Supplementary Material to

Mixed-integer optimization of distillation sequences with Aspen Plus: A practical approach

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1 Implementation of the mGBD Algorithm

The mGBD algorithm as described in the sections 3 and 5 of the main article has been implemented in Microsoft Excel VBA and the corresponding Excel files of Tab. 1, Tab. 2, Tab. 3, and Tab. 4 are available in the supplement. They are following the notation: "ExtractiveDist_x_y_z.xls", where x is the number of respective tables of the main article, y is the table row, and z is the initial integer set.

x

Tab. 1: Optimization results for four different optimization strategies (see section 3.2) for four sets of initial integer variables

		z Set 1	Set 2	Set 3	Set 4
Initial	TAC (T€/a)	840,58	801,51	860,34	862,03
	$(N_1,N_2,N_3,N_4,N_5)^*$	(23,12,30,17,25)	(30,8,39,12,25)	(23,12,39,17,25)	(23,3,27,4,11)
GBD Discard: Off Fix: Off Decomp.: Off	TAC (T€/a)	784,62	776,47	780,15	777,14
	$(N_1,N_2,N_3,N_4,N_5)^*$	(22,5,30,10,19)	(24,4,32,6,13)	(24,5,31,7,17)	(22,4,29,6,15)
	No. of outer iter. (l)	1	1	1	1
	No. of inner iter. (k)	24	23	12	17
	Non-converged runs	3	1	0	0
	Time (sens.) (min)	34,28 (15,33)	36,38 (18,35)	17,98 (8,91)	28,74 (12,95)
mGBD	TAC (T€/a)	775,76	776,47	775,93	776,43

To run the mGBD algorithm, an Aspen Plus installation and the Excel add-in OpenSolver are required. The Aspen Plus document file ("ExtractiveDistillation.apw"), the backup file ("ExtractiveDistillation.bkp"), and the Aspen Plus Problem Definition file ("ExtractiveDistillation.appdf") have been generated by Aspen Plus V8.8 and are provided in the supplement. To run the mGBD algorithm, only the Aspen Plus document file is needed.

The following steps to run the mGBD algorithm are required:

1. Copy the Excel and Aspen Plus files to the same folder

2. Add OpenSolver as Excel add-in

3. Configure VBA to work with the automation server

4. Run the mGBD algorithm

1.1   Copy Excel and Aspen Plus files

The Excel and Aspen Plus files have to copied to the same folder. To obtain a higher processing speed, it is recommended store the files locally on your machine.

1.2   Add OpenSolver as Excel add-in

Open the Excel file and add the OpenSolver as Excel add-in "Add-Ins" of the Developer tab.
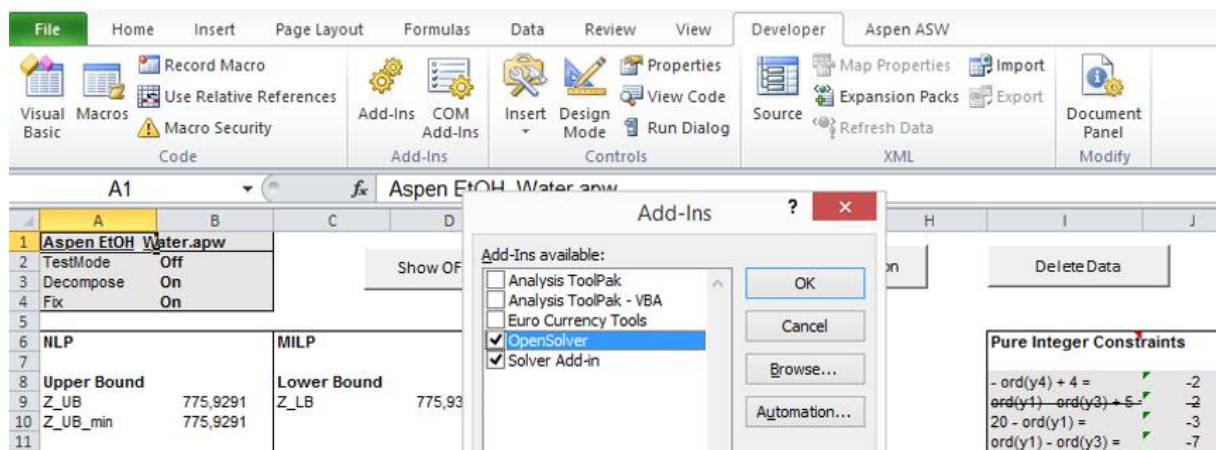
The OpenSolver for Excel (Mason, 2012) is an open source linear, integer, and non-linear optimizer for Microsoft Excel. The OpenSolver add-in can be downloaded from the *opensolver.org* website.

1.3   Configure VBA to work with the automation server

In "Visual Basic" of the Developer tab in Excel (Alt + F11), select the menu bar "Tools" and click "References".

Browse the drop-down menu and check "Aspen Plus GUI XX.X Type Library", where "XX.X" is the version of Aspen Plus installed on your machine. Click OK after your choice to complete the reference.

1.4 Run the mGBD algorithm

On the "Master" sheet of the Excel file, the grey cells can be modified, for example, the initial values in cells P8 to P12. The mGBD algorithm is started by clicking on the button "Start mGBD Algorithm".

It is not necessary to open Aspen Plus.

It is possible to run a single simulation separately by clicking on the button "Run Single Simulation".

In this case, the objective function and variable values and sensitivity information are copied to the

actual line of the Excel sheets "GBD" and "Sensitivities", respectively. The actual line L is always the line where the next empty cell of column F ("objective function Z") is located. The initial variables, that is the entrainer flow rate and the integer variables, are taken from the line above: cells G(L-1) and (CF(L-1):FB(L-1)), respectively.

It is also possible to run a single optimization run, where the entrainer flow rate is optimized at fixed integer values as entered in Aspen Plus ("Run Single Newton"). In this case, the Aspen Plus program should be open and no data will be copied to the Excel sheets.

The actual objective function values can be retrieved from Aspen Plus by clicking on the button "Show OF Values". After an optimization run the data can be erased by clicking on the button "Delete Data". The default parameters can be restored by clicking on the button "Set Default", while the default parameters are kept in the Excel worksheet "DefaultParameter".

2   Final Remarks

The main algorithm is stored in the VBA module "Algorithm_mGBD". Refer to the other modules for the sub procedures called in the main module.
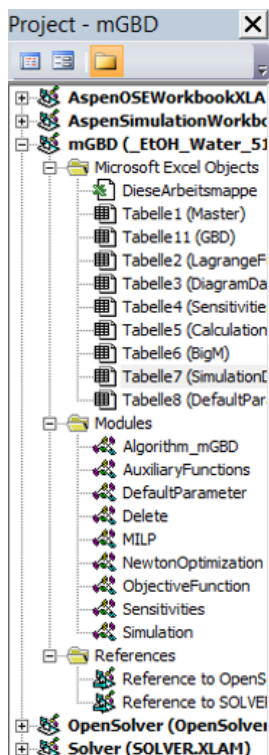
If an Aspen Plus error occurs,
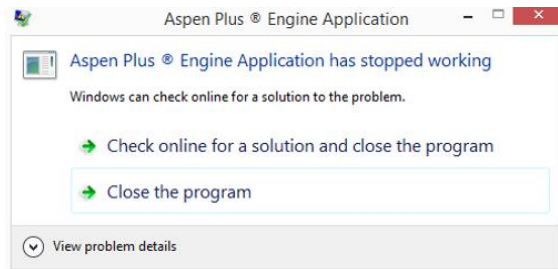
the algorithm can be continued by clicking "Close the program".

3 Literature

Mason, A. J. (2012). OpenSolver - An Open Source Add-in to Solve Linear and Integer Progammes in

Excel. In D. Klatte, H.-J. Lüthi, & K. Schmedders, *Operations Research Proceedings 2011* (S.

401-406). Berlin, Heidelberg: Springer.