**Input dataframe**

|  |  |  |  |
| --- | --- | --- | --- |
| **Parameter** | **Symbol** | **Unit** | **Value** |
| Depth |  | m | - |
| Concentration |  | mmol m-3 | - |
| Porosity (optional) |  | - | - |
| Electrical field (optional) |  | V m-1 | - |
| Advective velocity (optional) |  | m d-1 | - |
| First derivative of porosity (optional) |  | m-1 | - |
| First derivative of advective velocity (optional) |  | d-1 | - |
| First derivative of the effective diffusive coefficient (optional) |  | m d-1 | - |

**Env.parms list**

|  |  |  |  |
| --- | --- | --- | --- |
| **Parameter** | **Symbol** | **Unit** | **Value** |
| Temperature |  | °C | 10 |
| Salinity |  | PSU | 30 |
| Pressure |  | bar | 1.013 |
| Diffusive coefficient |  | m2 d-1 | - |
| Charge of the ion |  | - | 0 |

**gradient.parms list**

|  |  |  |  |
| --- | --- | --- | --- |
| **Parameter** | **Symbol** | **Unit** | **Value** |
| Limits between which gradient is calculated |  | m | - |

**discrete.parms list**

|  |  |  |  |
| --- | --- | --- | --- |
| **Parameter** | **Symbol** | **Unit** | **Value** |
| lower boundary of the integration domain |  | m | - |
| Upper boundary of the integration domain |  | m | - |
| Number of layers for the fitting function |  | - | 200 |
| Maximum number of discrete production zones |  | - | 12 |
| Number of zones to start lumping |  | - | - |
| Probability with which the null hypothesis is rejected |  | - | 0.01 |
| Upper boundary condition | UBC | - | Fixed concentration |
| Lower boundary conditions | LBC | - | Zero flux |
| Flux across the upper boundary | - | mmol m-2 d-1 | - |
| Flux across the lower boundary | - | mmol m-2 d-1 | - |

**continuous.parms list**

|  |  |  |  |
| --- | --- | --- | --- |
| **Parameter** | **Symbol** | **Unit** | **Value** |
| Order of the polynomial that is fitted |  | - | 3 |
| integer determining filter behaviour at the upstream (upper, left) boundary | Bnd.upper | - | 1\* |
| integer determining filter behaviour at the downstream (lower, right) boundary | Bnd.lower | - | 1\* |
| window size used in filtering the concentration C / flux J / production R, representing the number of data points to the left and right of the data midpoint | ,, | - | - |
| Determination of optimal window size | - | - | Automated\*\* |
| minimum value of the window size, used when scanning the optimal window size | Min.n | - | 2 |
| maximum value of the window size, used when scanning the optimal window size | Max.n | - | Nrow(input)/2-1 |
| keeps windows created by automated function | Keep.graphics | - | FALSE |
| Create equidistant data points | interpolation | - | Interpolate\*\*\* |

\*value is either 1, 2 or 3. Value = 1: no constraint on flux (default value). Value = 2: constant flux imposed. Value = 3: zero flux imposed.  
\*\* either "automated" or "interactive" (default).   
interactive allows user to select ideal filter size, automated lets function select ideal filter size  
\*\*\*\*\* either "average" or "interpolate" (default).   
average (take maximum stepsize) or interpolate (take minimum stepsize)