

Groundwater Pollution Concentration Estimation with Modified Kalman Filter Method

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ABSTRACT

The problem of groundwater pollution has an important effect on the quality of the environment and the quality of human life. Groundwater pollution can be caused by natural sources or human activities. Groundwater pollution problems can be modeled using the advection-dispersion equation. The model shows the concentration of pollutants in groundwater. Therefore, it is important to estimate groundwater pollutant concentrations. The estimation method can be used to predict groundwater pollutant concentrations in the future and maintain the stability of groundwater quality. This research collaborates the Kalman filter algorithm with the reduction method to estimate groundwater pollutant concentrations. The model is discretized first and then estimated using the Kalman filter algorithm. Next, model reduction was carried out using the Linear Matrix Inequality (LMI) method, then the reduced model was estimated using the Kalman filter algorithm. From the estimation results using the Kalman filter algorithm on the original system and the system that has been reduced by the LMI method, excellent estimation results are obtained, because it produces a very small error and is close to the real state variable. Accuracy is tested by calculating the average estimation error.

Keywords: Estimation, Groundwater pollution; Kalman filter; Linear Matrix Inequality; Reduced System

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INTRODUCTION

Groundwater, apart from being used for drinking water, is also one of the most important sources of water for irrigation. Unfortunately, groundwater is susceptible to pollutants. Groundwater pollution occurs when harmful substances (pollutants) enter the groundwater. These pollutants are practically limitless but can range from motor oil to chemicals from agriculture to untreated waste. Unlike surface water pollution, groundwater pollution is harder to detect and control which may cause the problem to persist for long periods of time.

Many researchers observed groundwater pollutant to determine the groundwater quality in an area as well controlling the groundwater quality stability. The research process is carried out by forming groundwater quality modeling and subsequently formed a control device to control or reduce the levels of groundwater pollutant substances. Because of the high cost of the control device and the amount of maintenance costs it cannot be placed as much as possible a tool to measure the concentration of groundwater pollutants. Therefore, estimation of groundwater pollutant concentration is necessary to predicting future groundwater pollutant concentrations.

Research on groundwater pollution concentration estimation has been conducted using the Kalman filter method, and the Ensemble Kalman Filter (EnKF) method [1]. Estimation is quite important in daily life because many life problems require estimation [2], such as estimation of river water level [3] [4] [5] [6], estimation of river water quality [7], estimation of air quality [8], etc.

The Kalman filter is a reliable estimation method in estimating and forecasting the state variables of a linear stochastic dynamical system. The advantage of the Kalman filter is its ability to estimate state variables in the past, present, and future. Estimation with the Kalman filter is done by predicting state variables based on the dynamics of the system, called the prediction stage and then making corrections to improve the estimation results based on data from the measurement results, called the correction stage. The prediction-correction stage is carried out recursively to obtain estimation results that are close to the true value by minimizing the estimation error covariance [9].

In general, the construction of estimation methods aims to obtain accurate results, that is, the estimation error is close to zero, with fast computation time. The problem of computation time is also strongly influenced by the order of the model, so to minimize computation time, it can be done by reducing the order of a large-order model so that a simple model with a smaller order is obtained without significant error, in the sense that the reduction error is very small. This model with a smaller order is called a reduced model. The way to get a reduced model is called model reduction [10]. Many model order reduction methods have been developed, including the Balanced Truncation (BA) method [11], the Singular Perturbation Approximation (SPA) method [12] and the Linear Matrix Inequality (LMI) method [10], [13], [14].

Research to find a better estimation method was also carried out by implementing the Kalman filter algorithm on the reduced model. This research discussed about a construction of Kalman Filter algorithm on the reduced model. It aimed to obtain accurate estimation with short computing time on the reduced model. The method that collaborates the Kalman filter estimation method with the model reduction method is called the modified Kalman filter method. The Kalman filter estimation method has been collaborated with the BT method [7] [15], the SPA method [5], and the LMI method [6], [16].

Based on previous research on the modified Kalman filter method, this research aims to estimate the concentration of groundwater pollution using the modified Kalman filter method, namely a method that collaborates the Kalman filter algorithm with the LMI method, to obtain accurate estimation results with short computing time.

METHODS

The steps in this research are as follows, beginning with obtaining a discrete linear time invariant (LTI) system of the mathematical model of groundwater pollution distribution problem. This is followed by reducing the system to obtain a reduced system using Linear Matrix Inequality (LMI) methods. It then implements the Kalman filter algorithm on the original discrete system i.e. the unreduced discrete LTI system, and implements the Kalman filter algorithm on the reduced system.

Mathematical model of groundwater pollution problem

The distribution of groundwater pollution for non-reactive solutes can be written as the advection-dispersion equation as follows [17].

$$\frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} - v_x \frac{\partial c}{\partial x}, \qquad (x, y) \in \Omega, \ t > 0,$$
(1)

with C(x, y, 0) = 0, $(x, y) \in \Omega$,

$$C(x, y, t) = \phi(x, y, t)(x, y) \in \partial \Omega$$

and $\Omega = (0, L_x) \times (0, L_y)$ is the observed area. C((x, y), t) is the pollution concentration at position x, y and time t. Parameters D_x, D_y and V_x, V_y are diffuse coefficient and groundwater flow velocity in x, y direction. It is assumed that $\phi(x, y, t)$ is a smooth function and D_x, D_y, v are constant.

Discretization of Model

Before we applied Modified Kalman Filter method to estimate the concentration of groundwater pollution, we discretize Eq. (1) respect to position x,y and time t and then we write in the state space form. The mathematical model of the groundwater pollution model in Eq. (1) is a dynamic system, so the time is continuous, so it must be discretized with change of state variable to time with Crank-Nicolson scheme. Then the discretization will be implemented to the Eq. (1), it can be :

$$[1 + 2(S_x + S_y)]c_{ij}^{n+1} + (S_v - S_x)c_{i+1,j}^{n+1} - (S_x + S_v)c_{i-1,j}^{n+1} - S_y(c_{i,j+1}^{n+1} + c_{i,j-1}^{n+1})$$
(2)
=[1 - 2(S_x + S_y)]c_{ij}^n + (S_x - S_v)c_{i+1,j}^n + (S_x + S_v)c_{i-1,j}^n + S_y(c_{i,j+1}^n + c_{i,j-1}^n) with $S_x = \frac{\tau D_x}{2h_1^2}$, $S_y = \frac{\tau D_y}{2h_2^2}$, $S_v = \frac{\tau v}{4h_1}$.

Given $\tau = \frac{T}{N}$, partition the interval [0, T] into *N* equal parts of width τ with *N* positive integers. Furthermore, it is obtained

$$\mathbf{A}c^{n+1} = \mathbf{B}c^n + c^* \tag{3}$$

with

$$c^{n+1} = [c_{11}^{n+1}, c_{21}^{n+1}, \dots, c_{M1}^{n+1}, c_{12}^{n+1}, c_{22}^{n+1}, \dots, c_{M2}^{n+1}, \dots, c_{1M}^{n+1}, c_{2M}^{n+1}, \dots, c_{MM}^{n+1}]_{M^2 \times 1}^T$$

$$\begin{split} c^{n} &= [c_{11}^{n}, c_{21}^{n}, \dots, c_{M1}^{n}, c_{12}^{n}, c_{22}^{n}, \dots, c_{M2}^{n}, \dots, c_{1M}^{n}, c_{2M}^{n}, \dots, c_{MM}^{n}]_{M^{2} \times 1}^{T} \\ c^{*} &= [(S_{x} + S_{v})c_{01}^{n+1} + S_{y}c_{10}^{n+1}, (S_{x} + S_{v})c_{02}^{n+1}, \dots, (S_{x} + S_{v})c_{0M}^{n+1} + S_{y}c_{1M+1}^{n+1}, \\ S_{y}c_{20}^{n+1}, 0, \dots, S_{y}c_{2,M+1}^{n+1}, \dots, (S_{x} - S_{v})c_{M+1,1}^{n+1} + S_{y}c_{M0}^{n+1}, (S_{x} - S_{v})c_{M+1,2}^{n+1}, \dots, (S_{x} - S_{v})c_{01}^{n+1} + S_{y}c_{10}^{n}, (S_{x} + S_{v})c_{02}^{n}, \dots, \\ (S_{x} - S_{v})c_{M+1,M}^{n} + S_{y}c_{M,M+1}^{n+1}]_{M^{2} \times 1}^{T} + [(S_{x} + S_{v})c_{01}^{n} + S_{y}c_{10}^{n}, (S_{x} + S_{v})c_{02}^{n}, \dots, \\ (S_{x} + S_{v})c_{0M}^{n} + S_{y}c_{1,M+1}^{n}, S_{y}c_{20}^{n}, 0, \dots, S_{y}c_{2,M+1}^{n}, \dots, (S_{x} - S_{v})c_{M+1,1}^{n} \\ &+ S_{y}c_{M0}^{n}, (S_{x} - S_{v})c_{M+1,2}^{n}, \dots, (S_{x} - S_{v})c_{M+1,M}^{n} + S_{y}c_{M,M+1}^{n}]_{M^{2} \times 1}^{T} \end{split}$$

The matrices **A** and **B** in Eq. (3) are matrices of size $M^2 \times M^2$ as follows:

$$\mathbf{A} = \begin{bmatrix} P_1 & Q_1 & 0 & \dots & 0 \\ Q_1 & P_1 & Q_1 & \dots & 0 \\ 0 & Q_1 & Q_1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & P_1 \end{bmatrix}, \qquad \mathbf{B} = \begin{bmatrix} P_2 & Q_2 & 0 & \dots & 0 \\ Q_2 & P_2 & Q_2 & \dots & 0 \\ 0 & Q_2 & Q_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & P_2 \end{bmatrix},$$

with matrices P_1 , P_1 , Q_1 , and Q_2 are matrices of size $M \times M$ as follows.

$$P_{1} = \begin{bmatrix} 1 + 2(S_{x} + S_{y}) & S_{v} - S_{x} & 0 & \dots & 0 \\ -(S_{x} + S_{v}) & 1 + 2(S_{x} + S_{y}) & S_{v} - S_{x} & \dots & 0 \\ 0 & -(S_{x} + S_{v}) & 1 + 2(S_{x} + S_{y}) & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 + 2(S_{x} + S_{y}) \end{bmatrix},$$
$$P_{2} = \begin{bmatrix} 1 - 2(S_{x} + S_{y}) & S_{x} - S_{v} & 0 & \dots & 0 \\ S_{x} + S_{v} & 1 - 2(S_{x} + S_{y}) & S_{x} - S_{v} & \dots & 0 \\ 0 & S_{x} + S_{v} & 1 - 2(S_{x} + S_{y}) & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 1 - 2(S_{x} + S_{y}) & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & -S_{y} \end{bmatrix} \text{ and } Q_{2} = \begin{bmatrix} S_{y} & 0 & 0 & \dots & 0 \\ 0 & S_{y} & 0 & \dots & 0 \\ 0 & 0 & S_{y} & \dots & 0 \\ 0 & 0 & S_{y} & \dots & 0 \\ 0 & 0 & S_{y} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & -S_{y} \end{bmatrix}.$$

From Eq. (3), we obtain Eq. (4) as follow :

$$c^{n+1} = \mathbf{A}^{-1}\mathbf{B}c^n + \mathbf{A}^{-1}c^*$$

(4)

Generally, the mathematic model in discrete time in Eq. (4) can be written as the discrete state space system of groundwater pollution modelling as follow :

$$c_{k+1} = Ac_k + Bu_k$$
with $A = \mathbf{A}^{-1}\mathbf{B}$ and $Bu_k = \mathbf{A}^{-1}c^*$. (5)

Furthermore, we construct the measurement equation at time k as follow:

 $y_k = Cc_k + Du_k$ (6) where *C* is a 5 × 16 matrix with elements C(1,2) = 1, C(2,5) = 1, C(3,7) = 1, C(4,11) = 1, C(5,15) = 1, and C(i, j) = 1 for other *i*, *j*. *D* is a 5 × 1 zero matrix.

So from Eq.(5) and Eq. (6), we have a discrete linear time invariant (LTI) system as follow $c_{k+1} = A c_k + B u_k$

$$y_k = C c_k + D u_k$$

with $c_k \in \mathbb{R}^{16}$ is called the state vector at time $k, u_k \in \mathbb{R}^{16}$ is called the input vector, $y_k \in \mathbb{R}^5$ is called the output vector, and A, B, C, D are each real constant matrices of corresponding size. Furthermore, the discrete LTI system is called the original discrete system (A, B, C, D).

RESULTS AND DISCUSSION

Actually, it is difficult to get real data, the concentration of groundwater pollution, because the measurement tools are limited, therefore, we concern on the algorithm Kalman Filter, and the Modified Kalman Filter method. So that the measurement data is generated from MATLAB program that represent Eq. (6). The simulation begins by reducing the system using the Linear Matrix Inequality (LMI) method to obtain the reduced system. Then implement the Kalman filter algorithm on the original discrete system and the reduced system.

Model reduction in the groundwater pollution model using Linear Matrix Inequality (LMI) method

The parameter values used in the simulation are assumed to be constant with M = 20; $D_x = 0.1$; $D_y = 0.1$; v = 10; $L_x = 20$; $L_y = 20$; T = 10; and N = 100. From the

simulation results, it is found that the original discrete system (A, B, C, D) is is an asymptotically stable system because all the eigenvalues of matrix A are less than 1.

From the original discrete system (A, B, C, D) we can obtain the controllability matrix **W** and the observability matrix **W** to obtain the Hankel singular values of the system the original discrete system (A, B, C, D) as follow:

 $\mathbf{W} \coloneqq \sum_{k=0}^{\infty} A^k B B^T (A^T)^k. \quad k = 0, 1, 2, 3, ...$ and $\mathbf{M} \coloneqq \sum_{k=0}^{\infty} (A^T)^k C^T C A^k. \quad k = 0, 1, 2, 3, ...$ It is obtained that all Hankel singular values of original discrete system (A, B, C, D), namely

 $\sigma_i = \sqrt{\lambda_i(\mathbf{WM})}, i = 1, \dots, 16$, where λ is the eigenvalue of matrix **WM**, are positive, i.e.:

6.9577 > 6.6006 > 5.6617 > 5.3606 > 0.3184 > 0.2880 > 0.2620 > 0.2208 > 0.0198 > 0.0166 > 0.0158 > 0.0141 > 0.0018 > 0.0015 > 0.0012 > 0.0011.

This means that the equilibrium gramian $\Sigma = diag(\sigma_1, \sigma_2, \dots, \sigma_n)$ is positive definite. Since the equilibrium gramian Σ is positive definite, it is guaranteed that the original discrete system (*A*, *B*, *C*, *D*) is a controllable and observable system.

Next, the original discrete system (A, B, C, D) is reduced using the Linear Matrix Inequality (LMI) method to obtain the reduced system (A_r, B_r, C_r, D_r) . It is found that the reduced system (A_r, B_r, C_r, D_r) is is an asymptotically stable system because all the eigenvalues of matrix A_r are less than 1. It is obtained that all Hankel singular values of reduced system (A_r, B_r, C_r, D_r) are positive. This means that the equilibrium gramian $\Sigma = diag(\sigma_1, \sigma_2, \dots, \sigma_r)$ is positive definite. Since the equilibrium gramian Σ is positive definite, it is guaranteed that the reduced system (A_r, B_r, C_r, D_r) is a controllable and observable system.

Furthermore, using the LMI method, we can find the supremum of the error $||G(z) - G_r(z)||_{\infty}$ denoted by a non-negative scalar γ that satisfies $\sigma_n \leq ||G(z) - G_r(z)||_{\infty} < \gamma \leq 2(\sigma_{r+1} + \cdots + \sigma_n)$, where G(z) and $G_r(z)$ are the transfer function of the original discrete system (A, B, C, D) and the reduced system (A_r, B_r, C_r, D_r) . The value of γ can be found to be the minimum possible as in **Table 1**.

R	Lower error limit reduction	error reduction using the LMI method	Upper error limit reduction	
	σ_{r+1}	γ	$2(\sigma_{r+1} + \cdots + \sigma_n)$	
3	5.3606	5.6	13.0434	
4	0.3184	0.45	2.3222	
5	0.288	0.4	1.6854	
6	0.262	0.35	1.1094	
7	0.2208	0.23	0.5854	
8	0.0198	0.025	0.1438	
9	0.0166	0.019	0.1042	
10	0.0158	0.018	0.071	
11	0.0141	0.0145	0.0394	
12	0.0018	0.0021	0.0112	
13	0.0015	0.0018	0.0076	
14	0.0012	0.0013	0.0046	
15	0.0011	0.00125	0.0022	

Table 1. Error $||G(z) - G_r(z)||_{\infty}$ obtained by the LMI method in groundwater pollution problems

Next, the estimation process is carried out using the Kalman filter algorithm on the LTI discrete system, either on the original discrete system or on the reduced system.

Construction of the Kalman Filter Algorithm in Reduced Systems

By using the transformation $z_k = P_{22} x_{r_k}$ on the reduced system (A_r, B_r, C_r, D_r) where

$$P_{22} = \text{diag}\left(\left(\sigma_{1} - \frac{\sigma_{m}^{2}}{\sigma_{1}}\right)^{-1} I_{k_{1}}, \dots, \left(\sigma_{m-1} - \frac{\sigma_{m}^{2}}{\sigma_{m-1}}\right)^{-1} I_{k_{m-1}}\right)_{n-k_{m} \times n-k_{m}}.$$

we obtain the reduced system $(P_{22}A_rP_{22}^{-1}, P_{22}B_r, C_rP_{22}^{-1}, D_r)$ which is similar to the reduced system (A_r, B_r, C_r, D_r) .

The representation of the state space for the reduced system $(P_{22}A_rP_{22}^{-1}, P_{22}B_r, C_rP_{22}^{-1}, D_r)$ of order r (r < n) is expressed as follows:

$$x_{r_{k+1}} = P_{22}A_r P_{22}^{-1} x_{r_k} + P_{22}B_r u_k, \tag{7}$$

$$z_{r_k} = C_r P_{22}^{-1} x_{r_k} + D_r u_k.$$
(8)

The reduced system $(P_{22}A_rP_{22}^{-1}, P_{22}B_r, C_rP_{22}^{-1}, D_r)$ in Eq. (7) and Eq. (8) does not contain any noise. Meanwhile, in real problems, a system is influenced by noise, namely noise in the system and noise in measurements. If the noise is taken into account in the system, then the reduced system $(P_{22}A_rP_{22}^{-1}, P_{22}B_r, C_rP_{22}^{-1}, D_r)$ becomes a stochastic reduced system as follows:

$$x_{r_{k+1}} = P_{22}A_r P_{22}^{-1} x_{r_k} + P_{22}B_r u_k + G_r w_{r_k},$$
(9)

$$z_{r_k} = C_r P_{22}^{-1} x_{r_k} + D_r u_k + v_{r_k}$$
(10)

with w_{r_k} and v_{r_k} being the system noise and measurement noise in the reduced system, respectively. The noise in the system w_{r_k} and the noise in the measurement v_{r_k} are assumed:

$$x_{r_0} \sim N\left(\bar{x}_{r_0}, P_{x_{r_0}}\right), w_{r_k} \sim N(0, Q_r) \text{ dan } v_{r_k} \sim N(0, R_r),$$

with Q_r being the system noise covariance w_{r_k} and R_r being the measurement noise covariance v_{r_k} , the Q_r matrix is assumed to be positive semi-definite, and the R_r matrix is assumed to be positive definite. Based on the initial conditions, it will apply

$$E[w_{r_k}] = 0, E[w_{r_k}^{T}] = 0, \text{ dan } E[w_{r_k}w_{r_k}^{T}] = Q_r$$
$$E[v_{r_k}] = 0, E[v_{r_k}^{T}] = 0, \text{ dan } E[v_{r_k}v_{r_k}^{T}] = R_r$$

Next, the construction of the Kalman filter algorithm on the stochastic reduced system $(P_{22}A_rP_{22}^{-1}, P_{22}B_r, C_rP_{22}^{-1}, D_r)$ is completely presented in **Figure 1**.

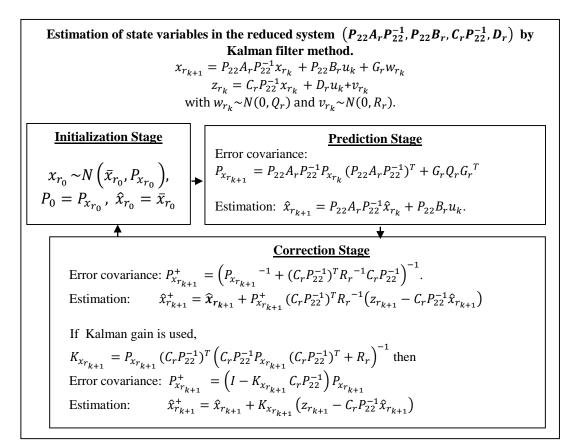


Figure 1. Schematic of Kalman filter algorithm on reduced system using Linear Matrix Inequality (LMI) method.

Since the system $(P_{22}A_rP_{22}^{-1}, P_{22}B_r, C_rP_{22}^{-1}, D_r)$ is similar to the reduced system (A_r, B_r, C_r, D_r) , then the system $(P_{22}A_rP_{22}^{-1}, P_{22}B_r, C_rP_{22}^{-1}, D_r)$ is also an asymptotically stable, controllable, observable reduced system. Furthermore, it is obtained that the estimation of the original discrete system (A, B, C, D) with the Kalman filter algorithm produces a very good estimation because the plot of the estimated variables is very close to the real state variables, as in **Figure 2**.

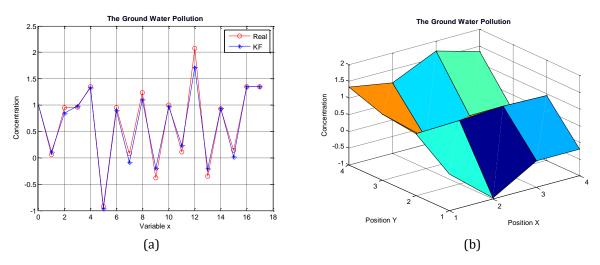


Figure 2. Original discrete system (*A*, *B*, *C*, *D*) estimation using Kalman filter algorithm on 2-D images (a) and 3-D images (b)

The same thing is also obtained from the estimation results of the reduced system with r = 9, which produces a very good estimate because it produces a very small error and is close to the real state variable, as in Figure 3.

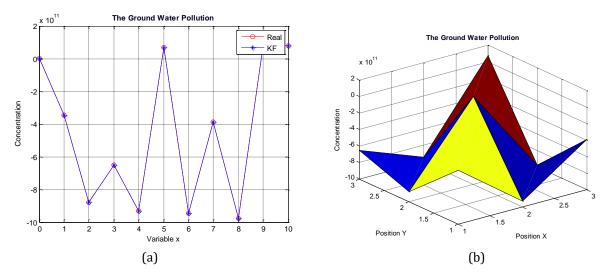


Figure 3. Estimation of reduced system with order r = 9 using Kalman filter algorithm in 2-D images (a) and 3-D images (b)

It is found that the estimation results on the reduced system are generally also very good, which is indicated by the very small error value as shown in **Table 2**.

System	Order	Average error	Average reduction	Average estimation
	System	estimation	time	time
Original	16	0.127958145772399		0.0277933
System				
	7	0.140664482209831	6.3500972	0.0202604
	8	0.278699717521668	6.9469524	0.0220778
	9	0.267349685322155	7.7447647	0.0232865
Reduced	10	0.190697644154231	9.7998875	0.0254702
System	11	0.248623319772574	13.6056212	0.0259470
	12	1.880960855844340	10.6206437	0.0255010
	13	0.888957187285023	15.0763490	0.0272671
	14	1.099929654411970	20.2884836	0.0265640
	15	1.771813543403840	21.5354403	0.0272022

From **Table 2**, the results show that the smallest estimation error is the original system estimation error. The estimation error in the reduced system increases as the reduction order increases. The longest estimation time is the estimation time for the original system. The larger the order of the reduced system, the longer the estimation time. Likewise for the reduction time, the larger the order of the reduced system, the longer the reduction time. The above results were obtained using the measurement matrix *C* with randomly generated measurement data.

CONCLUSIONS

Based on the analysis and discussion that has been done then can be drawn conclusion as follows, the Modified Kalman Filter Method can be applied in the estimation of state variables on the model of groundwater pollution process. The estimation results using the Kalman filter algorithm on the original system and the system that has been reduced by the LMI method, excellent estimation results are obtained, because it produces a very small error and is close to the real state variable.

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