Mathematics Taught in Chemical Engineering, What material should be covered? What should be the complexity?

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Abstract.

This material will discuss the contents of mathematics that should be taught in the undergraduate programs of chemical engineering in the country Mexico and eventually in other countries, what material should be covered, what is the complexity and where the boundary begins with the mathematics taught in graduate programs. Several exercises are presented and solved for students in the undergraduate program of chemical engineering in Universidad Autonoma de Zacatecas, Mexico.

The solved problems are the following: 1) A model of laminar flow through a lubricated tube. This is one problem of momentum transport more complicated than that for a tube filled with only one fluid; therefore it leads to the construction of one set of differential equations requiring the use of continuity boundary conditions for determining the velocity profiles of both fluids. 2) Slow flow over a solid sphere. It requests the analysis of momentum transport and more complicated procedures than those traditionally taught in the undergraduate programs. The deduction of Stokes law is performed. 3) Transient flow inside a cylindrical tube. It demands the solution of the partial differential equation that describes the starting of a liquid flow, due a pressure difference. The Sturm Liouville problem is solved, the variable separation method is used, and one of the differential equations is solved using Bessel functions because it has variable coefficients. The velocity profiles changing with time are found. 4) No stationary heat conduction in a cylindrical metallic bar. The partial differential equation describing the heating of a metallic bar in one of its ends is solved, with different boundary conditions, using the weighted residual methods and mainly, the orthogonal collocation method. 5.- Potential flow on a cylindrical tube. The partial differential equation is solved using the method of variable separation and the Euler equation to find the angular component of velocity.

Once the ability of the undergraduate students to solve this kind of problems is demonstrated, an optional undergraduate course is proposed about applied mathematics, including, among others, the indicated themes above. It is considered that the knowledge, dominion and familiarity with mathematics, will guide and motivate the students to pursue graduated studies and to do scientific research and the level of mathematics in the chemical engineering program should be indicated by those used in the main nucleus of subjects that distinguishes this career with respect to others.

Introduction.

With the goal of passing some subjects in the chemical engineering program in the UAZ – Zacatecas - Mexico, and to fulfill some requirements to graduate, so called Self Formation Seminars, several undergraduate students choose to solve problems related with Transport Phenomena and applied mathematics, involving mathematics more complicated that those traditionally taught in the undergraduate courses.

The advisor of these students, intrigued about the success of these actions, decided to investigate what are the contents of the programs of mathematics in the undergraduate programs in chemical engineering in other universities, in order to realize whether this is or not a risky task.

A survey was performed about the courses of mathematics taught in the undergraduate programs of chemical engineering of several universities of Mexico, USA and one of Canada. According to the collected information about that sample of universities, it was found that the common courses and topics are: Differential and integral calculus, with one or several variables, linear algebra, vectorial calculus, statistics and probability, differential equations of first, second and n-th order, linear, with constant coefficients, homogeneous and non homogeneous.

There were some differences among the programs in the most advanced courses from one university to another, and they indicate the border with the graduate courses. Some courses included and others no, the following topics: differential equations with variable coefficients, series of powers, systems of differential equations of first order, partial differential equations solved with the method of variable separation, etc. Then this set of topics is a non definite frontier between the undergraduate and graduate courses.

The focus of the courses of mathematics in chemical engineering.

Generally, all the undergraduate programs of chemical engineering have the following structure: Basic area, basic professional area, professional area and complementary area.

The basic area comprises the fundamental and scientific subjects for all the engineering, such as mathematics, chemistry, physics, physical – chemistry, etc. All of these subjects are common to all engineering careers. Basic professional area includes subjects such as transport phenomena, thermodynamics, chemical thermodynamics, etc, and these topics introduce to the student the fundamentals of chemical engineering, while the professional area contains chemical reactors, unit operations, etc. This last set of topics is the nucleus of the main subjects of chemical engineering career, which make the chemical engineering different from the other engineering.

Mathematics plays a very important role in this career and the way it is taught and its contents can be an important factor to give the student or not an adequate analytical capacity in solving problems during the career and later in the professional development, graduate studies and etc. In addition, students have a fear of mathematics and the instructor has to deal with it. This is the motivation to prepare this material.

All of these topics in mathematics can be taught with all mathematical rigor or just as mechanical applications without really understand the theorems and theory involved in the possibility of finding solutions of the equations in a region of the dominion, the uniqueness of the solution, etc. The collected documents in the survey did not allow us to see the focus of the programs, and although some of them included a lot of topics, it is possible to teach them using the mathematical rigor or just the mechanical applications of procedures or recipes. We believe one or other extremes are not convenient in chemical engineering. There are opinions that the mathematics in chemical engineering career should be taught by mathematicians, with the mathematical rigor, and taught as in the schools of mathematics. This focus has the risk of giving to the student a lot of specific and specialized information which is not supposed to be learned and be used in the career of chemical engineering, to distract the attention just in mathematics and to address his interest and concentration just in one area or subject, to deviate the students from the main objective of the career, and eventually they do not learn all the mathematical rigor, and just to pass the subject, and few or nothing of applications are illustrated, and the connection with chemical engineering is not done. Something similar could happen for example with the chemistry taught in chemical engineering. Eventually the professor feels like to teach it as if the career were of chemistry. Also the professor of physics would like to teach and concentrate in physics, forgetting the main objectives of the career of chemical engineering.

On the other hand, to teach mathematics just to let the student to learn how to use the formulas to calculate derivatives, integrals, how to apply the recipe of steps to solve a differential equations, etc, will deny the student to acquire a scientific background, necessary to get an analytical capacity and knowledge, useful to have a good development as chemical engineer, as a graduate student, as a scientific researcher, etc.

We consider that the mathematics needed by the chemical engineer should be a combination of both focuses and must be indicated by the objectives of the career. The nucleus of professional subjects of the career and those of the basic professional area, dictates the level and type of requested mathematics. These sets of subjects are referred to the topics that do distinct the chemical engineering from the other engineering and those that orient the student to the chemical engineering and contains: Balances of mass and energy, transport phenomena, thermodynamics, chemical kinetics, physical and chemical equilibrium, unit operations, chemical reactors, dynamics and control of processes, etc. The study of these subjects asks the analysis of physical or chemical processes in order to establish the mathematical model, to solve it and to interpret the solution, and to do changes in some variables and to understand the different behavior for each case, to analyze a system thermodynamically, to construct an equilibrium diagram, etc.

The analytical capacity can be reached once the student has good formation in mathematics, due it is an important analytical tool and the osseous skeleton of science, and he or she is not going to learn mathematics just using formulas without knowing how they were deducted. Then it is important to teach them something about the demonstration of easy theorems, deduction of formulas etc, because this formation is going to let them to use the mathematical tools to analyze the problems corresponding to other subjects such as transport phenomena, chemical reactors, unit operations, etc.

Once the under graduate students acquire this knowledge, they will be able to understand the deductions, and to realize analytical procedures and physical analysis. Of course, a graduate course should include more amounts of knowledge and with more deepness, due he or she is supposed to solve more complicated problems, than those solved by undergraduate student. Anyway, even in graduate courses for chemical engineering, they should hold the same focus, related with the applied mathematics and not with just mathematics, unless the interest of the student is to concentrate in a mathematical problem, for example a numerical method to solve a very complicated partial differential equation representing a physical problem with a lot of restrictions.

Border between graduate and undergraduate courses.

A typical graduate course of mathematics in chemical engineering include among other specific objectives: The acquisition of more deep knowledge of mathematics about matrices, eigenvalues, etc, the construction of mathematical models about a physical system, the solution of partial differential equations, using the Sturm Liouville theory, methods to discrete the solution of one equation, application of numerical methods to specific problems, etc. In other words, the graduate courses should provide the student the mathematical tools needed to do the thesis, and according to the thesis topic the needs can change.

Therefore, the border between the under graduate and graduate courses in mathematics is not clear and definite, and sometimes, several topics are common in both programs. The following topics belong to this common border: ordinary differential equations of variable coefficients, systems of ordinary first order differential equations, eigen values and eigen functions, auxiliary tools necessary to solve partial differential equations that represent the model of a physical phenomena, the separation method to solve partial differential equations, etc. Sometimes and in some schools, these topics are either taught in undergraduate and graduate courses.

Normally, in undergraduate courses the studied physical problems are related with convective problems and chemical reactions, which lead to ordinary differential equations and in the graduate courses, the studied physical problems (diffusion or diffusion + convection + chemical reaction) lead to partial differential equations or complicated systems of ordinary differential equations of first order, and because of that, the majority of the undergraduate courses have as last topic the ordinary differential equations of second order or higher with constant coefficients.

So far, in summary, it can be said that it is necessary to delimit the contents and focus of all the subjects taught in the undergraduate program of chemical engineer, to fulfill the general objective of the career. Consider besides that the certifying organisms of the chemical engineering programs request a number of courses and hours for each area and subject and it is not possible to dedicate an excess of hours just to mathematics, to chemistry, and etc.

The adequate use of mathematics in the establishment and solution of mathematical models will provide the undergraduate student a solid basis and to further develop with confidence in the graduate studies, to feel like to pursue graduate studies, etc. We believe however, that eventually the focus of rigorous mathematics is not necessary for the general formation of chemical engineer, unless the student is specifically interested in a deep analysis of a topic, a specific problem etc., where it is necessary to know under what conditions it is possible to solve a solution, the part of the dominion where the solution is stiff, the theorems that guarantee the uniqueness of the solution, etc. This knowledge may be acquired in a graduate course or in an optional undergraduate course, about selected topics of mathematics.

A proposal for a special undergraduate course for applied mathematics.

For those students interested in learning more mathematics, and to understand better its application in the problems rose from chemical engineering, it is possible to offer them a special course that will allow them to have more training and therefore more success when they study the graduate program.

The suggested title for the course is: Applied Mathematics in Selected Topics.

The general objective is to use specific physical problems, to analyze them to build the mathematical model, to solve it and to study all the mathematics behind the problem, in order to familiarize the student with the applied mathematics.

The proposal of contents is:

1) A model of laminar flow through a lubricated tube.

This problem involves the topics of formulation of mathematical model in transport phenomena, related with momentum transport more complicated than that for a tube filled with only one fluid and without lubrication; due it leads to the construction of one set of ordinary differential equations requiring the use of continuity boundary conditions for determining the velocity profiles of both fluids. (1)

2) Slow flow over a solid sphere. It requests the analysis of momentum transport and more complicated algebraic procedures than those traditionally taught in the undergraduate programs, it leads to the deduction of Stokes law. **(**1, 2, 5**)**

3) Transient flow inside a cylindrical tube. It asks the solution of the partial differential equation that describes the starting of a liquid flow caused by pressure difference. The Sturm Liouville problem is solved, the variable separation method is used, and one of the differential equations is solved using Bessel functions because of the variable coefficients. The velocity profiles changing with time are found**. (**1, 2**)**

4) No stationary heat conduction in a cylindrical metallic bar. The partial differential equation describing the heating of a metallic bar in one of its ends, with different boundary conditions, is solved using the orthogonal collocation method that belongs to the weighted residual methods (4, 6)

5. - Potential flow on a cylindrical tube. The partial differential equation is solved using the method of variable separation and the Euler equation to find the angular component of velocity. **(**3, 7**)**

6. - Multiple steady states of homogeneous and heterogeneous chemical reactors. **(8)**

7. - Liquid – Vapor Equilibrium. Construction of data for equilibrium diagrams using thermodynamic relations (9)**.**

Some illustration about the procedures and solutions is provided for two problems, worked by the students of UAZ. In this case, it is more important to give comments about the experiences of teaching these problems to the undergraduate students than to illustrate with detail the calculations and procedures, which can be found in the consulted books. Actually, the algebraic details are given as a guide to do comments.

Then the statement of the problem, some details about the algebra and some commentaries are given.

Problem One. - A model of laminar flow through a lubricated tube.

Statement: Important pressure drops are required to force viscous fluids to pass through tubes with small diameter. In this example we analyze a proposal to reduce the requested pressure by creating a thin layer of liquid lubricant on the internal surface of the tube. We assume that the thickness of the lubricant layer is constant and independent of the axial position and time. (1).

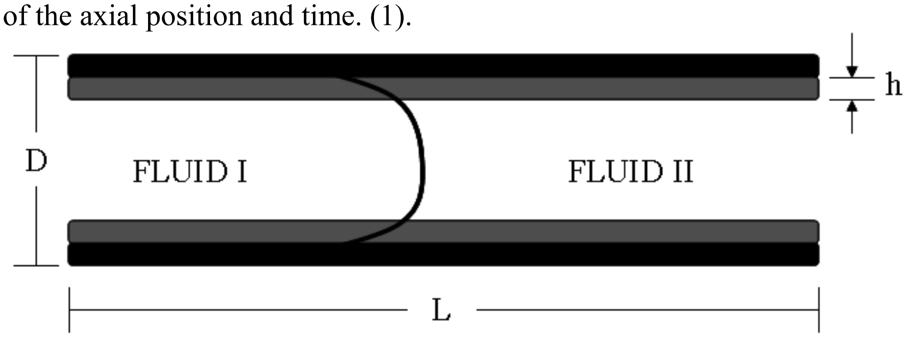

Figure 1. - Laminar flow of fluid I through a lubricated tube. Flow II is the lubricant with constant thickness h (1).

The solution for the velocity profile in fluid I is:

$$v_z^I = \frac{C^I}{4\mu^I} r^2 + F^I \, , \; 0 \le r \le \frac{D}{2} - h$$

Comment: Until now, to obtain the presented solution is easy and illustrated in undergraduate courses of transport phenomena, concretely, the problem of calculating the parabolic velocity profile for laminar viscous flow inside an empty circular tube. Then, the difficulty stars if the fluid contains a lubricating layer, where it is necessary to determine the expression for both fluids, and to achieve this goal, it is necessary to use additional boundary conditions, as it can be seen below.

The differential equation describing the change of velocity inside the lubricant layer, fluid II is:

$\mu^{II} \dfrac{dv_z^{II}}{dr} = \dfrac{C_r^{II}}{2} + \dfrac{E^{II}}{r}$, in the region: $\dfrac{D}{2} - h \le r \le \dfrac{D}{2}$

The solution is:

$$v_z^{II} = \frac{C^{II} r^2}{4\mu^{II}} r + \frac{E^{II}}{\mu^{II}} \ln r + F^{II}$$

Comment: To get this new differential equation for the lubricant layer, it is necessary to do an analysis in a differential volume element placed in the lubricant, or to analyze the Navier Stokes Equation.

There are five unknown constants, $\left(C^I, F^I, C^{II}, F^{II}, E^{II}\right)$ which will be determined using additional boundary conditions observed in the physical system.

So far we know that:

$C^I = \dfrac{\Delta P^I}{L}$ and $C^{II} = \dfrac{\Delta P^{II}}{L}$

The pressure drop is the same for fluids I and II, then:

$$C^I = C^{II} = \frac{\Delta P}{L}$$

Fluid II satisfies non slip condition because it is in touch with the tube wall.

$v_z^{II} = 0$, $r = R = D/2$

Substituting:

$$0 = \frac{C^{II} R^2}{4\mu^{II}} + \frac{E^{II}}{\mu^{II}} \ln R + F^{II} .$$

Also, a no slip condition is satisfied in the interface between the two fluids.

$$v_z^{II}\Big|_{R-h} = \frac{C^{II}(R-h)^2}{4\mu^{II}} + \frac{E^{II}}{\mu^{II}} \ln(R-h) + F^{II} = v_z^I\Big|_{R-h} = \frac{C^I}{4\mu^I}(R-h)^2 + F^I$$

Other boundary condition is the continuity of the shear stress in the interface between the fluids.

$\mu^{II} \dfrac{dv_z^{II}}{dr} = \mu^I \dfrac{dv_z^I}{dr}$ at $r = R - h$

$$\left(\frac{C^{II} r}{2} + \frac{E^{II}}{r}\right)\Bigg|_{R-h} = \left(\frac{C^I r}{2}\right)\Bigg|_{R-h}$$

Now we have five unknowns and five equations. After algebra we get:

$$C^I = C^{II} = \frac{\Delta P}{L}$$

$$E^{II} = 0$$

$$F^{II} = -\frac{\Delta P}{L} \frac{R^2}{4\mu^{II}}$$

$$F^I = -\frac{(R-h)^2}{4\mu^{II}} - \frac{R^2}{4\mu^{II}} - \frac{(R-h)^2}{4\mu^I}$$

Using these expressions we get the velocity profiles for both fluids.

$$\frac{v_z^I}{\Phi} = \left[(1-\eta)^2 + M\eta(2-\eta)\right] - s^2$$

$$\frac{v_z^{II}}{\Phi} = M\left(1-s^2\right)$$

Where:

$$\Phi = \frac{-CR^2}{4\mu^I} = \frac{\Delta PR^2}{4\mu^I L},\; s = \frac{r}{R},\; \eta = \frac{h}{R},\; M = \frac{\mu^I}{\mu^{II}}$$

Comment: Finally the dimensionless velocity profiles for both fluids were obtained. However note that this procedure requested to observe additional boundary conditions, to use them, to get the profile expressions asking the student to analyze and understand the problem to get the additional boundary conditions, to face them with a long algebraic procedure, and finally to attain the velocity profiles. Now the question is, and what is this for? Why to get this?. It is very important to illustrate the student what is the utility of all the obtained results to avoid frustration.

Now we use this information to evaluate the possibility of increasing the velocity of fluid I through the tube using the lubricant layer.
Volumetric flow velocity:

$$Q^I = \int_0^{R-h} 2\pi r v_z^I dr$$

$$\frac{Q^I}{2\pi R^2\Phi} = \frac{(1-\eta)^4}{4} + \frac{M\eta(2-\eta)(1-\eta)^2}{2}$$

The fluid velocity without lubricant is obtained with $\eta = 0$, (h = 0).
Then:

$$\Psi \equiv \frac{Q^I}{Q^I(\eta = 0)} = (1-\eta)^4 + 2M\eta(2-\eta)(1-\eta)^2$$

Figure 2 reports the plot of this last equation. Only for M > 1, when the lubricant is less viscous than the fluid I, there is an improvement in the fluid velocity. When η tends to one, even for a big value of M, the flow is reduced, since as the lubricant layer increases its thickness, and the area available for the flow is reduced.

Comment: To understand figure 2 will conclude the learning of the student about this problem the effort to reach these results, and avoid the frustration about to have performed a lot of algebra, without understanding the objective and the conclusions deducted from the results.

Problem Two: Transient flow inside a cylindrical tube

Statement: Consider a tube connected in the bottom of a big tank, and both are filled with water. The transversal section of the tube is circular. At time t < 0, the fluid is in repose and there is no flow. Suddenly, at t = 0, a constant pressure difference is applied in the ends of the tube, and the fluid starts to move from the tank to the tube and we want to estimate the necessary time in order the fluid reaches the new steady state. (1, 2)

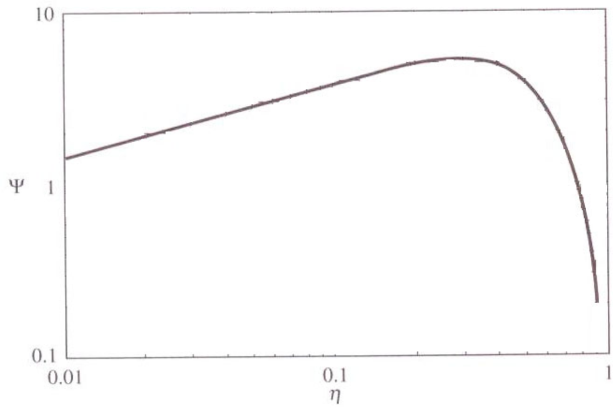

Figure 2.- Effect of a lubricant layer on the flow through a tube.

We assume laminar flow, a very long tube; the axial velocity is the only component of velocity. Using the continuity and Navier Stokes equations, it is possible to find the mathematical model describing this process.

$$\rho \frac{\partial u_z}{\partial t} = -\frac{\Delta P}{\Delta z} + \mu \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial u_z}{\partial r} \right)$$

Boundary conditions:

$u_z = 0$ at $r = R$ and $\dfrac{du_z}{dr} = 0,\ at\ r = 0$

Initial condition:

$u_z = 0\ at\ t = 0$

Using the following dimensionless variables:

$$s = \frac{r}{R} \qquad \Phi = \frac{u_z}{u_z^{\max}} \qquad \tau = \frac{\mu \cdot t}{\rho R^2}$$

We get the mathematical model without dimensions.

$$\frac{\partial \Phi}{\partial \tau} = \frac{1}{s}\frac{\partial}{\partial s}\left(s \frac{\partial \Phi}{\partial s} \right)$$

$\Phi = 0$ at $s = 1$, $\dfrac{\partial \Phi}{\partial s} = 0$ along $s = 0$

$\Phi = -(1 - s^2) \quad \tau = 0$

This is one example of the Sturm Liouville problem.

Comment: To reach this point demands the understanding of the student about the physical problem, the capacity to use the Navier Stokes equation, and the capacity to adimensionalize equations, and to understand how to propose the dimensionless variables.

To find the transient solution, we use the method of variable separation, proposing the following form of the solution:

$\Phi(s,\tau) = S \cdot (s) \cdot T(\tau) = ST$

Inserting it in the differential equation, we get the following system of differential equations:

$\frac{dT}{d\tau} = -\alpha^2 T$, $\quad \frac{d^2 S}{ds} + \frac{1}{s} \cdot \frac{dS}{ds} + \alpha^2 S = 0$

The solution of the first equation is:

$T = e^{-\alpha^2 t} \cdot A$

Comment: To reach this point, it is important to understand that the problem solution has two parts, one stationary and one dynamic. The variable separation method is used to reduce the original partial equation in one system of two differential ordinary equations.

The second equation is the Bessel type. A proposed solution is:

$S(s) = c_1 J_0(\alpha \cdot s) + c_2 Y_0(\alpha \cdot s)$

$$J_0(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(n!)^2} \left(\frac{x}{2}\right)^{2n} = 1 + \frac{x^2}{4} + \frac{x^4}{64} + \frac{x^6}{2304} + \ldots.. \qquad J_0(0) = 1$$

$$Y_0(\alpha^2 s) = \frac{2}{\pi}\left[\left(\gamma + \ln\left(\frac{\alpha^2 s}{2}\right)\right) J_0(\alpha^2 s) + \sum_{m=1}^{\infty} \frac{(-1)^{m+1} H_m}{2^{2m}(m!)^2}(\alpha^2 s)^{2m}\right], \quad \alpha^2 s > 0$$

Then,

$$\Phi_t(s,\tau) = \sum_{n=1}^{\infty} B_m \cdot e^{-\alpha_n^2 \cdot \tau} \cdot J_0(\alpha_n \cdot S) \qquad \tau = 0, \quad \Phi = -(1 - s^2)$$

$-(1 - s^2) = \sum_{n=1}^{\infty} B_m \cdot (1) \cdot J_0(\alpha_m \cdot S)$, to get B_m

$$\int_0^1 J_0(\alpha_m \cdot s)(1 - s^2) s ds = = \sum_{n=1}^{\infty} B_m \int_0^1 J_0(\alpha_m \cdot s) J_0(\alpha_m \cdot s) s ds$$

$$B_m = \frac{8}{\alpha_m^4 [J_1(\alpha_m)]}$$

$$\Phi = -8 \sum_{n=1}^{\infty} \frac{J_0(\alpha_n s)}{\alpha_n^3 J_1(\alpha_n)} \exp(-\alpha_n^2 \cdot \tau)$$

This equation is plotted in figure 3, showing the velocity profiles for different times. It is observed that at 140 seconds the second steady state has been reached, and the steady parabolic profile is attained by the fluid inside the tube.

Conclusions.

1.- The undergraduate students in chemical engineering have the capacity of solving more complicated problems than those traditionally taught in the undergraduate courses, if they want and are motivated, as it is demonstrated with the worked problems by the students of UAZ – Mexico.

2.- It is possible to offer a special course of applied mathematics to the undergraduate students with specific interests, with the main objective of going through the physical phenomena and all the involved mathematics.

3.- The undergraduate courses of mathematics in chemical engineering must maintain an equilibrium between the usage of the mechanical procedures and the mathematical rigor.

4.- The border between the under graduate and graduate courses of mathematics in chemical engineering is indicated by the objective of the career. Generally the tools for solving partial differential equations and others are the main content of graduate courses.

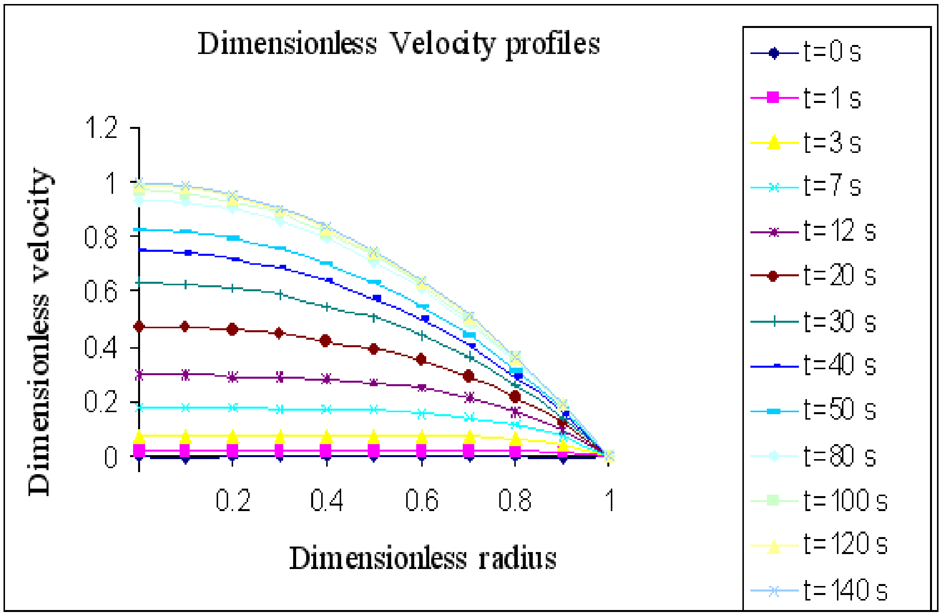

Figure 3.- Dimensionless radial velocity profiles at different times.

5.- According to the experience obtained, students that solved these problems are successful graduate students, which indicates that the dominion of mathematics prepare better the undergraduate students to pursue graduate studies.

References.

1.- Middleman Stanley, An Introduction to Fluid Mechanics, John Wiley and Sons Inc, 1998.

2.- Bird R. B., Stewart W. E., Lightfoot E. N., Transport Phenomena, Second Edition, John Wiley and Sons Inc., 2002.

3.- Welty J. R., Wicks C. E., Wilson R. E and Rorres G. L., Fundamentals of Momentum , Heat and Mass Transfer, John Wiley and Sons, Inc, Fifth Edition, 2008.

4.- O´ Neil Peter, Advanced Engineering Mathematics, Thomson, Sixth Edition, 2007.

5.- Bruce R. Munson, Donald F. Young, Theodore H. Okiishi, Fundamentals of Fluid Mechanics, Fifth Edition, John Willey and Sons, Inc. 2006.

6.- Finlayson Bruce A. The Method of Weighted Residuals and Variational Principles, with Application in Fluid Mexhanics, Heat and Mass Transfer, Academic Press, 1972.

7.- Merle C. Potter and David C. Wiggert, Mechanis of Fluids, Third Edition, Brooks/Cole Thomson Learning, 2002.

8.- H. Scott Fogler, Elements of Chemical Engineering, Second Edition, Perentice Hall, 1992

9.- Stanley I. Sandler, Chemical and Engineering Thermodynamics, Third Edition, John Wiley and Sons, 1999.