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# Finding appropriate model parameters for luminescence simulations: inverse modelling and model fitting with RLumModel

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Kinetic models of quartz luminescence have gained an important role for predicting experimental results and for better understanding charge transfers in (natural) quartz. Mathematically, the models comprise a set of several ordinary coupled first-order differential equations (ODEs), which describe the evolution of electron and hole populations on the time domain within quartz under various conditions, e.g., irradiation, light illumination or heating. In the last years, a number of parameter sets for modelling luminescence were presented in the literature. However, accurately simulating luminescence using this ODE approach first requires finding a set of numerical parameters (e.g., concentration of defects, transition probabilities, cross-sections, …), which best reflects the experimental data. The approaches applied in the past were mainly based on (a) manually changing model parameters via try and error and/or (b) using a genetic algorithm (Adamiec et al. 2004).

In our contribution, we present the newest version of the R-package 'RLumModel' (Friedrich et al. 2016). 'RLumModel' is an easy-to-use tool for simulating quartz luminescence signals based on the energy band model. The new version (0.3.0) enables 'sensitivity analysis' of model parameters and 'inverse modelling' via Markov-Chain Monte-Carlo (MCMC) methods. Own measurement results can be imported to R and used to fit model parameters.
Some model parameters have little effect on the model outcome, while other parameters are too similar and cannot be fitted simultaneously. A 'sensitivity analysis' estimates the sensitivity of the model output with regard to specific input parameter values.
Once parameters with large impact on the results were identified, this parameters can be fitted to experimental data using Markov-Chain Monte-Carlo (MCMC) methods which are a class of algorithms for sampling from a probability distribution based on constructing a Markov chain.
This results in good matches between simulated and experimentally measured TL and OSL signals. Whether the obtained results for the parameters are (physically) meaningful or whether this approach is only a mathematical technique fitting model parameters to experiments is critically discussed.

The approach of using sensitivity analysis and inverse modelling can be applied to other modelling problems in Earth Sciences, too.

References

Adamiec G. et al. (2004), Geochronometria 23: 9-14.
Friedrich J. et al. (2016), Quaternary Geochronology 35: 88-100.