CHAPTER 2

LITERATURE REVIEW

In this chapter, a brief overview of some recent approaches to modeling, state and parameter estimation and model predictive control from the chemical engineering literature has been presented.

2.1 MODELING

A model is a representation of a physical process. Mathematical models of chemical processes are especially useful for the designing of new processes, optimization of existing processes or control of a process. Models enable predictions about how a process will change when perturbed or modified. There are many different types of models that can be developed for a process. Data driven methods are developed from actual process data without assumptions about the details of the process, whereas the first principles models use understanding of the fundamental phenomena to create a model relationship.

The nonlinear modeling problem can be solved using the operating regime based modeling framework by:

- Decomposing the system's full range of operation into a number of overlapping operating regimes. This task includes a definition of the full operating range as well as the identification of variables that can be used to characterize the operating regimes.

- Developing local linear model for each operating regime.
- Combining the local models into global model using weighting functions.

Thus, it can be concluded that the operating regime based modeling framework provides a method to model nonlinear systems by an efficient interpolation of local linear models defined by operating regimes. Many different approaches have been proposed for using local models to approximate nonlinear systems. A detailed review is given in Johansen and Murray-Smith (1997), Foss, Johansen and Sorensen (1995) Johansen and Foss (1995) and Rueda (1996). In many cases the different approaches can be distinguished by the choice of the model weights:

- In Aufderheide and Bequette (2003), model weights have been computed using the recursive Bayesian algorithm. That is, given a set of models, the Bayesian algorithm recursively determines the likelihood that the i^{th} model is the true model of the plant based on the present residuals and the previous probabilities for each model.
- In Banerjee et al (1997), the multiple local models are combined into a single linear parameter varying global model. The parameters of the global models are selected to be model probabilities estimated using Bayesian approach.
- In T-S fuzzy model developed by Takagi and Sugeno (1985), the operating region is defined by the fuzzy set membership function and the weights are provided by the operating region

membership functions. The T-S fuzzy model provides a powerful way to model nonlinear dynamic systems. Moreover, fuzzy inference systems are universal approximators and a given mapping can be realized with an arbitrary degree of accuracy given enough number of rules over the universe of discourse.

The modeling framework that is based on combining a number of local models, where each local model has a predefined operating region in which the model is valid, is called operating regime model. The main advantage of this framework is its transparency. That is, the model structure not only is interpreted in terms of operating regimes, but also quantitatively, in terms of individual local models. Further, the operating regimes can be represented as a fuzzy set. This representation is appealing, since many systems change behavior smoothly as a function of the operating point and the soft transition between the regimes introduced by the fuzzy set representation captures this feature in elegant manner. However, probabilistic weighting chooses model or combination of models which best represent the current plant input/output behavior. Here, the local model weights are estimated on-line using a Bayesian approach.

In the paper by Banerjee et al (1997) the authors have stated that the Bayesian approach selects only the best model out of group of models. Since the study is concerned with state estimation during the plant transition, instead of just choosing the best single model, a better approach would be to construct a global model that interpolates between the local models as plant transforms itself.

Aufderheide and Bequette (2003) in their paper have stated that the Bayesian-MMAC results show convergence to a single model rather than combination of more than one model. Also, the probability estimation algorithm can get locked onto one model, so that its probability converges to one and that of other models converge to zero. Therefore, if the plant subsequently changes from one regime to another, it may take a very long time for the probabilities to reflect the change. For the above reasons, fuzzy rule base has been selected for combining the linear models.

Algorithms for the identification of T-S fuzzy model on the basis of data are described by Sugeno and Kang (1986) and several experimental and simulated examples are given in Takagi and Sugeno (1985), Sugeno and Kang (1986), Sugeno and Kang (1988). Gozard Karer etal(2007) have proposed a method to identify Hybrid fuzzy dynamic model for hybrid systems.

2.2 STATE AND PARAMETER ESTIMATION

State variables of a process are the variables that specify uniquely the state of the process at given time. Thus effective control and monitoring of a process requires reliable real-time information on the state variables of the process. State estimators are deterministic or stochastic, static or dynamic systems that are designed on the basis of a mathematical model and that can provide reliable frequent information on process state variables.

Luenberger (1971) observer has been used for state estimation of deterministic linear dynamic systems, whereas Kalman and Bucy (1961) filter has been extensively used for state estimation of noisy dynamic systems. But all real systems are noisy dynamic systems. That is why Kalman filter finds wide use in state estimation problems. Kalman filter is a recursive estimation approach where state estimates are obtained in two distinct steps. In the first step, a one step ahead prediction is obtained based on the latest state estimate and in the second step, the state estimate is refined by linearly combining the state prediction obtained in the first step with the new output measurement. The calculated result of the Kalman filter is the estimate of system states with minimum error variance. The rate of convergence of the Kalman filter can be adjusted by modifying the assumptions made about external system influences. The theoretical properties of the Kalman filter and the Luenberger observer can be found in estimation and/or systems theory text books by Chen (1984) and Friedland (1986). For parameter estimation, where system parameters change in a non-stationary manner, the parameter estimation problem can be transformed into a state estimation problem by augmenting the system states with the parameters to be estimated.

The motivation for nonlinear state estimation comes from the fact that the linear state estimators are often inadequate for nonlinear processes. It should be noted that, if the linear state estimator is not designed for the same steady state at which the process operates, then there will be an offset between the actual and estimated values of the state variables. There are many applications of the EKF presented in the literature and in Muske and Edgar (1997).

The Extended Kalman filter (EKF) is a natural extension of the linear filter to the nonlinear domain through local linearization. The Extended Kalman filter is probably the most widely used nonlinear filter. While EKF formulations have been successful in solving many industrial problems, its implementation is not always simple as the state error covariance prediction step requires analytical computation of jacobians at each time step.This can prove to be prohibitively complex and computationally demanding for high dimensional systems. Moreover this also implies that nonlinear function vectors appearing in system equations should be smooth and at least once differentiable. Recently the unscented Kalman filter(UKF) has been proposed as an alternative to the Extended Kalman filter where the above limitations has been overcome using the concept of sample statistics (Julier and Uhlmann 2004). The UKF uses a deterministic sampling technique to select a minimal set of sample points (called sigma points) around the mean. These Sigma points are then propagated through nonlinear functions and the covariance of the estimate is then recovered.

Vachanni et al (2005) have proposed a recursive constrained formulation called recursive nonlinear dynamic data reconciliation (RNDDR).This approach combines computational advantages of recursive estimation while handling constrained on states. The state and covariance propagation steps and the updated covariance computation in RNDDR are identical to EKF. The updated state estimates are obtained by solving a constrained optimization problem formulated only over one sampling interval, which significantly reduces the computational burden compared with MHE or NDDR formulations. Vachhani et al (2006) later developed a constrained version of the UKF (unscented recursive nonlinear dynamic data reconciliation or URNDDR) for state estimation and parameter estimation in nonlinear systems. This approach combines the advantages of the UKF and RNDDR formulations.

The notions of detectability and observability are of great importance in the state estimator design for dynamic systems. The detectability of a process is a necessary and sufficient condition for estimating the process state variables, whereas observability is a necessary and sufficient condition for the existence of an estimator with a completely adjustable rate of convergence. Observability existence indicates that measurable outputs contain useful information on all the state variables. For linear systems, the notions of observability and detectability are well-understood and precise criteria for their assessment are available in the linear system literature discussed by Chen (1984). For nonlinear systems, however, these notions are very complex and do depend on the region within which the system operates, that is, these system properties are local properties and difficult to assess in the general case.

Fuzzy state estimation is a topic that has received very little attention. There have been few papers published recently on fuzzy state estimator design; however, these papers usually deal with the noise free case. That is, fuzzy state estimators are designed for systems that are not affected by noise as discussed by Palm and Driankov (1999). Recently, Dan Simon has proposed a state estimator for noisy discrete time dynamic T-S fuzzy models and has shown that the state estimator generates accurate state estimates in the absence of unknown input Dan Simon (2003) and the presence of unknown input was discussed by Janarthanan (2006). Tanaka and Sugeno (1992) showed that the stability of a T-S fuzzy model could be shown by finding a common symmetric positive definite matrix (P) for N subsystems.

Mendonca et al (2007) have proposed a fault isolation scheme using fuzzy model based observer to detect and isolate several abrupt and incipient faults that are present in the control valves.

Francesco Pierri et al (2008) have proposed an observer based sensor fault detection and isolation for chemical batch reactors. The authors have designed the observers using H-infinity approach, to achieve fault detection and isolation even in the presence of external disturbance and modeling errors.

2.3 MODEL PREDICTIVE CONTROL

Model Predictive Control (MPC) is a general control methodology that has become an important research area in automatic control theory. MPC has emerged as one of the most attractive control techniques in the chemical and petrochemical industries during the past decade. MPC is characterized by the use of a process model to predict the process output at future discrete time instants over a specified prediction horizon, given the process inputs and the desired reference output.

The concept of predictive control was introduced in the eighties by Richalet et al (1978). The predictive controller calculates a sequence of future actuation signals by optimizing a cost function, which describes the control objectives. Due to their ability in explicitly handling of the constraints and easily extending to MIMO systems containing delays and inverse responses, this family of controllers has attracted good attention from large industrial manufacturers Ming He et al (2005) and Mark Camon (2004). It can be classified into LMPC and NMPC according to the employed predictive models.

Conventional MPC techniques are based on the use of linear models. LMPC can yield a satisfactory performance if the process is operated close to a nominal steady state or is fairly linear. The linear model is not adequate to describe a host of chemical engineering processes. Many times the dynamic characteristics of the process will change dramatically due to a large disturbance or significant setpoint changes. Also, batch processes typically operate over a wide operating range, making a linear control strategy ineffective.

Huang et al (2000) have shown that the LMPC may not assure satisfactory servo and regulatory control performances for wide range of operating conditions for highly nonlinear processes. Extended Dynamic Matrix Control (EDMC) has been proposed by Peterson et al (1992) to extend the existing version of the LMPC (i.e. Dynamic Matrix Control) to control nonlinear systems.

While LMPC was popular in early eighties, the 90s have witnessed a steadily increasing attention from control theoretists as well as control practitioners in the area of NMPC Qin et al (1997).

The need to achieve tighter control of strong nonlinear process has led to more general MPC formulation in which nonlinear dynamic model is used for prediction. It should be noted that the selection of suitable form of nonlinear model to represent system dynamics is a crucial step in the development of a NMPC scheme. These nonlinear models have led to NMPC algorithms and the survey on nonlinear control of chemical processes by Bequette (1991) summarizes different NMPC algorithms. Qin and Badgwell (2000) provide a good overview of nonlinear MPC applications that are currently available in industry.

Patwardhan et al (1992) described the application of NMPC to two distributed parameter processes which were a packed distillation column and a fixed-bed catalytic reactor. Over two thousand online applications of LMPC in the chemical process industry, mainly in the refining, petrochemical, and chemical industries as well as in pulp and paper and food processing have been reported in the paper by Qin and Badgwell (1997).

Nahas et al (1992) have proposed the use of internal model control using neural network for the control of chemical process. Since it is difficult to describe the complete system behavior using single linear model, the performance of control schemes based on single linear model being used to control nonlinear process can't yield satisfactory performance.

The multiple linear models concept has been used in the recent years for modeling of nonlinear systems. Also, multiple linear model based approaches for controller design has attracted the process control community and a plethora of multiple model adaptive control schemes have been proposed in the control literature (Gundala et al 2000, Yu et al 1992, Dougherty and Cooper 2003).

The method by Arkun et al (1998) uses the nonlinear first principles model to obtain the linear state space models at different operating points. These models are then weighted using a Bayesian estimator at each sampling instants to obtain an adaptive internal model and it is being used to develop internal model control schemes.

Townsend et al (1998) have represented the nonlinear system using local model network and have implemented dynamic matrix control using the local model network as an internal model. It should be noted that the local model network is limited to only NARX models and also, this technique can't be applied for multivariable control.

Ruiyao Gao et al (2002) has proposed a nonlinear PID controller for CSTR using local model networks. Recently they have used operating region recognition algorithm to obtain all the regions of the process and then linear models are identified for each regions. From the bank of linear models, the authors select the appropriate controller model for the dynamic matrix controller using the switching algorithm.

Multiple model approach based IMC controller has been proposed by chiu et al (2000). The authors’ have used transfer function model to describe the nonlinear system in each operating regime. The authors’ also have implemented the IMC algorithm on the simulated model of the CSTR and continuous fermenter.

Omar Galan et al (2004) have reported the real-time implementation of multi-linear model based control strategies on the laboratory scale process. The authors have implemented multi-linear MPC, scheduled proportional-integral controller and Robust H_∞ on the laboratory scale pH neutralization reactor. Rodriguez et al (1999) have described a supervisory approach based multiple model control design procedure for the binary pilot distillation column

Real time implementation of the multiple model predictive control scheme to control the mean arterial pressure and cardiac output has been reported in Ramesh Rao et al (1999). Predictive Control of nonlinear process using interpolated models have been proposed by Dharasakar and Gupta (2000). The authors have presented an approach to handle the nonlinearity of the process by using the step response models. The step response models are obtained for a few sub-regions of the operating region experimentally and the models for other sub-regions are determined through linear interpolation. The authors’ have validated the proposed control scheme on the simulated model of non-isothermal CSTR.

The application of linear and nonlinear long range predictive control based on linear and nonlinear generalized predictive control(NGPC)and linear and nonlinear generalized minimum variance (NGMV)algorithms to an open loop unstable continuous stirred tank reactor have been considered by Hale Hapoglu(2002)

Jenny and Rawlings (2004) have examined the control performance of the robust MPC(RMPC)method proposed by Wang and Rawlings(2004)on several examples. The authors have shown that the proposed RMPC method achieves satisfactory control for a system with time varying uncertainities in the process gain time constant and time delay . Further the proposed control scheme guarantees offset free non zero setpoint tracking and non zero disturbance rejection subject to input and output constraints.

A new predictive control framework for chemical processes namely stochastic closed loop model predictive control has been presented by Dennis Van Hessem and Okko Bosgra (2006).

A modified multiple model approach based state feedback control strategy has been proposed by Wang et al (2007) to achieve robust control with global stability. A simple model modification technique using state feedback to realize pole placement has been proposed by the authors' to ensure that the poles of the model are located in the left half of the complex plane. The proposed control scheme has been implemented on chaotic CSTR process and Zymomonas mobilis reactor. The authors have shown that the NMPC with a multi-model approach based on the modified model has led to improved performance.

A number of methods to incorporate fuzzy models into the MPC framework have been reported in the literature: Kim et al (1996), Martin Fischer et al (1998), Kothare et al (2000), Leyla et al (2000) and Li et al (2004) treated the fuzzy logic model as a collection of piecewise linear models, while Huang et al (2000) described the process by a fuzzy convolution model, consisting of number of quasi linear fuzzy implications. He et al (2005) has implemented multiple model predictive controller (MMPC) for temperature control of an Air-Heating Unit (AHU), using a

T-S fuzzy model. Abnoyi et al (2001) have proposed a linearization technique for product–sum crisp-type fuzzy model and designed a multi-step fuzzy predictive controller.

The use of Takagi Sugeno model in combination with MPC is described. In the paper by Roubos et al (1999). The authors have derived the process model form input output data by means of product space fuzzy clustering and the MIMO model is represented as a set of coupled multi input single output (MISO) models. The proposed fuzzy model based predictive controller has been evaluated with a simulated laboratory setup for a MIMO liquid level process with two inputs and four outputs

Haralambos Sarimveis and George Bafas(2003) have proposed fuzzy model predictive control for nonlinear processes using genetic algorithms. The authors have applied the method to a chemical reactor using a discrete Takagi-Sugeno model for predicting the behavior of the process. The proposed control scheme produced very good results and proved to be superior to the standard approach.

Hybrid fuzzy dynamic model based MPC on the batch reactor has been reported in Gorazd Karer et al (2007).

The advantage of using state estimation instead of the frequently used approach of the additive output disturbance has been reported by Ricker (1990). Ricker (1990) had used linear time-invariant state space models and applied state estimation theory. Recent trends in MPC favor the closed-loop approach, where the measurements are incorporated into the prediction. This feature necessitates an estimator to recover the states from noisy measurements and knowledge of a process model with uncertainty. State observer based MPC formulations make use of Kalman filters and EKF.

The application of state estimation based NMPC scheme to an unstable nonlinear process has been reported by Biagola and Figueroa (2004). The authors have considered the control of an open-loop unstable jacketed exothermic chemical reactor problem. Further, NMPC coupled with a state observer have been designed and finally, computer simulations were performed to illustrate the performance of both the nonlinear observer and the control strategy.

As suggested, one can also apply operating regime approaches to develop an operating regime based observer that can be applied in a model based controller. Since global information can be applied to determine the control input at each sampling instants, the nonlinear model based controller is expected to achieve better control performance.

In this work, a nonlinear state estimator is presented which will provide the estimated value of the internal states and the most significant disturbance of the process to the MPC. MPC strategies based on these nonlinear state estimators will allow tight control of the process and in addition, these control strategies may permit plant operation in a region that is economically attractive, whereas a linear controller will not be able to control the process satisfactorily.