

LJUNGSKILE - probabilistic speciation

The probabilistic speciation code LJUNGSKILE couples PHREEQC with a Latin Hypercube Sampling approach to allow an efficient calculation of species diagrams with uncertainties.

LJUNGSKILE has been developed by [A. Ödegaard-Jensen](#), [C. Ekberg](#) and [G. Meinrath](#) in a cooperation between Chalmers University of Technology at Göteborg/Sweden, RER Consultants Passau/ Germany and Technische Universität Bergakademie Freiberg/Germany.

The zipped code for the 2nd version LJUNGSKILE 2.0 is available for download (LJUNGSKILE 2.0). Unzip the package into one appropriate directory. The package includes all necessary programs, an example data base and example files for projects. Upon starting setup.exe, the user is guided through the installation process. The following files will be installed:

a) programs:

- phreeqc.exe (the public domain speciation code)
- simulation.exe (Borland C++)
- Ljungskile20.exe (Borland C++)
- LDP20.exe (Visual Basic 5.0)

b) example project files:

- example_Al.prj
- example_Fe.prj

c) data bases:

- example.dat

A manual for the 1st version LJUNGSKILE 1.0 is available from Swedish Nuclear Power Inspectorate ([SKI03_03.pdf](#)). This report gives a step-by-step description of a Ljungskile project setup, execution and analysis. The extensions for LJUNGSKILE20.exe and LDP20.exe are described in TALANTA. Coordinates of the manuscript will be given as soon as available.

step-by-step procedure:

- a) download the zipped file LDP20.zip
- b) download the Ljungskile 1.0 manual
- c) get the TALANTA paper "LJUNGSKILE - A computer program for assessing uncertainties in speciation calculations" (in press)
- d) unzip the LDP20.zip
- e) run the examples

Features of the LJUNGSKILE20 and LDP20:

- drastically improved stability
- allows to specify a solid phase and a gaseous phase simultaneously
- additional functionality in the Ljungskile Display Program
 - select different confidence regions
 - select/deselect species from the calculation