

**Computer Facilitated Mathematical Methods in Chemical Engineering –
Similarity Solution**

*Submitted for consideration to “Class and Home Problem” section of
Chemical Engineering Education*

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Abstract

High-performance computers coupled with highly efficient numerical schemes and user-friendly software packages have helped instructors to teach numerical solutions and analysis of various nonlinear models more efficiently in the class room. One of the main objectives of a model is to provide insight about the system of interest. Analytical solutions provide very good physical insight, as they are explicit in the system parameters. Having taught/co-taught applied math for both senior undergraduate and first-year graduate students for five years, the author feels that students do not appreciate the value of analytical solutions because (i) they wrongly feel that numerical methods can be used to solve complex problems using high-speed computers, (ii) they are not comfortable and confident of doing the complicated integrals, rigorous algebra, and transformations involved in obtaining analytical solutions. In the author's view, various techniques to obtain analytical solutions can be taught efficiently using computers. For example, the computer algebra systems such as Maple,¹ Mathematica,² MATLAB,³ REDUCE⁴ etc. can be used to perform the tedious algebra, manipulations, complicated integrals, variable transformations, differentiations etc. involved in applying various mathematical methods.

In this paper, we show how Maple can be used to facilitate similarity transformation techniques for solving chemical engineering problems. The purpose of this paper is to show the utility of Maple in performing the math, solving the equations and plotting the results. The readers are advised to refer to the cited references for understanding the physics of the problems solved. For the sake of readers not familiar with Maple, a brief introduction about Maple is given below

Maple

Maple¹ is a computer-algebra system capable of performing symbolic calculations. Although Maple can be used for performing number crunching or numerical calculations just like FORTRAN, the main advantage of Maple is its symbolic capability and the user-friendly graphical user interface. In a Maple program, commands are entered after “>”. Maple prints the results if “;” is used at the end of the statement. This helps in fixing the bugs or mistakes in the program after a particular step as the results are seen after every step or command. For brevity, most of the Maple commands are ended with colon (:) in this paper. In general, while Maple is very useful in doing the transformations, the user might have to manipulate the resulting expressions from a Maple command to obtain the equation in the simplest or desired form. Often, these manipulations can be done in Maple itself by “seeing” the resulting expressions. Hence, the author recommends that first-time users of Maple use “;” instead of “:” at the end of each statement to view the results after each command/statement. Many of the mistakes made by the students are identified and rectified easily if they replace (:) with (;) in all of the statements. Maple can be used to perform all the steps from setting up the equation to analyzing the final plots in the same sheet. All the mathematical steps and manipulations involved can be performed in the same program or file. For clarity, between the Maple commands and output, all the text describing the process or Maple commands are given within brackets “[]”.

Similarity Transformation for Partial Differential Equations

Similarity transformation is a powerful technique for treating partial differential equations arising from heat, mass, momentum transfer or other phenomena as it reduces the order of the governing differential equation (from partial to ordinary). Depending on the governing equation, boundary conditions, domain and complexity, the similarity transformation

technique might yield a closed-form solution, a series solution or a numerical solution. One of the major difficulties the students encounter is that they find it very difficult to convert the governing equation from the original independent variables to a similarity variable. The following examples illustrate the use of computers and software in teaching/obtaining similarity solutions for various chemical engineering problems.

Example 1: Diffusion/Heat Transfer in Semi-infinite Domains

Consider the transient heat conduction problem in a slab.^{1,2} The governing equation and initial/boundary conditions are:

$$\begin{aligned} \frac{\partial u}{\partial t} &= \alpha \frac{\partial^2 u}{\partial x^2} \\ u(x, 0) &= 0 \\ u(0, t) &= 1 \text{ and } u(\infty, t) = 0 \end{aligned} \quad (1)$$

where, u is the temperature, x is the distance from the surface of the slab and t is the time and α is the thermal diffusivity. Equation 1 is solved by using the transformation $\eta = x/(2\sqrt{\alpha t})$. The original partial differential equation is converted to an ordinary differential equation in the similarity variable η . The boundary conditions for U (u in the similarity variable) are:

$$\begin{aligned} U(0) &= 1 \\ U(\infty) &= 0 \end{aligned} \quad (2)$$

The steps involved in the similarity transformation method are illustrated below.

Typically, Maple programs are started with “restart” command to clear all the variables. Next, “with(student)” package is called to facilitate variable transformations:

```
> restart: with(student):
> eq:=diff(u(x,t),t)-alpha*diff(u(x,t),x$2);
      eq :=  $\left(\frac{\partial}{\partial t} u(x, t)\right) - \alpha \left(\frac{\partial^2}{\partial x^2} u(x, t)\right)$ 
```

[First, $u(x,t)$ is transformed to $U(\eta(x,t))$. Then the governing equation is converted to the similarity variable:]

```
>eq1:=changevar(u(x,t)=U(eta(x,t)),eq):eq2:=expand(simplify(subs(eta(x,t)=x/2/(alpha*t)^(1/2),eq1))):eq2:=expand(eq2*t):eq2:=subs(x=eta*2*(alpha*t)^(1/2),eq2):eq2:=convert(eq2,diff):
```

[The final form of the governing equation is:]

```
> eq2:=expand(-2*eq2);
```

$$eq2 := \left(\frac{d}{d\eta} U(\eta) \right) \eta + \frac{1}{2} \left(\frac{d^2}{d\eta^2} U(\eta) \right)$$

[The given boundary conditions are used to solve the governing equation:]

```
> bc1:=U(0)=1;
```

$$bc1 := U(0) = 1$$

```
> bc2:=U(infinity)=0;
```

$$bc2 := U(\infty) = 0$$

```
> U:=rhs(dsolve({eq2,bc1,bc2},U(eta))):
```

```
> U:=convert(U,erfc);
```

$$U := \text{erfc}(\eta)$$

```
> u:=subs(eta=x/2/(alpha*t)^(1/2),U);
```

$$u := \text{erfc}\left(\frac{x}{2\sqrt{\alpha t}}\right)$$

[The solution is plotted in Figure 1, which shows how the temperature u penetrates to progressively greater distances as the time t increases:]

```
>plot3d(subs(alpha=0.001,u),x=1..0,t=500..0,axes=boxed,labels=[x,t,"u"],orientation=[-60,60]);
```

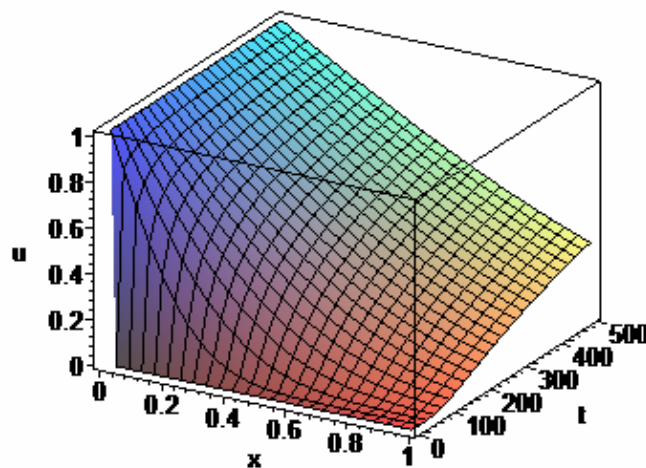


Figure 1: Dimensionless temperature distribution in a semi-infinite domain

Example 2 – Plane Flow Past a Flat Plate – Blasius Equation

The velocity distribution in the boundary layer of a plane laminar flow past a flat plate is given by³

$$\begin{aligned}\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} &= 0 \\ u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} &= \frac{\partial^2 u}{\partial y^2} \\ u(0,y) &= 1 \\ u(x,0) &= 0 \text{ and } u(x,\infty) = 1 \\ v(x,0) &= 0\end{aligned}\tag{3}$$

For this problem, first the velocities u and v should be converted to stream functions defined by $u = \partial\psi / \partial y$ and $v = -\partial\psi / \partial x$. The stream function by default satisfies the continuity equation (first equation). The second equation yields the governing equation for the stream function ψ . Next, the stream-function is expressed as $\psi = \sqrt{x} f(\eta)$, where $\eta = y/\sqrt{x}$ is the similarity variable. The boundary conditions for u and v yield the boundary conditions for ψ and finally for $f(\eta)$. Once the function $f(\eta)$ is obtained (numerically), both stream functions and velocity expressions can be expressed in terms of f and η . The steps involved in this example are more tedious compared to the previous example. All the complicated steps involved can be facilitated using Maple:

```
> restart:with(student):with(plots):
Warning, the name changecoords has been redefined
```

[The governing equation is entered:]

```
> eq:=u(x,y)*diff(u(x,y),x)+v(x,y)*diff(u(x,y),y)-
diff(u(x,y),y$2);
```

$$eq := u(x, y) \left(\frac{\partial}{\partial x} u(x, y) \right) + v(x, y) \left(\frac{\partial}{\partial y} u(x, y) \right) - \left(\frac{\partial^2}{\partial y^2} u(x, y) \right)$$

[Next, Stream functions ($u = \partial\psi / \partial y$ and $v = -\partial\psi / \partial x$) are introduced:]

```
> vars:={u(x,y)=diff(psi(x,y),y),v(x,y)=-diff(psi(x,y),x)}:
eq:=subs(vars,eq);
```

$$eq := \left(\frac{\partial}{\partial y} \Psi(x, y) \right) \left(\frac{\partial^2}{\partial x \partial y} \Psi(x, y) \right) - \left(\frac{\partial}{\partial x} \Psi(x, y) \right) \left(\frac{\partial^2}{\partial y^2} \Psi(x, y) \right) - \left(\frac{\partial^3}{\partial y^3} \Psi(x, y) \right)$$

[Next, the transformation $\psi = \sqrt{x} f(\eta)$ where $\eta = y/\sqrt{x}$ is used to obtain the equation for f:]

```
> eq := changevar (psi (x, y) = x^(1/2) * f (eta (x, y)) , eq) : eq1 := (simplify (subs (eta (x, y) = y/x^(1/2) , eq))) : eq1 := subs (y = eta * x^(1/2) , eq1) : eq1 := simplify (eq1 * x) : eq2 := convert (-eq1, diff) ;
```

$$eq2 := \frac{1}{2} \left(\frac{d^2}{d\eta^2} f(\eta) \right) f(\eta) + \left(\frac{d^3}{d\eta^3} f(\eta) \right)$$

[Next, the velocity variables u and v (i.e. derivatives of the stream function) are expressed in terms of f and the similarity variable η :]

```
> v (eta) :=-
```

```
diff (psi (x, y) , x) : v (eta) := changevar (psi (x, y) = x^(1/2) * f (eta (x, y)) , v (eta)) : v (eta) := expand (subs (eta (x, y) = y/x^(1/2) , v (eta))) : v (eta) := subs (y = eta * x^(1/2) , v (eta)) : v (eta) := factor (v (eta)) ;
```

$$v(\eta) := \frac{1}{2} \frac{f(\eta) - D(f)(\eta) \eta}{\sqrt{x}}$$

```
> u (eta) := diff (psi (x, y) , y) : u (eta) := changevar (psi (x, y) = x^(1/2) * f (eta (x, y)) , u (eta)) : u (eta) := expand (subs (eta (x, y) = y/x^(1/2) , u (eta))) : u (eta) := subs (y = eta * x^(1/2) , u (eta)) ;
```

$$u(\eta) := D(f)(\eta)$$

[D(f)(η) in Maple represents the derivative of f with respect to η . Next, the boundary conditions are expressed in terms of f:]

```
> bc1 := subs (eta = 0 , v (eta)) = 0 ;
```

$$bc1 := \frac{1}{2} \frac{f(0)}{\sqrt{x}} = 0$$

```
> bc1 := -bc1 * 2 * x^(1/2) ;
```

$$bc1 := f(0) = 0$$

```
> bc2 := subs (eta = 0 , u (eta)) = 0 ;
```

$$bc2 := D(f)(0) = 0$$

```
> bc3 := subs (eta = infinity , u (eta)) = 1 ;
```

$$bc3 := D(f)(\infty) = 1$$

[The length of the domain is taken to be 5 (to replace infinity). This number is found by trial and error. Increasing the length beyond 5 does not change the results.]

```
> bc3 := subs (infinity = 5 , bc3) ;
```

$$bc3 := D(f)(5) = 1$$

[For this problem, analytical solutions are not possible (though approximate solutions are possible). For this example, numerical solution for the Blasius equation is obtained as:]

```
> sol := dsolve ({eq2, bc1, bc2, bc3} , f (eta) , type = numeric) ;
```

$$sol := \text{proc } (x_bvp) \dots \text{end proc}$$

[The solution is plotted in Figure 2, which shows how the function, f (related to the stream function) varies with the similarity variable, η from 0 to 5]

```
> odeplot(sol, [eta, f(eta)], 0..5, thickness=3, axes=boxed);
```

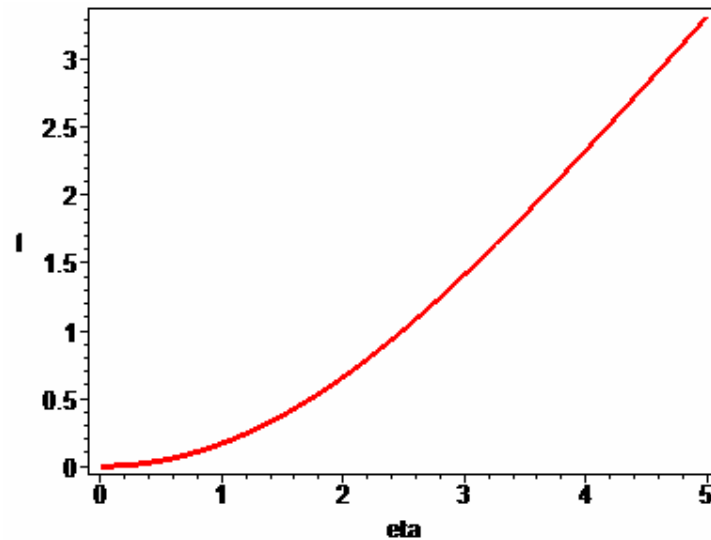


Figure 2: Function f as a function of the similarity variable, η

[Next, velocity profiles are obtained:]

```
> u(eta) := convert(u(eta), diff); v(eta) := convert(v(eta), diff);
```

$$u(\eta) := \frac{d}{d\eta} f(\eta)$$

$$v(\eta) := \frac{1}{2} \frac{f(\eta) - \left(\frac{d}{d\eta} f(\eta) \right) \eta}{\sqrt{x}}$$

[Figure 3 shows how the x component of velocity increases from zero at the wall and levels off at its main stream value for larger values of η from 0 to 5]

```
> odeplot(sol, [eta, u(eta)], 0..5, thickness=3, axes=boxed, labels=[eta, u]);
```

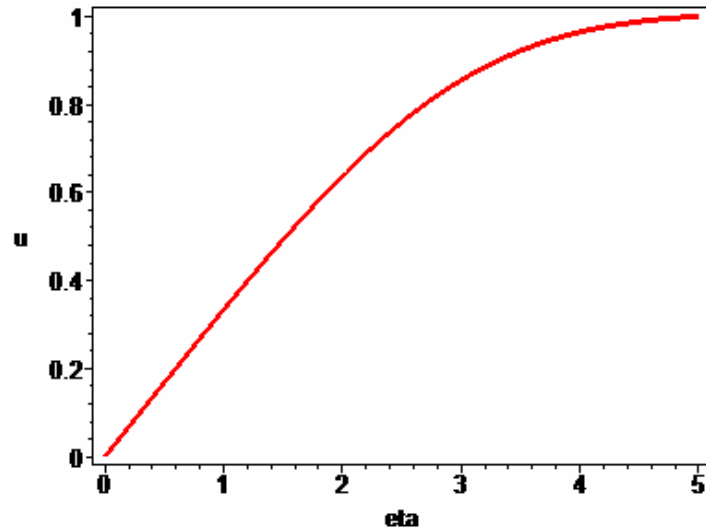


Figure 3: x-component velocity as a function of the similarity variable, η

[Since v is a function of x , $v*x^{1/2}$ is plotted. Figure 4 shows the y component of velocity (multiplied by $x^{1/2}$) increases from zero at the wall and levels off at its main stream value for larger values of η from 0 to 5]

```
>odeplot(sol, [eta, v(eta)*x^(1/2)], 0..5, thickness=3, axes=boxed, labels=[eta, "v*x^(1/2)"]);
```

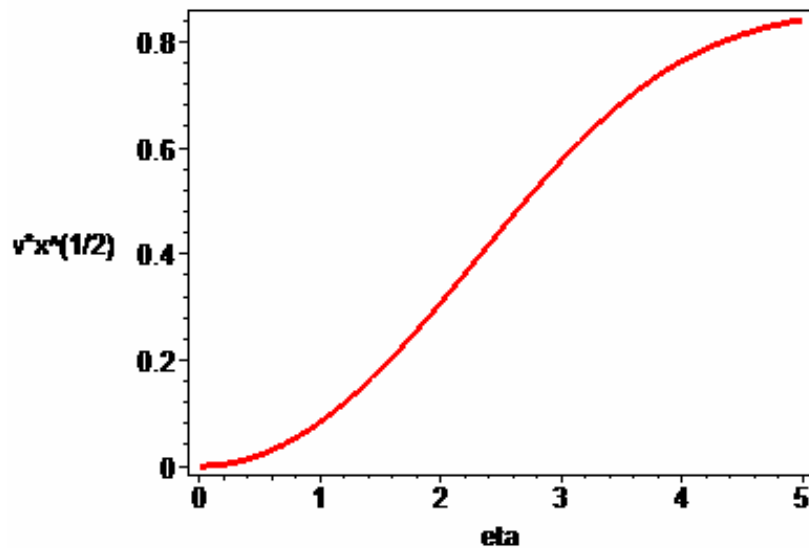


Figure 4: y-component velocity as a function of the similarity variable, η

[The solution at $\eta = 0$ is obtained as:]

```
> sol(0);
```

$$\left[\eta = 0., f(\eta) = 0., \frac{d}{d\eta} f(\eta) = 0., \frac{d^2}{d\eta^2} f(\eta) = 0.336152378983949952 \right]$$

[Stress is related to the Reynolds number (re) and the velocity gradient at $y = 0$:]

> **S:=re*diff(u(x,y),y);**

$$S := re \left(\frac{\partial}{\partial y} u(x, y) \right)$$

[The velocity gradient in terms of the stream function is:]

> **subs(u(x,y)=diff(psi(x,y),y),S);**

$$re \left(\frac{\partial^2}{\partial y^2} \psi(x, y) \right)$$

[The second derivative of the stream function (d) is expressed in terms of f and η :]

> **d:=diff(psi(x,y),y\$2):d:=changevar(psi(x,y)=x^(1/2)*f(eta(x,y)),d):d:=expand(subs(eta(x,y)=y/x^(1/2),d)):d:=subs(y=eta*x^(1/2),d):d:=convert(d,diff);**

$$d := \frac{\frac{d^2}{d\eta^2} f(\eta)}{\sqrt{x}}$$

> **S:=re*d;**

[The second derivative of f is found from the numerical solution:]

> **eqd3:=sol(0)[4];**

$$eqd3 := \frac{d^2}{d\eta^2} f(\eta) = 0.336152378983949952$$

[Hence, the stress-Reynolds number relationship becomes:]

> **S:=subs(diff(f(eta),`\$`(eta,2))=rhs(eqd3),S);**

$$S := \frac{0.336152378983949952 \text{ re}}{\sqrt{x}}$$

Example 3: Graetz Problem in Rectangular Coordinates

Consider the Graetz problem in *rectangular* coordinates (to simplify the mathematical complexity involved with a cylindrical geometry).⁴ The governing equation and initial/boundary conditions are:

$$\begin{aligned} (1-x^2) \frac{\partial u}{\partial z} &= \frac{\partial^2 u}{\partial x^2} \\ u(x,0) &= 1 \\ u(0,z) &= 0 \text{ and } \frac{\partial u}{\partial x}(1,z) = 0 \end{aligned} \quad (4)$$

For this problem, a similarity transformation cannot be used to reduce the partial differential equation to one ordinary differential equation (boundary value problem in η). To obtaining solutions very close to $z = 0$, Equation 4 is converted to the new coordinates defined by $\eta = x/(2\sqrt{z})$ and $z = z$ (note, some textbooks use $z = z_1$ as the second coordinate, but for simplicity it is left as z in this paper). In the new coordinates η and z , u is obtained using a perturbation technique by expressing u as $u = \sum_{i=0}^k z^k f_i(\eta)$. The boundary conditions for f (in the similarity variable η) are:

$$\begin{aligned} f_0(0) = 1; f_k(0) = 1, k = 1, 2, 3... \\ f_0(\infty) = 0; f_k(\infty) = 0, k = 1, 2, 3... \end{aligned} \quad (5)$$

The steps involved in the similarity transformation method are performed in Maple.

```
> restart:with(student):
> eq:=(1-x^2)*diff(u(x,z),z)-diff(u(x,z),x$2);
eq := (1 - x^2)  $\left(\frac{\partial}{\partial z} u(x, z)\right) - \left(\frac{\partial^2}{\partial x^2} u(x, z)\right)$ 
```

[First, the governing equation is converted to similarity variables (η and z):]

```
> eq1:=changevar(u(x,z)=U(eta(x,z),z),eq):eq2:=expand(simplify(subs(eta(x,z)=x/2/(z)^(1/2),eq1))):eq2:=expand(eq2*z):eq2:=subs(x=eta*2*(z)^(1/2),eq2):eq2:=convert(eq2,diff):eq2:=expand(-4*eq2);
eq2 := 2  $\left(\frac{\partial}{\partial \eta} U(\eta, z)\right) \eta - 4 z \left(\frac{\partial}{\partial z} U(\eta, z)\right) - 8 z \eta^3 \left(\frac{\partial}{\partial \eta} U(\eta, z)\right) + 16 z^2 \eta^2 \left(\frac{\partial}{\partial z} U(\eta, z)\right) + \left(\frac{\partial^2}{\partial \eta^2} U(\eta, z)\right)$ 
```

[For illustration, only terms up to z^2 are considered in the perturbation series:]

```
> N:=2;vars:={U(eta,z)=sum(z^k*f[k](eta),k=0..N)};
N:=2
vars := {U(eta, z) = f_0(eta) + z f_1(eta) + z^2 f_2(eta)}
```

[The governing equations for the dependent variables are obtained as:]

```
> eq3:=expand(subs(vars,eq2)):for i from 0 to 2 do
Eq[i]:=coeff(eq3,z,i);od;
```

$$Eq_0 := 2 \eta \left(\frac{d}{d\eta} f_0(\eta) \right) + \left(\frac{d^2}{d\eta^2} f_0(\eta) \right)$$

$$Eq_1 := 2 \eta \left(\frac{d}{d\eta} f_1(\eta) \right) - 4 f_1(\eta) - 8 \eta^3 \left(\frac{d}{d\eta} f_0(\eta) \right) + \left(\frac{d^2}{d\eta^2} f_1(\eta) \right)$$

$$Eq_2 := 2 \eta \left(\frac{d}{d\eta} f_2(\eta) \right) - 8 f_2(\eta) - 8 \eta^3 \left(\frac{d}{d\eta} f_1(\eta) \right) + 16 \eta^2 f_1(\eta) + \left(\frac{d^2}{d\eta^2} f_2(\eta) \right)$$

[The first three terms are obtained by solving these differential equations with the given boundary conditions (note that the boundary condition at $x = 1$ is solved approximately as $U = 0$ at $\eta = \infty$)]

```
> sol[0] := dsolve({Eq[0], f[0](0)=0, f[0](infinity)=1}); assign(sol[0]) :
```

$$sol_0 := f_0(\eta) = \text{erf}(\eta)$$

```
> sol[1] := dsolve({Eq[1]}) ;
```

$$sol_1 := \left\{ \begin{array}{l} f_1(\eta) = (1 + 2 \eta^2) _C2 + (1 + 2 \eta^2) \int \frac{e^{(-\eta^2)}}{(1 + 2 \eta^2)^2} d\eta _C1 + \frac{1}{3} \frac{(-3 \eta - 4 \eta^3) e^{(-\eta^2)}}{\sqrt{\pi}} \end{array} \right\}$$

[The constants have to be zero to satisfy the boundary conditions:]

```
> assign(sol[1]) : _C1:=0 : _C2:=0 : f[1](eta) := eval(f[1](eta)) ;
```

$$f_1(\eta) := \frac{1}{3} \frac{(-3 \eta - 4 \eta^3) e^{(-\eta^2)}}{\sqrt{\pi}}$$

[Similarly f_2 is obtained:]

```
> sol[2] := dsolve(Eq[2]) : assign(sol[2]) : _C3:=0 : _C4:=0 : f[2](eta) := eval(f[2](eta)) ;
```

$$f_2(\eta) := \frac{1}{180} \frac{(-285 \eta - 570 \eta^3 - 384 \eta^5 - 160 \eta^7) e^{(-\eta^2)}}{\sqrt{\pi}}$$

[Once the functions (the f 's) are obtained, the Sherwood number can be obtained:⁴]

```
> u := subs(vars, U(eta, z)) : u := subs(eta=x/2/sqrt(z), u) ;
```

$$u := \operatorname{erf}\left(\frac{x}{2\sqrt{z}}\right) + \frac{1}{3} \frac{z \left(-\frac{3x}{2\sqrt{z}} - \frac{x^3}{2z^{(3/2)}} \right) e^{\left(-\frac{x^2}{4z}\right)}}{\sqrt{\pi}}$$

$$+ \frac{1}{180} \frac{z^2 \left(-\frac{285x}{2\sqrt{z}} - \frac{285x^3}{4z^{(3/2)}} - \frac{12x^5}{z^{(5/2)}} - \frac{5x^7}{4z^{(7/2)}} \right) e^{\left(-\frac{x^2}{4z}\right)}}{\sqrt{\pi}}$$

[The dimensionless temperature distribution is plotted in Figure 5, which shows that the temperature increases from the center of the slab to the surface value along the x-coordinate. The increase in temperature is more rapid at the entrance and temperature increases are more gradual for higher values of z from 0 to 0.05, the distance along the flow]

```
>plot3d(u,x=1..0,z=0.05..0,axes=boxed,labels=[x,z,"u"],orientation=[120,60]);
```

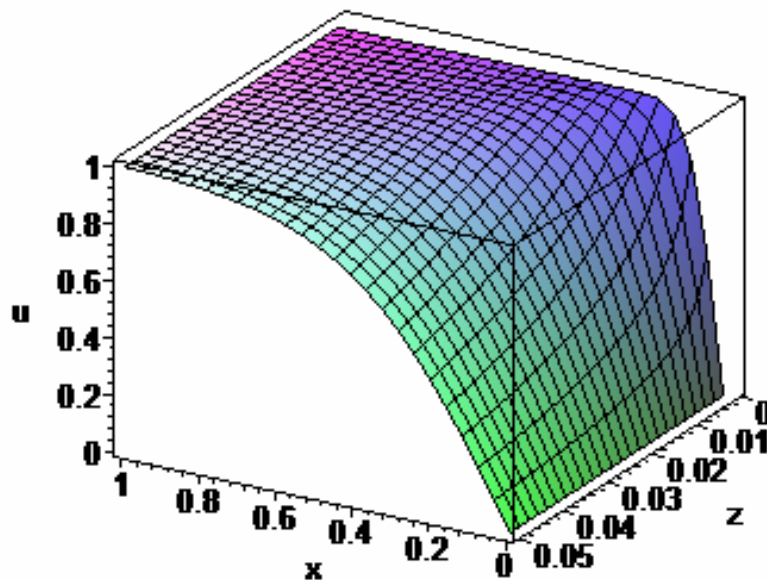


Figure 5: Dimensionless temperature distribution in rectangular coordinates, governed by the Graetz equation

Summary

The similarity solution approach is a very powerful technique for obtaining closed-form solutions for problems in heat, mass or momentum transfer and other disciplines in chemical engineering. A traditional approach to teach this technique would involve doing the complicated

variable transformations and integrals by hand. In this paper, we showed how an analytical technique could be facilitated using computers and software. While Maple has been used in this paper, Mathematica, MATLAB, REDUCE or other symbolic software packages can be used to obtain similar results. In addition to teaching numerical simulation, computers and software packages can be used to teach classical mathematical methods for a wide variety of problems. Mathematical methods such as those separations of variables, Laplace transform, perturbation, conformal mapping, Green's function, analytical method of lines, and series solutions for nonlinear problems (multiple steady states) can be facilitated using Maple. Interested readers can contact the author for further details or copies of related Maple programs. Some of these methods are illustrated in a book to be published.⁹

This paper illustrates that mathematical methods for non-trivial problems in chemical engineering can be taught efficiently in a class by using computers and user-friendly software.

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