CXT SIM-FIT Manual

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Abstract

This document is a user guide for the program CXT SIM-FIT. It contains the equations implemented in the program and describes the parameters that can be fitted.

1 Fundamentals and Program Usage

The program CXT SIM-FIT can be used for inverse-modeling and parametrization of convection-diffusion-reaction equations. Unlike the original CXTFit program, it solves the transport equations numerically. This allows consideration of additional effects:

- non-constant inlet concentrations (data file)
- non-constant parameters (e.g. sorption curves)
- kinetic transfer terms between mobile and immobile phases

In addition to the extended calculation capabilities, it allows monitoring and inspecting the transient profiles that are calculated at various time points during the integration.

1.1 Numerical Solution

The partial differential equation is transformed into a system of ordinary differential equations by using the control volume method. A central difference quotient approximation is used for the diffusion term Eqn. (1.1), and

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a first-order upwind discretization of the convection term Eqn. (1.2).

$$\frac{\partial c}{\partial x} = \frac{c_i - c_{i+1}}{\Delta x} \tag{1.1}$$

$$v\,c = v\,c_i \tag{1.2}$$

The time integration is done using a variable-order variable-step multi-step implementation of a BDF formulation, implemented in the SUNDIALS-CVODE[1] package. For the minimization a Levenberg-Marquardt algorithm is used, implemented in the LevMar library[2].

1.2 Program Usage

First load a break-through data file, with the following format:

```
# lines beginning with a '#' character are comments
# standard two-column layout is used, whitespace characters
# (space or tab characters) are used as separators between
# columns
# first column is the time point in [h]
# second column is the measured outlet concentration in [kg/m3s]
0  0
1  0
2  0.1
3  0.8
4  0.9
5  0.95
6  0.99
10  1
```

Then either specify the inlet concentration, or load a data file (same format as outlet data) for the inlet concentrations. Note that you can substitute any suitable concentration measure for the default kg/m^3. However, make sure that the outlet and inlet data files use the same unit!

Now estimate the parameters until you have a good initial guess!

Hint: While entering values you can hit Enter to run the simulation and update the current curve.

To optimize the fit, select/check one or more parameters and run the optimizer. It is useful to fit few parameters at a time until close to the best-fit.

[1] SUNDIALS, SUite of Nonlinear DIfferential ALgebraic equation Solvers, `www.llnl.gov/CASC/sundials`

[2] levmar: Levenberg-Marquardt nonlinear least squares algorithms in C/C++, `www.ics.forth.gr/ lourakis/levmar`

2 Model Description

For the current version, two models are implemented:

1. equilibrium sorption model (one balance equation)
2. mobile/immobile phases coupled with exchange term (two balance equations)

The implementation is straight-forward and can be easily extended. See Section 3 for details.

2.1 Model #1: Equilibrium Sorption

Instantaneous equilibrium between the mobile phase and adsorptive surfaces is assumed. Equation (2.1) is implemented. In addition to the parameters in the equation, the user interface allows input of the cross section, flow domain length, porosity and upstream volumetric flow rate. These input quantities are used to calculate, for instance, the convection velocity v inside the porous medium.

$$R_c \frac{\partial c}{\partial t} = -\frac{\partial}{\partial x}\left[-D\frac{\partial c}{\partial x} + v\,c\right] - \mu_c\,c + \gamma_c \tag{2.1}$$

with

Symbol	Dimension	Description
c	kg/m^3	Mass density/volume based concentration
t	s	Time
x	m	Spatial location
R_c	kg/kg	Retention coefficient
D	m^2/s	Diffusion coefficient
v	m/s	Convection velocity
μ_c	$1/s$	Linear reaction coefficient (1. Order reduction rate)
γ_c	$kg/m^3 s$	Mass production term (0. Order source/sink)

Parameters and notation are used as in [Parker & van Genuchten, 1984].

2.2 Model #2: Mobile/Immobile Phases

The component is transported in one phase as before in model #1. An concentration based exchange term controls transport to and from the immobile phase. There, instantaneous equilibrium between the mobile and adsorbed components is assumed. Equations (2.2) and (2.3) are implemented. The first equation is identical to the transport equation in model #1, except for

the additional mass exchange term.

$$R_c \frac{\partial c}{\partial t} = -\frac{\partial}{\partial x}\left[-D\frac{\partial c}{\partial x} + v\,c\right] - \beta\,(c-s) - \mu_c\,c + \gamma_c \tag{2.2}$$

$$R_s \frac{\partial s}{\partial t} = \beta\,(c-s) - \mu_s\,s + \gamma_s \tag{2.3}$$

with these symbols defined in addition to the ones already introduced in model #1.

Symbol	Dimension	Description
s	kg/m^3	Mass density/volume based concentration in immobile phase
R_s	kg/kg	Retention coefficient for the immobile phase
β	$1/s$	Mass transfer coefficient
μ_s	$1/s$	Linear reaction coefficient in immobile phase
γ_s	$kg/m^3 s$	Mass production term in immobile phase

For a very large β and $R_c = 0$, or $\beta = 0$ model #2 will give the same results as model #1.

3 Development

Development information are currently compiled and kept up-to-date on the webpage: `www.bauklimatik-dresden.de/cxtsimfit`

4 Licenses

The CXT SIM-FIT program is licensed under the GNU General Public License (GPL).

The CVODE library used in the program comes with the following license.

The Levenberg-Marquardt library used in the program comes with the following license.

```
(at your option) any later version.

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```