State Estimation in a CO_2 Capture Plant

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Abstract. Post combustion CO_2 capturing holds an important position in the area of carbon capture and sequestration (CCS). Research in this area range from experimental work to modeling work. Dynamic models are interesting since these describe the plant operation during variations, up-stream or down-stream, and due to their use-fulness in control design. To take full advantage of state space models in control design, it is necessary to have on-line knowledge of all states, also states that are not measured directly. Techniques for state estimation, such as Kalman filter based methods, thus form key technology for advancing control solutions. But state estimation is also of interest in its own right for making available on-line knowledge of states. In this study, a dynamic model of an amine based CO_2 capture plant is used as a basis for a state estimator. A high order version of the model is used to represent the "real" plant. A reduced order model of the plant is then used for state estimation, and the Ensemble Kalman filter is used.

Introduction

Power generation via fossil fuel-fired power plants is known to be the largest single source of CO_2 emission in the world [1]. The development of capture technologies targeting such sources therefore is important for achieving the goals in CO_2 emission reduction. Post-combustion capture, pre-combustion capture and oxy-fuel combustion are the three main technologies available at present [2], and much research is done with the prospect of developing those techniques further.

Post combustion capture is still the best known technique, possibly due to the large number of existing power plants, and the promising developments that are available. CO_2 capture by amine absorption and stripping is currently considered to be the most feasible option for the removal of carbon dioxide from the power plants' exhaust gases [3].

Modelling work related to CO_2 capture technologies plays an important role with respect to the design, control and optimization of the capture process. Steady state models are important for design and optimization purposes, and dynamic simulation models are important for control applications. Several dynamic models for simulating the amine based CO_2 absorption plants are presented in literature [4]-[6].

A model consisting of a set of first order differential equations to represent the system is referred to as a state space model. To take full advantage of state space models in control design, it is necessary to have on-line knowledge of all states, also states that are not measured directly. Techniques for state estimation, such as Kalman filter based methods, thus form a key technology for advancing control solutions. But state estimation is also of interest in its own right for making available on-line knowledge of states.

The Kalman filter based methods vary from basic Kalman filter (**KF**) to its extensions and generalizations such as the *Extended Kalman Filter* and *Unscented Kalman Filter*. The basic Kalman filter is applicable for linear dynamic systems, while the extensions and generalizations of the method are there to be used with the nonlinear dynamic systems [7]. The *Ensemble Kalman Filter* (**EnKF**) is another alternative to the traditional Kalman filter for better handling of nonlinear models with large number of states [8].

Use of traditional KF methods for models with high-dimensional state vectors is computationally difficult as an error covariance matrix for the model states needs to be stored and propagated in time. The Extended Kalman filter uses a linearized equation for the error covariance evolution when the model dynamics are nonlinear. This linearization can result in unbounded linear instabilities for the error evolution [8]. These two problems can be solved to a great extent by using the Ensemble Kalman filter.

In this study, a dynamic model of an amine based CO_2 capture plant is used as a basis for a state estimator. The model as developed and published by Jayarathna et al. ([6], [9] - [12]) is used in this study as the plant model. A high order version of the model is used to represent the 'real system' due to the absence of real plant data. A reduced order model of the plant is then used for state estimation, and the Ensemble Kalman filter is used.

1 Theory

The EnKF algorithm is presented in details with the derivation by Evensen [13]. Initialization of the estimator is done by providing values for the initial ensemble. When the number of simulations in an ensemble is N, the values of the initial ensemble are given according to the eq. 1.

$$x_{0|0} \sim \mathcal{N}(\bar{x}_0, P_0) \tag{1}$$

Having the initial ensembles available, the state estimator runs trough a propagation step and a measurement update step at each time step. The propagation step consists of three consecutive steps, the ensemble propagation, the estimated state-output propagation and the covariance calculation. For each simulation $i\,(i = 1, 2, \dots, N)$, the ensemble propagation step is given by eqs. 2 and 3.

$$x^i_{k|k-1} = f_{k-1}\left(x^i_{k-1|k-1}, u_{k-1}, w^i_{k-1}\right) \tag{2}$$

$$y^i_{k|k-1} = h_{k-1}\left(x^i_{k|k-1}, v^i_{k-1}\right) \tag{3}$$

Here w^i_{k-1} and v^i_{k-1} are the model disturbances $(w \sim \mathcal{N}(w_0, W))$ and the measurement noise $(v \sim \mathcal{N}(0, V))$.

The propagation of the estimated state and output is given by eqs. 4 and 5.

$$\hat{x}_{k|k-1} = \frac{\sum_{i=1}^{N} x^i_{k|k-1}}{N} \tag{4}$$

$$\hat{y}_{k|k-1} = \frac{\sum_{i=1}^{N} y^i_{k|k-1}}{N} \tag{5}$$

The covariance calculation is done according to eqs. 6 and 7.

$$e^i_{x,k|k-1} = \left(x^i_{k|k-1} - \hat{x}_{k|k-1}\right) \tag{6}$$

$$P_{k|k-1} = \frac{\sum_{i=1}^{N}\left(e^i_{x,k|k-1}\right)\left(e^i_{x,k|k-1}\right)^T}{N-1} \tag{7}$$

After completing the propagation step, the state estimator updates the predictions using the available measurements. The measurement update step consists of two consecutive stages in the used algorithm, Kalman gain calculation and state-out-covariance update. The Kalman gain calculations is performed according to the eqs. 8-11.

$$e^i_{y,k|k-1} = \left(y^i_{k|k-1} - \hat{y}_{k|k-1}\right) \tag{8}$$

$$P_y = \frac{\sum_{i=1}^{N}\left(e^i_{y,k|k-1}\right)\left(e^i_{y,k|k-1}\right)^T}{N-1} \tag{9}$$

$$P_{xy} = \frac{\sum_{i=1}^{N}\left(e^i_{x,k|k-1}\right)\left(e^i_{y,k|k-1}\right)^T}{N-1} \tag{10}$$

$$K_k = P_{xy} P_y^{-1} \tag{11}$$

The state-out-covariance update step is given by eqs. 12-14.

$$x^i_{k|k} = x^i_{k|k-1} + K_k\left(\left(y_k + v^i_k\right) - y^i_{k|k-1}\right) \tag{12}$$

$$\hat{x}_{k|k} = \frac{\sum_{i=1}^{N} x^i_{k|k}}{N} \tag{13}$$

$$P_{k|k} = P_{k|k-1} - K_k P_y K_k^T \tag{14}$$

Here $y_k = g(x_k)$.

Updated values of the states $(x^i_{k|k})$ are then taken as the initial values to run the estimator for the next time step. The averaged values $(\hat{x}^i_{k|k})$ are the estimates for the time step. The covariance matrix $(P_{k|k})$ can be used to get an idea about the uncertainty of the predictions.

2 Implementation

In the implementation of the state estimator, the number of ensembles is taken to be 60 ($N = 60$). The Parallel Computing Toolbox in MATLAB is used to work with 12 threads at the same time. This way, 12 simulations are performed simultaneously to complete each ensemble, and the time required for completing the simulations for an ensemble is reduced by five times. Initial state values (x_0) are taken from a simulation with sufficiently long simulation time, thus steady state is assumed. The covariance matrix of the initial states (P_0) is given according to the magnitude of the x_0 values (as a rule of thumb, the values of the diagonal matrix (P_0) are taken as a fraction of the initial state values).

A higher order model, i.e. with a higher number of control volumes than in the state estimator, is used to represent the "real" system due to the absence of real plant data. According to the assumptions made during the model development an infinite number of CVs should be used to represent the columns in the real system. But a finite number of CVs has to be used in practice.

Use of a finite number of control volumes introduces diffusion into the column models. Diffusion is a phenomenon that occur in the absorption and stripping columns. Therefore, it is acceptable to have a finite number of control volumes in the model that represents the real plant.

Several compositions and temperatures are taken as the measurements; we assume a total of 26 measurements. Measured compositions are the composition of the cleaned gas and the gas leaving the stripping column (can be measured by gas chromatography). The amount of dissolved CO_2 (total CO_2) and MEA (total MEA) in the solvent streams leaving the absorption tower, stripping tower and the buffer tank are also taken as measurements.

Mass flow rate of the amine solutions leaving the absorber, stripper and the buffer tank without the mass flow rate of the dissolved CO_2 are also included in the measurements. Temperatures of the liquid and vapor leaving the absorption tower, temperatures of the liquid and vapor streams leaving the stripping column, temperatures of the liquid streams leaving the heat exchangers and the temperature of the buffer tank are taken as the temperature measurements. Measurement noise is assumed to be white noise.

3 KF Predictions

An analysis related to the number of control volumes used in the tower models, given in Figure 1, showed that the execution time increases quadratically with the increasing number of control volumes. Therefore the number of control volumes to be used in the state estimator is chosen to be around 50 control volumes.

When the sensitivity of the model predictions to the number of control volumes used in the tower discretization is considered, from Figure 1 it is noticeable that the model predictions improves with the increasing number of control volumes up to about 100 CVs in towers. The predicted values remains with very little variations for higher number of control volumes than 100, but as can be seen from Figure 1 the execution time for the simulations increases very much for higher number of CVs than 100.

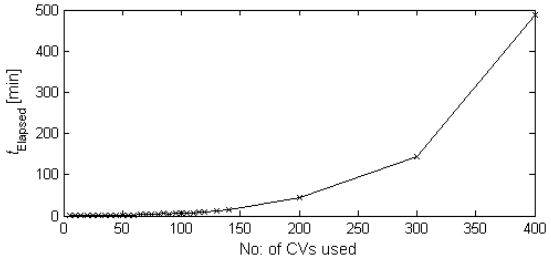

Figure 1: Execution time of the simulations with the number of control volumes used in the tower descretizations.

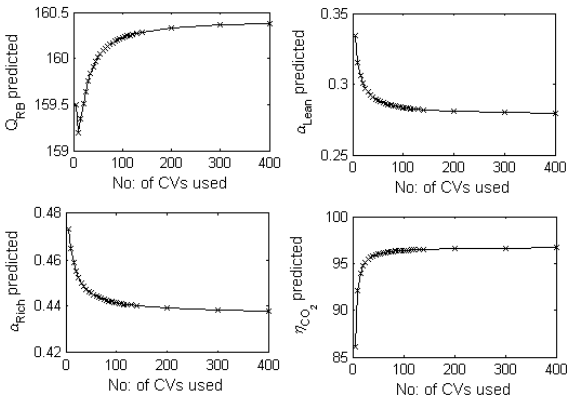

Figure 2: Dependancy of the model predictions on the number of control volumes in the tower descretizations. Q_{RB} predicted is the predicted re-boiler duty, α_{Lean} predicted is the predicted lean loading value, α_{Rich} predicted is the predicted rich loading value and η_{CO_2} predicted is the predicted CO_2 removal efficiency.

Therefore, 100 CVs is chosen as a rough limit for the maximum number of CVs that are used in the towers for the model that is used for representing the real system. The dependency of the model predictions with the number of control volumes used is shown in Figure 2.

Several different cases are studied to analyze the estimates of the EnKF to different scale of model errors. The model error was increased by increasing the difference between the number of control volumes used in the model that represents the real plant and the model used in the state estimator. One hour of the plant operation is simulated. Information about the cases performed for analyzing the sensitivity of the state estimator for the model error are given in the Table 1. Selected states are presented in Figures 3 - 8 for the four cases of Table 1 to analyse the quality of the estimates. Figures 3 - 5 show three measured states and Figures 6 - 8 show three unmeasured states.

Case no:	CVs in Model	CVs in Real System	Ratio	Computation time
1	15	15	1	2 h
2	50	50	1	20 h
3	40	50	1.25	6 h
4	40	100	2.5	6 h

Table 1: Details of the cases used for analyzing the sensitivity to the model error.

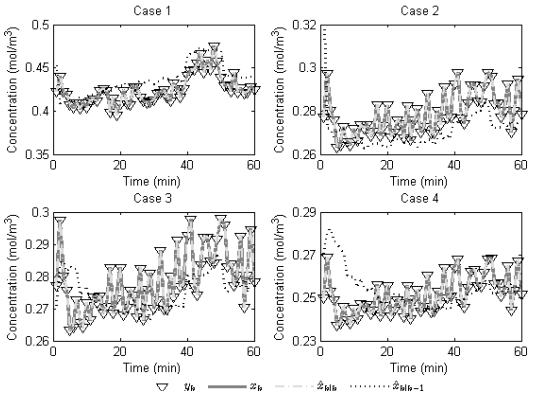

Figure 3: CO_2 concentration in the cleaned gas leaving the absorption tower. y_k: measurement, x_k: real state, $\hat{x}_{k|k}$: a posteriori state, $\hat{x}_{k|k-1}$: a priori state.

Prediction of CO_2 concentration in the cleaned gas leaving the absorption tower (Figure 3), which is a measured state, appear to be a good match with the real state in all four cases. Further, it can be seen that the measurement noise of this state is very small, and that should be the reason for this high quality prediction in all the cases. The other two measured states presented, the temperature of the rich amine steam leaving the absorber (Figure 4) and the temperature of the rich amine leaving the cross heat exchanger (Figure 5), are predicted with larger errors. The pattern of the predictions appears to follow the pattern of the real states, and the error of the prediction appears to be increasing with the model error.

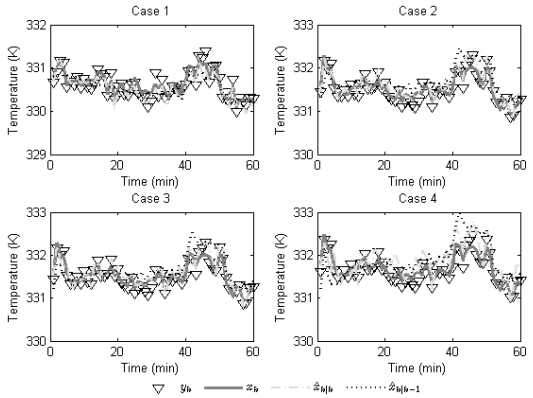

Figure 4: Temperature of the amine streams leaving theabsorption column. y_k: measurement, x_k: real state, $\hat{x}_{k|k}$: a posteriori state, $\hat{x}_{k|k-1}$: a priori state.

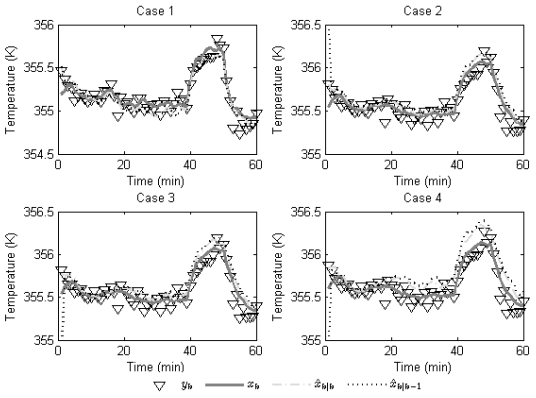

Figure 5: Temperature of the rich amine stream leaving the cross heat exchanger. y_k: measurement, x_k: real state, $\hat{x}_{k|k}$: a posteriori state, $\hat{x}_{k|k-1}$: a priori state.

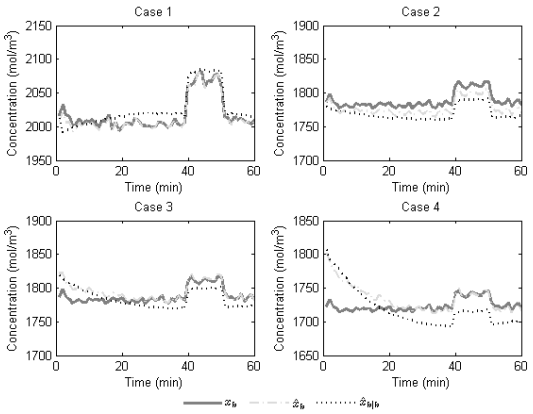

Figure 6: Total CO_2 concentration in the amine stream at 1/3 of the packing height of the absorption tower. x_k: real state, $\hat{x}_{k|k}$: a posteriori state, $\hat{x}_{k|k-1}$: a priori state.

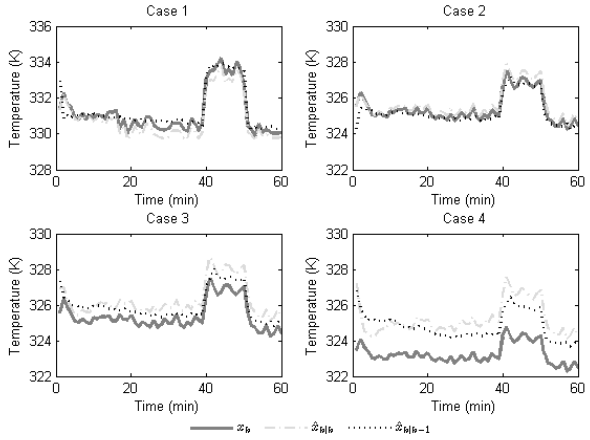

Figure 7: Liquid phase temperature at 1/3rd of the absorber packing height. x_k: real state, $\hat{x}_{k|k}$: a posteriori state, $\hat{x}_{k|k-1}$: a priori state.

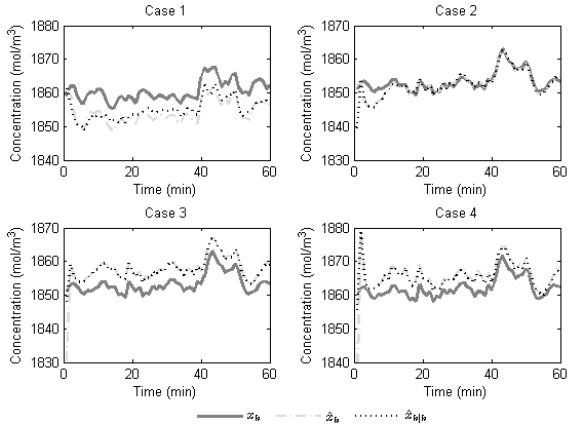

Figure 8: Total CO_2 concentration at 1/3rd of packing height of the stripping tower. x_k: real state, $\hat{x}_{k|k}$: a posteriori state, $\hat{x}_{k|k-1}$: a priori state.

Estimates of the states that are not measured are also in good accordance with the pattern of the real states (Figures 6 - 8). Similar to the observation with the measured states, it can be seen that the error in the estimated values are increasing with the increase in the model error.

When the computation time needed for each of the cases is considered, it can be seen that there will always be a time delay before the estimates are available.

4 Conclusions and Recommendations

A state estimator for making on-line predictions of the states of a CO_2 capture plant is developed. The Ensemble Kalman Filter algorithm is used in the state estimator, due to the suitability of the algorithm to handle nonlinear models with a large number of states. A simple model (with small number of control volumes) is used in the estimator while a high order model (with large number of control volumes) is used to represent the real system. Absence of real plant data is the reason for using a high order model as the real system. According to the assumptions of the model development, an infinite number of control volumes should be used in the tower discretization to represent the real system. In practice a finite number of control volumes is used, thought. Tower discretization into finite number of control volumes introduces diffusion into the system, which is also there in reality. Therefore, use of a finite number of control volumes in tower discretization is justified.

Sensitivity of the estimates to the model error is analyzed by performing simulations with increasing model error (by making the difference between the model and the system to increase). Some predictions seem very good and some predictions seems to be poorer. The observation from the results of the sensitivity analysis, in general, is that the deviation of the estimates from the real states increases with the increasing model error.

According to the simulation time needed for each of the cases considered in the sensitivity analysis, it can be seen that the estimates are available always with a time delay. This high computational time of the estimator is a problem for making available the timely estimates of the unmeasured states.

The use of iterations with the flash calculations in the model can be a reason for the computation time of the estimator. Making table look-up values available to be used instead of performing flash calculations, will be an option to speed up the estimator.

When the tendency to increase the error in the estimates with the increase of model error and the time delay of the estimates are considered, it is concluded that some restructuring of the model is required before the estimator is ready for on-line use.

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