# RADIOACTIVE DECAY MODELS IN A MATLAB E-LEARNING ENVIRONMENT

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**Abstract**

The Institute of Analysis and Scientific Computing at the Vienna University of Technology runs a web e-learning platform in an MATLAB environment for dynamical models. Teachers can use these online models for teaching and demonstrating in classes, whereas students can more understanding and increase their programming skills. Each module consists of a general introduction to the thematic, and a list of possible experiments with the model, with selected parameters. All examples are programmed and implemented in MATLAB whereby the underlying MATLAB *m-files* are also available for users.

Recently, the course *Modeling and Simulation* was enriched by modules concerning radioactive decay and diffusion, from basic radioactive decay via electron adsorption until contamination spread in the plane. This contribution describes details on the models used for these new modules (simple decay equation, decay with mother-daughter dynamics, nonlinear balance equation for agglomeration of atoms, and cellular automata model with global diffusion for radioactive spread) and shows adjoint web experiment modules in the e-learning platform.

**Keywords: Radioactive Decay, Migration Models, e-Learning, MATLAB**

**Presenting Author's biography**

**Peter Kristöfel.** He finished two master studies with distinction. He got one degrees in applied physics, where he studied a chaotic atomic system, and in applied mathematics, where he wrote his thesis on a model of the diabetes 2 prevalence in Austria. After that, he started his PhD work on semiconductor modeling. Besides that, he uses his interdisciplinary skills also in teaching and e-learning, where he works with the ARGE-SIM Group at TU Vienna.

# 1 MMT E-Learning System

The Institute of Analysis and Scientific Computing at the Vienna University of Technology runs a web e-learning platform in an MATLAB environment for dynamical models available for both, teachers and students. Teachers can use these online models for teaching and demonstrating in classes, whereas students can get more understanding and in-depth knowledge or increase their programming skills when getting over these examples at home; for details see [1, 2, 3].

All these dynamical models are available over the Mathematics, Modeling and Simulation (MMT) E-learning server, which provides suitable examples as well for lectures in basic mathematics (i.e. *Basic Mathematics for Surveillance and Mapping*) as for lectures given about modelling and simulation.

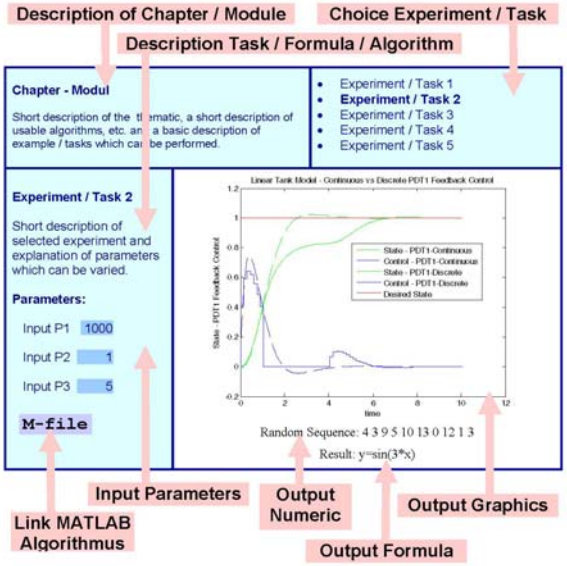


Fig. 1 The MMT organizer

The examples run at the *organizer* (Fig. 1) are organised in modules, whereas each module consists

- of a general introduction to the thematic with a short description of usable algorithms,
- of a list of tasks / experiments to be chosen from,
- of a short description of the chosen task / experiment with input of experiment parameters,
- of the output area with graphic output, numeric /textual output and formula output,
- and of the the m-file link, which when activated opens the m-file – the model description

In addition, the underlying MATLAB source codes (m-files; (Fig. 2).) of these models are available and provide sufficient advice when students start making their first experiences in programming MATLAB.

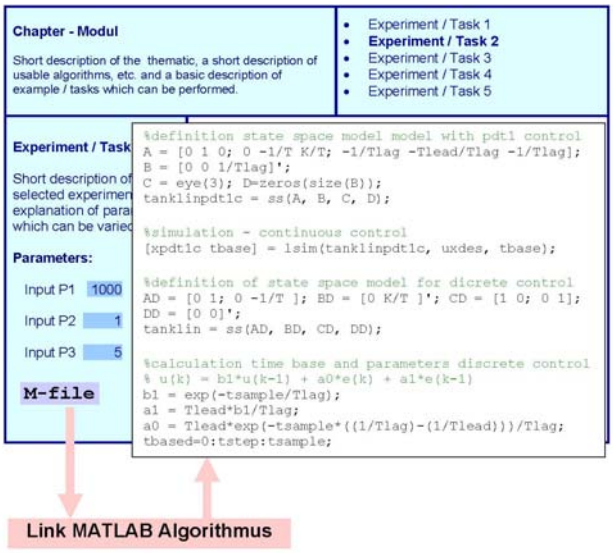


Fig. 2 The MMT organizer with model m-file opened

# 2 Modules Physics: Radiation and Absorption

Recently, the course *Modeling and Simulation* was enriched by modules concerning radioactive decay diffusion, and desorption, from basic radioactive decay via electron adsorption and desorption until contamination spread in the plane, with simple and complex models: simple decay equation, decay with mother-daughter dynamics, nonlinear balance equation for agglomeration of atoms, and cellular automata model with global diffusion for radioactive spread.

The modules address different levels of knowledge and different skills to be learned:

- Module *Radioactive Decay*
  level simple – medium,
  general modelling, modelling in physics

- Module *Desorption Kinetics Model Analysis*
  level medium
  general modelling, modelling in physics
  numerics

- Module *Desorption Kinetics Numerical Analysis*
  level medium - heavy
  general modelling, modelling in physics
  mathematical analysis, numerical analysis, approximation

- Module *Radioactive Migration*
  level medium - heavy
  general modelling, modelling in physics
  numerics, spatial modelling

## 3 Module Radioactive Decay

The module Radioactive Decay introduces the mathematical decay curve, and demonstrates the use of the logarithmic scaling of mathematical functions – a display mode that will become more important for them when facing more complex modelling tasks. A certain amount of a radioactive substance (particles, a certain mass, and a certain amount of substance) at a certain time (t) can be calculated from that particular substance at time 0 and an exponential factor that depends on the decay constant of the radioactive substance and the elapsing time.

Mathematics in behind in the exponential decay curve, and the half-life step function, in case of activity $A(t)$as variable with half-life parameter $\tau$ given by

$$A(t) = A_0 \exp(\frac{\ln 2}{\tau} t)$$

$$A(t_k + \tau) = \frac{1}{2} A(t_k)$$

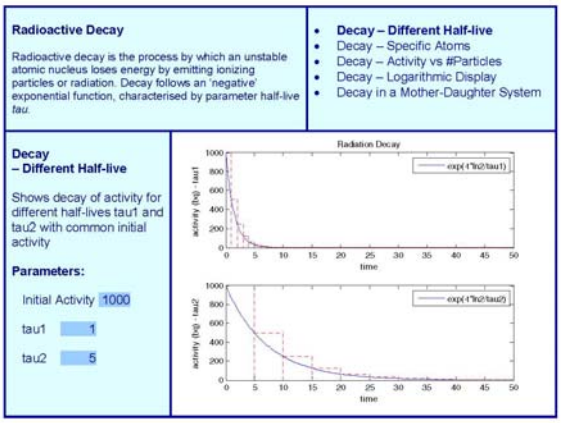


Fig. 3 Module *Radioactive Decay*, Experiment *Decay – Different Half-live*

The different tasks / experiments offered are

1. Decay – Different Half-live
2. Decay – Specific Atoms
3. Decay – Activity vs #Particles
4. Decay – Logarithmic Display
5. Decay in a Mother-Daughter System

Task (1) encourages students to compare different half-live parameters and to compare the exponential decay function with the decay step function which converges to the exponential decay function (Fig. 3).

Task (2) is intended to show the 'real life' in radioactivity: the decay of activity of different atoms is compared (Fig. 4), whereby half-life parameters in neighboured time scales can be chosen (Tab. 1).

Tab. 1 Half-live at different time scales for Experiment *Decay – Specific Atoms*

```
tau_c14 = 5730.0;   %years
tau_ra226 = 1600.0; %years

tau_u238 = 4.468e9; %years
tau_k40  = 1.28e9;  %years

tau_eu156 = 15.2  %days
tau_ge171 = 11.43 % days
tau_s35   = 87.5  % days

tau_cl39 = 56     %minutes
tau_fe61 =  6     % minutes
tau_br82 =  6.1   % minutes
```

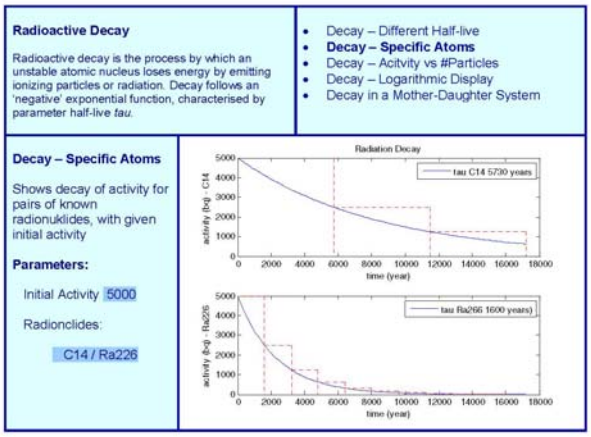


Fig. 4 Module *Radioactive Decay*, Experiment *Decay – Specific Atoms*

Task (3) outlines the connection between particle number $N(t)$, respective weight and the amount of substance:

$$N(t) = \frac{\ln 2}{\tau} A(t) = \frac{\ln 2}{\tau} A_0 \exp(\frac{\ln 2}{\tau} t)$$

It has been shown that the mole-concept and Avogadro's number are not that familiar to the students, but it is needed for the understanding of clearance models – which is intended by this experiment (Fig. 5).

Task (4) shows the decay at the logarithmic scale – resulting in 'simple' straight line. for many radionuclides. It is important for students to learn to read this type of decay documentation, because measurement devices produce such outputs.

Task (5) describes a so-called mother-daughter system. A radionuclide (mother) decays to another radionuclide (daughter), which then decays to a stable nuclide (granddaughter). The decrease/increase of the different nuclides, also in logarithmic scale is shown. The respective radionuclides are primarily preset, but the students have the possibility to fiddle about fictive decay constants to get a feeling of the system's behaviour.

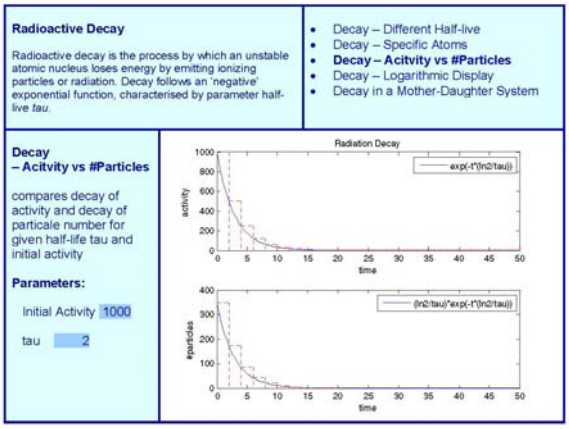


Fig. 5 Module *Radioactive Decay*,
Experiment *Decay – Activity vs. #Particles*

## 4 Module Desorption Kinetics

The models behind this module deal with the desorption kinetics of Lithium atoms from LiF. Lithium (Li) and fluoride (F) form a crystalline salt called an alkali halide ([4]).

When a LiF surface with a temperature of approx. 700 K is being irradiated by an electron beam, emission of lithium atoms can be measured. This typical behaviour of alkali halides is well known and due to their simple crystal structure this process is extensively studied. The specific dynamics depend on the temperature of the material, but at temperatures above 500 K the rate of evaporation from the surface is not the limiting factor in the experiment, so the effect of an electron beam can be studied in more detail.

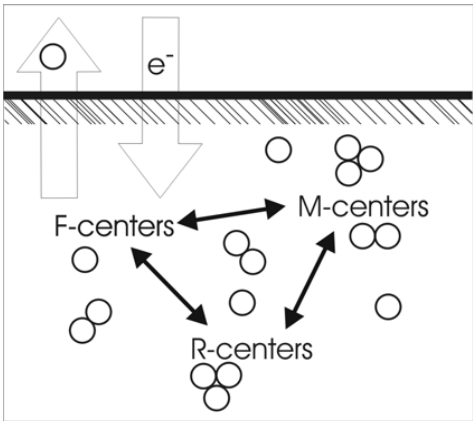


Fig. 6 Desorption and agglomeration of LiF atoms under electron bombardment

When electrons hit the surface with sufficient energy, so-called *F*-centers (a term from solid state physics) are formed in the crystal. Those can either immediately cause desorption of a lithium atom, or they agglomerate near the surface of the material and form aggregates of various sizes, called $F_{(i)}$-centers where $i = 1, \ldots, n$ denotes the size of the center, i.e. the number of aggregated atoms.

These break down after a characteristic time into $F_{(1)}$-centers (short: *F*-centers) again, which reach the surface and lead to emission of lithium atoms even after the electron beam has been turned off. This so-called *delayed emission* is depicted in Fig. 6.

Experiments described in [9] show that during electron bombardment the Li emission rate is constant but drops significantly in a very short time ( < 20 ms) when bombardment stops. It follows that during this short time interval one can still observe a delayed emission of Li atoms.

In order to build a model of the desorption dynamics some simplifications were made in [4]. These are justified by the small penetration depth of the electrons and the high temperature:

- The diffusion time of *F*-centers to the surface is very small and can be neglected.
- Every *F*-center reaching the surface causes desorption.
- There is no spatial dependence of the $F_i$-center concentration, i.e. centers are uniformly distributed
- Growth and decay of a center is only due to absorption or evaporation of an $F_{(1)}$-center, i.e. $F_{(i)} + F_{(1)} \leftrightarrow F_{(i+1)}$

The following system of differential equations is found to describe the dynamics of the $F_{(i)}$-centers accordingly, using nonlinear balance laws:

$$\frac{dF^{(1)}}{dt} = P - aF^{(1)} + \sum_{i=3}^{n} l_i F^{(i)} - \sum_{h=2}^{n-1} k_h F^{(1)} F^{(h)} + \\ + 2l_2 F^{(2)} - 2k_1 (F^{(1)})^2$$

$$\frac{dF^{(m)}}{dt} = l_{m+1} F^{(m+1)} - k_m F^{(1)} F^{(m)} - l_m F^{(m)} + \\ + k_{m-1} F^{(1)} F^{(m-1)}, \quad m = 2, \ldots, n-1$$

$$\frac{dF^{(n)}}{dt} = -l_n F^{(n)} + k_{n-1} F^{(1)} F^{(n-1)}$$

In the above *n-center desorption equations*, *m* ranges from 2 to *n*-1; *P* denotes the rate by which $F^{(1)}$-centers are formed, *a* the rate by which they get emitted from the surface. The $l_i$ and $k_h$ are constants describing the rate at which $F^{(i)}$-centers decay into $F^{(1)}$-centers and $F^{(h)}$-centers combine with $F^{(1)}$-centers to form $F^{(h+1)}$-centers, respectively. In the following this model is referred as nCM – n-center model.

The *n-center desorption equations* are made up of terms describing how each kind of center is formed by other centers and the electron beam and breaks down into smaller centers or gets desorbed. They represent a balance, with no centers entering or leaving the system except by electron bombardment (*P*) and atom absorption ($-a\,F^{(1)}$). The *3-center desorption equations* ($n = 3$, 3CM – 3-center model) are sufficient to get interesting results that can be validated by experimental data ([4]).

The variables and constants are renamed in order to be consistent with a more simple set of equations used in ARGESIM Comparison C1 Lithium Cluster Dynamics – [5]; [6, 7, 8] ($F^{(1)} \rightarrow f$, $F^{(2)} \rightarrow m$, $F^{(3)} \rightarrow r$; $a \rightarrow l_f$, $d_3 \rightarrow d_r$, $d_2 \rightarrow d_m$, $k_1 \rightarrow k_f$, $k_2 \rightarrow k_r$.):

$$\frac{df}{dt} = d_r r + 2d_m m - k_r mf - k_f f^2 - l_f f + p$$

$$\frac{dm}{dt} = d_r r - d_m m + k_f f^2 - k_r mf$$

$$\frac{dr}{dt} = -d_r r + k_r mf$$

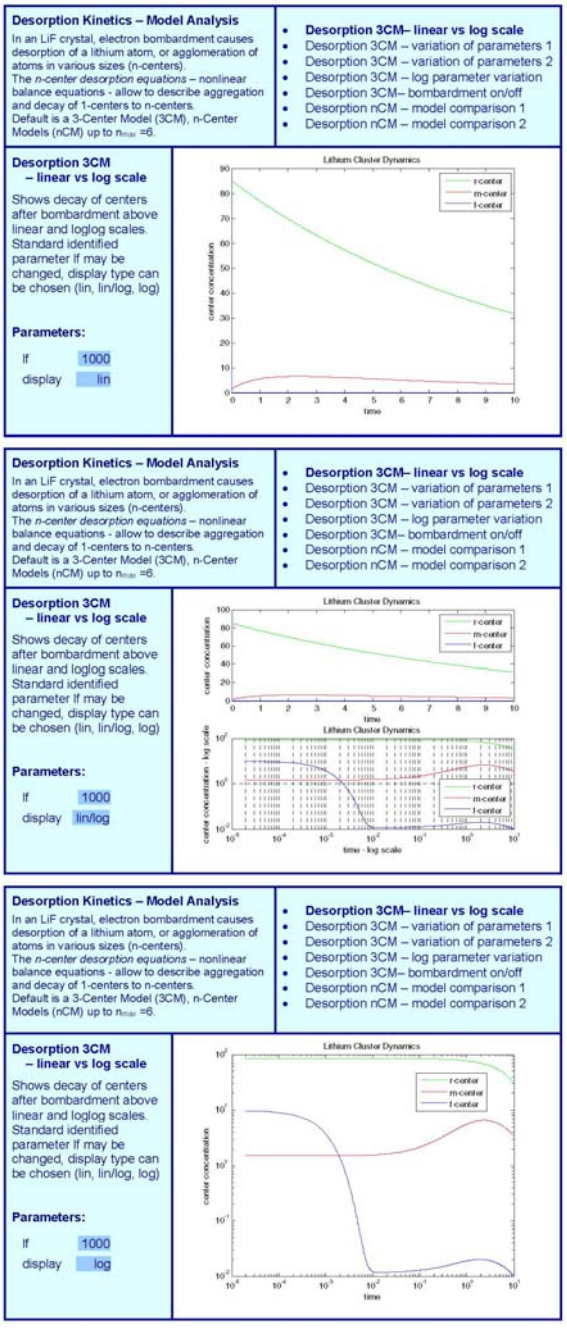


Fig. 7 Module *Desorption 3-center model* comparison of linear and logarithmic scales

In the MMT E-Learning System two variants of modules for the discussed desorption kinetics are implemented. One variant offers model analysis by simulation, parameter variation and model comparison, while the second variant checks numerical features of the ODE solvers and tests approximations. Tasks/experiments for the module *Desorption Kinetics – Model Analysis* are:

1. Desorption 3CM– linear vs log scale
2. Desorption 3CM – variation of parameters 1
3. Desorption 3CM – variation of parameters 2
4. Desorption 3CM – log parameter variation
5. Desorption 3CM– bombardment on/off
6. Desorption nCM – model comparison 1
7. Desorption nCM – model comparison 2

Task (1) simulates the 3-center model with identified, by also changeable parameter $l_f$ (situation after bombardment where center concentrations go back to zero) and shows the necessity of double logarithmic scales: while in the linear scale $f(t)$ is a straight line after an almost vertical decline at $t = 0$, the double logarithmic scale shows the type of the very fast decline at $t = 0$ and the relative maximum of $f(t)$ at $t = 1$ (Fig. 7). Task (2) and task (3) let the user experiment with different model parameters (parameters for behaviour of $f(t)$ or parameters for behaviour of $m(t)$ and $r(t)$, resp.), display in double logarithmic scales. It can be observed, that variation of e.g. $l_f$ shows a 'nonlinear' change of the results.

Task (4) explains the importance and impact of parameter $l_f$ : a logarithmic change of $l_f$ gives a 'linear' change in the results, on logarithmic scales (Fig. 8).

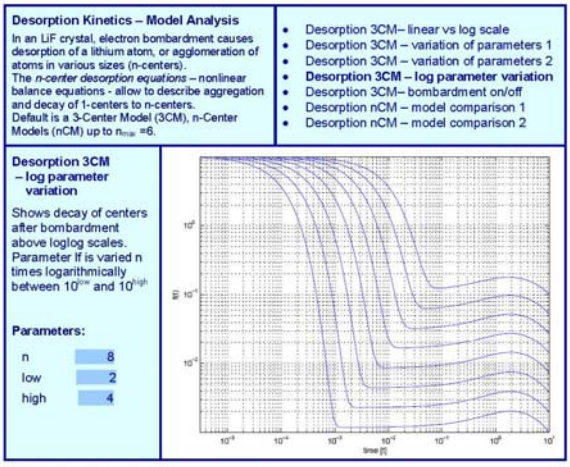


Fig. 8 Module *Desorption 3-center model* logarithmic parameter variation of $l_f$

Task (5) investigates another situation: with identified or smoothly changed 3-center model, bombardment is switched on and switched of – results show that *f*-centers follow almost immediately to the bombardment switching, that *r*-centers increase almost

linear and decrease almost exponentially, and that *m*-centers are only an intermediate stage between *f*-centers and *r*-centers (Fig. 9) – in linear scales.

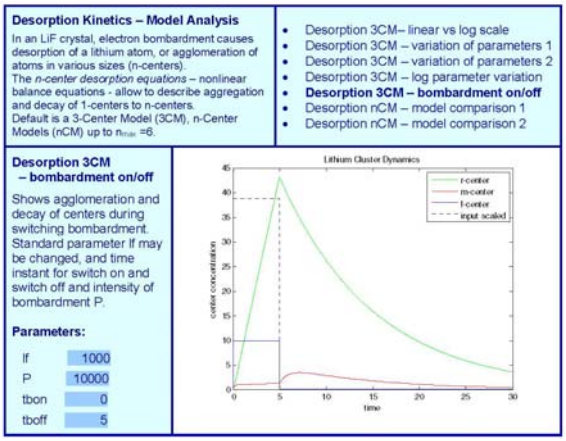


Fig. 9 Module *Desorption 3-center model* – bombardment switching on/off

Task (6) and task (7) compare different n-center models (situation after bombardment). Task (6) selects two nCMs and displays all states for comparison, task (7) compares dynamic of $F^{(1)}$ - centers for all nCMs, $n$=3, ..., 6 (Fig. 10).

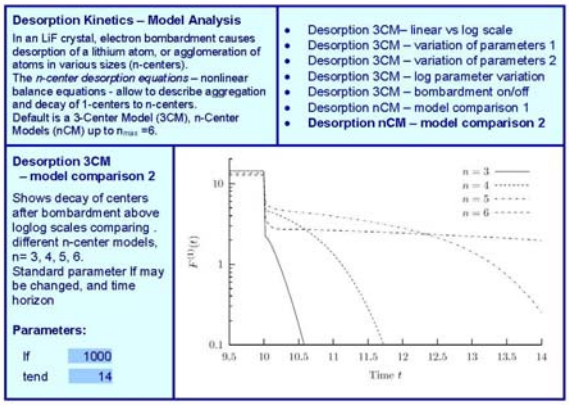


Fig. 10 Module *Desorption n-center model* – comparison for all n-center models, $n$=3, ..., 6

While module *Desorption Kinetics – Model Analysis* supports teaching and learning in the specified application, performing simulation with tuned ODE solvers, the module *Desorption Kinetics – Numerical Analysis* addresses the algorithms in behind and lets the user experiment with ODE solvers for the stiff system, with stiffness quality and with approximations with Taylor series and with linearisations using the Jacobian matrix, mainly with the 3-center model, and partly with the 5-center model. Tasks/experiments with this module are:

1. Desorption 3CM – ODE solver efficiency
2. Desorption 3CM – ODE solver comparison
3. Desorption 3CM – Stiffness analysis
4. Desorption 3CM – Taylor approximation
5. Desorption 3CM – Linearisation
6. Desorption 5CM – ODE solver comparison
7. Desorption 5CM – Stiffness analysis
8. Desorption 5CM – Taylor approximation
9. Desorption 5CM – Linearisation

Task (1) compares the efficiency of MATLAB's ODE solvers by measuring the computation time for a single run, whereby accuracy can be chosen. Fig. 11 shows clearly, that the stiff solvers are the fastest, but also the other solvers seem to work correctly. But Task (2), which compares the output of different solvers for different parameter values of $l_f$ (solver and accuracy to be chosen), shows, that non-stiff ODE solvers tend to overshoot and to oscillate – and to fail in some cases (Fig. 12).

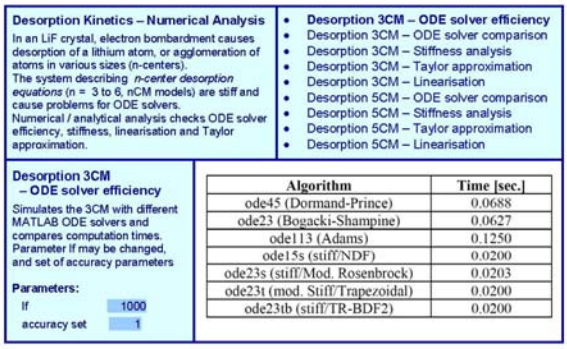


Fig. 11 Module *Desorption 3-center model* – ODE solver efficiency

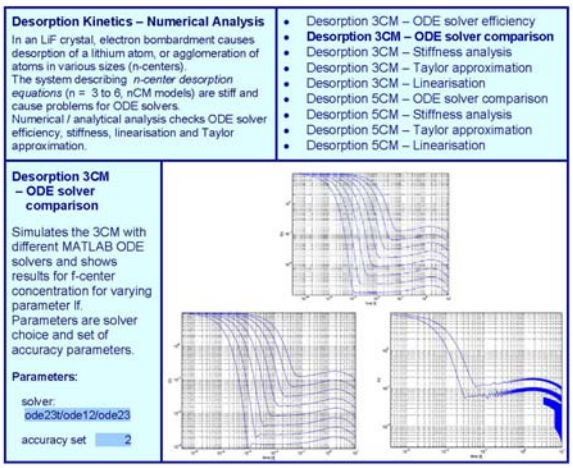


Fig. 12 Module *Desorption 3-center model* – ODE solver comparison for results with variation of $l_f$

While the first two tasks indicate only, that the system under investigation is a stiff system, task (3) checks the stiffness of the system in details and lets conclude, that the system is really stiff because of the size of the stiffness index $S_I(t)$.

The stiffness check is based on the eigenvalues of the linearised system, evaluated over time. For this module, a semi-analytical method is used, which evaluates the symbolically derived Jacobian matrix:

$$J(t) = \begin{pmatrix} -k_r m - 2k_f f - l_f & 2d_m - k_r f & d_r \\ 2k_f f - k_r f & -d_m - k_r f & d_r \\ k_r m & k_r f & -d_r \end{pmatrix}$$

An accurate and tuned ODE solver (for stiff systems) calculates the solutions for $f(t)$, $m(t)$, and $r(t)$ on a time grid, so that for each time instant the Jacobian matrix can be evaluated, and so that for each time instant the (three) eigenvalues can be calculated, resulting in 'eigenvalue function' and the stiffness index $S_I(t)$:

$$\lambda_1(t),\ \lambda_2(t),\ \lambda_3(t)$$

$$S_I(t) = \frac{\max_t \lambda_i(t)}{\min_t \lambda_i(t)}$$

Task (3) makes use of this approach and shows the eigenvalues changing over time, and the stiffness factor (Fig. 13): interestingly the eigenvalues for $f(t)$ remain almost constant (underlining the almost linear behaviour of $f(t)$ as very fast PT1 transfer function), while eigenvalues for $m(t)$ and $r(t)$ span over a range of $10^3$ – and compared with $f(t)$ the eigenvalues range between $10^{-1}$ and $10^3$, so that the stiffness factor $S_I(t)$ ranges between $10^5$ and $10^6$ – the system is really stiff ($S_I(t) > 10^4$). variation of $l_f$ within the reasonable range of 10 $l_f$ and $l_f$ /10 does not change the stiffness factor essentially.

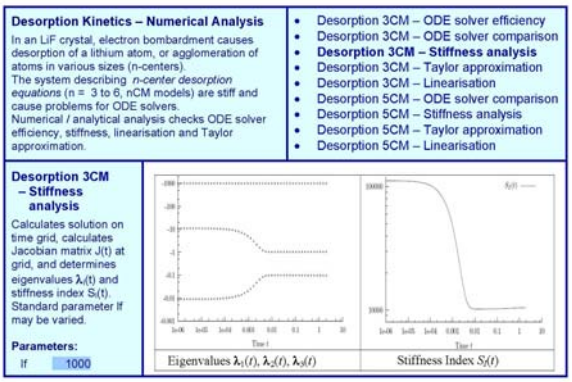


Fig. 13 Module *Desorption 3-center model* – Stiffness analysis

The semi-analytical approach is also used for task (5), where the Jacobian matrix represents the linearisation around the chosen linearisation point. Task (5) compares the nonlinear solutions with linearisations at different linearisation points.

Instead of linearisation, task (4) makes use of Taylor series expansion for approximation of the nonlinear system. The *3-center desorption equations* can be used to calculate semi-analytically the derivates of $f(t)$, $m(t)$ and $r(t)$ recursively for setting up the Taylor series, resp the Taylor polynomial of degree $k$:

$$T_k(f, \hat{t})(t) = \sum_{i=0}^{k} \frac{f^{(i)}(\hat{t})}{i!}(t - \hat{t})$$

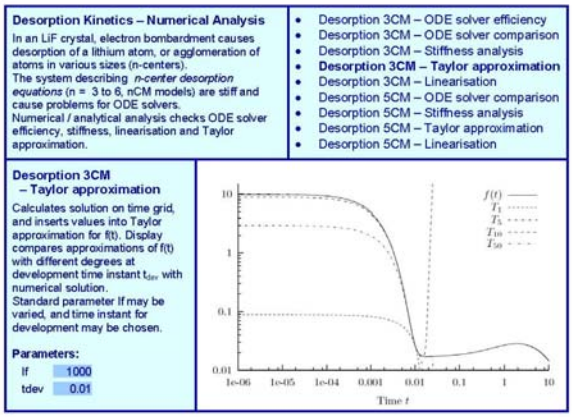


Fig. 14 Module *Desorption 3-center model* – Taylor approximation with different degrees at specified time instant

Task (4) allows choice of time instant for expansion and calculates taylor polynomials for fifferent degrees and compares with nonlinear solution over time (Fig. 14).

Task (6) – task (9) repeat tasks /experiments (1), (3)-(5) for a 5-center model. For details of mathematical back-ground, see [5].

## 5 Module Radioactive Migration

The basic Principles for the Migration of (radioactive) pollutants are diffusion, advection with groundwater flow or rain fall and sorption. When considering radioactive pollutants, radionuclides, also the radioactive decay of the respective radionuclides have to been taken into account.

Radionuclides might be released to the environment i.e. by fallout after nuclear weapons testing, or by a damaged satellite. They may be spread in the air for some meters by wind until they adhere to plants and crops. When it rains, these radio-elements are washed towards the grassroots, and deposition in the soil occurs. Now, further migration can take place via two different processes, which are basic key terms in the transport equation, namely diffusion in the soil, and advection with the rain water.

Diffusion is a physical equilibrium process, whereby molecules, atoms or ions move from areas having a high radioactive concentration $c(t, x, y, z)$to areas showing low radioactive concentration, caused by Brownian motion. The underlying three-dimensional equation is also known as Fick's Law, whereby $D_W$ represents the diffusion constant in the respective medium:

$$\frac{\partial c}{\partial t} = D_w\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}\right) = D_w \nabla^2 c$$

The second migration process, central advection, occurs due to the flow paths for groundwater within the soil and therefore enables another possibility of migration for pollutants. Advection by rainwater is the dominant migration process for trans-uranium elements. In this migration model advection is defined as the movement of dissolved particles in the flow of surrounding water and describes the dispersion of radionuclides. The advection term in the model is described has a certain velocity $\vec{u}$ and is defined as:

$$\frac{\partial c}{\partial t} = -\vec{u} \nabla c$$

Thereby $\vec{u}$ represents the fluid velocity, and $-\vec{u} \nabla c$ is the advective term.

Most radionuclides exhibit a very slow movement, with typical estimated travel times from a geological repository depth to the surface exceeding half-lives of many radionuclides. Thus, the migration process of pollutants in soil has to be described by the diffusion equation and advective term. Using empiric data for all constants used, this migration model works for any pollutant so far.

Now the special case of migration of radionuclides will be further investigated. The rate of decay of a radionuclide is described by its activity *A*, which is the number of atoms that decay per unit time. The probability of radioactive decay is represented by the decay constant $\lambda$, and depends on the half life of the respective radioculide.

$$A(t) = A_0 \exp(\lambda t)$$

The activity concentration depends on the respective radionuclide itself. If the released radionuclide decays to a stable product, the activity concentration will be decreased.

This model was implemented by a cellular automata approach. The CA-approach represents environmental condition on the release of radioactive elements at the best. Even though this approach is often referred as a simple black-box approach, it is shown that it is even able to conserve conservation quantities (i.e. amount of substance). The migration is described by using the transport equation, which is a combination of diffusion and advection. However, the spreading is blocked by different sorption processes, which can not described in a mathematical form. Therefore, they are realized by the help of retardation factors.

For more information on the model development see [9, 10, 11]. The development of the model is kernel of a PhD dissertation [12].

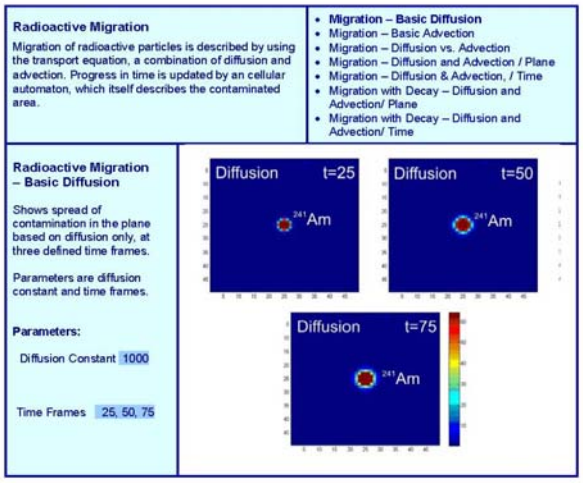


Fig. 15 Module *Radiactive migration* – Basic diffusion with three different time frames

The MMT module Radioactive Migration makes use of a simplifier 2D-implementation of the 3D- migration process, due to computation times, and shows the migration at certain time frames:

1. Migration – Basic Diffusion
2. Migration – Basic Advection
3. Migration – Diffusion vs. Advection
4. Migration – Diffusion and Advection / Plane
5. Migration – Diffusion & Advection, / Time
6. Migration with Decay – Diffusion and Advection/ Plane
7. Migration with Decay – Diffusion and Advection/ Time

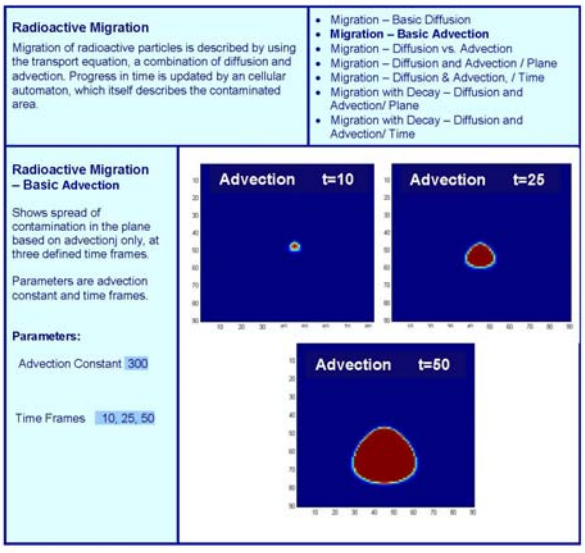


Fig. 16 Module *Radiactive migration* – Basic advection with three different time frames

Task (1) investigates migration with basic diffusion, experiments with diffusion parameter for chosen timeframes (Fig. A) – spread of circle type. As contrast, Task (2) investigates migration with basic advection, experiments with advection parameter for chosen timeframes (Fig. B) – spread of drop type. Task (3) compares pure diffusion and pure advection, with parameters for diffusion and advection, at same time frames.

## 6 References

Tasks (4) and (5) invite for experiments with both diffusion and advection, with display in the plane – like Task (1)-(3), or as function of time for one coordinate. And Tasks (6) and (7) add to experiments of type (4) and (5) decay of radiation.

This module may not only be used in physic's lectures, but also in lectures for modelling and simulation, in order to demonstrate modelling with cellular automata.


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