Chapter-4

MODEL DESCRIPTION AND APPLICATIONS

The chapter provides an overview of VP Model attained through the work described in the previous chapter, and presents two modelling problems pertaining to DDP solved through the developed VP Model. It also illustrates, use of VP Model for simulation and optimization and linking of VP Model with a reputed software, through examples pertaining to DDP.

4.1 Model Description

The developed VP Model has the following main parts:

A. **Simulation environment:** It is the main sheet for user's interface. It may be used to:

i. Define the independent and dependent variables and its units in order to attain a specific model correlating these variables.

ii. Go into the Training and Testing Sheets

iii. Check the readiness of the model for simulation and optimization

iv. Perform simulation and optimization

Snapshot of this sheet is provided in fig. 4.1 below. Fig 4.2 below provides a closer look of the 'simulation environment' of VP Model. It may be noted that in these figures other sheets namely Processing, Testing, Training and Model in addition to Simulation can be seen. But sheets other than Simulation are intended to be hidden for the end users.

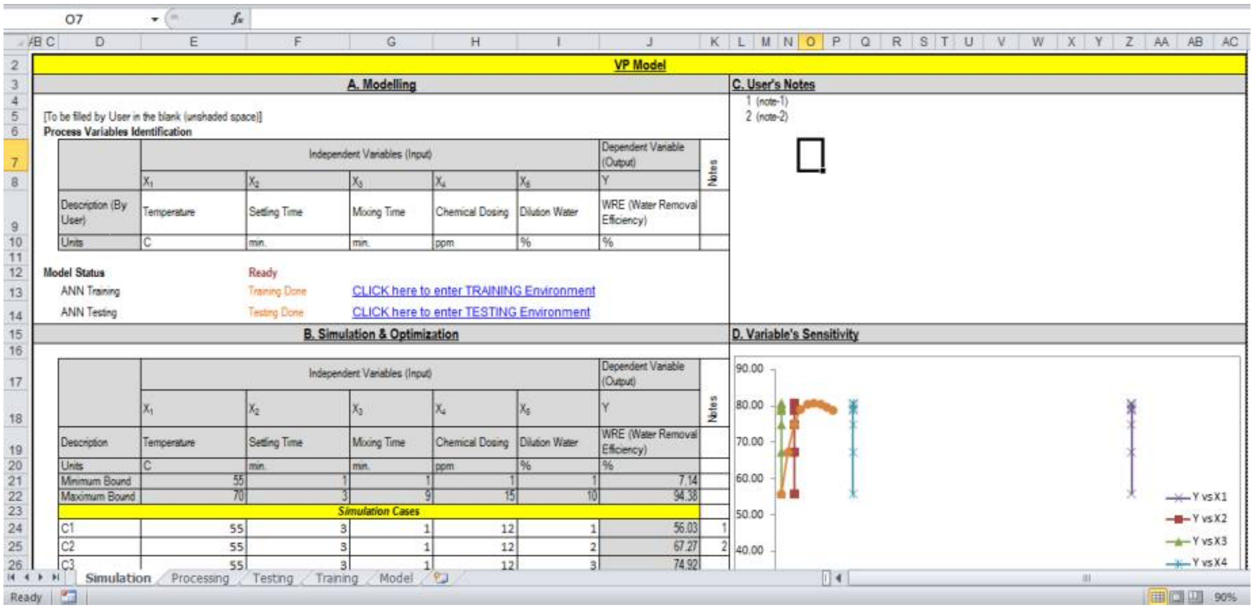


Fig. 4.1: Snapshot of the front-end sheet of VP Model

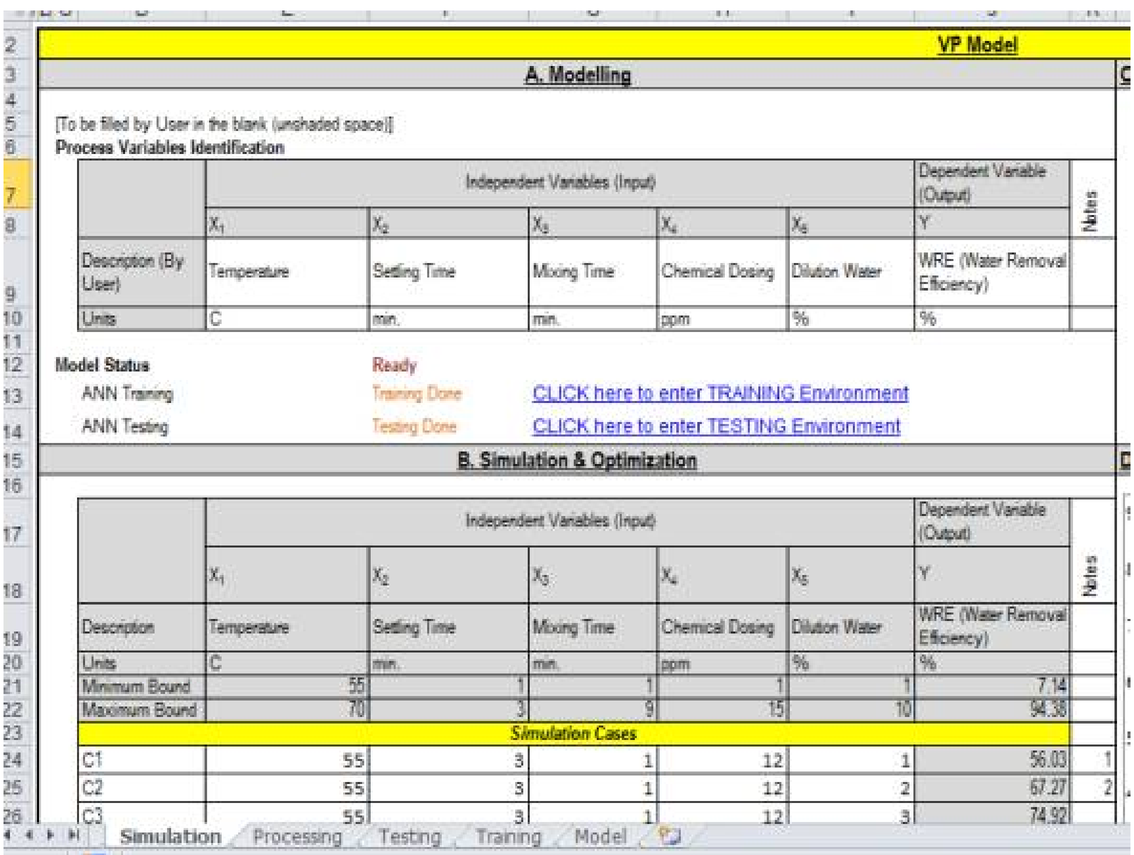


Fig. 4.2: Snapshot of the front-end sheet of VP Model: closer view

B. **Processing environment:** This is the hidden calculation sheet that provides means to transmit input to neural network from user's interface and to transmit output from the neural network to the user's interface after automatically performing scaling/normalization of input/output for accomplishing simulation and optimization. This is the 'back-end' tool not accessible to general end user.

C. **Training environment:** This can be accessed through the link provided in the 'simulation environment'. It can be used to populate the model with "Training Data" in order to train the ANN and retrieve and review the output generated by the model.

D. **Testing environment:** This can be accessed through the link provided in the 'simulation environment'. It can be used to feed the model with "Testing Data" and retrieve and review the output generated by the model.

E. **Model:** This can be accessed through the link provided in the "Training" Sheet. It contains the neural network computations including MSE, weights and biases.

4.2 Modelling Applications

As already mentioned previously, first an MLP type ANN was implemented in MS Excel, which by virtue of having inherent combined power and versatility of ANN and Excel spreadsheet can serve as a versatile process model (named VP Model). Thereafter, two process modelling problems pertaining to DDP was solved through the VP model, in order to be able to simulate and optimize operations. These two modelling problems are further described in the following sub-sections.

4.2.1. Modelling Problem-1: Modelling of DDP to predict SRE and WRE

<u>Problem Statement</u>: To model DDP, correlating performance of DDP (expressed in terms of SRE and WRE) with 5 process variables representing common operating factors as detailed below:

Dependent variables:

- Salt Removal Efficiency (expressed as %), SRE $= \left(1 - \frac{\text{outlet salt content}}{\text{inlet salt content}}\right) \times 100$
- Water Removal Efficiency (expressed as %), WRE $= \left(1 - \frac{\text{outlet water content}}{\text{inlet water content}}\right) \times 100$

Independent variables:

5 process variables representing common operating factors, namely, heating, chemical dosing, dilution, mixing and gravity settling:

- Temperature (^{o}C)
- Chemical injection (ppm)
- Fresh water injection (%)
- Mixing time (min.)
- Settling time (min.)

<u>Solution Method and Results</u>:

VP model was populated and trained with collected data from the literature [ref. Appendix-A2 for SRE; Appendix-A4 for WRE], separately, for determining SRE and WRE as output with above 5 process variables as input.

In general, data need to be pre-processed for outliers detection; however, to compare the result of the present model with the results obtained in the previous study, data was used 'as it is' from the literature.

After populating the model (that is, entering the data MS Excel sheet) for training data, it was normalized (scaled) from values 0 to 1 [10] . Thereafter, weights and biases were initialized with random numbers between -0.3 to 0.3 [10] in the "Model" sheet accessed through the "Training environment", though MS Excel can start iteration with any number. Then, Solver tool of Excel was run. After the model reached to some convergence, following values of model parameters were achieved, for SRE and WRE (as separate models).

Table 4.1: Model parameters for predicting SRE (%)

ANN Process Model Parameters											
i (down) / j (right)		1	2	3	4	5	6	7	8	9	10
w_{ij}	1	-12.6263	0.7582	-14.9015	-5.0235	4.5651	1.6923	-0.4025	7.9495	4.2642	9.5242
	2	24.3148	8.5870	15.3739	13.3558	16.9482	15.0946	15.3510	22.9725	15.4417	12.9918
	3	-10.6481	-0.8226	0.9016	9.9555	7.0863	0.5747	0.0929	8.8434	3.6772	0.1199
	4	-0.0622	-2.0029	-1.0860	0.0012	-0.1696	-0.4944	-1.0203	-4.9077	-3.8966	-0.5517
	5	0.1354	-0.2895	0.1854	-0.0598	0.0137	0.3066	-0.8527	0.4459	0.1062	0.3660
b_j		3.9290	-11.4582	3.5639	-3.7735	-11.7404	-2.8373	-1.0731	-10.3004	-1.3300	-9.7211
w_j		-8.3437	-4.0910	9.5657	-8.0860	14.6229	-10.4300	-3.1688	0.4425	0.5813	5.5897
b		0.3409									

Table 4.2: Model parameters for predicting WRE (%)

ANN Process Model Parameters											
i (down) / j (right)		1	2	3	4	5	6	7	8	9	10
w_{ij}	1	57.7841	-75.5347	1.9366	-0.2256	-13.3902	-6.1184	10.7764	-2.1404	0.1115	0.9743
	2	-38.2708	97.6506	15.4344	4.2559	3.2672	-0.4294	-1.3522	39.8944	-5.2743	0.6025
	3	2.0863	0.1806	8.3327	2.8828	-1.7233	5.8217	-8.6470	-55.2661	8.2321	-0.5325
	4	0.5544	97.3621	-4.5364	0.7124	-2.0782	0.3953	-1.1245	1.4520	0.7859	26.0496
	5	-114.8105	-0.0799	0.4044	10.5568	-7.1091	-0.3372	0.6378	-1.9100	0.6282	-0.2937
b_j		5.0953	-98.4017	2.2188	-2.0041	-1.7481	-0.7531	2.0516	1.2626	-0.0450	5.3534
w_j		-0.0459	-0.0746	0.4877	0.1635	-0.7286	-1.4188	-1.2716	0.5842	0.6445	30.2261
b		-29.4838									

As the model's parameters were found, it means modelling was accomplished. However, in case of ANN, it should be further tested for its output for unseen data. Accordingly, the model was tested with Testing data [ref. Appendix-A3 for SRE prediction; Appendix-A5 for WRE prediction].

To verify the performance of the achieved models (separate for SRE and WRE), outputs (SRE and WRE) of thus developed models in MS Excel were compared with:

- known experimental value (available in literature)

- known value computed from ANN model implemented through MATLAB (available in literature)

Results, discussed in next chapter, were found as encouraging.

Thereafter, one can enter different values of input variables as different simulation cases C1, C2, C3 etc. through the 'simulation environment' to know variation in SRE or WRE. Similarly one can use any simulation scenario as S1, S2 etc. to further optimize it using various tools available in Excel; which is further explained in the "Simulation and Optimization" sub-section of this thesis.

4.2.2. Modelling Problem-2: Modelling of DDP to predict Wash Water flowrate

Problem Statement: To model DDP to predict wash water flowrate based on 5 other variables representing common operating factors.

Dependent variable:

- Wash water flowrate (bbl/day i.e. barrel per day)

Independent variables:

5 variables representing common operating parameters in real plant, viz.:

- Crude production flow rate (bbl/day)
- Inlet temperature (^{o}F)
- Chemical dosing rate (bbl/day)
- Inlet salt content (ppm)
- Outlet salt content (ppm)

Note: Even though above two process-modelling problems are presented in regard to DDP, but both have different set of independent and dependent variables pertaining to different crude for different locations.

<u>Solution Method and Results</u>:

This modelling problem is unrelated to previous problem, except that both are pertaining to DDP. This is intended to demonstrate versatility of the developed VP Model, by getting the model populated, trained and tested, afresh, for different dependent and independent variables for another sets of data extracted from literature from another source.

More information regarding data is further detailed in section 3.2.3. Used data is annexed as appendix-A6 and A7.

Like solution to first problem, the VP Model was populated, trained and thus solved for predicting wash water flowrate based on the process variables indicated above for this problem. After the model reached to some convergence, following values of model parameters were achieved:

Table 4.3: Model parameters for estimating wash water flowrate

ANN Process Model Parameters											
i (down) / j (right)		1	2	3	4	5	6	7	8	9	10
w_{ij}	1	-13.9678	-96.0821	-7.7079	-157.0411	18.5960	3.7788	-215.5873	-21.8628	81.0235	9.4282
	2	4.5744	-30.1709	2.9642	52.6207	56.2546	5.9790	202.3798	-69.4241	-14.8663	-50.7040
	3	62.7162	-125.6250	116.2317	49.9733	33.4264	2.0586	-26.2680	3.1325	-11.0160	-63.0163
	4	4.3560	60.5267	3.8898	18.3727	4.8756	-2.8675	-183.5474	-7.3668	17.9194	0.9059
	5	2.5819	45.4958	2.7371	-10.5053	86.6214	-3.1115	77.6194	-82.1096	-13.1772	-18.9551
b_j		-1.8631	53.5763	-13.8674	132.1571	-31.6867	14.4653	43.3210	35.1020	-74.8899	5.4226
w_j		-0.3889	0.0985	0.5244	-8.2772	1.2305	4.0385	0.3954	1.1504	-0.1122	0.5890
b		3.2600									

Thereafter, the model was further tested.

To verify the performance of the model, output (predicted wash water flowrate) of thus developed model in MS Excel was compared with known plant values (available in literature). The results were found encouraging and are explained in the next chapter.

The converged and tested models may be utilized to simulate some scenarios in order to find optimal operating conditions, as indicated in the next section.

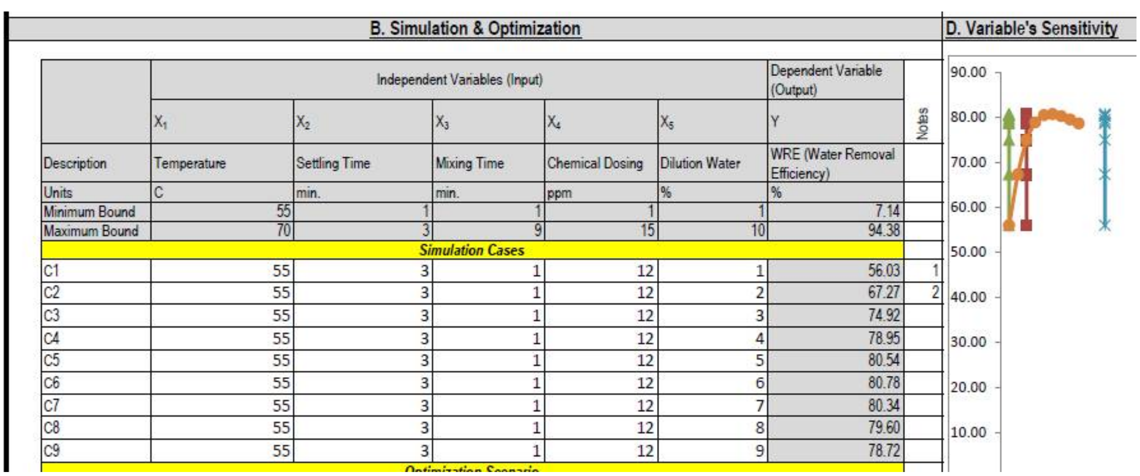
4.3 Simulation and Optimization

After satisfactory training and testing, thus created models through VP Model are ready for simulation and optimization. It may also be noted that the purpose of this work is to attain tools rather than finding optimal solutions to a specific numerical case.

4.3.1. Simulation

Several rows (ref. simulation cases C1, C2, C3 etc. in fig. 4.2) have been provided in the 'simulation environment' so that the user may like to simulate various operating scenarios by varying various independent variables (also ref. fig. 4.3 below). Plots of Y vs. X_1, X_2, X_3, X_4, and X_5 have been provided for sensitivity analysis (ref. fig. 4.3 below)

For example, in the screenshot provided in, it can be seen that by changing the value for dilution water and keeping the remaining independent variables same, impact on water removal efficiency was checked as simulation cases C1, C2, C3, C4, …… and C9. It is remarked that the obtained values, those appear in this screenshot are not the main focus but the developed framework / tool is the main issue of this thesis.


B. Simulation & Optimization

	Independent Variables (Input)					Dependent Variable (Output)	Notes
	X_1	X_2	X_3	X_4	X_5	Y	
Description	Temperature	Settling Time	Mixing Time	Chemical Dosing	Dilution Water	WRE (Water Removal Efficiency)	
Units	C	min.	min.	ppm	%	%	
Minimum Bound	55	1	1	1	1	7.14	
Maximum Bound	70	3	9	15	10	94.38	
Simulation Cases							
C1	55	3	1	12	1	56.03	1
C2	55	3	1	12	2	67.27	2
C3	55	3	1	12	3	74.92	
C4	55	3	1	12	4	78.95	
C5	55	3	1	12	5	80.54	
C6	55	3	1	12	6	80.78	
C7	55	3	1	12	7	80.34	
C8	55	3	1	12	8	79.60	
C9	55	3	1	12	9	78.72	

Fig. 4.3: Snapshot highlighting provision for simulation in VP Model

4.3.2. Optimization

For conducting optimization exercise, two rows (ref. optimization scenario S1 and S2 in fig. 4.4 below) have been dedicated in the 'simulation environment' in VP Model.

B. Simulation & Optimization

	Independent Variables (Input)					Dependent Variable (Output)
	X_1	X_2	X_3	X_4	X_5	Y
Description	Temperature	Settling Time	Mixing Time	Chemical Dosing	Dilution Water	WRE (Water Removal Efficiency)
Units	C	min.	min.	ppm	%	%
Minimum Bound	55	1	1	1	1	7.14
Maximum Bound	70	3	9	15	10	94.38
Simulation Cases						
C1	55	3	1	12	1	56.03
C2	55	3	1	12	2	67.27
C3	55	3	1	12	3	74.92
C4	55	3	1	12	4	78.95
C5	55	3	1	12	5	80.54
C6	55	3	1	12	6	80.78
C7	55	3	1	12	7	80.34
C8	55	3	1	12	8	79.60
C9	55	3	1	12	9	78.72
Optimization Scenario						
S1	65	2	1	2	1	60.23
S2	67	2	1	2	1	60.71

Fig. 4.4: Snapshot highlighting provision for optimization in VP Model

Provisions for two optimization scenarios (S1 and S2) have been dedicated in order to facilitate comparison. Various tools available in MS Excel can be used for performing optimization. For example, Solver may be used to maximize, minimize or to attain any value for any cell through iteration by adjusting remaining 5 cells (and even other cells anywhere). It is reminded that Solver has GRG2 algorithm for solving NLP type of optimization problem. At practical level, such optimization tool has numerous applications.

For the sake of demonstrating such optimization tool for model-based decision support at any plant, some examples are presented below:

<u>Example-1</u>:

Refer to fig. 4.4 above wherein some values for independent variables are entered for S1 and S2. Suppose, it was desired to increase WRE to 90 % by adjusting chemical dosing and dilution water for the plant, which was being operated as per the operating conditions indicated in scenario S1 in fig 4.4. Scenario S2 depicted in fig. 4.4 has been entered same as S1 (except some difference in temperature, which resulted little difference in WRE).

Solver was used (ref. fig. 4.5 below) to find the value of dilution water and chemical dosing in S2 (present in Excel row number 35) which may increase the efficiency from 60% to 90%. Corresponding WRE (present in Excel column number J) was set as objective function, and its target value was set as 90. It may be noted that Excel cell designated as J35 in the below fig. 4.5 represents WRE for scenario S2. Further, Excel cells H35 and I35 represents chemical dosing and dilution water respectively for scenario S2, which are the independent variables of interest for carrying out the optimization exercise. Constraints were set so that both independent variables may assume values between their maximum and minimum bounds. For illustrating different techniques, constraints for chemical dosing and dilution water were put in two different ways in fig 4.5: (i) constraints for dilution water was put using cell reference of the minimum and maximum bounds, and (ii) constraints for chemical dosing was put using the values of minimum and maximum bounds. GRG Nonlinear was selected as solving method and Solve button was pressed.

After carrying out several iterations, Excel returned the response, which is depicted in fig 4.6 below. Excel response indicates that it is not possible to attain the desired value of the efficiency (WRE) by only changing the chemical dosing and dilution rate within the given bounds, as it could increase up to around 82% (ref. fig. 4.6).

Such kind of model-based decision support tool would be helpful for optimizing plant operation, wherein various implicit constraints are present, and which involves aspects which may not be expressed quantitatively, at the hour of need. Such tool would be helpful in providing some instant answers pertaining to operational optimization exercise.

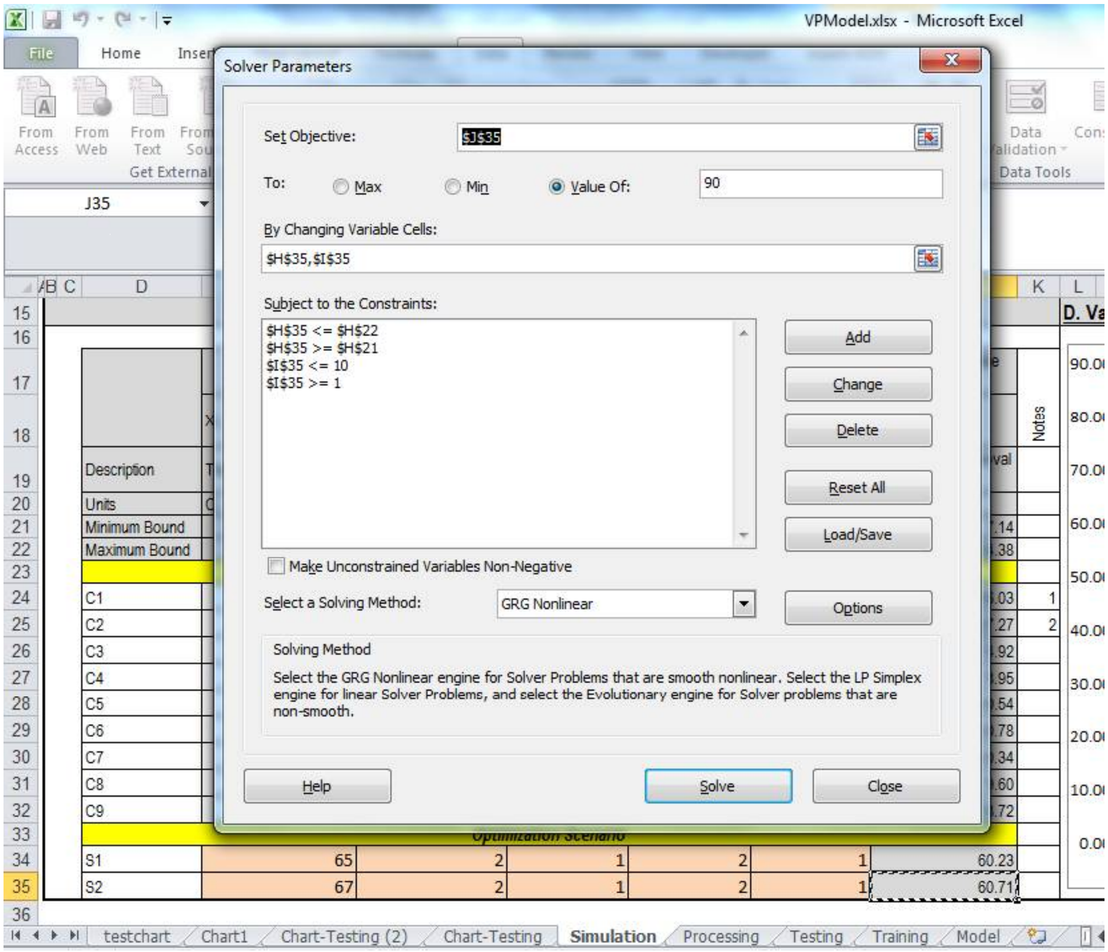


Fig. 4.5: Ex-1 for operational optimization through VP Model using Solver (Input)

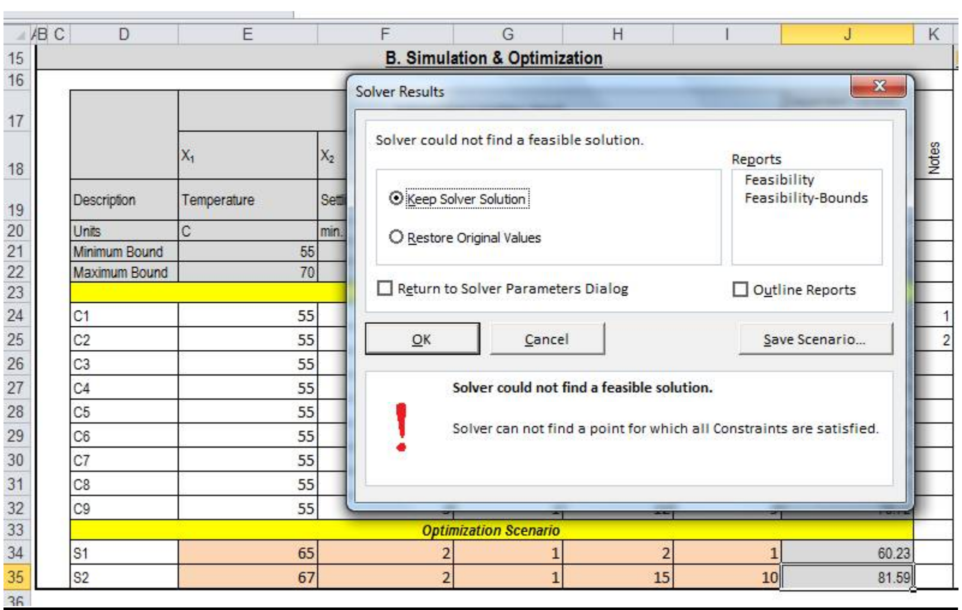
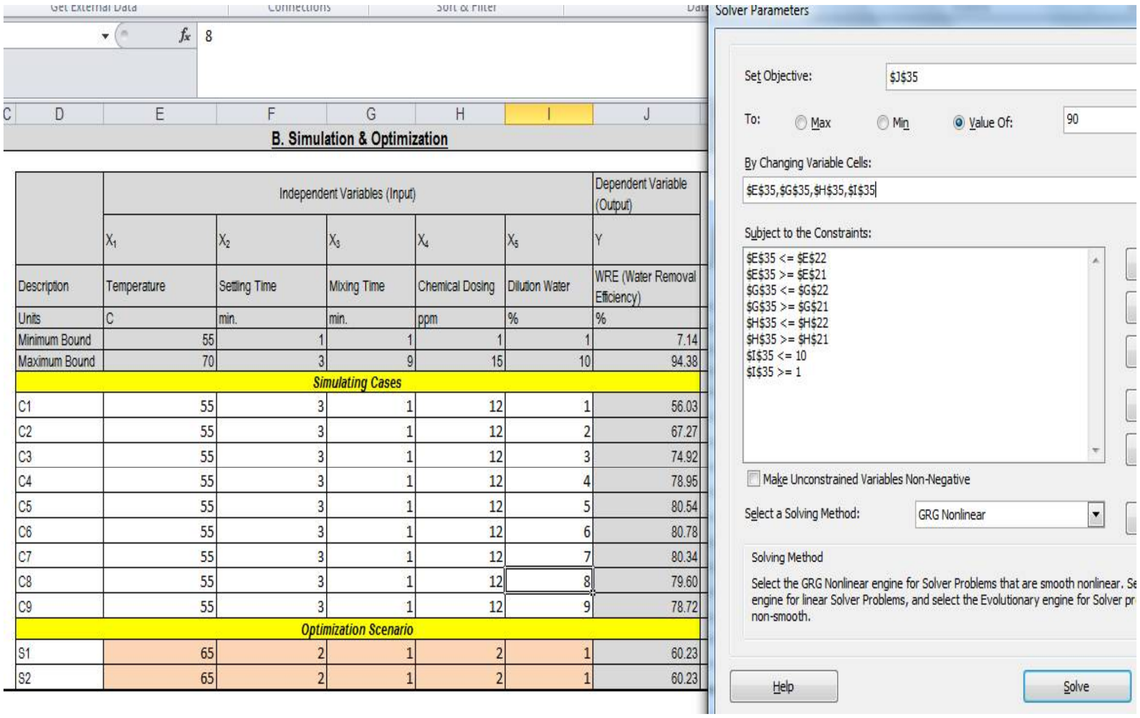


Fig. 4.6: Ex-1 for operational optimization through VP Model using Solver (Output)

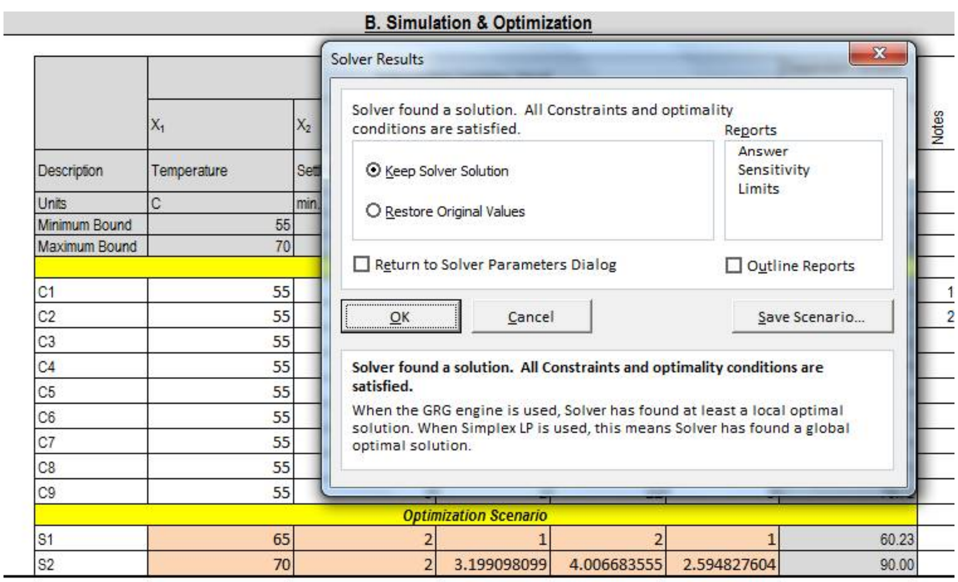
Example-2:

Same as example-1, but adjusting all variables except settling time. Again Solver was used to run its GRG2 optimization algorithm by setting objective function and constraints, as shown in fig. 4.7, and the result is depicted in fig 4.8 below:



	Independent Variables (Input)					Dependent Variable (Output)
	X_1	X_2	X_3	X_4	X_5	Y
Description	Temperature	Setting Time	Mixing Time	Chemical Dosing	Dilution Water	WRE (Water Removal Efficiency)
Units	C	min.	min.	ppm	%	%
Minimum Bound	55	1	1	1	1	7.14
Maximum Bound	70	3	9	15	10	94.38
Simulating Cases						
C1	55	3	1	12	1	56.03
C2	55	3	1	12	2	67.27
C3	55	3	1	12	3	74.92
C4	55	3	1	12	4	78.95
C5	55	3	1	12	5	80.54
C6	55	3	1	12	6	80.78
C7	55	3	1	12	7	80.34
C8	55	3	1	12	8	79.60
C9	55	3	1	12	9	78.72
Optimization Scenario						
S1	65	2	1	2	1	60.23
S2	65	2	1	2	1	60.23

Fig. 4.7: Ex-2 for operational optimization through VP Model using Solver (Input)



	X_1	X_2				
Description	Temperature					
Units	C	min.				
Minimum Bound	55					
Maximum Bound	70					
C1	55					
C2	55					
C3	55					
C4	55					
C5	55					
C6	55					
C7	55					
C8	55					
C9	55					
Optimization Scenario						
S1	65	2	1	2	1	60.23
S2	70	2	3.199098099	4.006683555	2.594827604	90.00

Fig. 4.8: Ex-2 for operational optimization through VP Model using Solver (Output)

As S2, initially was set almost as S1, notice the change in fig. 4.8: the Solver adjusted all except settling time to find the value of 90%. However, as a caution this could be only a local optimal solution. Trials can be done and arranged in Excel to apply more criteria.

Above examples, were shown as starter to demonstrate some simulation and optimization cases that may be applied on the model populated, trained and tested for predicting WRE.

There are many options to implement optimization problems including implementing other algorithm (e.g. LM) as well as utilizing ANN's mapping of entire data range to find a global maxima or minima, which are beyond the scope of present thesis.

4.4 VP Model linking with other reputed software (like Aspen Hysys)

Aspen Hysys has ASW (Aspen Simulation Workbook) add-in for Excel, which allows users to interact with the Hysys rigorous model at the back-end and Excel worksheet at the front-end. Therefore, the developed model in MS Excel may be linked to the Plant's Hysys model using ASW Excel add-in. As a simple example for simulation and optimization, to understand the framework, linking of the versatile process model (VP Model) developed in this study with Aspen Hysys is depicted in fig. 4.9 below:

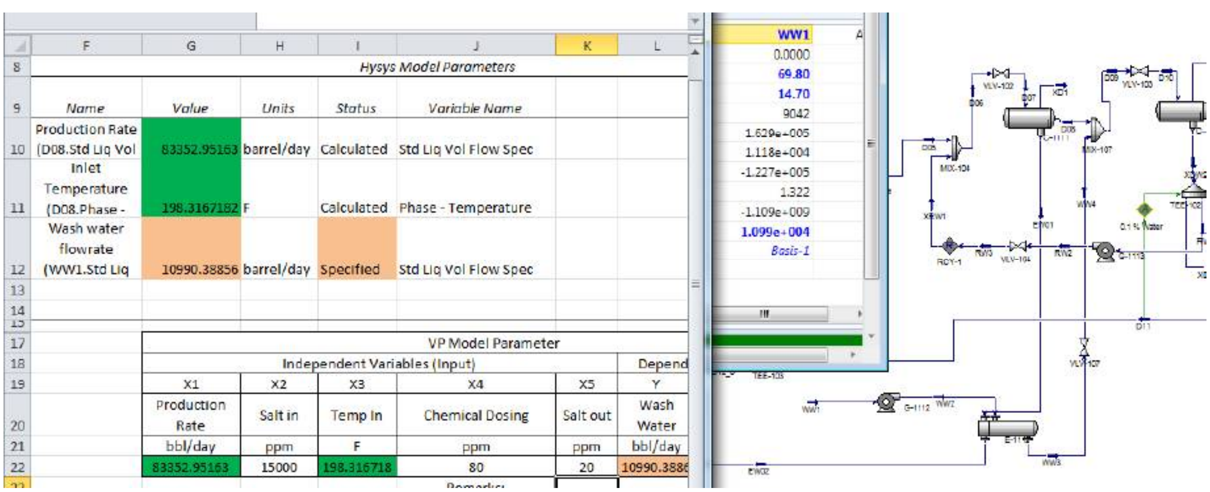


Fig. 4.9: Snapshot demonstrating VP Model linking with Hysys

In the above screen snapshot, Hysys PFD and Hysys worksheet for wash water pump and Excel worksheet providing interface between Hysys model and VP model of this study are all accommodated by minimizing and resizing views. These are further explained below:

a) On the right side of the fig. 4.9, the PFD of the Hysys model can be seen, in which desalters have been modelled as 3-phase separators, and there is a worksheet opened in the same Hysys environment showing wash water flow rate, which in this example is a specified input by the user. It may be noted that because Hysys does not predict performance of the desalter, user specified some value based on prevailing practice/experience regarding oil/wash water flow rates ratio to achieve desalting within the permissible range. To emphasize, this ratio was based on a general practice (typically within 3 to 7%) and does not represent specific optimal requirement depending upon actual operating scenario.

   Evidently, a modelling tool to predict wash water requirement for attaining a particular salt content in the outlet stream would save huge water (given the flow rate of total crude production in million barrels per day), particularly in a desert area like the middle-east. It will also minimize the energy consumption for pumping, could also minimize the nuisance to environment created during power generation, may minimize the chemical consumption causing huge savings and will reduce chemical entry to ecological system.

b) On the left side of the fig. 4.9, there is an Excel sheet, in the lower half of which, input and output variables of the present study model (VP Model) have been incorporated, so that wash water can be predicted based on the production rate, temperature, inlet salt content, chemical dosing rate and outlet salt content by linking cells of this Excel sheet to VP Model using normal procedure of linking cells of two different Excel sheet.

   Also in upper half of this Excel sheet, some of the process variables of Hysys, one as input to Hysys and some other as outputs from Hysys, have been incorporated by linking the Excel sheet with Hysys through the normal procedure of Excel and Hysys linking using ASW menus.

c) Further, some of the inputs to VP Model have been imported from the Hysys output by linking Excel cells of VP Model parameters with Excel cells representing corresponding Hysys model parameters, and output of the VP Model (i.e. wash water flowrate) is fed back to Hysys by linking this Excel cell of VP Model parameter with the cell of Hysys model parameter representing the specified input to Hysys model.

Thus, in this example, based on the production rate, inlet salt content, inlet temperature, chemical dosing and outlet salt specification, VP model predicted wash water flow rate, which was specified to Hysys using cell linking feature of Excel and ASW add-in from Hysys, whereas production rate and temperature for VP model was taken from the Hysys model. This is only for illustrating the framework and not to present any numerical value seen in the figure. This research provides a building block towards deployment of some model-based decision support, utilizing the modelling, simulation and optimization skills for DDP. Finding any specific values for any specific application is not the scope of this thesis.