DEVELOPMENT OF PARTIALLY SIMULATED CHEMICAL REACTOR FOR THE IMPLEMENTATION OF ADVANCED CONTROL SYSTEMS

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ABSTRACT

In this work, a partially simulated exothermic chemical reactor (PARS-EX) pilot plant available in our department is designed and utilized to implement and test various conventional and advanced control strategies. In this reactor, an exothermic chemical reaction is simulated, where heat energy generated from the reaction is replaced by a calculated and controlled steam flow rate through a coil immersed in the reactor. A control valve is used to regulate flow rate of fresh water into a heat exchanger. The heat exchanger then cools the process fluid and recycles it back to the reactor, hence controls the temperature of the reactor. Prior to the online implementation, several advanced controllers are simulated for tracking required temperature of the reactor. The online advanced control results are made possible due to the developed customized graphical user and process interface. The work also highlights the software development involved. The software is designed so that it is capable of implementing several advanced nonlinear control strategies such as genetic algorithm and fuzzy logic.

Keywords: Advanced nonlinear controllers; partially simulated; chemical reactor; process control.

INTRODUCTION

Chemical reactors are used in many industrial applications such as pharmaceutical and petrochemical processes. A good and reliable reactor containing an efficient temperature control system will contribute to the high quality end product for respective applications. Integrating conventional linear controllers has demonstrated challenges when dealing with nonlinear reactor behavior. Hence, other advanced nonlinear methods have been investigated for controlling these reactors (Geraldo *et* al., 2001). Nougues *et* al. (2002) demonstrated the use of genetic algorithm to get the best feeding profile to minimize reaction time with temperature constraint to increase the productivity in their online batch reactor. They have carried out online parameter estimation of the first principle reactor model and then successfully implemented optimal control for its temperature using genetic algorithm.

An intelligent modeling and control of pH value using genetic algorithm in a pH reactor is simulated by Mwembeshi *et* al, (2004) where they have optimized their controller parameters in order to regulate the pH value. In their study, they have determined the optimal values of the transform parameter in parallel with the model and controller parameters. An online implementation of pH control in a pilot scale pH plant using genetic algorithm for designing its controller was presented by Tan *et* al. (2005), concluded that the controller, where its parameters were evolved using genetic algorithm, is able to regulate the pH value with minimal overshoot and successfully rejected introduced feed disturbances.

As in the fuzzy logic, controllers have been successfully applied to a variety of plants since the pioneering work done by Mamdani and collaborators. A good starting review of fuzzy logic and its applications in process control can be referred to Wang, (1997). Fuzzy logic control systems have been developed as an alternative controller in industries, where it has proven itself in various applications. Various methods of integrating fuzzy logic in industries have been discussed by Van der Wal, (1995). Takashi *et* al., (1995) have proven that fuzzy logic control system can be applied and integrated to control components of complicated system such as a reactor feed water for a nuclear reactor.

In this paper, the study consists of using the advanced nonlinear control methods using the genetic algorithm and fuzzy logic controllers to control the temperature of a continuous stirred chemical reactor. The case study system described in the later section is divided into two main parts, i.e. the chemical reactor and its cooling jacket to remove heat from the system. The rest of the paper is organized as follows. In the first section, the introduction to the genetic algorithm and fuzzy logic are introduced. The second part mainly discussed about the software development, experimental work and some online implementation results followed by the discussions. Finally, conclusions are presented to conclude the findings for this work.

PROCESS DESCRIPTION

For our case study, it is assumed that a first order $A \xrightarrow{k_1} B$ irreversible exothermic reaction occurs in the process, where A is the reactant, B is the product and k_1 is the reaction rate. It is also assumed that the reactor is well mixed to give uniform concentration and temperature distribution in the reactor. The process is governed by the mass and the energy balance equations given by Bequette, (1999) as shown below: -

$$\frac{dC_a}{dt} = \frac{F}{V}\left(C_{af} - C_a\right) - k_o \exp\left(-\frac{E}{RT}\right)C_a \tag{1}$$

$$\frac{dT}{dt} = \frac{F}{V}\left(T_f - T\right) + \left(\frac{-\Delta H}{\rho C_p}\right)k_o \exp\left(-\frac{E}{RT}\right)C_a - \left(\frac{UA}{V\rho C_p}\right)\left(T - TC\right) \tag{2}$$

Where, C_a and T represent the reactant concentration and reactor temperature respectively. The manipulated variable for the system is the coolant jacket temperature, TC where it is directly manipulated by the fuzzy logic controller as its control action, u. The model operating parameters used in this work are as shown in Table 1 below.

Table 1: Process operating parameters

Process Parameters/Symbols/Values
Feed in = Feed out, F = 0.16 m^3/h
Reactor volume, V = 0.16 m^3
Pre-exponential factor, $k_o = 7.2 \times 10^{10}$ X 60 h^{-1}
Heat of reaction, $(-\Delta H)$ = 20 kcal/mol
Activation energy, $E = 1 \times 10^4$ $kcal.kg^{-1}.mol^{-1}$
Overall heat transfer coefficient, U = 4200 $kcal.m^{-2}h.K$
Heat transfer area, A=0.2 m^2
Feed concentration, C_{af} = 25 x 10^3 $kg.mol/m^{-3}$
Feed temperature, T_f = 308 .15 K
ρC_p =1000 kcal/(m^3K)
Ideal gas constant, R=1.987 cal/mol.K
Initial jacket temperature, TC_0 = 308.15 K
Initial reactant concentration, C_{a0}=23.9 x 10^3 kg.mol/liter
Initial reactor temperature, T_0=321.15 K

GENETIC ALGORITHMS

Genetic Algorithms are search algorithms based on the mechanics of natural selection and genetics. It has been developed by John Holland, his colleagues and students at the University of Michigan in 1960. Genetic Algorithms are particularly suitable for solving complex optimization problems and they are inherently parallel, since their search for the best solution is performed over genetic structures that can represent numbers of possible solutions. In order to search solutions for any problems, a typical genetic algorithm would do the followings iteratively:-

- Start with any initial random sets of individuals/strings/chromosomes, denoted by *P(0)*, which is called the initial population;
- Evaluate the objective function for each individuals in *P(0)*;
- Based on this evaluation, create a new set of population, i.e. *P(1)* using genetic operators; namely the selection, crossover and mutation;
- Repeat the procedure iteratively until a defined terminating condition is reached and satisfied.

Genetic Algorithm Model Based Control (GAMBC) Strategy

This section introduces a model based control scheme to provide the best control action to the process using genetic algorithm (Abdul Wahab *et* al., 2007). The GAMBC control structure is as highlighted in Figure 1. The following elements of the controller structure have to be defined prior to its implementation: an objective function, process model, parameter encoding to present the possible solution space and sets of genetic operators. A MATLAB toolbox by Chipperfield, (1994) was used throughout this work to implement the genetic operation to provide control action for the process.

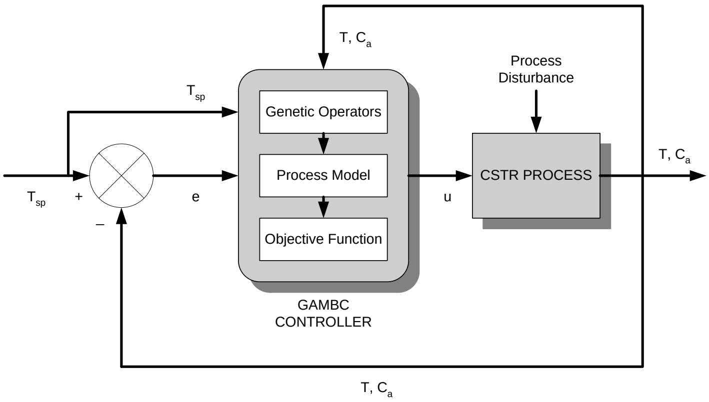


Fig.1: Genetic algorithm model based control structure.

Objective function used

The objective function used in this work is simply given by Eqn. (3) below, where T_{sp} is the desired reactor temperature set point and $\hat{T}$ is the reactor temperature from the first principle model optimized by the genetic algorithm. The genetic algorithm routine minimizes this fitness value, *J*.

$$J = \left| T_{sp}(k) - \hat{T}(k) \right| \qquad (3)$$

Parameter coding

The process control actions, T_C is identified as the variable that contributes directly to minimize the fitness value derived from objective function, hence providing the optimal control action to the process. The variable is encoded into the GA chromosomes. In order to limit the control action applied to the process, the encoding is quantified between u_{min}=298 and u_{max}=350 K in objective to maintain controller stability.

Genetic operators

The genetic operators used in this work are those described in the previous section where linear ranking, roulette wheel selection, single point crossover with rate P_c of 0.6 and mutation rate P_m of 0.05 were used through out the work. These genetic parameters are selected and inspired from examples cited in Goldberg, (1989) and also from simulation experiences. The flow chart showing the GAMBC control algorithm to continuously monitor the error between the reactor temperature set point, T_{sp} and the current temperature, *T* can be referred to Abdul Wahab et al, (2007).

If the error is below the defined value, i.e. 0.1 in this study, the system continues to monitor the process. The controller only starts to create the initial randomized population when the error is more than 0.1^{o}C. The initial 50 individuals are then evaluated using the objective function mentioned earlier (Eqn. 3) to obtain the fitness value, *J*. At this stage, the genetic algorithm operators will perform the selection, crossover and mutation at the assigned parameters as shown in Table 2. Using the evolved chromosomes that consist of 10-bits binary representation of the possible control action, T_C, the chromosomes are then decoded into real values before they are used to solve for the reactor temperature, T. A mean of checking the goodness of the proposed reactor temperature is then carried out. The evolution is then being checked for convergence and maximum allowable generation per sampling time, which is defined as 0.001 and 30 respectively. These terminating conditions are important as to make sure that complete generations are achievable between the sampling instants. The individual corresponds to the fittest value is then passed to the process as control action, u. Finally, the algorithm then monitors the user feedback to continue for the next iteration, otherwise stops the control loop.

Table 2: Genetic Algorithm Parameters Used (Abdul Wahab et al, 2007)

Parameters of GAMBC Controller	
Initial population, $P(0)$	100
Max generation per sampling time, (MAXGEN)	30
Control action limits	298 – 350 K
Crossover rate, P_c	0.6
Mutation rate, P_m	0.05
Length of encoding bits, L	10 bit

FUZZY LOGIC

The development of fuzzy logic in the late 70s has provoked many applications and implementation of fuzzy controllers. Further investigations pointed out certain advantages over the conventional PID controller. Besides satisfactory robustness in case of more complicated nonlinear and time varying systems, the most important advantage refers to the design principle, which is very similar to human reasoning. This principle is based on simple conditional rules. The design and tuning of the fuzzy logic controllers consists of membership function design and definition of fuzzy rules. Since the process requires at its input non-fuzzy values, the controller output fuzzy sets must be defuzzified, the result being a value u_s. In our case study consideration, the control system has to be designed to keep the reactor temperature, T at the desired value.

Fuzzy Logic Controller

For this study, a basic fuzzy logic configuration is used. A fuzzy logic control structure consists of fuzzifier to transform measured data into fuzzy sets, inference engine-fuzzy rule base to evaluate assigned fuzzy rules and defuzzifier to convert fuzzy sets into crisp value or real value. In this work, MATLAB and its Fuzzy Logic Toolbox have been used. In the design of the fuzzy logic temperature controller, fuzzy sets N(Negative), ZE(Zero), P(Positive), DEC(Decreasing), INC(Increasing), LO(Low) and HI(High) are assigned to universes $E_T=\{e_T\}$, $CE_T=\{ce_T\}$ and $U_T=\{u_T\}$ as specified by their membership functions. The range of values (universe of discourse) for a given inputs and output are shown in Figure 2. The actual values of the output variable are scaled with a scaling factor of G_u.

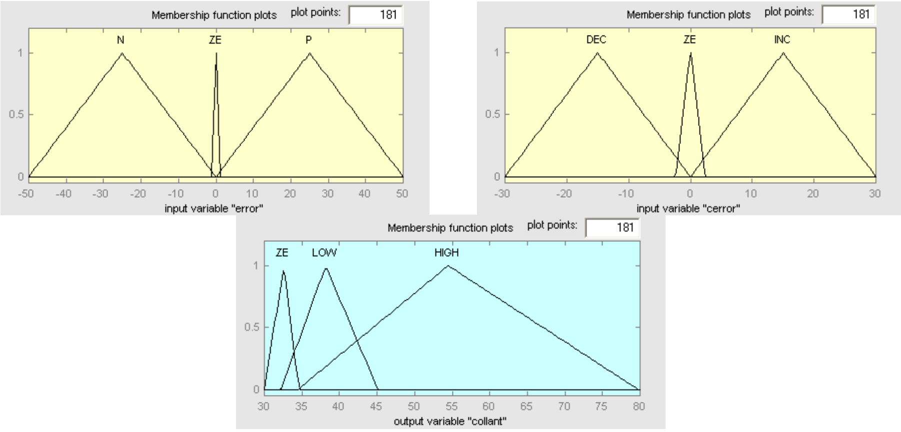


Fig. 2: Plot of membership functions using triangular function for **e**(top left), **ce**(top right) and **u**(below)

The rule-base table for reactor temperature control consisting of all 7 IF-THEN rules is summarized in Table 3, where the entries correspond to the values of the error, **e** and rate of error, **ce**. An example of a rule governing the system can be translated into "IF (**e** is N) AND (**ce** is DEC) THEN (**u** is ZE)" as shown in the highlighted row and column in the Table 3 below.

Table 3: Rule base for temperature control of the reactor

	Rate of error, ce			
Error, e		**DEC**	**ZE**	**INC**
	N	ZE		ZE
	ZE	ZE	ZE	ZE
	P	LO		HI

ONLINE IMPLEMENTATION

Details for the development of the pilot plant can be seen in Abdul Wahab *et* al, (2007 and 2008). The controller is tested to the pilot plant reactor available in our laboratory. The plant consists of the reactor and the cooling jacket where heat energy supplied from steam is used to simulate the exothermic reaction released by a studied chemical reaction. The pilot plant as shown in Figure 3 below is connected to a control room using OPTO22 module where a SCADA system is used to monitor and control the crucial control loops, i.e. reactor feeds and coolant flow rates.

Software development for online implementation

The information flowchart showing the computer control setup for the pilot plant system can be seen in Figure 4. The Paragon software manages the overall data acquisition and conventional control of the local control loops. This software is interfaced with the main data acquisition and the reactor simulation program, which is also interfaced to the fuzzy logic control algorithm program written in Visual Basic and running on an Intel Pentium computer. In order to implement the advanced control strategies for our partially simulated exothermic reactor, customized user graphical friendly interface software is developed to provide effective process monitoring and control for the pilot plant. The main objective is to test the strategies online in order to evaluate its performance for online set point tracking and load disturbance rejections.

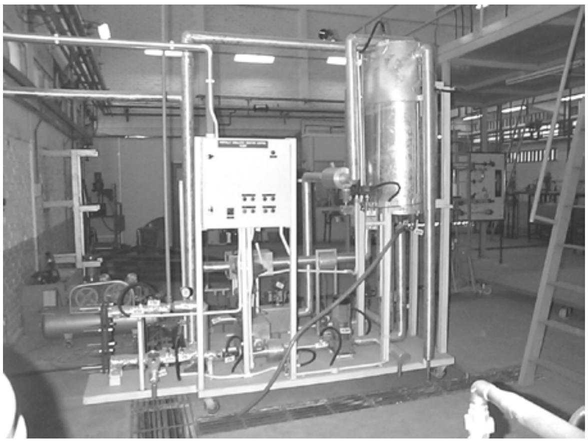


Fig. 3: PARS-EX pilot plant

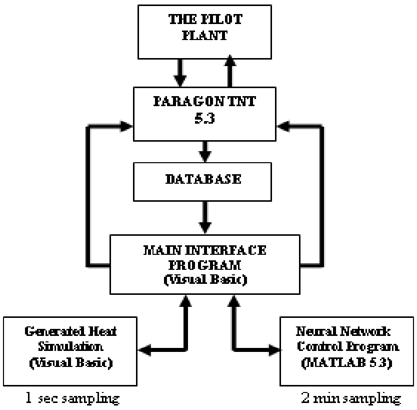
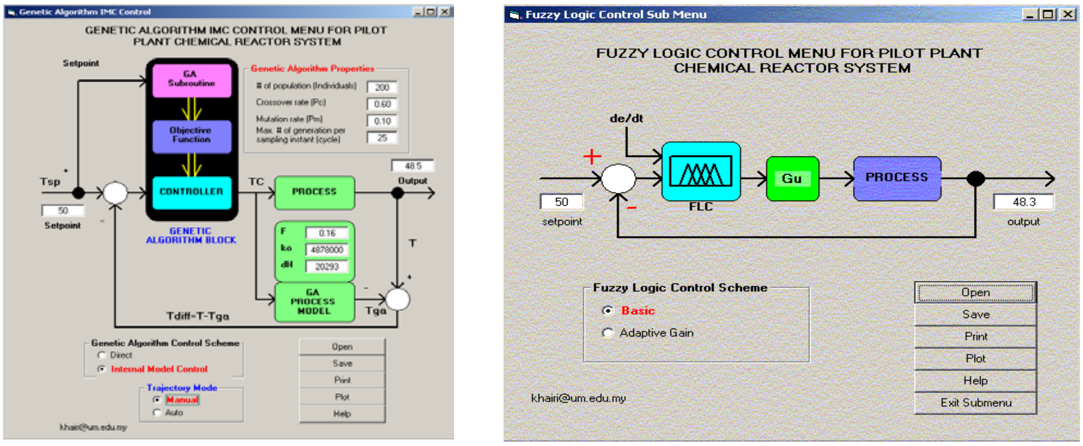


Fig. 4: Information flowchart

The graphical user interface menu for monitoring and control for previously discussed genetic algorithm and fuzzy logic are shown respectively in Figure 5. This control menu is used throughout the online implementation.



# of population (Individuals) 200
Crossover rate (Pc) 0.60
Mutation rate (Pm) 0.10
Max. # of generation per sampling instant (cycle) 25
Setpoint 50
Output 48.5
F 0.16
ko 4878000
dH 20293
Genetic Algorithm Control Scheme: ○ Direct ● Internal Model Control
Trajectory Mode: ● Manual ○ Auto

setpoint 50
output 48.3
Fuzzy Logic Control Scheme: ● Basic ○ Adaptive Gain

Fig. 5: Software development for implementing genetic algorithm model based control (left) and fuzzy logic control (right)

RESULTS AND DISCUSSIONS

In order to evaluate the performance of both genetic algorithm and fuzzy logic controllers implemented in this study, the controllers are tested with multiple point tracking and set point tracking with load disturbance rejection tests. The disturbance consists of feed flowrate, (*F*).

Multiple set point tracking

The genetic algorithm and fuzzy logic controllers are subjected to a multiple set point tracking demands from its nominal temperature values of 50 to 60, 45 and 55^{o}C. The reactor temperature demands were introduced with intervals of an hour respectively. Despite of measurement and process noises occurred during implementation, both of the controllers successfully tracked the demands as shown in the Figure 6 below.

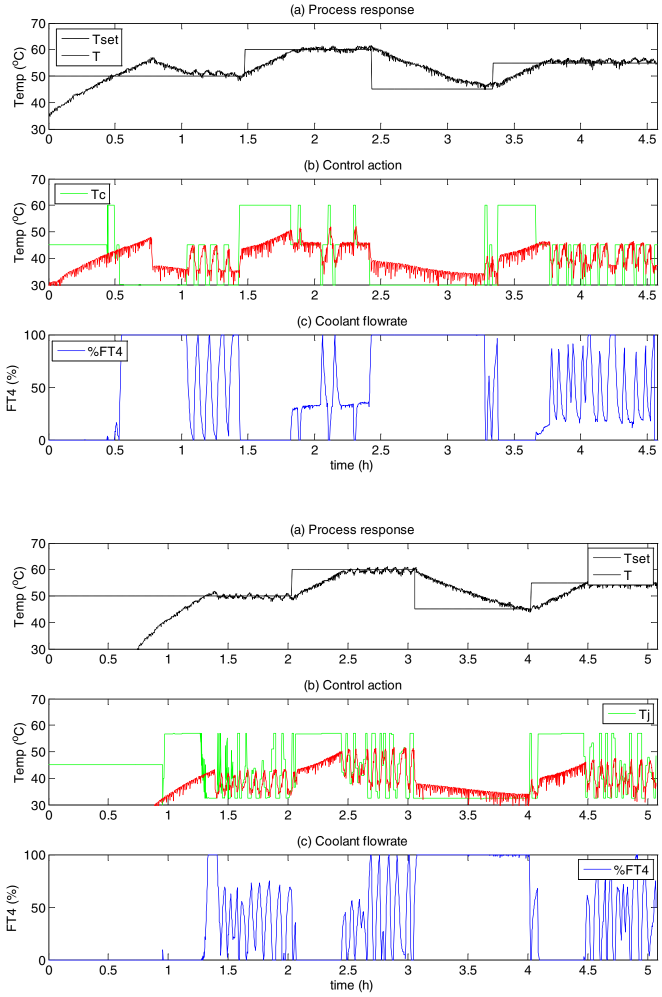
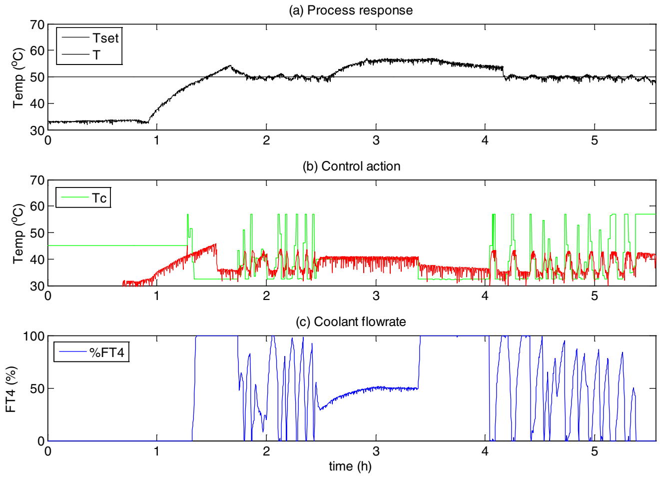


Fig. 6: Multiple set point tracking results with genetic algorithm model based (above) and fuzzy logic control approaches (below)

Set point tracking with load disturbance test

The controller is then tested further with introduced disturbance in feed in flowrate, *F* to the reactor where it was reduced to 85% from its nominal value. After startup, reactor temperature is left regulated by the fuzzy controller at T_{set} = 50^{o}C for about an hour. The disturbance is introduced and at the same time the controller was disconnected to let the process respond to the change of parameter introduced. After about an hour, the genetic algorithm model based controller is made to resume it control action. It was observed that the controller is capable in rejecting the disturbance as it successfully brought back the reactor temperature to the set point. Similar to the previous test and validation procedure, the fuzzy logic produce similar control response as shown in Figure 7.



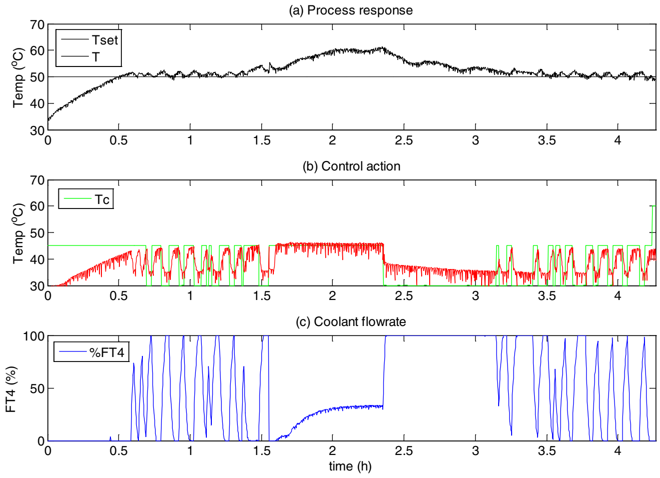


Fig. 7: Load disturbance rejection using genetic algorithm model based (above) and fuzzy logic control (below) due to changes in -15% of nominal feed in flow rate (*F*)

CONCLUSIONS

An advanced nonlinear control approaches using genetic algorithm and a fuzzy logic method to control temperature of the continuous stirred chemical reactor system was highlighted. The results show that it is possible to design a temperature control using fuzzy logic approach for accurate tracking for desired reactor temperature. It is shown that the controllers are capable to reject disturbances and to be independent to the mathematical model of the chemical reactor in various reactor operating regions. The software development carried out to implement the advanced control strategies such as fuzzy logic promises the possibilities of testing various and wide control techniques based on artificial intelligence methods.

ACKNOWLEDGMENTS

This work was fully supported by **Malaysia IRPA 09-02-03-0475** Project Grant and doctoral scholarship from The Ministry of Science, Technology and Innovations (MOSTI), Malaysia from 2003-2006 for first author is sincerely appreciated.

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