Beta µ |MODFLOW| | PEST

Spreadsheet Interface Workflow Documentation

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Beta µ |MODFLOW| | PEST

A mathematical, 3D numerical groundwater model converts precipitation into flow. Considers several different factors such as the soil moisture and evaporation rates, the permeability and declivity of a certain area, its materials distribution and so on. Then develops a cross-referencing function of all the available data with the water levels from monitoring wells. Once its math's rightness is ascertained, the model replicates a given problem on your computer scream.

As an application device (App); Dynamic in its openness to improvements; Modular and flexible in terms of quality, quantity and physical distribution of all utilized information: The numerical model aids the understanding of a problem. Forecasts future scenarios, therefore, supports the decision making, helping the management and dimensioning of an eventual intervention.

1. PURPOSE

This document discusses, strictly, the Beta µ initiative's technical, operative process.

Currently available in the format of a free of charge electronic spreadsheet (MS Excel plus some VBA shortcuts *.xlsm), Beta µ comes to facilitate the use of USGS|MODFLOW|PEST related codes.

So far, it may be viewed as a plugin of the renowned GMS|AQUAVEO graphical interface (GUI).

2. TECHNOLOGICAL SCENARIO

There is a perception that the MODFLOW, or, to put it more precisely, the PEST tools are not being exploited to its full potential. Apart to its well acknowledged, undeniable efficacy, the code still poses a reasonably complex challenge on its usage. Beta µ spreadsheet aims to make things easier.

PEST essentially automates the model parameters selection through mathematical regularization. Furthermore, according to recent studies, the PEST related mechanisms is also a suitable technique of assessing the uncertainty of numerical models, to the benefit of the decision-making process.

Beta µ provides a platform that addresses significant difficulties in dealing with extensive and varied amounts of MODFLOW | PEST related datasets.

GMS|AQUAVEO commercial platform was chosen here regarding its extensive [PEST] track record, and the prominent position of such GUI in the international scene. Indeed, the method can be adapted to others routines, as the USGS Model Muse, Feflow, FloPy or WST Vistas, among others.

Figure 1: What follows is the main Beta µ spreadsheet screen already in practice (at the IN tab).

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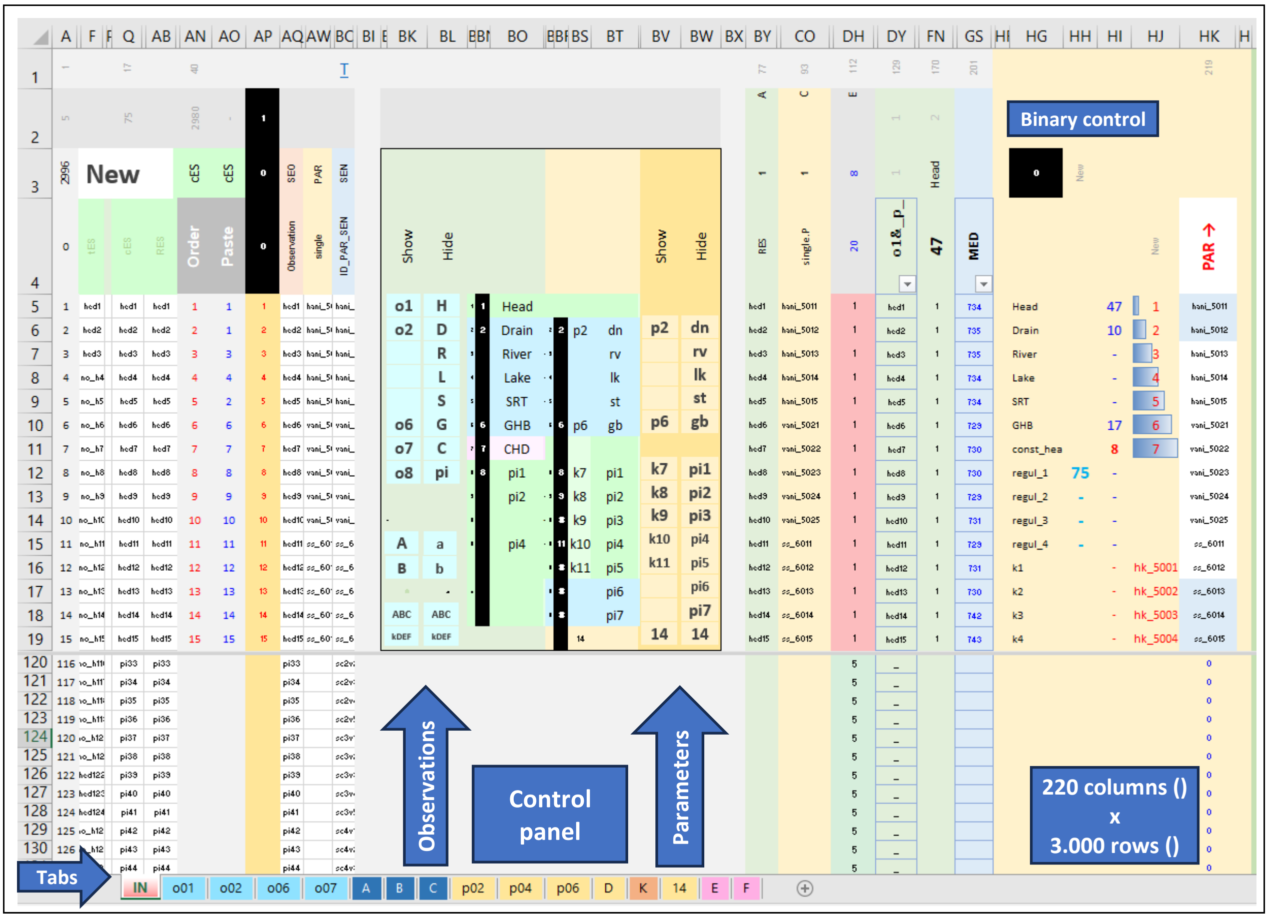

Figure 1: Summarizing the Beta µ spreadsheet; Control Panel & Global Account: Linked-In Tprogs project – Tab IN

https://shorturl.at/TYcYx - This example works out 47 hydraulic heads (m). Calibrates steady state water levels (RWL) and implements a routine to estimate all boundary conditions fluxes (m^3/d). 10 Drains, 17 GHB and 08 CHD boundary observed fluxes challenge a parameters dataset of mirrored 10 DRN and 10 GHB conductances, plus 05 pilot points of 05 hydrofacies together with its related horizontal and vertical anisotropy coefficients (HANI, VANI).

This main tab (**Figure 1**) displays the present case as a whole. Here observations o01-o02-o06-o07 compels the p02-p06, D-K parameters list. Mass balance and objective function Φ can be reached at the A, B, C tabs, while tab F discusses compiled sensitivities and susceptibilities (SEN - SEO).

Just out of curiosity, this procedure storages the data and does the processing of an [220 x 3,000] “Excel matrix”, the shortest routine with the required resourcefulness to deal with a wide variety of possible combinations, in different projects. More of its inner works will be shown in time.

The Beta µ spreadsheet goal is the identification of recurrent tasks, not waste any opportunity for its automatization. The user must be freed from each problem solved, to carry on in finding new insights on both, the geological problem at hand and the needed mechanisms to overcome it.

A nocode design, as open as possible, seeks to facilitate access to the implemented routines.

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3. THE BETA µ ROUTINE

The spreadsheet proposes an all-in-one environment to [handle back and front-end] information from any MODFLOW | PEST realization, regardless of all-possible combinations of inputs.

Ready to adapt to the use of diverse distributions of parameters and observations, it standardizes the data processing routines, so that the most varied tasks are subject to just a few manipulation mechanisms.

At Figure 2 observations [tabs H, DRN, GHB, CHD], from the “measured” and modeled datasets (MED, MOD), becomes charts containing different interrelated aspects of it, including sensitivities, which in its turn will have strong implications on any project. See objective function Φ afterwards.

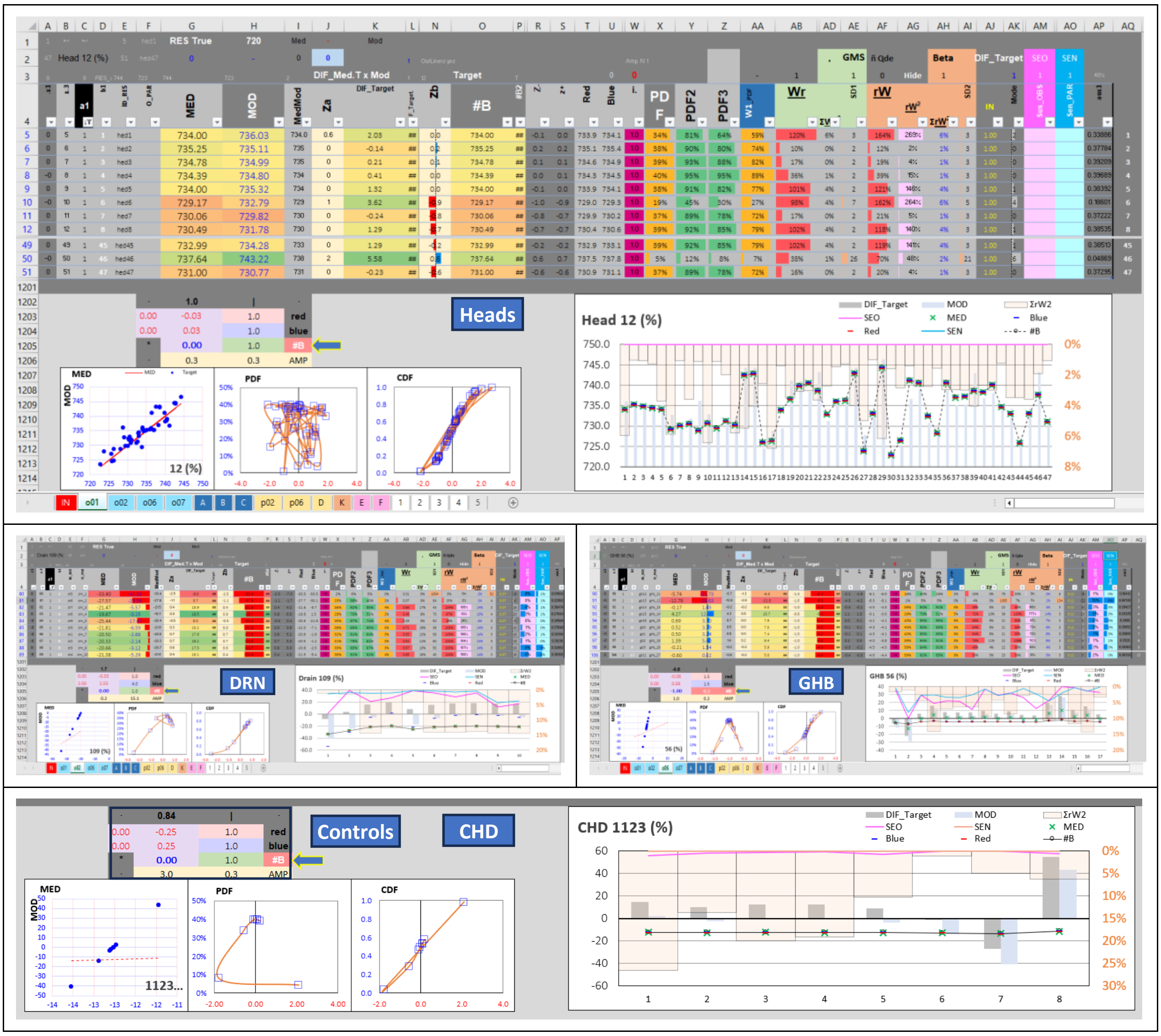

Figure 2: Observations – OBS – of Heads and all Boundary Conditions (H, DRN, GHB, CHD) – Tabs o01, o02, o06, o07

Figure 3 next presents the parameters (p02_DRN, p06_GHB, K) required to setup this scenario geological demands. The K tab summarizes five others, for pilot points. PEST is fed with initial

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values [not exactly "at random", but] a combination of field and specialist's expectations from a conceptual model (as knowledge constraints). All the decision-making occurs in the GMS. But early on, and paripassu, there are some opportunities for manual adjustments of parameters provided both by the Beta µ worksheets and by the adoption of structural measures that overcome what may eventually be limited by the validation of some initial configuration, as numerical constraints.

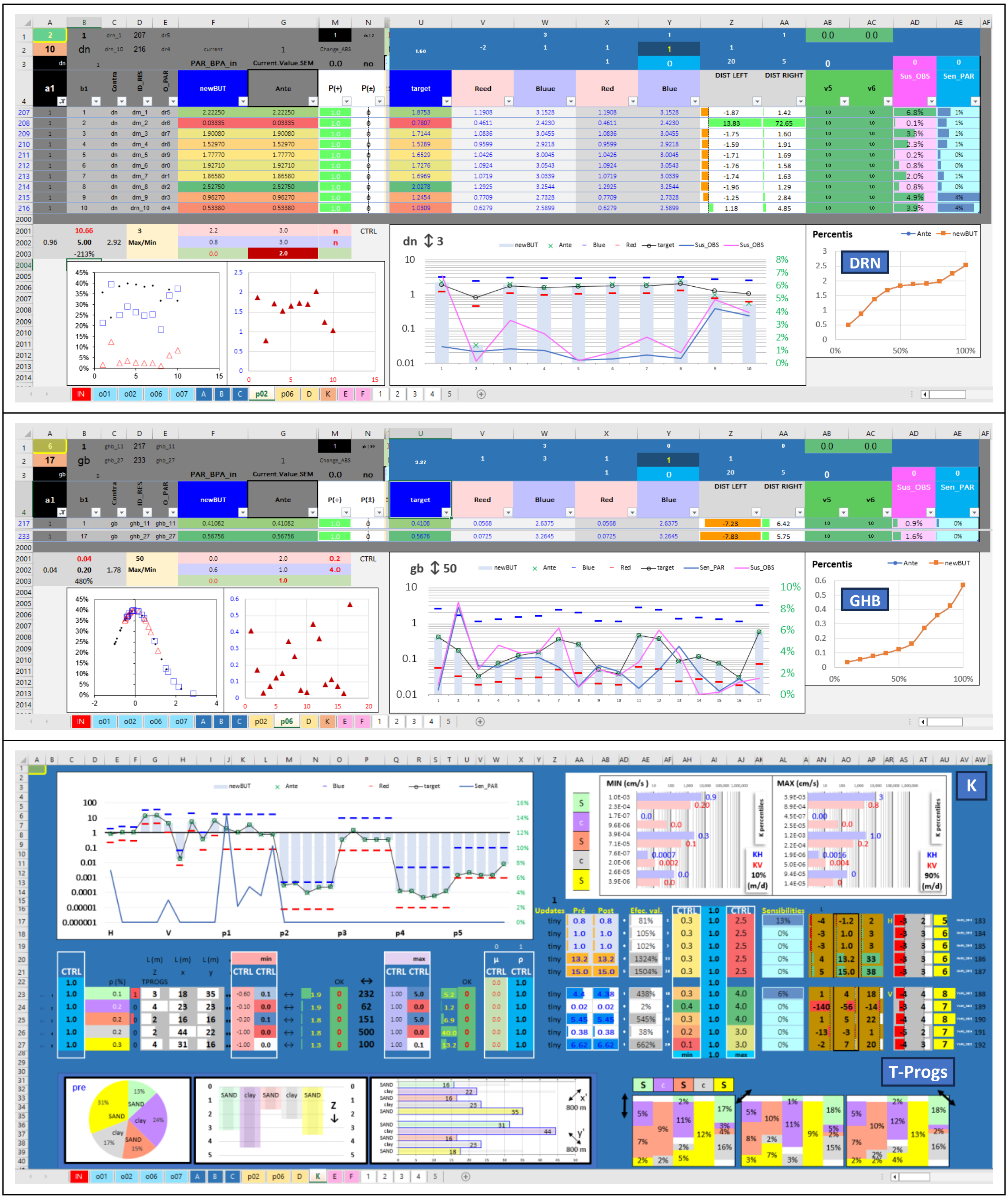

Figure 3: Parameters PAR – of Drains & General GHB, plus Hydraulic Conductivities by Pilot Points and Horizontal | Vertical Anisotropy Coefficients K 1, 2, 3, 4, 5 – Tabs p02, p06, K

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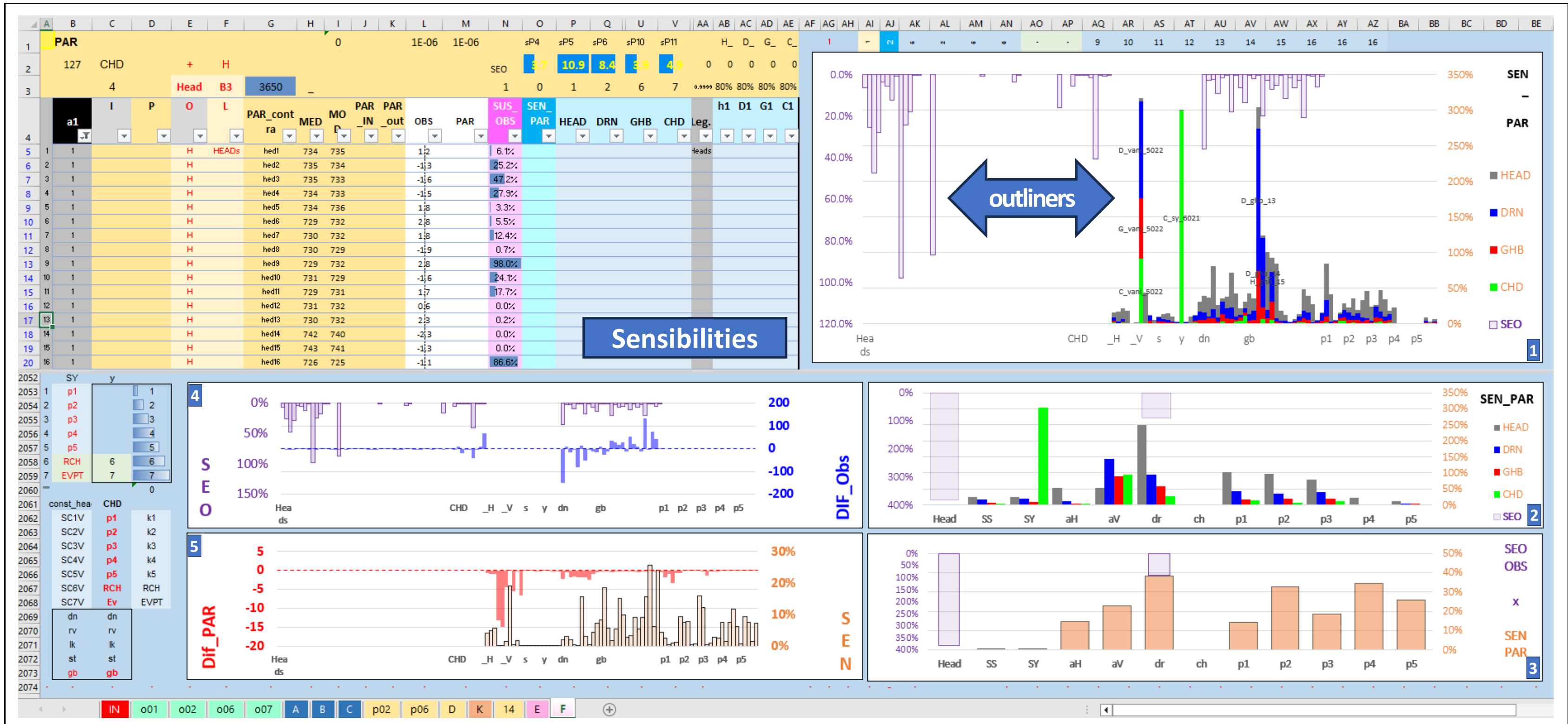
Figure 4: Here comes already the sensitivities, as PEST tries to change the elements magnitudes within each parameters list, to comply with the (weighed) observation demands and, conversely, also with the [susceptibilities] of a prior parameter distribution and delivered observations of an earlier realization.

This screen does nothing more than just summarize the consequences of a given MODFLOW| PEST setup, through GMS.



Last results of a late execution:

Chart 01:

- All OBS x PAR sensitivities.

Charts 02, 03:

- Grouped
- OBS x PAR

Chart 04:

- Changes OBS_SEO

Chart 05:

- Changes PAR_SEN

This 40MB spreadsheet is not dedicated to process numerical or differential equations.

- What are being advocating here is the need, or rather, the difficulty to understand what is being processed. In other words, this spreadsheet seeks to detail how the interaction between parameters and observations.
- From the so-called spatial covariance matrix, this is one of the fundamental numerical definitions.

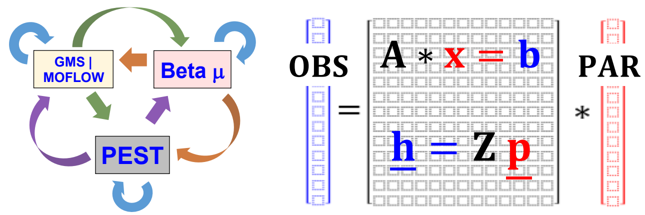


Figure 4: Parameters Sensitivities (SEN-PAR) versus observations susceptibilities (SUS-SEO) – Tab E

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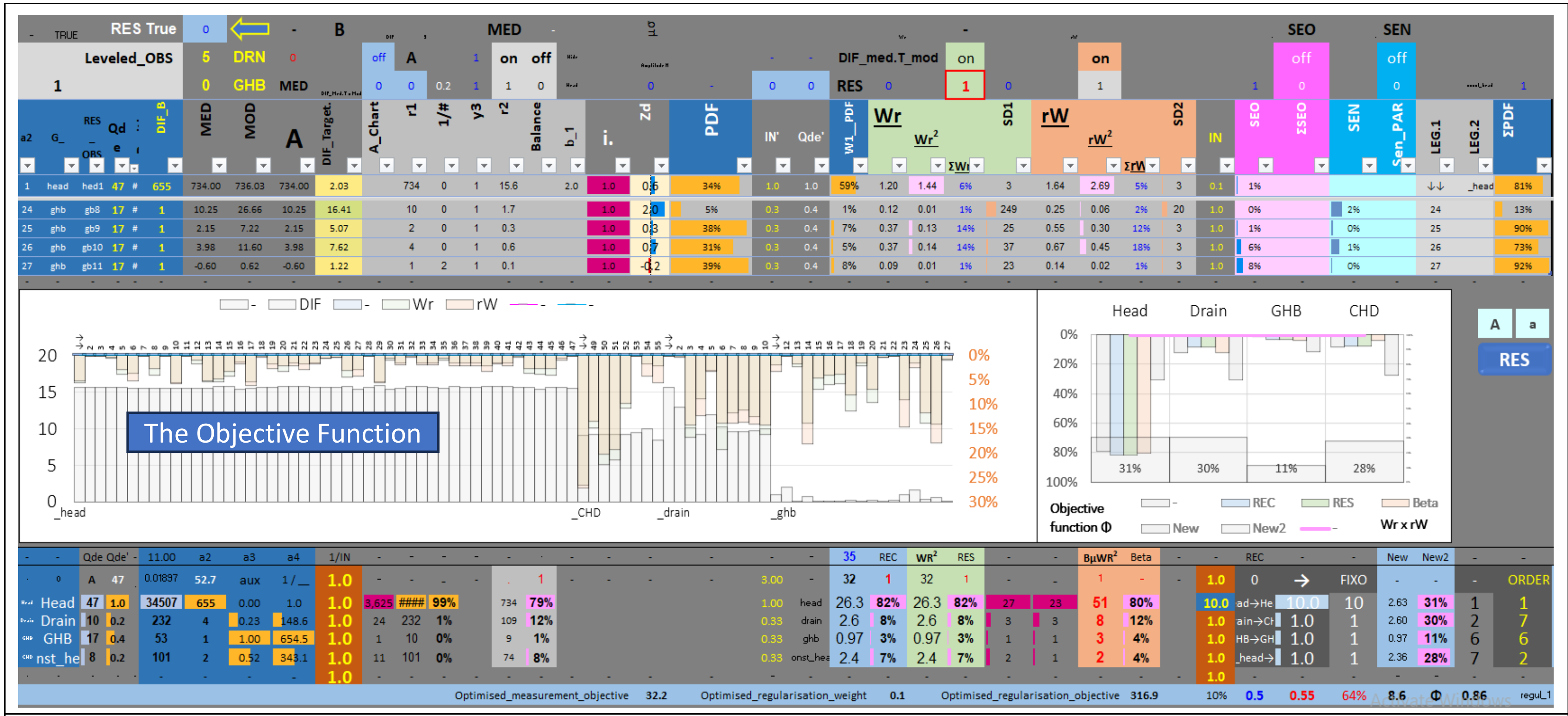
Figure 5: Measured Observations (MED) is a dubious term, given the frequently you just want to estimate a unknow variable (mainly for boundary fluxes). Actually, Bayes' theorem teaches that you need to guess at first (the prior). You get to know it only when Modflow informs you about its findings (MOD). So here starts the fun, when it's time to adjust all the expectations, (H, fluxes; - Do you got some?), by structural or parametrization (PEST) maneuvers.

At this scenario, there is the need to be at ease, to understand, accept and defend the advantages of Bayesian scheme. This is a circular reference: - The objectives guide the parameters selection as well as parameters implementation guides the definition of the objectives. As a trade-off, there is no difficulty in justifying credibility gains when all the modeled fluxes were accounted for, as long as it is balanced - even when using just a couple of real heads (H).



The mathematical regularization needs targets, amplitudes and weights.
In this opportunity, the user tries to guide the calibration towards a certain direction, according to his, her expectations from the conceptual model (OBS).

Be aware of commonly frustrations, in the form of restrictions imposed by structural inadequacies.

A Bayes Implication: The conceptual model is in cte. evolution. It must be subject to what may be proven by the mathematical conclusions.

Figure 5: Composed Objective function Φ, summarized accounts (Σ) for different observation groups – Tab A

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4. THE ELETRONIC TABLE MANAGEMENT MECHANISMS

All Beta µ routines resigns on a single statistical procedure, the dataset reconstruction of the Zscore analysis. Standardized Scores indicates the degree to which random distributions deviate from its own mean. A statistical proceeding best understood by the drawing of the Normal or Gaussian STD Distribution Curves, the PDF, CDF and p(x) functions for lists with variables of any kind.

Once all dataset is organized (a task fully automated in this spreadsheet), here's an illustration from our aquatinted DRN_PAR list. Instead, now with a fictitious referential distribution of 10 elements.

In ascending order, the dataset is reassembled in terms of its mean (µ) and standard deviations (σ). Then similar distributions become feasible to feed the next PEST realization. By comparison, this one (the target or real doted lines) has smaller ranges than the distribution of reference.

Figure 6 then also brings up two others, [µ] and [σ] induced, possibilities (the red and blue curves).

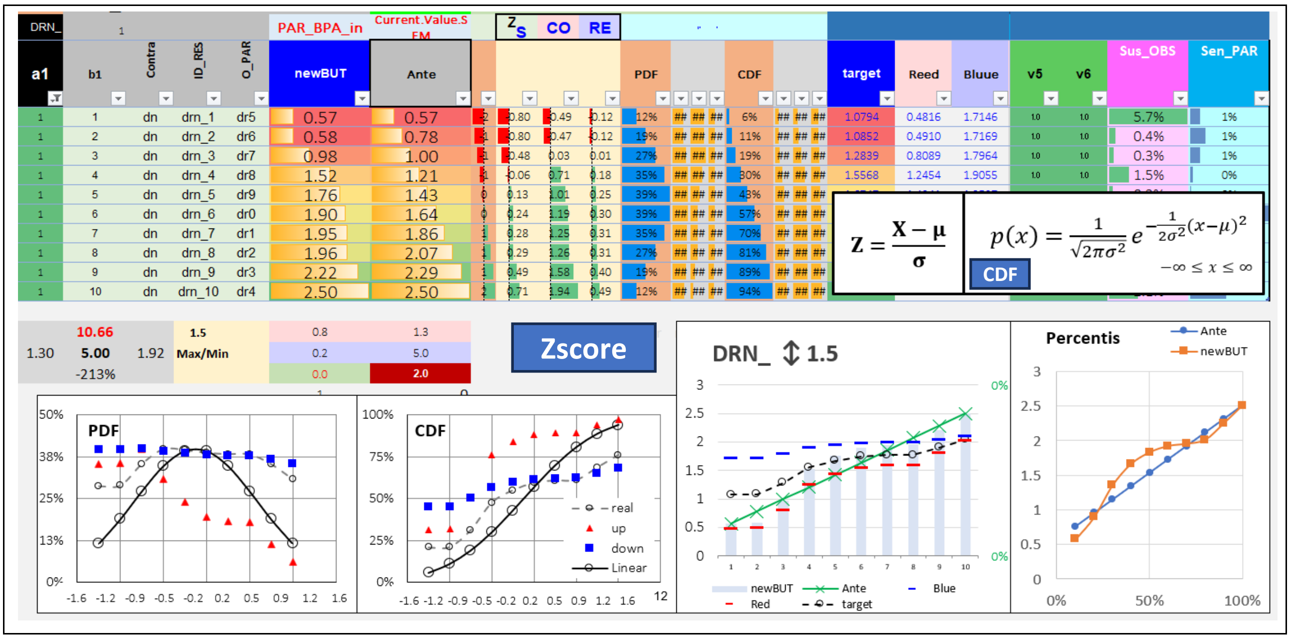

Figure 6: Changes and controls of an illustrative list of parameters, via STD analysis and Zscore – Tab p02'

Again, in light of what has been previously presented:

The next dataset goes in the same line of thought: A linear 1-20 ascending ordered distribution. But now which equidistant distances or leveled magnitudes, to be subjected to reconstructions as derived curves, varying its original (reference) curve mean (µ) and standard deviation (σ), by STD.

There **(Figure 7)** let's see how to reduce the range of any original distribution and, in doing so, how to reach the new spaces for each parameter independent variation point by point (within the red – blue lines of amplitude). In practice, each element is invariably connected with the sensitivities expressed due to its position, as relative weights of correspondent distances in relation to its mean.

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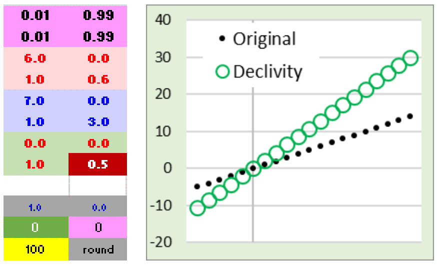
Perhaps stopping here would be suitable or worthwhile, to re-evaluate some possibilities in variating this new distribution of linear, sequential numbers ranging from 01 to 20.

A lower 6 – 15 unities variability was reached by 0.6 & 3.0 std deviations + (6, 7 µ). Being the red and blue curves amplitudes (?). The green one, … just an exercise for further thoughts.



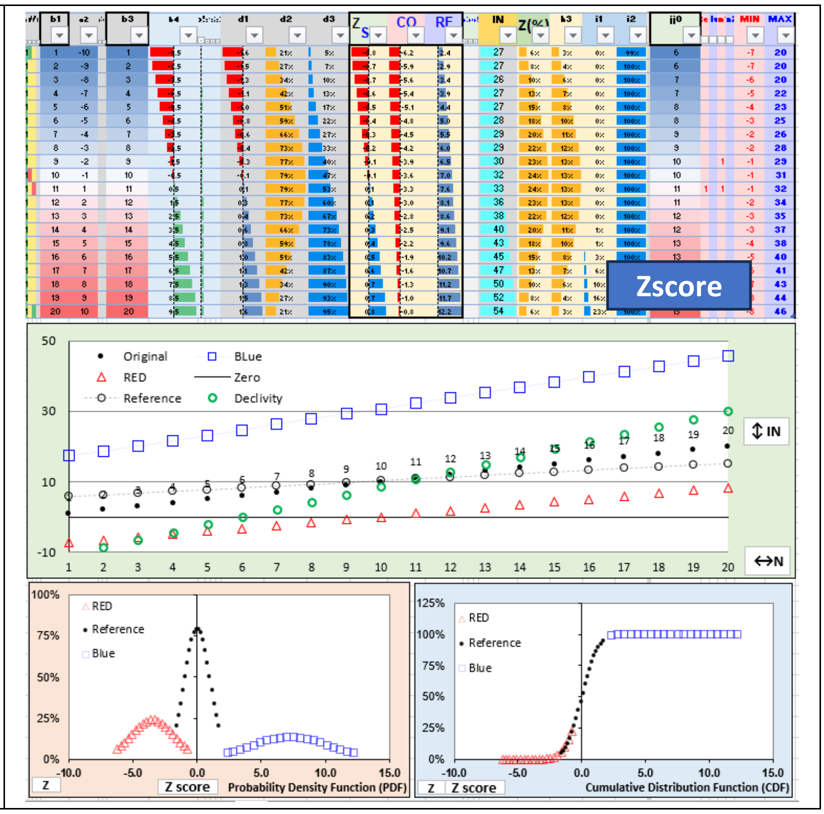


Figure 7: Didactical example of PDF, CDF distribution curves and the STD analysis

5. TERMS AND GUARANTEES

Accompanying this document, we plan to provide the complete, latest version of the Beta µ spreadsheet, as well as some case study situations - at no cost for the user.

Being the current solution embedded with the GMS | Aquaveo & MS Office interfaces, we suggested the installation of the MS Office Pro Plus 2019 or higher versions of Excel.

GMS can be found at: https://www.aquaveo.com/downloads?tab=1#TabbedPanels

GMS has a free trial period of 15 days that maybe requested at: https://evaluate.aquaveo.com/

After this period, a friendly request for 06 months to a 01-year student license is attainable, preferably by contacting Mr. Todd Wood (twood@aquaveo.com), referencing this Beta µ initiative's encouragement to establish a connection with the ongoing activity.

To formalize the deal, the availability of the Beta µ spreadsheet is subject to the following term:

I declare the intention to use the Beta µ spreadsheet for academic purposes only.
I agree with the undertake to notify the author of any commercial use.
The forms of remuneration for eventual commercial uses of the services provided by this code or associated algorithms is subject to a future agreement.

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Data: 04/10/2024 14:23:59-0300
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Your name:

The author: ____________________________

Rodrigo M Grossi Eng. MsC. | São Paulo | October - 10 - 2024

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6. MAIN INSTRUCTIONS

This text is intended for intermediate to advanced MODFLOW users, regardless the platform used.

When it comes to PEST, the user must be at least familiarized with its main concepts, which do not count as few. The theoretical documentation has more than 1,000 pages, and a large number of external routines and applications is also required. But that is the very motif for this project creation. To bridge these concepts to the user, in practice, together - what also has to be mentioned - together with the incommensurable contributions of the GMS shortcuts.

GMS does much of the work that would otherwise depend on numerous PEST applications, via Windows CMD Prompt commands, or prearranged files. *.txt → *.bat files.

There is still a long way to go in creating a more user-friendly routine, readily adaptable to various case demands. This is where the Beta µ spreadsheet comes in.

<u>**Figure 8 01:**</u> The spreadsheet, like any VBS file (*.xlsm) must be unlocked first; <u>**02:**</u> These are the inputs and outputs by any PEST configuration; <u>**03:**</u> These_Buttons calls the inputs; <u>**04:**</u> A simple routine (*.bat) transforms the need PEST files into [*.csv] which goes to Excel; <u>**05, 06:**</u> A Control Panel indicates which tabs were used and the main characteristics of a given case study scenario.

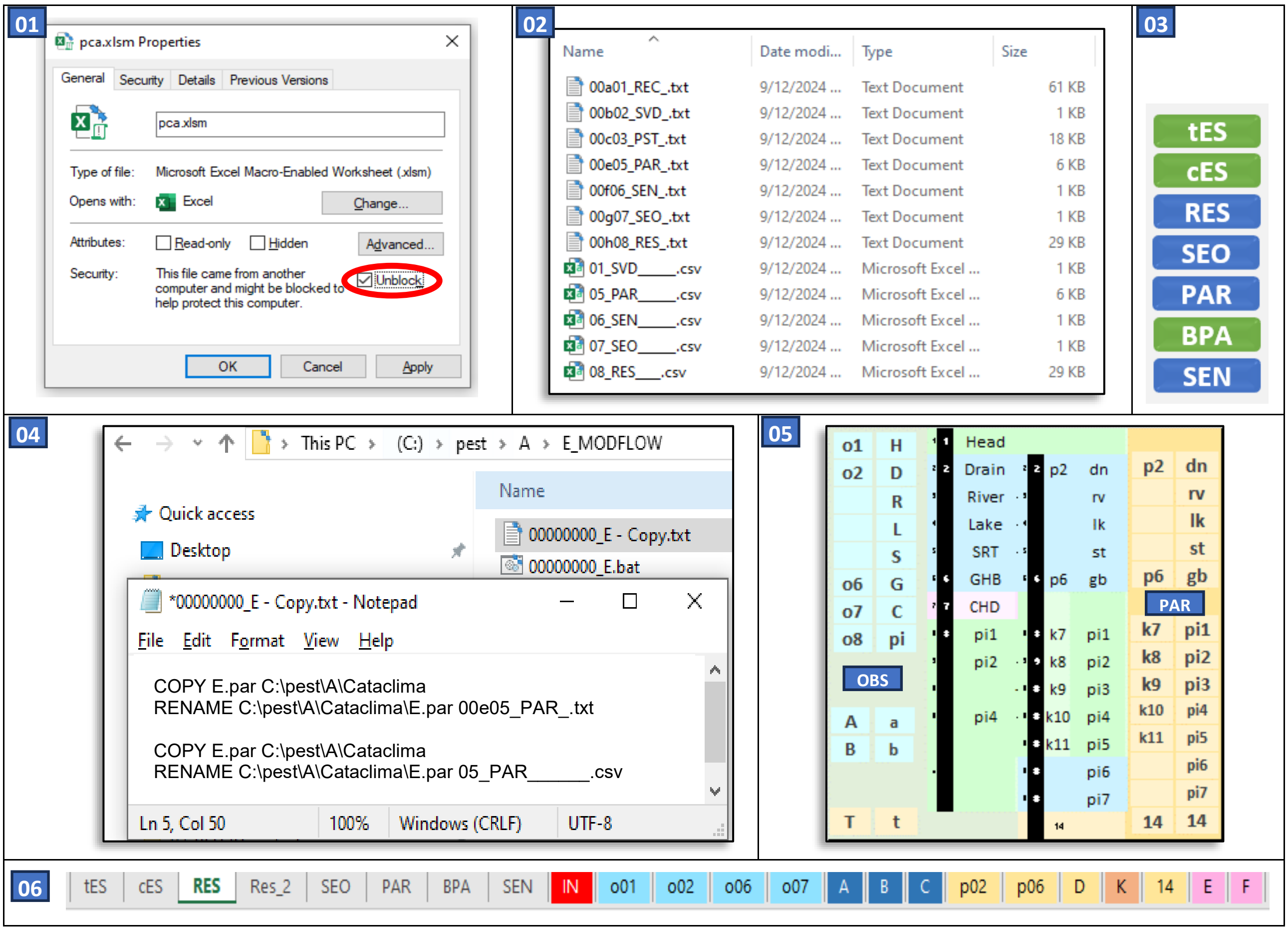

Figure 8: Setup Beta µ |GMS | PEST. *Some of it inspired by the Italians from https://kataclima.com/

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<u>The Figure 9</u> shown here below depicts the boundary conditions of the case study.

The domain comprehends a structure of 04 processing coverages. This case has 47 Hydraulic Heads (H_2); 10 segments for the drains (DRN); 17 segments for variable hydraulic Heads (GHB), plus 08 fixed (CHD) Heads downstream. MODFLOW | PEST runs it a first time, just to test the viability of each new scenario, precisely, by the numerical simulation.

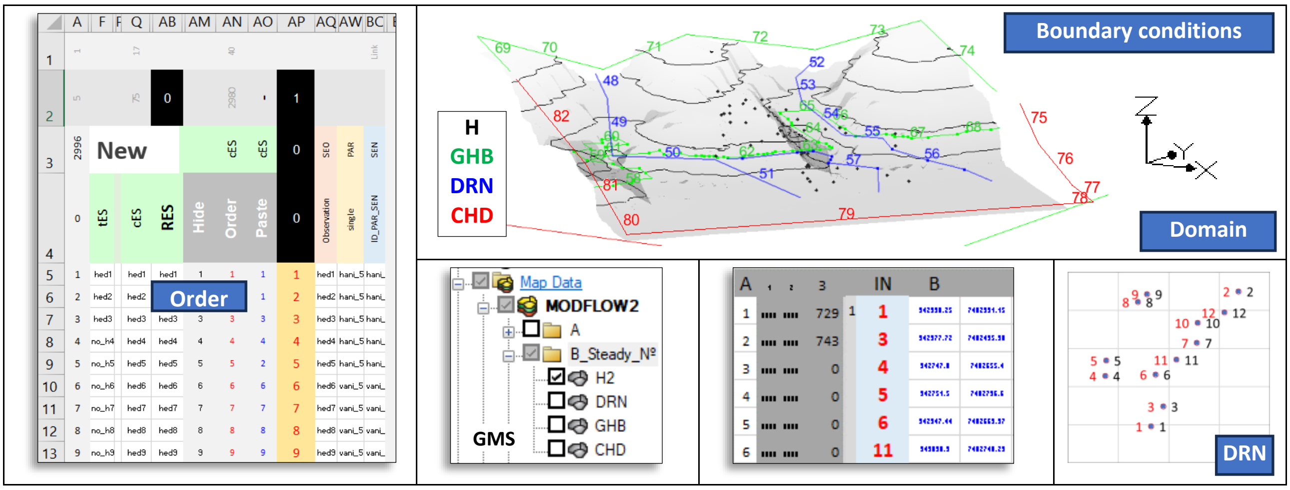

Figure 9: Boundary conditions, their sequential allocation and an organization device for future data crossing

6.1. Order, please

<u>Rule nº 1 of 2:</u> Beta µ [still] requires the user attention in providing a modelling structure with the same number of parameters and observations. For example, 10 conductances against 10 observed flows for the drains. In extension, there is the need to do a doble check. Make sure that the numerical model responds accordingly.

<u>Rule nº 2 of 2:</u> There are no restrictions on the possible configurations of new scenarios, although the final order of the mapped inputs (from conceptual to numerical form) is what matters most.

As presented (**<u>Figure 9</u>**) orders the observations to locations as: 1-47 Heads (H); 48-51, 52-56, 57 [Blue-DRN], 58-68, 69-74 [Green-GHB], 75-82 [Red CHD]. This is important because the goal is to remove misunderstandings of what is happening in the model and where, exactly. Beta µ provides an auxiliary worksheet (tab 4), which hopes to guide the correct 3D allocation of this information's.

From now on, no more harsh limitations exist (Get in touch if you find some).

<u>Instructions:</u> Place the boundary conditions in sequence 1-47H, 48-57DRN, GHB, and so on at a 1º GMS realization. Then make use this PEST "measured list" to effectively map the (already ordered) position. The data assumes the desired position from the Paste, fixed [cES-REs] columns (**<u>Figure 9</u>**).

The next task is, for the better or worse, how to answer one arising big question: - How to reconcile several sets of observations (heads & fluxes) of various orders of magnitude at the objective $f(\Phi)$?

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Figure 10 has a closer look of an already shown tables. The natural order, the very subject discussed a few lines above, assumed the correct positions now. A topic not so careful handled by GMS.

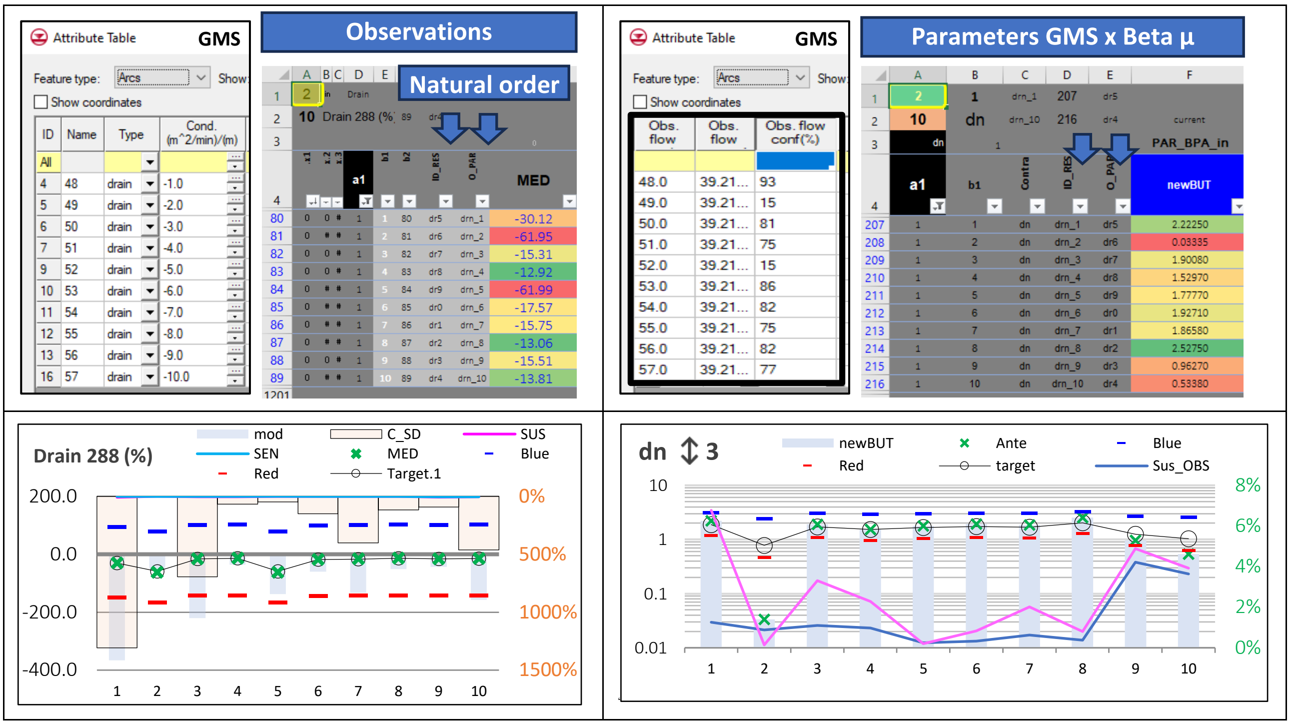

Figure 10: Organized sequence of parameter & observations for drains: Example (dr5 & drn_1); (dr0 & drn_6); ...

The greatest contribution of this (GUI) spreadsheet, perhaps a task placing itself even above or at the same level of importance as the objective function (Φ) understanding and illustration (Figure 5), is the deliverance of a routine that automatically adapts to different combinations, varied lists of parameters, observations…

01_ Observations _OBS (82 rows x 11 columns) + (75 rows, OBS pi$_{\pi_sn}$cv_pilot points)

1	hed1	15	hed15	29	hed29	43	hed43	57	dr9	71	gb13
2	hed2	16	hed16	30	hed30	44	hed44	58	gb0	72	gb14
3	hed3	17	hed17	31	hed31	45	hed45	59	gb1	73	gb15
4	hed4	18	hed18	32	hed32	46	hed46	60	gb2	74	gb16
5	hed5	19	hed19	33	hed33	47	hed47	61	gb3	75	ch0
6	hed6	20	hed20	34	hed34	48	dr0	62	gb4	76	ch1
7	hed7	21	hed21	35	hed35	49	dr1	63	gb5	77	ch2
8	hed8	22	hed22	36	hed36	50	dr2	64	gb6	78	ch3
9	hed9	23	hed23	37	hed37	51	dr3	65	gb7	79	ch4
10	hed10	24	hed24	38	hed38	52	dr4	66	gb8	80	ch5
11	hed11	25	hed25	39	hed39	53	dr5	67	gb9	81	ch6
12	hed12	26	hed26	40	hed40	54	dr6	68	gb10	82	ch7
13	hed13	27	hed27	41	hed41	55	dr7	69	gb11		
14	hed14	28	hed28	42	hed42	56	dr8	70	gb12		

02_ Parameters _PAR (72 rows x 04 columns)

1	hani_5011	13	ss_6013	25	drn_5	37	ghb_17	49	sc1v2	61	sc3v4
2	hani_5012	14	ss_6014	26	drn_6	38	ghb_18	50	sc1v3	62	sc3v5
3	hani_5013	15	ss_6015	27	drn_7	39	ghb_19	51	sc1v4	63	sc4v1
4	hani_5014	16	sy_6021	28	drn_8	40	ghb_20	52	sc1v5	64	sc4v2
5	hani_5015	17	sy_6022	29	drn_9	41	ghb_21	53	sc2v1	65	sc4v3
6	vani_5021	18	sy_6023	30	drn_10	42	ghb_22	54	sc2v2	66	sc4v4
7	vani_5022	19	sy_6024	31	ghb_11	43	ghb_23	55	sc2v3	67	sc4v5
8	vani_5023	20	sy_6025	32	ghb_12	44	ghb_24	56	sc2v4	68	sc5v1
9	vani_5024	21	drn_1	33	ghb_13	45	ghb_25	57	sc2v5	69	sc5v2
10	vani_5025	22	drn_2	34	ghb_14	46	ghb_26	58	sc3v1	70	sc5v3
11	ss_6011	23	drn_3	35	ghb_15	47	ghb_27	59	sc3v2	71	sc5v4
12	ss_6012	24	drn_4	36	ghb_16	48	sc1v1	60	sc3v3	72	sc5v5

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… this is done in order to facilitate the comparison, management, and final delivery of new lists (OBS | PAR) to feed back into future MODFLOW|PEST implementations, not to mention the tips provided to the user on where the present version of his model needs improvement. GMS|PEST finds the sensibilities, Beta µ points out where & how these influences is felt by the correspondent variables.

These archives [*.RES, *.SEO, *.PAR, *.SEN] are the channel of communication between all actors.

03_ Observation sensitivities or susceptibilities _SEO_OBS (82 rows x 05 columns)

1	hed1	15	hed15	29	hed29	43	hed43	57	dr9	71	gb13
2	hed2	16	hed16	30	hed30	44	hed44	58	gb0	72	gb14
3	hed3	17	hed17	31	hed31	45	hed45	59	gb1	73	gb15
4	hed4	18	hed18	32	hed32	46	hed46	60	gb2	74	gb16
5	hed5	19	hed19	33	hed33	47	hed47	61	gb3	75	ch0
6	hed6	20	hed20	34	hed34	48	dr0	62	gb4	76	ch1
7	hed7	21	hed21	35	hed35	49	dr1	63	gb5	77	ch2
8	hed8	22	hed22	36	hed36	50	dr2	64	gb6	78	ch3
9	hed9	23	hed23	37	hed37	51	dr3	65	gb7	79	ch4
10	hed10	24	hed24	38	hed38	52	dr4	66	gb8	80	ch5
11	hed11	25	hed25	39	hed39	53	dr5	67	gb9	81	ch6
12	hed12	26	hed26	40	hed40	54	dr6	68	gb10	82	ch7
13	hed13	27	hed27	41	hed41	55	dr7	69	gb11		
14	hed14	28	hed28	42	hed42	56	dr8	70	gb12		

04_Parameters sensitivities _ SEN_PAR (504 rows x 04 columns) (72) * 7 (-72)

_1______	ghb_27	drn_1	sc5v1	ghb_22	sy_6021	sc4v1	ghb_17	ss_6011	sc3v1	ghb_13
hani_5011	sc1v1	drn_2	sc5v2	ghb_23	sy_6022	sc4v2	ghb_18	ss_6012	sc3v2	ghb_14
hani_5012	sc1v2	drn_3	sc5v3	ghb_24	sy_6023	sc4v3	ghb_19	ss_6013	sc3v3	ghb_15
hani_5013	sc1v3	drn_4	sc5v4	ghb_25	sy_6024	sc4v4	ghb_20	ss_6014	sc3v4	ghb_16
hani_5014	sc1v4	drn_5	sc5v5	ghb_26	sy_6025	sc4v5	ghb_21	ss_6015	sc3v5	ghb_17
hani_5015	sc1v5	drn_6	_3_DRAIN_	ghb_27	drn_1	sc5v1	ghb_22	sy_6021	sc4v1	ghb_18
vani_5021	sc2v1	drn_7	hani_5011	sc1v1	drn_2	sc5v2	ghb_23	sy_6022	sc4v2	ghb_19
vani_5022	sc2v2	drn_8	hani_5012	sc1v2	drn_3	sc5v3	ghb_24	sy_6023	sc4v3	ghb_20
vani_5023	sc2v3	drn_9	hani_5013	sc1v3	drn_4	sc5v4	ghb_25	sy_6024	sc4v4	ghb_21
vani_5024	sc2v4	drn_10	hani_5014	sc1v4	drn_5	sc5v5	ghb_26	sy_6025	sc4v5	ghb_22
vani_5025	sc2v5	ghb_11	hani_5015	sc1v5	drn_6	_5_CHD__	ghb_27	drn_1	sc5v1	ghb_23
ss_6011	sc3v1	ghb_12	vani_5021	sc2v1	drn_7	hani_5011	sc1v1	drn_2	sc5v2	ghb_24
ss_6012	sc3v2	ghb_13	vani_5022	sc2v2	drn_8	hani_5012	sc1v2	drn_3	sc5v3	ghb_25
ss_6013	sc3v3	ghb_14	vani_5023	sc2v3	drn_9	hani_5013	sc1v3	drn_4	sc5v4	ghb_26
ss_6014	sc3v4	ghb_15	vani_5024	sc2v4	drn_10	hani_5014	sc1v4	drn_5	sc5v5	ghb_27
ss_6015	sc3v5	ghb_16	vani_5025	sc2v5	ghb_11	hani_5015	sc1v5	drn_6	hani_5011	sc1v1
sy_6021	sc4v1	ghb_17	ss_6011	sc3v1	ghb_12	vani_5021	sc2v1	drn_7	hani_5012	sc1v2
sy_6022	sc4v2	ghb_18	ss_6012	sc3v2	ghb_13	vani_5022	sc2v2	drn_8	hani_5013	sc1v3
sy_6023	sc4v3	ghb_19	ss_6013	sc3v3	ghb_14	vani_5023	sc2v3	drn_9	hani_5014	sc1v4
sy_6024	sc4v4	ghb_20	ss_6014	sc3v4	ghb_15	vani_5024	sc2v4	drn_10	hani_5015	sc1v5
sy_6025	sc4v5	ghb_21	ss_6015	sc3v5	ghb_16	vani_5025	sc2v5	ghb_11	vani_5021	sc2v1
drn_1	sc5v1	ghb_22	sy_6021	sc4v1	ghb_17	ss_6011	sc3v1	ghb_12	vani_5022	sc2v2
drn_2	sc5v2	ghb_23	sy_6022	sc4v2	ghb_18	ss_6012	sc3v2	ghb_13	vani_5023	sc2v3
drn_3	sc5v3	ghb_24	sy_6023	sc4v3	ghb_19	ss_6013	sc3v3	ghb_14	vani_5024	sc2v4
drn_4	sc5v4	ghb_25	sy_6024	sc4v4	ghb_20	ss_6014	sc3v4	ghb_15	vani_5025	sc2v5
drn_5	sc5v5	ghb_26	sy_6025	sc4v5	ghb_21	ss_6015	sc3v5	ghb_16	ss_6011	sc3v1
drn_6	_2_HEAD_	ghb_27	drn_1	sc5v1	ghb_22	sy_6021	sc4v1	ghb_17	ss_6012	sc3v2
drn_7	hani_5011	sc1v1	drn_2	sc5v2	ghb_23	sy_6022	sc4v2	ghb_18	ss_6013	sc3v3
drn_8	hani_5012	sc1v2	drn_3	sc5v3	ghb_24	sy_6023	sc4v3	ghb_19	ss_6014	sc3v4
drn_9	hani_5013	sc1v3	drn_4	sc5v4	ghb_25	sy_6024	sc4v4	ghb_20	ss_6015	sc3v5
drn_10	hani_5014	sc1v4	drn_5	sc5v5	ghb_26	sy_6025	sc4v5	ghb_21	sy_6021	sc4v1
ghb_11	hani_5015	sc1v5	drn_6	_4_GHB__	ghb_27	drn_1	sc5v1	ghb_22	sy_6022	sc4v2
ghb_12	vani_5021	sc2v1	drn_7	hani_5011	sc1v1	drn_2	sc5v2	ghb_23	sy_6023	sc4v3
ghb_13	vani_5022	sc2v2	drn_8	hani_5012	sc1v2	drn_3	sc5v3	ghb_24	sy_6024	sc4v4
ghb_14	vani_5023	sc2v3	drn_9	hani_5013	sc1v3	drn_4	sc5v4	ghb_25	sy_6025	sc4v5
ghb_15	vani_5024	sc2v4	drn_10	hani_5014	sc1v4	drn_5	sc5v5	ghb_26	drn_1	sc5v1
ghb_16	vani_5025	sc2v5	ghb_11	hani_5015	sc1v5	drn_6	_6_REGU_	ghb_27	drn_2	sc5v2
ghb_17	ss_6011	sc3v1	ghb_12	vani_5021	sc2v1	drn_7	hani_5011	sc1v1	drn_3	sc5v3
ghb_18	ss_6012	sc3v2	ghb_13	vani_5022	sc2v2	drn_8	hani_5012	sc1v2	drn_4	sc5v4
ghb_19	ss_6013	sc3v3	ghb_14	vani_5023	sc2v3	drn_9	hani_5013	sc1v3	drn_5	sc5v5
ghb_20	ss_6014	sc3v4	ghb_15	vani_5024	sc2v4	drn_10	hani_5014	sc1v4	drn_6	
ghb_21	ss_6015	sc3v5	ghb_16	vani_5025	sc2v5	ghb_11	hani_5015	sc1v5	drn_7	
ghb_22	sy_6021	sc4v1	ghb_17	ss_6011	sc3v1	ghb_12	vani_5021	sc2v1	drn_8	
ghb_23	sy_6022	sc4v2	ghb_18	ss_6012	sc3v2	ghb_13	vani_5022	sc2v2	drn_9	
ghb_24	sy_6023	sc4v3	ghb_19	ss_6013	sc3v3	ghb_14	vani_5023	sc2v3	drn_10	
ghb_25	sy_6024	sc4v4	ghb_20	ss_6014	sc3v4	ghb_15	vani_5024	sc2v4	ghb_11	
ghb_26	sy_6025	sc4v5	ghb_21	ss_6015	sc3v5	ghb_16	vani_5025	sc2v5	ghb_12	

End

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6.2. The GMS x Beta µ interaction

On the one hand, this routine works with values placed as "Targets" of the objective function, as well its connected amplitudes and standard deviation, becoming the weights of each distribution.

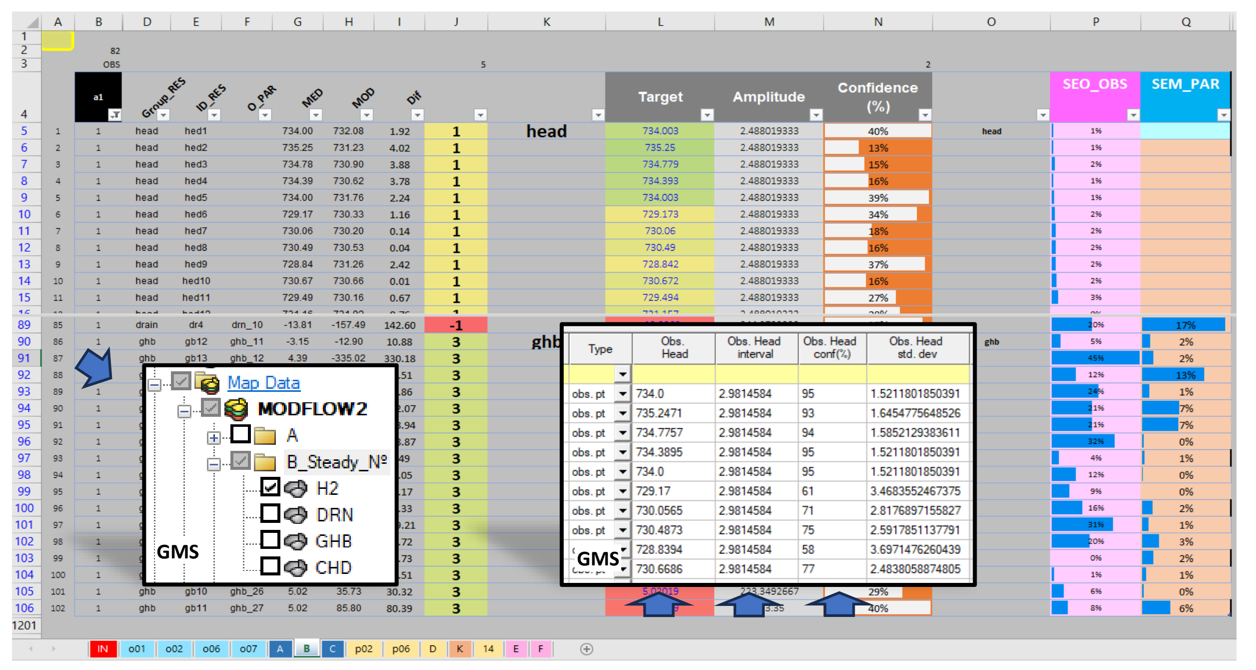

Figure 11: Objective function Targets, amplitudes of variation and standard deviation of the observations – Tab B

On the other hand, faster than in the previous item, the direct loading of parameters is enabled from the Beta µ spreadsheet to GMS, including those related to the pilot points, via a *.prn file.

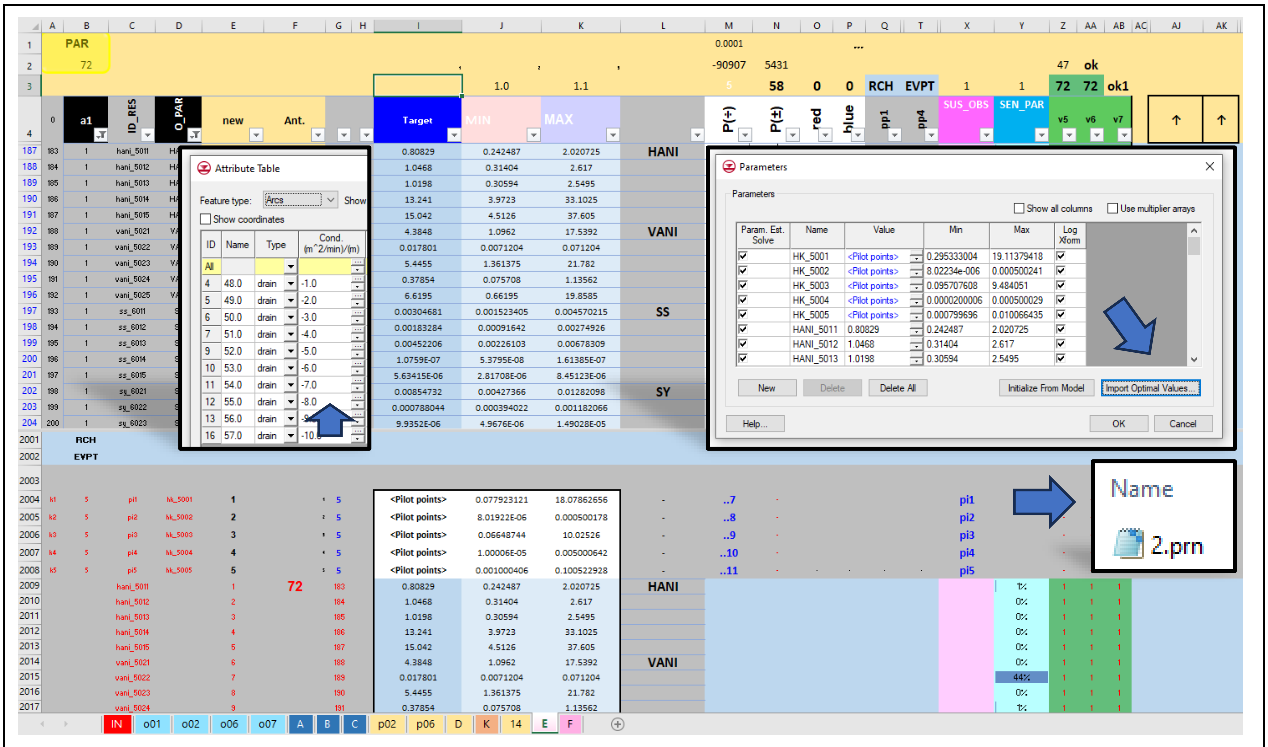

Figure 12: Setting input distributions of parameters and its amplitudes (min, max) of each new realization – Tab E

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6.3. Hydraulic conductivities and pilot points

This variation of the parameter dataset routine, exclusively for hydraulic conductivities, is due to the need of understanding it and its “distribution” within the model domain, … in a unique grasp.

Tab K summarises five others [7,8,9,10,11, &D]. And it also gives the user an expedite notion of the three-dimensional arrangements, of how the materials (hydrofacies) fill the model. Tab 01 brings on a mechanism to improve the [T-Progs] interpolation strategy management.

Figure 13: This tab contains the same control mechanisms, based on STD | Zscore reconstructions.

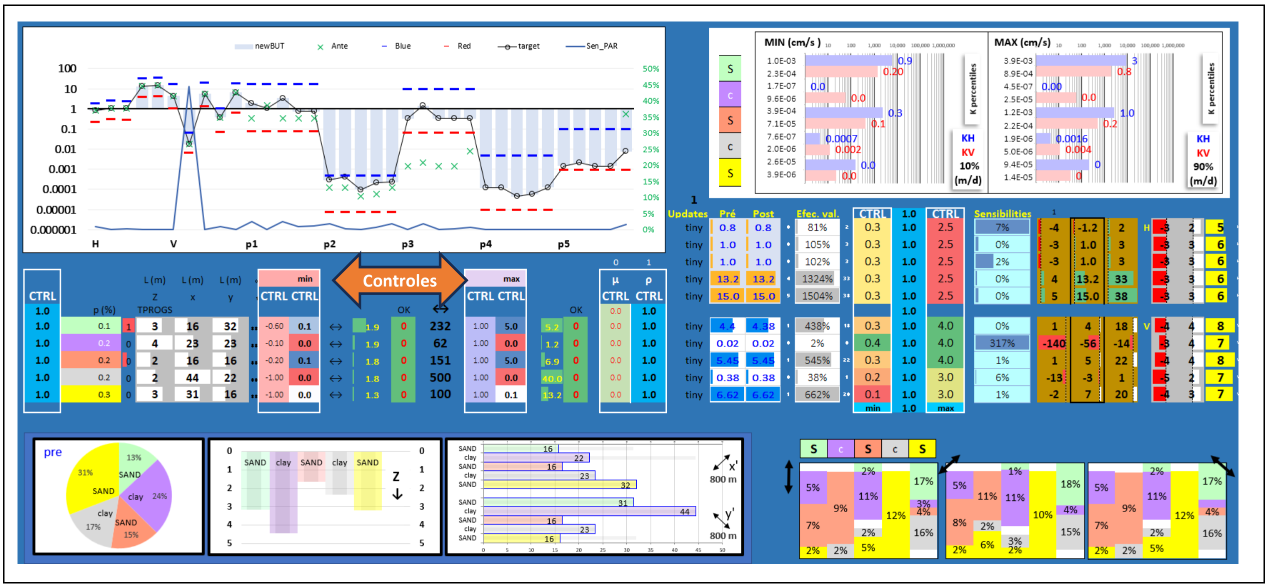

Figure 13: Summary of results, sensitivities and control mechanism of hydraulic conductivities – Tab K

This last Beta µ tab is a screen that reports the flow rates recorded in each new PEST run.

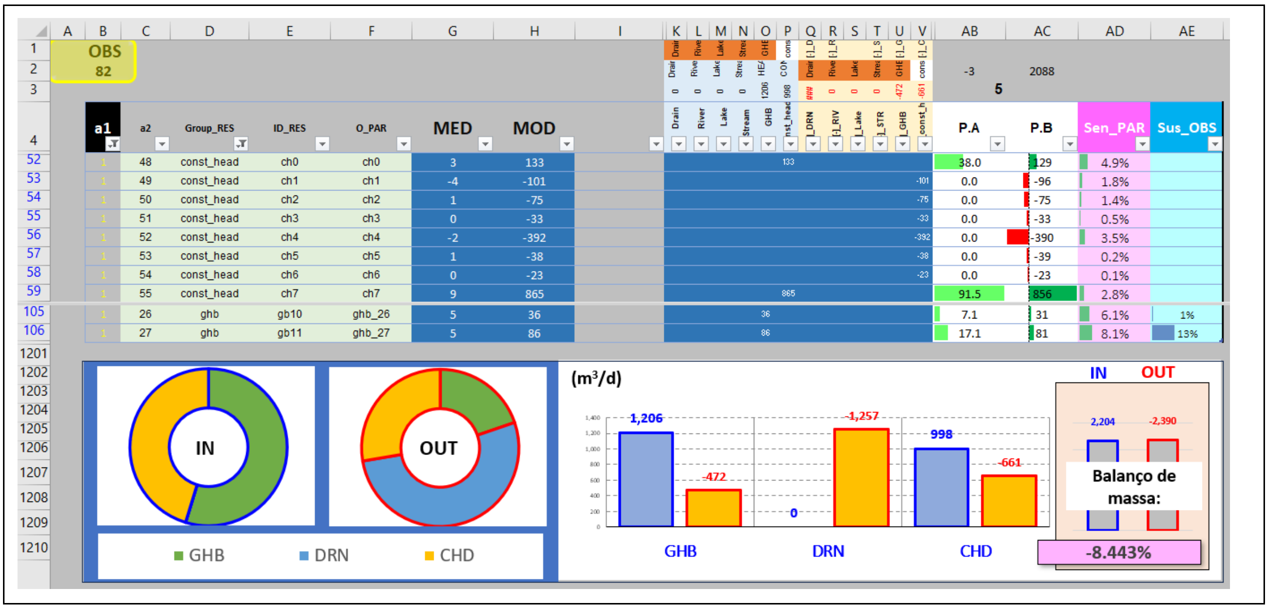

Figure 14: A final worksheet compares the flow rates recorded for all boundary conditions – Tab C

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7. AUXILIARY TABS

One of the fundamental strategies of this proposal, ((to extract the most of the relation between GMS and PEST software architectures)), is to place all the needed information in a single screen.

Great importance is also deposited on teaching the user to respect the standard logic rules of the electronic spreadsheet. For instance, among the 07 layers| 08 surfaces of Figure 15, the user is encouraged to change this vertical spatialization without disturbing the implemented logic.

7.1. Redistributing the thickness of the 3D Grid layers

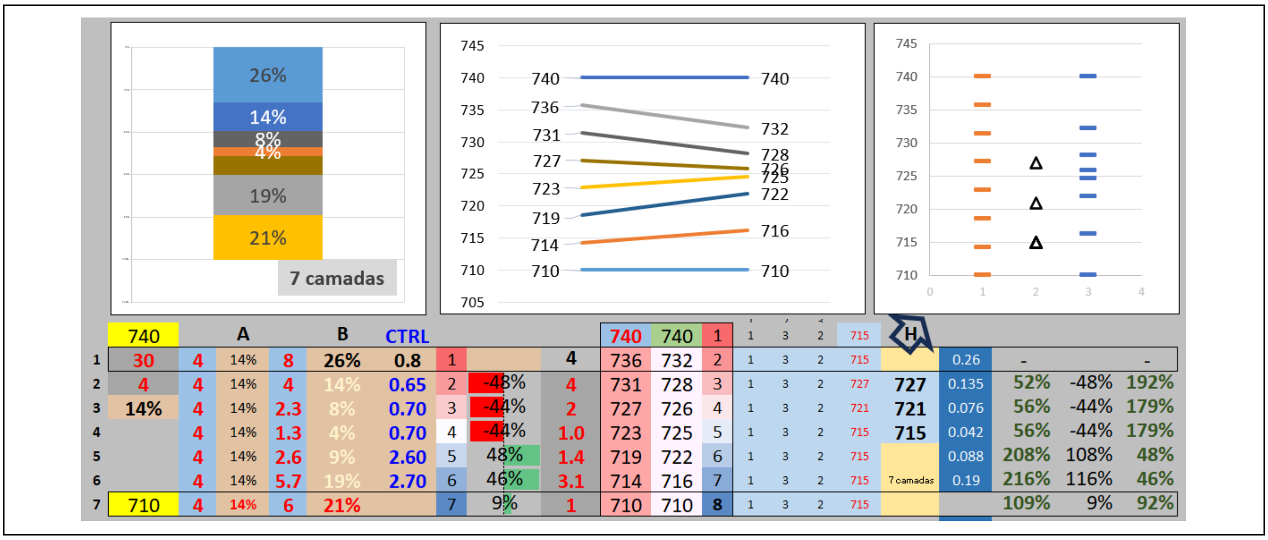

Figure 15: 3D Grid layer redistribution mechanism – Tab 02

7.2. Position and topography (elevation) of boundary conditions

Then here comes a humble suggestion on dealing with the position, elevations, nodes of this case.

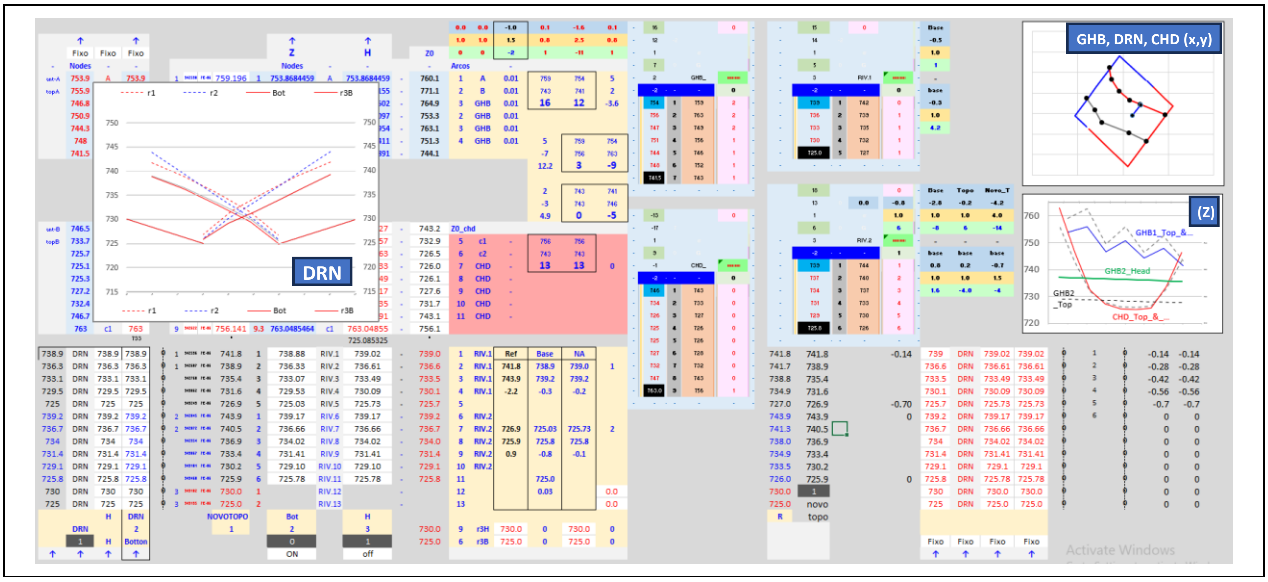

Figure 16: Positioning and math's to rearrange elevations (z) of utilized boundary conditions – Tab 04

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7.3. T-Progs

Let's see a fundamental worksheet, the last one, I promise. The Transitional Probability Software (T-Progs) is an interpolation engine. It efficiently and accurately distributes the hydraulic properties within any chosen modelling domain. Beta μ dedicates an interface to it. And due to its relationship with one of the main MODFLOW|PEST functionalities, the SVD routine, it is recommended a certain immersion by part of the user, on this subject.

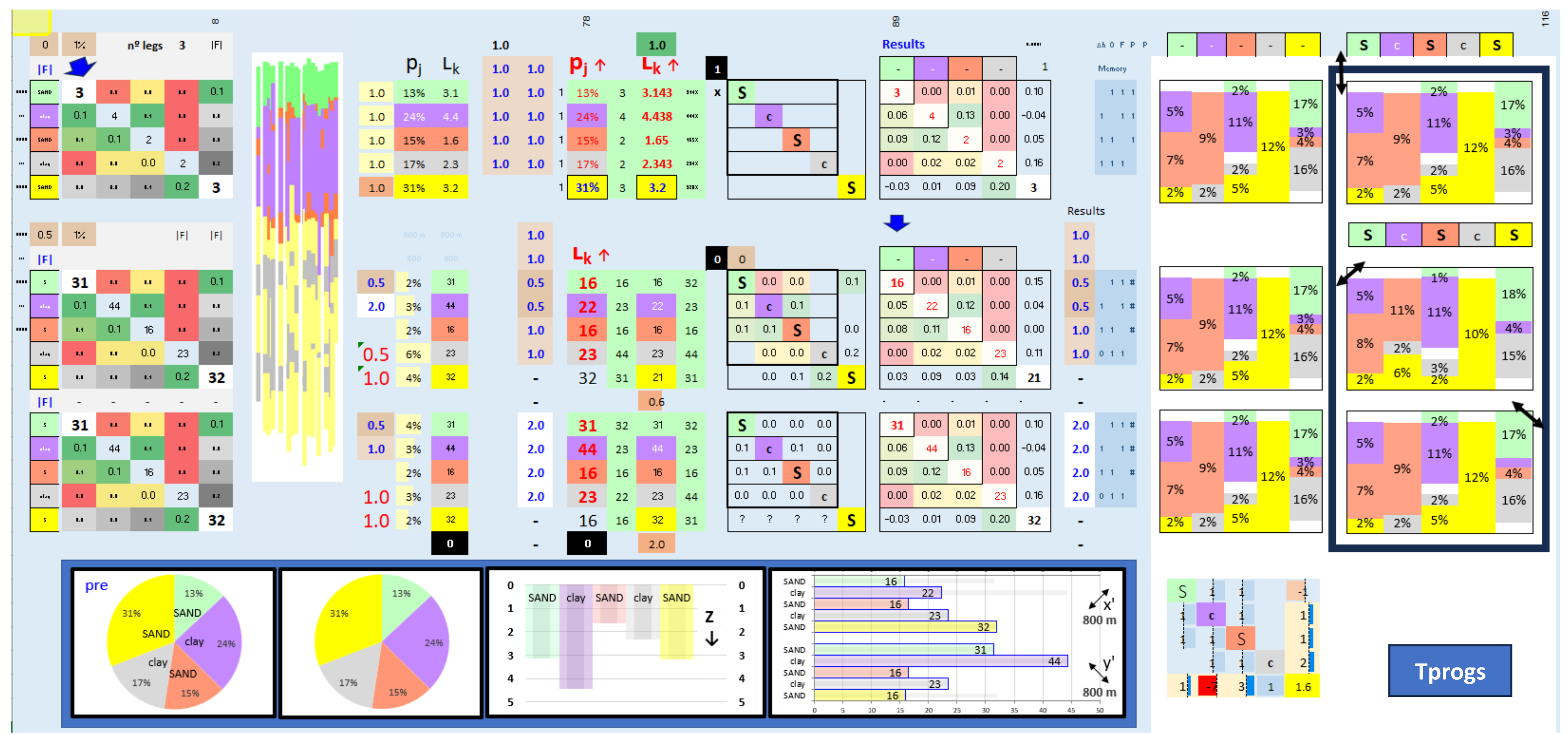

Figure 17: Interpretation of the this very case study resolution. T-Progs initial configurations – Tab 01

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8. OBJECTIVE FUNCTION - Φ

Fast forward, discussing what matters most: - A fifth PEST file (the *.REC archive, not previously mentioned), records the final math's of any realization. As shown below (Figure 18) the spreadsheet compares the contents of *.REC x *.RES files, with the intent to see this problem's weights distribution. This kind of comparison is very important, given the Bayesian need of prior observations to run the code (a prep mere guessing exercise). The PDF function directs the parametrization towards a given predefined objective, as long as measures were taken to level the weights of varied observation groups.

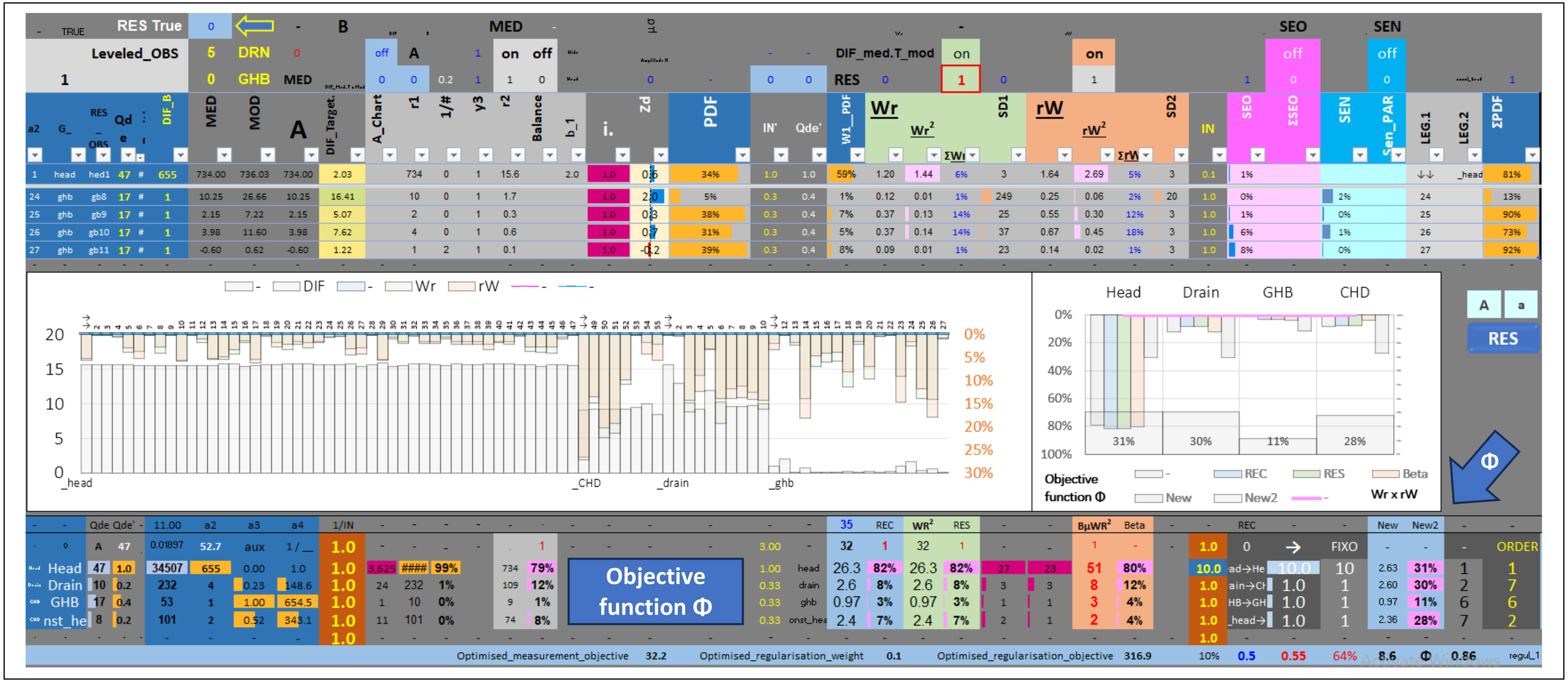

Figure 18: Composed Objective Function Φ Management – Real dataset 01 – Tab A

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8.1. Objective function – CHD boundary condition

Fluxes within each boundary condition is provided at the corresponded tab. Here the CHD elements at columns MOD & #B face each other in reaching the precious DIF_Target info. In its turn, a derived combination of Za (from DIF_Target) & PDF (from Za) gives the individual rW weights for the next run.

Note the parity of MED and #B columns here, cause this reconstruction at #B relies on zero mean and no standard deviation (µ=0, σ=1) from MED.

The comprehension of **GMS columns** inner workflow (*.REC & RES files) emerged from **the Beta columns**. Next page provides additional analogies.

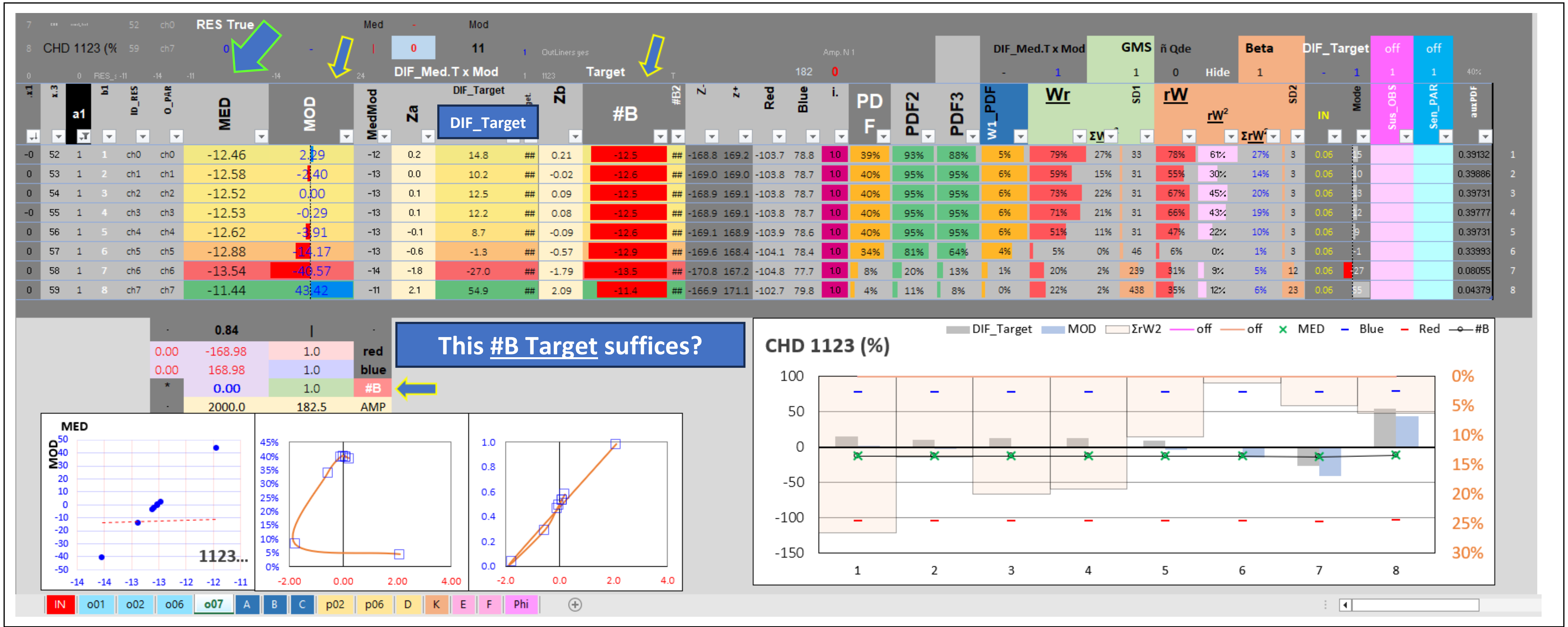

Figure 19: Composed Objective Function Φ Management – Real dataset details nº 02 – CHD – Tab o07

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8.2. Objective function – GHB boundary condition

Now alternatively, the binomial MED & #B(Target) datasets diverges because it was chosen to diminish the discrepancy within the “expected” OBS, in a scale or [σ = 0.2 & µ = -1]. The main chart points that out (MED x @#B). Ans yes, this kind of information needs to be fed in the model next afterwards.

Here, PDF (thus rW & SD2) is much less variable. The GMS columns being turned off, as we did not have the GMS *.REC [Wr] math for this realization yet.

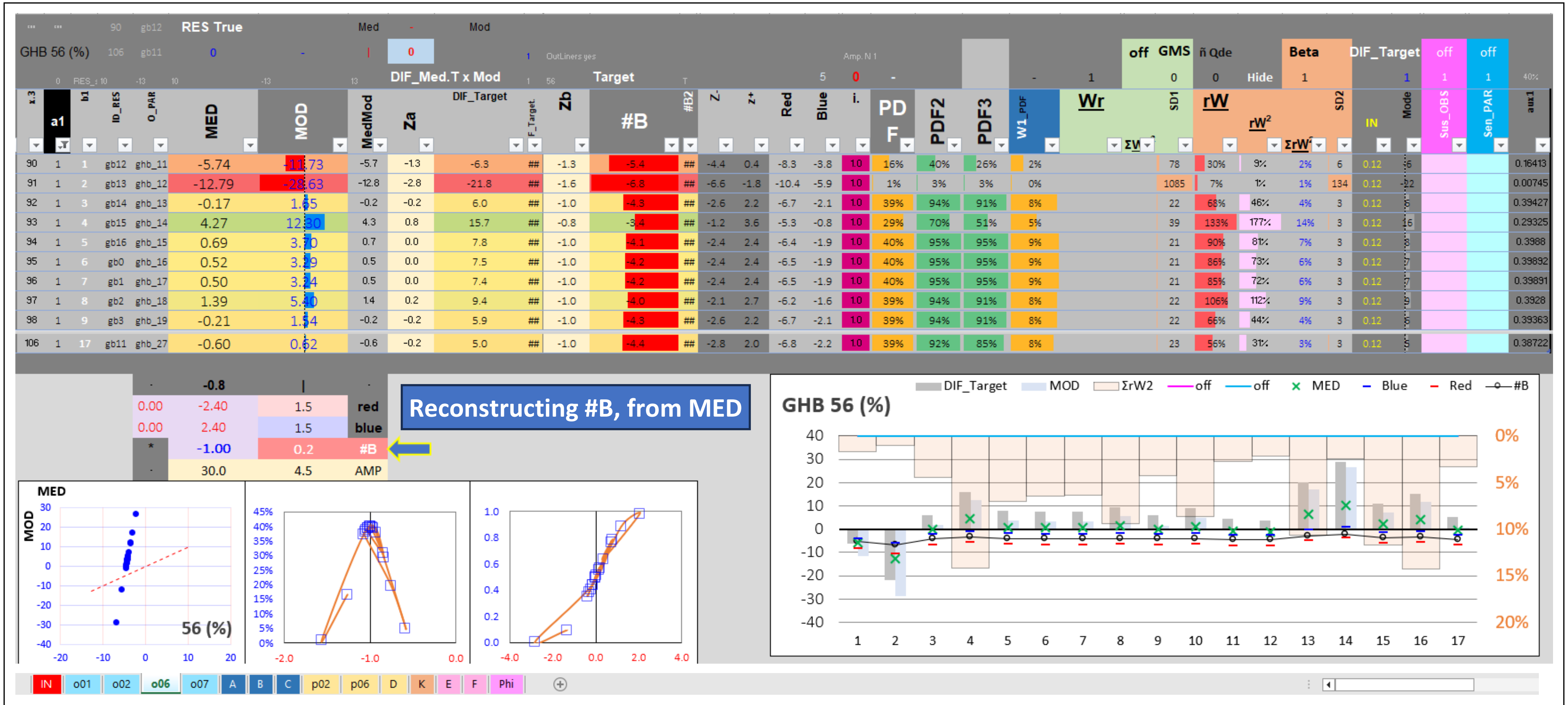

Figure 20: Composed Objective Function Φ Management – Real dataset details nº 03 – GHB – Tab o06

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8.3. Objective function – DRN (fluxes m^3/d) combines with Hidraulic Heads (m)

Complementing all the related information, here comes the last two components of this problem.

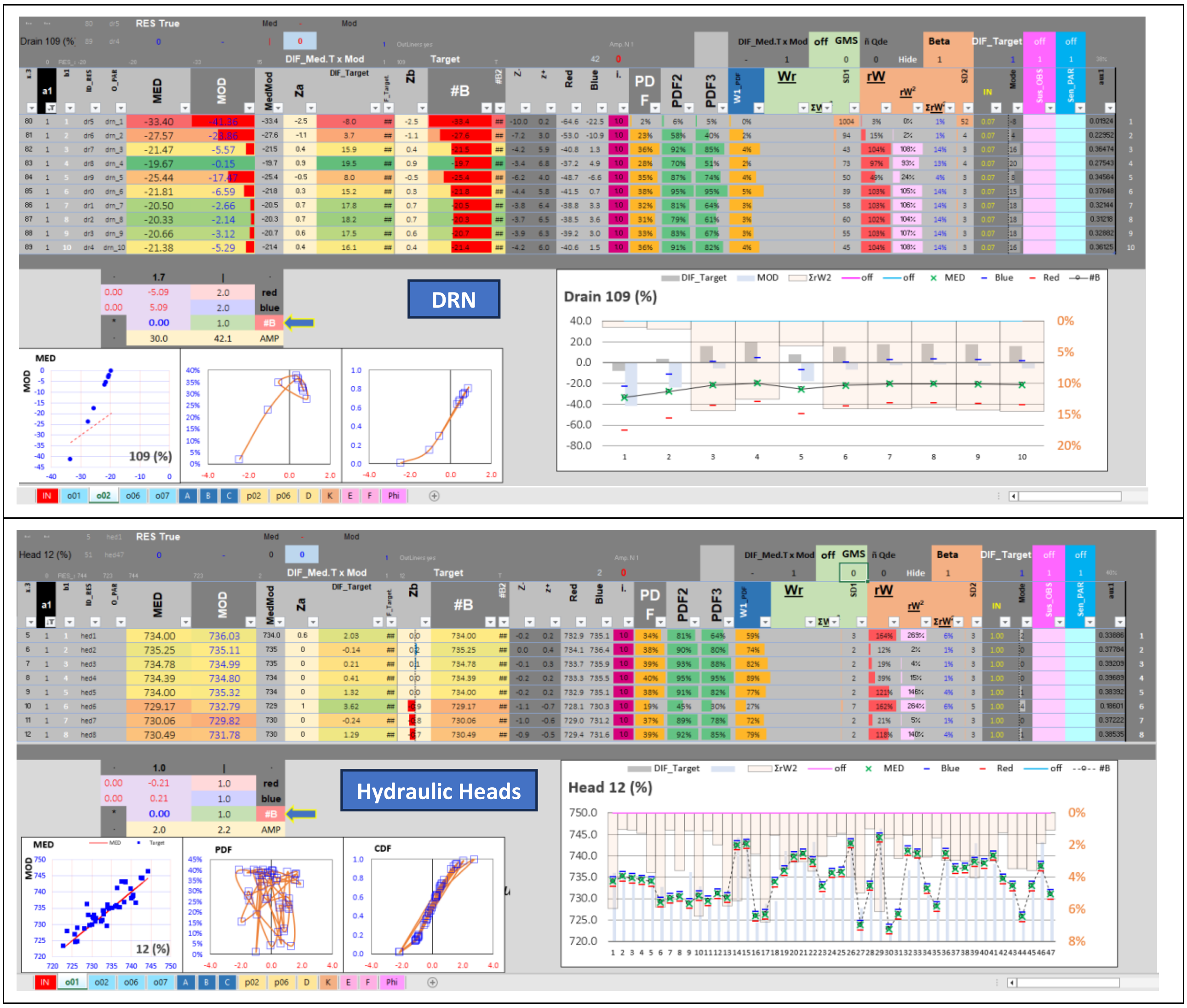

Figure 21: Composed Objective Function Φ Management – Real dataset details 04 and 05 – Tabs o02 and o01

As is there to be seen, this routine gives similar opportunity to change [expected] amplitudes of Red & Blue columns as well. There is, the same patronized routine through STD reconstruction (of µ, σ), creates an associated space for deviations on the allowed fluctuations of measures observations in the next MODFLOW|PEST contest. These amplitudes, again, comes from Targets, thus, from MED.

The dedicated PDF|CDF chats of Probability Density and Cumulative Distribution Functions points out scrambled curves, taking into account a Z-score analysis being done on muddled distributions.

Then the remaining left and right main small and big visualization charts delivers the same content, both for a cross-correlated and a patronized clustered columns format, accordingly.

Still, assuming that the present justification alone was insufficient to demonstrate, unequivocally, the envisioned weights (PDF| Wr | rW), let us dig a litter deeper. Be careful not to get wounded.

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Perhaps the best way to comprehend the somewhat intricate controls of the weight's quantification (Wr | rW) from the Z-score distribution of DIF_Target (MED), multiplied by the same distribution that originates it, is towards the apagogical arguments of the ***Reductio ad absurdum.***

So here we go with a very simple case where, let us say, for the first distribution of Heads the [expected] MED variables goes linearly from 01 to 47. Them we have the same, but in a decrescent order for the enforced negative drains (DRN), plus a 13^{th} fold increase in its contents (-1,-14,-27, …). Accounted, each group separately, with the expectations of GHB, and the ones (OBS) of CHD (+/-).

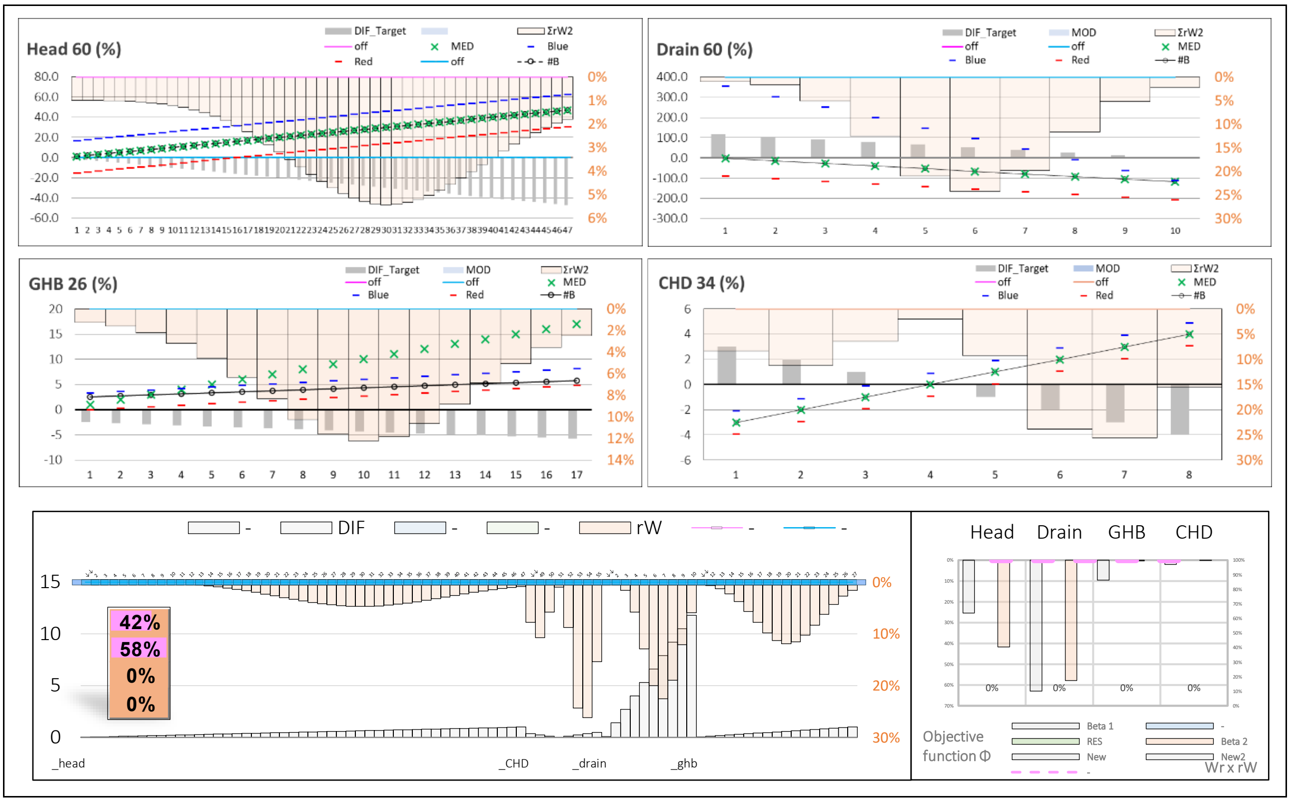

Figure 22: Composed Objective Function Φ Management – Synthetic dataset details – Example 01 – Tab A

Above, assumed also that the MOD column is zero, gives a magnitude of DIF_Target components equalling MED, if there is no change in its inner [MED µσ STD attributes], right?

Note the chat's absence of MOD. Also in these chats, DIF_Target depicts the inverse of MED.

Them a secondary analysis, after this database preliminary description's, supresses the bell curve and, in detriment of the Normal Gaussian distribution of DIF_Target, goes instead strait to formalize the assuming weights (wR^2) of PDF multiplied by MED. That is why we do not see a regular format of ΣwR^2, because the implicit bell curve becomes slightly modified by the utilized regularly crescent values of it. As we see in 1 – 47 for Heads, then in GHB, CHD, but differently in DRN – Drains. …

DRN wR^2 distributions goes back to the bell shape because, alternatively, its PDF suffers a counter-measure, varying amplitudes. A forward step foreseeing the parameter selection results (on MOD).

Summing up, the last chat (Figure 22) brings the overhaul of all these synthetic datasets combined.

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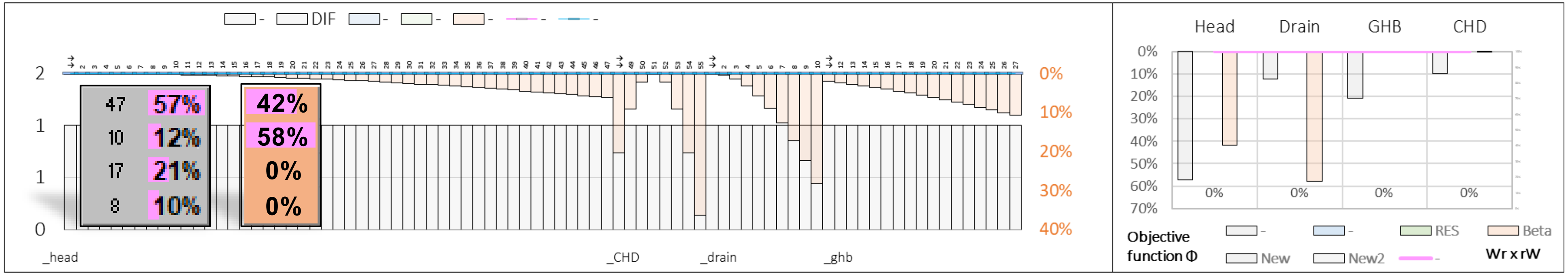
In here, the PDF columns/chart become reflected as original distributions (ID) when there are zero STD deviation. I.e. All observations being the same =1.



Following suit this line of thought, suppose a situation where the earlier equalized datasets (all expectations MED=1) need to be also leveled further, also in relation to the number or quantity of data they deliver to the objective function (Φ).

The greater the amount of info. (ID), the lower in magnitude (MED).

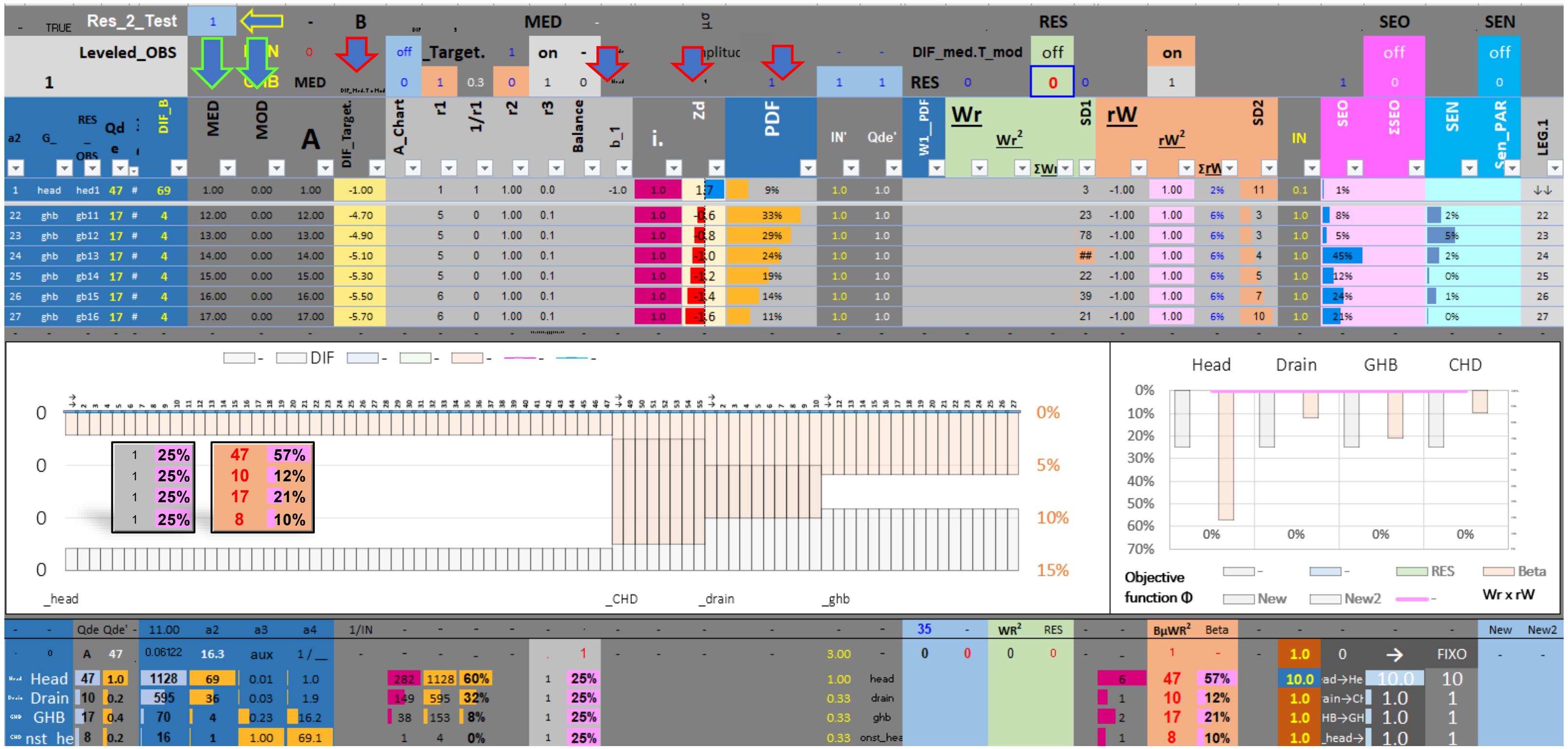


Figure 23 - Composed Objective Function (Φ) Management – Synthetic dataset details – Examples 02 and 03 – Tab A

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Thus, in the end, coming back to Figure 24 of our case study scenario, there is the need on user's end to apply certain coefficients (Q_n) to correct how the "observed" MED "expectations" groups will be understood by the PEST algorithm, in its effort to direct the parameters selection in a way consistent with the very choices OBS-MOD (hydraulic heads or boundary condition fluxes) he, she requests the model to perform. A quite bayesian this statement, right?

Besides proved the REC | RES parity, the Beta2 report did not meet the same values, but just approximated magnitudes. Indeed, this still gives the user a good enough tool to pre-arrange components (observations / expectations) for the groundwater problem on screen.

PS: Beta1 doesn't the same, because this simpler report avoids purposely, the PDF statistics. PPS: The need of "IN*Qde" on [RES True] remains a bit blurry.

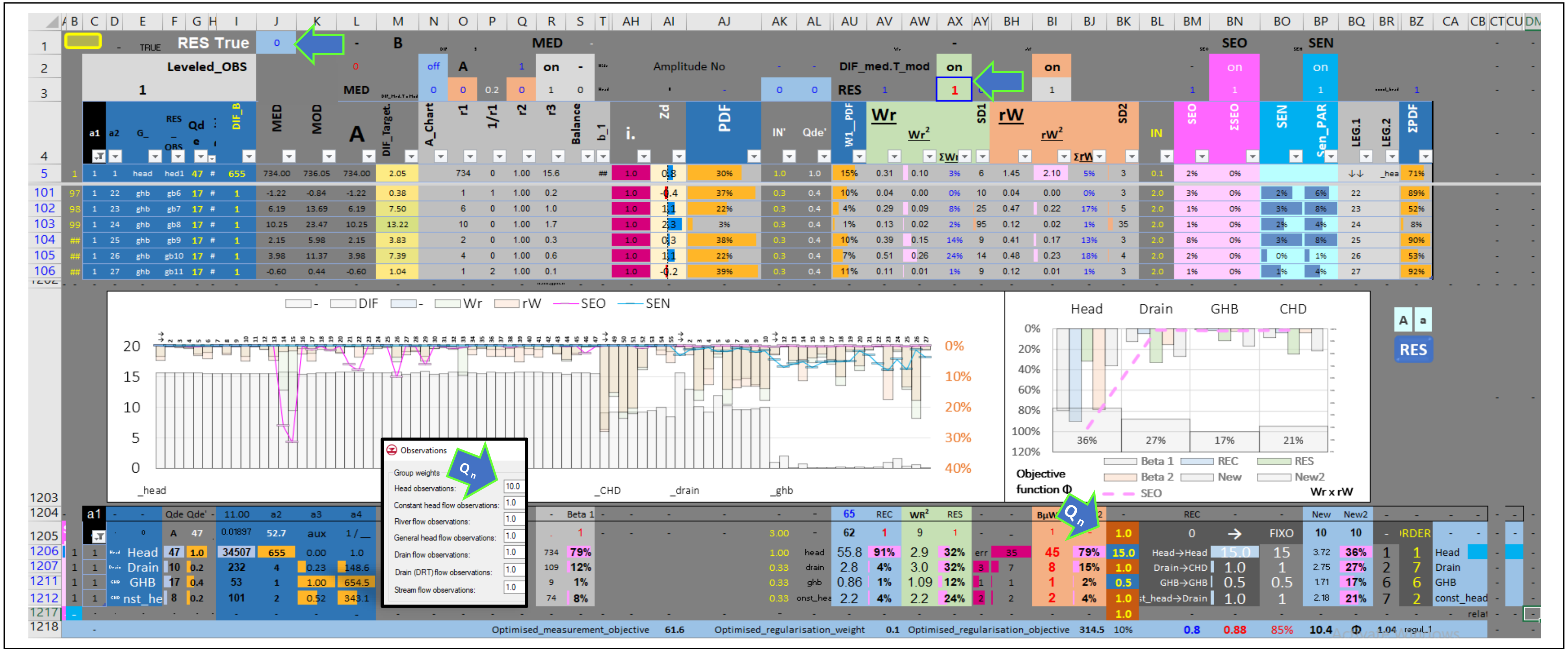

Figure 24: - Composed Objective Function Φ Management – final values for a given realization – Tab A

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Again, we can't afford being tired of it, after all the mathematical regularization is an issue with circular references: **Figure 25a** has what have just turned into earlier insights. With these sensibilities on sight, the decision making goes back to the user. A model structure (boundary conditions modifications, mainly), and or other parameter's list (**Figure 25b**), and or even new observations – MED expectations for boundary flux merely estimations – is required.

Figure 25: Sensibilities and some results for the Parameter Selection Strategy – Tab F

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9. PARAMETER SELECTION STRATEGY

This initiative tries, sincerely, to carry on with no regards on how things get done in GMS. Because the aim is to quickens the evolution of the PEST methodology in itself. A code which, in the humble opinion Beta µ developers, got indeed a great impulse by GMS | Aquaveo GUI software.

As presented at **Figure 9**, them a bit further at **Figure 16**, the structural part, the [x, y] positions, and elevations (z) of all modeled element starts from a doble effort which requires two MODFLOW coverages for each boundary condition.

Instructions: From the first coverage of river, drain, ghb drawn dispositions: (01): A brand-new coverage with just one Arc is required; (02) Redistribute its vertices in a (lets say) 20% greater value then the preceding one; (03) Transform its vertices into nodes; (04) End finally use the results of Beta µ worksheet auxiliary **TAB – 04 (Figure 26a)** to rearrange, and this is very important, the GMS sequential coverage IDs in the correct, crescent order. PS: Paste the coverage positions at [IN] and extract at [OUT], after the need correction selecting manually the [↓] adequate values / positions.

PPS: Usually by convention, the black / blue colors receive the inputs, the red one gives the results.

Next **(Figure 26b)** dealing with arcs | nodes elevations: Better explained by a comparison of GHB and CHD, here we have besides the elevations at stake (Z_i), a routine to derive the new elevations from the original topographic positions, (guess what?) by DPF reconstructions (µ, σ).

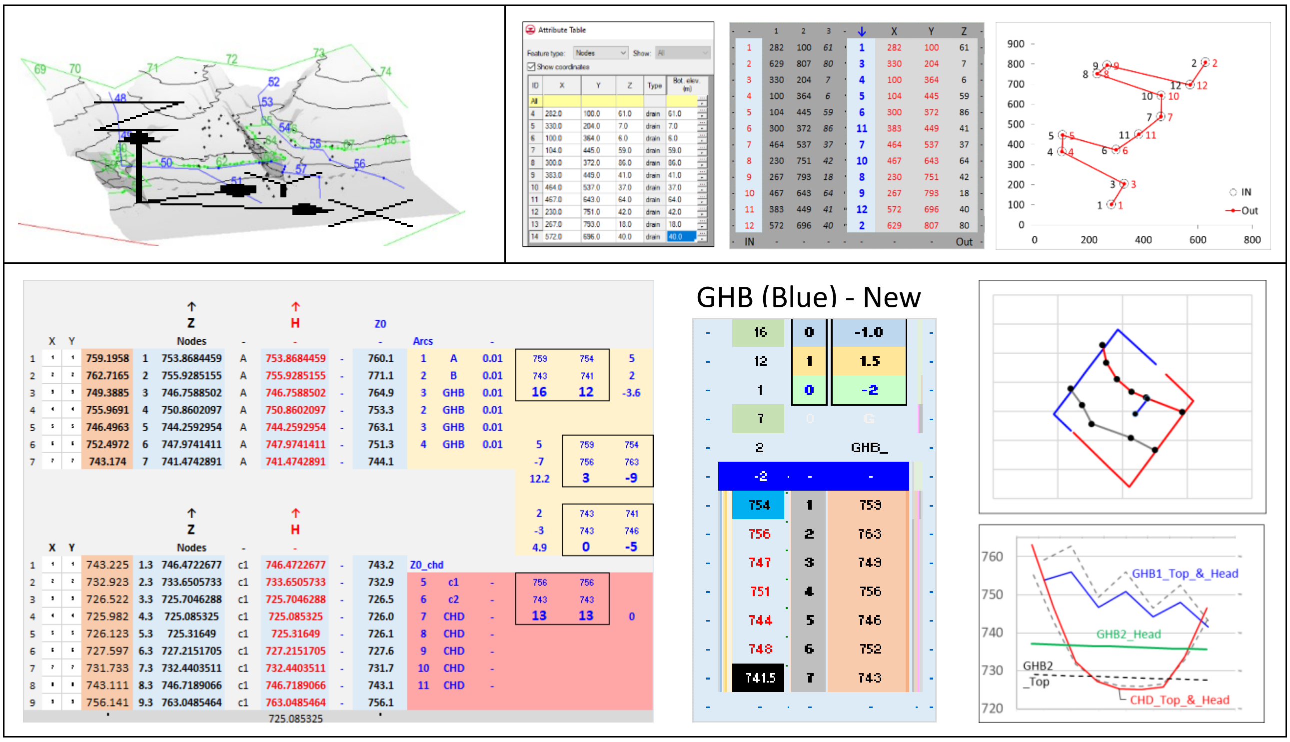

Figure 26: Two routines to organize the data positions (x, y) and boundary conditions elevations (z) – Tab 4

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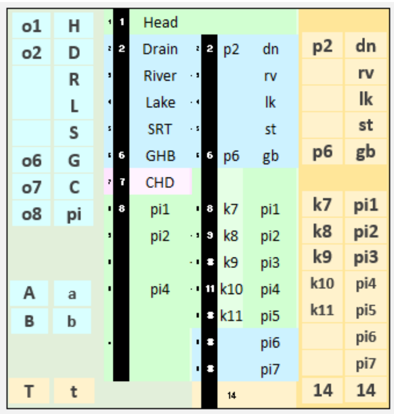
9.1. The spreadsheet main controls

As a matter of fact, Beta µ deals with at least two advanced open-source routines, MODFLOW|PEST, powered by this commercial Graphical User Interface, the Aquaveo Groundwater Modelling System®.

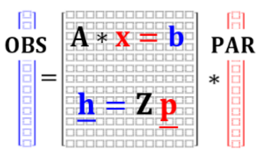
Everything was organized by the GMS team in a single *.gpr file, which afterwords comes with an accompanying [*. MODFLOW] folder and almost a hundred subfiles. Our case is named just [E.gpr].

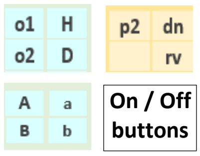
This study case archives were stored in the simples form as [C:\pest\A\E_MODFLOW].

To make things more efficient, we recommend to implement a simple Bath file routine inside the E_MODFLOW folder, as already describe at the Figure 8_04 (Thanks Franchesca!).



Theoretically, everything relies on the covariance matrix, the model per si.





There is to say, this matrix format contains all interrelated, relationship between Parameters and Observations Vectors.

This spreadsheet primary duty to contrast related information's (plus SEO & SEN, for instance) in every possible way. But even so, not ignoring possible impacts of cross correlations from a given parameter to another of its kind, as observations.

Another fundamental empowerment Beta µ believes being able to deliver as a contribution to the GMS|PEST calibration efforts come from the need of a self-organized way to automatically understands mapped observations (OBS), from the GMS to MODFLOW to PEST, which then goes to be placed side by side with the correspondent parameter's setlists. In various end formats.

So, Beta µ automatically matches the two given lists of parameters and observations through the simple uploading of the individual [Res, Seo, Par, Bpa, Sen] Beta µ tabs. Thus, the need to honor the **Rule nº 1 of 2**, described in the item 6.1 of this document. PS. To open up the inputs tabs, the [A, a] buttons need to be activated first. 

Beta µ advocates that lots of conceivably inspiring relationships are presently detached from each other. Then there is a bottleneck in figuring out the objective function (meaning) and construction mechanism. Not to mention the lack of accountability for all boundary "expectations" (MED).

Figure 27: Main Beta µ controls, some working conditions and general specifications

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9.2. The Beta µ spreadsheet internal mechanisms (IN Tab)

The reader is invited to duck on the Beta µ IN_tab on its own benefit, to learn how to get rid of eventual new bugs, and following suit, not to throw away any chance of improvement.

<u>**IN_tab**</u> has three parts: <u>**01-Arriving Columns; 02-Processing Columns; 03-References (Figure 28).**</u> For the sake of clarity, the first columns just repeat, condenses the <u>**[Res, Seo, Par, Bpa, Sen]**</u> info.

Following the spreadsheet protocol, data storage and processing capabilities are deployed, didactically, trying to reach the acutest way in handle most of MODFLOW possible scenarios in the GMS platform. There is presently the 1|55|77|112|129|171|202|219 routines. Some guidelines:

[A] The 40th column or thereabouts fix the essential trouble of having the mapped information in the expected order. In accomplishing that, it is necessary to reinforce <u>**Rule nº 2 of 2**</u>**:** Having taken all necessary precautions to reach an organized disposition of Boundary Conditions, this was not enough. A first MODFLOW|PEST <u>[referential realization]</u> is required, using the identifications (IDs) on the place of "measured expectations", Hydraulic Heads & Fluxes in the crescent order, 1,2,3,4. Doble check the PEST files and you'll be thanking me later. This preliminary realization rearranges all information in the right order (from the ID coverage), applying the <u>**Order | Fixo | Pronto**</u> routines.

[B] Observational PEST results (RES file | column) arrive in two flavors: with and without Tikhonov Regularization indices (a too ethereal subject to discuss here). Beta µ routine just gets it out of sight.

[C] From the next five sets of processing columns, the first one is subdivided indeed, in two sections:
- A, B, C, D columns receive the required data sequence. Now on, Beta µ does another automatized key routine: It takes charge of taming the long SEN_PAR file to match the preceding list.

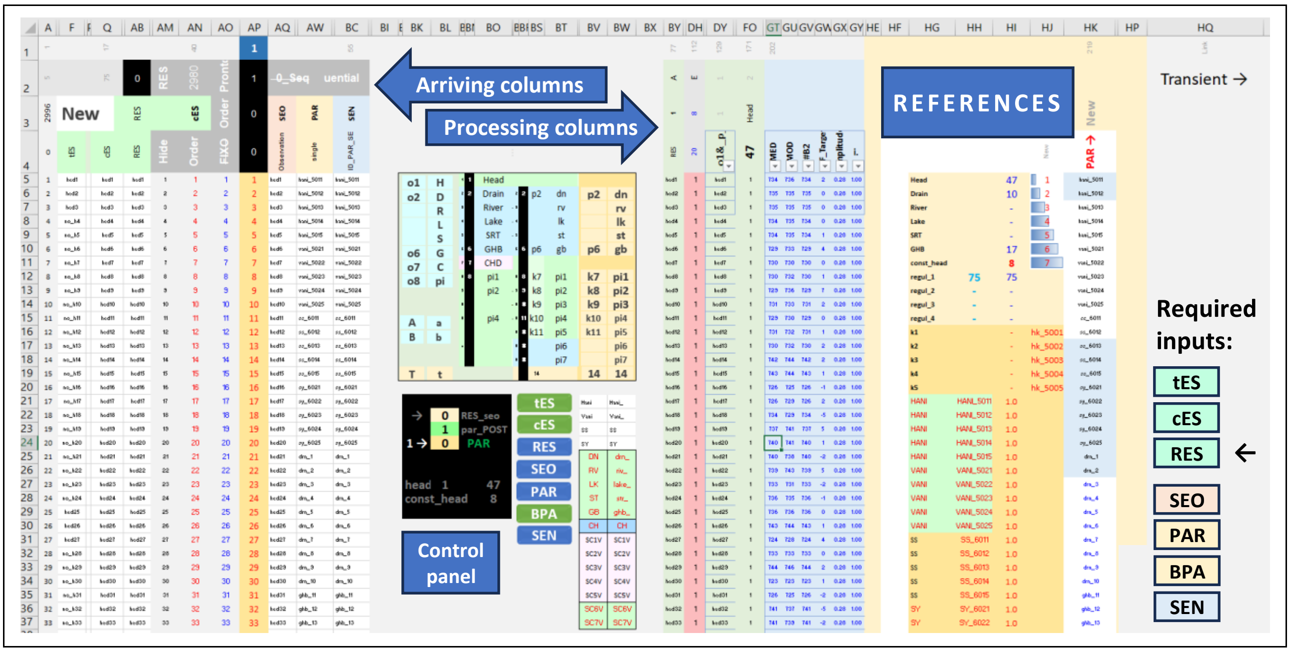

Figure 28: Organizational aspects of the main Beta µ IN Tab

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9.2.1. Indentation

[D] Beta µ was once thought, settled, to unveil the objective function. But then it assumed a pivotal role, evolving as a data processing back & front-end tool. **Figure 29** on its own clarifies the situation.

Comparing – before | after – the established main BETA µ protocol – left | right.

RES	SEO	PAR	SEN
1	head	1	HANI
2	head	2	HANI
3	head	3	HANI
4	head	4	HANI
5	head	5	HANI
6	head	6	VANI
7	head	7	VANI
8	head	8	VANI
9	head	9	VANI
10	head	10	VANI
11	head	11	SS
12	head	12	SS
13	head	13	SS
14	head	14	SS
15	head	15	SS
16	head	16	SY
17	head	17	SY
18	head	18	SY
19	head	19	SY
20	head	20	SY
21	head	21	drn 1
22	head	22	drn 2
23	head	23	drn 3
24	head	24	drn 4
25	head	25	drn 5
26	head	26	drn 6
27	head	27	drn 7
28	head	28	drn 8
29	head	29	drn 9
30	head	30	drn 10
31	head	31	ehb 11
32	head	32	ehb 12
33	head	33	ehb 13
34	head	34	ehb 14
35	head	35	ehb 15
36	head	36	ehb 16
37	head	37	ehb 17
38	head	38	ehb 18
39	head	39	ehb 19
40	head	40	ehb 20
41	head	41	ehb 21
42	head	42	ehb 22
43	head	43	ehb 23
44	head	44	ehb 24
45	head	45	ehb 25
46	head	46	ehb 26
47	head	47	ehb 27
48	drain	48	sc1v1
49	drain	49	sc1v2
50	drain	50	sc1v3
51	drain	51	sc1v4
52	drain	52	sc1v5
53	drain	53	sc2v1
54	drain	54	sc2v2
55	drain	55	sc2v3
56	drain	56	sc2v4
57	drain	57	sc2v5
58	ehb	58	sc3v1
59	ehb	59	sc3v2
60	ehb	60	sc3v3
61	ehb	61	sc3v4
62	ehb	62	sc3v5
63	ehb	63	sc4v1
64	ehb	64	sc4v2
65	ehb	65	sc4v3
66	ehb	66	sc4v4
67	ehb	67	sc4v5
68	ehb	68	sc5v1
69	ehb	69	sc5v2
70	ehb	70	sc5v3
71	ehb	71	sc5v4
72	ehb	72	sc5v5
73	ehb	-	-
74	ehb	-	-
75	CHD	-	-
76	CHD	-	-
77	CHD	-	-
78	CHD	-	-
79	CHD	-	-
80	CHD	-	-
81	CHD	-	-
82	CHD	END	END

RES	SEO	-	-	PAR	SEN	-	-
1	head	62	ehb	-	-	35	ehb 15
2	head	63	ehb	-	-	36	ehb 16
3	head	64	ehb	-	-	37	ehb 17
4	head	65	ehb	-	-	38	ehb 18
5	head	66	ehb	-	-	39	ehb 19
6	head	67	ehb	-	-	40	ehb 20
7	head	68	ehb	-	-	41	ehb 21
8	head	69	ehb	-	-	42	ehb 22
9	head	70	ehb	-	-	43	ehb 23
10	head	71	ehb	-	-	44	ehb 24
11	head	72	ehb	-	-	45	ehb 25
12	head	73	ehb	-	-	46	ehb 26
13	head	74	ehb	-	-	47	ehb 27
14	head	75	CHD	-	-	-	-
15	head	76	CHD	-	-	-	-
16	head	77	CHD	-	-	-	-
17	head	78	CHD	-	-	-	-
18	head	79	CHD	-	-	-	-
19	head	80	CHD	-	-	-	-
20	head	81	CHD	-	-	-	-
21	head	82	CHD	-	-	-	-
22	head	-	-	-	-	48	sc1v1
23	head	-	-	-	-	49	sc1v2
24	head	-	-	-	-	50	sc1v3
25	head	-	-	-	-	51	sc1v4
26	head	-	-	-	-	52	sc1v5
27	head	-	-	-	-	53	sc2v1
28	head	-	-	-	-	54	sc2v2
29	head	-	-	-	-	55	sc2v3
30	head	-	-	-	-	56	sc2v4
31	head	-	-	-	-	57	sc2v5
32	head	-	-	-	-	58	sc3v1
33	head	-	-	-	-	59	sc3v2
34	head	-	-	-	-	60	sc3v3
35	head	-	-	-	-	61	sc3v4
36	head	-	-	-	-	62	sc3v5
37	head	-	-	-	-	63	sc4v1
38	head	-	-	-	-	64	sc4v2
39	head	-	-	-	-	65	sc4v3
40	head	-	-	-	-	66	sc4v4
41	head	-	-	-	-	67	sc4v5
42	head	-	-	-	-	68	sc5v1
43	head	-	-	-	-	69	sc5v2
44	head	-	-	-	-	70	sc5v3
45	head	-	-	-	-	71	sc5v4
46	head	-	-	-	-	72	sc5v5
47	head	-	-	-	-	-	-
-	-	-	-	1	HANI	-	-
-	-	-	-	2	HANI	-	-
-	-	-	-	3	HANI	-	-
-	-	-	-	4	HANI	-	-
-	-	-	-	5	HANI	-	-
-	-	-	-	6	VANI	-	-
-	-	-	-	7	VANI	-	-
-	-	-	-	8	VANI	-	-
-	-	END	END	9	VANI	END	END
-	-			10	VANI		
-	-			11	SS		
-	-			12	SS		
-	-			13	SS		
-	-			14	SS		
-	-			15	SS		
-	-			16	SY		
-	-			17	SY		
-	-	Next	1	18	SY	Next	2
-	-	-	-	19	SY	-	-
-	-	-	-	20	SY	-	-
48	drain	-	-	21	drn 1	-	-
49	drain	RES	SEO	22	drn 2	PAR	SEN
50	drain			23	drn 3		
51	drain	PAR	SEN	24	drn 4	RES	SEO
52	drain			25	drn 5		
53	drain	-	-	26	drn 6	-	-
54	drain	-	-	27	drn 7	-	-
55	drain	-	-	28	drn 8	-	-
56	drain	-	-	29	drn 9	-	-
57	drain	-	-	30	drn 10	-	-
58	ehb	-	-	31	ehb 11	-	-
59	ehb	-	-	32	ehb 12	-	-
60	ehb	-	-	33	ehb 13	-	-
61	ehb	-	-	34	ehb 14	-	-
-	-	END	END	-	-	END	END

Figure 29 – Indentation - Matching Observations and Parameters, the main logic behind the spreadsheet frame.

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Complementing the guidelines above: The next two sets from **02-Processing Columns at Figure 28** performs no more than being simply repositories to the preceding logic, besides some help in making the data movements within the various Beta µ worksheets a bit more palatable to the user.

Then finally comes a data recapture from the various specific processes from the others worksheets.

So far, at REFERENCES, most of it displays fixed contents aiding, steering the algorithm as a whole.

Here, cells of variations nomenclatures to related functions are harmonized, then the code rearranges what can be taken as interconnected or interchangeable elements. Then it uses some malleable maneuvers accounting for observations & parameters wherever the modelling demands.

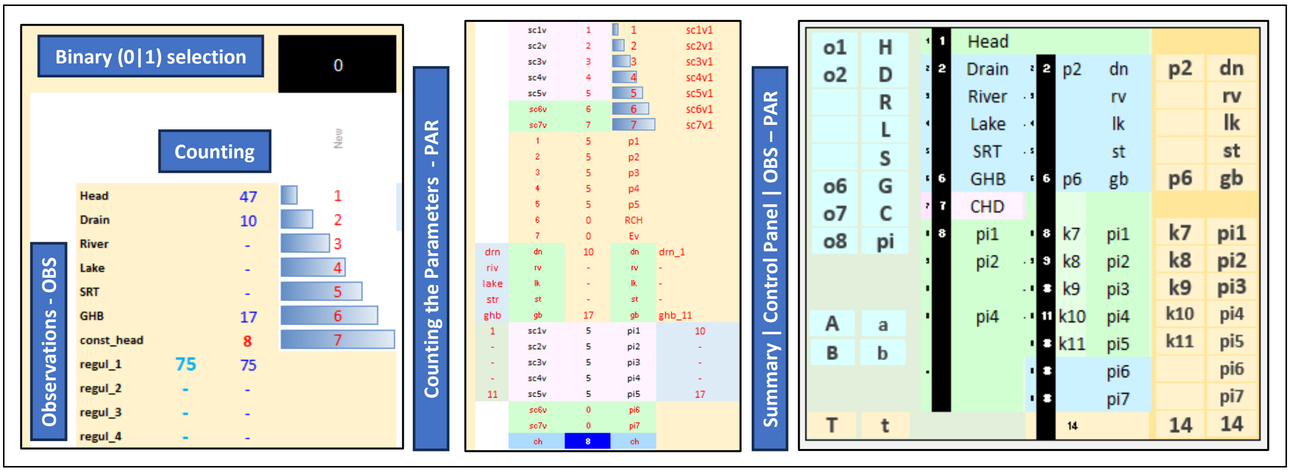

Figure 30: Referential cells – controlling the whole spreadsheet logic – IN tab

Coming soon, this new routine addresses the transient scenarios (Figure 31). That's why the set of parameters Specific storage (SS) and Specific yield (SY) have already been foreseen for the present spreadsheet steady state format. An automatized code for it is still under development (Figure 31).

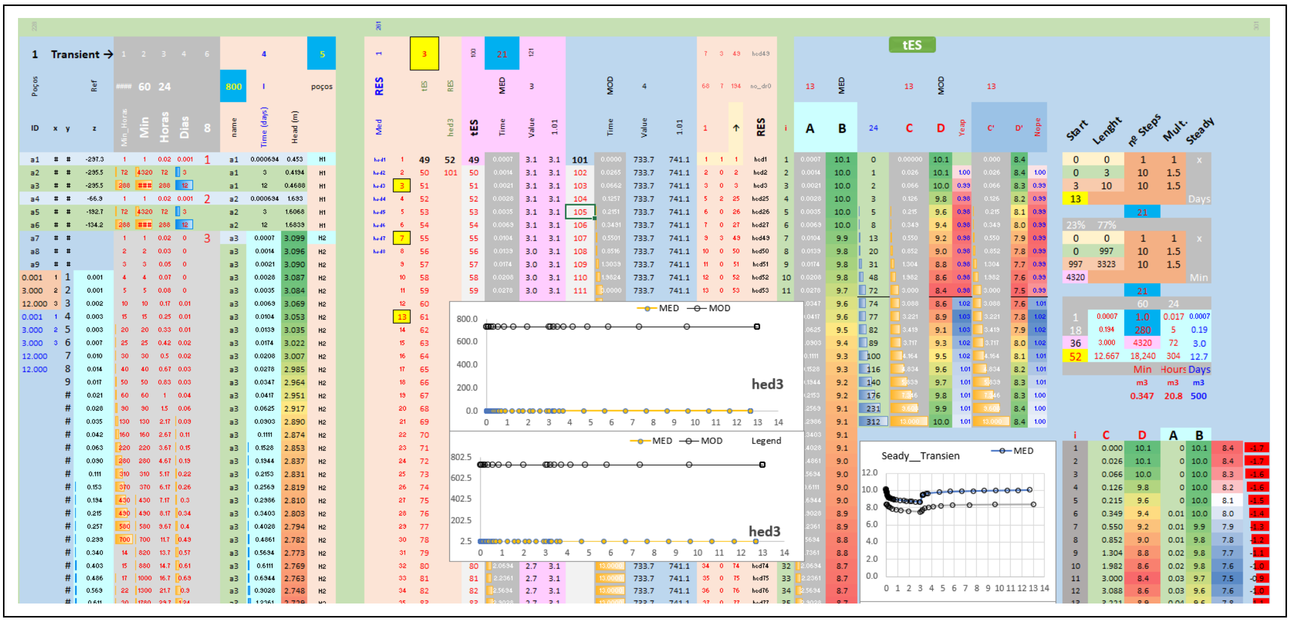

Figure 31: Handling the transient scenarios – Final, extra part still under development – IN tab

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TABLE OF FIGURES

End

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