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A Geometric Level Set Method for Transcendental Equations from Chemical Engineering

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When trying to solve a single transcendental equation $f(x, a) = 0$ that depends on two parameters x and a, we have found the standard root finders such as bisection and Newton's method lacking within the parameter range of a with multiple roots. Here we propose, implement, and test a level set method for solving parameterized transcendental equations with bifurcation. We create the elevation matrix data $Z = f(x, a) \in \mathbb{R}^{n,n}$ for x and a data vectors in $\mathbb{R}^n$ and draw the level zero contour curve for the associated surface $(x, a, f(x, a)) \in \mathbb{R}^3$ via data interpolation. The method is very simply implemented via MATLAB's built-in `contour` command. It works exceedingly well and is much faster than using standard root finders that generally fail do give useful information near the bifurcation points or using continuation methods.

Introduction

The modeling and design of chemical plants and processes relies on solving equations, algebraic, rational, transcendental, differential, integral etc. Equations in a single real variable x have been solved successfully for a long time by using inclusion/bisection algorithms or tangent inspired algorithms such as the secant and more sophisticated methods that use derivative information as Newton's method and all of its variants. We refer to Fausett (1999) and Engeln-Müllges and Uhlig (1996) for example.

When studying parameterized transcendental equations for simple chemical engineering processes, a shortcoming of the classical root finding algorithms becomes apparent when there are multiple roots. This is the case whenever the plant is operated at a point with multiple steady states. In this case, the classical root finders Cheney and Kincard (2004), Sastry (2006), and Balaji and Seader (1995) generally fail to find all the steady states and they cannot find the bifurcation points reliably. This leads us to investigate graphical means, to elevation matrices for the equation and to the level set method for transcendental equations.

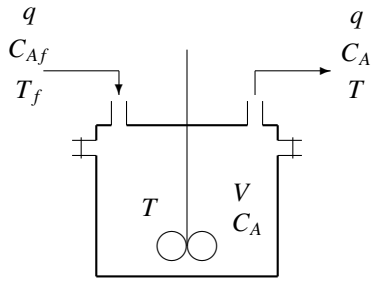
Chemical Engineering Framework for Problems with Static Bifurcation

Almost all problems faced by chemical and biochemical engineers are non linear. One of the simplest practical examples is the homogeneous non-isothermal and adiabatic *continuous stirred tank reactor*, called CSTR for short.

The steady states of a CSTR are described by non linear transcendental equations. If we consider the simple reaction

$$A \implies B$$

Figure 1. Schematic diagram of an adiabatic CSTR



in an adiabatic CSTR, then the rate of reaction is given by

$$r \;=\; k_0 \cdot e^{-E/(R\cdot T)} \cdot C_A \;.$$

Assuming a constant volume V and a constant volumetric flow rate q in the CSTR, the steady state equations are

$$q \cdot C_A = q \cdot C_{Af} - V \cdot k_0 \cdot e^{-E/(R\cdot T)} \cdot C_A \qquad (1)$$

and

$$q \cdot \rho \cdot C_p \cdot (T - T_f) \;=\; V \cdot k_0 \cdot e^{-E/(R\cdot T)} \cdot C_A \cdot (-\Delta H) \qquad (2)$$

Here

q = volumetric flow rate, in l/min ;
C_A = reactant concentration at the exit and at every point in the CSTR, in mole/l ;
ρ = mixture average (constant) density, in g/l ;
C_p = mixture average (constant) specific heat, in cal/g·K ;
C_{Af} = reactant feed concentration, in mol/l ;
V = active reactor volume; in l ;
k_0 = frequency factor for the reaction, in 1/min ;

E = reaction activation energy, in J/mole ;
R = general gas constant, in J/(mole·K) ;
T = temperature at the exit and at every point in the CSTR, in K ;
T_f = feed temperature, in K ;
ΔH = heat of reaction, in J/mole .
By multiplying the material balance design equation by $(-\Delta H)$ and adding it to the heat balance design equation we obtain a simple linear relation between T and C_A, namely

$$C_A = C_{Af} + \rho \cdot C_p \cdot (T_f - T)/(-\Delta H) . \quad (3)$$

Thus the two model equations (1) for our problem can be replaced by the following simple equation in T:

$$q \cdot \rho \cdot C_p \cdot (T - T_f) = \quad (4)$$
$$V \cdot k_0 \cdot e^{-E/(R \cdot T)} \cdot \{C_{Af} + \rho \cdot C_p \cdot (T_f - T)/(-\Delta H)\} \quad (5)$$
$$\cdot(-\Delta H) \quad (6)$$

And C_A can be retrieved from the solution of (4) by using formula (3).

Our single model equation (4) has the the form

$$R(T) = G(T) ,$$

where $G(T)$ is the transcendental heat generating function of the reaction on the right hand side and $R(T)$ is the linear heat removal function on the left hand side of the previous heat design equation. To illustrate the behavior of the solutions to this transcendental heat balance design equation, we plot both $G(T)$ and $R(T)$ against T.

Figure 2. Heat generation function $G(T)$ and heat removal function $R(T)$

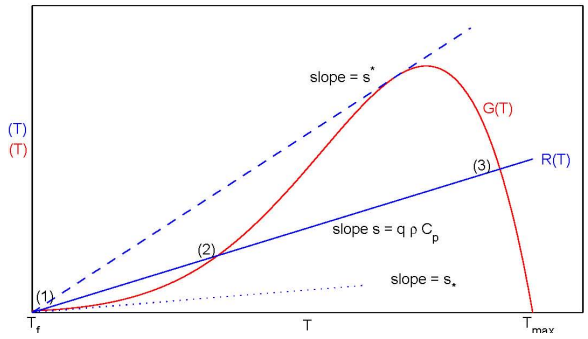


Figure 2 shows that in a certain region of the parameter $s = q \cdot \rho \cdot C_p$, the adiabatic CSTR has three steady states, marked by (1), (2), (3) in the plot, where the line $R(T)$ and the curve $G(T)$ intersect. From a steady state analysis point of view, the steady states (1) and (3) are stable, while the middle steady state (2) is unstable. The solution behavior in Figure 2 is called bifurcation. The **bifurcation points** for the parameter s are determined by the tangent lines that represent $R(T)$ in the plot with dashed and dotted extreme slopes s^* and s_*. For any slope $s_* < s < s^*$ there are three steady states, while for any $s > s^*$ there is only one low temperature steady state near (1) and for any $s < s_*$ there is only one steady state solution for a large temperature T near T_{max}.

The equation $R(T) = G(T)$ can be put into dimensionless form by dividing both sides by $q \cdot \rho \cdot C_p \cdot T_f$ to become

$$y - 1 = \alpha e^{-\gamma/y}(1 + \beta - y) . \quad (7)$$

Here we have set $y = \dfrac{T}{T_f}$, $\alpha = \dfrac{V \cdot k_0}{q}$, $\gamma = \dfrac{E}{R \cdot T_f}$, and $\beta = \dfrac{(-\Delta H) \cdot C_{Af}}{\rho \cdot C_p \cdot T_f}$, where y denotes the dimensionless temperature, α is the dimensionless pre-exponential factor, β is the thermicity factor, and γ is the dimensionless activation energy.

Given CSTR specific β and γ values, our task is to solve the transcendental equation (7) for y on an interval of α values for which there are multiple solutions.

Solution by Classical Root Finders

In this section, we try to find the values of y in equation (7) that correspond to the points labeled (1), (2), and (3) in Figure 2 for a given interval $(\alpha_1, \alpha_2) \subset \mathbb{R}$ with multiplicity and fixed β and γ. We first use a generic root finder such as the bisection method that is available as the built-in MATLAB function `fzero`.
The standard form $f(y) = 0$ of equation (7) is

$$f(y) = y - 1 - \alpha e^{-\gamma/y}(1 + \beta - y) = 0 . \quad (8)$$

Figure 3. Solutions to equation (8) using MATLAB's bisection method `fzero` for $\beta = 1$ and $\gamma = 8.5$

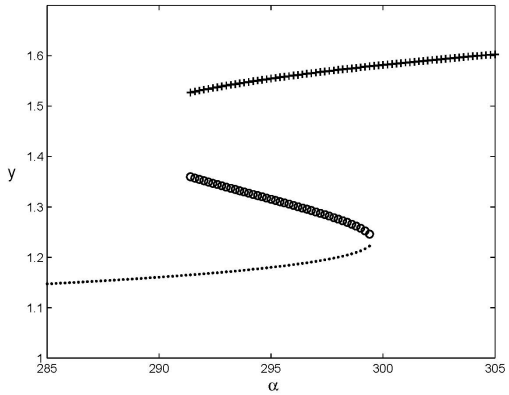


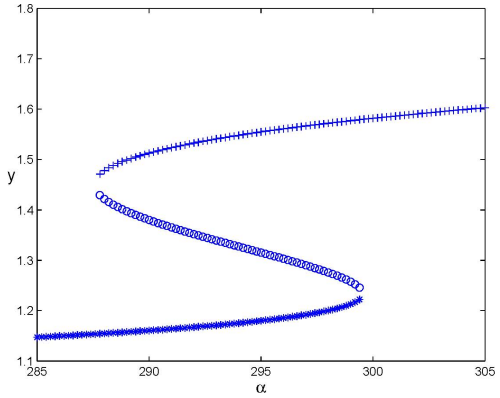
Figure 3 was obtained by starting `fzero` from the extreme relative temperature values $y = 1$ and $y = 1 + \beta$ and fixed

α. If `fzero` finds two separate roots of equation (8) for one α, then `fzero` is again used to look for the middle root starting from the average of the two solutions. This is executed for $n = 100$ linearly increasing α values from $\alpha_1 = 285$ to $\alpha_2 = 305$ for the fixed CSTR parameters $\beta = 1$ and $\gamma = 8.5$ in Figure 3. For approximately all $\alpha < 292$, the bisection algorithm fails to find any roots of (8) other than the low y value one, even when starting from $y = 1 + \beta$. Similarly for all $\alpha > 299$, the only solutions found from the low temperature starting point $y = 1$ by bisection are the high temperature ones. This gives rise to the disconnected solution curve of Figure 3. Note also that as soon as two distinct solutions are found for one α, then the middle solution guess of $\frac{y_{sol_{top}} + y_{sol_{bot}}}{2}$ produces a middle solution of (8) when using MATLAB's `fzero`. Refining the size of α steps by choosing $n = 1000$ and smaller α steps, for example, does not affect the size of the gaps in Figure 3 at all.

The relatively large gaps in Figure 3 between the three branches of the bifurcation curve are typical of inclusion/bisection algorithms in the face of multiple roots. These algorithms generally fail to supply any useful information on the bifurcation points.

Our next classical trial method for solving the transcendental equation (8) is Newton's method. The following figure is obtained in MATLAB when using Newton's method for equation (8).

Figure 4. Solutions to equation (8) using Newton's method for $\beta = 1$ and $\gamma = 8.5$



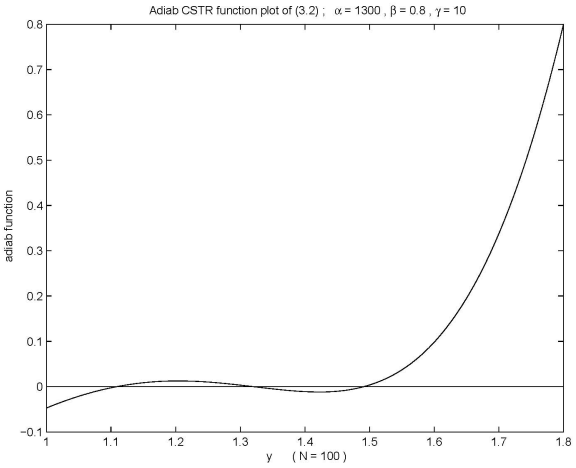
The graph above looks much better since the gaps between the three branches are smaller than those in Figure 3. But the gaps near the bifurcation points can apparently not be filled via Newton's method either.

Graphical Solution via the Level Set Method

Here we develop a faster and more reliable method, the *level set method*, for finding all y values that solve equation (8) for a given α parameter interval. We proceed in three stages.

First we determine the range of α for which there are multiple steady states. To illustrate, we look at Figure 5 with the graph of f in equation (8) with $\alpha = 1300$, $\beta = 0.8$, and $\gamma = 10$.

Figure 5. Graph of f in equation (8) for $\alpha = 1300$, $\beta = 0.8$ and $\gamma = 10$



To solve equation (8) for this data we need to find the roots of the graph depicted in Figure 5. There are three shallow intersections of the horizontal axis $(y, 0)$ in the plane with the graph $(y, f(y)) \in \mathbb{R}^2$ of f. The more shallow these intersections become, the more unsatisfactory our computation of roots becomes, using standard root finding methods such as the inclusion/bisection method or the Newton root finder.

Therefore we turn to graphical solution methods in this section. We *first* find the bifurcation limits for a given data set α, β, γ semi-graphically by using the previous figure as our guide and relying on a slight variant of equation (7), namely

$$\frac{1}{\alpha}(y-1) \;=\; e^{-\gamma/y}(1+\beta-y) \;\; (\,=\;\tilde{f}(y))\,. \qquad (9)$$

The left hand side of equation (9) describes a line with slope $1/\alpha$ in the variable y that contains the point $(y, \tilde{f}) = (1, 0)$. The right hand side is exponential in y with $(y, \tilde{f}) = (1, e^{-\gamma} \cdot \beta)$ on its graph and $e^{-\gamma} \cdot \beta > 0$. The MATLAB algorithm that we use to find the range of α values with multiple crossings limits the search for tangents from $(1, 0) \in \mathbb{R}^2$ to the graph of the exponential curve $\tilde{f}$ to y values below the maximum of the right hand side of equation (9). It then slides backwards along the curve, computing the

maximal and minimal ratios of $\tilde{f}$ and y, i.e., it effectively computes good approximations to the two extreme slopes $1/\alpha_1$ and $1/\alpha_2$ of tangent lines to the graph of $\tilde{f}$ that pass through the point $(1, 0)$, see Figure 6. The essential lines of our MATLAB code for finding the bifurcation points are

```
y = [1:(bt/N):1+bt];   b = 1;
   % y partition, N steps;
   %   b is a bifurcation marker
if bt < 0, y = y(1:N); N = N-1; end
   % if bt < 0, we avoid division by zero
f = exp(-ga./y).*((1+bt)-y);
   % exponential part of adiabatic non-iso
   %   equation (right side of (3) )
F = max(f); i = find(f == F);
   % limit search for bifurcation to
   %   1 <= y <= max(f) location
if i == 1, disp('no bifurcation alphas for this
    data'),
   % if no bifurcation
    al1 = 50; al2 = 1000; b = 0; end
   % set default output
y = y - 1;
   % shift y by 1
foyold = f(2)/y(2); k = 3; mi = 1;  ma = 1;
   % initialize
while (k < i & mi == 1)
   % search for a min (=al2) of 1/al
    if f(k)/y(k) < foyold, foyold = f(k)/y(k);
    k=k+1; else mi = 0; end, end,
if (k >= N | k >= min(i)), disp('no bifurcation
   alphas for this data'),
    al1 = 50; al2 = 1000; b = 0; else,
   % no bifurcation: set default output
    al2 = (y(k-1))/f(k-1); y0 = y(k-1)+1;
    f0 = f(k-1); end
while (k < i & ma == 1)
   % search for a max (=al1) of 1/al
    if f(k)/y(k) > foyold, foyold = f(k)/y(k);
    k=k+1; else, ma = 0; end, end
al1 = (y(k-1))/f(k-1);
```

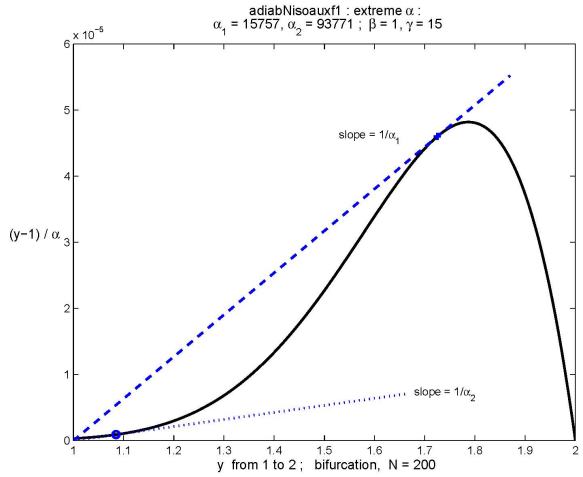
The reciprocals of the extreme slopes then give us the extreme parameters α_1 and α_2 as the bifurcation points for equation (9). In Figure 6 the bifurcation limits α_1 and α_2 are displayed numerically in the plot's title, as well as drawn out on the graph by a little o and + mark, respectively, for $\beta = 1$ and $\gamma = 15$.

Following our first step of finding the bifurcation points α_1 and α_2, we *secondly* form the *elevation matrix*

$$Z = F(\alpha, y) = y - 1 - \alpha e^{-\gamma/y}(1 + \beta - y) \in \mathbb{R}^{n,n} \qquad (10)$$

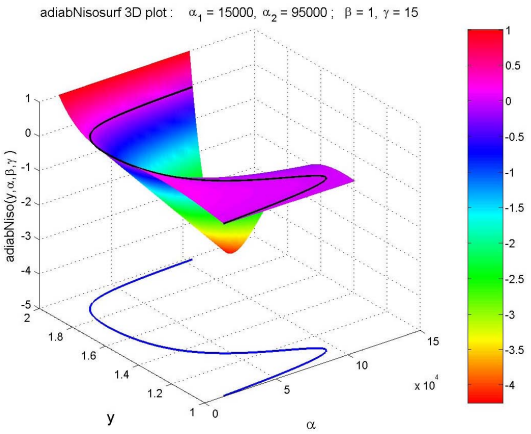
as a function of two discrete variable n-vectors in α and y for the physically relevant range $0.9 \cdot \alpha_1 \le \alpha \le 1.1 \cdot \alpha_2$ and $1 \le y \le 1 + \beta$. This includes the parameter interval $(\alpha_1, \alpha_2) \subset \mathbb{R}$ in which there is bifurcation. The equation (10) with $z = F(\alpha, y) = 0$ re-interprets our earlier equation (8) $f(y) = 0$ by replacing the repeated 1-dimensional root finding attempts with varying α values in bisection or

Figure 6. Bifurcation limits for equation (8) for $\beta = 1$ and $\gamma = 15$



Newton by a 2-dimensional direct approach to root finding in the two variables α and y. The elevation matrix $Z \in \mathbb{R}^{n,n}$ is displayed graphically in MATLAB as a 3D surface over the relevant α-y rectangle in Figure 7. *Thirdly*, the bifurcation curve of all solutions to the four equivalent equations (7) to (10) relate y and α. This curve is the projection of the level zero curve $F(\alpha, y) = 0$ of the elevation matrix surface Z onto the α-y plane where the height $z = 0$. Our 3D plot of the surface $(\alpha, y, F(\alpha, y))$ in Figure 7 contains this level curve marked in black on the surface, as well as a second, isolated plot of it below the surface in blue.

Figure 7. Surface of the elevation matrix $Z = F(\alpha, y)$ and its level zero contour plots for $15000 \le \alpha \le 95000$, $\beta = 1$ and $\gamma = 15$ obtained from equation (10)



In Figure 7 note the very shallow and flat topography of the elevation surface for F above the sub-rectangle $1 \le y \le 1.2$ and $50,000 \le \alpha \le 100,000$ that is problematic for the classical root finders.

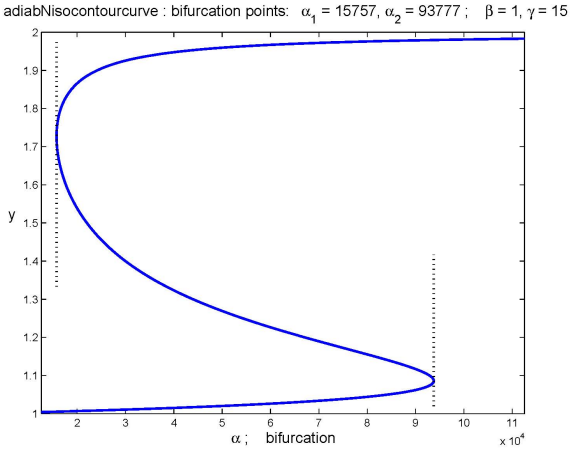
MATLAB finds a contour curve of a surface by interpolating the surface data and it does so very efficiently and accurately, even for "shallow or flat data". On the other hand, the relatively steep slopes at surface points with high y values near $1+\beta$ in our plot help explain why the classical root finding methods can easily overshoot the high or low y value roots near the bifurcation points.

Figure 8 gives a detailed plot of the level zero curve of the solutions to $F(\alpha, y) = 0$.
The numerically active part of the MATLAB code that draws the bifurcation curve plot in Figures 7 and 8 consists of four lines

```
[y,al] =
meshgrid([1:bt/N:1+bt],[0.8*a11:(1.2*a22-0.8*a11)/
   N:1.2*a22]);
 % make grids for y and alpha in relevant ranges
     for y and beta
z = adiabNiso(y,al,bt,ga);
   % z = adiab Non-iso function value
C = contour(al,y,z,[0 0],'b');
```

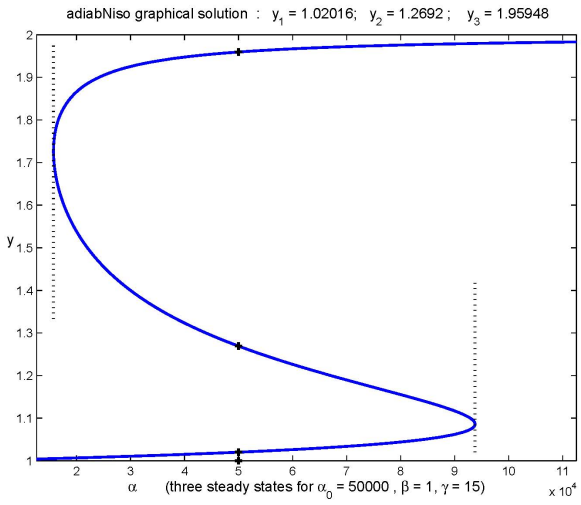
once the bifurcation points α_1 (= $a11$) and α_2 (= $a22$ in the above code) have been found as detailed earlier.

Figure 8. Level zero contour plot for F in equation (10) for $10,000 \le \alpha \le 110,000$, with $\beta = 1$ and $\gamma = 15$



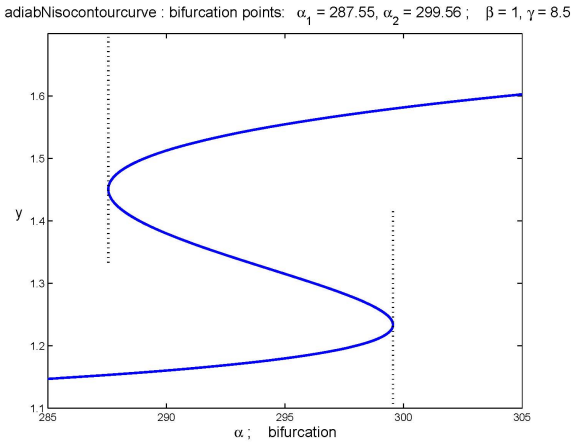
The numerical values for the steady state temperatures y at one specific α value can be found by further 2D interpolation of the level zero curve. A typical result is depicted in red in Figure 9 for $\alpha = 50,000$ and $\beta = 1$, $\gamma = 15$.
For a comparison of the methods, in Figure 11 we have superimposed the data from the bisection algorithm of Figure 3 (with circle symbols) on top of the level set method's graphical output depicted by the solid line in Figure 10 below which depicts the level method solution curve for $\beta = 1$ and $\gamma = 8.5$.

Figure 9. Level zero contour plot for F in equation (10) for $10,000 \le \alpha \le 110,000$, $\beta = 1$ and $\gamma = 15$; with steady state temperatures y_1, y_2, and y_3 for $\alpha = 50,000$



And likewise in Figure 12 for the output of Newton's algorithm from Figure 4 (with star symbols) and the level set method result, both times for $\beta = 1$ and $\gamma = 8.5$.

Figure 10. Bifurcation curve of the level set method for $\beta = 1$ and $\gamma = 8.5$



Figures 10 to 12 make it obvious that the level set method gives much more meaningful numerical results and a clearer graphical representation of the multiple steady state solutions of the CSTR problem described by equations (7) to (10).
By all appearances the level set method is far more reliable near the bifurcation points and surpasses and supersedes our initial more generic root finding attempts.
In Figures 10 to 12, the bifurcation points were determined

Figure 11. Bifurcation curve: level set method (solid line –); bisection method (circles ∘)

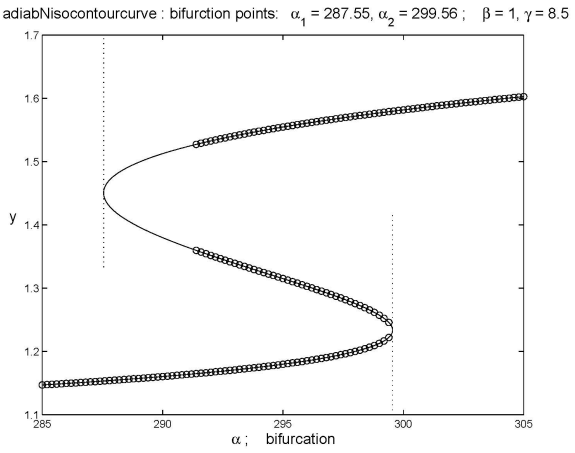
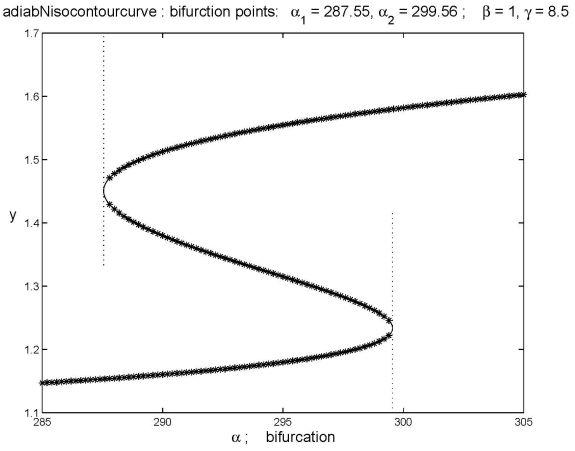


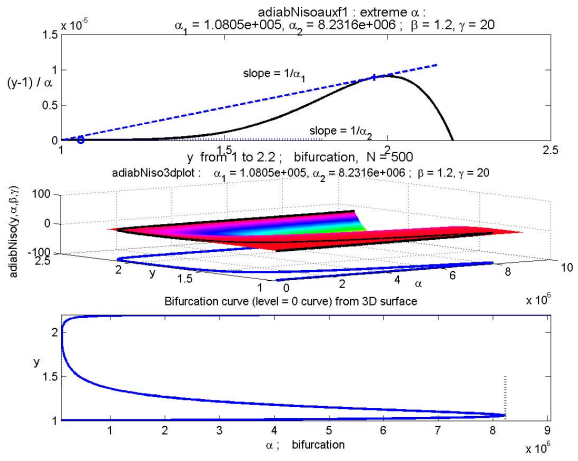
Figure 12. Bifurcation curve: level set method (solid line –); Newton method (stars ∗)



numerically by exploiting the graphical situation of Figure 6. The two bifurcation points for α are indicated by two dotted vertical lines. A visual inspection shows a perfect match between the computed bifurcation points α_1 and α_2 and the extremes of the solution function excursions. Moreover, our graphically obtained data and that obtained from the bisection or Newton's algorithm are perfectly consistent with the part of the graph where bisection data or Newton data are available.

Finally, we depict the three level curve generating plots in one composite figure. Having given consideration to relatively low parameter values, such as $\beta = 1$ and $\gamma = 8.5$ which have a small α range with bifurcation, we now choose a set of relatively large parameters $\beta = 1.2$ and $\gamma = 20$ that shows the wide dynamic range of the bifurcation points α_i, depending on the particular CSTR reaction.

Figure 13. Combined plot of the function graph, the elevation matrix graph, and the level zero contour plot for F in equation (10) for $10,000 \le \alpha \le 9,000,000$, $\beta = 1.2$ and $\gamma = 20$



Conclusions

It has become customary to try and use continuation methods to solve parameterized equations with bifurcation. However, one drawback to continuation, especially for these equations from chemical engineering is the relative difficulty of finding feasible starting values for the continuation process itself, i.e, to obtain one point on each branch of the family of solution curves. This generally requires a user interface and may be difficult to accomplish.
In contrast, the *level set method* needs no user interface, no knowledge of feasible starting points for continuation, nor any knowledge of the number of branches of the solution curve. The level set method is entirely self-contained in the three MATLAB code lines

```
... meshgrid ...;
... surface ....;
...contour ...
```

that were mentioned earlier. These three code lines automatically give the right answers to all such problems and they do so very quickly.

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