CHAPTER 7

OPTIMISATION OF A PACKED COLUMN USING THE DYNAMIC TRAJECTORY METHOD

1. INTRODUCTION

Reactor 6 as described in Chapter 1 could consist of any type of vessel in which the mixture could be heated and well mixed. The reaction that takes place is the transferral of solid particles from the aqueous phase to the hydrocarbon phase. A good choice of reactors would be a packed column heated from the outside. The packed column should provide ample area for the phase transfer. The column as discussed in this chapter is constructed from glass and is packed with glass beads which provide a large surface area for reaction. In order to achieve the phase transfer, heat is required to be input into the system. The column would therefore be heated via electrical heating bands wound around the shell. To obtain the maximum heat transfer at the maximum allowable temperature, the surface area in the column should be at a maximum.

The condition for the optimum temperature progression in a given type of reactor is that the system should be maintained at a temperature where the rate is a maximum. [38] The peptization reaction is endothermic i.e. heat is required to be input into the reaction mixture for most efficient phase transfer. For endothermic reactions, a rise in temperature increases both the equilibrium conversion and the rate of reaction. The maximum possible temperature should thus be used in the process (subject to constraints e.g. no liquid should be boiled off in the process). The heat is transferred to the mixture via the glass beads. The conduction rate (q) is given by eq. (7.1):

$$q = -kA\frac{dT}{dx} \tag{7.1}$$

where k is the thermal conductivity, A is the cross sectional area and $\frac{dT}{dx}$ is the temperature gradient.

From eq. (7.1) it can be seen that to obtain the maximum heat transfer at the maximum allowable temperature, the surface area in the column should be at a maximum.

This chapter documents the procedure of mathematical optimisation using the dynamic trajectory method to determine the optimum column geometry for maximum heat transfer. In this investigation, the reliability of the optimisation algorithm is also tested.

2. AN OVERVIEW OF MATHEMATICAL OPTIMISATION

Mathematical optimisation involves converting a verbal description of a problem into a well-defined mathematical statement. This transcription occurs in three steps: [39]

- identifying the set of variables that describe the system,
- establishing a criterion called the objective function f to determine whether or not a given design is better than another and
- specifying the set of constraints governing the system.

The optimisation problem has the following general mathematical form: [40]

$$\underset{\text{with respect to } x}{minimise}\ f(\mathbf{x}),\ \mathbf{x} = (x_1, x_2, ..., x_n) \in R^n \tag{7.2}$$

and is subject to the following constraints:

$$g_j(\mathbf{x}) \leq 0 \quad j = 1,2,...,m \tag{7.3}$$

$$h_j(\mathbf{x}) = 0 \quad j = 1,2,...,r < n \tag{7.4}$$

where $f(\mathbf{x})$, $g_j(\mathbf{x})$ and $h_j(\mathbf{x})$ are scalar functions of $\mathbf{x}$.

$f(\mathbf{x})$ is the objective function where $\mathbf{x} = (x_1, x_2, ... x_n)$ represents the vector of the design variables i.e. all the possible solutions

$g_j(\mathbf{x})$ represents the jth inequality constraint

$h_j(\mathbf{x})$ represents the jth equality constraint0

The vector $\mathbf{x}$ that minimises $f(\mathbf{x})$ subject to the given constraints is denoted by $\mathbf{x}^*$ with the corresponding optimum function value $f(\mathbf{x}^*)$.

The values of $f(\mathbf{x})$, $g_j(\mathbf{x})$ and $h_j(\mathbf{x})$ at any point, $\mathbf{x} = (x_1, x_2, ... x_n)$, may be obtained from analytical known formulae, from a computational process or from measurements of the physical process.

Solving engineering optimisation problems may be difficult for a number of reasons: [40]

- evaluation of the objective and constraint functions may be computationally very expensive,
- numerical noise may exist in the objective and constraint functions,
- there may be discontinuities in the functions,
- the objective and constraint functions may possess areas where they are undefined and
- the problem to be solved may have more that one local minimum.

In order to address these problems, a number of different optimisation algorithms and methods have been developed. For this optimisation problem, the dynamic trajectory methods for unconstrained minimisation by Snyman (also called the "leap-frog" method) will be used. The code LFOPCV3 (leap-frog algorithm for constrained problems) used in the problem was modified for the application. [40]

3. DYNAMIC TRAJECTORY METHOD FOR UNCONSTRAINED MINIMISATION

The basic dynamic trajectory model is based on the following argument:

Assume a particle of unit mass in an n-dimensional conservative force field, with the potential energy at $\mathbf{x}$ given by $f(\mathbf{x})$. The particle can "roll" up or down a "hill". The hill represents the function. The objective is for the particle to roll down to the bottom of the hill i.e. to a minimum. At $\mathbf{x}$, the force on the particle is given by $\mathbf{a} = \ddot{\mathbf{x}} = -\nabla f(\mathbf{x})$. For the time interval [0,t], the conservation of energy holds

$$\frac{1}{2}\|\dot{\mathbf{x}}(t)\|^2 - \frac{1}{2}\|\dot{\mathbf{x}}(0)\|^2 = -[f(\mathbf{x}(t)) - f(\mathbf{x}(0))] \quad (7.5)$$

$$\frac{1}{2}\|\dot{\mathbf{x}}(t)\|^2 - \frac{1}{2}\|\dot{\mathbf{x}}(0)\|^2 = f(\mathbf{x}(0)) - f(\mathbf{x}(t)) \quad (7.6)$$

or $$\frac{1}{2}\|\dot{\mathbf{x}}(t)\|^2 + f(\mathbf{x}(t)) = \frac{1}{2}\|\dot{\mathbf{x}}(0)\|^2 + f(\mathbf{x}(0)) \quad (7.7)$$

$$\begin{aligned}\|\mathbf{x}\| &= \|(x_1, x_2, \ldots, x_n)\| \\ &= \sqrt{x_1^2 + x_2^2 + \ldots + x_n^2}\end{aligned} \quad (7.8)$$

let $$\frac{1}{2}\|\dot{\mathbf{x}}(t)\|^2 = T(t) \quad (7.9)$$

and $$\frac{1}{2}\|\dot{\mathbf{x}}(0)\|^2 = T(0) \quad (7.10)$$

then $$T(t) + f(t) = T(0) + f(0) = constant \quad (7.11)$$

or $$\Delta f = -\Delta T \quad (7.12)$$

From (7.11) it can be seen that as long as T increases, the potential energy f decreases as the particle rolls down the hill (function) with increasing velocity, moving to a region of lower potential energy. This is the basis of the dynamic trajectory algorithm.

The dynamic trajectory method has the following properties:

- It uses only function gradient information and no explicit line searches are performed to determine the value of the function at a particular point. The method is robust and can handle discontinuities in functions and gradients and steep valleys in terms of the shape of the function.
- This algorithm seeks a low local minimum and can therefore be used in a methodology for global optimisation.
- The method is, however, not as efficient on smooth and near quadratic functions as some of the more classical optimisation methods. [40]

3.1 Basic algorithm for unconstrained problems

For unconstrained problems i.e. where no constraints exist and all points $\mathbf{x}$ are feasible where the function is defined, the code LFOP1(b) may be used. With $f(\mathbf{x})$ defined and a starting point, $\mathbf{x}(0) = \mathbf{x}^0$ given, the dynamic trajectory is computed by solving the initial value problem:

$$\ddot{\mathbf{x}} = -\nabla f(\mathbf{x}(t)) \tag{7.13}$$

$$\dot{\mathbf{x}}(0) = 0 \tag{7.14}$$

$$\mathbf{x}(0) = \mathbf{x}^0 \tag{7.15}$$

In computing the trajectory, $\dot{\mathbf{x}}(t)$ must be monitored because as long as T (which is $\frac{1}{2}\|\dot{\mathbf{x}}(t)\|^2$) increases, $f(\mathbf{x}(t))$ decreases. When $\|\dot{\mathbf{x}}(t)\|$ decreases i.e. the particle starts rolling up the hill (function), an interfering strategy must be applied to extract some energy to increase the likelihood of descent of the particle to the bottom of the hill.

In practice the numerical integration of the initial value problem by the "leap-frog" method is performed as follows:

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \mathbf{v}^k \Delta t \tag{7.16}$$

$$\mathbf{v}^{k+1} = \mathbf{v}^k + \mathbf{a}^{k+1} \Delta t \tag{7.17}$$

where $\mathbf{a}^k = -\nabla f(\mathbf{x}^k)$ and $v^0 = \frac{1}{2} a^0 \Delta t$ for k=0, 1, 2, ... and time step Δt.

A typical interfering strategy would be as follows:

If $\|\mathbf{v}^{k+1}\| \geq \|\mathbf{v}^k\|$ continue, else set $\mathbf{v}^k = \dfrac{\mathbf{v}^{k+1} + \mathbf{v}^k}{4}$ and $\mathbf{x}^k = \dfrac{\mathbf{x}^{k+1} + \mathbf{x}^k}{2}$ to compute a new $\mathbf{v}^{k+1}$ before continuing.

3.2 Basic algorithm for constrained problems

In certain problems, constraints are imposed on the feasible region via expressions (7.3) and (7.4). When constraints exist, the unconstrained optimisation algorithm LFOP1(b) can be applied to the constrained problem if this problem is reformulated in terms of the penalty function formulation. $P(\mathbf{x})$, the penalty function, is a combination of the original function and the constraints i.e.

$$\text{Minimise} \qquad P(\mathbf{x}) \tag{7.18}$$

$$\text{where} \quad P(\mathbf{x}) = f(\mathbf{x}) + \sum_{i=1}^{m} \rho_i h_i^2(\mathbf{x}) + \sum_{j=1}^{r} \beta_j g_j^2(\mathbf{x}) \tag{7.19}$$

$$\text{and} \qquad \rho_i >> 0 \qquad \beta_j = \begin{cases} 0 & \text{if } g_j(\mathbf{x}) \le 0 \\ \mu_j >> 0 & \text{if } g_j(\mathbf{x}) > 0 \end{cases} \tag{7.20}$$

ρ_i and μ_j are penalty parameters. Often $\rho_i = \mu_j =$ constant $= \rho$ for all i and j and the penalty function is then denoted by $P(\mathbf{x}, \rho)$ where typically, $\rho = 10^4$.

The code used for constrained optimisation is LFOPCV3. LFOPCV3 is the application of LFOP1(b) to the penalty function formulation. There are three phases in this code as described below.

In the first phase, the overall penalty parameter $\rho = \rho_0$ is set to equal 10^2. Using some $\mathbf{x}^0$, LFOP1(b) is applied to $P(\mathbf{x}, \rho_0)$ to give $\mathbf{x}^*(\rho_0)$.

In the second phase, $\mathbf{x}^0 = \mathbf{x}^*(\rho_0)$. The penalty parameter is increased, $\rho = \rho_1 = 10^4$ and LFOP1(b) is applied to $P(\mathbf{x}, \rho_1)$ to give $\mathbf{x}^*(\rho_1)$. The active constraints are identified $i_a = 1, 2, \ldots n_a$; $g_{i_a}(\mathbf{x}^*(\rho_1)) > 0$.

In the third phase, $\mathbf{x}^0 = \mathbf{x}^*(\rho_1)$ and LFOP1(b) is used to minimise $P_a(\mathbf{x}, \rho_1) = \sum_{i=1}^{m} \rho_1 h_i^2(\mathbf{x}) + \sum_{i_a=1}^{n_a} \rho_1 g_{i_a}^2(\mathbf{x})$ (including active constraints) to give $\mathbf{x}^*$.

The derivatives of the objective function and the constraints are again required as for the unconstrained problem (Section 3.1).

4. PACKED COLUMN PROBLEM DEFINITION

The total available surface area in the packed column (assuming all surface areas are at the same temperature) is a function of the area of one bead (a_{bead}) multiplied by the total number of beads (n_{beads}). (The contact area between the beads and between the beads and the column wall has not been included. Furthermore, the inner surface area of the column has been excluded. Additional comments regarding this exclusion are given in Section 7.)

$$Total\ surface\ area = n_{beads} a_{bead} \tag{7.21}$$

where

$$a_{bead} = \pi d_{bead}^2 \tag{7.22}$$

and d_{bead} represents the bead diameter.

The number of beads can be calculated as the volume in the column occupied by the beads divided by the volume of one bead (with the voidage taken into consideration). The volume of a single bead is given by

$$v_{bead} = \frac{\pi d_{bead}^3}{6} \tag{7.23}$$

ε is the voidage in the column i.e. the volumetric fraction that is not occupied by beads but through which liquid can flow. A common value selected for the voidage is 0.4 [41]. (1- ε) therefore represents the volumetric fraction occupied by the beads (V_{beads}). The height of the column is H_{column} and ϕ_{column} is the diameter of the column.

$$V_{beads} = \frac{\pi \phi_{column}^2 H_{column}(1-\varepsilon)}{4} \tag{7.24}$$

The number of beads (n_{beads}) is given by:

$$n_{beads} = \frac{V_{beads}}{v_{bead}} = \frac{3\phi_{column}^2 H_{column}(1-\varepsilon)}{2d_{bead}^3} \tag{7.25}$$

The surface area is therefore given by:

$$Total\ surface\ area = n_{beads} a_{bead} = \frac{3\pi\phi_{column}^2 H_{column}(1-\varepsilon)}{2d_{bead}} \tag{7.26}$$

It was assumed that the diameter and height of the column would be restricted by space limitations if the column were to be used in an application on a plant and glass columns of diameter between 0.1 and 1 metre and heights of between 0.5 and 3 metres were considered. The size of glass beads that were considered is in the range of 5 to 75 mm.

The following equations are obtained when translating into inequality constraints:

$$0.1 \leq \phi_{column} \leq 1 \tag{7.27}$$

$$0.5 \leq H_{column} \leq 3 \tag{7.28}$$

$$0.005 \leq d_{bead} \leq 0.075 \tag{7.29}$$

Rearranging eqs (7.27) to (7.29) gives

$$\phi_{column} - 1 \leq 0 \tag{7.30}$$

$$0.1 - \phi_{column} \leq 0 \tag{7.31}$$

$$H_{column} - 3 \leq 0 \tag{7.32}$$

$$0.5 - H_{column} \leq 0 \tag{7.33}$$

$$d_{bead} - 0.075 \leq 0 \tag{7.34}$$

$$0.005 - d_{bead} \leq 0 \tag{7.35}$$

A further important parameter is the time required for the mixture to react and for the reaction to go to completion. Experimental work has indicated that a residence time (τ) of approximately 15 minutes is required to ensure that the solid particles are transferred in the reaction. It has also been noticed that the residence time should be less than 30 minutes in order to prevent the reaction mixture from becoming viscous.

The residence time, τ, (in hours) can be determined from eq. (7.36) where $V_{liquid\ in\ column}$ is the volume through which liquid can flow in the column, and Q is the volumetric flow rate through the column. The volumetric flow rate for this investigation was taken to be 58 l/h ($1.6*10^{-5}$ m^3/s).

$$\tau = \frac{V_{liquid\ in\ column}}{Q} = \frac{\pi \phi_{column}^2 H_{column} \varepsilon}{4Q} \tag{7.36}$$

Taking the residence times into account gives

$$\frac{15}{60} \leq \frac{\pi \phi_{column}^2 H_{column} \varepsilon}{4Q} \leq \frac{30}{60} \tag{7.37}$$

or, rearranged,

$$\frac{15}{60}\frac{4Q}{\pi\varepsilon} \leq \phi_{column}^2 H_{column} \leq \frac{30}{60}\frac{4Q}{\pi\varepsilon} \tag{7.38}$$

Often the optimum length to diameter ratio of vessels is in the range of 2.5 to 5. [42] It was decided that the ratio of the column height to the diameter should be at least less than 3/2 which gives a value in the same area as the recommended ratio. The equation indicating this proportion is given by

$$\frac{\phi_{column}}{H_{column}} \leq \frac{2}{3} \tag{7.39}$$

or

$$\frac{\phi_{column}}{H_{column}} - \frac{2}{3} \leq 0 \tag{7.40}$$

The constraints in terms of the geometry limitations are taken into account and an additional constraint arises, namely that the diameter of the glass beads must be less than that of the column.

$$d_{bead} \leq \phi_{column} \tag{7.41}$$

or

$$d_{bead} - \phi_{column} \leq 0 \tag{7.42}$$

5. DEFINITION OF OBJECTIVE FUNCTION AND CONSTRAINTS

The design variables chosen for this problem are the column diameter, the diameter of the glass beads and the height of the column. The diameter of the glass beads is orders of magnitude smaller than the diameter and height of the column. This variable should therefore be scaled. [40]

Let

$$x_1 = \phi_{column} \tag{7.43}$$

$$x_2 = 100 * d_{bead} \tag{7.44}$$

$$x_3 = H_{column} \tag{7.45}$$

The design variables are substituted into eq. (7.26) to give

$$f(\mathbf{x}) = \frac{300\pi x_1^2 x_3 (1-\varepsilon)}{2x_2} \tag{7.46}$$

5.1 Reaction excluding residence time and column proportion

Initially, for interest, the simple case for reaction where the residence time and column proportion are not taken into account was considered.

The objective is to maximise the surface area for reaction and heat transfer. This is equivalent to minimising the negative of the objective function:

$$\text{Minimise } f(\mathbf{x}) = -\frac{300\pi x_1^2 x_3 (1-\varepsilon)}{2x_2} \tag{7.47}$$

The objective function must be minimised subject to the following inequality constraints from eqs (7.30), (7.31), (7.34), (7.35), (7.32), (7.33) and (7.42).

$$\begin{aligned}
g_1(\mathbf{x}) &= x_1 - 1 \le 0 \\
g_2(\mathbf{x}) &= 0.1 - x_1 \le 0 \\
g_3(\mathbf{x}) &= x_2 - 7.5 \le 0 \\
g_4(\mathbf{x}) &= 0.5 - x_2 \le 0 \\
g_5(\mathbf{x}) &= x_3 - 3 \le 0 \\
g_6(\mathbf{x}) &= 0.5 - x_3 \le 0 \\
g_7(\mathbf{x}) &= x_2 - 100x_1 \le 0
\end{aligned} \tag{7.48}$$

The derivatives of the objective function with respect to the three design variables are given by

$$\frac{\partial f}{\partial x_1}(\mathbf{x}) = -\frac{300\pi x_1 x_3(1-\varepsilon)}{1x_2}$$
$$\frac{\partial f}{\partial x_2}(\mathbf{x}) = \frac{300\pi x_1^2 x_3(1-\varepsilon)}{2x_2^2} \tag{7.49}$$
$$\frac{\partial f}{\partial x_3}(\mathbf{x}) = -\frac{300\pi x_1^2(1-\varepsilon)}{2x_2}$$

The derivatives of the inequality constraints are given by

$$\begin{aligned} &g_1'(\mathbf{x}) = 1 \\ &g_2'(\mathbf{x}) = -1 \\ &g_3'(\mathbf{x}) = 1 \\ &g_4'(\mathbf{x}) = -1 \\ &g_5'(\mathbf{x}) = 1 \\ &g_6'(\mathbf{x}) = -1 \\ &g_7'(\mathbf{x}, x_1) = -100 \\ &g_7'(\mathbf{x}, x_2) = 1 \end{aligned} \tag{7.50}$$

5.2 Reaction including residence time and column proportion

For the case where the residence time and the column proportion were taken into account, the equation for the objective function remained the same but additional inequality constraints were added. The inequality constraint for the residence time is derived as shown by

$$\frac{15}{60}h*\frac{4}{\pi\varepsilon}*58\frac{l}{h}*\frac{1}{1000\frac{l}{m^3}} \le \phi_{column}^2 H_{column} \le \frac{30}{60}h*\frac{4}{\pi\varepsilon}*58\frac{l}{h}*\frac{1}{1000\frac{l}{m^3}} \tag{7.51}$$
$$\frac{0.058}{\pi\varepsilon} \le x_1^2 x_3 \le \frac{0.116}{\pi\varepsilon}$$

or

$$x_1^2 x_3 - \frac{0.116}{\pi\varepsilon} \le 0 \tag{7.52}$$

$$\frac{0.058}{\pi\varepsilon} - x_1^2 x_3 \le 0 \tag{7.53}$$

The additional inequality constraints are given by

$$g_8(\mathbf{x}) = x_1^2 x_3 - \frac{0.116}{\pi\varepsilon} \le 0$$

$$g_9(\mathbf{x}) = \frac{0.058}{\pi\varepsilon} - x_1^2 x_3 \le 0 \tag{7.54}$$

$$g_{10}(\mathbf{x}) = \frac{x_1}{x_3} - \frac{2}{3} \le 0$$

The derivatives of the objective function remain the same.

The derivatives of the additional inequality constraints are given by

$$\begin{aligned} g_8'(\mathbf{x}, x_1) &= 2x_1 x_3 \\ g_8'(\mathbf{x}, x_3) &= x_1^2 \\ g_9'(\mathbf{x}, x_1) &= -2x_1 x_3 \\ g_9'(\mathbf{x}, x_3) &= -x_1^2 \\ g_{10}'(\mathbf{x}, x_1) &= \frac{1}{x_3} \\ g_{10}'(\mathbf{x}, x_3) &= -\frac{x_1}{x_3^2} \end{aligned} \tag{7.55}$$

6. RESULTS

The objective function, equations for the inequality constraints, derivatives of the objective function with respect to the design variables and derivatives for the constraints were entered into LFOPCV3. A portion of the Fortran source code for the investigation into the optimisation of the surface area with residence time and geometric constraints is given in the appendix.

6.1 Reaction excluding residence time and column proportion

The number of variables was specified as three. The initial guess was chosen as X(1) = 0.3 (column diameter = ϕ_{column} = 0.3 m), X(2) = 0.5 (bead diameter = d_{bead} = 5 mm) and X(3) = 1.5 (column height = H_{column} = 1.5 m). The number of inequalities was specified as 7 (as given by eq. (7.48)) and the number of equalities as zero. The penalty function parameters were specified as 10^2 for (ρ_0) and 10^4 for (ρ_1). The tolerance, XTOL was specified to be 10^{-9} and EG (the value against which the gradient vector of the penalty function is compared) set to 10^{-8}. The maximum step size was set to be 1 and the maximum number of iterations was set at 100 000.

The objective function was input into SUBROUTINE FUN of LFOPCV3 and the inequality constraints were input into SUBROUTINE CONIN. SUBROUTINE CONEG for equality constraints was left blank. The gradient vectors of the objective function and the inequality constraints were input into SUBROUTINE GRADF and SUBROUTINE GRADC respectively while SUBROUTINE GRADH (for the gradient vectors of the equality constraints) was left blank.

The solution was found to converge in 295 iterations. The optimum for the surface area was found where $x_1^* = 1$; $x_2^* = 0.5$ and $x_3^* = 3$. This means that the column diameter is equal to 1 m; the bead diameter is equal to 5 mm and the height is equal to 3 m. The resultant surface area was found to be 1696.5 m^2 and the number of beads required is 21 600 000. Figure 7.1 shows the plots of the values of the variables at each iteration.

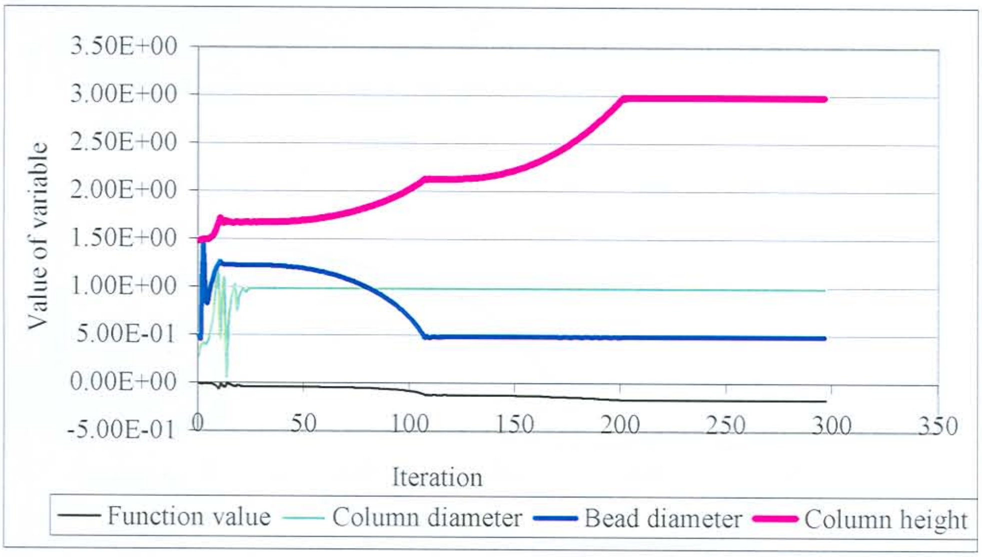

Figure 7.1 Plots of the values of the variables at each iteration

These results make sense as the largest column with the smallest bead size would give the greatest area. A larger column would be able to accommodate a larger number of beads and more beads of a smaller size would fit into the column giving a greater surface area for reaction.

6.1.1 Investigation into the effect of different starting conditions

Different starting conditions were chosen to determine whether or not the solution converged to the same answer and whether or not the minimum of the previous solution was a local or a global minimum. These starting conditions along with the number of iterations required to obtain convergence are shown in Table 7.1. Figures 7.2, 7.3 and 7.4 show the plots of the values of the variables at each iteration for run 1, 2 and 3 respectively.

For all runs, the same solution is obtained. For run 1, arbitrary initial values were selected for the three variables. In run 2, the initial variables are those furthest away from the solution. The solution is obtained in 1688 iterations which is greater than the 388 and the 102 required for conditions 1 and 3 respectively. The solution converged relatively quickly in run 3 as the starting conditions chosen were those values of the converged solution.

Table 7.1 Values of the variables for different starting conditions

Run no.	Starting value for variable			Iteration
	X(1)	X(2)	X(3)	
1	1	2	1	388
2	0.1	7.5	0.5	1688
3	1	0.5	3	102

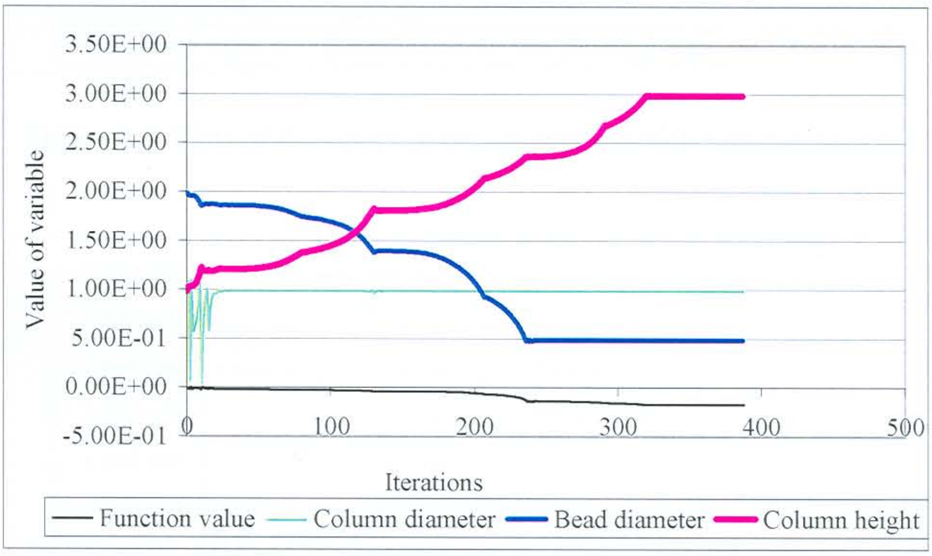

Figure 7.2 Plots of the values of the variables at each iteration for run 1

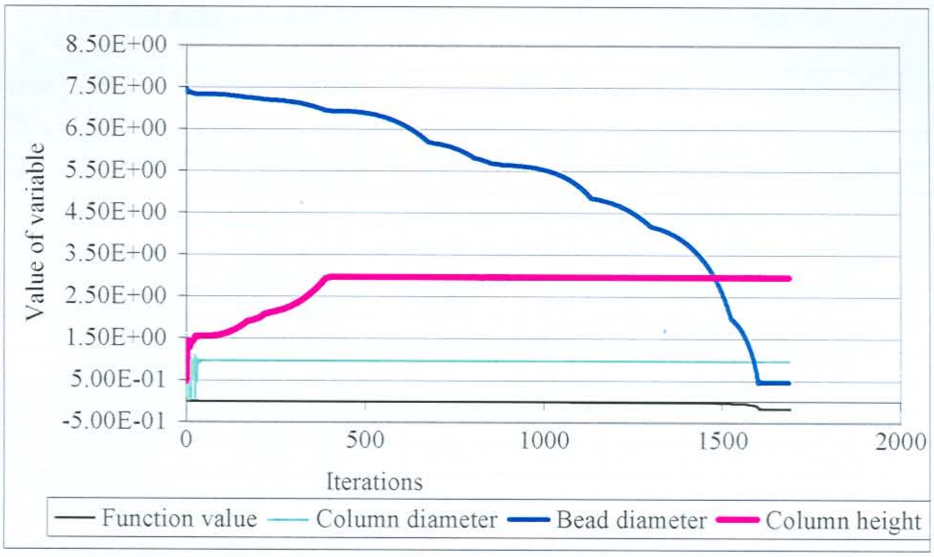

Figure 7.3 Plots of the values of the variables at each iteration for run 2

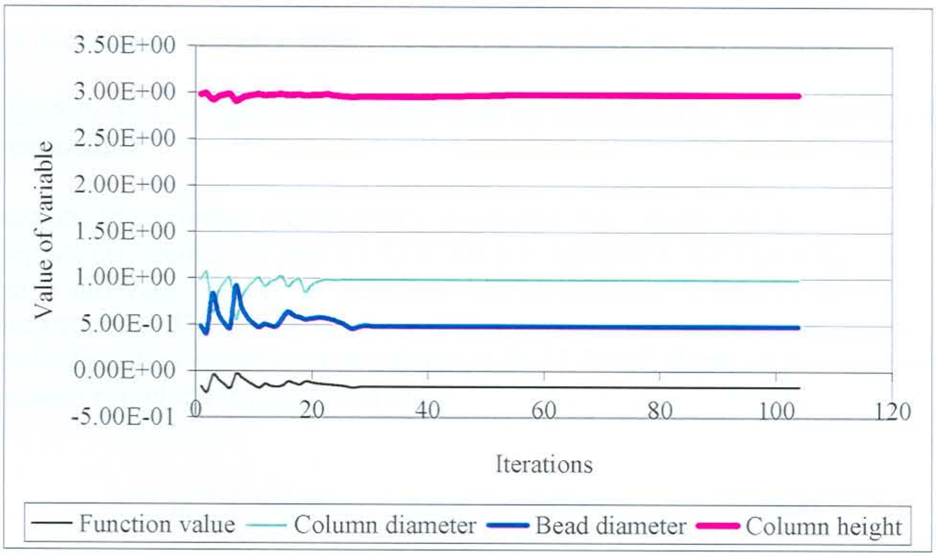

Figure 7.4 Plots of the values of the variables at each iteration for run 3

6.1.2 Investigation into the effect of changing the step size, DELT

The effect of changing the step size, DELT and with X(1) = 1, X(2) = 0.5 and X(3) = 3 was investigated. The results are given in Table 7.2. The results are rounded off where necessary for presentation in the table.

Table 7.2 Effect of DELT on the solution obtained

DELT	Iterations	Obj. func.	Final x-values			Final inequality constraint function values						
		F	X(1)	X(2)	X(3)	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)
100	1075	-0.17	1	0.5	3	$2.7e^{-11}$	-0.9	-7	$2.7e^{-11}$	$4.5e^{-12}$	-2.5	-99.5
10	153	-0.17	1	0.5	3	$5.8e^{-9}$	-0.9	-7	$5.8\ e^{-9}$	$9.6\ e^{-10}$	-2.5	-99.5
1	102	-0.17	1	0.5	3	$-1.0e^{-9}$	-0.9	-7	$-1.0e^{-9}$	$-1.6e^{-10}$	-2.5	-99.5
0.1	107	-0.17	1	0.5	3	$8.5e^{-9}$	-0.9	-7	$8.6e^{-9}$	$1.4e^{-9}$	-2.5	-99.5
0.01	76	-0.17	1	0.5	3	$1.8e^{-10}$	-0.9	-7	$1.8e^{-10}$	$2.9\ e^{-11}$	-2.5	-99.5
0.005	57	-0.17	1	0.5	3	$5.2e^{-9}$	-0.9	-7	$5.3e^{-9}$	$8.7e^{-10}$	-2.5	-99.5
0.004	49	-0.17	1	0.5	3	$5.6e^{-9}$	-0.9	-7	$5.6e^{-9}$	$9.3e^{-10}$	-2.5	-99.5
0.001	49	-0.17	1	0.5	3	$1.0e^{-8}$	-0.9	-7	$1.0e^{-8}$	$1.7e^{-9}$	-2.5	-99.5
0.0001	109	-0.17	1	0.5	3	$1.0e^{-8}$	-0.9	-7	$1.0e^{-8}$	$1.7e^{-9}$	-2.5	-99.5
0.00001	474	-0.17	1	0.5	3	$-3.7e^{-12}$	-0.9	-7	$-3.7e^{-12}$	$-6.2e^{-13}$	-2.5	-99.5

The solution converged to the same final value for the objective function value with the minimum number of iterations for DELT equal to 0.004. The same number of iterations was required for DELT equal to 0.001 but DELT equal to 0.004 gave the lowest value for the final inequality constraint function values.

6.2 Reaction including residence time and column proportion

6.2.1 Investigation into the effect of different starting conditions for the problem with inequality constraints

For this reaction, the number of inequality equations was increased to 10 (as given by the additional equations shown in eqs (7.53)). DELT remained set equal to 1. The solution converged in a different number of iterations and to different solutions for differing starting values for the variables. The results for these different conditions are given in Tables 7.3 and 7.4. The resultant surface area for all runs was found to be 52.20 m^2. Some of the values in Tables 7.3 and 7.4 have been rounded off for presentation.

Table 7.3 Solution obtained for different starting values

Run no.	Starting value for variable			Iterations	Obj. func.	Final x-values		
	X(1)	X(2)	X(3)		F	X(1)	X(2)	X(3)
1	0.3	0.5	1.5	126	-0.00522	0.25	0.5	1.5
2	1	2	1	394	-0.000249	-0.038	0.5	3
3	0.1	7.5	0.5	18974	-0.00522	0.39	0.5	0.61
4	1	0.5	3	122	-0.00522	0.18	0.5	2.88
5	0.39	0.5	0.61	230	-0.00522	0.38	0.5	0.64
6	0.38	0.5	0.64	373	-0.00522	0.38	0.5	0.64

Table 7.4 Values for the final inequality constraint functions

Run no.	Final inequality constraint function values									
	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)
1	-0.75	-0.14	-7	$-1.4e^{-9}$	-1.5	-1.4	-24	$-4.2e^{-9}$	$-4.6e^{-2}$	-0.50
2	-1	0.14	-7	$4.3e^{-4}$	$1.2e^{-3}$	-2.9	4	$-8.8e^{-2}$	$4.2e^{-2}$	-0.69
3	-0.61	-0.28	-7	$7.2e^{-11}$	-2.4	-0.81	-38	$9.8e^{-11}$	$-4.6e^{-2}$	$-3.0e^{-2}$
4	-0.82	$-7.9e^{-2}$	-7	$7.5e^{-13}$	-0.12	-2.8	-17	$5.4e^{-12}$	$-4.6e^{-2}$	-0.60
5	-0.63	-0.28	-7	$1.5e^{-10}$	-2.4	-0.62	-38	$2.1e^{-10}$	$-4.6e^{-2}$	$-7.1e^{-2}$
6	-0.62	0.28	-7	$2.0e^{-11}$	-2.4	-0.6	-37	$2.8e^{-10}$	$-4.6e^{-2}$	$-7.4e^{-2}$

Run 2 did not appear to reach a solution as two of the final inequality constraint function values were contravened (C(2) and C(7)). It appears that a number of different local optima were obtained in this problem. This probably comes about as a result of the flexibility in the design for the column proportion. There are a number of different possible combinations for the optimum surface area for a column diameter to height ratio of less than 2/3. Runs 5 and 6 converged to approximately the same answer possibly as a result of the similar starting variables.

6.2.2 Investigation into the solution obtained with one equality constraint and inequality constraints

The effect of adding the ratio of column diameter to height as an equality constraint instead of an inequality constraint was investigated. The ratio was set to 2/3. The number of inequality equations was decreased to 9 and the number of equality constraints to 1. The equality constraint is given by

$$h_1(\mathbf{x}) = \frac{x_1}{x_3} - \frac{2}{3} = 0 \qquad (7.56)$$

For these conditions, DELT remained set equal to 1. The solution converged in 157 iterations for starting values of X(1) = 0.3, X(2) = 0.5 and X(3) = 1.5. The optimum for the surface area was found where $x_1^* = 0.39480761$; $x_2^* = 0.5$ and $x_3^* = 0.59221141$. This means that the column diameter is equal to approximately 0.39 m; the bead diameter is equal to 5 mm and the height is equal to approximately 0.59 m. The resultant surface area was found to be 52.20 m^2. The values of the final inequality constraints were:

C(1) = –0.61
C(2) = -0.29
C(3) = -7
C(4) = $6.5e^{-10}$
C(5) = -2.4
C(6) = -0.49
C(7) = -39
C(8) = $1.2e^{-10}$
C(9) = $-4.6e^{-2}$

for the nine equations respectively. The final equality constraint function value was $-5.6e^{-9}$.

6.2.3 Investigation into the effect of changing the step size, DELT with inequality and one equality constraint

The effect of changing DELT and with starting values of X(1) = 0.3, X(2) = 0.5 and X(3) = 1.5 was investigated. The results are given in Tables 7.5 and 7.6. Some of the results are rounded off where necessary for presentation in the table.

Table 7.5 Effect of DELT on the solution obtained

Run no.	DELT	Iteration	Obj. func.	Final x-values		
				X(1)	X(2)	X(3)
1	100	407	-0.00522	0.39	0.5	0.59
2	10	508	-0.00522	0.39	0.5	0.59
3	5	179	-0.00522	0.39	0.5	0.59
4	1	157	-0.00522	0.39	0.5	0.59
5	0.1	195	-0.00522	0.39	0.5	0.59
6	0.01	268	-0.00522	0.39	0.5	0.59
7	0.001	1288	-0.00522	0.39	0.5	0.59
8	0.0001	11122	-0.00522	0.39	0.5	0.59

Table 7.6 Values for the final inequality constraint functions

Run no.	Final inequality constraint function values									Fin. equal constr. funct.
	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)	C(8)	C(9)	H(1)
1	-0.61	-0.29	-7	$3.0e^{-10}$	-2.4	-0.49	-39	$5.6e^{-10}$	$-4.6e^{-2}$	$-1.7e^{-9}$
2	-0.61	-0.29	-7	$4.1e^{-10}$	-2.4	-0.49	-39	$-2.2e^{-10}$	$-4.6e^{-2}$	$7.4e^{-10}$
3	-0.61	-0.29	-7	$6.7e^{-10}$	-2.4	-0.49	-39	$9.8e^{-10}$	$-4.6e^{-2}$	$-4.5e^{-9}$
4	-0.61	-0.29	-7	$6.5e^{-10}$	-2.4	-0.49	-39	$1.2e^{-10}$	$-4.6e^{-2}$	$-5.6e^{-10}$
5	-0.61	-0.29	-7	$-3.1e^{-10}$	-2.4	-0.49	-39	$4.5e^{-11}$	$-4.6e^{-2}$	$-1.1e^{-9}$
6	-0.61	-0.29	-7	$-3.1e^{-10}$	-2.4	-0.49	-39	$2.1e^{-10}$	$-4.6e^{-2}$	$-1.1e^{-9}$
7	-0.61	-0.29	-7	$-4.9e^{-10}$	-2.4	-0.49	-39	$4.9e^{-10}$	$-4.6e^{-2}$	$-1.6e^{-9}$
8	-0.61	-0.29	-7	$3.5e^{-10}$	-2.4	-0.49	-39	$7.6e^{-11}$	$-4.6e^{-2}$	$-3.9e^{-9}$

Figure 7.5 gives the plot of the values of the variables at each iteration for the DELT that gives the lowest number of iterations. This is run 4 where DELT equals 1. The fact that the fewest iterations are obtained when DELT is less than 10 and greater than 0.99 can possibly be explained by the following. DELT should be of the same order of magnitude as the "diameter" of the region if interest [43] i.e. $DELT = \sqrt{N} * variable - range$ where N is the number of variables. DELT can be calculated to be in the region of:

$$\sqrt{3}*1-0.9=0.8$$
$$\sqrt{3}*3-2.5=2.7 \qquad (7.57)$$
$$\sqrt{3}*5-7=1.7$$

for the column height and diameter and bead diameter respectively (taking a random value for the variable in the range provided).

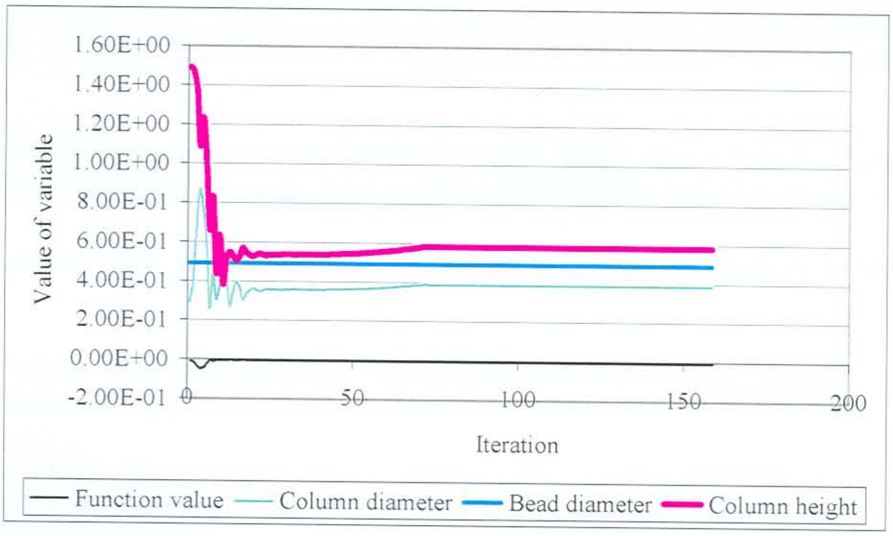

Figure 7.5 Plots of the values of the variables at each iteration

6.2.4 Investigation into the effect of different starting conditions with one equality constraint and inequality constraints

With the new system of equations and with DELT equal to 1, solutions were obtained for differing starting values for the variables. The results for these different conditions are given in Tables 7.7 and 7.8. Once again, the resultant surface area was found to be 52.20 m^2 for all runs. Some of the values in Table 7.7 have been rounded off for presentation.

Table 7.7 Solution obtained for different starting values

Run no.	Starting value for variable			Iterations	Obj. func.	Final x-values		
	X(1)	X(2)	X(3)		F	X(1)	X(2)	X(3)
1	0.3	0.5	1.5	157	-0.00522	0.39	0.5	0.59
2	1	2	1	1360	-0.00522	0.39	0.5	0.59
3	0.1	7.5	0.5	32845	-0.00522	0.39	0.5	0.59
4	1	0.5	3	189	-0.00522	0.39	0.5	0.59
5	0.39	0.5	0.59	352	-0.00522	0.39	0.5	0.59

Table 7.8 Values for the final inequality constraint functions

Run no.	Final inequality constraint function values									Fin. equal constr. funct.
	C(1)	**C(2)**	**C(3)**	**C(4)**	**C(5)**	**C(6)**	**C(7)**	**C(8)**	**C(9)**	**H(1)**
1	-0.61	-0.29	-7	$6.5e^{-10}$	-2.4	-0.49	-39	$1.2e^{-10}$	$-4.6e^{-2}$	$-5.6e^{-10}$
2	-0.61	-0.29	-7	$1.4e^{-10}$	-2.4	-0.49	-39	$2.8e^{-10}$	$-4.6e^{-2}$	$1.05e^{-10}$
3	-0.61	-0.29	-7	$5.8e^{-11}$	-2.4	-0.49	-39	$4.1e^{-11}$	$-4.6e^{-2}$	$-8.8e^{-10}$
4	-0.61	-0.29	-7	$3.5e^{-10}$	-2.4	-0.49	-39	$7.1e^{-10}$	$-4.6e^{-2}$	$-1.6e^{-10}$
5	-0.61	-0.29	-7	$2.1e^{-10}$	-2.4	-0.49	-39	$-4.8e^{-10}$	$-4.6e^{-2}$	$-1.6e^{-9}$

All runs converged to the same values for the variables. Those runs where the starting values of the variables were chosen close to the final x-values exhibited the lowest number of steps.

6.2.5 Investigation into the solution obtained using finite differences to determine the gradients

Instead of using the analytical gradients, finite differences were used to determine the gradients i.e. the gradient was computed as:

$$f'(x) = \frac{f(x+\Delta x) - f(x)}{\Delta x} \tag{7.58}$$

The solution obtained using this method was then compared to that obtained when using the analytical gradients.

With starting values of X(1) = 0.3, X(2) = 0.5 and X(3) = 1.5, 203 iterations were required to obtain a solution when finite differences were used to calculate the gradients with Δx (the step size used to find the gradient) or DELX equal to 10^5. Figure 7.6 gives the plot of the values of the variables at each iteration for DELT equal to 1 (see Table 7.5). This value resulted in the lowest number of iterations required for run 4. The solution obtained is the same as that obtained for the gradients by the analytical derivatives.

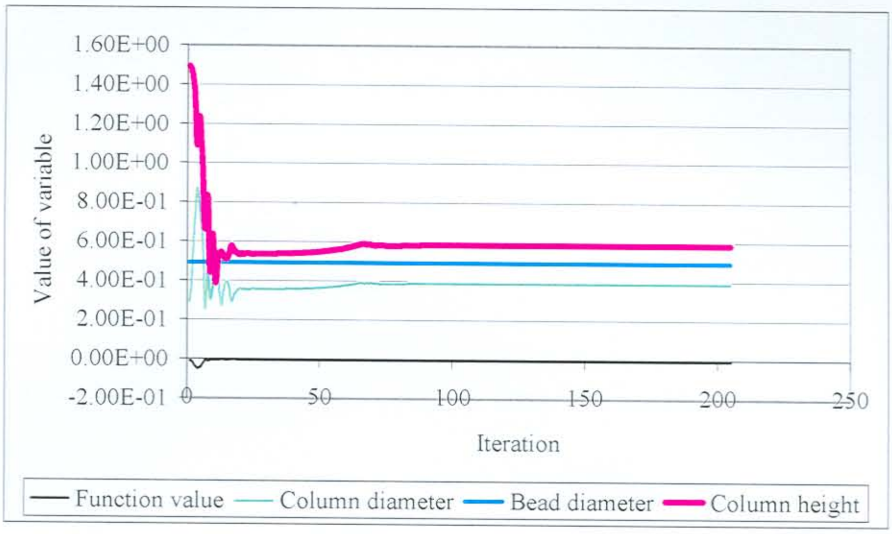

Figure 7.6 Plots of the values of the variables at each iteration

The value of DELX was varied to determine the effect on the number of iterations required to obtain the solution. The results are given in Table 7.9.

Table 7.9 Effect of DELX on iterations required to obtain solution

Run no.	Size of DELX	Iteration
1	$1e^{-6}$	157
2	$1e^{-5}$	157
3	$1e^{-4}$	161
4	$1e^{-3}$	201
5	$1e^{-2}$	203
6	$1e^{-1}$	195
7	0.5	848
8	1	848
9	10	149
10	100	133

All runs converged to the same solution. As the size of DELX decreased (below 1), the number of iterations required to reach the solution also decreased possibly because the value of the gradient was more accurate and the solution was approached more quickly. Figure 7.7 gives the plot of the values of the variables at each iteration for DELX equal to 10^{-5} that gives the lowest number of iterations.

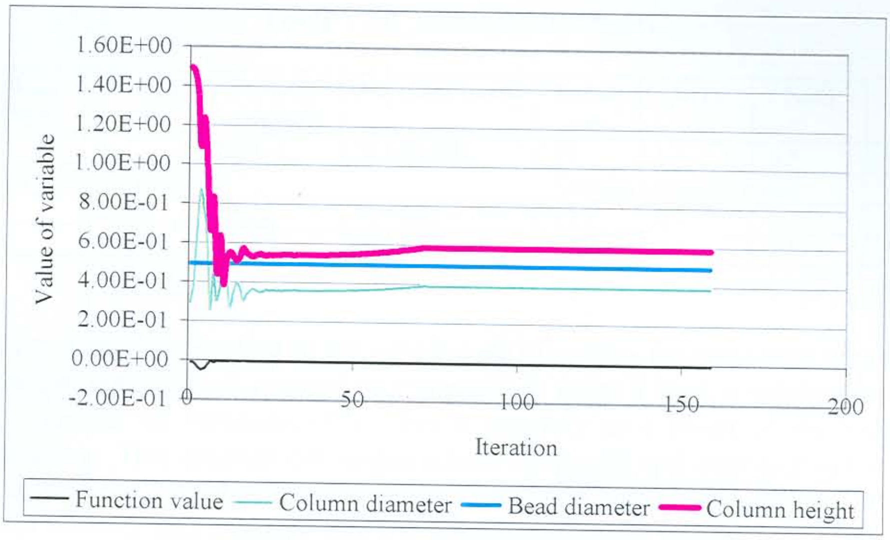

Figure 7.7 Plots of the values of the variables at each iteration

As DELX increased above 1, the number of iterations required for convergence also decreased. This is probably because, as the gradient is calculated, the constraints are encountered and the solution is forced to convergence more quickly.

7. CONCLUSIONS AND RECOMMENDATIONS

A number of investigations were conducted to determine what the dimensions of a packed column should be to obtain maximum heat transfer at the maximum allowable temperature for the manufacture of ferrofluid. The solutions obtained with the least number of steps for the various cases considered are summarised in Table 7.10.

1 = Optimisation where the residence time and geometric column height to diameter constraint is ignored
2 = Optimisation where the residence time and geometric column height to diameter constraint is taken into consideration as an inequality constraint
3 = Optimisation where the residence time is considered and the geometric column height to diameter constraint is taken as an equality consideration
4 = Optimisation where the residence time is taken into account, geometric column height to diameter constraint is taken as an equality consideration and finite differences are used to calculate derivatives

Table 7.10 Summary of results

	ϕ_{column} (m)	d_{bead} (mm)	H_{column} (m)	Surface area (m^2)	No. glass beads	Iterations	X(1)	X(2)	X(3)	DELT
1	1	5	3	1696.5	21 600 000	57	1	0.5	3	0.004
2	Various valid solutions obtained					Various variables tested				
3	0.39	5	0.59	52.22	664 630	157	0.3	0.5	1.5	1
4	0.39	5	0.59	52.22	664 630	157	0.3	0.5	1.5	1

From the results it can be seen that in the simple case (1) where the residence time and geometric diameter to height constraint is ignored as compared to cases 2 to 4, a solution is obtained with the minimum number of iterations (57). This is possibly as a result of the lower number of constraint equations. This solution converges where the height and diameter of the column are a maximum and the bead diameter is a minimum. This would provide the greatest surface area thus promoting heat transfer and ensuring that the solid particles are transferred from the aqueous to the organic phase. The residence time in this case if the values of the variables obtained as a solution are substituted back into the equations would, however, result in a completely unacceptable residence time of more than 16 hours. The resultant product would be viscous and much of the organic phase may have evaporated.

When including the residence time considerations and the height to diameter ratio as an inequality constraint, various valid solutions were obtained for different starting values of the variables. This is because there are a number of combinations of height to diameter that would be below 2/3 that would still give the same surface area and acceptable residence time. (In fact, from calculations, it is seen that for the solutions obtained in Table 7.3, the residence time is a maximum.) In further work that was conducted but not reported in this dissertation, it was found that when the inner surface area was included, different starting conditions converged to one solution where a maximum was obtained for the inner surface area.

When the height to diameter ratio is included as an equality constraint and when finite differences are used for calculation of the gradient, the solution is obtained in 157 iterations when DELT equals 1. The column diameter would be approximately 0.39 m, the height would be approximately 0.59 m and the bead diameter 5 mm. The bead diameter is at its smallest size to give the largest surface area. The surface area available for reaction is approximately 52.22 m^2. With the additional constraints, there is approximately 32 times less surface area available for reaction and heat transfer.

An area for further study would be to consider the number of beads required to fill the column to be a discrete value. The bead diameter could also be considered a discrete variable, as the glass beads are available commercially in certain specific sizes. The problem could be reformulated accordingly. The column height and diameter are relatively flexible as a glass blower could manufacture a column to a required specification. It would, however, be cheapest to purchase a standard commercially available glass column. In addition, experimental verification of the computed results would prove interesting.