORTRAN 90/95 was implemented. For sake of illustration, Fig. 6 shows how routine MOLCH is call from computational module programmed in FORTRAN 90 95.

```
    CALL MOLCH (IDO, FCNUT, FCNBC, NPDES, t, tprox, Nx, xnodal, TOL, dt, Y, LDY)

    Y(1,Nx) = Y(1,Nx-1)
ENDDO

! Print results

    WRITE (*,100) t, IDO
100 format('Solution at t = ',F8.0, '     IDO = ',I2)

I = 1
write (*,200) I, xnodal(I), Y(1,I)
DO I = 5, Nx, 5
    write (*,200) I, xnodal(I), Y(1,I)
200 format('I = ',I3, '   x = ',F6.2, '   T(x) = ',F6.1)
ENDDO

END

! ***********************************************************************************

SUBROUTINE FCNUT (NPDES, x, t, u, dudx, d2udx2, dudt)

INTEGER NPDES                                         ! SPECIFICATIONS FOR ARGUMENTS
REAL    x, t, u(*), dudx(*), d2udx2(*), dudt(*) ! termos padronizados
REAL    sT                                            ! termo fonte

! Define the PDE: nonlinear diffusion-convection with discontinuous coefficients

alfa = 1.38e-7
vx   = 0.0
sT   = 0.0

dudt(1) = alfa*d2udx2(1) - vx*dudx(1) + sT

RETURN
END

! ***********************************************************************************
```

Figure 6. Example of routine MOLCH call from a program in FORTRAN 90/95.

In order to familiarize to such IMSL routine, an existing (application) example similar to the problem of interest was studied aiming at future implementation of the numerical solution. At this point, it is worth mentioning that in IMSL Math / Library “Users’ Handbook” one is able to find at least one demonstration (application) example for each routine. Accordingly, in order to test the resulting computational code, a 1-D transient heat transfer problem was selected from (Incropera & DeWitt, 1998) basically consisting of solid bar whose half-length was buried in the ground (soil). Bar ends were subjected to distinct temperatures, namely, exposed end (above ground, corresponding to $x = 0$) was subjected to air at −15°C while buried end ($x = 1$ m) was at 20°C. Further details can be found in (Incropera & DeWitt, 1998).

Figure 7 shows the output screen (window opened by the program) with some simulated results with the help of routine MOLCH, setting 30 days for the heat exchange process. The first column contains identification numbers for grid points, the corresponding x position within the 1-D solution domain, and simulated values for temperature at the final simulation instant. Simulated results agreed with the solution presented in (Incropera & DeWitt, 1998).

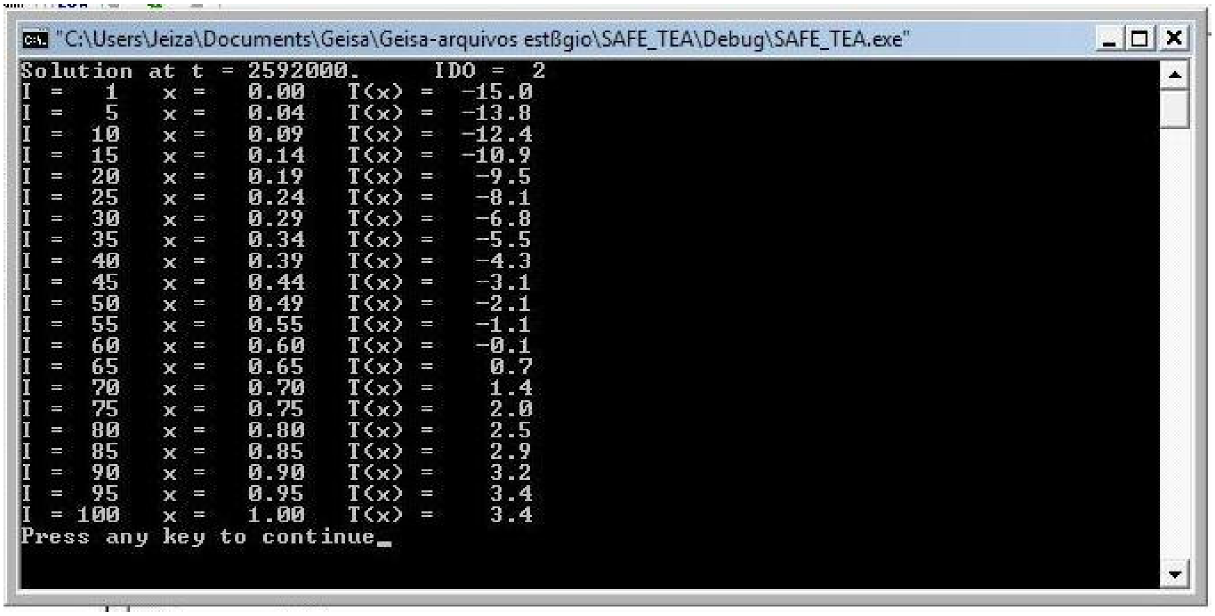

Figure 7. Initial tests with routine MOLCH aiming at the numerical solution of the PDE of interest.

5. CONCLUDING REMARKS

The search for didactic software for Transport Phenomena education suggested some deficiency not only regarding Food Engineering but also with respect to other Engineering branches. As far as authors' knowledge is concerned, there is an academic software for heat transfer simulation aiming at Mechanical Engineering education, which suggests some lack of (non-commercial) didactic software to help and support the education of such basic Engineering courses. On its turn, the search for case-studies involving Food Engineering allowed one to identify necessary aspects for the proper development of a software of such nature, including fundamental user-provided parameters (e.g., density, specific heat, thermal conductivity, etc.).

The choice for FORTRAN 90/95 programming was important inasmuch as it allowed the use of a suitable IMSL Math / Library routine (namely, MOLCH) able to numerically solve the differential equation that governs the transport phenomenon of interest (namely, heat transfer), this way dismissing detailed knowledge of its inner logic. On its turn, the choice for Visual Basic to build up the graphical user interface (GUI) was convenient bearing in mind its friendly environment. The didactic simulator proposed in this project is fully operational yet. As far as future work is concerned, it is worth citing the accomplishment of new tests aiming at routine MOLCH validation, coupling between FORTRAN code (program) and GUI (elaborated in Visual Basic), and the extension of the simulator towards further Transport Phenomena interesting to Food Engineering.

6. ACKNOWLEDGEMENTS

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