

# Genetic Algorithms for Estimating Heat Transfer Parameters in Trickle Bed Reactors

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## 1. INTRODUCTION

Trickle bed reactors(TBR's) are the most widely used multiphase reactors used extensively in petroleum and petrochemical industries and to a lesser extent in waste water treatment plants and biochemical industries. In the reactor the liquid and gas phases move concurrently downward through a packed bed. Different flow regimes are encountered depending on the velocity of fluid phases and the type of packing used viz. Trickle flow regime(at low liquid and low gas rates), spray flow regime(at low liquid and high gas rates), pulse flow regime(at intermediate liquid and gas rates) and dispersed bubble regime(at high liquid and gas rates). Industrially TBR's are operated in trickle or pulse flow regimes.

The two dimensional, two parameter pseudo homogeneous model has been widely accepted as a heat transfer model for a TBR in which heat transfer in radial direction is characterized by the effective radial thermal conductivity of the bed( $k_{er}$ ) and the effective wall-to-bed

heat transfer coefficient( $h_w$ ). Assuming that there is no temperature difference between the solid and fluid phases at any point in the packed bed, neglecting heat losses in the axial direction and considering  $k_{er}$  and  $h_w$  to be constant within the layer, a heat balance on a volume element of the bed leads to the following differential equation:

$$(LCp_l + GCp_g^*) \frac{dT}{dz} = k_{er} \left[ \frac{1}{r} \frac{dT}{dr} + \frac{d^2T}{dr^2} \right]$$

with boundary conditions

$$\begin{aligned} T &= T_1 & ; & & z=0, r \geq 0 \\ \frac{dT}{dr} &= 0 & ; & & z \geq 0, r=0 \\ h_w(T_w - T_R) &= k_{er} \frac{dT}{dr} & ; & & z \geq 0, r=R \end{aligned}$$

the analytical solution is of the form

$$\frac{(T_{C_1} - T_1)}{(T_C - T_w)} = 1 - 2 \sum (J_0(b_n r/R) \exp(-Ab_n^2 z)) / (b_n J_1(b_n) [1 + (b_w/B_1)^2]) \quad (2)$$

where

$$\begin{aligned} A &= k_{er} / (R^2 (LCp_l + GCp_g^*)); \\ Bi &= \text{Biot no} = h_w R / k_{er} \end{aligned}$$

$b_n$  are the roots of the equation  $Bi J_0(b_n) = b_n J_1(b_n)$  for a constant wall temperature. Radial temperature profile

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method has been widely used for estimation of  $k_{er}$  and  $h_w$  in trickle bed reactors (Specchia and Basldi, 1979; Babu 1993). In the present study a robust optimisation technique called Genetic algorithm (GA) is used for estimating  $k_{er}$  and  $h_w$  in conjunction with the measured radial temperature profile with an objective function.

$$F = \frac{1}{M} \sum (T_{cal} - T_{exp})^2$$

where 'M' is the no. of measurement points.

## 2. GENETIC ALGORITHMS

Genetic algorithms (GA) are non-traditional optimisation routines that make use of the principles of natural selection and genetics (Goldberg, 1989; Davis 1991) and have been successfully applied in various fields (Moros et al., 1996; Wolf and Moros., 1997; Upreti and Deb, 1996; Chakraborty and Sastry, 1997; 1998). The variables of the objective function are string coded of a certain length depending on the accuracy required. GA always deal with a population of points. The points in the population are subjected to operations like reproduction, cross-over and mutation till we get the desired optimum.

A few advantages of GA over other traditional techniques are:

- \*Search space is discretized by using string coded structures even though the objective function may be continuous.

- \*We always deal with a population of points and so global optimum values can be trapped easily and multiple optimums can be captured in a single run.

- \*Suitable for multimodal applications.

## 3. EXPERIMENTAL SETUP AND PROCEDURE

The experimental setup to obtain the data on radial temperature profile is shown in Fig.1. the detailed explanation of the experimental setup, the data collection and reduction procedures are reported elsewhere (Babu, 1993; Babu and Rao, 1998; Babu and Sastry, 1999).

Air and water were fed to the column from the top at the desired flowrates by means of precalibrated rotameters. Hot water was circulated through the jacket around the test section at sufficiently high flowrates (25-30 l/min) in order to maintain nearly constant wall temperature, and the minimum and maximum temperature difference between the inlet and outlet hot water streams were 0.3 deg.c at low flow rates to 2 deg.c at high flow rates respectively of the following fluids. After steady state was attained the flow rates of air and water and the temperatures were recorded. The average of the three angular positions was taken as the temperature of each radial position. This procedure was repeated for a wide range of air (0.01-0.898 kg/m<sup>2</sup>s) and water flow rates (3.16-71.05 kg/m<sup>3</sup>), covering trickle, pulse and dispersed bubble flow regimes. The length of the heat transfer test section used for heat transfer experiments was 0.715m. the packing employed were 2.59mm ceramic spheres, 4.05 and 6.75mm glass spheres and 4.0 and 6.75mm ceramic rasching rings.

#### 4. RESULTS AND DISCUSSION

The pseudo code for the implementation of GA for an objective function:

$$\text{Min } F = \sum_{i=1}^3 (T_{\text{calc}(i)} - T_i)^2$$

where  $T_1, T_2, T_3$  are the temperatures at three different radial positions is as follows:

1. Input length of chromosome(lchrom), mutation and cross-over probabilities.
2. Formulation of mating pool(oldpop)
3. Select strings for crossover-select()
4. Crossover()
5. Mutation() for the required no. Of of bits----- $\rightarrow$ newpop
6. Oldpop=newpop
7. Repeat steps 3 to 6 till desired optimum ( $F > 0.03$ ) is obtained.

The 'rand' function in Borland C++ library was used for the generation of random numbers which helped as initial guesses. After the steps of the algorithm were performed, the following graphs viz. No. of function evaluations (vs) sample experimental data pts (Fig.2) and error (vs) Generation no. (Figs.3,4) were plotted. From the figs.3 and 4 it is evident that as the number of generations reaches a value around 20 the error remains constant and hence the value of  $T_{\text{calc}}$  converges to the experimentally determined values.

The values of  $k_{\text{eff}}$  and  $h_w$  converges within a maximum of 14 generations for different packings with the maximum population size being 12. The graphs are plotted for two different packings. Initially the values of inputs to the code were:

Lchrom(chromosome length)=8  
Population size=8;  
Max.number of generations=8

Since the convergence of the heat transfer parameters to the experimental values was very slow, these inputs were subsequently altered and checked for faster convergence so as to minimise the number of iterations. The chromosome length was varied from 8 to 12, population size from 8 to 12 and maximum number of generations from 8 to 15. It was found out that the convergence is the fastest for the following values of these parameters:- lchrom=12, population size=12 and maximum number of generations=14.

#### 5. CONCLUSIONS

The present study shows that the estimation of heat transfer parameters in a TBR can be effectively done using genetic algorithms-a non-traditional optimisation technique. The number of iterations using GA was found out to be much lesser to the conventional RTP (Radial temperature profile) method.

It was also found that the values- lchrom=12, Population size=12, Maximum number of generations=14 the heat transfer parameters converge to the optimum with a higher accuracy.

## NOTATION

L	Liquid flow rate
G	Gas flow rate
$C_{p_l}$	Specific heat of the liquid
$C_{p_g}$	Rate of change of enthalpy with respect to rise in temperature of the gas phase.
T	Temperature
R	Radius of the bed
r	Radial position in the bed
Bi	Biot number
$k_{er}$	Effective radial thermal conductivity of the bed
$h_w$	Effective wall-to-bed heat transfer coefficient

## REFERENCES

Babu B.V (1993). "Hydrodynamics and heat transfer in single phase liquid and two phase gas-liquid co-current downflow through packed bed columns" Ph.D. thesis.IIT, Bombay.

Babu B.V. and Rao V.G. (1998). "Prediction of effective bed thermal conductivity and wall-to-bed heat transfer coefficient in a packed bed under no flow conditions" Journal of Energy, Heat and Mass transfer vol.20, pp 43-50

Babu B.V. and K.K.N.Sastry (1999). "Estimation of heat transfer parameters in a trickle bed reactor using differential evolution and orthogonal collocation", Computers and Chemical Engg. Vol.23, pp 327-339.

Chakraborty. C and Sastry K.K.N (1997). "Genetic Algorithm-an effective

alternative for proving logical arguments" Evonews,5,17-18.

Chakraborty.C and Sastry K.K.N (1998). "The genetic algorithms approach for proving logical arguments in natural language." In:J.R.Koza,K.Deb, D.E.Goldberg(Eds.) Genetic programming 1998: Proceedings of 3<sup>rd</sup> annual conference (pp463-470): San Mateo, CA.

Davis.L 1991). "Handbook of genetic algorithms" New York: Van Nostrand Reinhold

Goldberg D.E.(1989): "Genetic algorithms in search, optimisation and machine learning" Reading MA: Addison-Wesley

Moros,R; Kalies,H; Rex,H.G; and Schaffarczyk,St.(1996) "A genetic algorithm for generating initial parameter estimations for kinetic models of catalytic processes" Comp and Chemical engg.20,1257-1270

Specchia V and Baldi G(1979). "Heat transfer in trickle bed reactors", Chem.engg. commun.3;483-499

Upreti S.R. and Deb.K (1996). "Optimal design of an ammonia synthesis reactor using genetic algorithms",Comp.&Chemical engg.;21,87-93.

Wolf D and Moros R (1997). "Estimating the rate constant of heterogeneous catalytic reactions without supposition of rate determining surface steps-an application of genetic algorithms"Chem engg sci.52,1189-1199.

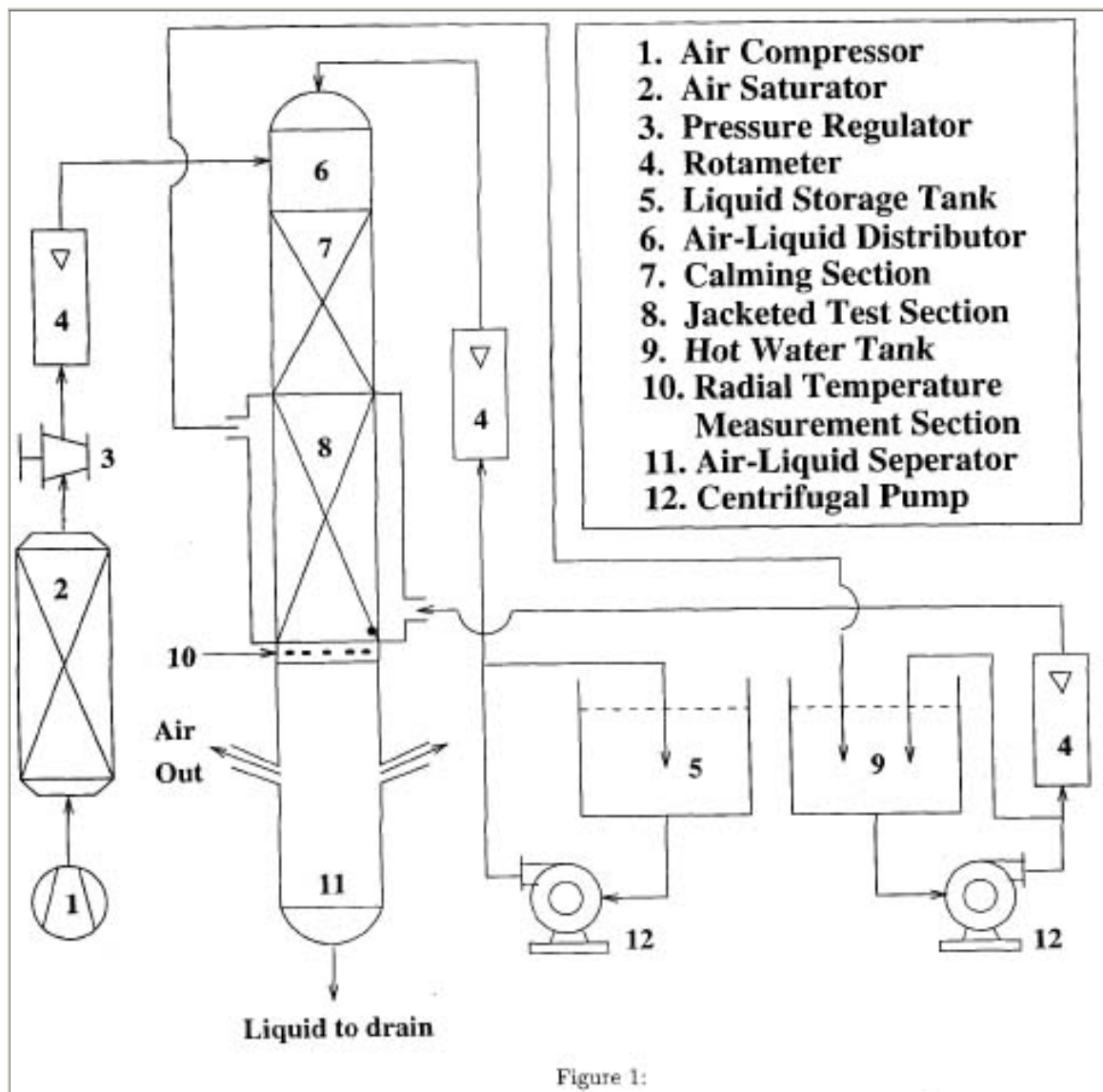
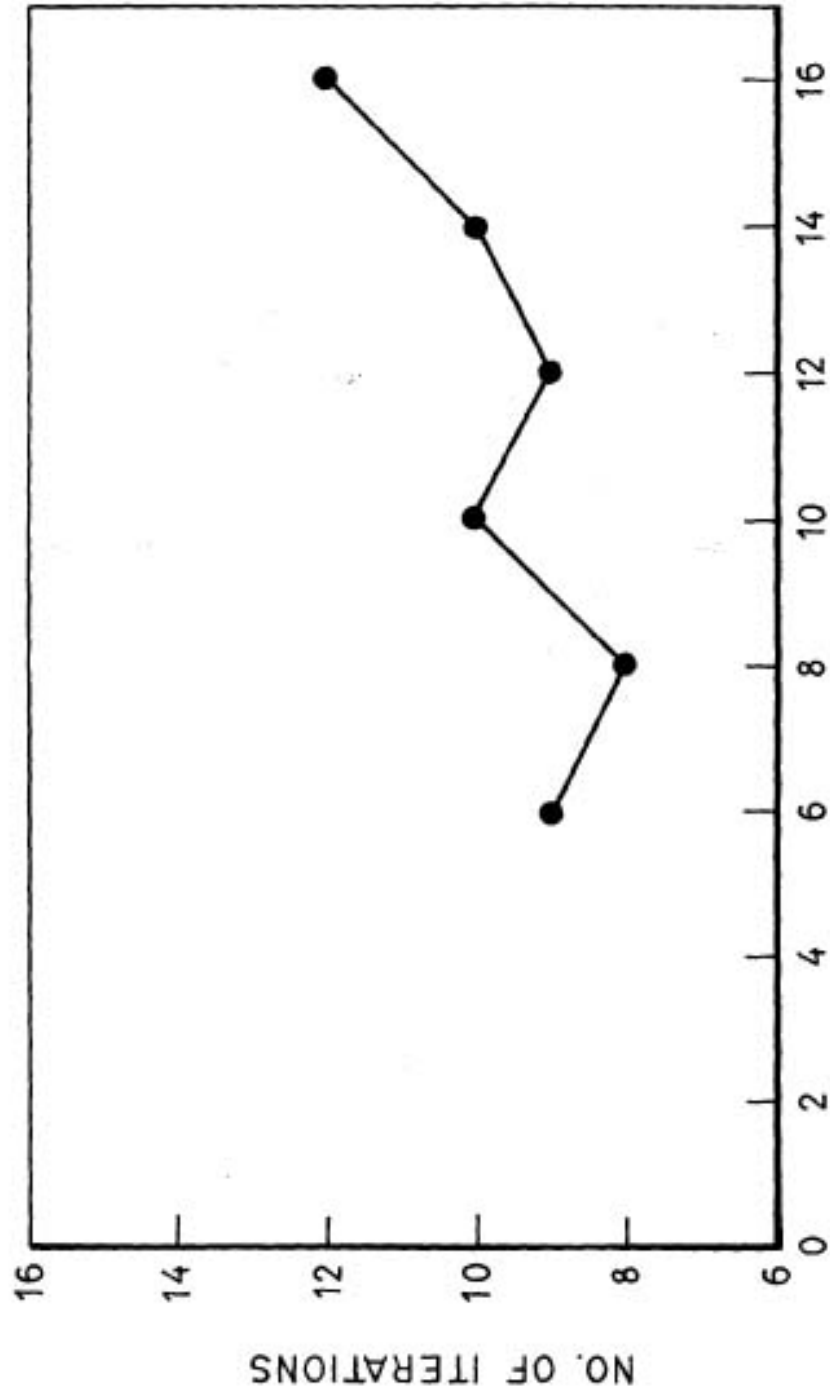


Figure 1:

FIG.2 NO. OF ITERATIONS Vs SAMPLE EXPT. DATA POINTS



SAMPLE EXPT. DATA POINTS

FIG.3 ERROR Vs GENERATION NUMBER CURVE

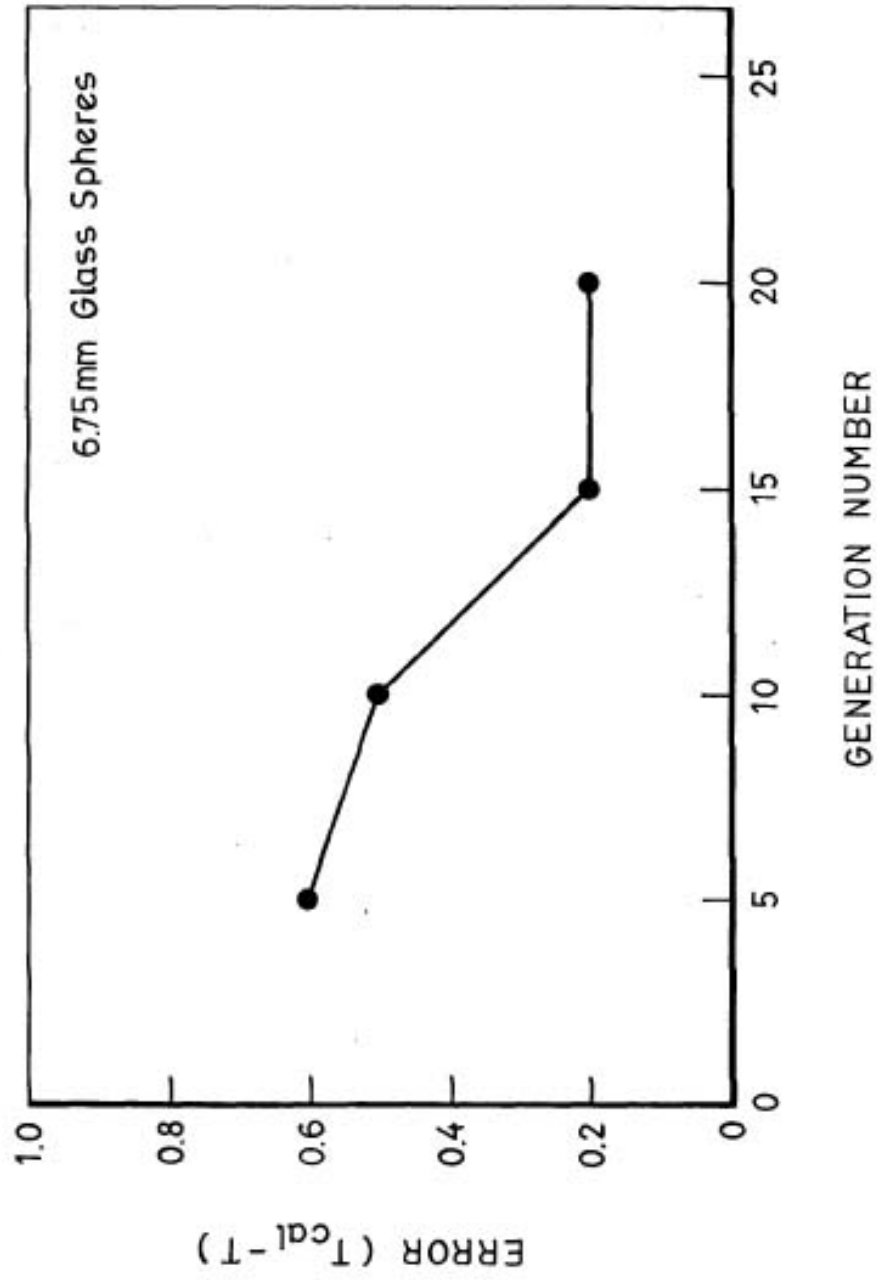
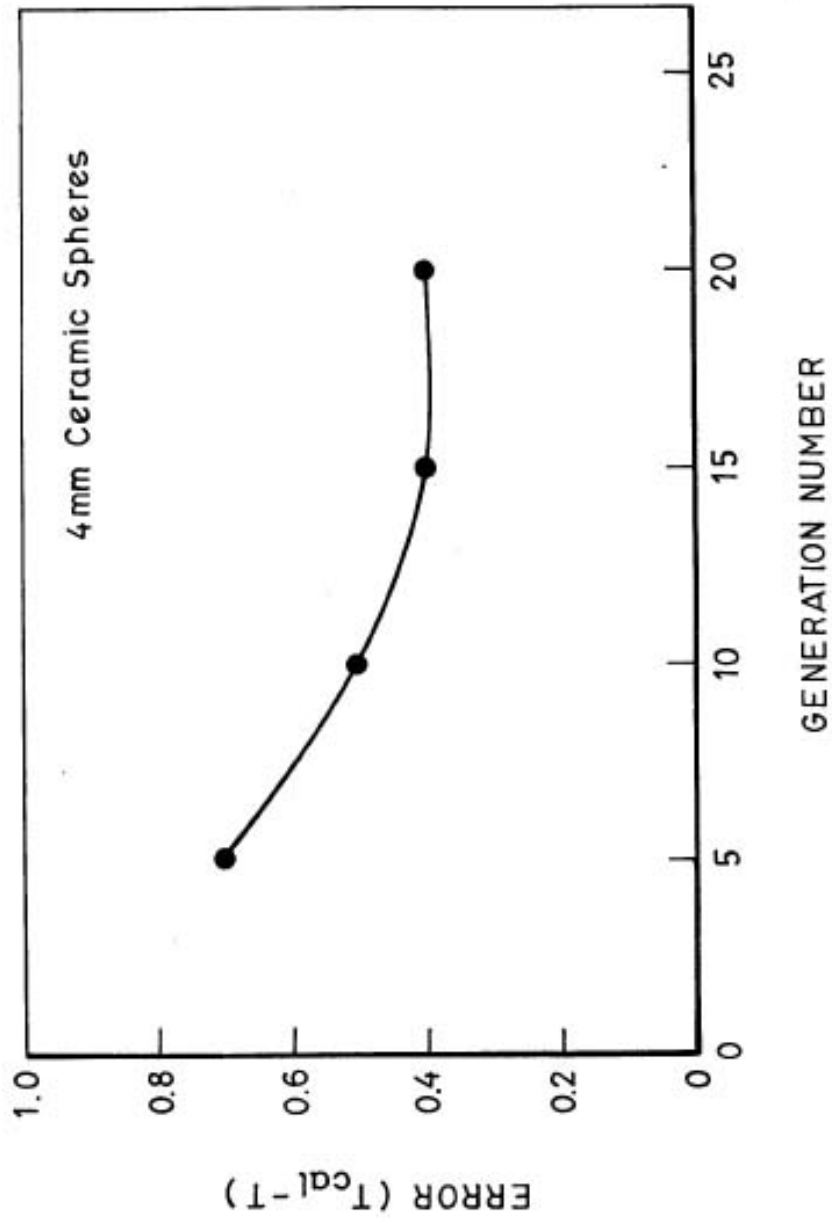


FIG.4 ERROR Vs GENERATION NUMBER CURVE



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