Parameter estimation using multiparametric programming for implicit Euler's method based discretization

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ABSTRACT

This work presents a study that aims to compare two discretization methods for solving parameter estimation using multiparametric programming. In our earlier work, parameter estimation using multiparametric programming was presented where model parameters were obtained as an explicit function of measurements. In this method, the nonlinear ordinary equations (ODEs) model was discretized by using explicit Euler's method to obtain algebraic

equations. Then, a square system of parametric nonlinear algebraic equations was obtained by formulating optimality condition. These equations were then solved symbolically to obtain model parameters as an explicit function of measurements. Thus, the online computation burden of solving optimization problems for parameter estimation is replaced by simple function evaluations. In this work, we use implicit Euler's method for discretization of nonlinear ODEs model and compare with the explicit Euler's method for parameter estimation using multiparametric programming. Complexity of explicit parametric functions, accuracy of parameter estimates and effect of step size are discussed.

1. INTRODUCTION

In process systems, the accuracy of parameter estimates is important for the development of mathematical models and requires reliable parameter estimation techniques. In these models, ordinary differential equations (ODEs) or differential-algebraic equations (DAEs) are widely used to describe the processes. Most commonly used parameter estimation techniques involve solving an optimization problem for minimization of the sum of squared differences between the measurements and the model predictions. Parameter estimation is also used in fault detection (Jiang et al., 2008, Isermann, 1993, Huang, 2001, Garatti and Bittanti, 2012, Park and Himmelblau, 1983, Pouliezos et al., 1989). The principle involved in parameter estimation based fault detection is that the specific parameters of the model can be associated with faults. For example, heat transfer coefficient in heat exchanger model can be related to fouling (Delmotte et al., 2013), cross section of outlet holes related to the tank leakage (Johansson, 2000) and specific growth rate, half saturation coefficient and inhibition coefficient which affect the respiration rate in the wastewater treatment (Wimberger and Verde, 2008). With this assumption, parameters of a system are estimated on-line repeatedly using well known parameter estimation methods. If there is a discrepancy between the estimated parameters and the 'true' parameters, it gives an indication of faults. An overview for fault detection using parameter estimation can be found in (Venkatasubramanian et al., 2003, Hwang et al., 2010).

Parameter estimation of the nonlinear ODE system, requires solving a dynamic optimization problem, where the optimization is difficult due to the presence of nonconvexities (Vassiliadis, 1994, Papamichail and Adjiman, 2002, Papamichail and Adjiman, 2004, Sakizlis et al., 2003). Several approaches for parameter estimation have been presented and can be categorized as decomposition and sequential / simultaneous approaches. In the decomposition method, the direct integration of ODEs model is not required and the parameter estimation is solved in two steps. Firstly to fit the experimental data and secondly solve the optimization problem to minimize the difference between estimates of the derivatives obtained from fitted model and the derivatives evaluated from the equations in the given ODEs model at the experimental data points. Varah (1982) has developed a parameter estimation technique where they fitted the measurement data using splines method. Principal differential analysis (PDA) has been extended to nonlinear ODEs and improved by repeating the two steps, introducing iterated PDA (iPDA) to overcome the issues of precision (Poyton et al., 2006, Varziri et al., 2008). Dua (2011) has proposed a method using artificial neural network (ANN) model to fit the data and utilized differential derivatives of ANN approximation to estimate the parameters of nonlinear ODE systems. Least squares support vector machines (LV-SVM) (Mehrkanoon et al., 2014) and two stage (TS) method (Chang et al., 2015, Chang et al., 2016) are other proposed methods for parameter estimation involving fitting the data and solving the optimization problem. In Bhagwat et al. (2003), nonlinear process is decomposed into multiple local-linear regimes using a multi-linear model-based fault detection approach.

The parameter estimates which explicitly require theintegral of ODEs model can be categorized as sequential and simultaneous approach. In the sequential approach (Hwang and Seinfeld, 1972, Kim et al., 1991, Bilardello et al., 1993), the optimization problem is solved separately from numerical solution of ODEs model whilst in the simultaneous approach, the optimization problem of parameter estimation is solved together with differential equations model which is converted into algebraic equations (Chen et al., 2016, De et al., 2013). A collocation approaches for parameter estimation has been demonstrate in (Chen et al., 2016, Villadsen, 1982, Tjoa and Biegler, 1991) and ANN implementation is used in Dua and Dua (2011) for simultaneous parameter estimation.

However, the above mentioned approaches are computationally expensive and may not converge in a reasonable time. Hence, a multiparametric programming approach was proposed to overcome these limitations by obtaining model parameters as an explicit function of measurements in our earlier work (Che Mid and Dua, 2017). Multiparametric programming provides the optimization variables as an explicit function of the parameter (Dua and Pistikopoulos, 1999, Pistikopoulos, 2009, Oberdieck et al., 2016, Pistikopoulos et al., 2007b, Pistikopoulos et al., 2007a, Charitopoulos and Dua, 2016). In that work, the model parameters were considered as optimization variables and the measurements as the parameters in the context of multiparametric programming. The nonlinear ODEs model was discretized to obtain algebraic equation using explicit Euler's method. Then, a square system was formulated by writing the Karush-Kuhn-Tucker (KKT) conditions and the symbolic solution of model parameters as an explicit function of measurements is obtained. Thus, the computational burden of online parameter estimation problem is replaced by computing the model parameters as an explicit function of measurement.

In this work, for the discretization of nonlinear ODEs we use implicit Euler's method instead of the explicit Euler's method. The explicit Euler's method has simple calculations per time step, which are relatively easier to implement and the implicit method on the other hand is relatively more difficult, which makes it computationally intensive. However, the advantages of the implicit method include that it is usually more numerically stable for solving stiff differential equations and provides more accurate approximate solution (Acary and Brogliato, 2009, Acary and Brogliato, 2010, Benko et al., 2009, Hasan et al., 2014, Koch et al., 2000, Sun et al., 2014). Once the nonlinear ODEs are converted to the algebraic equations using implicit Euler's method, then the model parameters will be obtained as an explicit function of measurements. The rest of this paper is organized as follows: Section 2 presents the parameter estimation algorithm using multiparametric programming and in Section 3, three examples are presents to illustrate the proposed works. Concluding remarks are presents in Section 4.

2. PROBLEM STATEMENT AND SOLUTION APPROACH

2.1. Problem definition

The objective of the fault detection problem is to estimate the model parameters, $\mathbf{\Theta}$, such that the error, ε_{FD}, between the measurements, $\hat{x}_j(t_i)$, and model predicted values of state variables, $x_j(t_i)$, is minimised as follows follows (Dua and Dua, 2011):

Problem 1:

$$\varepsilon_{PE} = \min_{\boldsymbol{\theta},\mathbf{x}(t)} \sum_{j\in J} \sum_{i\in I} \left\{ \hat{x}_j(t_i) - x_j(t_i) \right\}^2 \tag{1}$$

Subject to:

$$\frac{dx_j(t)}{dt} = f_j\left(\mathbf{x}(t),\mathbf{u}(t),\boldsymbol{\theta},t\right),\ \ j \in J \tag{2}$$

$$x_j(t=0) = x_j^0,\ j \in J \tag{3}$$

$$t \in [0,t_f] \tag{4}$$

where $\mathbf{x}(t_i)$ is the J-dimensional vector of state variables in the given ODE system, $\hat{x}_j(t_i)$ represents the measurements of the state variables at the time points, t_i, $\mathbf{u}(t)$ is the vector of control variables and $\boldsymbol{\theta}$ is the vector of parameters.

2.2. Discretization of Ordinary Differential Equations

In this work, we propose an implicit Euler's method to discretize nonlinear ODEs to algebraic equations. Consider the ODE initial value problem where Equations (2) to (3) are to be solved on the interval, $t \in [0,t_f]$, thus the discretization of an ODE model using an implicit Euler's method is given by

$$x_j(i+1) = x_j(i) + \Delta t f_j\left(\mathbf{x}(i+1),\mathbf{u}(i),\boldsymbol{\theta}\right), i \in I\ ,\ j \in J \tag{5}$$

where step size is given by Δt .

2.3. Parameter Estimation using Multiparametric Programming

The algorithm to obtain the model parameters as an explicit function of measurements using multiparametric programming is summarized as below:

(i) Formulate the optimization in Problem 1 as a Nonlinear Programming (NLP) problem.

Problem 2:

$$\varepsilon_{MPP} = \min_{\boldsymbol{\theta},\mathbf{x}(i)} \sum_{j\in J}\sum_{i\in I}\left\{\hat{x}_j(i+1) - x_j(i+1)\right\}^2 \tag{6}$$

Subject to:

$$h_j = x_j(i+1) - x_j(i) - \Delta t f_j\left(\mathbf{x}(i+1), \mathbf{u}(i), \boldsymbol{\theta}\right) = 0, i \in I, j \in J \tag{7}$$

$$x_j(0) = x_j^0, j \in J \tag{8}$$

where h_j represents the set of nonlinear algebraic equations obtained by discretizing the ODEs given by Equation (5) and we consider $I = \{0,1\}$ in this work.

(ii) Formulate Karush-Kuhn-Tucker (KKT) conditions for Problem 2. The Lagrangian function is given by

$$L = g + \sum_{j\in J}\lambda_j h_j \tag{9}$$

where

$$g = \sum_{j\in J}\sum_{i\in I}\left\{\hat{x}_j(i+1) - x_j(i+1)\right\}^2 \tag{10}$$

$$h_j = 0, j \in J \tag{11}$$

and λ_j represents the Lagrange multipliers. The KKT conditions are given by the Equality Constraints as follows

$$\nabla_{\boldsymbol{\theta}} L = \nabla_{\boldsymbol{\theta}} g + \nabla_{\boldsymbol{\theta}} \sum \lambda_j h_j = 0, j \in J \tag{12}$$

$$h_j = 0 \tag{13}$$

(iii) Solve the Equality Constrains in Equations (12) and (13) of the KKT conditions parametrically using a symbolic solution technique to obtain Lagrange multiples. The model parameters, $\boldsymbol{\theta}$, as a function of measurements, $\hat{\mathbf{x}}$, i.e., $\boldsymbol{\theta}(\hat{\mathbf{x}})$ are obtained. For systems involving simultaneous polynomial equations techniques, such as Groebner Basis can be used for obtaining symbolic solution using software such as Mathematica. Note that for the case $I = \{0,1\}$ considered in this work, the initial conditions ($i = 0$) would be given and the state variables at $i = 1$ can be eliminated by using equation (11). Therefore, $\mathbf{x}$ and $\boldsymbol{\theta}$ appear as optimisation variables in (1) and (6) but $\mathbf{x}$ can be eliminated using (11) and the gradient of L is obtained only with respect to $\boldsymbol{\theta}$ as shown in (12).

(iv) Screen the solutions obtained in the previous step and ignore solutions with imaginary parts.

(v) Calculate the estimated model parameters, $\boldsymbol{\theta}$, using the measurements, $\hat{\mathbf{x}}$, by simple evaluation of $\boldsymbol{\theta}(\hat{\mathbf{x}})$.

3. ILLUSTRATIVE EXAMPLES

We present three examples using both the implicit and explicit Euler's methods for discretizing the nonlinear ODEs for parameter estimation using multiparametric programming. The comparison results are described next.

3.1. Example 1: Irreversible Liquid–phase Reaction of the First Order

Consider the following first-order irreversible chain reactions (Dua, 2011, Esposito and Floudas, 2000, Dua and Dua, 2011) :

$$A \xrightarrow{\theta_1} B \xrightarrow{\theta_2} C$$

where the nonlinear ODE model is described by two differential equations given by:

$$\frac{dx_1}{dt} = -\theta_1 x_1 \tag{14}$$

$$\frac{dx_2}{dt} = \theta_1 x_1 - \theta_2 x_2 \tag{15}$$

where x_1 and x_2 are concentrations of A and B respectively and θ_1 and θ_2 are the rate constant parameters. The objective of parameter estimation is to solve the following problem:

Problem 3:

$$\varepsilon_{PE} = \min_{\theta_1, \theta_2} \sum_{i \in I} \left\{ (\hat{x}_1(t_i) - x_1(t_i))^2 + (\hat{x}_2(t_i) - x_2(t_i))^2 \right\} \tag{16}$$

Subject to:

Equations (14) - (15)

where the estimates of model parameters, θ_1 and θ_2, are obtained by minimizing the sum of squares of the differences between measurements and model predicted values.

3.1.1. Discretization of Ordinary Differential Equations

The nonlinear ODE model in Equations (14) and (15) is discretized using both the implicit and explicit Euler's methods and reformulated as the following algebraic equations:

<u>Implicit Euler's method:</u>

$$x_1(i+1) = \frac{x_1(i)}{1+\Delta t\theta_1} \tag{17}$$

$$x_2(i+1) = \frac{\Delta t\theta_1 x_1(i+1) + x_2(i)}{1+\Delta t\theta_2} \tag{18}$$

<u>Explicit Euler's method:</u>

$$x_1(i+1) = x_1(i) - \Delta t\theta_1 x_1(i) \tag{19}$$

$$x_2(i+1) = x_2(i) + \Delta t\theta_1 x_1(i) - \Delta t\theta_2 x_2(i) \tag{20}$$

3.1.2. Parameter Estimation Problem

The parameter estimation problem is reformulated as the following NLP problem for both the discretization methods to estimate the model parameters, θ_1 and θ_2, such that the error, ε_{MPP}, between the measurement of state variables, $\hat{x}_i(i+1)$, and model predicted value of state variables, $x_i(i+1)$, is minimized. Problem 4 describes the parameter estimation problem using the implicit Euler's method for discretization of ODEs (Equations 17 and 18) as follows:

Problem 4:

$$\varepsilon_{MPP} = \min_{\theta_1,\theta_2} \sum_{i\in I} \left\{ (\hat{x}_1(i+1) - x_1(i+1))^2 + (\hat{x}_2(i+1) - x_2(i+1))^2 \right\} \tag{21}$$

Subject to:

$$h_1 = x_1(i+1) - \frac{x_1(i)}{1+\Delta t\theta_1} = 0 \tag{22}$$

$$h_2 = x_2(i+1) - \frac{\Delta t\theta_1 x_1(i+1) + x_2(i)}{1+\Delta t\theta_2} = 0 \tag{23}$$

Equations (22) and (23) are substituted into Equation (21) to obtain:

$$g = \left(\hat{x}_1(i+1) - \frac{x_1(i)}{1+\Delta t\theta_1} \right)^2 + \left(\hat{x}_2(i+1) - \frac{\Delta t\theta_1 x_1(i+1) + x_2(i)}{1+\Delta t\theta_2} \right)^2 \tag{24}$$

The gradients of g with respect to θ_1 and θ_2 are given by:

$$\begin{aligned} \frac{\partial g}{\theta_1} &= (2\Delta t\ x_1(i)(-(x_1(i)/(1+\Delta t\theta_1)) + \hat{x}_1(i+1)))/(1+\Delta t\theta_1)^2 - (2(-((\Delta t^2\theta_1\ x_1(i))/ \\ &(1+\Delta t\theta_1)^2) + (\Delta t\ x_1(i))/(1+\Delta t\theta_1))(-(((\Delta t\theta_1\ x_1(i))/(1+\Delta t\theta_1) + x_2(i))/ \\ &(1+\Delta t\theta_2)) + \hat{x}_2(i+1)))/(1+\Delta t\theta_2) \\ &= 0 \end{aligned} \tag{25}$$

$$\frac{\partial g}{\theta_2} = (2\Delta t((\Delta t\theta_1 x_1(i))/(1+\Delta t\theta_1) + x_2(i))(-(((\Delta t\theta_1 x_1(i))/(1+\Delta t\theta_1) + x_2(i))/ \\ (1+\Delta t\theta_2)) + \hat{x}_2(i+1)))/(1+\Delta t\theta_1)^2 \\ = 0 \tag{26}$$

Equality Constraints in Equations (25) and (26) are solved analytically in Mathematica, and the solution for Example 1 with discretization using **implicit Euler's method** is given by

Solution 1:

$$\theta_1 = -\frac{x_2(i)}{\Delta t\,(x_1(i) + x_2(i))};\theta_2 = \frac{-x_1(i) + \hat{x}_1(i+1) - x_2(i) - \hat{x}_2(i+1)}{\Delta t\,(x_1(i) - \hat{x}_1(i+1) + x_2(i))} \tag{27}$$

Solution 2:

$$\theta_1 = \frac{x_1(i) - \hat{x}_1(i+1)}{\Delta \text{t}\,\hat{x}_1(i+1)};\theta_2 = \frac{x_1(i) - \hat{x}_1(i+1) + x_2(i) - \hat{x}_2(i+1)}{\Delta \text{t}\,\hat{x}_2(i+1)} \tag{28}$$

The discretization of nonlinear ODEs using implicit Euler's method for parameter estimation using multiparametric programming provides the parameter estimates as given by solutions 1 and 2. Considering the positive values of model parameters in this example, $\theta_1 \geq 0$ and $\theta_2 \geq 0$; solution 1 is ignored because it implies that the concentration of B, $x_2(i)$ is negative, which is not true. Hence, model parameters are evaluated using solution 2. Next, we provide the NLP problem formulation using explicit Euler's method as given in Equations (19) and (20).

Problem 5:

$$\varepsilon_{MPP} = \min_{\theta_1,\theta_2} \sum_{i \in I} \{(\hat{x}_1(i+1) - x_1(i+1))^2 + (\hat{x}_2(i+1) - x_2(i+1))^2\} \tag{21}$$

Subject to:

$$h_1 = x_1(i+1) - x_1(i) + \Delta t\theta_1 x_1(i) = 0 \tag{29}$$

$$h_2 = x_2(i+1) - x_2(i) - \Delta t\theta_1 x_1(i) + \Delta t\theta_2 x_2(i) = 0 \tag{30}$$

Equations (29) and (30) are substituted into Equation (21) to obtain:

$$g = (\hat{x}_1(i+1) - x_1(i) + \Delta t \theta_1 x_1(i))^2 + ((\hat{x}_2(i+1) - x_2(i) - \Delta t \theta_1 x_1(i) + \Delta t \theta_2 x_2(i))^2 \tag{31}$$

The gradients of g with respect to θ_1 and θ_2 are given by

$$\begin{aligned}\frac{\partial g}{\partial \theta_1} &= 2\Delta t x_1(i)(-x_1(i) + \Delta t \theta_1 x_1(i) + \hat{x}_1(i+1)) - 2\Delta t x_1(i)(-\Delta t \theta_1 x_1(i) - x_2(i) + \\ &\quad \Delta t \theta_2 x_2(i) + \hat{x}_2(i+1)) \\ &= 0\end{aligned} \tag{32}$$

$$\begin{aligned}\frac{\partial g}{\partial \theta_2} &= 2\, \Delta t\, x_2(i)\, (-\Delta t\, \theta_1\, x_1(i) - x_2(i) + \Delta t\, \theta_2\, x_2(i) + \hat{x}_2(i+1)) \\ &= 0\end{aligned} \tag{33}$$

Equality Constraints in Equations (32) and (33) are solved analytically in Mathematica, and the solution of parameter estimation with discretization using **explicit Euler's method** is given by

$$\theta_1 = -\frac{-x_1(i) + \hat{x}_1(i+1)}{\Delta t\, x_1(i)}; \ \theta_2 = -\frac{-x_1(i) + \hat{x}_1(i) - x_2(i) + \hat{x}_2(i+1)}{\Delta t\, x_2(i)} \tag{34}$$

Next, a comparison between solution in Equation (28) and Equation (34) is carried out for analyzing the accuracy of parameter estimates and effect of step size.

3.1.3. Results for Example 1

In this example, three different step size are used to estimate model parameters. The simulated data for state variables profile, x_1 and x_2, is generated at $t = t_i$ with initial values given by $x_1(0) = 1$ and $x_2(0) = 0$. The model parameters, θ_1 and θ_2, obtained in Equations (28) and (34) are calculated and compared for effectiveness and accuracy between the two discretization methods of ODEs. The comparison of model parameters for different step size, $\Delta t = [0.10, 0.05, 0.01]$ is shown in Figures 1 and 2 for θ_1 and θ_2, respectively. From these figures, we can see that for the smallest step size, $\Delta t = 0.01$, the estimated model parameters, θ_1

and θ_2 are close to the actual true values of the model parameters ($\hat{\theta}_1 = 5$ and $\hat{\theta}_2 = 1$). Table 1 shows that percentage error (%) of the implicit Euler's method is smaller than that obtained by explicit Euler method for $\Delta t = 0.01$. This figure indicates that the present method provides better results than that obtained by explicit Euler method. (Note: The time (t_i) in Table 1 only show the selected time for the purpose of presenting the percentage error results).

3.2. Example 2: Lotka–Volterra model

Consider the following Lotka–Volterra model (Dua, 2011, Dua and Dua, 2011, Esposito and Floudas, 2000) where the nonlinear ODE model is model is described by two differential equations:

$$\frac{dx_1}{dt} = \theta_1 x_1 (1 - x_2) \tag{35}$$

$$\frac{dx_2}{dt} = \theta_2 x_2 (x_1 - 1) \tag{36}$$

where θ_1 and θ_2 are the model parameters to be estimated. The objective of parameter estimation is to solve the following problem:

Problem 6:

$$\varepsilon_{PE} = \min_{\theta_1, \theta_2} \sum_{i \in I} \left\{ (\hat{x}_1(t_i) - x_1(t_i))^2 + (\hat{x}_2(t_i) - x_2(t_i))^2 \right\} \tag{37}$$

Subject to:

Equations (35)-(36)

where the parameters, θ_1 and θ_2 must be estimated such that the error, ε_{PE} between measurements and model predicted values is minimized.

3.2.1. Discretization of Ordinary Differential Equations

The nonlinear ODE model in Equations (35) and (36) is discretized using implicit and explicit Euler's methods and reformulated as the following algebraic equations:

<u>Implicit Euler's method:</u>

$$x_1(i+1) = \frac{x_1(i)}{1 - \Delta t\theta_1 + \Delta t\theta_1 x_2(i+1)} \tag{38}$$

$$x_2(i+1) = \frac{x_2(i)}{-1 - \Delta t\theta_2 + \Delta t\theta_2 x_1(i+1)} \tag{39}$$

<u>Explicit Euler's method:</u>

$$x_1(i+1) = x_1(i) + \Delta t\theta_1 x_1(i) - \Delta t\theta_1 x_1(i) x_2(i) \tag{40}$$

$$x_2(i+1) = x_2(i) - \Delta t\theta_2 x_2(i) + \Delta t\theta_2 x_1(i) x_2(i) \tag{41}$$

3.2.2. Parameter Estimation Problem

The parameter estimation problem is formulated as the following NLP problem such that the error, ε_{MPP}, between the measurement of state variables, $\hat{x}_i(i+1)$ and model predicted value of state variables, $x_i(i+1)$ is minimized to estimate model parameters, θ_1 and θ_2. Problem 7 is the parameter estimation problem using proposed discretization of an ODE using implicit Euler's method given in Equations (38) and (39).

Problem 7:

$$\varepsilon_{MPP} = \min_{\theta_1,\theta_2} \sum_{i \in I} \left\{ (\hat{x}_1(i+1) - x_1(i+1))^2 + (\hat{x}_2(i+1) - x_2(i+1))^2 \right\} \tag{42}$$

Subject to:

$$h_1 = x_1(i+1) - \frac{x_1(i)}{1 - \Delta t\theta_1 + \Delta t\theta_1 x_2(i+1)} = 0 \tag{43}$$

$$h_2 = x_2(i+1) - \frac{x_2(i)}{-1 - \Delta t\theta_2 + \Delta t\theta_2 x_1(i+1)} = 0 \tag{44}$$

The Equations (43) and (44) are substituted into Equation (42) to obtain:

$$\begin{aligned} g = {} & (\hat{x}_1(i+1) - x_1(i)/(1 - \Delta t\theta_1 + \Delta t\theta_1 x_2(i+1)))^2 + ((\hat{x}_2(i+1) - x_2(i)/ \\ & (-1 - \Delta t\theta_2 + \Delta t\theta_2 (x_1(i)/(1 - \Delta t\theta_1 + \Delta t\theta_1 x_2(i+1)))))^2 \end{aligned} \tag{45}$$

The gradients of g with respect to θ_1 and θ_2 are given by:

$$\begin{aligned} \frac{\partial g}{\theta_1} = {} & (2x_1(i)(-\Delta t + \Delta t x_2(i+1))(\hat{x}_1(i+1) - x_1(i)/(1 - \Delta t\theta_1 + \Delta t\theta_1 x_2(i+1))))/ \\ & (1 - \Delta t\theta_1 + \Delta t\theta_1 x_2(i+1))^2 + (2\Delta t\theta_2 x_1(i) x_2(i)(-\Delta t + \Delta t x_2(i+1))(\hat{x}_2(i+1) + \\ & x_2(i)/(-1 - \Delta t\theta_2 + (\Delta t\theta_2 x_1(i))/(1 - \Delta t\theta_1 + \Delta t\theta_1 x_2(i+1)))))/((1 - \Delta t\theta_1 + \\ & \Delta t\theta_1 x_2(i+1))^2 (-1 - \Delta t\theta_2 + (\Delta t\theta_2 x_1(i))/(1 - \Delta t\theta_1 + \Delta t\theta_1 x_2(i+1)))^2) \\ = {} & 0 \end{aligned} \tag{46}$$

$$\begin{aligned} \frac{\partial g}{\theta_2} = {} & -((2x_2(i)(-\Delta t + (\Delta t\ x_1(i))/(1 - \Delta t\theta_1 + \Delta t\theta_1 x_2(i+1)))(\hat{x}_2(i+1) + x_2(i)/ \\ & (-1 - \Delta t\theta_2 + (\Delta t\theta_2 x_1(i))/(1 - \Delta t\theta_1 + \Delta t\theta_1 x_2(i+1)))))/(-1 - \Delta t\theta_2 + \\ & (\Delta t\theta_2 x_1(i))/(1 - \Delta t\theta_1 + \Delta t\theta_1 x_2(i+1)))^2) \\ = {} & 0 \end{aligned} \tag{47}$$

Equality Constrains in Equations (46) and (47) are solved analytically in Mathematica, and the solution for Example 2 with discretization **using implicit Euler's method** is given by

Solution 1:

$$\theta_1 = \frac{-1-x_1(i)}{\Delta t\,(-1+x_2(i+1))}\,;\theta_2 = \frac{-1+\hat{x}_1(i+1)}{\Delta t x_2(i)\,(x_2(i)-\hat{x}_2(i+1))} \tag{48}$$

Solution 2:

$$\theta_1 = \frac{x_1(i)-\hat{x}_1(i+1)}{\Delta \mathrm{t}\;\hat{x}_1(i+1)(-1+x_2(i+1))}\,;\theta_2 = \frac{-x_2(i)+\hat{x}_2(i+1)}{\Delta \mathrm{t}\;(-1+\hat{x}_1(i+1))\;\hat{x}_2(i+1)} \tag{49}$$

The solution for Example 2 using implicit Euler's method gives two set of model parameters as explicit function of measurements as given in solutions 1 and solution 2. Considering the positive values of model parameters in this example, $\theta_1 \geq 0$ and $\theta_2 \geq 0$, the solution 1 is ignored because it implies that the concentrations of A, $x_1(i)$ is negative which is not true. Hence, model parameters are evaluated using solution 2. Next, we describe the similar NLP problem using explicit Euler's method.

Problem 8 describes the parameter estimation problem using explicit Euler's method for discretization of ODEs given in Equations (40) and (41), as follows:

Problem 8:

$$\varepsilon_{MPP} = \min_{\theta_1,\theta_2} \sum_{i\in I} \{(\hat{x}_1(i+1)-x_1(i+1))^2 + (\hat{x}_2(i+1)-x_2(i+1))^2\} \tag{42}$$

Subject to:

$$h_1 = x_1(i+1) - x_1(i) - \Delta t\theta_1 x_1(i) + \Delta t\theta_1 x_1(i)x_2(i) = 0 \tag{50}$$

$$h_2 = x_2(i+1) - x_2(i) + \Delta t\theta_2 x_2(i) - \Delta t\theta_2 x_1(i)x_2(i) = 0 \tag{51}$$

The Equations (50) and (51) are substituted into Equation (42) to obtain:

$$g = (\hat{x}_1(i+1) - x_1(i) - \Delta t\theta_1 x_1(i) + \Delta t\theta_1 x_1(i)x_2(i))^2 + (\hat{x}_2(i+1) - x_2(i) + \Delta t\theta_2 x_2(i) - \Delta t\theta_2 x_1(i)x_2(i))^2 \quad (52)$$

The gradients of g with respect to θ_1 and θ_2 are given by:

$$\frac{\partial g}{\partial \theta_1} = 2(-\Delta t x_1(i) + \Delta t x_1(i)x_2(i))(-x_1(i) - \Delta t\theta_1 x_1(i) + \hat{x}_1(i+1) + \Delta t\,\theta_1 x_1(i)x_2(i)) = 0 \quad (53)$$

$$\frac{\partial g}{\theta_2} = 2(\Delta t x_2(i) - \Delta t x_1(i)x_2(i))(-x_2(i) + \Delta t\theta_2 x_2(i) - \Delta t\theta_2 x_1(i)x_2(i) + \hat{x}_2(i+1)) = 0 \quad (54)$$

Equality Constrains in Equations (53) and (54) are solved analytically in Mathematica, and the solution for Example 2 with discretization using **explicit Euler's method** is given by

$$\theta_1 = \frac{x_1(i) - \hat{x}_1(i+1)}{\Delta t\, x_1(i)(-1 + x_2(i))};\ \theta_2 = \frac{-x_2(i) + \hat{x}_2(i+1)}{\Delta t(-1 + x_1(i))x_2(i)} \quad (55)$$

Next, a comparison between solution from Equation (49) and Equation (55) is carried out for investigating accuracy of parameter estimates and effect of step size

3.2.3. Results for Example 2

In Example 2, the simulated data for state variables profile, x_1 and x_2, is generated at $t = t_i$ with initial values given by $x_1(0) = 1.2$ and $x_2(0) = 1.1$. The model parameters are estimated using the explicit function as given in Equations (49) and (55). Three different step size are used to estimate model parameters, $\Delta t = [0.10, 0.05, 0.01]$. The estimated model parameters, θ_1 and θ_2, for different step size, Δt are shown in Figures 3 and 4. As the step size decreased, the estimated model parameter values for θ_1 and θ_2 become closer to the true values of the model parameters ($\hat{\theta}_1 = 3$ and $\hat{\theta}_2 = 1$). Table 2 shows that percentage error of the implicit Euler's method is smaller than that obtained by explicit Euler methods for $\Delta t = 0.01$. Thus, the discretization using implicit Euler's method gave more accurate model parameters estimates as compared to explicit Euler's method. (Note: The time (t_i) in Table 2 only show the selected time for the purpose of presenting the percentage error results)

3.3. Example 3: Single-stage evaporator system

A mathematical model of a single-stage evaporator system (Dalle Molle and Himmelblau, 1987) is given as :

$$\frac{dW}{dt} = F - \left(\delta W + E_c\right) - V \tag{56}$$

$$\frac{dT}{dt} = \frac{\beta F x_F + (V - F)(T - T_B)}{W} \tag{57}$$

where

$$V = \left(\frac{UA(T_S - T) - FC_p(T - T_F) - Q_L}{\Delta H_V}\right) \tag{58}$$

Here, W and T are the state variables representing the holdup and temperature, respectively, and the model parameters for this process system are heat transfer coefficient, UA, and composition of feed, x_F. Also, V is the vapor flow rate from the evaporator, F is the feed flow rate, T_S is the steam temperature, T_B is the temperature for normal boiling point of the solvent, T_F is the temperature of the feed system, C_p is the heat capacity of the solution, Q_L is the rate of heat loss to the surroundings, and ΔH_V is the heat of vaporization of the solvent.

The objective of parameter estimation is to solve the following problem:

Problem 9:

$$\varepsilon_{PE} = \min_{UA, x_f} \sum_{i \in I} \{(\hat{W}(t_i) - W(t_i))^2 + (\hat{T}(t_i) - T(t_i))^2\} \quad (59)$$

Subject to:

Equations (56)-(58)

where the parameters, UA and x_F, must be estimated such that the error, ε_{PE} between measurements and model predicted values is minimized.

3.3.1. Discretization of Ordinary Differential Equations

The nonlinear ODE model in Equations (56) to (58) is discretized using implicit and explicit Euler's methods and reformulated as the following algebraic equations:

<u>Implicit Euler's method:</u>

$$W(i+1) = (-(F - E_c - ((UA(T_S - T(i+1) - FC_p(T(i+1) - T_F) - Q_L) / \Delta H_V)\Delta t - W(i)) / (-\delta \Delta t - 1) \quad (60)$$

$$T(i+1) = \frac{1}{2}\frac{1}{\Delta t(C_pF+UA)}(C_pFT_B\Delta t - C_pFT_F\Delta t - F\Delta H_V\Delta t + T_BUA\Delta t +$$
$$T_SUA\Delta t - Q_L\Delta t - \Delta H_V W(i+1) - (C_p^2F^2T_B^2\Delta t^2 - 2C_p^2F^2T_BT_F\Delta t^2 +$$
$$C_p^2F^2T_F^2\Delta t^2 + 4C_pF^2\beta\Delta H_V\Delta t^2 x_F + 2C_pF^2T_B\Delta H_V\Delta t^2 -$$
$$2C_pF^2T_F\Delta H_V\Delta t^2 + 2C_pFT_B^2UA\Delta t^2 - 2C_pFT_BT_FUA\Delta t^2 -$$
$$2C_pFT_BT_SUA\Delta t^2 + 2C_pFT_FT_SUA\Delta t^2 + 4FUA\beta\Delta H_V\Delta t^2 x_F +$$
$$2C_pFQ_LT_B\Delta t^2 - 2C_pFQ_LT_F\Delta t^2 + 4C_pFT(i)W(i+1)\Delta H_V\Delta t -$$
$$2C_pFT_BW(i+1)\Delta H_V\Delta t - 2C_pFT_FW(i+1)\Delta H_V\Delta t + F^2\Delta H_V{}^2\Delta t^2 +$$
$$2FT_BUA\Delta H_V\Delta t^2 + 2FT_SUA\Delta H_V\Delta t^2 + T_B{}^2UA^2\Delta t^2 - 2T_BT_SUA^2\Delta t^2 -$$
$$T_S{}^2UA^2\Delta t^2 + 2FQ_L\Delta H_V\Delta t^2 + 2FW(i+1)\Delta H_V{}^2\Delta t + 2Q_LT_BUA\Delta t^2 -$$
$$2Q_LT_SUA\Delta t^2 + 4T(i)UAW(i+1)\Delta H_V\Delta t - 2T_BUAW(i+1)\Delta H_V\Delta t -$$
$$2T_SUAW(i+1)\Delta H_V\Delta t + Q_L{}^2\Delta t^2 + 2Q_LW(i+1)\Delta H_V\Delta t +$$
$$W(i+1)^2\Delta H_V{}^2)^{1/2}) \tag{61}$$

<u>Explicit Euler's method:</u>

$$W(i+1) = W(i) + \Delta t(F - (\delta W(i) + E_c) - ((UA(T_S - T(i)) - FC_p(T(i) - T_F) - Q_L)/\Delta H_V)) \tag{62}$$

$$T(i+1) = T(i) + \Delta t(\beta F x_F + (((UA(T_S - T(i)) - FC_p(T(i) - T_F) - Q_L)/\Delta H_V) -$$
$$F)(T(i) - T_B)/W(i)) \tag{63}$$

3.3.2. Parameter Estimation Problem

The parameter estimation problem is formulated as the following NLP problem such that the error, ε_{MPP}, between the measurement of state variables, $\hat{W}(i+1)$ and $\hat{T}(i+1)$, and model predicted value of state variables, $W(i+1)$ and $T(i+1)$, is minimized to estimate model parameters, UA and x_F. Problem 10 is the parameter estimation problem using proposed discretization of an ODE using implicit Euler's method given in Equations (60) and (61).

Problem 10:

$$\varepsilon_{MPP} = \min_{UA, x_f} \sum_{i \in I} \{(\hat{W}(i+1) - W(i+1))^2 + (\hat{T}(i+1) - T(i+1))^2\} \tag{64}$$

Subject to:

$$\begin{aligned} h_1 &= W(i+1) - (-(F - E_c - ((UA(T_S - T(i+1) - FC_p(T(i+1) - T_F) - Q_L) / \Delta H_V)\Delta t - W(i)) / \\ &\quad (-\delta\Delta t - 1) \\ &= 0 \end{aligned} \tag{65}$$

$$\begin{aligned} h_2 &= T(i+1) - (\frac{1}{2}\frac{1}{\Delta t(C_p F + UA)}(C_p F T_B \Delta t - C_p F T_F \Delta t - F\Delta H_V \Delta t + T_B UA\Delta t + T_S UA\Delta t - \\ &\quad Q_L \Delta t - \Delta H_V W(i+1) - (C_p^2 F^2 T_B^2 \Delta t^2 - 2C_p^2 F^2 T_B T_F \Delta t^2 + C_p^2 F^2 T_F^2 \Delta t^2 + \\ &\quad 4C_p F^2 \beta \Delta H_V \Delta t^2 x_F + 2C_p F^2 T_B \Delta H_V \Delta t^2 - 2C_p F^2 T_F \Delta H_V \Delta t^2 + 2C_p F T_B^2 UA\Delta t^2 - \\ &\quad 2C_p F T_B T_F UA\Delta t^2 - 2C_p F T_B T_S UA\Delta t^2 + 2C_p F T_F T_S UA\Delta t^2 + 4FUA\beta\Delta H_V \Delta t^2 x_F + \\ &\quad 2C_p F Q_L T_B \Delta t^2 - 2C_p F Q_L T_F \Delta t^2 + 4C_p F T(i) W(i+1)\Delta H_V \Delta t - 2C_p F T_B W(i+1)\Delta H_V \Delta t - \\ &\quad 2C_p F T_F W(i+1)\Delta H_V \Delta t + F^2 \Delta H_V{}^2 \Delta t^2 + 2FT_B UA\Delta H_V \Delta t^2 + 2FT_S UA\Delta H_V \Delta t^2 + T_B{}^2 UA^2 \Delta t^2 - \\ &\quad 2T_B T_S UA^2 \Delta t^2 - T_S{}^2 UA^2 \Delta t^2 + 2FQ_L \Delta H_V \Delta t^2 + 2FW(i+1)\Delta H_V{}^2 \Delta t + 2Q_L T_B UA\Delta t^2 - \\ &\quad 2Q_L T_S UA\Delta t^2 + 4T(i) UAW(i+1)\Delta H_V \Delta t - 2T_B UAW(i+1)\Delta H_V \Delta t - 2T_S UAW(i+1)\Delta H_V \Delta t + \\ &\quad Q_L{}^2 \Delta t^2 + 2Q_L W(i+1)\Delta H_V \Delta t + W(i+1)^2 \Delta H_V{}^2)^{1/2})) \\ &= 0 \end{aligned} \tag{66}$$

The Equations (65) and (66) are substituted into Equation (64) to obtain:

$$
\begin{aligned}
g = {} & (\hat{W}(i+1) - ((-(F - E_c - ((UA(T_S - T(i+1) - FC_p(T(i+1) - T_F) - Q_L)/\Delta H_V)\Delta t - \\
& W(i))/(-\delta\Delta t - 1)))^2 + (\hat{T}(i+1) - (\frac{1}{2}\frac{1}{\Delta t(C_p F + UA)}(C_p F T_B \Delta t - C_p F T_F \Delta t - F\Delta H_V \Delta t + \\
& T_B UA\Delta t + T_S UA\Delta t - Q_L \Delta t - \Delta H_V W(i+1) - (C_p^2 F^2 T_B^2 \Delta t^2 - 2C_p^2 F^2 T_B T_F \Delta t^2 + C_p^2 F^2 T_F^2 \Delta t^2 + \\
& 4C_p F^2 \beta \Delta H_V \Delta t^2 x_F + 2C_p F^2 T_B \Delta H_V \Delta t^2 - 2C_p F^2 T_F \Delta H_V \Delta t^2 + 2C_p F T_B^2 UA\Delta t^2 - \\
& 2C_p F T_B T_F UA\Delta t^2 - 2C_p F T_B T_S UA\Delta t^2 + 2C_p F T_F T_S UA\Delta t^2 + 4FUA\beta\Delta H_V \Delta t^2 x_F + \\
& 2C_p F Q_L T_B \Delta t^2 - 2C_p F Q_L T_F \Delta t^2 + 4C_p F T(i) W(i+1)\Delta H_V \Delta t - 2C_p F T_B W(i+1)\Delta H_V \Delta t - \\
& 2C_p F T_F W(i+1)\Delta H_V \Delta t + F^2 \Delta H_V{}^2 \Delta t^2 + 2FT_B UA\Delta H_V \Delta t^2 + 2FT_S UA\Delta H_V \Delta t^2 + T_B{}^2 UA^2 \Delta t^2 - \\
& 2T_B T_S UA^2 \Delta t^2 - T_S{}^2 UA^2 \Delta t^2 + 2FQ_L \Delta H_V \Delta t^2 + 2FW(i+1)\Delta H_V{}^2 \Delta t + 2Q_L T_B UA\Delta t^2 - \\
& 2Q_L T_S UA\Delta t^2 + 4T(i) UAW(i+1)\Delta H_V \Delta t - 2T_B UAW(i+1)\Delta H_V \Delta t - 2T_S UAW(i+1)\Delta H_V \Delta t + \\
& Q_L{}^2 \Delta t^2 + 2Q_L W(i+1)\Delta H_V \Delta t + W(i+1)^2 \Delta H_V{}^2)^{1/2})))^2
\end{aligned}
\qquad (67)
$$

The gradients of g with respect to UA and x_F are given by:

$$
\begin{aligned}
\frac{\partial g}{UA} = & -(1/2)T_B\Delta t + T_S\Delta t - (1/2)(2C_PFT_B{}^2\Delta t^2 - 2C_PFT_BT_F\Delta t^2 - 2C_PFT_BT_S\Delta t^2 + \\
& 2C_PFT_FT_S\Delta t^2 + 4F\beta\Delta H_V\Delta t^2 x_F + 2FT_B\Delta H_V\Delta t^2 - 2FT_S\Delta H_V\Delta t^2 + 2T_B{}^2UA\Delta t^2 - \\
& 4T_BT_SUA\Delta t^2 + 2T_S{}^2UA\Delta t^2 + 2Q_LT_B\Delta t^2 - 2Q_LT_S\Delta t^2 + 4T(i)W(i+1)\Delta H_V\Delta t - \\
& 2T_BW(i+1)\Delta H_V\Delta t - 2T_SW(i+1)\Delta H_V\Delta t)/sqrt(C_P{}^2F^2T_B{}^2\Delta t^2 - 2C_P{}^2F^2T_BT_F\Delta t^2 + \\
& C_P{}^2F^2T_F{}^2\Delta t^2 + 4C_PF^2\beta\Delta H_V\Delta t^2 x_F + 2C_PF^2T_B\Delta H_V\Delta t^2 - 2C_PF^2T_F\Delta H_V\Delta t^2 + \\
& 2C_PFT_B{}^2UA\Delta t^2 - 2C_PFT_BT_FUA\Delta t^2 - 2C_PFT_BT_SUA\Delta t^2 + 2C_PFT_FT_SUA\Delta t^2 + \\
& 4FUA\beta\Delta H_V\Delta t^2 x_F + 2C_PFQ_LT_B\Delta t^2 - 2C_PFQ_LT_F\Delta t^2 + 4C_PFT(i)W(i+1)\Delta H_V\Delta t - \\
& 2C_PFT_BW(i+1)\Delta H_V\Delta t - 2C_PFT_FW(i+1)\Delta H_V\Delta t + F^2\Delta H_V{}^2\Delta t^2 + 2FT_BUA\Delta H_V\Delta t^2 - \\
& 2FT_SUA\Delta H_V\Delta t^2 + T_B{}^2UA^2\Delta t^2 - 2T_BT_SUA^2\Delta t^2 + T_S{}^2UA^2\Delta t^2 + 2FQ_L\Delta H_V\Delta t^2 + \\
& 2FW(i+1)\Delta H_V{}^2\Delta t + 2Q_LT_BUA\Delta t^2 - 2Q_LT_SUA*\Delta t^2 + 4T(i)UAW(i+1)\Delta H_V\Delta t - \\
& 2T_BUAW(i+1)\Delta H_V\Delta t - 2T_SUAW(i+1)\Delta H_V\Delta t + Q_L{}^2\Delta t^2 + Q_LW(i+1)\Delta H_V\Delta t + \\
& W(i+1)^2\Delta H_V{}^2))/(\Delta t(C_PF + UA)) + (1/2)(C_PFT_B\Delta t + C_PFT_F\Delta t - F\Delta H_V\Delta t + \\
& T_BUA\Delta t + T_SUA\Delta t - Q_L\Delta t - \Delta H_VW(i+1) - sqrt(C_P{}^2F^2T_B{}^2\Delta t^2 - 2C_P{}^2F^2T_BT_F\Delta t^2 + \\
& C_P{}^2F^2T_F{}^2\Delta t^2 + 4C_PF^2\beta\Delta H_V\Delta t^2 x_F + 2C_PF^2T_B\Delta H_V\Delta t^2 - 2C_PF^2T_F\Delta H_V\Delta t^2 + \\
& 2C_PFT_B{}^2UA\Delta t^2 - 2C_PFT_BT_FUA\Delta t^2 - 2C_PFT_BT_SUA\Delta t^2 + 2C_PFT_FT_SUA\Delta t^2 + \\
& 4FUA\beta\Delta H_V\Delta t^2 x_F + 2C_PFQ_LT_B\Delta t^2 - 2C_PFQ_LT_F\Delta t^2 + 4C_PFTW(i+1)\Delta H_V\Delta t - \\
& 2C_PFT_BW(i+1)\Delta H_V\Delta t - 2C_PFT_FW(i+1)\Delta H_V\Delta t + F^2\Delta H_V{}^2\Delta t^2 + 2FT_BUA\Delta H_V\Delta t^2 - \\
& 2FT_SUA\Delta H_V\Delta t^2 + T_B{}^2UA^2\Delta t^2 - 2T_BT_SUA^2\Delta t^2 + T_S{}^2UA^2\Delta t^2 + 2FQ_L\Delta H_V\Delta t^2 + \\
& 2FW(i+1)\Delta H_V{}^2\Delta t + 2Q_LT_BUA\Delta t^2 - 2Q_LTsUA\Delta t^2 + 4T(i)UAW(i+1)\Delta H_V\Delta t - \\
& 2T_BUAW(i+)\Delta H_V\Delta t - 2T_SUAW(i+1)\Delta H_V\Delta t + Q_L{}^2\Delta t^2 + 2Q_LW(i+1)\Delta H_V\Delta t + \\
& W(i+1)^2\Delta H_V{}^2))/(\Delta t(C_PF + UA)^2) \\
= & \ 0
\end{aligned} \qquad (68)
$$

$$
\begin{aligned}
\frac{\partial g}{x_F} &= (1/2)(\hat{T}(i+1) - (1/2)(C_P F T_B \Delta t + C_P F T_F \Delta t - F\Delta H_V \Delta t + T_B UA\Delta t + T_S UA\Delta t - \\
&Q_L \Delta t - \Delta H_V W(i+1) - sqrt(C_P{}^2 F^2 T_B{}^2 \Delta t^2 - 2C_P{}^2 F^2 T_B T_F \Delta t^2 + C_P{}^2 F^2 T_F{}^2 \Delta t^2 + \\
&4C_P F^2 \beta \Delta H_V \Delta t^2 x_F + 2C_P F^2 T_B \Delta H_V \Delta t^2 - 2C_P F^2 T_F \Delta H_V \Delta t^2 + 2C_P F T_B{}^2 UA\Delta t^2 - \\
&2C_P F T_B T_F UA\Delta t^2 - 2C_P F T_B T_S UA\Delta t^2 + 2C_P F T_F T_S UA\Delta t^2 + 4FUA\beta \Delta H_V \Delta t^2 x_F + \\
&2C_P F Q_L T_B \Delta t^2 - 2C_P F Q_L T_F \Delta t^2 + 4C_P F T(i) W(i+1) \Delta H_V \Delta t - 2C_P F T_B W(i+1) \Delta H_V \Delta t - \\
&2C_P F T_F W(i+1) \Delta H_V \Delta t + F^2 \Delta H_V{}^2 \Delta t^2 + 2F T_B UA\Delta H_V \Delta t^2 - 2F T_S UA\Delta H_V \Delta t^2 + \\
&T_B{}^2 UA^2 \Delta t^2 - 2T_B T_S UA^2 \Delta t^2 + T_S{}^2 UA^2 \Delta t^2 + 2FQ_L \Delta H_V \Delta t^2 + 2FW(i+1)\Delta H_V{}^2 \Delta t + \\
&2Q_L T_B UA\Delta t^2 - 2Q_L T_S UA\Delta t^2 + 4T(i) UAW(i+1)\Delta H_V \Delta t - 2T_B UAW(i+1)\Delta H_V \Delta t - \\
&2T_S UAW(i+1)\Delta H_V \Delta t + Q_L{}^2 \Delta t^2 + 2Q_L W(i+1)\Delta H_V \Delta t + W(i+1)^2 \Delta H_V{}^2)) / \\
&(\Delta t(C_P F + UA)))(4C_P F^2 \beta \Delta H_V \Delta t^2 + 4FUA\beta \Delta H_V \Delta t^2) / (sqrt(C_P{}^2 F^2 T_B{}^2 \Delta t^2 - \\
&2C_P{}^2 F^2 T_B T_F \Delta t^2 + C_P{}^2 F^2 T_F{}^2 \Delta t^2 + 4C_P F^2 \beta \Delta H_V \Delta t^2 x_F + 2C_P F^2 T_B \Delta H_V \Delta t^2 - \\
&2C_P F^2 T_F \Delta H_V \Delta t^2 + 2C_P F T_B{}^2 UA\Delta t^2 - 2C_P F T_B T_F UA\Delta t^2 - 2C_P F T_B T_S UA\Delta t^2 + \\
&2C_P F T_F T_S UA\Delta t^2 + 4FUA\beta \Delta H_V \Delta t^2 x_F + 2C_P F Q_L T_B \Delta t^2 - 2C_P F Q_L T_F \Delta t^2 + \\
&4C_P F T W(i+1)\Delta H_V \Delta t - 2C_P F T_B W(i+1)\Delta H_V \Delta t - 2C_P F T_F W(i+1)\Delta H_V \Delta t + \\
&F^2 \Delta H_V{}^2 \Delta t^2 + 2F T_B UA\Delta H_V \Delta t^2 - 2F T_S UA\Delta H_V \Delta t^2 + T_B{}^2 UA^2 \Delta t^2 - 2T_B T_S UA^2 \Delta t^2 + \\
&T_S{}^2 UA^2 \Delta t^2 + 2FQ_L \Delta H_V \Delta t^2 + 2FW(i+1)\Delta H_V{}^2 \Delta t + 2Q_L T_B UA\Delta t^2 - 2Q_L T_S UA\Delta t^2 + \\
&4T(i) UAW(i+1)\Delta H_V \Delta t - 2T_B UAW(i+1)\Delta H_V \Delta t - 2T_S UAW(i+1)\Delta H_V \Delta t + \\
&Q_L{}^2 \Delta t^2 + 2Q_L W(i+1)\Delta H_V \Delta t + W(i+1)^2 \Delta H_V{}^2)\Delta t(C_P F + UA)) \\
&= 0
\end{aligned}
\tag{69}
$$

Equality Constrains in Equations (68) and (69) are solved analytically in Mathematica, and the solution for Example 3 with discretization **using implicit Euler's method** is given by

$$\begin{aligned}UA = (&C_P F T_F \Delta t - C_P F T(i+1)\Delta t + \hat{W}(i+1)\Delta H_V \delta\Delta t + E_C \Delta H_V \Delta t - F\Delta H_V \Delta t - Ql\Delta t - \\ &W(i)\Delta H_V + \hat{W}(i+1)\Delta H_V)/(\Delta t(T(i+1) - T_S))\end{aligned} \tag{70}$$

$$\begin{aligned}x_F = -(&C_P F T_B T_F \hat{T}(i+1)\Delta t - C_P F T_B T_F T(i+1)\Delta t - C_P F T_B \hat{T}(i+1) T_S \Delta t + C_P F T_B T(i+1) T_S \Delta t - \\ &C_P F T_F \hat{T}(i+1)^2 \Delta t + C_P F T_F \hat{T}(i+1) T(i+1)\Delta t + C_P F \hat{T}(i+1)^2 T_S \Delta t - \\ &C_P F \hat{T}(i+1) T(i+1) T_S \Delta t + T_B \hat{T}(i+1)\hat{W}(i+1)\Delta H_V \delta\Delta t - T_B T_S \hat{W}(i+1)\Delta H_V \delta\Delta t - \\ &\hat{T}(i+1)^2 \hat{W}(i+1)\Delta H_V \delta\Delta t + \hat{T}(i+1) T_S \hat{W}(i+1)\Delta H_V \delta\Delta t + E_C T_B \hat{T}(i+1)\Delta H_V \Delta t - \\ &E_C T_B T_S \Delta H_V \Delta t - E_C \hat{T}(i+1)^2 \Delta H_V \Delta t + E_C \hat{T}(i+1) T_S \Delta H_V \Delta t - F T_B \hat{T}(i+1)\Delta H_V \Delta t + \\ &F T_B T(i+1)\Delta H_V \Delta t + F\hat{T}(i+1)^2 \Delta H_V \Delta t - F\hat{T}(i+1) T(i+1)\Delta H_V \Delta t - Q_L T_B \hat{T}(i+1)\Delta t + \\ &Q_L T_B T(i+1)\Delta t + Q_L \hat{T}(i+1)^2 \Delta t - Q_L \hat{T}(i+1) T(i+1)\Delta t + T(i) T(i+1) W(i+1)\Delta H_V - \\ &T(i) T_S W(i+1)\Delta H_V - T_B \hat{T}(i+1) W(i)\Delta H_V + T_B \hat{T}(i+1)\hat{W}(i+1)\Delta H_V + T_B T_S W(i)\Delta H_V - \\ &T_B T_S \hat{W}(i+1)\Delta H_V + \hat{T}(i+1)^2 W(i)\Delta H_V - \hat{T}(i+1)^2 \hat{W}(i+1)\Delta H_V - \\ &\hat{T}(i+1) T(i+1) W(i+1)\Delta H_V - \hat{T}(i+1) T_S W(i)\Delta H_V + \hat{T}(i+1) T_S \hat{W}(i+1)\Delta H_V + \\ &\hat{T}(i+1) T_S W(i+1)\Delta H_V)/((T(i+1) - T_S) F\beta\Delta H_V \Delta t)\end{aligned} \tag{71}$$

In (Che Mid and Dua, 2017), the explicit parametric model parameters for single-stage evaporator system with the discretization of ODEs model using **explicit Euler's method** is given as :

$$\begin{aligned}UA = -(&1/(\Delta t\,(T(i) - T_S)))(-\Delta H_V \Delta t E_c + \Delta H_V \Delta t F + \Delta t Q_L + C_P \Delta t F T(i) - C_P \Delta t F T_F + \\ &\Delta H_V W(i) - \delta\Delta H_V \Delta t W(i) - \Delta H_V \hat{W}(i+1))\end{aligned} \tag{72}$$

$$\begin{aligned}x_F = -(&1/(\beta\Delta t F))(-\Delta t E_c T(i) + \Delta t E_c T_B + 2T(i) W(i) - \delta\Delta t T(i) W(i) - T_B W(i) + \delta\Delta t T_B W(i) - \\ &\hat{T}(i+1) W(i) - T(i)\hat{W}(i+1) + T_B \hat{W}(i+1))\end{aligned} \tag{73}$$

The comparison between solutions from Equations (70) to (73) is carried out for investigating accuracy of parameter estimates and effect of step size.

3.3.3. Results for Example 3

The simulated data for state variables profile, $W(i)$ and $T(i)$, is generated at $t = t_i$ with initial values, $W(0) = 13.8$ kg and $T(0) = 107$ °C, and parameter values in Table 3 (Dalle Molle and Himmelblau, 1987). Two different step size are used to estimated model parameters, $\Delta t = [0.10, 0.05]$. The estimated model parameters, UA and x_F, are calculated using the explicit function as given in Equations (70) to (73) and shown in Figures 5 and 6. As the step size decreased to 0.05, the estimated model parameter values for UA and x_F become closer to the true values of the model parameters ($\hat{UA} = 40.548$ and $\hat{x}_F = 0.032$). Table 4 shows that percentage error of the implicit Euler's method is smaller than that obtained by explicit Euler methods for $\Delta t = 0.05$. Thus, the discretization using implicit Euler's method gave more accurate model parameters compared to explicit Euler's method where the estimated model parameters are close to the true values. (Note: The time (t_i) in Table 4 only show the selected time for the purpose of presenting the percentage error results).

4. CONCLUDING REMARKS

In this work, we proposed the discretization of the nonlinear ODEs using implicit Euler's method for implementing parameter estimation using multiparametric programming. An implementation of proposed method is demonstrated through three case studies. The results show that the implementation of multiparametric programming for parameter estimation successfully obtained model parameters as an explicit function of measurements. Differences in step size were investigated for effectiveness of the proposed method and a small step size gave values close to the true values of model parameters. The parametric expressions obtained for the implicit Euler's method were more complex than that obtained for the explicit Euler's method. However, compared with the explicit discretization, the implicit Euler's gave more accurate parameter estimates for the same step size.

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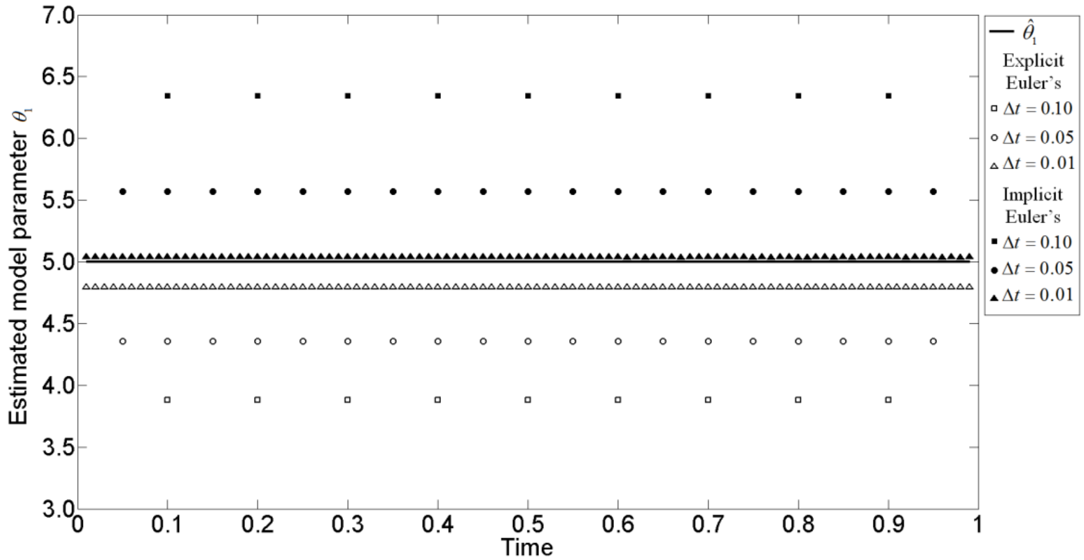

Figure 1. Estimated model parameter, θ_1, for different step size, Δt

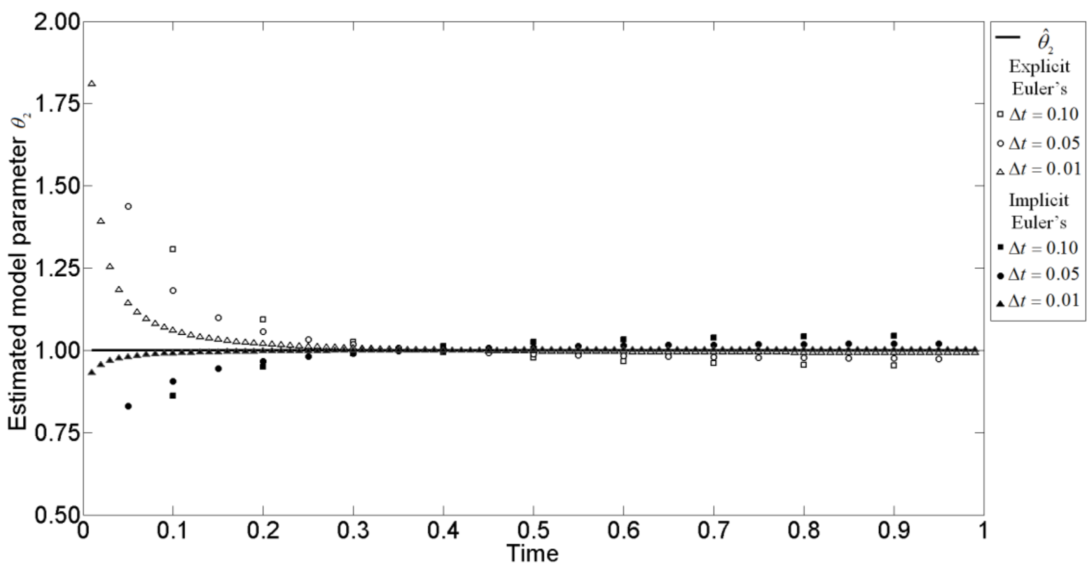

Figure 2. Estimated model parameter, θ_2, for different step size, Δt

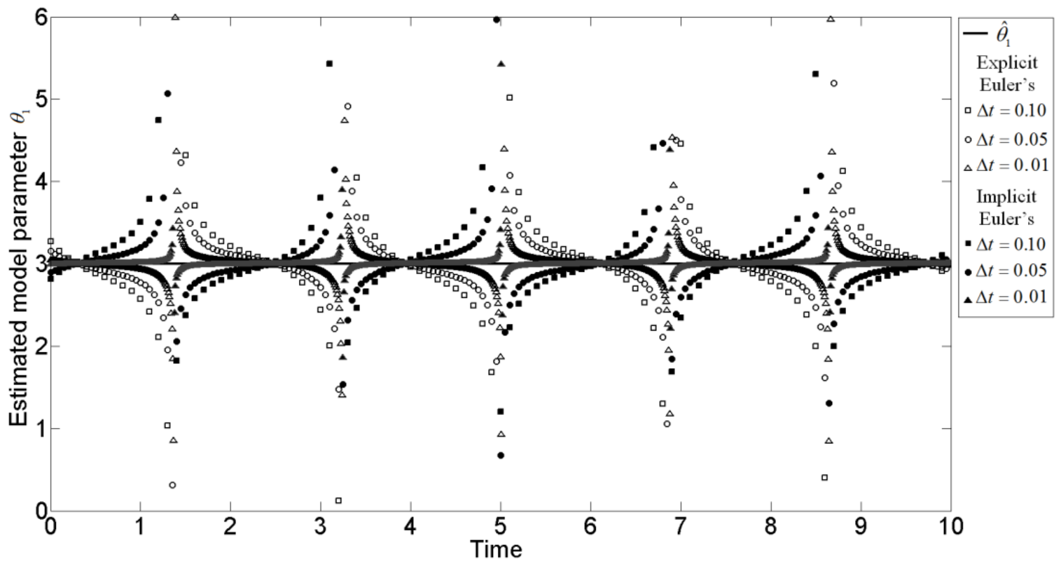

Figure 3. Estimated model parameter, θ_1, for different step size, Δt

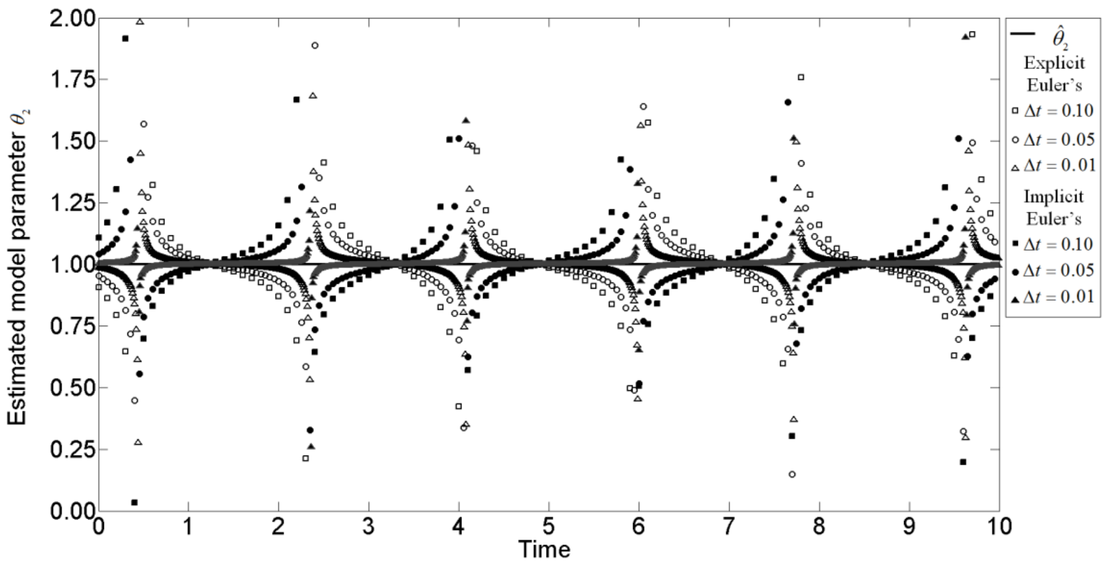

Figure 4. Estimated model parameter, θ_2, for different step size, Δt

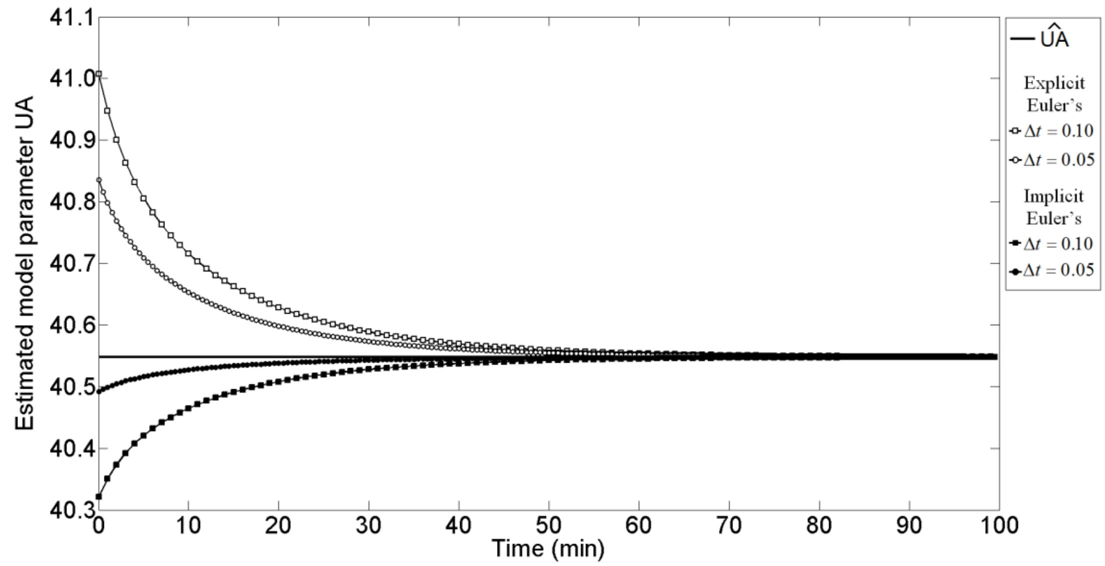

Figure 5. Estimated model parameter, UA for different step size, Δt

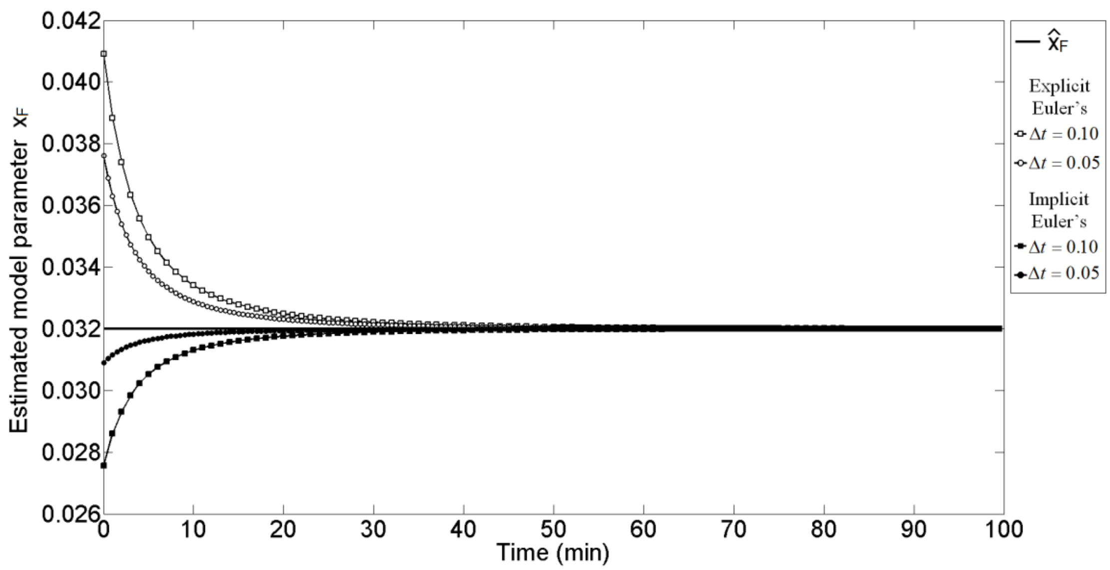

Figure 6. Estimated model parameter, x_F for different step size, Δt

Table 1. Comparison of the estimated model parameters, θ_1 and θ_2, for step size $\Delta t = 0.01$

Time (t_i)	Implicit Euler's Method				Explicit Euler's Method			
	Estimated model parameters		% Error		Estimated model parameters		% Error	
	θ_1	θ_2	θ_1	θ_2	θ_1	θ_2	θ_1	θ_2
0.10	5.03682	0.99098	0.7364	0.9020	4.79529	1.05976	4.0942	5.9760
0.20	5.03682	0.99714	0.7364	0.2860	4.79529	1.01915	4.0942	1.9150
0.30	5.03682	0.99921	0.7364	0.0790	4.79529	1.00628	4.0942	0.6280
0.40	5.03682	1.00019	0.7364	0.0190	4.79529	1.00030	4.0942	0.0300
0.50	5.03682	1.00073	0.7364	0.0730	4.79529	0.99706	4.0942	0.2940
0.60	5.03682	1.00105	0.7364	0.1050	4.79529	0.99514	4.0942	0.4860
0.70	5.03681	1.00125	0.7362	0.1250	4.79528	0.99394	4.0944	0.6060
0.80	5.03679	1.00138	0.7358	0.1380	4.79526	0.99318	4.0948	0.6820
0.90	5.03682	1.00146	0.7364	0.1460	4.79529	0.99269	4.0942	0.7310

Table 2. Comparison of the estimated model parameters, θ_1 and θ_2, for step size $\Delta t = 0.01$

Time (t_i)	Implicit Euler's Method				Explicit Euler's Method			
	Estimated model parameters		% Error		Estimated model parameters		% Error	
	θ_1	θ_2	θ_1	θ_2	θ_1	θ_2	θ_1	θ_2
0.00	2.99132	1.00291	0.289	0.291	3.04693	0.98652	1.564	1.348
0.01	2.99174	1.00303	0.275	0.303	3.04472	0.98593	1.491	1.407
0.02	2.99216	1.00316	0.261	0.316	3.04259	0.98531	1.420	1.469
0.03	2.99255	1.00329	0.248	0.329	3.04055	0.98468	1.352	1.532
0.04	2.99294	1.00342	0.235	0.342	3.03857	0.98403	1.286	1.597
0.05	2.99331	1.00356	0.223	0.356	3.03667	0.98335	1.222	1.665
0.06	2.99367	1.0037	0.211	0.370	3.03482	0.98265	1.161	1.735
0.07	2.99402	1.00385	0.199	0.385	3.03304	0.98192	1.101	1.808
0.08	2.99435	1.00401	0.188	0.401	3.03130	0.98116	1.043	1.884
0.09	2.99468	1.00417	0.177	0.417	3.02963	0.98037	0.988	1.963
0.10	2.99500	1.00434	0.167	0.434	3.02800	0.97955	0.933	2.045

Table 3. Model parameters for single-stage evaporator system

Parameter	Value	Description
U	43.6 kJ/(min m ˚C)	heat transfer coefficient
A	0.93 m^2	area of heat transfer
x_F	0.032 mass fraction	the composition of the feed
T_S	136 ˚C	the steam temperature in the steam chest
T_B	100 ˚C	normal boiling point of the solvent
C_p	4.18 kJ/(kg ˚C)	the heat capacity of the solution
T_F	88 ˚C	the temperature of the feed system
Q_L	400.0 kJ/min	the rate of heat loss to the surroundings
ΔH_V	2240 kJ/kg	the heat of vaporization of the solvent
β	8.33 ˚C	boiling point elevation per mass fraction of solute
δ	0.06 (kg/min)/kg holdup	constant
E_c	0.0454 kg/min	constant
F	2.27 kg/min	feed flow rate

Table 4. Comparison of the estimated model parameters, UA and x_F , for step size $\Delta t = 0.05$

Time (t_i)	Implicit Euler's Method				Explicit Euler's Method			
	Estimated model parameters		% Error		Estimated model parameters		% Error	
	UA	x_F	UA	x_F	UA	x_F	UA	x_F
0.00	40.4915	0.03089	0.138	3.416	40.8357	0.03761	0.704	17.296
0.50	40.4954	0.03103	0.129	2.983	40.8155	0.0369	0.655	15.095
1.00	40.4988	0.03115	0.120	2.623	40.7979	0.0363	0.612	13.276
1.50	40.5019	0.03125	0.113	2.323	40.7825	0.03581	0.575	11.754
2.00	40.5045	0.03133	0.107	2.069	40.7687	0.03539	0.541	10.471
2.50	40.507	0.0314	0.101	1.853	40.7563	0.03503	0.511	9.378
3.00	40.5091	0.03146	0.095	1.668	40.7451	0.03473	0.484	8.441
3.50	40.5111	0.03151	0.090	1.509	40.7349	0.03447	0.459	7.632
4.00	40.513	0.03156	0.086	1.370	40.7256	0.03424	0.436	6.929
4.50	40.5146	0.0316	0.082	1.249	40.717	0.03404	0.415	6.315
5.00	40.5162	0.03163	0.078	1.142	40.709	0.03386	0.395	5.776
5.50	40.5176	0.03166	0.074	1.048	40.7017	0.03371	0.377	5.299
6.00	40.519	0.03169	0.071	0.964	40.6948	0.03357	0.360	4.878
6.50	40.5203	0.03171	0.068	0.890	40.6884	0.03345	0.345	4.501
7.00	40.5214	0.03173	0.065	0.824	40.6823	0.03334	0.330	4.164
7.50	40.5226	0.03175	0.062	0.764	40.6767	0.03325	0.316	3.863
8.00	40.5236	0.03177	0.060	0.711	40.6713	0.03316	0.303	3.590
8.50	40.5246	0.03179	0.057	0.662	40.6663	0.03308	0.291	3.344
9.00	40.5255	0.0318	0.055	0.617	40.6616	0.03301	0.279	3.122
9.50	40.5264	0.03181	0.053	0.578	40.6571	0.03294	0.268	2.919
10.00	40.5273	0.03183	0.051	0.541	40.6528	0.03288	0.257	2.734

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