Package 'EleChemr'

October 12, 2022

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` *Chrono amperometry digital simulation*

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^2/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^2
`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"))
```

CV *Cyclic voltammetry digitial simulation*

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^2/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 sweepexpressed 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^2
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

```
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^2/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^-1
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^2
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

```
CVEC(Co = 0.001, DerApprox = 2, Dm = 0.45, kc = 0.00001, errCheck = FALSE, Method = "Euler")
```

CVEE *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^2/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^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
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^2
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

```
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,
  Vi = 0.3,
  Vf = -0.3,
  Vs = 0.001,
  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 speciesexpressed 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^2
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 digitial 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^2/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^2
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

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

OneMat *Starting Matrix of oxidazed 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 dimention 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.	numer 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^2/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^2
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 dimention ixj filled with 1 value

Examples

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

Index