INTRODUCTION

Batch reactor is an essential unit operation in almost all batch-processing industries. The control of a batch reactor in a simple case consists of charging the reactor, controlling the reactor temperature to meet some processing criterion, and shutting down and emptying the reactor (Figure 1). Operating batch reactors efficiently and economically is very important as far as overall profitability is concerned.

The dynamic optimization (optimal control) of batch reactors has received major attention in the past. The objective was to determine the optimum reactor temperature profiles for cases where there are competing side reactions, so that an increase in the yield (productivity, profit and so on) may be obtained using the optimal profiles (Logsdon and Biegler, 1993; Luss, 1994). However, all these researchers considered only the off-line optimization problems. None of them have implemented these results on-line. The focus of this paper is to obtain optimal operating policies of batch reactors in terms of reactor temperature and to track these temperatures on-line by designing controllers based on non-linear model.

In recent years, neural networks have been extensively used in process systems (Chen and Weigand, 1994; Aziz et al., 2000; Cabassud and LeLann, 2001). For a given set of inputs, NNs are able to produce a corresponding set of outputs according to some mapping relationship.

This relationship is encoded into the network structure during a period of training (also called learning), and is dependant upon the parameters of the network, i.e., weights and biases. Once the network has been trained (on the basis
of known sets of input/output data), the input/output mapping
is produced in a time that is orders of magnitude lower
than the time needed for rigorous deterministic modelling
(Greaves et al., 2003).

In this work, we used neural networks as both dynamic
estimator for heat release due to exothermic reactions in
a control strategy and also as controllers in batch reactors
(described later).

There are various neural network architectures but all the
applications considered in this work have utilized the feed
forward multi-layered neural network (Figure 2). The numbers
of hidden layers and nodes may vary in different applications
and depend on the user specifications. There are
various types of activation functions available but in this
work, the log-sigmoid function has been used in both the
hidden and output layers. No specific technique is available to decide the optimum number and it is usually carried
out through trial-and-error procedure (Aziz, 2001). Since the
process being studied is a dynamic system, it is necessary
to feed the network with past historical data.

The multi-layered feed forward network shown in
Figure 2 is trained using the back-propagation method.
This method is chosen because it is the most well known
and widely used algorithm associated with the training of
a feed forward neural network. Basically it is a gradient
descent, parallely distributed optimization technique to
minimise the error between the network and target output
by manipulation of the connection weights (parameters)
of the network (Aziz, 2001).

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