# Identification of Dynamics of a Distillation Column

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# IDENTIFICATION OF DYNAMICS OF A DISTILLATION COLUMN †

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ABSTRACT

Linear models of distillation column dynamics have been computed from plant data by the maximum likelihood method. The models are compared with results obtained by other identification techniques, the least squares method, the generalised least squares method and cross correlation analysis. The different methods give comparable results for these data depending on a low noise level.

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## 1. INTRODUCTION

This work is a part of a systematic investigation of various identification methods with respect to practical applications to industrial processes. The purpose of this paper is to show how the maximum likelihood method for parameter estimation can be used for plant modelling. The process studied is a binary distillation column. The maximum likelihood (M.L.) estimates are also compared with cross correlation analysis and with estimates obtained by the generalized least squares (G.L.S.) method and by the least squares (L.S.) method.

The data, for which the identification is performed, have been received from National Physical Laboratory in London, where the practical experiments have been carried out. Cross correlation and G.L.S. models have also been computed at the National Physical Laboratory. Those models have been referred to in this report.

The purpose of the experiments was to apply recent ideas of control theory to a practical situation. Both modelling and control calculations were therefore entirely performed in the time domain. The received discrete time models are well suited for on-line control applications.

The experiments were performed with a six-plate pilot-scale binary distillation column. Perturbations were introduced either to the reflux ratio or to the boiler heat supply. The perturbations were PRBS-sequences. The output signals were the temperatures T1-T6 from the lowest plate (1) to the top plate (6) and also a composition measurement at the output stream. In this work four experiments are investigated and some of the typical results are shown. In all the four experiments the input signal is the reflux ratio and the output is either the temperature T6 or the top-product composition. The M.L. identification gives models, which do not differ much from experiment to experiment. It turns out that a second order model is sufficient to define the plant behaviour from the reflux ratio to the temperature T6, but that a second or a third order model is appropriate to describe the relation between the reflux ratio and the top-product composition. Furthermore the last model has a non-minimum phase character.

It also turns out that for this case cross correlation analysis gives results comparable with the results obtained from M.L. or G.L.S. methods. The parametric methods are perhaps preferable because they can be used direct for the control computations. However, cross correlation analysis is a good method to obtain a fast, rough estimate of the process. On the other hand the M.L. method seems to give better models when the noise-signal ratio is high. Notice also that even if the G.L.S. method worked very well for these experiments, no theoretical proof is available of the statistical goodness of the results. The M.L. estimates, on the other hand, are unbiassed, consistent and efficient. The L.S. method often gives a high order model when the noise is correlated.

## 2. THE DISTILLATION COLUMN AND THE MEASUREMENTS

A laboratory distillation process separating a mixture of ethanol and water is investigated. A simplified flow diagram of the distillation column is shown in Fig. 1. Furthermore a digital computer is coupled to the distillation column, ref {6}. The distillation column is described in ref {2}. The column has six plates, numbered 1 to 6 from below. As input signals the power supply to the reboiler, the feed composition and the reflux ratio can be chosen. The output signals from the column are the plate temperatures T1-T6, the mass flow of the top product and the composition of the top product. The reboiler liquid level is under local closed loop control.

During these identification experiments perturbations were introduced either to the heat supply to the reboiler or to the reflux ratio. The temperatures of the plates and the top product composition were recorded. The input signals are PRBS-signals of 2- or 3-level type, ref {1}. In this work four experiments have been investigated. The experimental conditions are given in Table 1. In these four experiments the only interesting relations were the relation between the reflux ratio and the temperature T6 (A) and the relation between the reflux ratio and the top product composition (B). The other input signals were constant during the experiment. By 1A we mean the input-output samples obtained from experiment 1, and where the input is the reflux ratio and the output the temperature T6. Other notations follow straight forward.

| Experiment | Input | Number of periods of the input | Heat in kW | Reflux perturbed between | Sampling interval in seconds | Feed |
|---|---|---|---|---|---|---|
| 1 | 63 bits prbs | 5 | 1.73 | 2.95:1 & 5:1 | 96 | 90cc/min 4%BM |
| 2 | 127 bits prbs | 2 | 1.7 | 2.95:1 & 5:1 | 64 | 95cc/min 4%BM |
| 3 | 127 bits prbs | 2 | 1.56 | 5:1 & 10:1 | 96 | 46.5cc/min 5.75%BM |
| 4 | 80 bits 3-level m-sequence | 3 | 1.56 | 5: 1&7:1&10:1 | 96 | 46.5cc/min 5.75%BM |



Table 1 - Experimental conditions

## 3. OUTLINE OF THE MAXIMUM LIKELIHOOD ESTIMATION METHOD

The problem is to determine an appropriate model of a process from which we have input-output samples. Assuming the process to be linear of n-th order and to be subject to disturbances that are stationary random processes with rational power spectra, we choose the model

$$A(z^{-1})\ y(t) = B(z^{-1})\ u(t) + \lambda\ C(z^{-1})\ e(t) \qquad (1)$$

where $\{u(t), y(t), t = 1,2,\ldots,N\}$ is the input-output sequence and where $\{e(t), t = 1,2,..,,N\}$ is a sequence of independent normal (0,1) random variables. z denotes the shift operator

$$z\ x(t) = x(t+1) \qquad (2)$$

and A(z), B(z) and C(z) are polynomials

$$A(z) = 1 + a_1 z + \ldots + a_n z^n$$

$$B(z) = b_1 z + \ldots + b_n z^n$$

$$C(z) = 1 + c_1 z + \ldots + c_n z^n \qquad (3)$$

Since the identification is described elsewhere {4}, {9} the details are not given here. However, a short summary is presented.

The problem is solved by determining the maximum likelihood estimate of the parameters $\theta = (a_1,\ldots,a_n,b_1,\ldots,b_n,c_1,\ldots,c_n)$. The maximum likelihood estimate is consistent, asymptotically normal and efficient under mild conditions given in {10}. Maximizing the likelihood function is equivalent to minimizing the loss function

$$V(\theta) = \frac{1}{2} \sum_{t=1}^{N} \varepsilon^2(t) \qquad (4)$$

where the residuals $\varepsilon(t)$ are obtained from

$$C(z^{-1})\ \varepsilon(t) = A(z^{-1})\ y(t) - B(z^{-1})\ u(t) \qquad (5)$$

The identification problem is then reduced on a problem of minimizing a function of several variables.

We solve this problem by a recursive technique, which uses both the gradient with respect to the parameters, $V_\theta$, and the matrix of the second partial derivatives, $V_{\theta\theta}$. Other minimization methods do not use the second derivatives but the work to compute these is not of essential importance because the computations of $V_{\theta\theta}$ are done very economically and increase only linearly with the order of the model for large N. Furthermore this method directly gives the accuracy of the parameters, because an estimate of the inverse of the information matrix is available ($\lambda^2\{V_{\theta\theta}\}^{-1}$). The parameter $\lambda$ is determined from

$$\hat{\lambda} = \frac{2}{N} V(\hat{\theta}) \qquad (6)$$

where $\hat{\theta}$ is such that $V(\hat{\theta})$ is minimal.

To obtain a starting value for the minimizing algorithm we put $c_i = 0$, $i = 1,\ldots,n$. The loss function $V(\theta)$ is quadratic in $a_i$ and $b_i$ and the algorithm converges in one step to the least squares estimate of the a- and b-parameters.This estimate is then taken as the starting point for the gradient routine. By taking different starting values of $c_i$, $i = 1,\ldots,n$ we investigate whether $V(\theta)$ has several local minima.

This method of identification also gives a possibility to test the order of the model, when it is unknown. The identification is repeated for increasing order of the model. Now let $V_n$ denote the minimal value of the loss function for the n-th order model. It follows from {9} that the parameter estimates for large N are asymptotically normal $(\theta_o, \lambda^2 V_{\theta\theta}^{-1})$, where $\theta_o$ stands for the correct value of $\theta$. Assuming that asymptotic theory may be applied we test the hypothesis that the system is of order n, that is the null hypothesis is

$$H_o: a_{n+1}^o = \ldots = a_{n+k}^o = b_{n+1}^o = \ldots = b_{n+k}^o = c_{n+1}^o = \ldots = c_{n+k}^o = 0$$

($\theta_i^o$ stands for the correct value of $\theta_i$).

Then

$$F_{n+k,n} = \frac{V_n - V_{n+k}}{V_{n+k}} \cdot \frac{N - 3(n+k)}{3 \cdot k} \qquad (7)$$

has an F(3k, N - 3(n+k)) distribution under null hypothesis. When N is large $3k \cdot F_{n+k,n}$ tends to a $\chi^2$-distribution with 3k degrees of freedom. Most often the test is used with k = 1, that is we test the model of order (n+1) against the model of order n. It is used at a risk level of 5%, that is if the test quantity is greater than 2.6 (N is supposed to be larger than 100), the loss function has been reduced significantly and the order of the model is at least (n+1). However, this statistical test often seems to give a too high order model when identifying industrial processes, ref {5}. For simulated data, on the other hand, the test works very well.

FORTRAN programs for the identification procedure are available. The programs are described in {4}. They can handle the multiple-input, single output case and are in this sense a bit more general than what has been described in this section. But principally there is no difference. There is no loss in generality for the identification procedure by assuming the constant term of the B-polynomial, $b_o$, to be zero or by assuming the time delay k in the model

$$A(z^{-1})\, y(t) = B(z^{-1})\, u(t-k) + \lambda\, C(z^{-1})\, e(t) \qquad (8)$$

to be zero. These cases can be handled with by shifting input/output signals appropriately.

## 4. RESULTS OF THE MAXIMUM LIKELIHOOD IDENTIFICATION AND COMPARISON WITH OTHER IDENTIFICATION TECHNIQUES

In this section typical results from the identification of the four experiments are presented. First we give an example showing the results of the maximum likelihood identification of experiment 1B for increasing order of the system (Table 2).

| n | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| $a_1$ | -0.808±0.032 | -1.208±0.015 | -1.461±0.239 | -0.568±0.218 |
| $a_2$ | | 0.234±0.015 | 0.497±0.292 | -0.909±0.066 |
| $a_3$ | | | 0.015±0.061 | 0.556±0.204 |
| $a_4$ | | | | -0.042±0.057 |
| $b_1$ | 0.499±0.046 | 0.104±0.013 | 0.106±0.013 | 0.109±0.013 |
| $b_2$ | | -0.806±0.015 | -0.842±0.030 | -0.749±0.026 |
| $b_3$ | | | 0.233±0.191 | -0.527±0.154 |
| $b_4$ | | | | 0.286±0.165 |
| $c_1$ | 0.553±0.055 | -0.624±0.061 | -0.891±0.244 | 0.027±0.224 |
| $c_2$ | | 0.111±0.057 | 0.238±0.172 | -0.677±0.022 |
| $c_3$ | | | -0.004±0.063 | 0.258±0.126 |
| $c_4$ | | | | 0.015±0.064 |
| $\lambda$ | 42.39 | 12.49 | 12.26 | 12.11 |
| V | 283079 | 24569 | 23668 | 23092 |

Table 2 - Results of M.L. identification of experiment 1B for increasing order of the model. In the table the estimated values of the parameters are given together with the estimated standard deviations of parameter estimates. Furthermore the estimated values of $\lambda$ and V for each model are given.

If we try to test the order with a statistical F-test we get the following test quantities

$F_{2,1} = 1083$
$F_{3,2} = 3.9$
$F_{4,3} = 2.5$

If the test is performed at a risk level of 5%, we conclude that the system is of third order. However, there are other facts that lead to the conclusion that perhaps a second order model is sufficient to describe the process. There is a large increase of the uncertainty of the parameters when going from n = 2 to n = 3, and this indicates the presence of redundant parameters in the third order model. But the parameters $a_3$ and $c_3$ do not differ significantly from zero. Therefore putting these parameters zero we identify the other parameters by the ML-method. We get results according to Table 3.

| | |
|---|---|
| $a_1$ | -1.403 ± 0.052 |
| $a_2$ | 0.426 ± 0.051 |
| $b_1$ | 0.106 ± 0.013 |
| $b_2$ | -0.836 ± 0.018 |
| $b_3$ | 0.187 ± 0.051 |
| $c_1$ | -0.834 ± 0.078 |
| $c_2$ | 0.201 ± 0.060 |
| $\lambda$ | 12.26 |
| V | 23672 |

Table 3 - Results of M.L. identification of experiment 1B; $n = 3^{*}$ ($a_3 = c_3 = 0$)

From Tables 2 and 3 it is obvious that there is only a very small increase in the lossfunction when the parameters $a_3$ and $c_3$ are omitted. The test quantity $F_{3^{*},2}$ is 11.7. The resulting model is thus

$$y(t) = \frac{0.106z^{-1}-0.836z^{-2}+0.187z^{-3}}{1-1.403z^{-1}+0.426z^{-2}}\,u(t)+12.3\frac{1-0.834z^{-1}+0.201z^{-2}}{1-1.403z^{-1}+0.426z^{-2}}\,e(t)$$

For the further comparisons we, however, use the second order model

$$y(t) = \frac{0.104z^{-1}-0.806z^{-2}}{1-1.208z^{-1}+0.234z^{-2}}\,u(t)+12.5\,\frac{1-0.624z^{-1}+0.111z^{-2}}{1-0.208z^{-1}+0.234z^{-2}}\,e(t)$$

and the third order model from Table 2. The reasons are the small difference between the dynamics of the models and the structure of the models from the other identification methods.

Furthermore the assumptions about the sequence {e(t)} to be normal and independent should also be tested. Tests of the residuals show that they are independent and normally distributed with good accuracy already for the second order model (Fig. 2 and 3).

In Fig. 4 and 5 the results of the M.L. identification of experiment 1B are shown. In these figures we show

1. The input signal
2. The output signal, y(t)
3. The residuals, $\varepsilon(t)$
4. The deterministic output, $y_d(t)$, defined by

   $$y_d(t) = \frac{B(z^{-1})}{A(z^{-1})} u(t)$$

   where $B(z^{-1})/A(z^{-1})$ is the obtained model.
5. The error of the deterministic model, $e_d(t)$, where

   $$e_d(t) = y(t) - y_d(t)$$

   This error is a sum of for instance the disturbances in the process and the measurements and the error introduced by the model approximation of the real process (unlinearities, other inputs etc).

Notice the different scales.

The error of the deterministic model is rather small. The improvement of the model when going from second order to third order seems to be negligible. Notice that the residuals also are the errors of the one-step-ahead predictor.

As a comparison the least squares (L.S.) estimates are given in Table 4.

| n | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| $a_1$ | -0.923 | -1.133 | -0.713 | -0.612 |
| $a_2$ | | 0.160 | -0.370 | -0.299 |
| $a_3$ | | | 0.124 | -0.101 |
| $a_4$ | | | | 0.061 |
| $b_1$ | 0.138 | 0.111 | 0.111 | 0.108 |
| $b_2$ | | -0.809 | -0.762 | -0.751 |
| $b_3$ | | | -0.374 | -0.435 |
| $b_4$ | | | | -0.165 |
| $\lambda$ | 45.86 | 14.40 | 12.71 | 12.41 |
| V | 331309 | 32669 | 25446 | 24263 |

Table 4 - Least squares estimates for experiment 1B

In Fig. 6 and 7 the results of the L.S. identification are shown for the second and third order model. From Fig. 4-7 it is not easy to determine if there are significant differences between the models. However, in Fig. 3 we can see that the residuals from the L.S. models are not independent to the same extent as the residuals from the M.L. models.

A G.L.S. estimation of a model for the process has been performed at the National Physical Laboratory using the same measurements. The second order pulse transfer function was

$$y(t) = \frac{0.103z^{-1} - 0.805z^{-2}}{1 - 1.204z^{-1} + 0.230z^{-2}} u(t)$$

and the parameters of this model are almost equal to the second order M.L. model. The G.L.S. method is described in ref {3}. More models obtained by the G.L.S. method can be found in ref {7}. For instance we give examples where there are larger differences between the G.L.S. and M.L. estimates, Table 5.

| Experiment | 3B | | 4B | |
|---|---|---|---|---|
| Method | G.L.S. | M.L. | G.L.S. | M.L. |
| $a_1$ | -1.552 | -1.586 | -1.531 | -1.537 |
| $a_2$ | 0.567 | 0.601 | 0.551 | 0.554 |
| $b_1$ | 0.240 | 0.220 | 0.245 | 0.225 |
| $b_2$ | -0.602 | -0.566 | -0.604 | -0.598 |
| Gain | 24.1 | 23.1 | 18.0 | 21.9 |

Table 5 - Comparison between models obtained by G.L.S. and M.L. identification of experiments 3B and 4B

Experiments 3 and 4 were carried out under the same operating conditions but with different input signals. From Table 5 we notice that the G.L.S. estimates of the plant gain, defined by

$$|H(z)| = \frac{\sum_{i=1}^{n} b_i}{1 + \sum_{i=1}^{n} a_i}$$

(the final value theorem applied to H(z), the pulse transfer function), differ much more than the M.L. estimates. However, since $\sum_{i=1}^{n} a_i$ is close to -1 any small variations in the parameters $a_i$ will result in significant changes in $|H(z)|$. Therefore no definitive conclusion can be drawn from this comparison of the two identification methods.

In Fig. 8 we show the results of cross correlation analysis compared with M.L. estimates. When the input signal is a PRBS-sequence as in this case, the cross correlation function is approximative equal to the impulse response, ref {1 } and {8}.A parameter model can be estimated using the cross correlation function. When the signal to noise ratio is high the cross correlation analysis seems to give reasonable estimates. But when this ratio is low cross correlation analysis may give bad estimates. On the other hand the M.L. method still works very well. In this case there is no large difference between the impulse response of the 2nd or 3rd order models and the cross correlation function.

In Fig. 9 the impulse response of the 3rd M.L. model is compared with those of the 2nd and 3rd order L.S. models. The impulse responses from the 3rd order M.L. model and from the M.L. model with $a_3$ and $b_3$ equal zero are practically the same.

Below some more results from the M.L. identification of the four experiments are given.In Table 6 some of the obtained models are presented.

| Experiment | 1A | | 3B | | 4A | |
|---|---|---|---|---|---|---|
| Order | 1 | 2 | 2 | 3 | 1 | 2 |
| $a_1$ | -0.974±0.005 | -1.464±0.067 | -1.586±0.039 | -1.331±0.223 | -0.978±0.007 | -1.531±0.111 |
| $a_2$ | | 0.486±0.065 | 0.601±0.038 | 0.296±0.358 | | 0.546±0.108 |
| $a_3$ | | | | 0.052±0.144 | | |
| $b_1$ | -0.032±0.001 | -0.030±0.001 | 0.220±0.033 | 0.212±0.032 | -0.031±0.001 | -0.029±0.001 |
| $b_2$ | | 0.011±0.003 | -0.566±0.034 | -0.470±0.060 | | 0.013±0.004 |
| $b_3$ | | | | -0.215±0.128 | | |
| $c_1$ | -0.471±0.060 | -1.103±0.083 | -0.597±0.069 | -0.333±0.288 | -0.398±0.068 | -1.004±0.121 |
| $c_2$ | | 0.328±0.068 | 0.111±0.064 | 0.088±0.153 | | 0.208±0.077 |
| $c_3$ | | | | -0.015±0.073 | | |
| $\lambda$ | 0.772 | 0.684 | 26.04 | 25.53 | 0.730 | 0.693 |
| V | 93.86 | 73.73 | 86120 | 82803 | 64.01 | 57.71 |

Table 6 - Results from the maximum likelihood identification of experiments 1A, 3B and 4A

In Fig. 10-17 typical results are shown. From Tables 2 and 6 we see that the models for the two different processes respectively do not differ very much from experiment to experiment. The only large difference is the b-coefficients for experiments 1B and 3B, but this is probably due to the different experiment conditions. F-test gives a third order model for experiment 3B, but the accuracies are increasing very much from the second order model. The accuracies of the parameters of the models from experiments 1A and 4A are much larger for the second order models. But in this second case the F-test significantly gives a second order model. For both processes therefore a second order model seems to be appropriate.

## 5. ACKNOWLEDGEMENT

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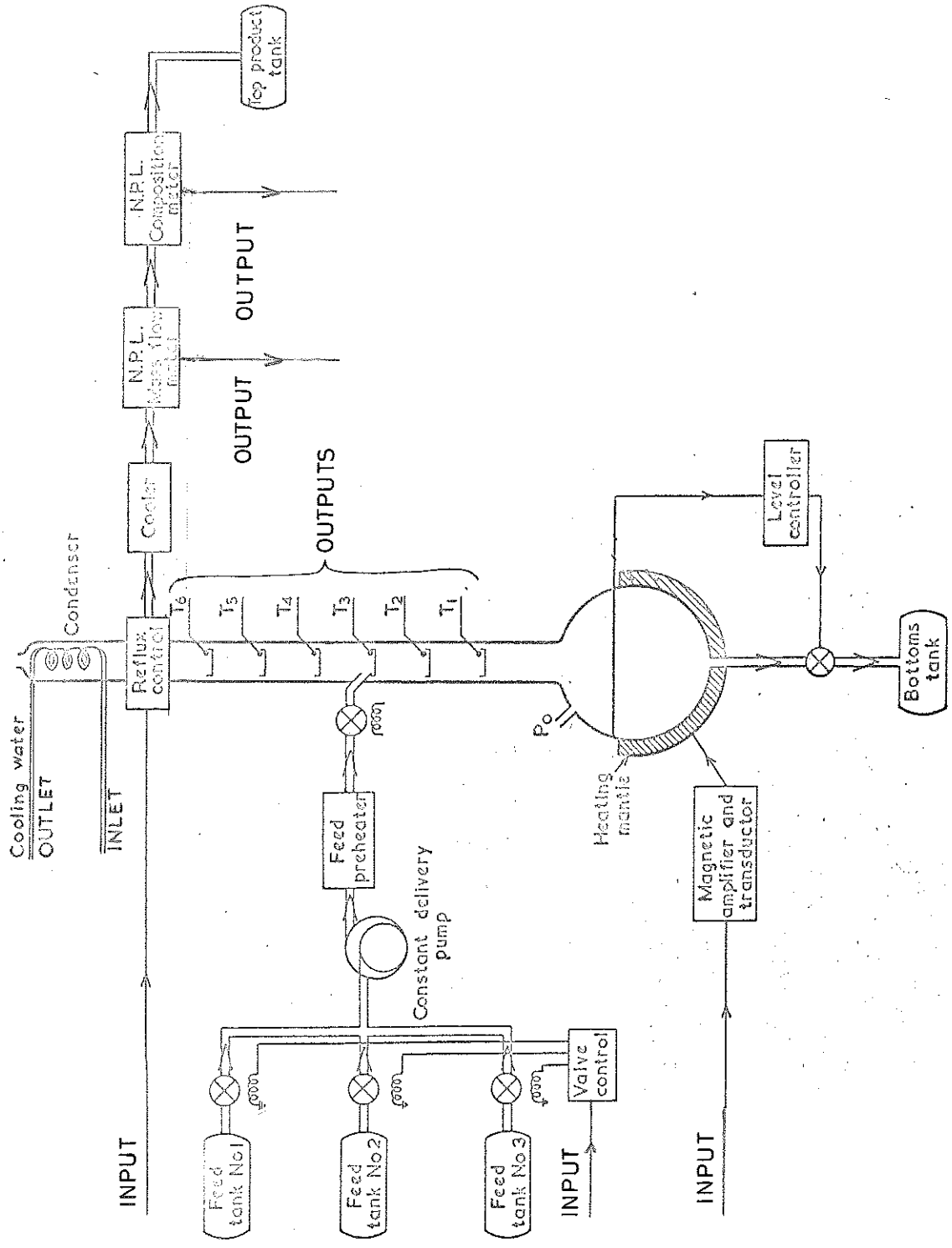


Fig. 1 - Simplified flow diagram of the distillation column

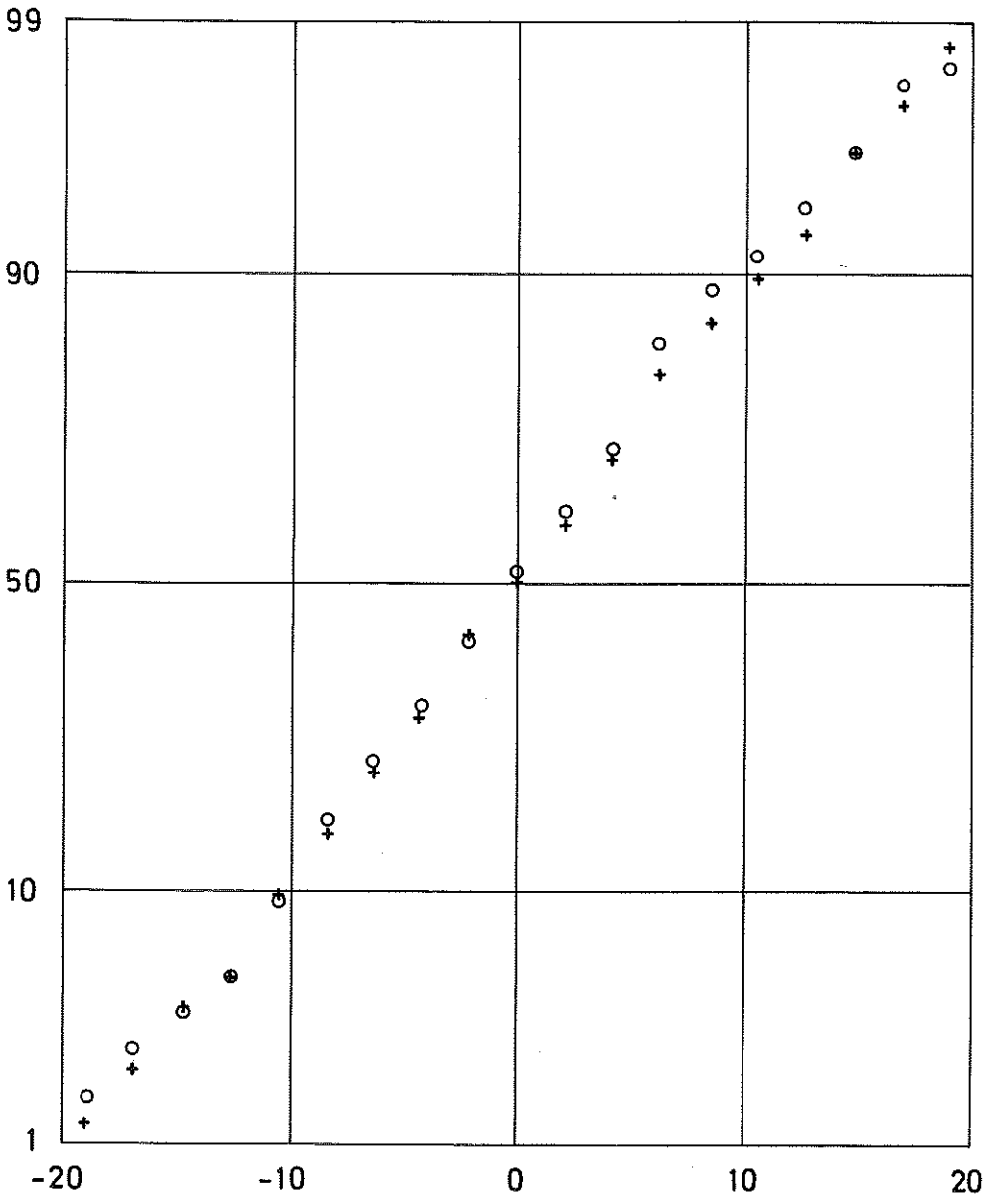


Fig. 2 - Test of normality of the residuals of the M.L. models of order 2(+) and 3(0) for experiment 1B. The residuals have been divided into class intervals and in this diagram the cumulative frequencies are plotted with a vertical scale corresponding to a normal distribution, that is a perfect normally distributed variable gives a straight line.

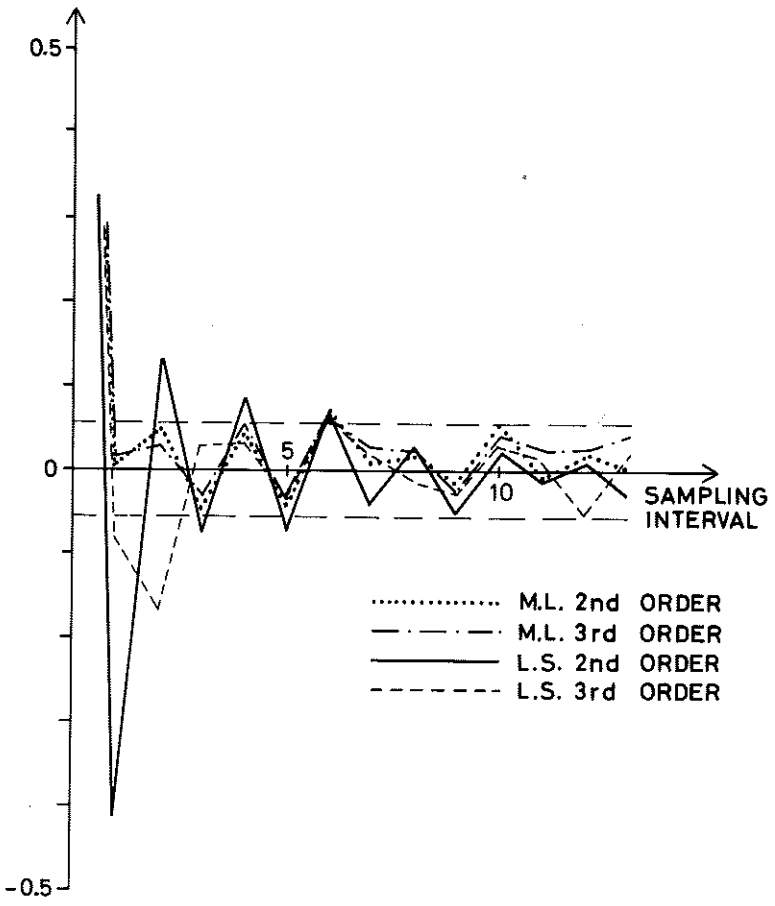


Fig. 3 - Sample covariance functions, $r(\tau)$ for the residuals for different models for experiment 1B. The dashed lines give the one sigma limit for $r(\tau)$, $\tau \neq 0$. According to the assumptions $r(\tau)$ should equal zero, $\tau \neq 0$.

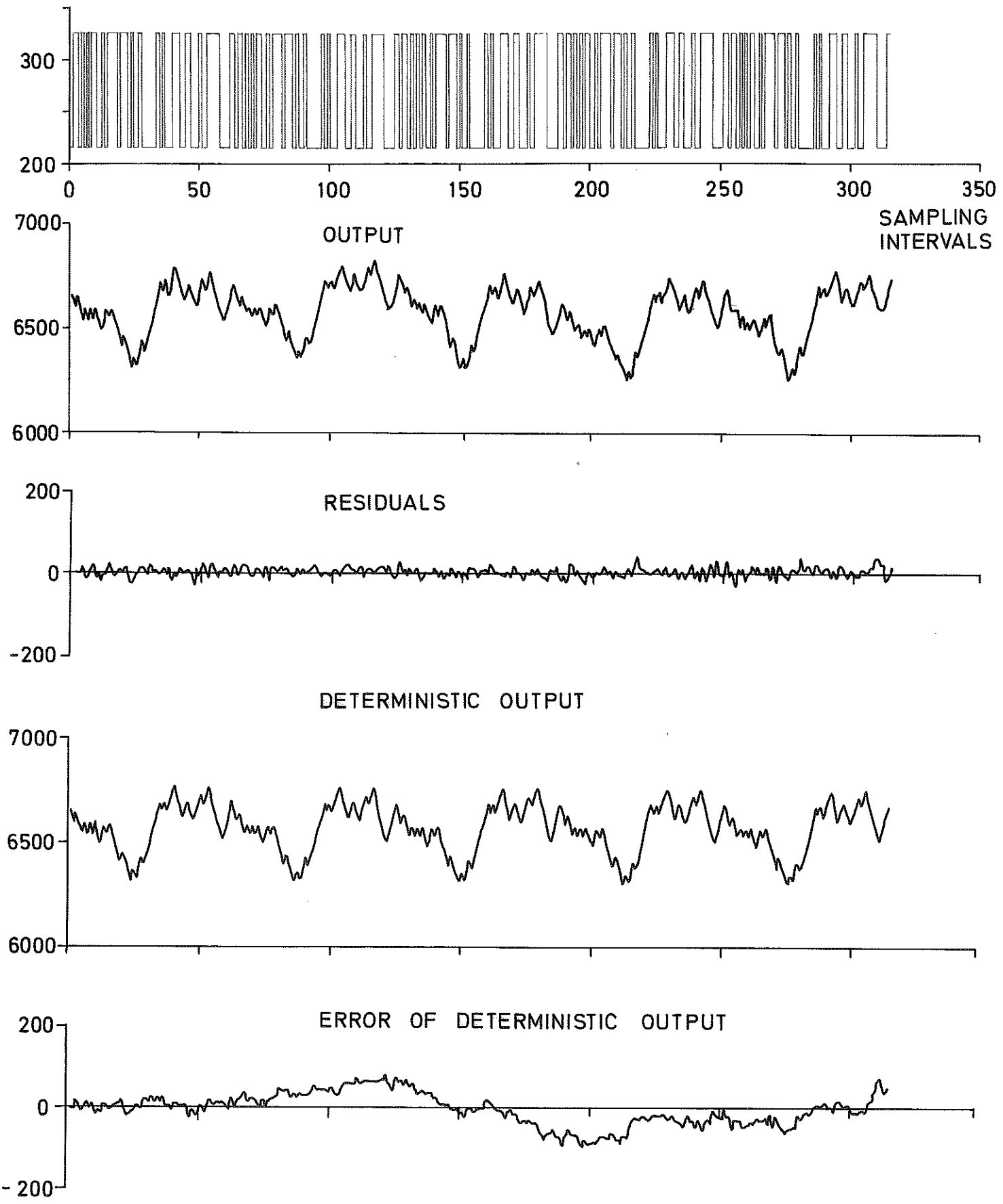


Fig. 4 - Results from identification of experiment 1B, M.L. 2nd order

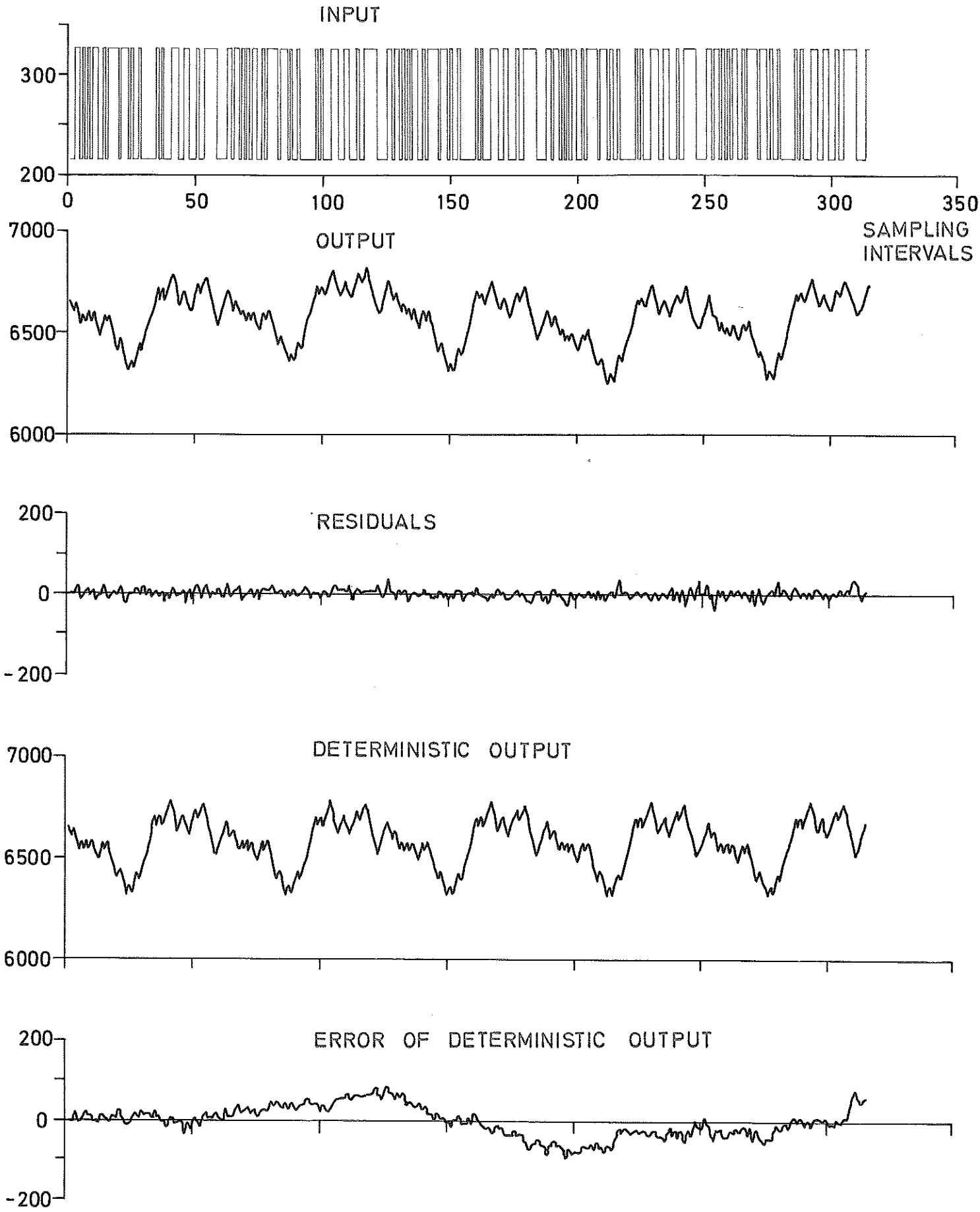


Fig. 5 - Results of identification of experiment 1B, M.L. 3rd order

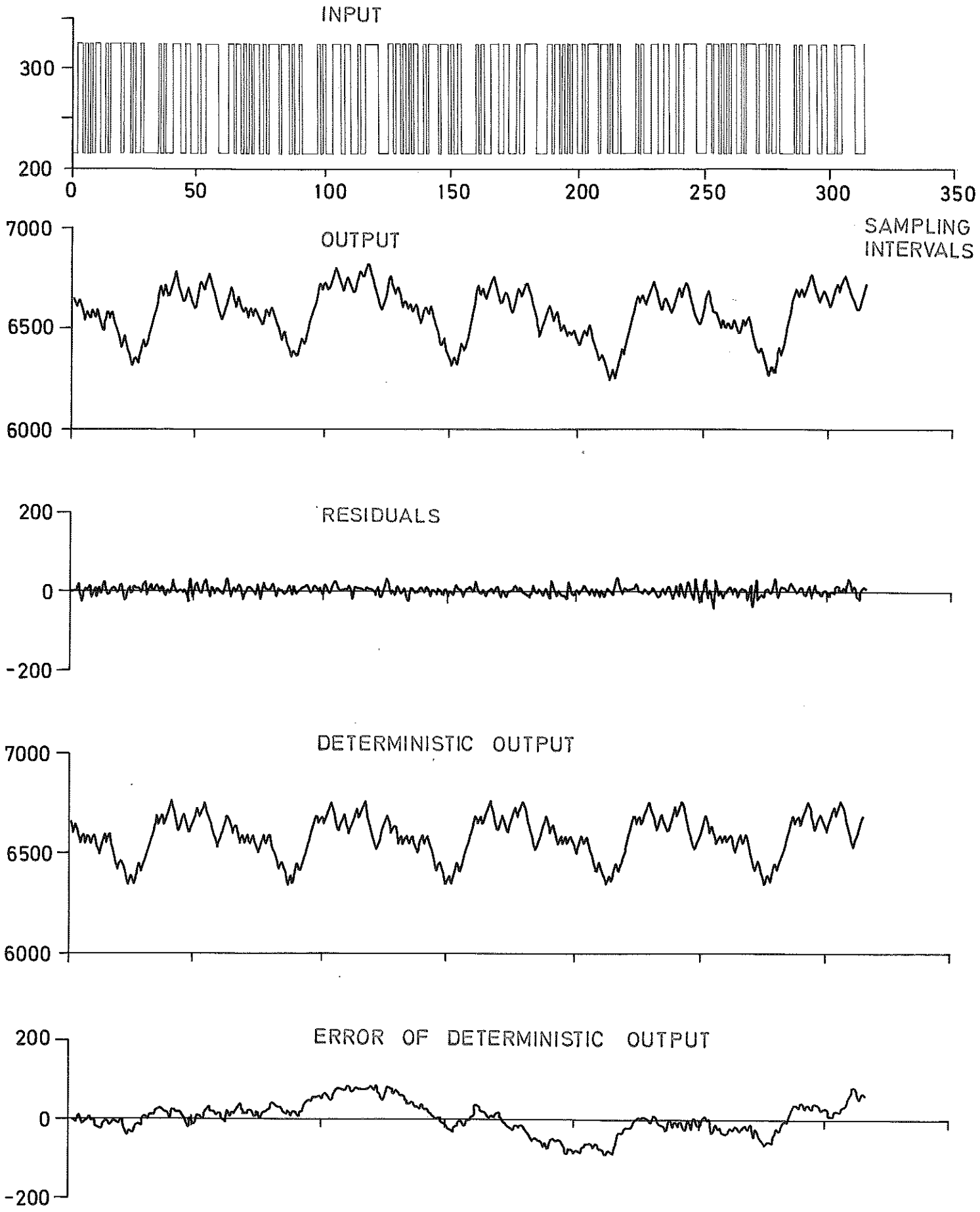


Fig. 6 - Results of identification of experiment 1B, L.S. 2nd order

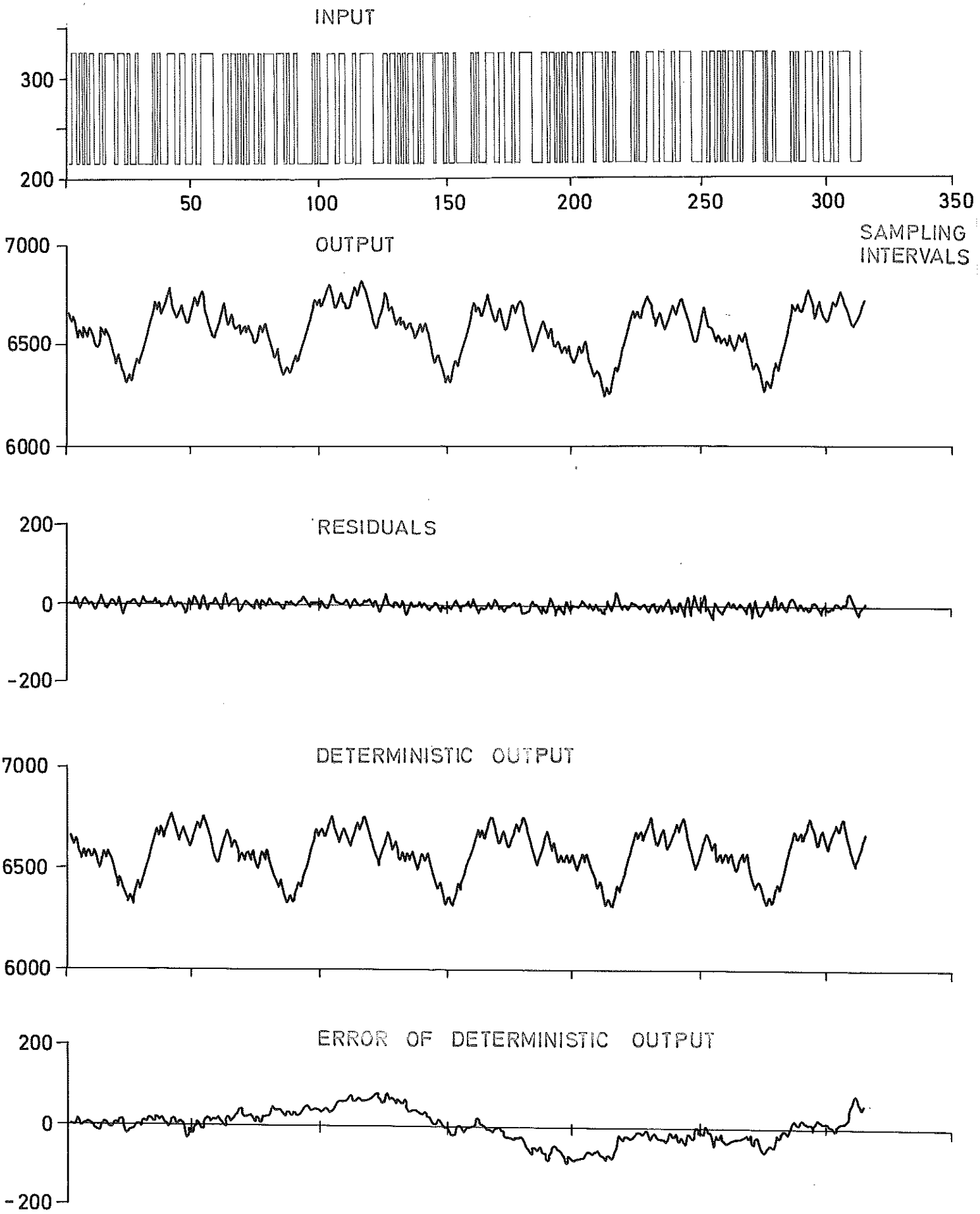


Fig. 7 - Results of identification of experiment 1B, L.S. 3rd order

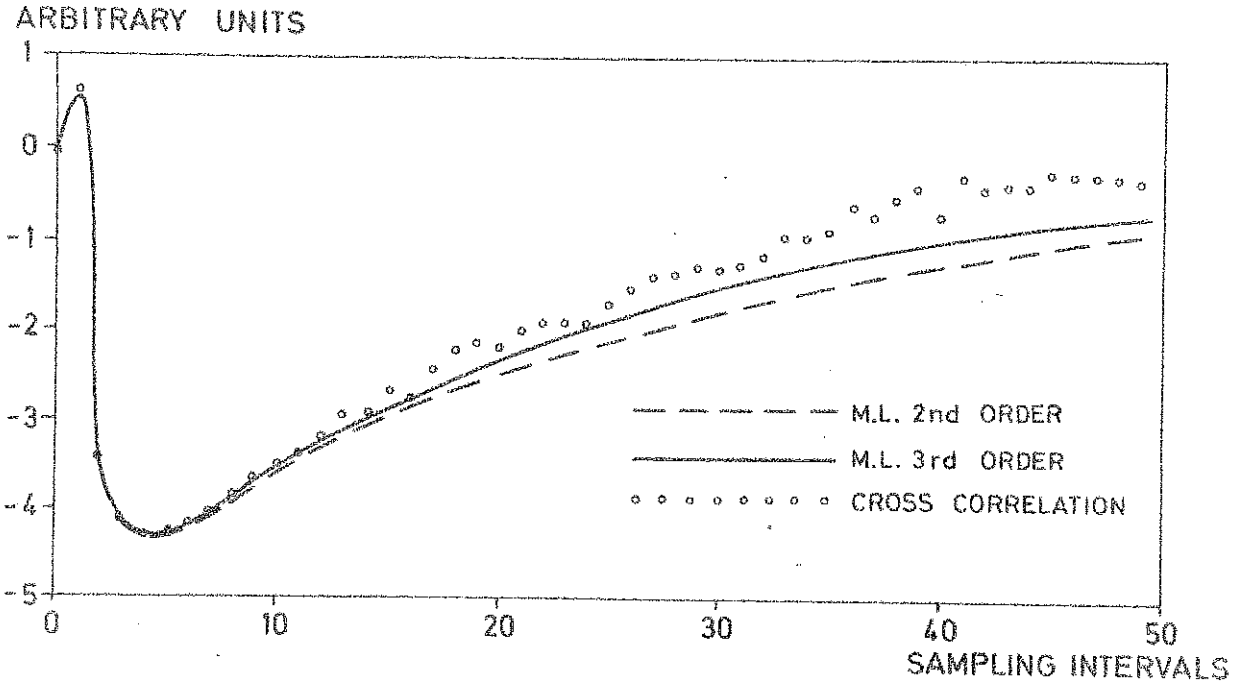


Fig. 8 - Impulse response from the 2nd and 3rd order M.L. models and the cross correlation function (experiment 1B)

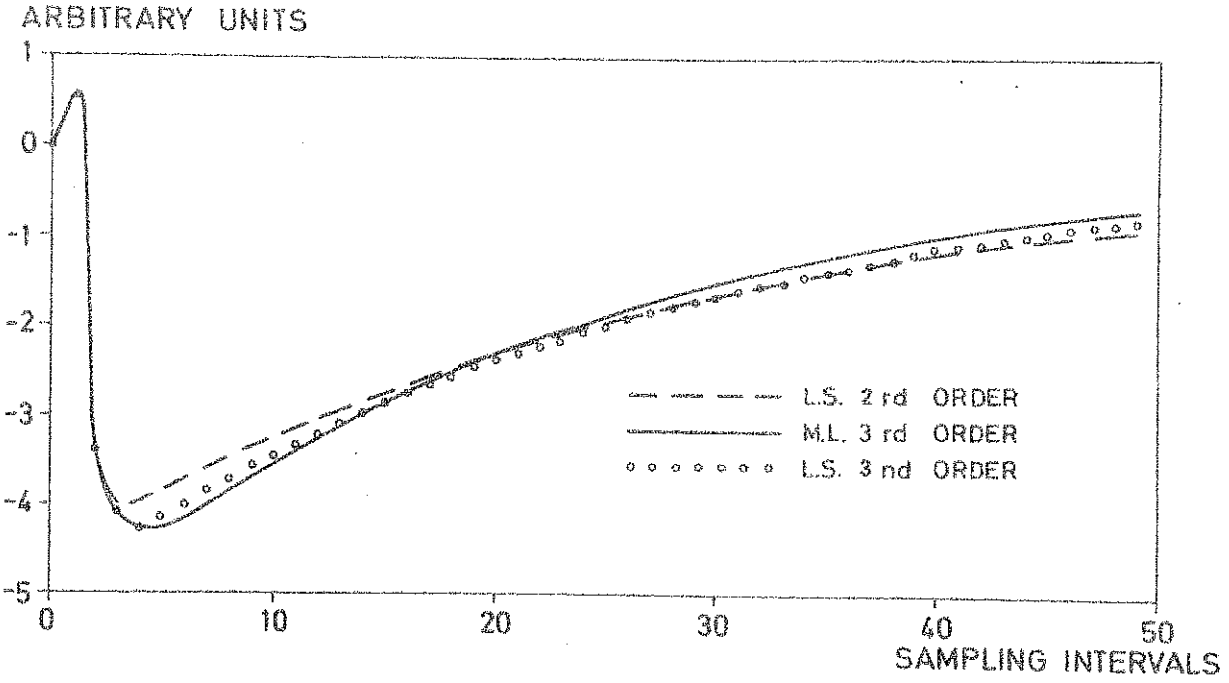


Fig. 9 - Impulse response from 2nd and 3rd order L.S. models and 3rd order M.L. model (experiment 1B)

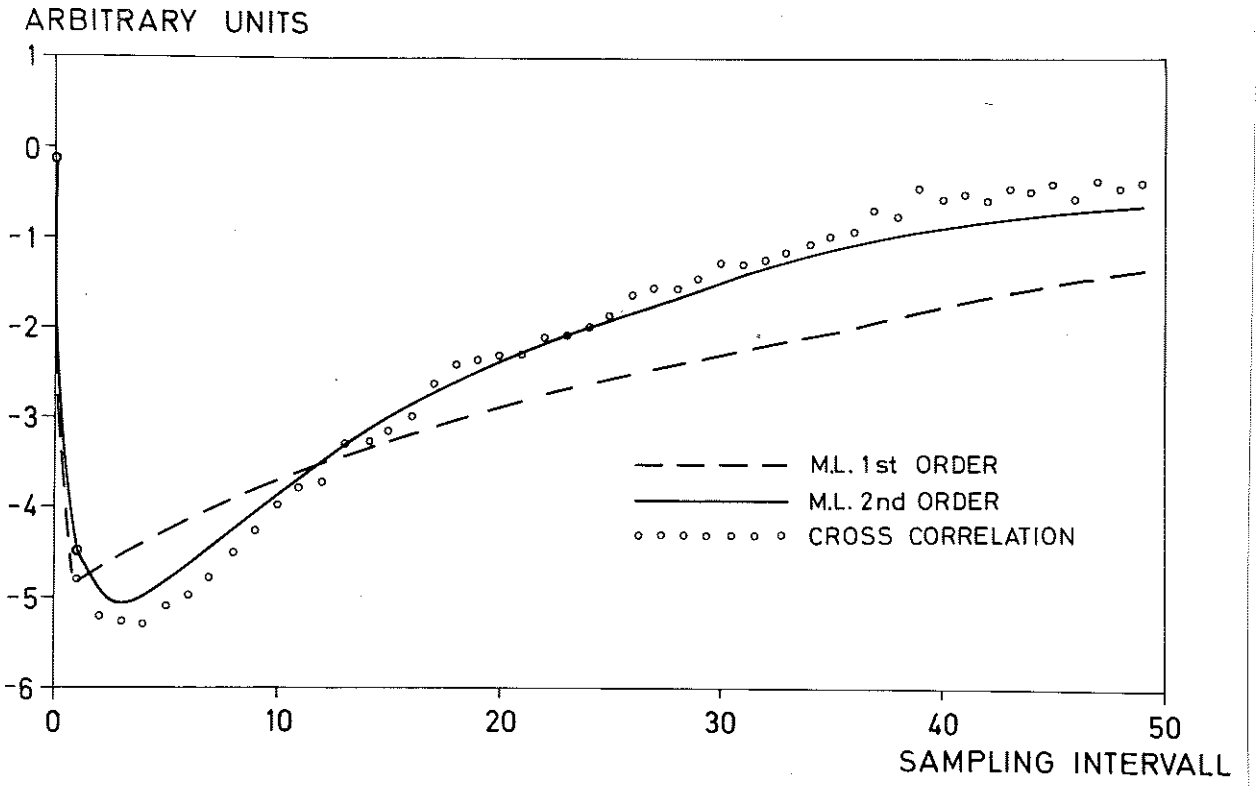


Fig. 10 - Impulse response from 1st and 2nd order M.L. models and the cross correlation function (experiment 1A)

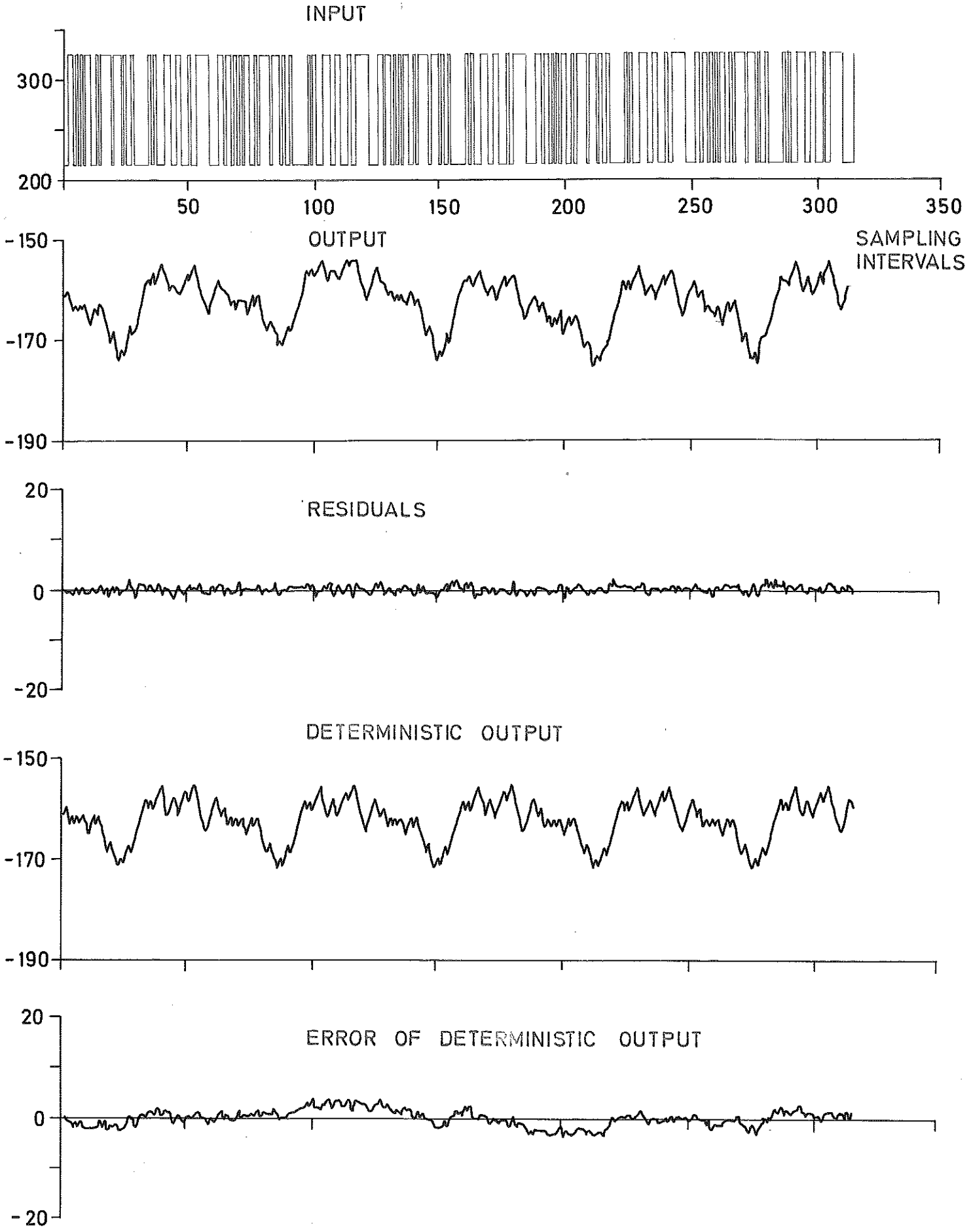


Fig. 11 - Results of identification of experiment 1A, M.L. 1st order

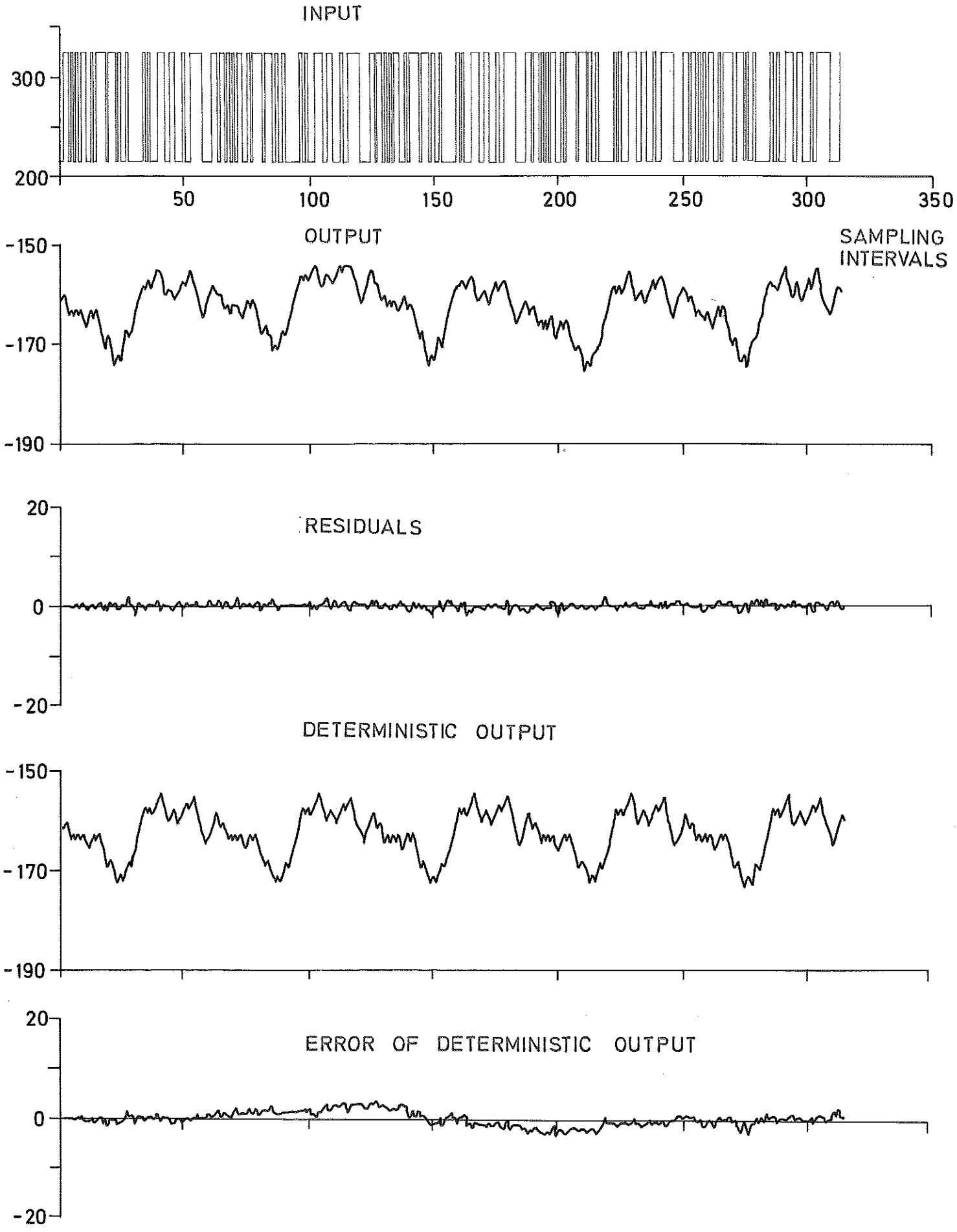


Fig. 12 - Results of identification of experiment 1A, M.L. 2nd order

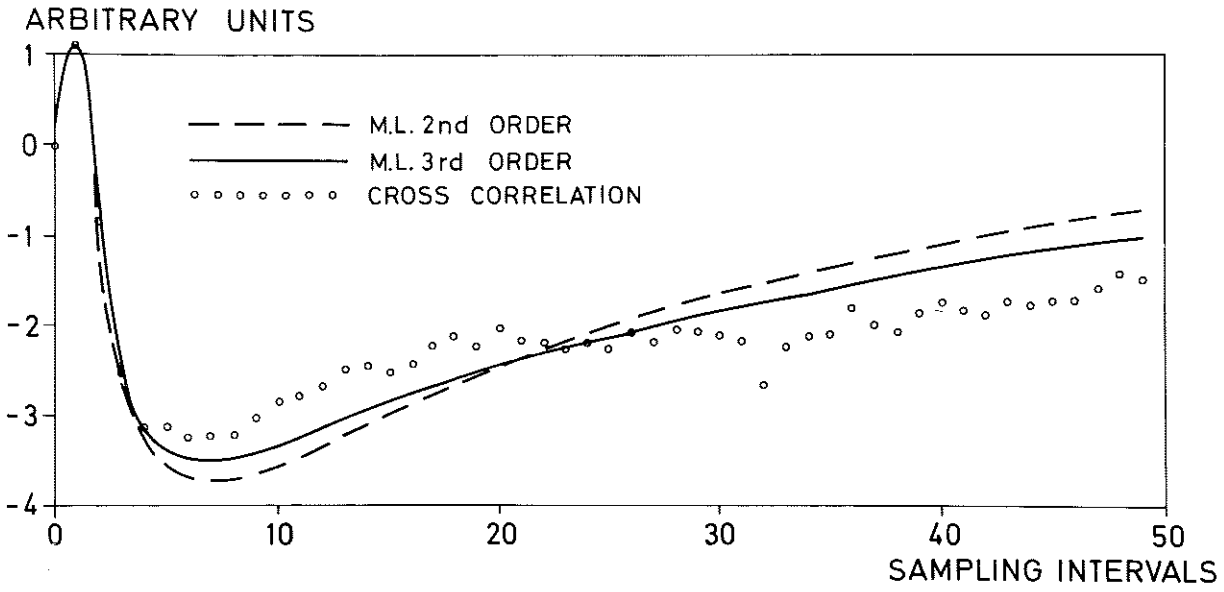


Fig. 13 - Impulse response from 2nd and 3rd order M.L. models and the cross correlation function (experiment 3B)

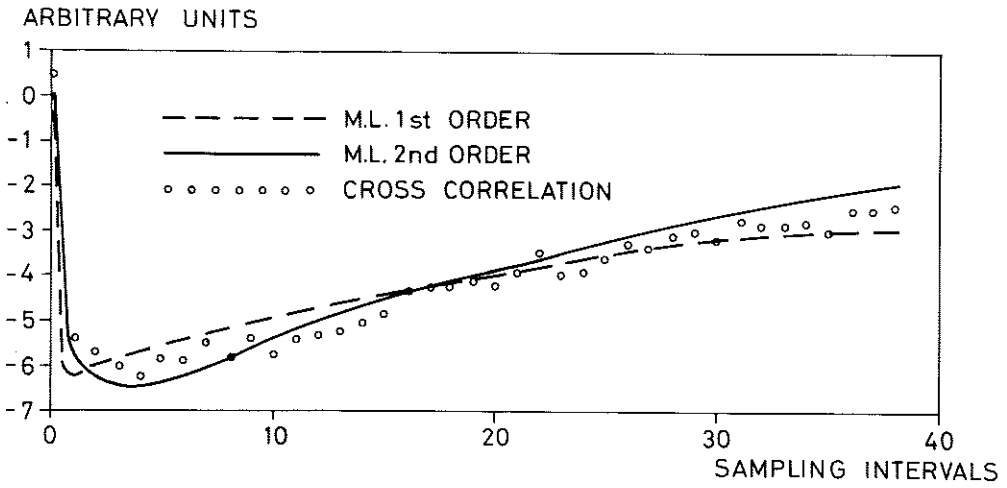


Fig. 15 - Impulse response from 1st and 2nd order M.L. models and the cross correlation function (experiment 4A)

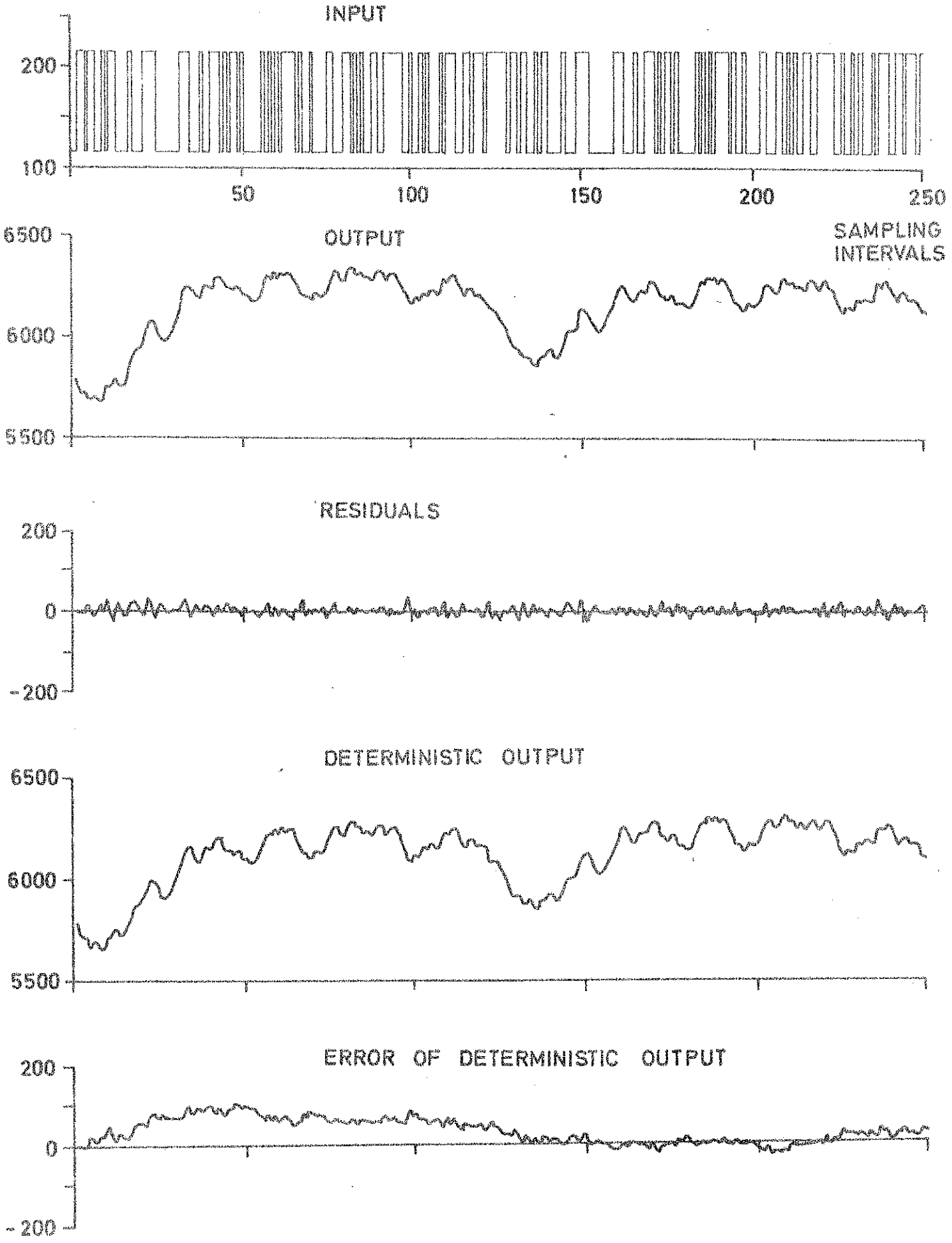


Fig. 14 - Results of identification of experiment 3B, M.L. 3rd order

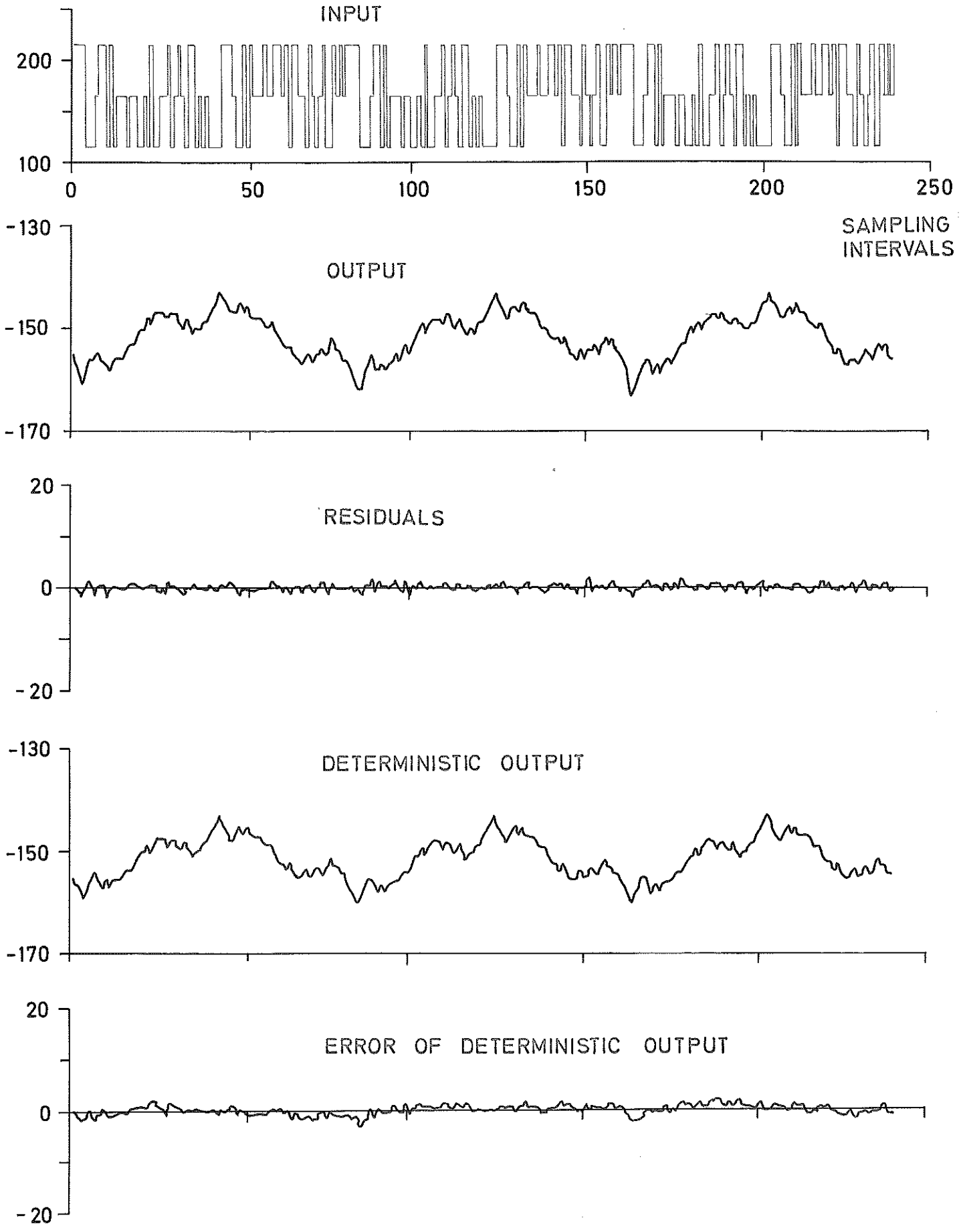


Fig. 16 - Results from identification of experiment 4A, M.L. 1st order

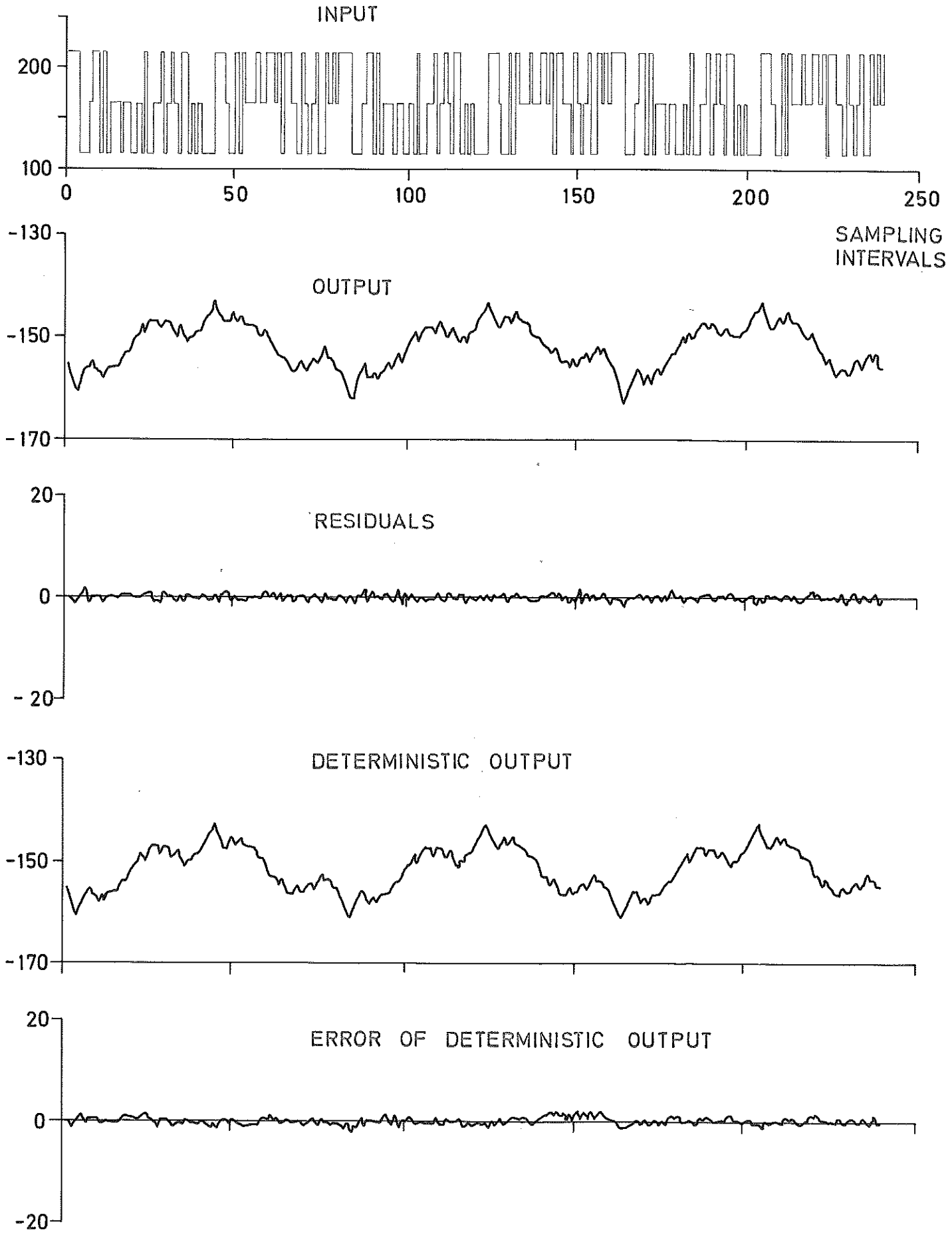


Fig. 17 - Results from identification of experiment 4A, M.L. 2nd order