optpar.txt

The file holds additional model options to info.txt and is therefore located in the same folder as info.txt. The file is used to define what kind of optimisation to be done if calibration is set in info.txt. There are several different methods to chose from, each with their settings. Which model parameters to calibrate and within which boundaries are information also given in *optpar.txt*.

Maximum 100 model parameters may be optimised simultaneously. To optimise more parameters, the code needs to be changed (set *maxoptpar* to a higher value). All parameters are described in the section on par.txt, but not all of them can be calibrated. The objective function of the optimization is defined in info.txt as the combination of criteria chosen, see Performance criteria options.

There are eight methods of optimisation implemented in HYPE as detailed in the table below. Additionally, there are two other tasks for output generation, WA and WS, which produce detailed performance and simulation results for all runs performed during optimisation. Tasks WA and WS are compatible with selected optimisation methods only, a denoted in the table. The task of organized scanning SC is a parameter investigation method.

Task	Description
MC	Monte Carlo (MC) simulation with parameter values randomly distributed over the intervals (basic MC-method)
ВР	progressive Monte Carlo simulation with parameter space limited by best found so far (alternative MC-method)
SM	progressive Monte Carlo simulation with parameter space reduced in stages (alternative MC-method)
DE	Differential Evolution Markov Chain method (alternative MC-method)
BN	optimisation with Brent method
Q1	optimisation with QuasiNewton DFP gradient-based method
Q2	optimisation with QuasiNewton BFGS gradient-based method
SD	optimisation with QuasiNewton steepest descent method
SC	organised scanning of two parameters
WA	write performance result for all simulations (MC, SM or DE)
WS	write simulation results (basin-, time- or map-files) for all ensembles in Monte Carlo simulation (MC, BP, or DE) (maximum 9999999 ensembles total)

File content

The first row is for general comments. It is ignored by the program when reading the file. Next comes a section with calibration settings. It reaches from second to 21st row, and are used to define tasks and other settings. Last comes a section defining the parameters to be calibrated. These occupy row 22 and onward.

In the calibration setting section a row starts with a code indicating a task or other settings. Argument of the code is listed from position 12 and forward on each row. The following options are available for the calibration setting section:

Code	Argument	Default value	Description
task	two letter word	FALSE	define what kind of optimisation to do (see methods above), and if additional results are to be written for the MC-methods
cal_log	Y/N	YES	flag for writing a calibration.log file
scan_numx	integer	1	number of steps taken for the first parameter (SC method)
scan_numy	integer	1	number of steps taken for the second parameter (SC method)
num_mc	integer	1000	number of Monte Carlo simulations (per centre point and stage for progressive MC)
num_ens	integer	1	number of best Monte Carlo simulations to keep and print results from (and use as centre points for next stage of progressive MC) (maximum 999)
num_bpmc	integer	200	number of simulations per reduced parameter space which the best simulations shall be selected from (BP MC-method)
num_bpmax	integer	100	number of reductions of the parameter space for MC simulation (BP MC-method)
num_stages	integer	1	number of stages for progressive Monte Carlo (SM MC-method)
num_zoom	real	0.9	reduction of parameter space (0-1) for each stage of progressive MC (BP MC-method)
DEMC_ngen	integer	100	number of generations for DEMC method
DEMC_npop	integer	25	number of populations for DEMC method
DEMC_gammascale	real	1	scaling of the mutation strength for DEMC method. A new (next generation) parameter candidate is proposed as a mutation of the parent parameter value based on the difference between two random members of the parent population. DEMC_gammascale is a scaling factor for the resulting parameter jump width. Small values will cause smaller mutations, which potentially stabilises the search through large parameter spaces at the cost of convergence speed. A value of 1 will result in no scaling.
DEMC_crossover	real	1	crossover probability for DEMC method. Probability that the proposed candidate is chosen instead of the parent parameter. Large DEMC_crossover values mean larger probability that the proposal is chosen. Set to 1, all proposals are accepted. This makes it harder to find an acceptable overall proposal because all parameters are changed in every generation. Set to 0.5, each parameter candidate has only a 50% chance to be accepted into the next proposal.
DEMC_sigma	real	0.1	sample error standard deviation for DEMC method. Base for the standard deviation of the random perturbation, which adds random noise to the proposed parameter in addition to the gamma-mutation. This value is multiplied with 3rd-row value for each parameter (see description of parameter rows below).

Code	Argument	Default value	Description
DEMC_accprob	integer	0	scaling factor for probabilistic acceptance for DEMC method (0 = off (default); >0 = on). If set to off, parameter proposals will only (and always) be accepted if the likelyhood score decreases (= better performance). If turned on, also proposals with higher likelyhood score can be accepted; better performance will give higher probability of acceptance. High values of the scaling factor will also increase the probability of acceptance.
BR_diagStp	Y/N	YES	flag for taking a diagonal step at the end of each iteration (BN method)
num_maxItr	integer	500	max amount of iterations (interrupt non-MonteCarlo methods)
num_maxTim	integer	72	max calibration time (hours) (interrupt non-MonteCarlo methods)
num_parItr	integer	10	number of iterations taken into account for parameter change tolerance (interrupt non-MonteCarlo methods)
num_criItr	integer	10	number of iterations taken into account for criterium change tolerance (interrupt non-MonteCarlo methods)
num_criTol	real	0.001	tolerance for criteria relative change over last iterations (interrupt non-MonteCarlo methods)
lnS_maxItr	integer	500	max amount of line search iterations (per line) (non- Monte Carlo methods)
lnS_tol	real	0.001	general relative tolerance for line search (non-Monte Carlo methods)
QN_nrmTol	real	0.001	tolerance for gradient norm to be considered zero (QN methods)
QN_pctDerv	real	0.02	factor to offset current parameter values for numerical derivative (QN methods)
QN_stencil	integer	2	numerical derivative stencil type (2, 4, 6 and 8 allowed) (QN methods)
QN_lambMax	real	0.9	factor of parameter interval, used to limit the step length of the line search within given parameter intervals (QN methods)
QN_lambAcc	real	1.618	factor increasing the step length of the line search (QN methods)

From row 22 and onward, model parameters to be calibrated are listed. The parameter is given as it is or with single quotation marks (e.g. 'cevp') followed by its values. For non-general parameters, values for all soil types/land uses/subbasins/parameterregions/etc have to be provided.

Each parameter is defined on three rows:

- Row 1 specifies lower boundaries of the parameter range
- **Row 2** specifies upper boundaries of the parameter range (the model actually accepts lower and upper boundaries in any order)
- **Row 3** specifies either a minimum step width for parameter change *or*, in case of the DE method, a parameter specific factor to scale the random noise added to the proposed next-generation parameter, see description of DEMC settings code DEMC_sigma in table above.

NOTE: If lower and upper boundaries are identical, the parameter is omitted. This allows to calibrate a selection of the values for dependent parameters.

Example of parameter rows in *optpar.txt*:

```
wcfc
    0.100 0.020 0.120 0.050 0.250 0.250 0.150 0.050 0.500 0.500 0.050
wcfc
    0.100 0.120 0.120 0.050 0.250 0.250 0.150 0.050 0.500 0.500 0.050
wcfc
    0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
ttmp    0.0    0.0
ttmp    2.0    2.0
ttmp    0.01 0.01
```

Explaination of example: The rows starting with wcfc are representing field capacity for 11 soil types, where the second soil type's wcfc is calibrated. Parameter ttmp is threshold temperature for 2 land uses, which are both calibrated.