Software development and numerical simulation of the heterogeneity in transport diffusion with nutrients

Pascale Cuevas

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Supervisor: Dr. Alain Rapaport rapaport@inra.supagro.fr
Trainee: Pascale Cuevas pascale.cuevas@usach.cl.

1   Introduction

In our environment, we can frequently identify phenomena that can be well studied under single input / single output representation (from now on SISO), for example in the fields of Biotechnology (case of the study of Landfills) or Geosciences (propagation of water through cracks), when researchers fill a tracer in an determined area. In the first case, many reactions take part in the area, but since a landfill is usually huge, it is difficult to know what happens in the inside of it. The only thing that we know is that the re-circulation leachate increases the bio-reaction rates since it improves the system mixing. So, we would like to study what happens if we put an inert substrate in the leachate to understand the behaviour of this fluid. In the second case, it could be interesting to study how the water or any source propagates in an area, in order to know for instance what could happen in case of a natural disaster as a big rain or a melting of glaciers and this way to know where to install an urban settlement. So, the idea here is as before, to put an inert substrate in a source and to measure the output response.

Figure 1: Geosciences researchers filling a tracer near Montpellier, France.

The motivation for this work is to characterize these two phenomena exposed above, assuming that initially biological interaction does not happen or considering an inert chemical tracer. These phenomena can be well modelled as a SISO compartimental system with a large network of many tanks, to capture the spatial inhomogeneity and the complex routes of water through the media. It has been proved in the work of Alejandro Rojas and Alain Rapaport (not published yet but with two presentations made), that a large network of tanks in a SISO compartimental system, can be well approximated and studied as a smaller network, let us say of two or more tanks in Serial, Parallel or Mixed SISO.[1]

Consider, as a first approximation, a network consisting of two tanks that can have a Serial, Parallel or Mixed configuration. Define the total volume $V = V_1 + V_2$ as the sum of the volumes of the two tanks (which will be a fixed parameter), and define $a := V_1/V$ the proportion of volume in the first tank. Let S_1 and S_2 be the concentration of the substrate in the first and second tanks, and Q be the input flow rate. The problem consist of, given certain data as a time series $\{tdata_i, Soutdata_i\}_{i=1}^N$ of the output response of the observed system and the input function $u = S_{in} = S_{in}(t)$ for the substrate, to determine the 3-tuple of parameters (a, α, d) (involved in the respective ODE system for the Serial, Parallel or Mixed configuration) and the system configuration that best fits to the data.

This will be done by the least squares method in a numerical way in **Python** and a graphic interface for the problem will be also developed.

The three possible configurations for the two tanks network with one input and one output are the following:

The serial configuration, where there is a linear order, a diffusion rate d, and also an advection rate Q. Notice that here $S_{out} = S_2$:
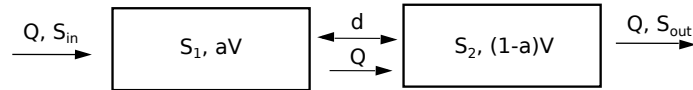

Figure 2: Serial configuration for the two tanks network

The parallel configuration, which is a little more complex than the serial because it has more parameters. Here we have a diffusion rate d and input goes directly to the two tanks with a rate αQ and $(1 - \alpha)Q$ respectively. Notice that here $S_{out} = \alpha S_1 + (1 - \alpha)S_2$

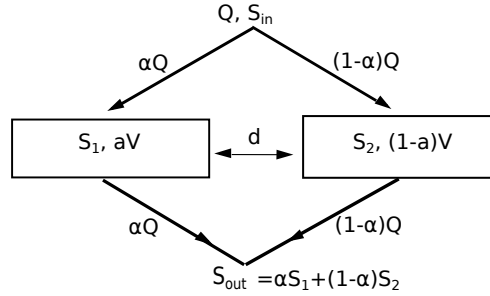Figure 3: Parallel configuration for the two tanks network

The mixed configuration, where the input goes directly to the two tanks with a rate αQ and $(1 - \alpha)Q$ respectively as in the parallel configuration, but with an advection term between the first and the second tank as in the series configuration. In this case $S_{out} = S_1$.
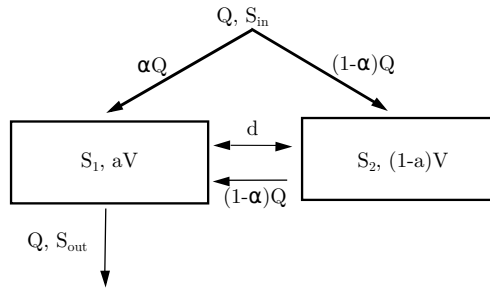
Figure 4: Mixed configuration for the two tanks network

2 The Model

Always under the assumption that the content in each tank is perfectly mixed, and the total volume V and the rate Q are constant; we have three models that represent the configuration Serial, Parallel and Mixed of the two tanks network. As a result of the mass balance equations [2], we have the following system of ODE with initial condition $(S_1(0), S_2(0)) = (0, 0)$ that we consider to be null (absence of former tracer):

Serial Configuration

$$\begin{cases} \dot{S}_1 = \dfrac{Q}{aV}(S_{in}(t) - S_1) + \dfrac{d}{aV}(S_2 - S_1), \\ \dot{S}_2 = \dfrac{Q}{(1-a)V}(S_1 - S_2) + \dfrac{d}{(1-a)V}(S_1 - S_2); \end{cases}$$

Parallel Configuration

$$\begin{cases} \dot{S}_1 = \dfrac{\alpha Q}{aV}(S_{in}(t) - S_1) + \dfrac{d}{aV}(S_2 - S_1), \\ \dot{S}_2 = \dfrac{(1-\alpha)Q}{(1-a)V}(S_{in}(t) - S_2) + \dfrac{d}{(1-a)V}(S_1 - S_2); \end{cases}$$

Mixed Configuration

$$\begin{cases} \dot{S}_1 = \dfrac{Q}{aV}((\alpha S_{in}(t) + (1-\alpha)S_2) - S_1) + \dfrac{d}{aV}(S_2 - S_1), \\ \dot{S}_2 = \dfrac{(1-\alpha)Q}{(1-a)V}(S_{in}(t) - S_2) + \dfrac{d}{(1-a)V}(S_1 - S_2); \end{cases}$$

where $(S_1, S_2) \in \mathbb{R}_+ \times \mathbb{R}_+$ and $S_{in}(\cdot)$ is supposed to be a positive and bounded function of time (Heaviside or Periodic), where the parameters $(a, \alpha, d) \in (0, 1) \times (0, 1) \times \mathbb{R}_+$.

Notice that any of the three configurations can be written in the form

$$\dot{x} = f(x, u, p), \quad \text{with} \quad x_0 = 0,$$

where x is the state variable with $x = (S_1, S_2)$, u represents the input control $S_{in}(t)$, and p represents the vector of parameters (a, α, d). It is also important to notice that for the three cases, we have that the dynamics f is linear with respect to the state variable x and with respect to the control variable u.

This fact becomes clearer if we write the equations in the SISO representation in the state space [3]

$$\begin{cases} \dot{x} = Ax + Bu, \\ y = Cx + Du, \end{cases}$$

which is called *controlled dynamical system* and where A is the dynamics matrix, B is the control matrix, C is called the sensor matrix and D the direct term. Here y represents the output response. In this work, we will see that the term D does not appear in the equations, concluding that the input signal does not have a direct influence in the output response.

We are going to choose $x = (S_1, S_2)^t$ and $u = S_{in}(t)$ for the three configurations. In each case we have that

- **in Serial Network**

$$A = \begin{pmatrix} \frac{-(Q+d)}{aV} & \frac{d}{aV} \\ \frac{(Q+d)}{(1-a)V} & \frac{-(Q+d)}{(1-a)V} \end{pmatrix} \qquad B = \begin{pmatrix} \frac{Q}{aV} \\ 0 \end{pmatrix}, \qquad C = \begin{pmatrix} 0 \\ 1 \end{pmatrix}^t$$

- **in Parallel Network**

$$A = \begin{pmatrix} \frac{-(\alpha Q+d)}{aV} & \frac{d}{aV} \\ \frac{d}{(1-a)V} & \frac{-((1-\alpha)Q+d)}{(1-a)V} \end{pmatrix}, \qquad B = \begin{pmatrix} \frac{\alpha Q}{aV} \\ \frac{(1-\alpha)Q}{(1-a)V} \end{pmatrix}, \qquad C = \begin{pmatrix} \alpha \\ (1-\alpha) \end{pmatrix}^t$$

- **in Mixed Network**

$$A = \begin{pmatrix} \frac{-(Q+d)}{aV} & \frac{(1-\alpha)Q+d}{aV} \\ \frac{d}{(1-a)V} & \frac{-((1-\alpha)Q+d)}{(1-a)V} \end{pmatrix}, \qquad B = \begin{pmatrix} \frac{\alpha Q}{aV} \\ \frac{(1-\alpha)Q}{(1-a)V} \end{pmatrix}, \qquad C = \begin{pmatrix} 1 \\ 0 \end{pmatrix}^t$$

It is easy to see that the linearity of f with respect to the state and control variables inmediately implies that the usual Cauchy-Lipschitz condition guarantees the uniqueness of the Cauchy problem. Furthermore, the solutions are defined for all time as the vector $x(t)$ and can be bounded by an exponential function by Gronwall Lemma [4]. Then, there exists a unique solution for each of this initial value problems, and to numerically solve them it is used the Runge Kutta 4 Scheme in all the scripts.

2.1 Runge Kutta 4 Scheme

The Runge Kutta method is used to solve numerically nonlinear ODE systems. It comes from the Euler Scheme, but it has order 4th and It use information of 4 points [5].

Given a *Cauchy Problem* of the form $\dot{x} = f(t, x)$, $x(0) = x_0$, with the dynamics $f \in C^1$ we have that if $t_{k+1} = t_k + h$, then the *Runge Kutta 4* Scheme is given by

$$
\begin{cases}
k_1 = hf(t_n, x_n), \\
k_2 = hf(t_n + \dfrac{h}{2}, x_n + \dfrac{k_1}{2}), \\
k_3 = hf(t_n + \dfrac{h}{2}, x_n + \dfrac{k_2}{2}), \\
k_4 = hf(t_n + h, x_n + k_3), \\
x_{n+1} = x_n + \dfrac{k_1}{6} + \dfrac{k_2}{3} + \dfrac{k_3}{3} + \dfrac{k_4}{6}.
\end{cases}
$$

2.2 Transfer Function and Equivalence

We introduce the concept of equivalence between two controlled dynamical systems and the concept of transfer function [4]. Let us consider a linear system of the form

$$
\begin{cases}
\dot{x} = Ax(t) + Bu(t), \\
y = Cx(t),
\end{cases}
$$

where $x(t) \in \mathbb{R}^n$, $u(t) \in \mathbb{R}^m$, $y(t) \in \mathbb{R}^p$, $A \in \mathbb{M}_n(\mathbb{R})$, $B \in \mathbb{M}_{n,m}(\mathbb{R})$ and $C \in \mathbb{M}_{p,n}(\mathbb{R})$. The following expression of the output $y(t)$ is called *input-output Relation* or also *Inner Representation*

$$
y(t) = Ce^{tA}x(0) + Ce^{tA}\int_0^t e^{-sA}Bu(s)ds.
$$

The Impulsional Response of a linear system is its Output signal with null initial conditions, when the Input signal is excited by a Dirac Impulsion. In this context, The Impulsional Response Matrix W is given by

$$
W(t) = \begin{cases}
Ce^{tA}B, & \text{if } t \leq 0, \\
0, & \text{if } t < 0.
\end{cases}
$$

The Transfer Matrix H is the Laplace Transform of the Impulsional Response Matrix W

$$
H(s) = \mathcal{L}(W)(s) = \int_0^{+\infty} W(t)e^{-st}dt
$$

where if $Y(s) = \mathcal{L}(y)(s)$ and $U(s) = \mathcal{L}(u)(s)$, with $y(t) = 0$ and $u(t) = 0$ if $t < 0$.

We have that

$$Y(s) = H(s)U(s)$$

with

$$Y(s) = C(sI - A)^{-1}BU(s)$$

where

$$H(s) = C(sI - A)^{-1}B.$$

In this context, we have that two linear systems are said equivalent if they have the same transfer function of minimal realization, i.e. with irreducible numerator and denumerator polynomns in s. The matrices A, B and C depend on the coordinate system. Since the transfer function relates input to outputs the transfer function should also be invariant to coordinate changes in the state space.

3 The Least Squares Method

The least squares method for this problem can be expressed by

$$\min_p l_2, \quad l_2(p) := ||\, r[x(t_1), \cdots, x(t_N), p]\, ||_2^2 = \sum_{k=1}^{N} [r_k(p)]^2, \text{ with } r(\cdot) \in \mathbb{R}^N,$$

where p is the vector of parameters (a, α, d) and N is the length of the vector of time and the length of the solution of the ODE system. In this case, each residual is given by the difference between $r_k(p) = Soutdata_k - Sout_k(p)$, where $Sout_k(p)$ is the solution of the ODE system for the serial, parallel or mixed network, and $Soutdata_k$ is the output response of the given time series.

The problem of the Least Squares has been well studied in Statistics, for different functions to fit to some observable data, such as the linear function, polynomial function and other kind of given functions. The important thing here is to notice, that for some of these cases we can assure the existence of a unique minimum if the dependancy on the parameters is linear.

In this problem, the existence of local extrema points is guaranteed if the objective function is coercive. We cannot guarantee uniqueness, but the existence of local minimum points and to characterize them by computing the gradient with respect to p and to see if it is near to 0 in these extreme points. We also know that the objective function is positive since it is a sum of squares or errors so it means that the function is bounded below by 0 [6].

4   Numerics and results

As a first step, we need to generate different sets of data as a Parallel, Serial and Mixed time series and we do this in **python** using the modules **numpy, scipy** (even though the initial motivation has always been and will be to apply these results to real data). We generate the data $\{t_i, S_{out}(t_i)\}_{i=1}^N$ with parameters $(a^\star, \alpha^\star, d^\star)$ by solving the associated dynamics and saving the results in a text file with the two columns of the time series, one of them corresponding to the time variable and the other one corresponding to the output response of the parallel, serial or mixed network configurations, considering this 3-tuple of parameters. We do this using a positive input signal which makes the solutions of the dynamics to remain positive [8]. The function that we use is a step function of the form

$$f(x) = \left\{ \begin{array}{ll} a & \text{si } 0 \leq t \leq 40, \\ 0 & \text{si } t \in (-\infty, 0) \cup (40, +\infty), \end{array} \right.$$

where $a > 0$.

Then, we would like to find as we said before, which of the three solutions of the parallel, serial and mixed dynamics best fits to the time series. This is done by the Least Squares Method and we use a module developed at MIT that is called **lmfit** [7], wich allows contraint problems as in this case where with $(a, \alpha, d) \in (0, 1) \times (0, 1) \times \mathbb{R}_+$ and uses the Levenberg-Marquardt algorithm.

4.1   Generation of a Parallel time series test

We generate the data in a parallel configuration $\{t_i, S_{out}(t_i)\}_{i=1}^N$ with parameters (0.9, 0.6, 0.1). If we consider 5 random initial guesses for the fit, we obtain the following results in the console

```
 Initial Guess

(0.38355791130094807, 0.40486097469859972, 0.062432747793508603)

 Parallel Config

[[Variables]]
    a:        0.72142292 +/- 0.422246 (58.53%) (init= 0.3835579)
    alpha:    0.27312399 +/- 0.630804 (230.96%) (init= 0.404861)
    d:        0.89809848 +/- 1.777452 (197.91%) (init= 0.06243275)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                    =  1.000
    C(alpha, d)                    = -1.000
    C(a, d)                        = -1.000
[[Value of the residual]]
2.534988359e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
```

(7.0006365455048316, 6.91453357288857, 0.96521269468228721)

 Serial Config

[[Variables]]
    a: 0.09586256 +/- 0   (0.00%) (init= 0.3835579)
    alpha: 0.40486097 +/- 0   (0.00%) (init= 0.404861)
    d: 0.89854593 +/- 0   (0.00%) (init= 0.06243275)
[[Correlations]] (unreported correlations are < 0.100)
[[Value of the residual]]
2.06828927057
[[Partial Derivatives with respect (a,alpha,d)]]
(3.9659123064452739, 0.0, 0.023108647076330868)

 Mixed Config

[[Variables]]
    a: 0.25819653 +/- 0.016877 (6.54%) (init= 0.3835579)
    alpha: 0.51639312 +/- 0.033754 (6.54%) (init= 0.404861)
    d: 0.26709852 +/- 0.120107 (44.97%) (init= 0.06243275)
[[Correlations]] (unreported correlations are < 0.100)
    C(a, alpha)   = 1.000
    C(alpha, d)   = 1.000
    C(a, d)   = 1.000
[[Value of the residual]]
2.53498519041e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(8.0274331630254974, 7.2814383808320491, 1.0125344166948045)

 Initial Guess

(0.93818076528214878, 0.66934022597267129, 0.26413897755245941)

 Parallel Config

[[Variables]]
    a: 0.20348238 +/- 0.000240 (0.12%) (init= 0.9)
    alpha: 0.60606541 +/- 0.000419 (0.07%) (init= 0.6693402)
    d: 0.56696741 +/- 0.001097 (0.19%) (init= 0.264139)
[[Correlations]] (unreported correlations are < 0.100)
    C(a, alpha)   = 1.000
    C(alpha, d)   = 1.000
    C(a, d)   = 1.000

```
[[Value of the residual]]
1.80611293293e-05
[[Partial Derivatives with respect to (a,alpha,d)]]
(8.0982295485427223, 7.4249987648971896, 1.1932868686438374)


 Serial Config

[[Variables]]
    a:         0.89999637 +/- 0         (0.00%) (init= 0.9)
    alpha:    0.66934022 +/- 0         (0.00%) (init= 0.6693402)
    d:         0.84564081 +/- 0         (0.00%) (init= 0.264139)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
2.09086821677
[[Partial Derivatives with respect (a,alpha,d)]]
(6.6706562156022109, 0.0, -0.18590491117227437)


 Mixed Config

[[Variables]]
    a:         0.36690725 +/- 0.569273 (155.15%) (init= 0.9)
    alpha:    0.58759676 +/- 3.165701 (538.75%) (init= 0.6693402)
    d:         0.73048435 +/- 5.423665 (742.48%) (init= 0.264139)
[[Correlations]] (unreported correlations are <  0.100)
    C(alpha, d)                    =  1.000
    C(a, alpha)                    =  1.000
    C(a, d)                        =  0.999
[[Value of the residual]]
0.618813737838
[[Partial Derivatives with respect to (a,alpha,d)]]
(5.7988446253771642, -5.1908789467117078, 0.48589952524116242)


 Initial Guess

(0.18105675972234747, 0.87384353692801664, 0.45185221737716141)


 Parallel Config

[[Variables]]
    a:         0.10237893 +/- 0.024785 (24.21%) (init= 0.1810568)
    alpha:    0.40552496 +/- 0.057298 (14.13%) (init= 0.8738435)
    d:         0.11007976 +/- 0.105366 (95.72%) (init= 0.4518522)
[[Correlations]] (unreported correlations are <  0.100)
```

```
    C(a, alpha)                      =   1.000
    C(alpha, d)                      =   1.000
    C(a, d)                          =   1.000
[[Value of the residual]]
2.53498608957e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(12.325962262488231, 8.5276922378803643, 2.0977179038089968)


 Serial Config

[[Variables]]
    a:          0.09587160 +/- 0        (0.00%) (init= 0.1810568)
    alpha:   0.87384353 +/- 0           (0.00%) (init= 0.8738435)
    d:          0.89877834 +/- 0        (0.00%) (init= 0.4518522)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
2.06828927128
[[Partial Derivatives with respect (a,alpha,d)]]
(3.9656502226996793, 0.0, 0.023047450253077528)


 Mixed Config

[[Variables]]
    a:          0.35451045 +/- 0.066948 (18.88%) (init= 0.1810568)
    alpha:   0.70902099 +/- 0.133897 (18.88%) (init= 0.8738435)
    d:          0.89274323 +/- 0.393343 (44.06%) (init= 0.4518522)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                      =   1.000
    C(alpha, d)                      =   1.000
    C(a, d)                          =   1.000
[[Value of the residual]]
2.53498534233e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(6.4205968383044461, 5.5111530781806488, 0.84822301790264643)


 Initial Guess

(0.38040712747315997, 0.20153001119767155, 0.23938753336350715)


 Parallel Config

[[Variables]]
    a:          0.72120806 +/- 0.089419 (12.40%) (init= 0.3804071)
```

```
    alpha:    0.27280307 +/- 0.133532 (48.95%) (init= 0.20153)
    d:        0.89900283 +/- 0.376301 (41.86%) (init= 0.2393875)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                      =  1.000
    C(alpha, d)                      = -1.000
    C(a, d)                          = -1.000
[[Value of the residual]]
2.53498574367e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(6.9979028413175612, 6.9138212565344972, 0.96475953876956377)


 Serial Config

[[Variables]]
    a:        0.09451119 +/- 0          (0.00%) (init= 0.3804071)
    alpha:    0.20153001 +/- 0          (0.00%) (init= 0.20153)
    d:        0.86200221 +/- 0          (0.00%) (init= 0.2393875)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
2.06828927251
[[Partial Derivatives with respect (a,alpha,d)]]
(4.0378168332161568, 0.0, 0.023954234076484227)


 Mixed Config

[[Variables]]
    a:        0.35523210 +/- 0.582184 (163.89%) (init= 0.3804071)
    alpha:    0.71046429 +/- 1.164368 (163.89%) (init= 0.20153)
    d:        0.89697972 +/- 3.415002 (380.72%) (init= 0.2393875)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                      =  1.000
    C(alpha, d)                      =  1.000
    C(a, d)                          =  1.000
[[Value of the residual]]
2.53498528794e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(6.4126065452100578, 5.5017619343548985, 0.84745077141004155)


 Initial Guess

(0.28528037798100547, 0.82329119924041705, 0.82635823601592162)


 Parallel Config
```

```
[[Variables]]
    a:        0.27895859 +/- 0.004074 (1.46%) (init= 0.2852804)
    alpha:    0.72744576 +/- 0.006082 (0.84%) (init= 0.8232912)
    d:        0.89970410 +/- 0.017140 (1.91%) (init= 0.8263582)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                   =  1.000
    C(alpha, d)                   =  1.000
    C(a, d)                       =  1.000
[[Value of the residual]]
2.53498518995e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(6.8592955267725157, 7.0583864539666861, 0.9644084824135063)


 Serial Config

[[Variables]]
    a:        0.90000000 +/- 0          (0.00%) (init= 0.2852804)
    alpha:    0.82329119 +/- 0          (0.00%) (init= 0.8232912)
    d:        0.89999999 +/- 0          (0.00%) (init= 0.8263582)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
2.0810212464
[[Partial Derivatives with respect (a,alpha,d)]]
(91.441733086945916, 0.0, -0.17017586877532409)


 Mixed Config

[[Variables]]
    a:        0.35548344 +/- 0.012204 (3.43%) (init= 0.2852804)
    alpha:    0.71096698 +/- 0.024409 (3.43%) (init= 0.8232912)
    d:        0.89845366 +/- 0.071554 (7.96%) (init= 0.8263582)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                   =  1.000
    C(alpha, d)                   =  1.000
    C(a, d)                       =  1.000
[[Value of the residual]]
2.5349851896e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(6.4098345695363479, 5.4985007929533083, 0.8471833252749309)
```

We can notice in these results that, for the 5 random initial conditions, the serial configuration is not good for the parallel time series because the value of the residual is $r \geq 2$ with partial derivatives close to $0_{\mathbb{R}^3}$.

We can also notice that the mixed and the parallel configuration are good approximations of the parallel time series, and this is a non intuitive result. For each of the 5 random initial guesses, the value of the residual for each configuration is of the order of 10^{-5} o 10^{-6}, but the value of the partial derivatives aren't so close of the vector $0_{\mathbb{R}^3}$. The candidates to local minimum found with more coincidences are $(0.27, 0.72, 0.89)$, $(0.72, 0.27, 0.89)$ for the parallel configuration and $(0.35, 0.71, 0.89)$ for the mixed configuration. Even though, we know that a value near to the 3-tuple of parameters chosen to generate the time series has to be found, but it seems that the parallel dynamics depends strongly on the initial guess.

This situation is illustrated in the following figures, where it is possible to see 4 curves with different tuples of parameters. In black crosses we have the experimental data; in blue, green, and red, we have the solutions of the parallel, mixed, and serial ODE systems respectively, from which the mixed configuration seems to be the closest to the experimental data, using the 3-tuple (a, α, d) found in the search of a local minimum by the Least Squares method.
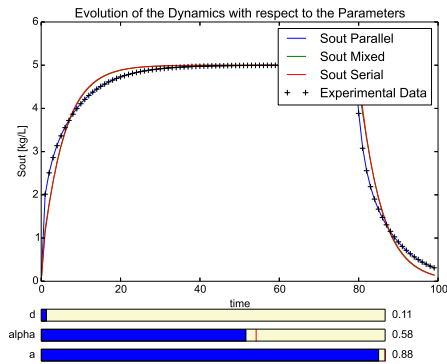

Figure 5: Local Minimum at $(0.89, 0.58, 0.11)$ Parallel Configuration
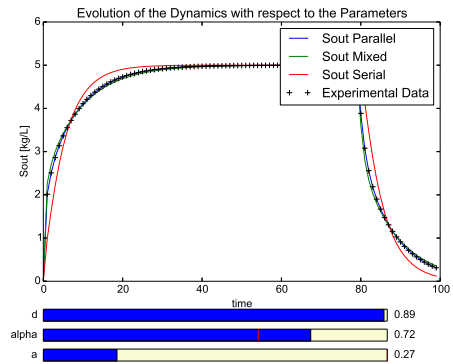

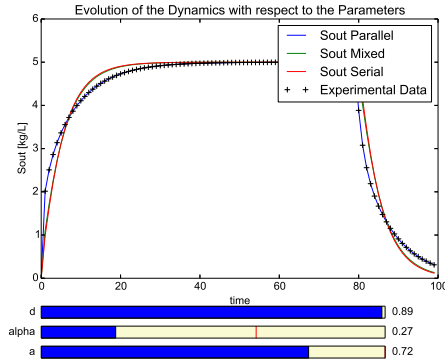Figure 6: Local Minimum at $(0.27, 0.72, 0.89)$ Parallel Configuration

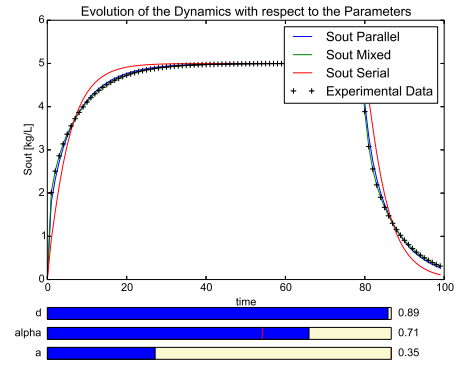Figure 7: Local Minimum at (0.72, 0.27, 0.89) Parallel Configuration

Figure 8: Local Minimum at (0.35, 0.71, 0.89) Mixed Configuration

4.2 Serial Experimental Data

We generate the data in a serial configuration $\{t_i, S_{out}(t_i)\}_{i=1}^N$ with parameters $(a, d) = (0.5, 0.1)$. If we consider 5 random initial guesses for the parameters we obtain the following results

```
 Initial Guess

(0.6322444961620276, 0.12466967744882029, 0.24922045654726677)


 Parallel Config

[[Variables]]
    a:        0.62586632 +/- 5.25e+05 (83958685.96%) (init= 0.6322445)
    alpha:    0.62585570 +/- 5.05e+05 (80689574.22%) (init= 0.1246697)
    d:        0.66932790 +/- 1.45e+07 (2171618843.16%) (init= 0.2492205)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                   =  1.000
    C(alpha, d)                   =  0.248
    C(a, d)                       =  0.245
[[Value of the residual]]
1.86473531841
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.10038847063060796, 0.099787253190974923, -5.8846261197231797e-10)


 Serial Config
```

```
[[Variables]]
    a:        0.39655530 +/- 0          (0.00%) (init= 0.6322445)
    alpha:    0.12466967 +/- 0          (0.00%) (init= 0.1246697)
    d:        0.01011291 +/- 0          (0.00%) (init= 0.2492205)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
2.7863420143e-06
[[Partial Derivatives with respect (a,alpha,d)]]
(1.6795648030742876, 0.0, 1.0104043523445863)


 Mixed Config

[[Variables]]
    a:        0.59566256 +/- 1.327511 (222.86%) (init= 0.6322445)
    alpha:    0.01000000 +/- 0.019228 (192.29%) (init= 0.1246697)
    d:        0.01000009 +/- 1.898074 (18980.57%) (init= 0.2492205)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, d)                   = -1.000
    C(alpha, d)               =  0.999
    C(a, alpha)               = -0.999
[[Value of the residual]]
0.0157716808366
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.70290349709393074, 1.8982344039116974, 0.31405528320978432)


 Initial Guess

(0.83630373497318544, 0.66255434137164582, 0.6589677498628117)


 Parallel Config

[[Variables]]
    a:        0.74946479 +/- 1.30e+05 (17337137.04%) (init= 0.8363037)
    alpha:    0.74945393 +/- 1.24e+05 (16517951.46%) (init= 0.6625543)
    d:        0.27487412 +/- 2.73e+06 (993239265.49%) (init= 0.6589677)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)               = -0.516
    C(a, d)                   =  0.228
[[Value of the residual]]
1.8647353184
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.1502850045426829, 0.14822747856717555, -1.106492675262416e-09)
```

```
 Serial Config

[[Variables]]
    a:         0.39743342 +/- 0          (0.00%) (init= 0.8363037)
    alpha:     0.66255434 +/- 0          (0.00%) (init= 0.6625543)
    d:         0.01163249 +/- 0          (0.00%) (init= 0.6589677)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
2.7863451885e-06
[[Partial Derivatives with respect (a,alpha,d)]]
(1.6633220404641116, 0.0, 1.0096459581509412)


 Mixed Config

[[Variables]]
    a:         0.59566262 +/- 14.48835 (2432.31%) (init= 0.8363037)
    alpha:     0.01000000 +/- 0.011746 (117.47%) (init= 0.6625543)
    d:         0.01000000 +/- 12.62627 (126262.78%) (init= 0.6589677)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, d)                       = -1.000
    C(alpha, d)                   =  1.000
    C(a, alpha)                   = -1.000
[[Value of the residual]]
0.0157716791163
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.70290499827721298, 1.8982343400912016, 0.31405574092486754)


 Initial Guess

(0.57608858417469677, 0.90891311569352884, 0.36509756722516973)


 Parallel Config

[[Variables]]
    a:         0.89964568 +/- 1.16e+04 (1293305.05%) (init= 0.5760886)
    alpha:     0.89955888 +/- 2.15e+04 (2392821.05%) (init= 0.9)
    d:         0.70415516 +/- 7.44e+05 (105620924.48%) (init= 0.3650976)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                   =  0.997
    C(alpha, d)                   = -0.496
    C(a, d)                       = -0.489
[[Value of the residual]]
1.86473531917
```

```
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.15577115499028071, 0.15170667682713468, -1.1513665576501353e-07)


 Serial Config


[[Variables]]
    a:        0.49006838 +/- 0          (0.00%) (init= 0.5760886)
    alpha:    0.90000000 +/- 0          (0.00%) (init= 0.9)
    d:        0.09917110 +/- 0          (0.00%) (init= 0.3650976)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
2.78634188548e-06
[[Partial Derivatives with respect (a,alpha,d)]]
(0.080304389289425834, 0.0, 0.96772867859970091)


 Mixed Config


[[Variables]]
    a:        0.58977569 +/- 673.5588 (114205.94%) (init= 0.5760886)
    alpha:    0.01000565 +/- 13.07552 (130681.37%) (init= 0.9)
    d:        0.01867549 +/- 934.2440 (5002514.16%) (init= 0.3650976)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, d)                    = -1.000
    C(alpha, d)                =  1.000
    C(a, alpha)                = -1.000
[[Value of the residual]]
0.0159397278534
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.61952512228376744, 1.9292917843885624, 0.30873191422941676)


 Initial Guess


(0.47353965926462938, 0.53559937648661859, 0.80496894103776184)


 Parallel Config


[[Variables]]
    a:        0.50446171 +/- 2.89e+04 (5733496.96%) (init= 0.4735397)
    alpha:    0.50447180 +/- 2.88e+04 (5707267.56%) (init= 0.5355994)
    d:        0.01322907 +/- 2.71e+05 (2046213252.10%) (init= 0.8049689)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                = -0.380
    C(a, d)                    = -0.281
```

```
[[Value of the residual]]
1.8647353184
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.12747220141038351, 0.12791559235907357, -3.3479885530596221e-10)


 Serial Config


[[Variables]]
    a:         0.60350331 +/- 0          (0.00%) (init= 0.4735397)
    alpha:     0.53559937 +/- 0          (0.00%) (init= 0.5355994)
    d:         0.01001101 +/- 0          (0.00%) (init= 0.8049689)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
2.78634275689e-06
[[Partial Derivatives with respect (a,alpha,d)]]
(1.8513078914105008, 0.0, 1.01045584178669)


 Mixed Config


[[Variables]]
    a:         0.59566262 +/- 0.213973 (35.92%) (init= 0.4735397)
    alpha:     0.01000000 +/- 0.003244 (32.44%) (init= 0.5355994)
    d:         0.01000000 +/- 0.020411 (204.11%) (init= 0.8049689)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, d)                      =  1.000
    C(alpha, d)                  = -0.970
    C(a, alpha)                  = -0.969
[[Value of the residual]]
0.0157716791047
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.70290450674445437, 1.8982341219193775, 0.31405540962435202)


 Initial Guess


(0.94814012821816906, 0.77659502500081745, 0.15867223825873666)


 Parallel Config


[[Variables]]
    a:         0.82754886 +/- 955.1720 (115421.83%) (init= 0.9)
    alpha:     0.82420778 +/- 774.7447 (93998.72%) (init= 0.776595)
    d:         0.56901149 +/- 1.24e+03 (217957.01%) (init= 0.1586722)
[[Correlations]] (unreported correlations are <  0.100)
```

```
    C(a, alpha)                         =   1.000
    C(alpha, d)                         = -0.999
    C(a, d)                             = -0.999
[[Value of the residual]]
1.86489425509
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.24094935839573672, 0.047922052648186053, -0.000129227948120203)


 Serial Config

[[Variables]]
    a:          0.51026669 +/- 0          (0.00%) (init= 0.9)
    alpha:      0.77659502 +/- 0          (0.00%) (init= 0.776595)
    d:          0.79262414 +/- 0          (0.00%) (init= 0.1586722)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
0.505689491318
[[Partial Derivatives with respect (a,alpha,d)]]
(0.18593744763312214, 0.0, 0.54294360937714448)


 Mixed Config

[[Variables]]
    a:          0.26904375 +/- 7.129365 (2649.89%) (init= 0.9)
    alpha:      0.01068730 +/- 0.830477 (7770.69%) (init= 0.776595)
    d:          0.73922213 +/- 22.11993 (2992.33%) (init= 0.1586722)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, d)                             =   1.000
    C(a, alpha)                         =   1.000
    C(alpha, d)                         =   1.000
[[Value of the residual]]
0.311280258793
[[Partial Derivatives with respect to (a,alpha,d)]]
(-2.8256922095596715, 3.3086492542728219, 0.42442871994985421)
```

It is not difficult to see that for the 5 initial guess, the two configuration that best fit to the experimental data are the serial and the mixed ones. In the case of the parallel configuration, we have that the residual value is $r \geq 1$ with partial derivatives in the minimum point very close to 0. The candidates to be local minimum point are $(a^\star, d^\star) = (0.49, 0.09)$ for the serial configuration with residual value of the order of 10^{-6} and partial derivatives are close to $\vec{0}$. For the mixed configuration we have the candidate $(a^\star, \alpha^\star, d^\star) = (0.59, 0.01, 0.01)$ with a residual value of the order of 10^{-2}. In this case, the fact that the mixed configuration fits good to the serial data is more intuitive, because if we see the ODE system that models this configuration, we see that if $\alpha \approx 0$ the equations are the same that the equations for the serial configuration. In any case, the configuration that best fits the time series is the serial one.
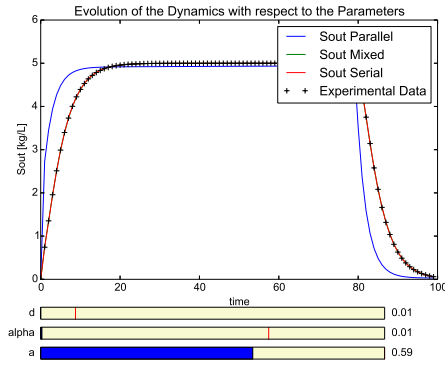

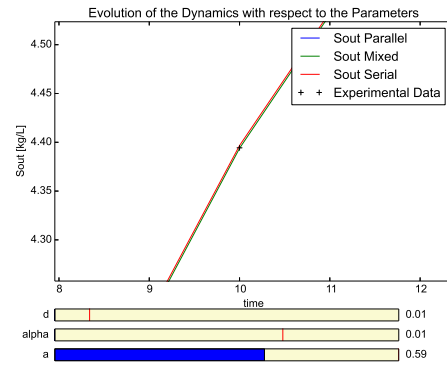Figure 9: Minimum value (0.59, 0.01, 0.01) Mixed Dynamics

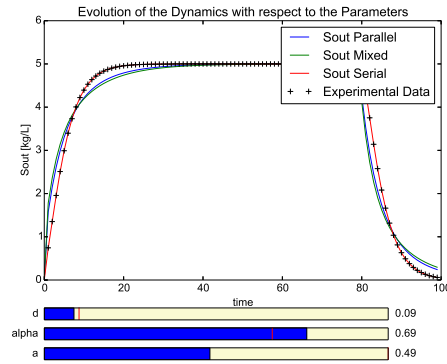Figure 10: Minimum value (0.59, 0.01, 0.01) Mixed Dynamics Zoom

Figure 11: Minimum value (0.49, 0.09) Serial Dynamics

4.3 Mixed Experimental Data

As before, we generate a time series using the Mixed configuration with parameters (0.7, 0.6, 0.1) and we to explore the results of the fitting with the three configurations for 5 random initial guesses.

```
 Initial Guess

(0.64049356957553172, 0.64911355449204633, 0.2232518845546223)

 Parallel Config

[[Variables]]
    a:        0.64481046 +/- 1.43e+04 (2221233.19%) (init= 0.6404936)
    alpha:    0.64478765 +/- 1.57e+04 (2427989.13%) (init= 0.6491136)
    d:        0.80912635 +/- 7.00e+04 (8649132.90%) (init= 0.2232519)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                   = -0.270
    C(alpha, d)                   = -0.223
    C(a, d)                       = -0.133
[[Value of the residual]]
0.391510900669
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.096040208612679923, 0.095284717465282665, -3.1251390364417375e-09)

 Serial Config

[[Variables]]
    a:        0.88619817 +/- 0          (0.00%) (init= 0.6404936)
    alpha:    0.64911355 +/- 0          (0.00%) (init= 0.6491136)
    d:        0.79705934 +/- 0          (0.00%) (init= 0.2232519)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
0.390126232855
[[Partial Derivatives with respect (a,alpha,d)]]
(1.4259152867592551, 0.0, 0.0020307118967721749)

 Mixed Config

[[Variables]]
    a:        0.83431506 +/- 0.077053 (9.24%) (init= 0.6404936)
    alpha:    0.71512720 +/- 0.066045 (9.24%) (init= 0.6491136)
    d:        0.02268413 +/- 0.088714 (391.08%) (init= 0.2232519)
[[Correlations]] (unreported correlations are <  0.100)
```

```
    C(a, alpha)                   =  1.000
    C(alpha, d)                   = -1.000
    C(a, d)                       = -1.000
[[Value of the residual]]
3.06984044246e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(1.6977576843226132, 2.6010484937981264, 0.55660202136867665)


 Initial Guess

(0.61933055187414621, 0.9308260135341071, 0.54372248679531909)


 Parallel Config

[[Variables]]
    a:       0.67129604 +/- 2.24e+04 (3330297.54%) (init= 0.6193306)
    alpha:   0.65911846 +/- 7.65e+04 (11599103.43%) (init= 0.9)
    d:       0.73766862 +/- 3.31e+04 (4487929.55%) (init= 0.5437225)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                   =  1.000
    C(a, d)                       = -0.577
    C(alpha, d)                   = -0.577
[[Value of the residual]]
0.391511862967
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.49922910994872338, -0.14527030020028975, -0.00099348825706169208)


 Serial Config

[[Variables]]
    a:       0.89931235 +/- 0           (0.00%) (init= 0.6193306)
    alpha:   0.90000000 +/- 0           (0.00%) (init= 0.9)
    d:       0.51144247 +/- 0           (0.00%) (init= 0.5437225)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
0.390126232857
[[Partial Derivatives with respect (a,alpha,d)]]
(2.0460973466874699, 0.0, 0.0025707683262432557)


 Mixed Config

[[Variables]]
    a:       0.84545984 +/- 0.124174 (14.69%) (init= 0.6193306)
```

```
    alpha:    0.72467998 +/- 0.106466 (14.69%) (init= 0.9)
    d:        0.01230441 +/- 0.155683 (1265.27%) (init= 0.5437225)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                    =  1.000
    C(alpha, d)                    = -1.000
    C(a, d)                        = -1.000
[[Value of the residual]]
0.000383545925329
[[Partial Derivatives with respect to (a,alpha,d)]]
(1.3873016762356469, 2.4517427772746685, 0.58408088624689702)


 Initial Guess

(0.87132383353105913, 0.44425697957586985, 0.42779048261228525)


 Parallel Config

[[Variables]]
    a:        0.89624396 +/- 2.35e+05 (26217423.18%) (init= 0.8713238)
    alpha:    0.89624391 +/- 2.35e+05 (26266956.66%) (init= 0.444257)
    d:        0.84287703 +/- 2.02e+06 (240231608.83%) (init= 0.4277905)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                    =  1.000
[[Value of the residual]]
0.391510900669
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.12305159151302369, 0.12547538052676832, -2.7755575615628914e-13)


 Serial Config

[[Variables]]
    a:        0.88839645 +/- 0          (0.00%) (init= 0.8713238)
    alpha:    0.44425697 +/- 0          (0.00%) (init= 0.444257)
    d:        0.74976069 +/- 0          (0.00%) (init= 0.4277905)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
0.390126239113
[[Partial Derivatives with respect (a,alpha,d)]]
(1.5080133422144704, 0.0, 0.002070669464487862)


 Mixed Config

[[Variables]]
```

```
    a:          0.81553096 +/- 0.108382 (13.29%) (init= 0.8713238)
    alpha:      0.69902654 +/- 0.092900 (13.29%) (init= 0.444257)
    d:          0.04279762 +/- 0.107321 (250.77%) (init= 0.4277905)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                  =  1.000
    C(alpha, d)                  = -1.000
    C(a, d)                      = -1.000
[[Value of the residual]]
3.06984044338e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(1.8624334614202716, 2.7374582753668721, 0.51193850634075111)


 Initial Guess


(0.50317895765129494, 0.87002975610844158, 0.24301409040633959)


 Parallel Config


[[Variables]]
    a:          0.10981715 +/- 1.00e+05 (91370199.95%) (init= 0.503179)
    alpha:      0.10982001 +/- 9.60e+04 (87423183.03%) (init= 0.8700298)
    d:          0.01020525 +/- 8.90e+03 (87179884.71%) (init= 0.2430141)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                  =  1.000
    C(alpha, d)                  =  0.436
    C(a, d)                      =  0.436
[[Value of the residual]]
0.391510900685
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.36581205812628581, 0.37693257558947812, -4.8953063824797027e-10)


 Serial Config


[[Variables]]
    a:          0.88371543 +/- 0          (0.00%) (init= 0.503179)
    alpha:      0.87002975 +/- 0          (0.00%) (init= 0.8700298)
    d:          0.85034021 +/- 0          (0.00%) (init= 0.2430141)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
0.390126235243
[[Partial Derivatives with respect (a,alpha,d)]]
(1.3432103616005608, 0.0, 0.0020615363060361158)
```

```
 Mixed Config

[[Variables]]
    a:         0.84244135 +/- 0.444970 (52.82%) (init= 0.503179)
    alpha:     0.72209258 +/- 0.381401 (52.82%) (init= 0.8700298)
    d:         0.01304553 +/- 0.543356 (4165.08%) (init= 0.2430141)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                    =  1.000
    C(alpha, d)                    = -1.000
    C(a, d)                        = -1.000
[[Value of the residual]]
3.06984044288e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(1.632543373280295, 2.5394018523156974, 0.57937324277541624)


 Initial Guess

(0.33699678167553571, 0.71157382993011853, 0.1140635735291029)


 Parallel Config

[[Variables]]
    a:         0.79582371 +/- 5.90e+05 (74180454.27%) (init= 0.3369968)
    alpha:     0.79581023 +/- 1.24e+06 (156283011.36%) (init= 0.7115738)
    d:         0.77897284 +/- 4.19e+06 (537463985.85%) (init= 0.1140636)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                    =  1.000
    C(alpha, d)                    =  0.553
    C(a, d)                        =  0.551
[[Value of the residual]]
0.39151090067
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.11377680324409223, 0.11379909431830093, -1.6355805598777806e-09)


 Serial Config

[[Variables]]
    a:         0.11775271 +/- 0          (0.00%) (init= 0.3369968)
    alpha:     0.71157382 +/- 0          (0.00%) (init= 0.7115738)
    d:         0.88140164 +/- 0          (0.00%) (init= 0.1140636)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
0.3901262331
```

```
[[Partial Derivatives with respect (a,alpha,d)]]
(0.6699823263839888, 0.0, 0.0019666314819699604)


 Mixed Config


[[Variables]]
    a:        0.83495303 +/- 2.235995 (267.80%) (init= 0.3369968)
    alpha:    0.71567403 +/- 1.916553 (267.80%) (init= 0.7115738)
    d:        0.02194791 +/- 2.586645 (11785.38%) (init= 0.1140636)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                   =  1.000
    C(alpha, d)                   = -1.000
    C(a, d)                       = -1.000
[[Value of the residual]]
3.06984044333e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(1.6924467450517764, 2.5962735464453059, 0.55830568324310959)
```

It is interesting to notice that in this case the three configurations are good approximation of the time series. For the 5 random initial guesses we found that the best candidates to be local minimum value, due to its residual value and partial derivatives, are those corresponding to the mixed configuration $(a^\star, \alpha^\star, d^\star) = (0.84, 0.71, 0.021)$ with residual value of the order of 10^{-6} and partial derivatives near to $\vec{0}$, for the serial configuration $(a^\star, d^\star) = (0.11, 0.88)$ and $(0.88, 0.85)$ with a residual value of the order of 10^{-1} and partial derivatives close to $\vec{0}$, for the parallel configuration $(a^\star, \alpha^\star, d^\star) = (0.1, 0.1, 0.01)$ and $(0.79, 0.79, 0.77)$ with residual value of the order of 10^{-1} and partial derivatives in the local minimun candidates near to $\vec{0}$.

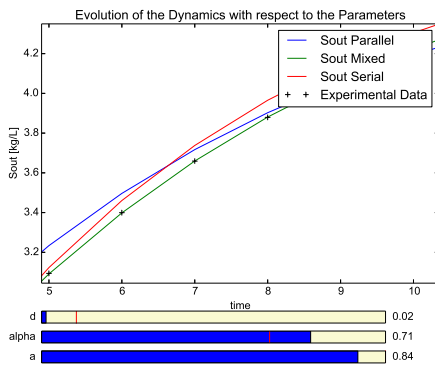We illustrate this situation in the following figures:

Figure 12: Minimum Value Mixed Configuration (0.84, 0.71, 0.021)
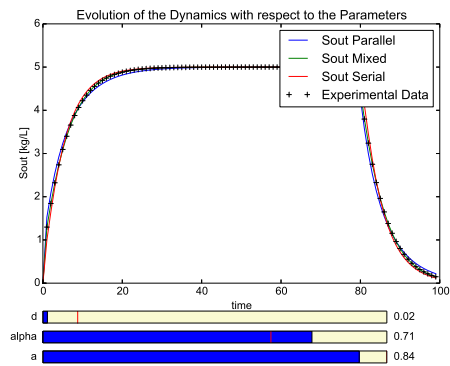

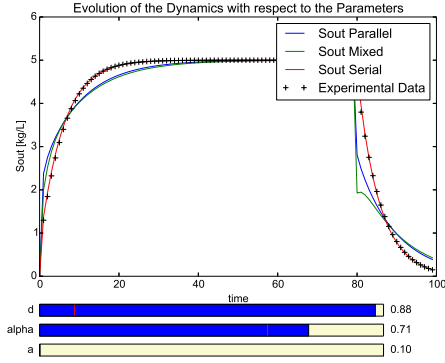Figure 13: Minimum Value Mixed Configuration (0.84, 0.71, 0.021)

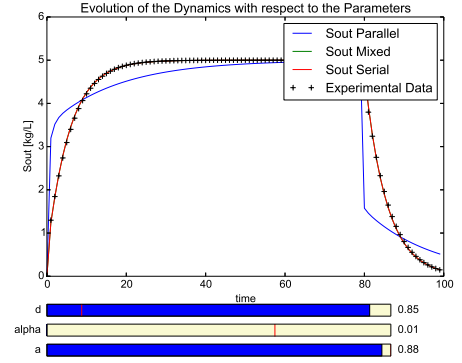Figure 14: Minimum Value Serial Configuration (0.11, 0.88)

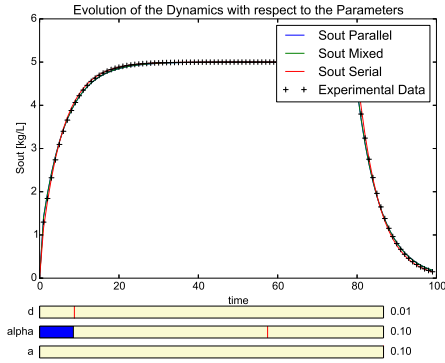Figure 15: Minimum Value Serial Configuration (0.88, 0.85)

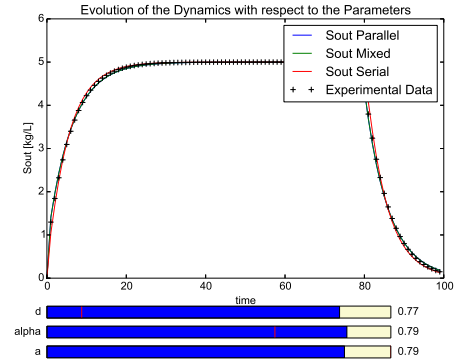Figure 16: Minimum Value Parallel Configuration (0.1, 0.1, 0.01)

Figure 17: Minimum Value Parallel Configuration (0.79, 0.79, 0.77)

5   The influence of the input signal

We consider now another time series given by an experiment with a signal of the type $S_{in}(t) = a(1 + \sin(2\pi t))$, with $a > 0$ and $t \in [0, 40]$. This signal is positive and continuous, so the solution of the ODE system remains positive [8].

In this case we can see that the residual value grows, but in all the cases the behaviour is similar. The interesting cases are those in which, given a time series, we can find more than one dynamics that best fits the time series, but the idea is to see what happens with a new input Signal, because this will show which dynamics achieves the best fit.

Such as we did before, we generate the data $\{t_i, S_{out}(t_i)\}_{i=1}^{N}$ with parameters (a, α, d), i.e to save in a file the two vector columns, one of them the time and the other one the output response considering this 3-tuple of parameters. We apply the least squares method to the three configurations

in serial, parallel and mixed, and we are going to use the module **lmfit**, the class **Parameters** and the function **minimize** which works with the algorithm *Levenberg-Marquardt* for constraint optimization problems, with $(a, \alpha, d) \in (0, 1) \times (0, 1) \times \mathbb{R}_+$.

5.1   Parallel Experimental Data

We generate 5 random initial guesses and as we do before for the first input Signal, we will obtain a candidate to be a local minimum for the parameters in the dynamics.

If we consider the same parameters as before, i.e., (0.9, 0.6, 0.1) we obtain that

```
 Initial Guess

(0.37396099786170756, 0.64501639983899717, 0.13089714291828092)

 Parallel Config

[[Variables]]
    a:        0.27794145 +/- 0.012346 (4.44%) (init= 0.373961)
    alpha:    0.72592584 +/- 0.018466 (2.54%) (init= 0.6450164)
    d:        0.89542079 +/- 0.052024 (5.81%) (init= 0.1308971)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                  =  1.000
    C(alpha, d)                  =  1.000
    C(a, d)                      =  1.000
[[Value of the residual]]
2.94277426909e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(15.116724722240143, 12.037106137910975, 0.97071193313600368)

 Serial Config

[[Variables]]
    a:        0.89999999 +/- 0          (0.00%) (init= 0.373961)
    alpha:    0.64501639 +/- 0          (0.00%) (init= 0.6450164)
    d:        0.89999997 +/- 0          (0.00%) (init= 0.1308971)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
4.27476282614
[[Partial Derivatives with respect (a,alpha,d)]]
(24.973016004921522, 0.0, -0.2769454856305309)

 Mixed Config
```

```
[[Variables]]
    a:        0.35566436 +/- 0.004826 (1.36%) (init= 0.373961)
    alpha:    0.71132876 +/- 0.009652 (1.36%) (init= 0.6450164)
    d:        0.89951327 +/- 0.028278 (3.14%) (init= 0.1308971)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                    =  1.000
    C(alpha, d)                    =  1.000
    C(a, d)                        =  1.000
[[Value of the residual]]
2.94277426797e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(13.182832001996209, 8.2989691625378121, 0.85061512601905942)


 Initial Guess

(0.071662826025287396, 0.31775620517684644, 0.46386064614043088)


 Parallel Config

[[Variables]]
    a:        0.08456453 +/- 0.016542 (19.56%) (init= 0.07166283)
    alpha:    0.36279714 +/- 0.041243 (11.37%) (init= 0.3177562)
    d:        0.03653555 +/- 0.065942 (180.49%) (init= 0.4638606)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                    =  1.000
    C(alpha, d)                    =  1.000
    C(a, d)                        =  1.000
[[Value of the residual]]
2.94277426942e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(35.860074487860331, 17.775170929391091, 2.4957752590137958)


 Serial Config

[[Variables]]
    a:        0.09457950 +/- 0           (0.00%) (init= 0.07166283)
    alpha:    0.31775620 +/- 0           (0.00%) (init= 0.3177562)
    d:        0.89888778 +/- 0           (0.00%) (init= 0.4638606)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
4.24974989795
[[Partial Derivatives with respect (a,alpha,d)]]
```

```
(6.2515175759900288, 0.0, 0.022064447276726185)


 Mixed Config


[[Variables]]
    a:         0.27695904 +/- 0.040762 (14.72%) (init= 0.07166283)
    alpha:     0.55391810 +/- 0.081525 (14.72%) (init= 0.3177562)
    d:         0.39835407 +/- 0.280233 (70.35%) (init= 0.4638606)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                   =  1.000
    C(alpha, d)                   =  1.000
    C(a, d)                       =  1.000
[[Value of the residual]]
2.94277426814e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(16.466537084655616, 10.487788379221175, 0.97282087449551358)


 Initial Guess


(0.61548960295661825, 0.68005931392515062, 0.13711189205260654)


 Parallel Config


[[Variables]]
    a:         0.78308335 +/- 0.083019 (10.60%) (init= 0.6154896)
    alpha:     0.37093795 +/- 0.140040 (37.75%) (init= 0.6800593)
    d:         0.62799217 +/- 0.375197 (59.75%) (init= 0.1371119)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                   =  1.000
    C(alpha, d)                   = -1.000
    C(a, d)                       = -1.000
[[Value of the residual]]
2.94277426959e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(19.4327141181119, 12.581148491093211, 1.145816204732353)


 Serial Config


[[Variables]]
    a:         0.06884557 +/- 0           (0.00%) (init= 0.6154896)
    alpha:     0.68005931 +/- 0           (0.00%) (init= 0.6800593)
    d:         0.17022682 +/- 0           (0.00%) (init= 0.1371119)
[[Correlations]] (unreported correlations are <  0.100)
```

```
[[Value of the residual]]
4.24974996256
[[Partial Derivatives with respect (a,alpha,d)]]
(10.003327727465372, 0.0, 0.04107756345410607)


 Mixed Config


[[Variables]]
    a:        0.35567289 +/- 0.016045 (4.51%) (init= 0.6154896)
    alpha:    0.71134581 +/- 0.032090 (4.51%) (init= 0.6800593)
    d:        0.89956325 +/- 0.093986 (10.45%) (init= 0.1371119)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                  =  1.000
    C(alpha, d)                  =  1.000
    C(a, d)                      =  1.000
[[Value of the residual]]
2.94277426944e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(13.182558452269314, 8.2987864358385988, 0.8506060221326045)


 Initial Guess


(0.43351926774696392, 0.77987752392857379, 0.6345287732331838)


 Parallel Config


[[Variables]]
    a:        0.24656721 +/- 0.073161 (29.67%) (init= 0.4335193)
    alpha:    0.67757979 +/- 0.116179 (17.15%) (init= 0.7798775)
    d:        0.76026562 +/- 0.321502 (42.29%) (init= 0.6345288)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                  =  1.000
    C(alpha, d)                  =  1.000
    C(a, d)                      =  1.000
[[Value of the residual]]
2.94277426852e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(16.461148764600971, 12.406388622922506, 1.0482380439540397)


 Serial Config


[[Variables]]
    a:        0.90000000 +/- 0          (0.00%) (init= 0.4335193)
```

```
    alpha:    0.77987752 +/- 0          (0.00%) (init= 0.7798775)
    d:        0.89999999 +/- 0          (0.00%) (init= 0.6345288)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
4.27476278439
[[Partial Derivatives with respect (a,alpha,d)]]
(24.973532093679118, 0.0, -0.27694525910213486)


 Mixed Config


[[Variables]]
    a:        0.35369981 +/- 0.017951 (5.08%) (init= 0.4335193)
    alpha:    0.70739966 +/- 0.035903 (5.08%) (init= 0.7798775)
    d:        0.88797549 +/- 0.105654 (11.90%) (init= 0.6345288)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                 =  1.000
    C(alpha, d)                 =  1.000
    C(a, d)                     =  1.000
[[Value of the residual]]
2.94277426876e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(13.246228594661607, 8.3413135601627975, 0.85273049397611489)


 Initial Guess


(0.45698021079744799, 0.54039782182217422, 0.32228621551769343)


 Parallel Config


[[Variables]]
    a:        0.10114969 +/- 0.377779 (373.49%) (init= 0.4569802)
    alpha:    0.40267655 +/- 0.877495 (217.92%) (init= 0.5403978)
    d:        0.10486264 +/- 1.600438 (1526.22%) (init= 0.3222862)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                 =  1.000
    C(alpha, d)                 =  1.000
    C(a, d)                     =  1.000
[[Value of the residual]]
2.94277426973e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(31.461333726707412, 16.634333751651042, 2.1293476482851408)


 Serial Config
```

```
[[Variables]]
    a:        0.09266204 +/- 0          (0.00%) (init= 0.4569802)
    alpha:    0.54039782 +/- 0          (0.00%) (init= 0.5403978)
    d:        0.84616639 +/- 0          (0.00%) (init= 0.3222862)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
4.24974990375
[[Partial Derivatives with respect (a,alpha,d)]]
(6.4552221842428814, 0.0, 0.023075144148076987)


 Mixed Config

[[Variables]]
    a:        0.29472189 +/- 0.048544 (16.47%) (init= 0.4569802)
    alpha:    0.58944381 +/- 0.097090 (16.47%) (init= 0.5403978)
    d:        0.51843591 +/- 0.322620 (62.23%) (init= 0.3222862)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                 =  1.000
    C(alpha, d)                 =  1.000
    C(a, d)                     =  1.000
[[Value of the residual]]
2.94277427413e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(15.567051378937544, 9.8882018930130382, 0.93738626960624771)
```

In the same way as we saw before, we can see that for the 5 random initial guesses we have that for the serial configuration, the residual value remains $r \geq 4$ with partial derivatives near to $\vec{0}$ so this configuration remains actually far from the time series. The best configurations are the mixed and the parallel one with residual value of the order of 10^{-6} and candidates to be local minimun with more concidences being $(0.27, 0.72, 0.89)$ for the parallel configuration and for the mixed configuration we have $(0.35, 0.71, 0.89)$. Notice that the 3-tuple of parameters has been found in the case of the first Input.

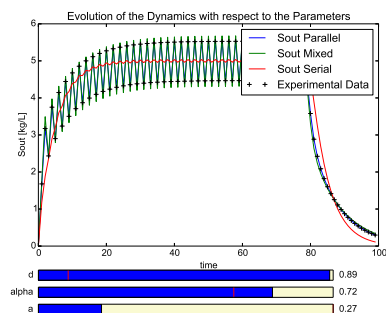This situation can be seen in the following Figures:

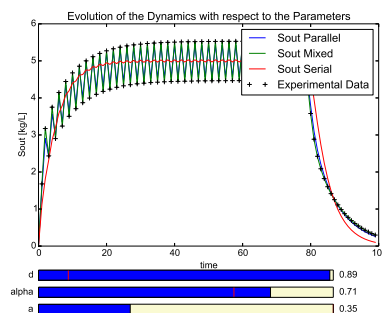Figure 18: Minimum Value Parallel Configuration $(0.27, 0.72, 0.89)$

Figure 19: Minimum Value Mixed Configuration $(0.35, 0.71, 0.89)$

5.2   Serial Data

If we generate the time series with the parameters $(a, \alpha) = (0.5, 0.1)$ as we did before for the first input Signal, we obtain the following set of results:

```
 Initial Guess

(0.898147033875766, 0.87546700869026339, 0.6497321529546165)

 Parallel Config

[[Variables]]
    a:        0.88163845 +/- 5.85e+04 (6639125.24%) (init= 0.898147)
    alpha:    0.88165181 +/- 5.85e+04 (6639684.23%) (init= 0.875467)
    d:        0.88268077 +/- 1.85e+05 (20934098.03%) (init= 0.6497322)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                      =  1.000
```

```
    C(a, d)                      =  0.424
    C(alpha, d)                  =  0.419
[[Value of the residual]]
2.91903275056
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.24767915938861407, 0.23902827407260574, -1.5143886145096985e-09)


 Serial Config

[[Variables]]
    a:         0.60339309 +/- 0          (0.00%) (init= 0.898147)
    alpha:     0.87546700 +/- 0          (0.00%) (init= 0.875467)
    d:         0.01020261 +/- 0          (0.00%) (init= 0.6497322)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
2.99495292819e-06
[[Partial Derivatives with respect (a,alpha,d)]]
(1.8535848235569994, 0.0, 1.0127008822482073)


 Mixed Config

[[Variables]]
    a:         0.59458858 +/- 614.3427 (103322.32%) (init= 0.898147)
    alpha:     0.01000000 +/- 11.42412 (114241.20%) (init= 0.875467)
    d:         0.01000015 +/- 837.3710 (8373580.01%) (init= 0.6497322)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, d)                      = -1.000
    C(alpha, d)                  =  1.000
    C(a, alpha)                  = -1.000
[[Value of the residual]]
0.038907169276
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.3319056677566663, 4.1193910378697831, 0.17386467083232507)


 Initial Guess

(0.047972817379432042, 0.24166515556623713, 0.77560776824961941)


 Parallel Config

[[Variables]]
    a:         0.89480691 +/- 3.78e+06 (422273986.25%) (init= 0.04797282)
    alpha:     0.89478259 +/- 3.76e+06 (420706213.05%) (init= 0.2416652)
```

```
    d:         0.85516153 +/- 1.04e+08 (12115447933.10%) (init= 0.7756078)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                    =   1.000
    C(alpha, d)                    =   0.234
    C(a, d)                        =   0.234
[[Value of the residual]]
2.91903275072
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.27216183761678003, 0.2571524993693064, -5.7629012673032776e-09)


 Serial Config

[[Variables]]
    a:         0.60171152 +/- 0          (0.00%) (init= 0.04797282)
    alpha:     0.24166515 +/- 0          (0.00%) (init= 0.2416652)
    d:         0.01309986 +/- 0          (0.00%) (init= 0.7756078)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
2.99510463086e-06
[[Partial Derivatives with respect (a,alpha,d)]]
(1.822207537608439, 0.0, 1.0112610987162014)


 Mixed Config

[[Variables]]
    a:         0.04625772 +/- 4.64e-08 (0.00%) (init= 0.04797282)
    alpha:     0.04625772 +/- 4.64e-08 (0.00%) (init= 0.2416652)
    d:         0.65989346 +/- 2.19e-06 (0.00%) (init= 0.7756078)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                    =   1.000
    C(a, d)                        =   0.999
    C(alpha, d)                    =   0.999
[[Value of the residual]]
4.84596394973e+93
[[Partial Derivatives with respect to (a,alpha,d)]]
(-4.8459639497294368e+95, 1.2525661460615068e+108, 2.2988609600264858e+96)


 Initial Guess

(0.33562802923675084, 0.91997476060319328, 0.16059688133902905)


 Parallel Config
```

```
[[Variables]]
    a:        0.88387384 +/- 3.59e+04 (4066675.42%) (init= 0.335628)
    alpha:    0.89968846 +/- 2.62e+04 (2914411.83%) (init= 0.9)
    d:        0.88883945 +/- 1.98e+05 (22317944.88%) (init= 0.1605969)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                  =  1.000
    C(alpha, d)                  = -1.000
    C(a, d)                      = -1.000
[[Value of the residual]]
2.91918345737
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.070519990733064475, 1.0140510900559008, -0.0022028352989700295)


 Serial Config

[[Variables]]
    a:        0.52618872 +/- 0          (0.00%) (init= 0.335628)
    alpha:    0.90000000 +/- 0          (0.00%) (init= 0.9)
    d:        0.09423858 +/- 0          (0.00%) (init= 0.1605969)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
2.99495279964e-06
[[Partial Derivatives with respect (a,alpha,d)]]
(0.51171310026309658, 0.0, 0.97224404116468821)


 Mixed Config

[[Variables]]
    a:        0.54119137 +/- 938.6039 (173432.91%) (init= 0.335628)
    alpha:    0.01027907 +/- 18.16012 (176670.81%) (init= 0.9)
    d:        0.08831535 +/- 603.6527 (683519.55%) (init= 0.1605969)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, d)                      = -1.000
    C(alpha, d)                  =  1.000
    C(a, alpha)                  = -1.000
[[Value of the residual]]
0.0501068716534
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.29377188821619393, 4.7756616050475902, 0.53463872904203757)


 Initial Guess

(0.14516215836077739, 0.062094628411814456, 0.49840307812174844)
```

```
 Parallel Config

[[Variables]]
    a:          0.10505868 +/- 8.44e+04 (80319664.84%) (init= 0.1451622)
    alpha:      0.10505867 +/- 8.44e+04 (80327783.93%) (init= 0.06209463)
    d:          0.81104012 +/- 1.93e+05 (23769298.86%) (init= 0.4984031)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                     =  1.000
    C(a, d)                         = -0.695
    C(alpha, d)                     = -0.695
[[Value of the residual]]
2.91903275015
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.24907687560293823, 0.25987017420714409, -1.7763568394002505e-13)


 Serial Config

[[Variables]]
    a:          0.46061340 +/- 0          (0.00%) (init= 0.1451622)
    alpha:      0.06209462 +/- 0          (0.00%) (init= 0.06209463)
    d:          0.08696876 +/- 0          (0.00%) (init= 0.4984031)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
2.99495281787e-06
[[Partial Derivatives with respect (a,alpha,d)]]
(0.56616448716806, 0.0, 0.97561586933612576)


 Mixed Config

[[Variables]]
    a:          0.59458876 +/- 20.84641 (3506.02%) (init= 0.1451622)
    alpha:      0.01000000 +/- 0.349810 (3498.11%) (init= 0.06209463)
    d:          0.01000002 +/- 31.69183 (316917.54%) (init= 0.4984031)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, d)                         = -1.000
    C(alpha, d)                     = -1.000
    C(a, alpha)                     =  1.000
[[Value of the residual]]
0.0389071609683
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.33191218859979499, 4.1193920782833775, 0.1738680179154968)
```

```
 Initial Guess

(0.54560832845147234, 0.18598231926019237, 0.21940050831925306)


 Parallel Config

[[Variables]]
    a:        0.89968986 +/- 4.25e+05 (47224523.54%) (init= 0.5456083)
    alpha:    0.89968030 +/- 4.52e+05 (50236666.66%) (init= 0.1859823)
    d:        0.84700162 +/- 1.25e+07 (1478842621.77%) (init= 0.2194005)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                  =  1.000
    C(alpha, d)                  =  0.107
    C(a, d)                      =  0.107
[[Value of the residual]]
2.91903275258
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.28083214935961109, 0.2662082327611337, -9.3853813609712233e-10)


 Serial Config

[[Variables]]
    a:        0.50483084 +/- 0          (0.00%) (init= 0.5456083)
    alpha:    0.18598231 +/- 0          (0.00%) (init= 0.1859823)
    d:        0.09980368 +/- 0          (0.00%) (init= 0.2194005)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
2.9949527994e-06
[[Partial Derivatives with respect (a,alpha,d)]]
(0.16066078062406658, 0.0, 0.96967867936454455)


 Mixed Config

[[Variables]]
    a:        0.59458872 +/- 0.879105 (147.85%) (init= 0.5456083)
    alpha:    0.01000000 +/- 0.001720 (17.21%) (init= 0.1859823)
    d:        0.01000000 +/- 0.817409 (8174.10%) (init= 0.2194005)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, d)                      = -1.000
    C(alpha, d)                  =  0.998
    C(a, alpha)                  = -0.998
[[Value of the residual]]
0.0389071606731
```

```
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.33190873035081819, 4.1193908554301935, 0.17386596090336048)
```

We can notice that the parallel configuration is not the best again, because of the value of the residuals for the 5 random initial guesses are $r \geq 2$ with partial derivatives very close to $\vec{0}$.

In this case the serial configuration fits the best to the serial time series with residual values of the order of 10^{-6}, candidate to be local minimum being $(a^\star, d^\star) = (0.52, 0.09)$ and partial derivatives close to $\vec{0}$. After that, the mixed configuration is the second best fit, with residual values of the order of 10^{-2}, candidate to be local minimum $(a^\star, \alpha^\star, d^\star) = (0.59, 0.01, 0.01)$ with partial derivatives near to $\vec{0}$. The values found are almost the same that the value found for the first input signal. We have to emphasize the fact that the candidate to be local minimum for the mixed configuration is such that the value of $\alpha \approx 0$, and as we said before when $\alpha = 0$ in the equations for the mixed dynamics, we get the serial dynamics.

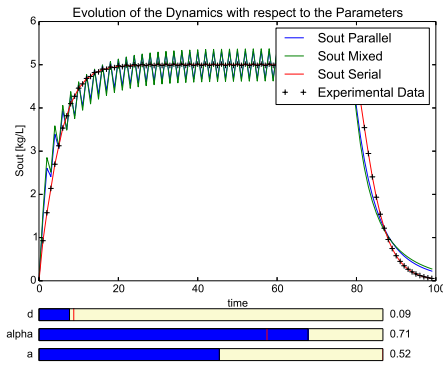This situation is illustrated in the following figures

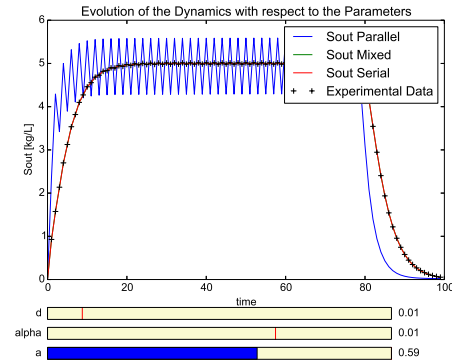Figure 20: Local Minimum at (0.52, 0.09) Serial Configuration

Figure 21: Local Minimum at (0.59, 0.01, 0.01) Parallel Configuration

5.3 Mixed Experimental Data

We generate data in this configuration with parameters $(a, \alpha, d) = (0.7, 0.6, 0.1)$. If we consider again 5 random initial guesses we obtain the following results

```
Initial Guess

(0.24731536882756289, 0.73016632608760612, 0.027155181981844967)

Parallel Config
```

```
[[Variables]]
    a:         0.05269855 +/- 1.55e+04 (29319789.25%) (init= 0.2473154)
    alpha:     0.05269854 +/- 1.55e+04 (29325581.21%) (init= 0.7301663)
    d:         0.02605377 +/- 1.58e+05 (607784293.85%) (init= 0.02715518)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                  =  1.000
    C(alpha, d)                  =  0.536
    C(a, d)                      =  0.536
[[Value of the residual]]
0.509752927101
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.74193317553217231, 0.80759080775214542, 4.4408920985006262e-14)


 Serial Config

[[Variables]]
    a:         0.89999999 +/- 0          (0.00%) (init= 0.2473154)
    alpha:     0.73016632 +/- 0          (0.00%) (init= 0.7301663)
    d:         0.89999997 +/- 0          (0.00%) (init= 0.02715518)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
1.23111698721
[[Partial Derivatives with respect (a,alpha,d)]]
(72.749333386623064, 0.0, -0.26383333990189772)


 Mixed Config

[[Variables]]
    a:         0.72253938 +/- 1.875185 (259.53%) (init= 0.2473154)
    alpha:     0.61931943 +/- 1.607301 (259.53%) (init= 0.7301663)
    d:         0.09782245 +/- 0.361963 (370.02%) (init= 0.02715518)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                  =  1.000
    C(alpha, d)                  = -1.000
    C(a, d)                      = -1.000
[[Value of the residual]]
2.74022735312e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(3.7764692860304376, 4.6050022606742793, 0.38625457697539478)


 Initial Guess
```

(0.58091555914630755, 0.1784773238640156, 0.13632167239754367)

 Parallel Config

[[Variables]]
    a: 0.02832382 +/- 9.99e+03 (35278668.71%) (init= 0.5809156)
    alpha: 0.02832693 +/- 9.99e+03 (35257316.24%) (init= 0.1784773)
    d: 0.86259324 +/- 2.75e+04 (3186006.80%) (init= 0.1363217)
[[Correlations]] (unreported correlations are < 0.100)
    C(a, alpha)   = 1.000
    C(a, d)   = -0.599
    C(alpha, d)   = -0.594
[[Value of the residual]]
0.509752927229
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.4011172124653184, 245.11347236167973, 2.3313451169570953e-08)

 Serial Config

[[Variables]]
    a: 0.90000000 +/- 0   (0.00%) (init= 0.5809156)
    alpha: 0.17847732 +/- 0   (0.00%) (init= 0.1784773)
    d: 0.90000000 +/- 0   (0.00%) (init= 0.1363217)
[[Correlations]] (unreported correlations are < 0.100)
[[Value of the residual]]
1.23111698361
[[Partial Derivatives with respect (a,alpha,d)]]
(72.749651922132472, 0.0, -0.26383323486267596)

 Mixed Config

[[Variables]]
    a: 0.84484810 +/- 0.215281 (25.48%) (init= 0.5809156)
    alpha: 0.72415547 +/- 0.184526 (25.48%) (init= 0.1784773)
    d: 0.01008133 +/- 0.267246 (2650.90%) (init= 0.1363217)
[[Correlations]] (unreported correlations are < 0.100)
    C(a, alpha)   = 1.000
    C(alpha, d)   = -1.000
    C(a, d)   = -1.000
[[Value of the residual]]
2.74023324234e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(2.7621883739898636, 3.6794771693499824, 0.58817029799383735)

```
 Initial Guess

(0.21365604761835966, 0.046561239810539057, 0.87601156867141305)

 Parallel Config

[[Variables]]
    a:         0.16757179 +/- 2.01e+04 (11983249.22%) (init= 0.213656)
    alpha:     0.16758851 +/- 2.01e+04 (11980235.82%) (init= 0.04656124)
    d:         0.89985501 +/- 2.58e+03 (287047.37%) (init= 0.8760116)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                  =   1.000
    C(a, d)                      =  -0.514
    C(alpha, d)                  =  -0.513
[[Value of the residual]]
0.509752928634
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.17847758248055179, 0.18301379855369948, -2.0910162490395123e-09)

 Serial Config

[[Variables]]
    a:         0.90000000 +/- 0           (0.00%) (init= 0.213656)
    alpha:     0.04656123 +/- 0           (0.00%) (init= 0.04656124)
    d:         0.90000000 +/- 0           (0.00%) (init= 0.8760116)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
1.23111698362
[[Partial Derivatives with respect (a,alpha,d)]]
(72.749651766454889, 0.0, -0.26383323491678823)

 Mixed Config

[[Variables]]
    a:         0.84486233 +/- 0.980364 (116.04%) (init= 0.213656)
    alpha:     0.72416766 +/- 0.840312 (116.04%) (init= 0.04656124)
    d:         0.01006364 +/- 1.217159 (12094.62%) (init= 0.8760116)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                  =   1.000
    C(alpha, d)                  =  -1.000
    C(a, d)                      =  -1.000
[[Value of the residual]]
```

```
2.74022736906e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(2.7620914083324251, 3.6793656347928492, 0.5882115889333599)

 Initial Guess

(0.74525062311904178, 0.053823604379000245, 0.57290349697215681)

 Parallel Config

[[Variables]]
    a:         0.12498469 +/- 1.38e+06 (1107200032.95%) (init= 0.7452506)
    alpha:     0.12498457 +/- 1.40e+06 (1121662909.99%) (init= 0.0538236)
    d:         0.45012898 +/- 1.70e+07 (3785119392.95%) (init= 0.5729035)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                      =  1.000
    C(a, d)                          =  0.493
    C(alpha, d)                      =  0.492
[[Value of the residual]]
0.509752927101
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.26328711803800253, 0.26998809725448103, -2.7755575615628914e-13)

 Serial Config

[[Variables]]
    a:         0.89999999 +/- 0          (0.00%) (init= 0.7452506)
    alpha:     0.05382360 +/- 0          (0.00%) (init= 0.0538236)
    d:         0.89999988 +/- 0          (0.00%) (init= 0.5729035)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
1.23111698366
[[Partial Derivatives with respect (a,alpha,d)]]
(72.749009490677508, 0.0, -0.26383346318699097)

 Mixed Config

[[Variables]]
    a:         0.61001138 +/- 1.634672 (267.97%) (init= 0.7452506)
    alpha:     0.52286686 +/- 1.401148 (267.97%) (init= 0.0538236)
    d:         0.06529415 +/- 1.260819 (1930.98%) (init= 0.5729035)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                         =  1.000
```

```
    C(a, d)                          =   1.000
    C(alpha, d)                      =   1.000
[[Value of the residual]]
2.74022733953e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(4.8280686076140773, 5.6011914688922264, 0.32590186082696609)


 Initial Guess

(0.18528200894722269, 0.3025050300461819, 0.61307201528385524)


 Parallel Config

[[Variables]]
    a:        0.42781256 +/- 1.28e+05 (30032081.22%) (init= 0.185282)
    alpha:    0.42781426 +/- 1.27e+05 (29771574.81%) (init= 0.302505)
    d:        0.02792362 +/- 1.82e+05 (651526830.24%) (init= 0.613072)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, alpha)                      =   1.000
    C(alpha, d)                      =   0.567
    C(a, d)                          =   0.566
[[Value of the residual]]
0.509752927152
[[Partial Derivatives with respect to (a,alpha,d)]]
(0.17774744590088876, 0.17843711385574501, -2.1260770921571748e-11)


 Serial Config

[[Variables]]
    a:        0.07186989 +/- 0          (0.00%) (init= 0.185282)
    alpha:    0.30250503 +/- 0          (0.00%) (init= 0.302505)
    d:        0.22213834 +/- 0          (0.00%) (init= 0.613072)
[[Correlations]] (unreported correlations are <  0.100)
[[Value of the residual]]
1.21509017112
[[Partial Derivatives with respect (a,alpha,d)]]
(10.288708285695613, 0.0, 0.049473406369959783)


 Mixed Config

[[Variables]]
    a:        0.78648038 +/- 1.211010 (153.98%) (init= 0.185282)
    alpha:    0.67412599 +/- 1.038014 (153.98%) (init= 0.302505)
```

```
    d:         0.06794748 +/- 0.897648 (1321.09%) (init= 0.613072)
[[Correlations]] (unreported correlations are <  0.100)
    C(a,  alpha)                      =  1.000
    C(alpha, d)                       = -1.000
    C(a, d)                           = -1.000
[[Value of the residual]]
2.74022734082e-06
[[Partial Derivatives with respect to (a,alpha,d)]]
(3.2280513857940187, 4.1189940714924678, 0.46038940637596187)
```

In this case, we have that the configuration that best fits the time series is the mixed config-uration with residual values of the order of 10^{-6} and the candidate to be local minimum being (0.72, 0.61, 0.097) and then the parallel configuration with residual values of the order of 10^{-1} and candidate to be local minimum (0.427, 0.427, 0.027) and partial derivatives near to $\vec{0}$. The serial configuration is not good to approximate the mixed configuration because for this 5 random initia guesses we have that $r \geq 1$ with partial derivatives near to $\vec{0}$.
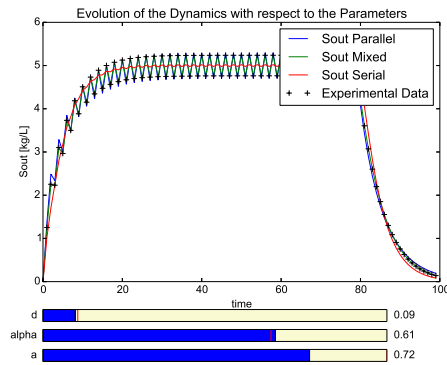
We show this results in the following pictures

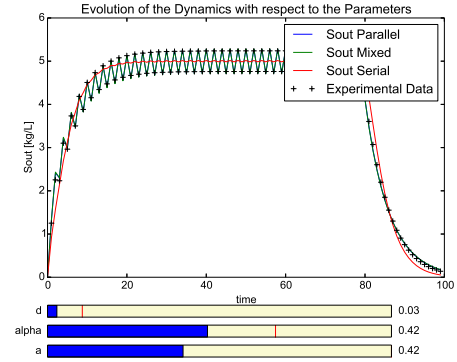Figure 22: Local Minimum at (0.72, 0.61, 0.097) Mixed Cnfiguration

Figure 23: Local Minimum at (0.427, 0.427, 0.027) Parallel Con-figuration

6   Conclusions

Through the results of the previous sections, we have seen the behaviour of the results for the fitting process for data generated as time series by the three different configurations of two tanks, succesfully obtaining the original configuration. For this, we implemented in **python** a discretization of the corresponding ODE systems, and then used the **lmfit** package (as well as other mathematical and computational tools).

It is relevant to emphasize the importance of the Input Signal to be able to identify what kind of configuration is better than other to fit to the given data. In the case of the mixed time series this fact is clearer, because with the first input signal, the serial configuration could be a good approximation to the data, but with the second input signal we have seen that this is not the case, because the value of the residual for the 5 random initial guesses is large ($r \geq 1$).

It is also relevant to emphasize that for the parameter d and for certain value of the parameters a and α, even though we supposed that $d \in (0, +\infty)$, we could see numerically that if $d*$ is too large with respect to the parameter d taken to generate the time series, the solutions of the ODE systems goes far from the experimental data, which means that any tuple in the form (a, α, d) with $d >> d^*$ drives the solutions to diverge from the experimental data. This result, could be interesting to be explored in the future in order to improve the fitting method, specially concerning to the algorithms used to minimize the residuals.

The following images show the situation when d is larger than the value for which the time series is generated. In these cases, $d = 0.1$.
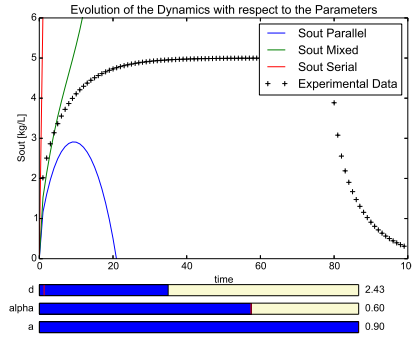

Figure 24: Values of the parameters for which the solutions of the ODE escape from Parallel Data
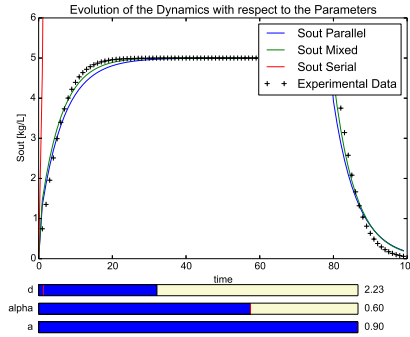

Figure 25: Values of the parameters for which the solutions of the ODE escape from Serial Data
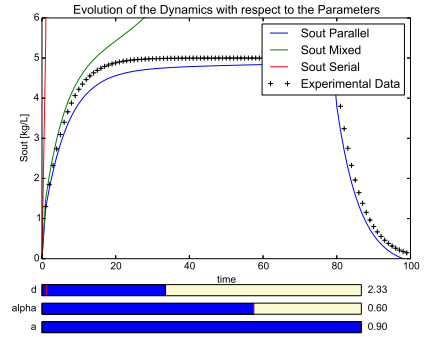

Figure 26: Values of the parameters for which the solutions of the ODE escape from Mixed Data

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