



Optimization of arsenic extraction in rice samples by Plackett-Burman design and response surface methodology

The objective of this research paper is to optimize the extraction condition of arsenic species and dimethylarsonic acid in paddy rice by a simple solvent extraction using water as an extraction reagent. Design of experiments (DoE) methodology is implemented for the estimation of the variable effects.

The factors (independent variables) examined are: T = extraction temperature (°C), t = shaking time (min), R = rotation speed (rpm), V = solvent volume (mL) and D = dummy factor. All the factors are continuous. The responses (dependent variables) examined are: Y_1 = As (III) extraction (mg/kg), Y_2 = As (V) (mg/kg), Y_3 = DMA extraction (mg/kg) and Y_4 = sum of arsenic species (mg/kg). The applied DoE method is Plackett Burman design.

Isalos version used: 2.1.2

Scientific article: <https://www.sciencedirect.com/science/article/abs/pii/S0308814616302977>

Step 1: Plackett Burman Design

In the first tab named “Action” define the factors in the column headers and fill each column with the low and high levels of the corresponding factors. This tab can be renamed “Plackett Burman”. Afterwards, apply the Plackett Burman method: *DOE* → *Screening* → *Plackett Burman*

	Col1	Col2 (I)	Col3 (I)	Col4 (I)	Col5 (I)	Col6 (I)
User Header	User Row ID	T	t	V	R	D
1		30	30	10	100	-1
2		70	90	20	120	1


DoE Plackett Burman
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×

Number of Center Points per Block

Number of Replicates

Number of Blocks

☐ Random Standard order

Excluded Columns

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Included Columns

Col2 -- T
Col3 -- t
Col4 -- V
Col5 -- R
Col6 -- D

Number of Runs

Results (right spreadsheet):

	Col1	Col2 (I)	Col3 (S)	Col4 (S)	Col5 (S)	Col6 (I)	Col7 (I)	Col8 (I)	Col9 (I)	Col10 (I)
User Header	User Row ID	Standard Order	Block Number	Replicate Number	Point Type	T	t	V	R	D
1		1	Block: 1	Replicate: 1	Design Point	30	90	10	100	-1
2		2	Block: 1	Replicate: 1	Design Point	70	30	10	100	1
3		3	Block: 1	Replicate: 1	Design Point	30	30	10	120	1
4		4	Block: 1	Replicate: 1	Design Point	30	30	20	120	1
5		5	Block: 1	Replicate: 1	Design Point	30	90	20	120	-1
6		6	Block: 1	Replicate: 1	Design Point	70	90	20	100	1
7		7	Block: 1	Replicate: 1	Design Point	70	90	10	120	1
8		8	Block: 1	Replicate: 1	Design Point	70	30	20	120	-1
9		9	Block: 1	Replicate: 1	Design Point	30	90	20	100	1
10		10	Block: 1	Replicate: 1	Design Point	70	90	10	120	-1
11		11	Block: 1	Replicate: 1	Design Point	70	30	20	100	-1
12		12	Block: 1	Replicate: 1	Design Point	30	30	10	100	-1

Step 2: Definition of response variables

Create a new tab named “Responses” and define the responses in the column headers. Fill each column with the values of the corresponding responses that were observed and make sure the values follow the order of the experiments as given by the Plackett Burman method. Then, select all columns to be transferred to the right spreadsheet: *Data Transformation* → *Data Manipulation* → *Select Column(s)*

	Col1	Col2 (D)	Col3 (D)	Col4 (D)	Col5 (D)
User Header	User Row ID	Y1	Y2	Y3	Y4
1		10.3	20.4	12.6	43.3
2		54.1	26.75	13.5	94.4
3		8.1	18.3	12.6	39.1
4		7.6	25.1	12.9	45.6
5		9.7	21.3	12	43.9
6		56.3	31.1	15.4	102.8
7		61.5	27	14.3	102.8
8		56.6	26.6	15.4	98.6
9		9.5	17.7	13.8	40.9
10		60.5	27.4	15.4	103.3
11		45.8	26.4	14.1	86.2
12		9.6	19.5	12.6	41.7


Select Column(s)
? ×

Excluded Columns

Included Columns

Col2 -- Y1
Col3 -- Y2
Col4 -- Y3
Col5 -- Y4

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Execute

Cancel

Step 3: Data selection

Create a new tab named “Data” and import the results from the “Plackett Burman” and “Responses” spreadsheets by right clicking on the left spreadsheet. Then, select only the factors and responses columns to be transferred to the right spreadsheet: *Data Transformation* → *Data Manipulation* → *Select Column(s)*

	Col1	Col2	Col3	Col4	Col5	Col6
User Header	User Row ID					
1						
2						
3						
4						
5						
6						
7						
8						
9						
10						

Multiple Spreadsheet Joiner

Join Configuration Steps

Step 1: Plackett Burman X Responses (C

Add

Delete

Join Type

☒ Concatenation ☐ Left Join ☐ Right Join ☐ Inner Join ☐ Full Outer Join

Left Spreadsheet

Plackett Burman

Right Spreadsheet

Responses

Join Column

☒ Common header name ☐ Different header names

Execute

Cancel

Select Column(s)

Excluded Columns

Col2 -- Standard Order
Col3 -- Block Number
Col4 -- Replicate Number
Col5 -- Point Type

Included Columns

Col6 -- T
Col7 -- t
Col8 -- V
Col9 -- R
Col10 -- D
Col11 -- Y1
Col12 -- Y2
Col13 -- Y3
Col14 -- Y4

Execute

Cancel

Results:

	Col1	Col2 (I)	Col3 (I)	Col4 (I)	Col5 (I)	Col6 (I)	Col7 (D)	Col8 (D)	Col9 (D)	Col10 (D)
User Header	User Row ID	T	t	V	R	D	Y1	Y2	Y3	Y4
1		30	90	10	100	-1	10.3	20.4	12.6	43.3
2		70	30	10	100	1	54.1	26.75	13.5	94.4
3		30	30	10	120	1	8.1	18.3	12.6	39.1
4		30	30	20	120	1	7.6	25.1	12.9	45.6
5		30	90	20	120	-1	9.7	21.3	12	43.9
6		70	90	20	100	1	56.3	31.1	15.4	102.8
7		70	90	10	120	1	61.5	27	14.3	102.8
8		70	30	20	120	-1	56.6	26.6	15.4	98.6
9		30	90	20	100	1	9.5	17.7	13.8	40.9
10		70	90	10	120	-1	60.5	27.4	15.4	103.3
11		70	30	20	100	-1	45.8	26.4	14.1	86.2
12		30	30	10	100	-1	9.6	19.5	12.6	41.7

Step 4: Pareto analysis

Create a new tab named “Pareto Analysis – Y1” and import the results from the spreadsheet “Data”. Then, conduct pareto analysis for the first response variable, Y1: *DOE* → *Post DoE Analysis* → *Pareto Analysis*

Pareto Analysis

Dependent Variable

Col7 -- Y1

Analysis Type

Main Effects

Level Of Significance

0.05

Excluded Columns

Col8 -- Y2

Col9 -- Y3

Col10 -- Y4

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Factors

Col2 -- T

Col3 -- t

Col4 -- V

Col5 -- R

Covariates

DOE type:

☒ Factorial / Screening
 ☐ Response Surface

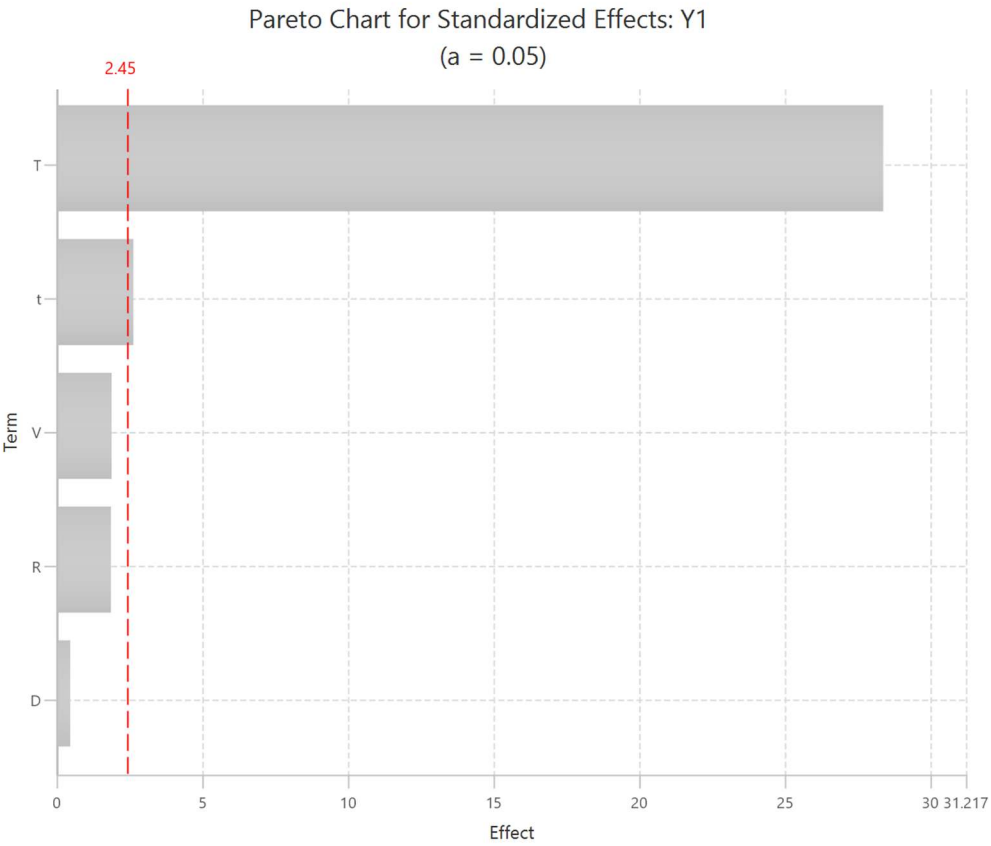
☐ Include Center Points

Execute

Cancel

Results:

	Col1	Col2 (S)	Col3 (S)
User Header	User Row ID	Pareto Analysis of :	Standardized Effects
1		Variable	Effect
2		T	28.3790262
3		t	2.6351953
4		V	1.8851782
5		R	1.8649074
6		D	0.4662269
7		Significance Value	2.4469119

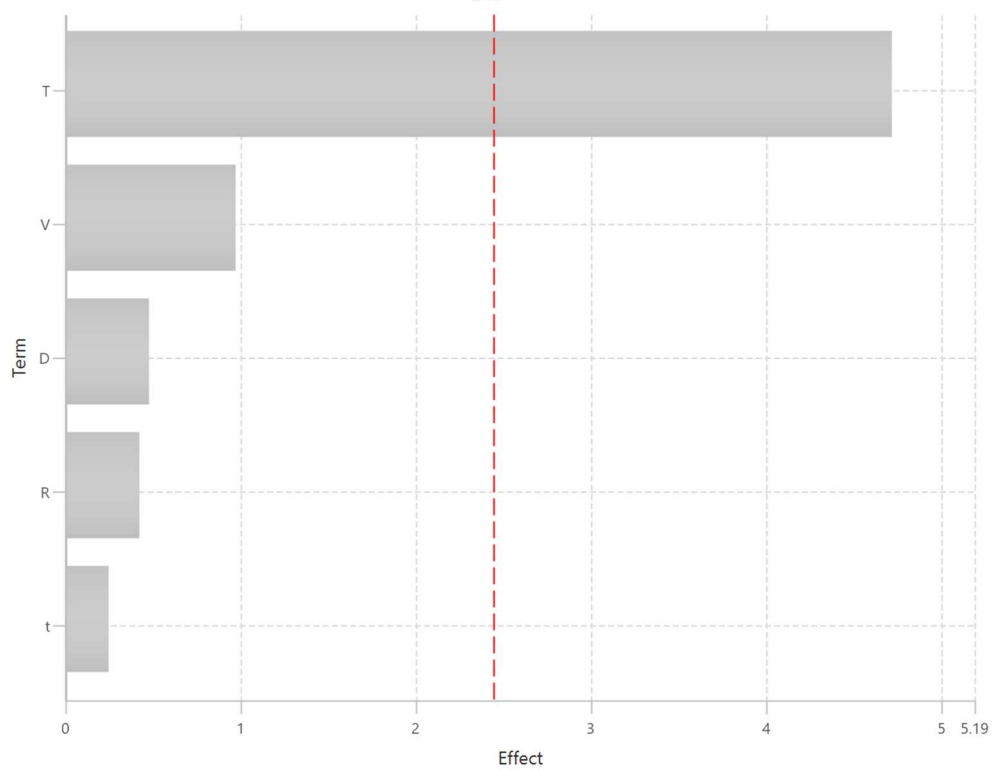


Repeat this step for the rest of the response variables. Results, Y₂:

	Col1	Col2 (S)	Col3 (S)
User Header	User Row ID	Pareto Analysis of :	Standardized Effects
1		Variable	Effect
2		T	4.7178104
3		V	0.9721216
4		D	0.4778225
5		R	0.4229003
6		t	0.2471496
7		Significance Value	2.4469119

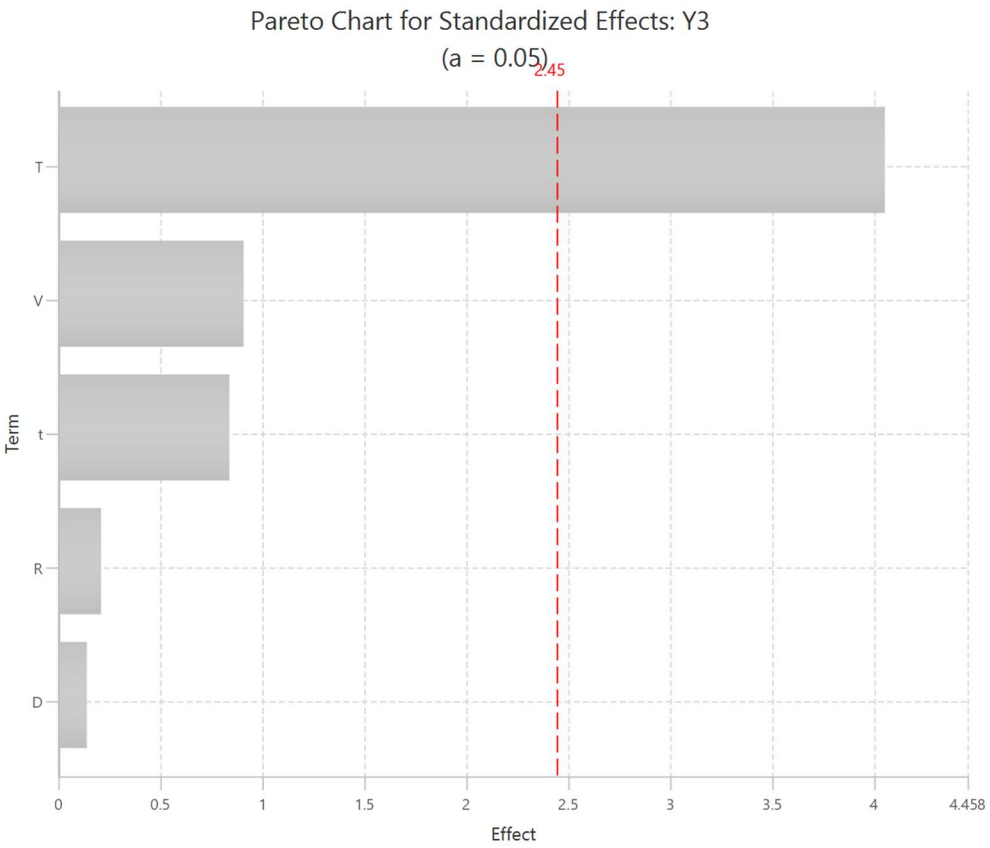
Pareto Chart for Standardized Effects: Y2

($\alpha = 0.05$)



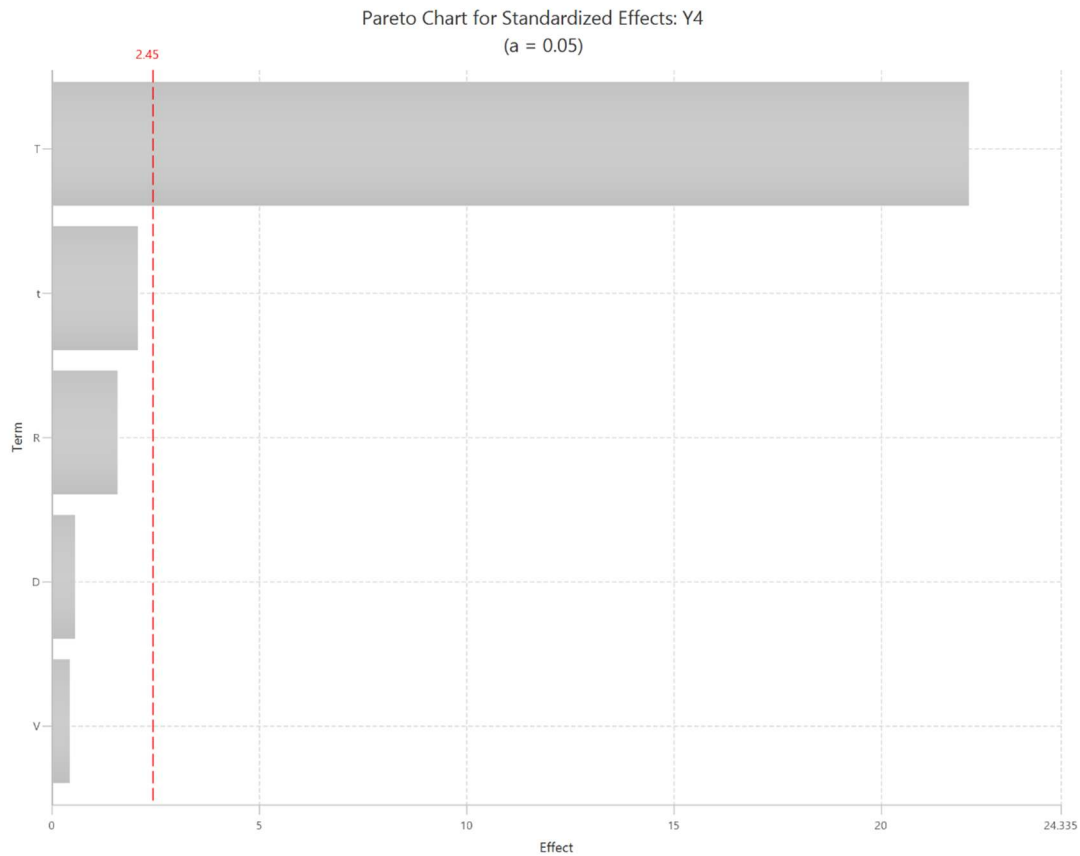
Results, Y₃:

	Col1	Col2 (S)	Col3 (S)
User Header	User Row ID	Pareto Analysis of :	Standardized Effects
1		Variable	Effect
2		T	4.0525434
3		V	0.9083287
4		t	0.8384573
5		R	0.2096143
6		D	0.1397429
7		Significance Value	2.4469119



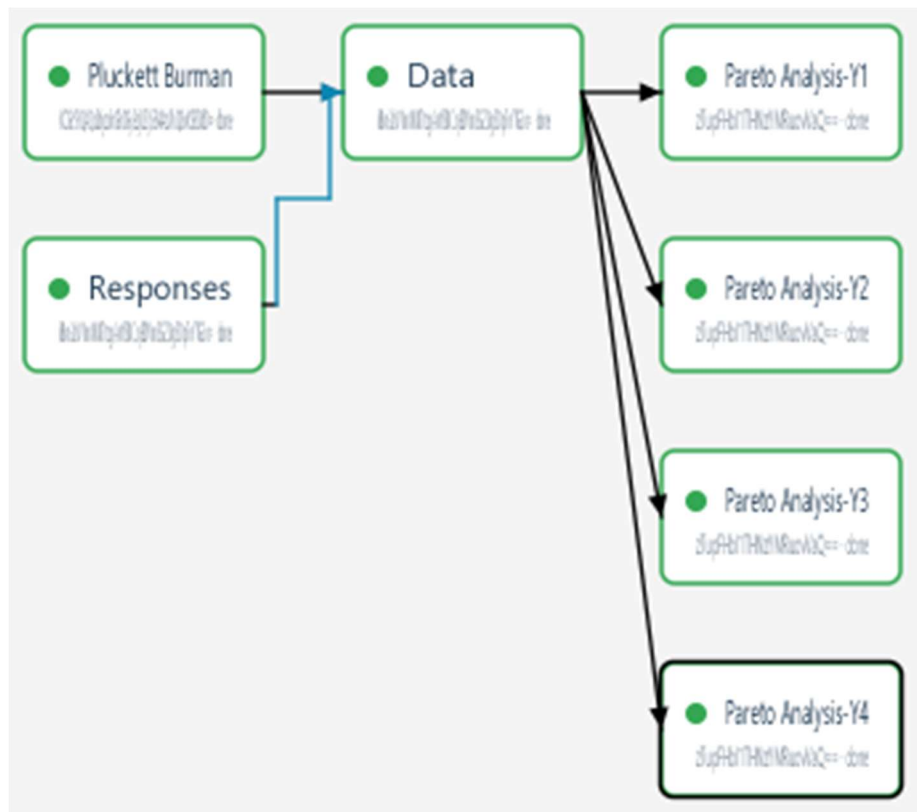
Results, Y₄:

	Col1	Col2 (S)	Col3 (S)
User Header	User Row ID	Pareto Analysis of :	Standardized Effects
1		Variable	Effect
2		T	22.1223272
3		t	2.0822574
4		R	1.5915343
5		D	0.5702998
6		V	0.4376719
7		Significance Value	2.4469119



Final Isalos Workflow

The final workflow is presented below:



References

- (1) Ma, L.; Wang, L.; Tang, J.; Yang, Z. Optimization of Arsenic Extraction in Rice Samples by Plackett–Burman Design and Response Surface Methodology. *Food Chemistry* **2016**, *204*, 283–288. <https://doi.org/10.1016/j.foodchem.2016.02.126>.