

# Package ‘EleChemr’

February 9, 2021

**Title** Electrochemical Reactions Simulation

**Version** 1.2.0

**Description** Digital simulation of electrochemical processes.

Each function allows for implicit and explicit solution of the differential equation using methods like Euler, Backwards implicit, Runge Kutta 4, Crank Nicholson and Backward differentiation formula as well as different number of points for derivative approximation. Several electrochemical processes can be simulated such as: Chronoamperometry, Potential Step, Linear Sweep, Cyclic Voltammetry, Cyclic Voltammetry with electrochemical reaction followed by chemical reaction (EC mechanism) and CV with two following electrochemical reaction (EE mechanism). In update 1.1.0 has been added a general purpose CV function that allow to simulate up to 4 EE mechanism combined with chemical reaction for each species. Update 1.2.0 improved the accuracy of the measurements and allow personalized data resolution for simulation.

Bibliography regarding this methods can be found in the following texts.

Dieter Britz, Jorg Strutwolf (2016) <ISBN:978-3-319-30292-8>.

Allen J. Bard, Larry R. Faulkner (2000) <ISBN:978-0-471-04372-0>.

**License** GPL-3

**Encoding** UTF-8

**LazyData** true

**Imports** ggplot2

**RoxygenNote** 7.1.1

**NeedsCompilation** no

**Author** Federico Maria Vivaldi [aut, cre]

**Maintainer** Federico Maria Vivaldi <federico-vivaldi@virgilio.it>

**Repository** CRAN

**Date/Publication** 2021-02-09 14:20:03 UTC

## R topics documented:

ChronAmp	2
CottrCheck	3
CV	4

CVEC . . . . .	5
CVEE . . . . .	6
Derv . . . . .	8
Gen_CV . . . . .	9
invMat . . . . .	11
LinSwp . . . . .	12
OneMat . . . . .	13
ParCall . . . . .	14
PotStep . . . . .	16
ZeroMat . . . . .	17

<b>Index</b>	<b>18</b>
--------------	-----------

---

ChronAmp	<i>Chrono amperometry digital simulation</i>
----------	--

---

## Description

Return a graph I vs t of the electrochemical process

## Usage

```
ChronAmp(
  Co = 0.001,
  exptime = 1,
  Dx = 1e-05,
  Dm = 0.45,
  Temp = 298.15,
  n = 1,
  Area = 1,
  DerApprox = 2,
  l = 100,
  errCheck = FALSE,
  Method = "Euler"
)
```

## Arguments

Co	bulk concentration expressed in Molar
exptime	experimental time to be simulated expressed in seconds
Dx	diffusion coefficient expressed in cm <sup>2</sup> /s
Dm	simulation parameter, maximum 0.5 for explicit methods
Temp	temperature in kelvin
n	number of electrons involved in the process
Area	area of the electrode expressed in cm <sup>2</sup>
DerApprox	number of point for the approximation of the first derivative

l                    number of time steps of the simulation  
 errCheck            if true the function returns a list with parameters for CottrCheck function  
 Method              method to be used for the simulation = "Euler" "BI" "RK4" "CN" "BDF"

**Value**

if errCheck == F a graph I vs t, if errCheck == T a list

**Examples**

ChronAmp(Co = 0.001, exptime = 1, DerApprox = 2, Dm = 0.45, errCheck = FALSE, Method = "Euler")

---

CottrCheck                    *Cottrel current check for the Chronoamperometric simulation*

---

**Description**

Return a graph G/Gcot vs t of the electrochemical process

**Usage**

CottrCheck(Elefun)

**Arguments**

Elefun                  the function to be checked = ChronAmp, PotStep

**Value**

A graph G/Gcot vs t for the simulation data selected

**Examples**

CottrCheck(ChronAmp(errCheck = TRUE, Method = "BI"))

**Description**

Return a graph I vs E of the electrochemical process

**Usage**

```
CV(  
  Co = 0.001,  
  Dx = 1e-05,  
  Eo = 0,  
  Dm = 0.45,  
  Vi = 0.3,  
  Vf = -0.3,  
  Vs = 0.001,  
  ko = 0.01,  
  alpha = 0.5,  
  Temp = 298.15,  
  n = 1,  
  Area = 1,  
  l = 100,  
  DerApprox = 2,  
  errCheck = FALSE,  
  Method = "Euler"  
)
```

**Arguments**

Co	bulk concentration expressed in Molar
Dx	diffusion coefficient expressed in cm <sup>2</sup> /s
Eo	reduction potential of the species expressed in Volts
Dm	simulation parameter, maximum 0.5 for explicit methods
Vi	initial potential of the sweep expressed in Volts
Vf	final potential of the sweep expressed in Volts
Vs	potential scan rate of the simulation expressed in V/s
ko	heterogeneous electron transfer rate constant expressed in m/s
alpha	charge transfer coefficient
Temp	temperature in kelvin
n	number of electrons involved in the process
Area	area of the electrode expressed in cm <sup>2</sup>
l	number of time steps of the simulation

DerApprox	number of point for the approximation of the first derivative
errCheck	if true the function returns a list with parameters for Cottrell function
Method	method to be used for the simulation = "Euler" "BI" "RK4" "CN" "BDF"

**Value**

if errCheck == F a graph I vs E, if errCheck == T a list

**Examples**

```
CV(Co = 0.001, DerApprox = 2, Dm = 0.45, errCheck = FALSE, Method = "Euler")
```

---

 CVEC

---

*EC behaviour cyclic voltammetry simulator*


---

**Description**

Return a graph I vs E of the electrochemical process

**Usage**

```
CVEC(
  Co = 0.001,
  Dx = 1e-05,
  Eo = 0,
  Dm = 0.45,
  Vi = 0.3,
  Vf = -0.3,
  Vs = 0.001,
  ko = 0.01,
  kc = 0.001,
  l = 100,
  alpha = 0.5,
  Temp = 298.15,
  n = 1,
  Area = 1,
  DerApprox = 2,
  errCheck = FALSE,
  Method = "Euler"
)
```

**Arguments**

Co	bulk concentration expressed in Molar
Dx	diffusion coefficient expressed in cm <sup>2</sup> /s
Eo	reduction potential of the species expressed in Volt
Dm	simulation parameter, maximum 0.5 for explicit methods
Vi	initial potential of the sweep expressed in Volt
Vf	final potential of the sweep expressed in Volt
Vs	potential scan rate of the simulation expressed in V/s
ko	heterogeneous electron transfer rate constant expressed in m/s
kc	rate constant of the reaction Red → C expressed in s <sup>-1</sup>
l	number of time steps of the simulation
alpha	charge transfer coefficient
Temp	temperature in kelvin
n	number of electrons involved in the process
Area	area of the electrode expressed in cm <sup>2</sup>
DerApprox	number of point for the approximation of the first derivative
errCheck	if true the function returns a list with parameters for Cottrell function
Method	method to be used for the simulation = "Euler" "BI" "RK4" "CN" "BDF"

**Value**

if errCheck == F a graph I vs E, if errCheck == T a list

**Examples**

C<sub>VEE</sub>(Co = 0.001, DerApprox = 2, Dm = 0.45, kc = 0.00001, errCheck = FALSE, Method = "Euler")

---

C<sub>VEE</sub>

*EE behaviour cyclic voltammetry simulator*

---

**Description**

Return a graph I vs E of the electrochemical process

**Usage**

```

CVEE(
  Co = 0.001,
  Dx1 = 1e-05,
  Eo1 = 0,
  Vi = 0.3,
  Vf = -0.3,
  Vs = 0.001,
  ko1 = 0.01,
  alpha1 = 0.5,
  Dred = 1e-05,
  Dred2 = 1e-05,
  Eo2 = 0,
  ko2 = 0.01,
  alpha2 = 0.5,
  Dm = 0.45,
  l = 100,
  Temp = 298.15,
  n = 1,
  Area = 1,
  DerApprox = 2,
  errCheck = FALSE,
  Method = "Euler"
)

```

**Arguments**

Co	bulk concentration expressed in Molar
Dx1	diffusion coefficient of the oxidized species expressed in cm <sup>2</sup> /s
Eo1	reduction potential of the first electrochemical reaction expressed in Volt
Vi	initial potential of the sweep expressed in Volt
Vf	final potential of the sweep expressed in Volt
Vs	potential scan rate of the simulation expressed in V/s
ko1	heterogeneous electron transfer rate constant of the first electrochemical reaction expressed in m/s
alpha1	charge transfer coefficient of the first electrochemical reaction
Dred	diffusion coefficient of the first reduced species expressed in cm <sup>2</sup> /s
Dred2	diffusion coefficient of the second reduced species expressed in cm <sup>2</sup> /s
Eo2	reduction potential of the second electrochemical reaction expressed in Volt
ko2	heterogeneous electron transfer rate constant of the second electrochemical reaction expressed in m/s
alpha2	charge transfer coefficient of the second electrochemical reaction
Dm	simulation parameter, maximum 0.5 for explicit methods
l	number of time steps of the simulation

Temp	temperature in kelvin
n	number of electrons involved in the process
Area	area of the electrode expressed in cm <sup>2</sup>
DerApprox	number of point for the approximation of the first derivative
errCheck	if true the function returns a list with parameters for CottrellCheck function
Method	method to be used for the simulation = "Euler" "BI" "RK4" "CN" "BDF"

**Value**

if errCheck == F a graph I vs E, if errCheck == T a list

**Examples**

```
CVEE(Co = 0.001, DerApprox = 2, Dm = 0.45, errCheck = FALSE, Method = "Euler")
CVEE(Co = 0.001, Eo2 = -0.15, Dm = 0.45)
```

---

Derv

*Derivative calculation of concentration profile*


---

**Description**

Return a the derivative of the concentration profile simulated

**Usage**

```
Derv(
  npoints = 2,
  h,
  Ox,
  mode = "Forward",
  Derivative = "First",
  CoefMat = FALSE
)
```

**Arguments**

npoints	number of points to be used for the derivative
h	space for the finite difference
Ox	data upon the derivative is calculated
mode	"Forward" or "Backward" the derivative will be calculated for the npoints
Derivative	"First" or "Second" derivative to calculate
CoefMat	if T return the derivative coefficient matrix for selected derivative



**Value**

a vector with the derivative requested or the coefficient of such derivative

**Examples**

```
Derv(npoints = 2, h = 0.13, Ox = matrix(c(1,2), nrow = 1), mode = "Forward", Derivative = "First")
```

---

Gen\_CV

*General Purpose CV simulation*

---

**Description**

Return a graph I vs E of the electrochemical process, up to 4 EE mechanisms and CE mechanisms can be simulated

**Usage**

```
Gen_CV(  
  Co = 0.001,  
  Cred = 0,  
  kco = 0,  
  Dx1 = 1e-05,  
  Eo1 = 0,  
  kc1 = 0,  
  ko1 = 0.01,  
  alpha1 = 0.5,  
  Dred = 1e-05,  
  Dred2 = 1e-05,  
  Eo2 = 0,  
  kc2 = 0,  
  ko2 = 0,  
  alpha2 = 0.5,  
  Dm = 0.45,  
  Dred3 = 1e-05,  
  Eo3 = 0,  
  kc3 = 0,  
  ko3 = 0,  
  alpha3 = 0.5,  
  Dred4 = 1e-05,  
  Eo4 = 0,  
  kc4 = 0,  
  ko4 = 0,  
  alpha4 = 0.5,  
)
```

```

Temp = 298.15,
n = 1,
Area = 1,
l = 100,
DerApprox = 2,
errCheck = FALSE,
Method = "Euler"
)

```

### Arguments

Co	bulk concentration oxidated species expressed in Molar
Cred	bulk concentration of reduced species expressed in Molar
kco	Chemical rate constant for Ox Species expressed in $s^{-1}$
Dx1	diffusion coefficient of the oxidized species expressed in $cm^2/s$
Eo1	reduction potential of the first electrochemical reaction expressed in Volt
kc1	Chemical rate constant for Red Species expressed in $s^{-1}$
Vi	initial potential of the sweep expressed in Volt
Vf	final potential of the sweep expressed in Volt
Vs	potential scan rate of the simulation expressed in $V/s$
ko1	heterogeneous electron transfer rate constant of the first electrochemical reaction expressed in $m/s$
alpha1	charge transfer coefficient of the first electrochemical reaction
Dred	diffusion coefficient of the first reduced species expressed in $cm^2/S$
Dred2	diffusion coefficient of the second reduced species expressed in $cm^2/s$
Eo2	reduction potential of the second electrochemical reaction expressed in Volt
kc2	Chemical rate constant for second Red Species expressed in $s^{-1}$
ko2	heterogeneous electron transfer rate constant of the second electrochemical reaction expressed in $m/s$
alpha2	charge transfer coefficient of the second electrochemical reaction
Dm	simulation parameter, maximum 0.5 for explicit methods
Dred3	diffusion coefficient of the third reduced species expressed in $cm^2/s$
Eo3	reduction potential of the third electrochemical reaction expressed in Volt
kc3	Chemical rate constant for third Red Species expressed in $s^{-1}$
ko3	heterogeneous electron transfer rate constant of the third electrochemical reaction expressed in $m/s$
alpha3	charge transfer coefficient of the third electrochemical reaction
Dred4	diffusion coefficient of the fourth reduced species $cm^2/s$
Eo4	reduction potential of the fourth electrochemical reaction expressed in Volt
kc4	Chemical rate constant for fourth Red Species expressed in $s^{-1}$

ko4	heterogeneous electron transfer rate constant of the fourth electrochemical reaction expressed in m/s
alpha4	charge transfer coefficient of the fourth electrochemical reaction
Temp	temperature in kelvin
n	number of electrons involved in the process
Area	area of the electrode expressed in cm <sup>2</sup>
l	number of time steps of the simulation
DerApprox	number of point for the approximation of the first derivative
errCheck	if true the function returns a list with parameters for CottrCheck function
Method	method to be used for the simulation = "Euler" "BI" "RK4" "CN" "BDF"

**Value**

if errCheck == F a graph I vs E, if errCheck == T a list

**Examples**

```
Gen_CV(Co = 0.001, DerApprox = 2, Dm = 0.45, errCheck = FALSE, Method = "Euler")
Gen_CV(Co = 0.001, Eo2 = -0.15, Dm = 0.45, kc1 = 0.0001)
```

---

 invMat

*Inverse matrix*


---

**Description**

Returns the inverse matrix of the selected one

**Usage**

```
invMat(A)
```

**Arguments**

A                    matrix to be inverted

**Value**

inverse matrix of the selected

**Examples**

```
invMat(A = matrix(c(1,2,6,14), nrow = 2))
```

---

 LinSwp

*Linear Sweep digital simulation*


---

**Description**

Return a graph I vs E of the electrochemical process

**Usage**

```

LinSwp(
  Co = 0.001,
  Dx = 1e-05,
  Eo = 0,
  Dm = 0.45,
  Vi = 0.3,
  Vf = -0.3,
  Vs = 0.001,
  ko = 0.01,
  alpha = 0.5,
  Temp = 298.15,
  n = 1,
  Area = 1,
  l = 100,
  DerApprox = 2,
  errCheck = FALSE,
  Method = "Euler"
)

```

**Arguments**

Co	bulk concentration expressed in Molar
Dx	diffusion coefficient expressed in cm <sup>2</sup> /s
Eo	reduction potential of the species expressed in Volt
Dm	simulation parameter, maximum 0.5 for explicit methods
Vi	initial potential of the sweep expressed in Volt
Vf	final potential of the sweep expressed in Volt
Vs	potential scan rate of the simulation expressed in V/s
ko	heterogeneous electron transfer rate constant expressed in m/s
alpha	charge transfer coefficient
Temp	temperature in kelvin
n	number of electrons involved in the process
Area	area of the electrode expressed in cm <sup>2</sup>
l	number of time steps of the simulation

DerApprox      number of point for the approximation of the first derivative  
errCheck      if true the function returns a list with parameters for CottCheck function  
Method      method to be used for the simulation = "Euler" "BI" "RK4" "CN" "BDF"

**Value**

if errCheck == F a graph I vs E, if errCheck == T a list

**Examples**

```
LinSwp(Co = 0.001, Dm = 0.45, DerApprox = 2, errCheck = FALSE, Method = "Euler")
```

---

OneMat      *Starting Matrix of oxidized species*

---

**Description**

Return a matrix  $ixj$  filled with 1 value

**Usage**

```
OneMat(i, j = i)
```

**Arguments**

i      number of rows  
j      number of columns

**Value**

a matrix of dimension  $ixj$  filled with 1 value

**Examples**

```
OneMat(2,2)
```

---

ParCall

*Parameters call*

---

### **Description**

Returns a list with the parameters necessary for the simulation

### **Usage**

```
ParCall(  
    Fun,  
    n.,  
    Temp.,  
    Dx1.,  
    eta.,  
    exptime.,  
    Eo1.,  
    ko1.,  
    ko2.,  
    kc.,  
    Dm.,  
    Vf.,  
    Vi.,  
    Vs.,  
    alpha1.,  
    Eo2.,  
    Dred1.,  
    Dred2.,  
    alpha2.,  
    Dred3.,  
    Dred4.,  
    ko3.,  
    ko4.,  
    kco.,  
    kc1.,  
    kc2.,  
    kc3.,  
    kc4.,  
    alpha3.,  
    alpha4.,  
    Eo3.,  
    Eo4.,  
    l.  
)
```

### **Arguments**

Fun                      Name of the function this function is called to. Must be a string.

n.	Number of electrons
Temp.	Temperature for the simulation
Dx1.	Diffusion coefficient of species One
eta.	OverPotential for potential step
exptime.	experimental time for the simulation
Eo1.	reduction potential of the first electrochemical reaction
ko1.	heterogeneous electron transfer rate constant of the first electrochemical reaction
ko2.	heterogeneous electron transfer rate constant of the second electrochemical reaction
kc.	Chemical rate constant for first Ox Species, used in simulation with just one species
Dm.	Simulation parameter, maximum 0.5 for explicit methods
Vf.	Final potential of the sweep
Vi.	Initial potential of the sweep
Vs.	Scan rate of the simulation
alpha1.	charge transfer coefficient of the first electrochemical reaction
Eo2.	reduction potential of the second electrochemical reaction
Dred1.	diffusion coefficient of the first reduced species
Dred2.	diffusion coefficient of the second reduced species
alpha2.	charge transfer coefficient of the second electrochemical reaction
Dred3.	diffusion coefficient of the third reduced species
Dred4.	diffusion coefficient of the fourth reduced species
ko3.	heterogeneous electron transfer rate constant of the third electrochemical reaction
ko4.	heterogeneous electron transfer rate constant of the fourth electrochemical reaction
kco.	Chemical rate constant for first Ox Species
kc1.	Chemical rate constant for first Red Species
kc2.	Chemical rate constant for second Red Species
kc3.	Chemical rate constant for third Red Species
kc4.	Chemical rate constant for fourth Red Species
alpha3.	charge transfer coefficient of the third electrochemical reaction
alpha4.	charge transfer coefficient of the fourth electrochemical reaction
Eo3.	reduction potential of the third electrochemical reaction
Eo4.	reduction potential of the fourth electrochemical reaction
l.	num of time steps

**Value**

inverse matrix of the selected

**Examples**

```
ParCall("ChronAmp", n. = 1, Temp. = 298, Dx1. = 0.0001, exptime. = 1, Dm. = 0.45, l. = 100)
```

---

 PotStep

---

*Chrono amperometry with a finite step digital simulation*


---

**Description**

Return a graph I vs t of the electrochemical process

**Usage**

```
PotStep(
  Co = 0.001,
  exptime = 1,
  Dx = 1e-05,
  Dm = 0.45,
  eta = 0,
  Temp = 298.15,
  n = 1,
  Area = 1,
  l = 100,
  DerApprox = 2,
  errCheck = FALSE,
  Method = "Euler"
)
```

**Arguments**

Co	bulk concentration expressed in Molar
exptime	experimental time to be simulated expressed in seconds
Dx	diffusion coefficient expressed in cm <sup>2</sup> /s
Dm	simulation parameter, maximum 0.5 for explicit methods
eta	overpotential of the step expressed in Volt
Temp	temperature in kelvin
n	number of electrons involved in the process
Area	area of the electrode expressed in cm <sup>2</sup>
l	number of time steps of the simulation
DerApprox	number of point for the approximation of the first derivative
errCheck	if true the function returns a list with parameters for CottrCheck function
Method	method to be used for the simulation = "Euler" "BI" "RK4" "CN" "BDF"



**Value**

if errCheck == F a graph I vs t, if errCheck == T a list

**Examples**

```
PotStep(Co = 0.001, exptime = 1, Dm = 0.45, DerApprox = 2, errCheck = FALSE, Method = "Euler")
```

---

ZeroMat

*Starting Matrix of reduces species and fluxes*

---

**Description**

Return a matrix  $ixj$  filled with 0 value

**Usage**

```
ZeroMat(i, j = i)
```

**Arguments**

i	number of rows
j	number of columns

**Value**

a matrix of dimation  $ixj$  filled with 1 value

**Examples**

```
ZeroMat(2,2)
```

# Index

ChronAmp, [2](#)  
CottrCheck, [3](#)  
CV, [4](#)  
CVEC, [5](#)  
CVEE, [6](#)  
  
Derv, [8](#)  
  
Gen\_CV, [9](#)  
  
invMat, [11](#)  
  
LinSwp, [12](#)  
  
OneMat, [13](#)  
  
ParCall, [14](#)  
PotStep, [16](#)  
  
ZeroMat, [17](#)