Available online at www.sciencedirect.com
ScienceDirect
Journal of Process Control 18 (2008) 347–360
JOURNAL OF PROCESS CONTROL
www.elsevier.com/locate/jprocont

A continuous stirred tank heater simulation model with applications

Nina F. Thornhill [a,*], Sachin C. Patwardhan [b], Sirish L. Shah [c]

[a] Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London SW7 2AZ, UK
[b] Department of Chemical Engineering, I.I.T. Bombay, Powai, Mumbai 400 076, India
[c] Department of Chemical and Materials Engineering, University of Alberta, Edmonton, Canada T6G 2G6

Received 18 December 2006; received in revised form 2 July 2007; accepted 11 July 2007

Abstract

This article presents a first principles simulation of a continuous stirred tank heater pilot plant at the University of Alberta. The model has heat and volumetric balances, and a very realistic feature is that instrument, actuator and process non-linearities have been carefully measured, for instance to take account of the volume occupied by heating coils in the tank. Experimental data from step testing and recordings of real disturbances are presented. The model in Simulink and the experimental data are available electronically, and some suggestions are given for their application in education, system identification, fault detection and diagnosis.

Keywords: Benchmark simulation; Disturbance; Experimental validation; First-principles model; Hybrid model; Performance analysis; System identification

1. Introduction

Process simulations are of value to university teachers and academic researchers because they allow comparisons and demonstrations of the merits of different approaches in areas such as control design, system identification and fault diagnosis.

This paper has an educational purpose. It describes a simulation of an experimental continuous stirred tank heater (CSTH) pilot plant. Volumetric and heat balance equations are presented along with algebraic equations derived from experimental data for calibration of sensors and actuators and unknown quantities such heat transfer through the heating coils. Many of these relationships have non-linearities, and hard constraints such as the tank being full are also captured. A valuable feature is that the model uses measured, not simulated, noise and disturbances and therefore provides a realistic platform for data-driven identification and fault detection. Code and data for the simulation presented in this article are available from the CSTH simulation website [38]. The model has been implemented in the Simulink simulation platform with a view to easy accessibility by students and researchers.

The next section of the paper reviews benchmark models from the process systems literature and places the CSTH model in context. Section 3 presents the pilot plant, relevant equations and the calibrations. Section 4 describes implementation of the model in the Simulink simulation platform. Section 5 presents experimental data for model validation while Section 6 shows the time trends of process and measurement disturbances captured from the experimental plant. All of these data sets are available at the CSTH web site. The model is then explored mathematically to give a linearized state-space representation at the operating point and also an input–output transfer function matrix representation. Finally, Section 8 suggests some applications for the simulation and presents a challenge in the form of a system identification problem.

* Corresponding author. Tel.: +44 0 20 7594 6622; fax: +44 0 20 7594 6606.
E-mail address: n.thornhill@imperial.ac.uk (N.F. Thornhill).

0959-1524/$ - see front matter
doi:10.1016/j.jprocont.2007.07.006

2. Background and context

2.1. Introduction

Process simulations in the public domain have been used in education and academic research for many years to compare the performance and applicability of methods for control, identification and diagnosis. Broadly speaking, the simulations fall into two categories: (i) models in which the dynamics are captured through first principles, and (ii) linear models presented as transfer functions or in state-space form. Also available are detailed models for individual components of a process such as control valves and rotating machinery. Commercial training simulators are a further important category of process simulation. The following sections review the literature and place the CSTH simulation in the context of other work.

2.2. First principles models

A very widely used model is the classic continuous stirred tank reactor simulation with Van de Vusse reaction kinetics [39]. It appears in text books [26,10] and has been used for demonstration of control schemes and fault diagnosis. The reaction equations are non-linear because they include the bilinear products of flow rates, composition and temperature as well as the temperature dependence of reaction rate [26]. Other authors have made realistic additions such as the dynamics of a reactor with a cooling jacket [31,32].

At the time of writing, more than 150 articles in the Science Citation index are using the Tennessee Eastman challenge problem [9]. This simulation represents a complete process comprising a reactor and several separation columns and heat exchangers. The process presents significant plant-wide multivariable control challenges and the authors also provided simulations of process faults. A baseline control system was reported by [24] and the simulation has been widely used for demonstration of advanced control schemes (e.g. [23,30,22,20,40]), and for testing of fault detection and diagnosis schemes, both data driven and model-based [19,12,5,14–16,34]. The original code was written in Fortran, while [29] has made an implementation in Simulink available to other researchers.

Other first principles models from the literature are:

- The vinyl acetate process [4];
- The reactor/regenerator section of a Model IV fluid catalytic cracking unit [25];
- Emulsion polymerization with population and particle balance [11];
- The ALSTOM gasifier that produces gas from carbon-based feedstock [8,7];
- Non-linear distillation model [35]. Matlab code is available for this simulation [36].

2.3. Linear dynamic models

The non-linear distillation model paper of [35] offered transfer function models linearized at different operating points as well as the first principles model.

Models expressed in the form of a transfer function matrix are helpful for demonstrating multivariable problems where interactions are the key issue. Their clear capture of these effects also gives them value for teaching purposes. For instance, [33] use the Wood–Berry two-by-two transfer function model of a pilot-scale distillation [42]. The model relates plant inputs (reflux rate and steam flow rate) to outputs (top and bottom product compositions). It is expressed as transfer functions in the form of first order lags plus time delays (FOPTD). [21] used the Wood–Berry model to demonstrate performance monitoring of a model predictive controller.

The Shell challenge problem [28] is a transfer function representation of an industrial debutanizer. Again, each transfer function is a first order lag with delay where some of the delays are very long, giving a considerable challenge for multivariable control. The paper by [3] concerned worst-case bounds and statistical uncertainty in the evaluation of the Relative Gain Array. It presented results from several transfer function benchmark models including a simplified model for the Shell challenge problem and a three-by-three model for a pilot scale distillation column which originated with [27].

State-space benchmarks are used for the testing of model reduction algorithms in which the aim is to derive a smaller representation with many fewer states which has almost the same dynamic input–output behaviour as the original problem. The SLICOT collection [37] created as part of the European Union's BRITE-EURAM III NICONET programme gives some huge state-space models as challenges for this purpose and the Oberwolfach model reduction benchmark collection [18] has similar uses.

2.4. Hybrid and data-based models

An issue with the use of simulations for applications in fault diagnosis and robust control can be that noise and disturbances are difficult to model accurately. There is a tendency to model these as filtered or integrated Gaussian random noise or as piecewise linear disturbances, but in many case such simple signals fail to capture real effects. For instance, time trends of instruments measuring the output of a non-linear system typically have a non-Gaussian distribution and a spectrum characterized by phase coupling. Real data captured from processes provide more realistic tests than simulated data.

[41] provided benchmark data for a non-linear dynamic model identification challenge problem. The data are from a laboratory surge tank which generated non-linear input–output data for the comparison of non-linear modeling methods. A specific issue was that models should be robust to noise in the identification data.