Run Dyssol using command line

1. Running with command line

With the help of provided *DyssolC* tool the command line calculations can be performed. The command *DyssolC* can be started from the command prompt. As the single input argument a configuration file must be provided:

```
> DyssolC.exe script.txt
```

The *DyssolC.exe* file can be found in the installation directory of Dyssol.

2. Configuration file

The configuration file is a text file with the format described in Table 1.

Only 3 parameters from the list are mandatory parameters: SOURCE_FILE, MODELS_PATH, MATERIALS_DATABASE. The rest are optional and will override parameters set in initial file, specified as SOURCE_FILE. If RESULT_FILE parameter is not specified, results of the simulation will be written to a SOURCE_FILE.

Parameters MODELS_PATH, DISTRIBUTION_GRID, UNIT_PARAMETER, UNIT_HOLDUP_* can be mentioned several times in the script file, the rest should be places only ones.

An exemplary configuration file *ExampleConfigFile.txt* is available in the installation directory of Dyssol.

Table 1 – Available parameters

Identifier	Parameters
General	
SOURCE_FILE *Full path to the *dflw file with initial flowsheet*	`C:\Path\to\source\file.dflw`
RESULT_FILE *Full path to the file where simulation results will be written*	`C:\Path\to\result\file.dflw`
MODELS_PATH *Path to the directory where *.dll libraries of units and solvers can be found*	`C:\Path\to\dir\with\models\`
MATERIALS_DATABASE	`C:\Path\to\database.dmdb`

Full path to the file with materials database	
Simulation	
SIMULATION_TIME *End simulation time in [s]*	<value>
Options	
RELATIVE_TOLERANCE	<value>
ABSOLUTE_TOLERANCE	<value>
MINIMAL_FRACTION	<value>
INIT_TIME_WINDOW	<value>
MIN_TIME_WINDOW	<value>
MAX_TIME_WINDOW	<value>
MAX_ITERATIONS_NUM	<value>
WINDOW_CHANGE_RATE	<value>
ITER_UPPER_LIMIT	<value>
ITER_LOWER_LIMIT	<value>
ITER_UPPER_LIMIT_1	<value>
CONVERGENCE_METHOD *Convergence method*	<method> <method> = 0 – Direct substitution; <method> = 1 – Wegstein; <method> = 2 – Steffensen;
ACCEL_PARAMETER *Parameter of Wegsten's method*	<value>
RELAX_PARAMETER *Parameter of Direct Substitution method*	<value>
EXTRAPOL_METHOD *Extrapolation method*	<method> <method> = 0 – Linear; <method> = 1 – Cubic spline; <method> = 2 – Nearest neighbor;
Grids	
DISTRIBUTION_GRID *Specification of meshes for distributed parameters of solids*	General form: <distribution> <type> <classes> [<grid>] (<min> <max> | <boundaries> | <names>) For Continuous not Manual: <distribution> <type> <classes> <grid> <min> <max> For Discrete or Continuous Manual: <distribution> <type> <classes> <boundaries> For Symbolic: <distribution> <type> <classes> <names> <distribution> – index of the distribution as it stated in Grid Specification window <type> – distribution type: 0 – Continuous 1 – Discrete 2 – Symbolic <classes> – number of classes <grid> – type of the grid (if <type> = 0): 0 – Manual 1 – Equidistant 2 – Geometric increasing 3 – Logarithmic increasing

	4 – Geometric decreasing 5 – Logarithmic decreasing <min> – min value (if <type> = 0 and <grid> != 0) <max> – max value (if <type> = 0 and <grid> != 0) <boundaries> – class boundary values ((if <type> = 0 and <grid> = 0) or (if <type> = 1)) <names> – names of classes boundary values (if <type> = 2)
Unit parameters	
UNIT_PARAMETER *Specification of unit parameters*	General form: <unit> <parameter> (<value> | <time> <value> [<time> <value> […]] | <string> | <solver>) For constant parameter: <unit> <parameter> <value> For time-dependent parameter: <unit> <parameter> <time> <value> [<time> <value> […]] For string parameter: <unit> <parameter> <string> For solver parameter: <unit> <parameter> <solver> <unit> – index of the unit <parameter> – index of the parameter <value> – numerical value of the parameter <time> – value of the time point (for time-dependent parameters) <string> – numerical value of the parameter (for string parameters) <solver> – name of a *.dll file with solver (for solver parameter)
Holdups	
UNIT_HOLDUP_MTP *Specification of holdups: mass, temperature and pressure*	<unit> <holdup> <timepoint> <mass> <temperature> <pressure> <unit> – index of the unit <holdup> – index of the holdup in the unit <timepoint> – index of the time point <mass> – mass value <temperature> – temperature value <pressure> – pressure value
UNIT_HOLDUP_PHASES *Specification of holdups: phase fractions*	<unit> <holdup> <timepoint> <fraction> [fraction […]] <unit> – index of the unit <holdup> – index of the holdup in the unit <timepoint> – index of the time point <fraction> – mass fraction of the phase, number of parameters must correspond to the number of phases
UNIT_HOLDUP_COMP *Specification of holdups: compound fractions in phase*	<unit> <holdup> <phase> <timepoint> <fraction> [fraction […]] <unit> – index of the unit <holdup> – index of the holdup in the unit <phase> – index of the phase <timepoint> – index of the time point <fraction> – mass fraction of the compound, number of parameters must correspond to the number of compounds
UNIT_HOLDUP_SOLID *Specification of holdups: distributed parameters of solids*	<unit> <holdup> <distribution> <compound> <timepoint> <psdtype> <function> <psdgridtype> (<param1> <param2> | <values>) <unit> – index of the unit <holdup> – index of the holdup in the unit <distribution> – index of the distribution as specified in Distributions Sequence

	<compound> – index of the compound, 0 – for total mixture <timepoint> – index of the time point <psdtype> – PSD type, if <distribution> corresponds to a PSD: -1 – Not a PSD 0 – q3 1 – Q3 2 – q0 3 – Q0 4 – Mass fraction 5 – Number 6 – q2 7 – Q2 <function> – index of the distribution function: 0 – Manual 1 – Normal distribution 2 – RRSB 3 – GGS 4 – Logarithmic Normal <psdgridtype> – type of the grid if <distribution> corresponds to a PSD: -1 – Not a PSD 0 – Diameters 1 – Volumes <param1>, <param2> – parameters of the distribution function (only if <function> != 0) <values> – list of distribution values (only if <function> = 0)