CHAPTER III

PROCEDURE OF SIMULATION AND OPTIMIZATION

The objective of this research is for finding optimal batch scheduling of suspension polyvinyl chloride production process. To meet maximum production in time horizon, the newly feeding proposal is proposed and trialed both simulation and plant production. Therefore, it is limited by every technical constrained. The optimization by Differential evolutionary algorithm techniques is selected to apply for model simulation in optimization part.

This chapter is presented about system overview of batch production, batch time estimation, conjunction between batch and continuous process, utilities constrained, feeding proposal and optimization.

3.1 System overview

Calculation of the production rate in function of batch timing and line limitations in order to find optimal line production rates and estimation of the times at which batches are discharged in the DGZ is necessary. An average autoclave cycle is 6 hours, thus the average between two batches is around 3 hours. Production rate (m^3/h) corresponds to downwards slope of stock volume (m^3) in DGZ. Production rate has MIN and MAX limitations and speed of variation limitations depending on the used control structure and the available element in operations of down stream equipment such as centrifugal decanter, fluidized bed dryer and sieve screens. Every autoclave has to wait until there is sufficient room in the DGZ. In the other hand, the improper starting batch could be emptied DGZ, and the equipment down stream must be shut down. Therefore, to keep slurry after finish polymerization in autoclave too long period (in experience means over 20 min) will lead to quality problem in finish product which is PVC resin. The enough space volume in DGZ at the moment of AC discharge time is always required. A chart description is in Fig 3.1.
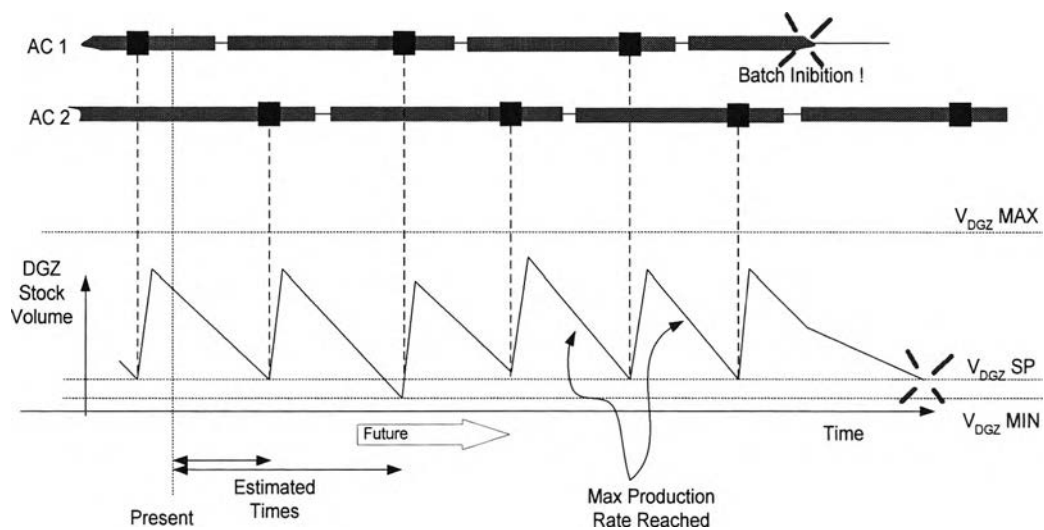

Figure 3.1 Batch switching from AC1 and AC2 to DGZ

Where

- Green bar: Autoclave Batch Operations.
- Blue boxes: Time at which an AC is discharged into the DGZ.
- Red bar: Waiting time when the AC is ready to discharge but the DGZ is occupied.

It can be made some key observations.

- Production rate (m³/h) corresponds to downwards slope of stock volume (m³) in Fig 2.1. Mass PVC resin production rate (ton/h) can be converted by multiplied production rate (m³/h) with density (ton/ m³).
- Production rate has MIN and MAX limitations and speed of variation limitations depending on the used control structure and on the available elements in operation (Such as centrifuges, sieve screens, ...).
- Every autoclave has to wait until there is sufficient room in DGZ to discharge. If the production rate is not determined in a predictive way, then the volume in DGZ may become too high generating waiting times for the next AC.
- If an important problem occurs in the line (batch inhibition, run away reaction, AC out of order and control), stripper and dryer production rates are not decreased in a predictive way, then any of them could be emptied and that unit operation must to be shut down.

3.2 Autoclave time estimation

For identified autoclave time estimation, it needs to be arranged each step of production in to Gantt chart following utilities consumption (kg/min) activities and batch time duration (min). The utilities consumption rate is plotted with time in minute along autoclave time estimation. Utilities flow rate requested are raw materials of production which are comprised of antioxidant agent (RMB), dispersing agent (RMX), vinyl chloride monomer (VCM), demineralised water (WD), initiator (INI), hot water (WH) and ammonium hydroxide (INH). Utilities supply unit is single ones, so it can not supply utilities to both autoclaves, AC1 and AC2, at the same time. This constrained was taken in to account in the condition of simulation to be one constrained function.

Therefore, reactor volume of AC1 is 120 m³ and AC2 is 140 m³ accordingly. Both reactors are equipped with the difference surface area of VCM gas condensers which are directly impacted to process and batch control. Production recipes, utilities consumptions and time consumed for each line operation is difference. So, Gantt chart of both reactors is different. The result of arrangement for suspension PVC resin grade 266RC from AC1 and AC2 are here in table 3.1 and table 3.2.

By Gantt chart of both reactors, it can be summarized as table 3.3 and table 3.4 following here below.

Table 3.1: Gantt chart of suspension polyvinyl chloride production grade 266RC in AC1.

Plant : Map Ta Phut
Quality : 266RC
Line : S1
Reactor volume (m3) : 120
Condensor surface (m2) : 78

PVC-S : Sequence timing

Operation / Time (minutes)	To be filled	Amount of feeding (kg)	Start at time (T1)	Stop at time (T2)	Total (min)	Feeding rate (kg/min)	Note
AC preparation and initial loadings							
- AC check	-	-	1	3	3	0.0	Control
- AC check inhibition system	-	-	1	3	3	0.0	PLC check
- Initial water charging (WD)	-	27000.0	4	11	8	3375.0	Feed cool WD at 27 ton
- Anti-oxydant agent(s) loading	-	25.2	4	31	28	0.9	Masterbatch preparation and feed
- Dispersing agent(s) loading	-	1898.1	5	19	15	126.5	Feed S21,S23 and anticrust S56
- VCM charging	-	51500.0	10	23	14	3678.6	Flow depend on pumps
- Initiator loading	-	22.4	12	20	9	2.5	Do not count transfer from PSX only feed
AC heating up	-						
- Hot water charging (Hot WD)	-	22000.0	32	43	12	1833.3	Feed hot water 180C at flow 185 ton/hr
- AC heat-up	-	-	-	-	-	0	Nil
Polymerisation	-	-	44	318	275	-	In normal operation
Amount of VCM (t)	51.5						
Amount of initial water (m3)	51.5						
Filling ratio (%)	-						
Use of KI	no						
Non isothermal polymerisation	no						
Kind of cooling water for the AC (TRG,chilled	chilled water						
Temperature at the double jacket inlet (°C)	5 c						
Flow of the double jacket inlet water (m3/h)	700						
Kind of cooling water for the CD (TRG,chilled	chilled water						
Temperature at the condensor inlet (°C)	5 c		Polym time: If double jacket temp. lower than #jack.ts-cd# 40 'c start ramp with initial temp at #cd in.ts# 45'c				
Flow of the condensor water (m3/h)	380						
Start of the CD at conversion rate (%)	0						
with a ramp of	0.013'c/sec						
Polymerisation time in winter (min)	275						
Polymerisation time in summer (min)	275						
Stop the reaction at conversion rate (%)	90						
Calculated at pressure (b)	2.0 P.drop						
Calculated at temperature (°C)	68						
Final operations							
- NH4OH loading	-	10.3	322	323	2	5.2	-
- Anti-oxydant agent(s) loading	-	-	319	321	3	0.0	-
AC discharge and preparation							
- AC discharge	-	-	323	334	12	0.0	-
- CD rinsing	-	-	325	333	9	0.0	-
- AC cleaning	20 m3/h	-	323	342	20	356.0	-
- AC antifouling pulverisation	800 l/h		343	359	17	5.6	-
- AC inhibition line rinsing	-		334	338	5	0.0	-
- AC degassing	-	-	-	-	-	-	No degassing from autoclave
- Final checking	-	-	343	346	4	0.0	-

102446   kg

AC preparation and initial loadings	31
AC heating up	12
Polymerisation	275
Final operations	5
AC discharge and preparation	36
TOTAL BATCH CYCLE (min)	359

Table 3.2: Gantt chart of suspension polyvinyl chloride production grade 266RC in AC2.

Plant : Map Ta Phut
Quality : 266RC
Line : S1
Reactor volume (m3) : 140
Condensor surface (m2) : 320

PVC-S : Sequence timing

Operation / Time (minutes)	To be filled	Amount of feeding (kg)	Start at time (T1)	Stop at time (T2)	Total (min)	Feeding rate (kg/min)	Note
AC preparation and initial loadings							
- AC check	-	-	1	3	3	0	Control
- AC check inhibition system	-	-	1	3	3	0	PLC check
- Initial water charging (WD)	-	33000.0	4	13	10	3300.0	Feed cool WD at 27 ton
- Anti-oxydant agent(s) loading	-	25.7	4	31	28	0.9	Masterbatch preparation and feed
- Dispersing agent(s) loading	-	1990.3	5	20	16	124.4	Feed S21,S23 and anticrust S56
- VCM charging	-	54000.0	10	24	15	3600.0	Flow depend on pumps
- Initiator loading	-	23.5	12	21	10	2.3	Do not count transfer from PSX only feed
AC heating up	-						
- Hot water charging (Hot WD)	-	22000.0	32	43	12	1833.3	Feed hot water 180C at flow 185 ton/hr
- AC heat-up	-	-	-	-	-	0	Nil.
Polymerisation	-	-	44	263	220	-	In normal operation
Amount of VCM (t)	51.5						
Amount of initial water (m3)	51.5						
Filling ratio (%)	-						
Use of KI	no						
Non isothermal polymerisation	no						
Kind of cooling water for the AC (TRG,chilled,...)	chilled water						
Temperature at the double jacket inlet (°C)	5 'c						
Flow of the double jacket inlet water (m3/h)	700						
Kind of cooling water for the CD (TRG,chilled,...)	chilled water			Polym time: If double jacket temp. lower than #jack.ts-cd# 40 'c start ramp with initial temp at #cd in.ts# 45'c			
Temperature at the condensor inlet (°C)	5 'c						
Flow of the condensor water (m3/h)	380						
Start of the CD at conversionrate (%)	0						
with a ramp of	0.013'c/sec						
Polymerisation time in winter (min)	220						
Polymerisation time in summer (min)	220						
Stop the reaction at conversion rate (%)	90						
Calculated at pressure (b)	2.0 P.drop						
Calculated at temperature (°C)	68						
Final operations							
- NH4OH loading	-	10.8	267	268	2	5.4	-
- Anti-oxydant agent(s) loading	-	-	264	266	3	0	-
AC discharge and preparation							
- AC discharge	-	-	269	294	26	0	Make take model for calculation
- AC rinsing	-	-	295	324	30	0	-
- CD rinsing	-	-	271	279	9	0	-
- AC antifouling pulverisation	800 l/h	-	325	342	18	5.6	-
- AC inhibition line rinsing	-	-	280	284	5	0	-
- Final checking	-	-	331	334	4	0	-

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AC preparation and initial loadings	31
AC heating up	12
Polymerisation	220
Final operations	5
AC discharge and preparation	73
TOTAL BATCH CYCLE (min)	334

Table 3.3 Summary of Gantt chart from batch AC1

No	Operation	Variable name	Start at time (T1)	Stop at time (T2)	Feeding rate (kg/min)
1	Initial water charging (WD)	WD	4	11	3375.000
2	Anti-oxydant agent(s) loading	RMB	4	31	0.898
3	Dispersing agent(s) loading	RMX	5	19	126.543
4	VCM charging	VCM	10	23	3678.571
5	Initiator loading	INI	12	20	2.489
6	Hot water charging (Hot WD)	WH	32	43	1833.333
7	WD Polymerisation	WDS	44	318	0.002
8	NH4OH loading	INH	322	323	5.150
9	Mass flow AC discharge	SYO	323	342	*See discharge model*
10	AC cleaning	HP	323	342	336.000
11	AC antifouling pulverisation	NOX	343	359	5.600

Table 3.4 Summary of Gantt chart from batch AC2

No	Operation	Variable name	Start at time (T1)	Stop at time (T2)	Feeding rate (kg/min)
1	Initial water charging (WD)	WD	4	13	3300.00
2	Anti-oxydant agent(s) loading	RMB	4	31	0.92
3	Dispersing agent(s) loading	RMX	5	20	124.39
4	VCM charging	VCM	10	24	3600.00
5	Initiator loading	INI	12	21	2.35
6	Hot water charging (Hot WD)	WH	32	43	1833.33
7	WD Polymerisation	WDS	44	263	0.002
8	NH4OH loading	INH	267	268	5.40
9	Mass flow AC discharge	SYO	269	294	*See discharge model*
10	AC cleaning	HP	295	324	336.000
11	AC antifouling pulverisation	NOX	325	342	5.600

A batch scheduling estimation for an autoclave is based on the information coming from the batch management program modules. One complete cycle of the autoclave has been divided in phases for which the starting time can be defined from

the autoclave state and duration is almost constant. Phases can be separated by 5 phases following.

- AC preparation and initial loadings
- AC heating up
- Polymerization
- Final operations
- AC discharge and preparation

Operations module that acts in difference time along batch is shown in Fig 3.2 By the meaning of each block is shown in table 3.3 and 3.4.
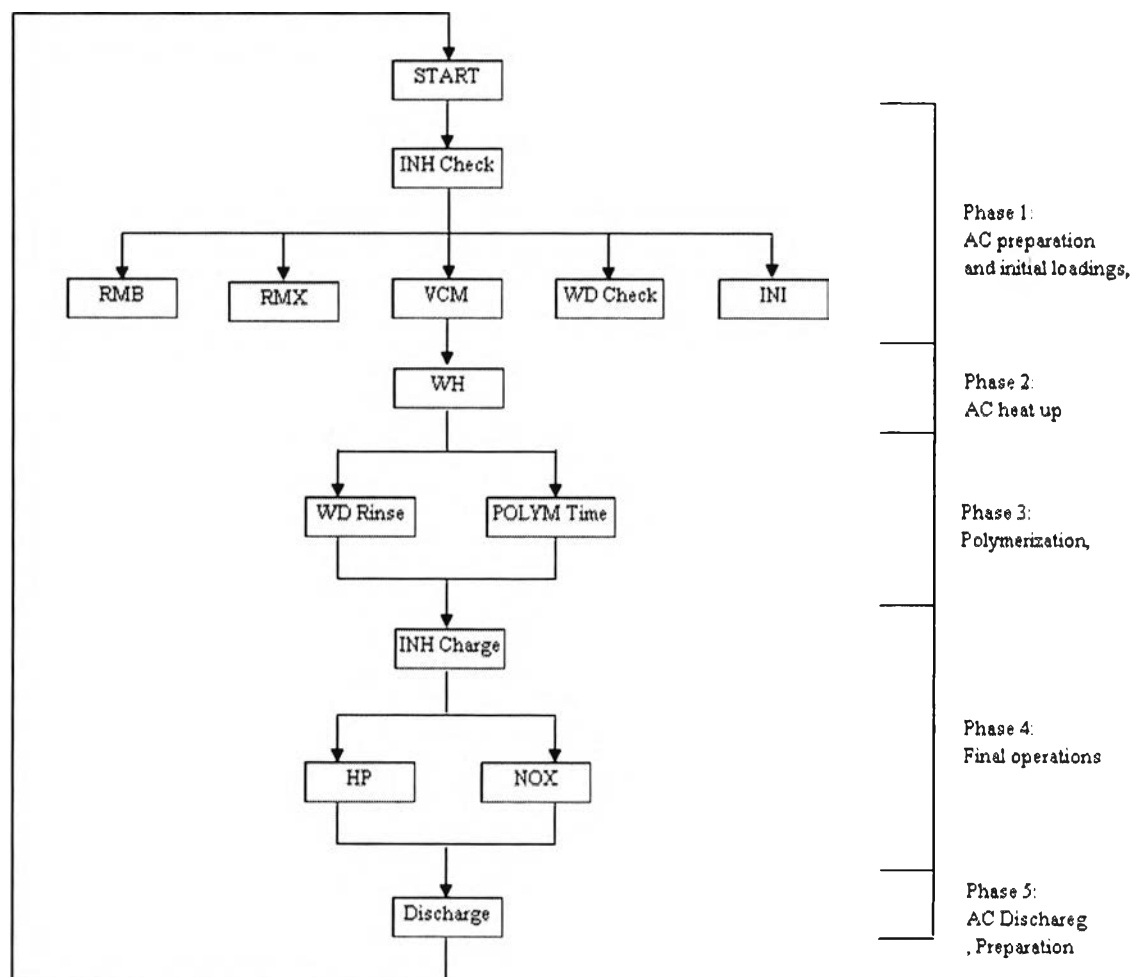

Figure 3.2 Operation module along batch separates by phase.

The phases from 1 to 5 are used to make the estimation for calculation the time which the batch will arrive to DGZ. The remaining time for autoclave until beginning discharge in the DGZ is obtained as the time remaining for the current phase plus the sum of the time durations for the remaining phases. In case the current phase is lasting longer than expected, then the estimation is maintained constant to the sum of the remaining phase durations. This allows re-synchronizing the estimation if a phase has taken more or less time than the expected value.
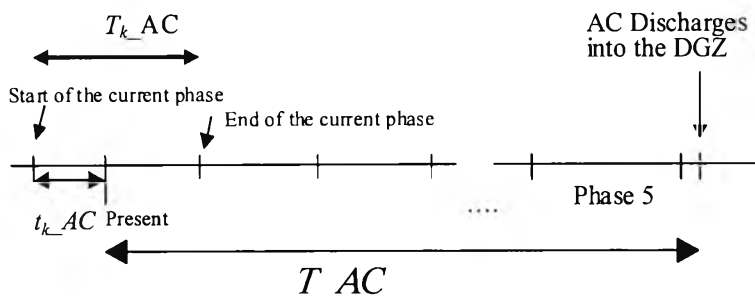
Figure 3.3 Phase time estimation diagram

$$T\_AC = \max(T_k\_AC - t_k\_AC, 0) + \sum_{j=k+1}^{5} T_j\_AC + \sum_{j=k}^{5} T_j\_AC - \min(t_k\_AC, T_k\_AC)$$

$$(3.1)$$

Where

T_AC: Estimated time remaining for the AC batch to begin the discharge to DGZ

k:　　Autoclave recipe current phase index (1...5)

t_k_AC: Elapsed time in the current phase in the current batch

T_j_AC: Expected value for the duration of the phase *j*

This formula 2.1 will be allowed us to know AC time estimation that slurry from AC1 and AC2 will be readily discharged to degasser. Following section 1.7 (Assumption) which is the condition for this studying, the process is assumed to be in normal operation and conversion rate (CR) is become constant for both AC1 and AC2. It does not take in to account abnormal operation such as run away reaction. So, AC time estimation can be calculated following table 2.5. These values are used in simulation model.

Table 3.5 AC time estimation from reactor 1 and 2

Reactor	AC time estimation (min)
AC1	322
AC2	268

3.3 Utilities constrained

The utilities supply unit is the common one which is supplied for both reactors. By the limitation of equipment such as utilities charge pumps, common line supplies, the same utilities can not be fed to both reactors at the same time. The impact of this limitation to AC1 and AC2 is here below.

- It is leaded to both reactors can not be started batch at the same time.
- It is also can not request to consume the same utilities at the same time.

This constrained is taken in to account for the maximum flow rate utilities that can be supplied in the same period (The same period means the same minute of absolute time counted from T_0 along time horizon). If the simulation requests more flow rate than the data in table 3.6, the simulation will be generated "FALSE". It means production in this horizon equals to zero because, that production can not be occurred in real process.

Table3.6 Summary of utilities limitation supply for both reactors

No	Operation	Variable name	Feeding rate (kg/min)
1	Initial water charging (WD)	WD	3543.75
2	Anti-oxydant agent(s) loading	RMB	0.96
3	Dispersing agent(s) loading	RMX	132.87
4	VCM charging	VCM	3780.00
5	Initiator loading	INI	2.61
6	Hot water charging (Hot WD)	WH	1925.00
7	NH4OH loading	INH	0.002
8	AC cleaning	HP	352.80
9	AC antifouling pulverisation	NOX	5.88

Note: WDS is separation unit for each reactor and SYO is not utility.

3.3.1   Verify formula of utilities limitation input in model simulation

Refer to section 3.3 (Utilities constrained), it needs to be adapted data in table 3.6 in order to input in simulation model. The utility limitation is checking function before let model calculates slurry feed rate out off DGZ, and calculates production.

Specify

T_{11}, T_{12}, T_{13}, T_{14}, ... are absolute time of starting batch from AC1.

T_{21}, T_{22}, T_{23}, T_{24}, ... are absolute time of starting batch from AC2.

The highest T value from AC1 and AC2 plus batch time of its line shall not be over than *Time horizon* following formula below.

$$T_{xx} + AC \ time \ (Batch \ time) \leq Time \ horizon \qquad (3.2)$$

Example

Time horizon of one day = 1440 min

Time horizon of one week = 10080 min

If T_{xx} plus batch time is over time horizon, it means that discharge slurry to DGZ of that batch is over than period of interested. Time horizon is set at 1440 min in this case studying.

Supposing T_{11} is starting, it means that AC1 is started 1st batch in time horizon. This batch will pass progressively by minute in phase from 1 to 5. Each phase will request to consume utilities in time and consumption as presented in table 3.3 Summary of Gantt chart for AC1.

Next, T_{21} is starting. It means that AC2 is started 1st batch. This batch will go in the same path, consume utilities in the period following table 3.4. Summary of Gantt cheat for AC2 likes as described for T_{11}.

Model will make summation for consumption of every utility in every minute. If the result of consumption over than limitation of supply which is specified in Table 3.6, it means utilities are not enough for supply. So, that batch can not be occurred in real process. Model will be generated "FALSE" and shown production equal to zero.

3.4 Discharge time and flow rate estimation

It is applied mass-material balance and dynamic model of tank discharge by gravity and Bernoulli's equation to simulate volume flow rate discharge from autoclave to DGZ which is gradually decreased when liquid head in autoclave decreases. The simple diagram is shown in Fig 3.4 and model is here below in formula.
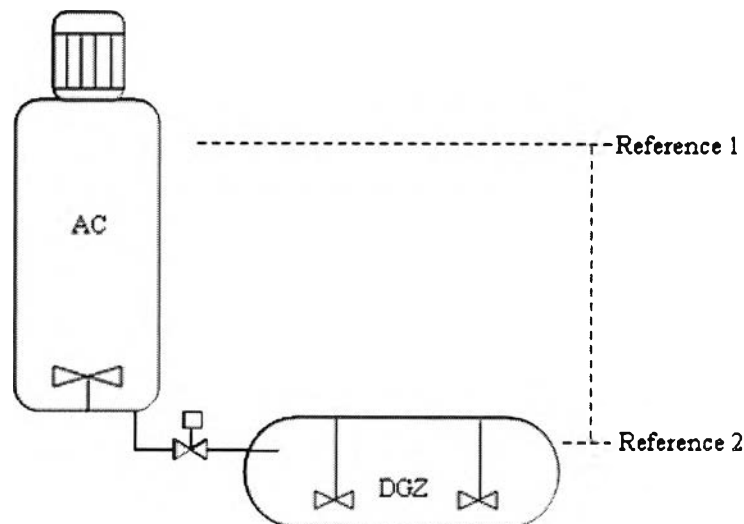

Figure 3.4 Diagram of slurry discharging from AC to DGZ

Bernoulli's equation

$$\left[\frac{P_1}{\rho g} + \frac{V_1^2}{2g} + H_1\right] = \left[\frac{P_2}{\rho g} + \frac{V_2^2}{2g} + H_2 + Loss\right]$$ (3.3)

After derived equation, the final form is here below.

$$\frac{dh}{dt} = -2.5\sqrt{h}$$ (3.4)

Where

P:	Pressure at reference point (Pa)
V:	Velocity of liquid at reference point (m/s)
ρ:	Density of slurry (kg/m^3)
H:	High from reference point (m)
h:	Level of slurry inside autoclave (m)
t:	Time (s)

By discharging model, slurry flow rate out off reactor can be calculated. Flow rate is assumed to be linear during period in one minute in order to be easier for making simulation. Mass flow rate versus time from both autoclaves are in table 3.7 and table 3.8 Time is continued count from the minute after finish batch time which is described on topic 3.2 (Autoclave time estimation). They are plotted in graphs in Fig 3.5 and 3.6.

Table 3.7 Discharge flow rate from AC1

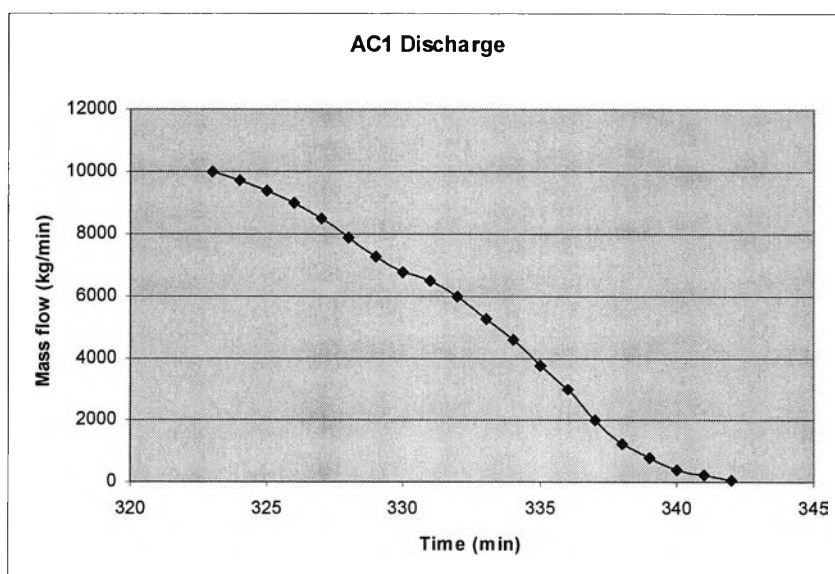| Time	Mass out (kg/min)	Volume flow (m³/min)
323	10000	10.504
324	9700	10.189
325	9400	9.874
326	9000	9.454
327	8500	8.929
328	7900	8.298
329	7300	7.668
330	6800	7.143
331	6500	6.828
332	6000	6.303
333	5300	5.567
334	4600	4.832
335	3800	3.992
336	3000	3.151
337	2000	2.101
338	1200	1.261
339	800	0.840
340	400	0.420
341	200	0.210
342	50	0.053
	102450	**107.616**

Figure 3.5 Graph shows discharge flow rate from AC1

Table 3.8 Discharge flow rate from AC2

| Time	Mass out (kg/min)	Volume flow (m³/min)
269	11000	11.555
270	10700	11.239
271	10200	10.714
272	9600	10.084
273	9200	9.664
274	8400	8.824
275	7800	8.193
276	7000	7.353
277	6500	6.828
278	5900	6.197
279	5100	5.357
280	4800	5.042
281	4300	4.517
282	3900	4.097
283	3400	3.571
284	2800	2.941
285	2400	2.521
286	1900	1.996
287	1300	1.366
288	900	0.945
289	600	0.630
290	500	0.525
291	400	0.420
292	200	0.210
293	100	0.105
294	50	0.053
	118950	**124.947**
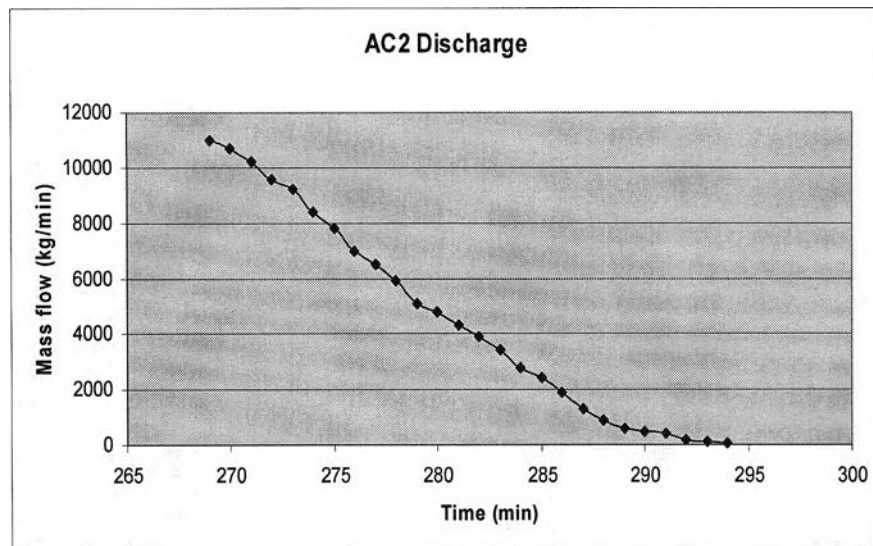
AC2 Discharge

Figure 3.6 Graph shows discharge flow rate from AC2

Flow rate of slurry from autoclave to DGZ is varied following head inside autoclave. Volume flow rate out from autoclave is equaled to volume increased in DGZ. Mass flow rate is also the same with volume flow rate.

3.5 Mass and volume calculation in DGZ

We derive formula for calculation volume of the horizontal vessel with ellipsoidal head (2:1) in order to check the volume of DGZ. The detail of calculation is shown in Appendix 2. As we known the volume of DGZ is equaled to 180 m^3, so set volume 0 m^3 equals to 0% and 100 m^3 equals to 100%. Apply linear regression programming to find the relation between volume and percentage and plots in graph following Fig 3.7. From now on, The DGZ volume is called V_{DGZ}.

Graph of relation between volume and level in DGZ

$y = 1.8171x + 8E-14$
$R^2 = 1$
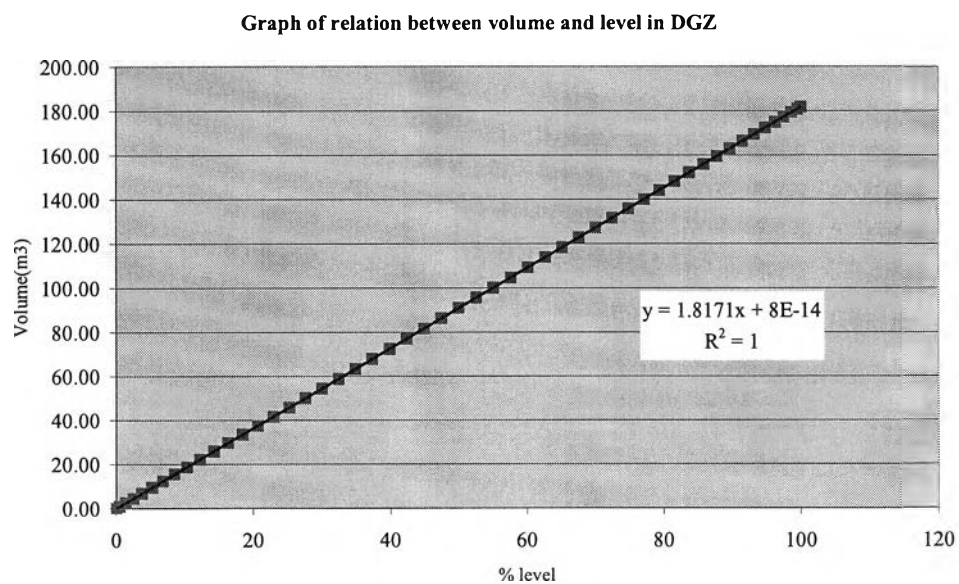
Figure 3.7 Volume versus percentage in DGZ

Therefore, V_{DGZ} has operating range MIN and MAX. Max operating volume is set at 150 m^3 because, it needs to have enough available volume for evacuated unconverted VCM gas out to VCM recovery unit. MIN operating volume is set at 10 m^3 because the level inside DGZ at volume below $10m^3$ is lover than agitator level. Slurry is suspended liquid, so it will be suspended and blocked discharge line. This incident will lead to process interruption and shut down. So, Flow rate is set following condition below in model.

V_MAX   = 150 m^3

V_MIN   = 10 m^3

3.6 Introduction of flow control and volume estimation

From the batch scheduling, scenario, it is possible to calculate an optimal line production rate following the subsequent objectives 1.) Maximize the line production rate and 2.) Insure that DGZ will never be emptied and that there is sufficient room to discharge the autoclave at the discharge time. The principle is in Fig. 3.8.
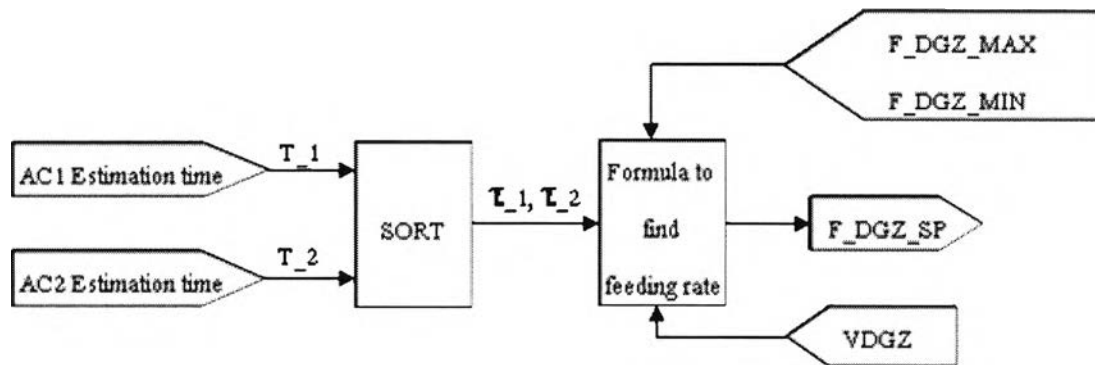

Figure 3.8 Block diagram of optimal DGZ feeding

This step is considered in order to find F_DGZ_SP (Flow rate of slurry out off degasser) which optimal in the constrained condition.

The formula is proposed to solve by minimizing the following cost function (J) as following equation 3.5.

$$\min_{\substack{F < F\_DGZ\_MAX \\ F > F\_DGZ\_MIN}} \left[\frac{V_{DGZ\,\tau(n-1)} + \left(\Delta V_{n-1} - F_n \cdot \left(\tau_{n-1} - \tau_n\right)\right)}{\left(\tau_n - \tau_{n-1}\right)} \right] \tag{3.5}$$

Where

F: Line production rate
F_DGZ_MIN: Line production rate minimal constraint
F_DGZ_MAX: Line production rate maximal constraint
V_{DGZ} :   Current volume in DGZ
V_{SP}:   Minimal level set point (Current volume in DGZ (30 m^3)
ΔV: Future level variation of DGZ

τ: Absolute time which batch arrive in DGZ.

Line physical constrains are due to

- Stock constraints of the degasser, DGZ (10 m^3 - 150 m^3).
- Degasser minimum and maximum production rate flow out (35 m^3/h to 90m^3/h).

Production rate constraints are depending on DGZ stock, F_DGZ_MIN and F_DGZ_MAX. They are chosen to insure (in case of no other limitations) that:

- The stock in DGZ will never be emptied (to avoid line shut down).
- There is sufficient room to discharge an autoclave at the discharge time. Otherwise, autoclave will have to wait and impact to reduce the throughput of the whole PVC production line. The other constrain is quality problem. In the experience, slurry which is kept in DGZ over than 20 minute will be observed quality problem in finish resin.

These two constraint equations are given by

$$F\min_n = \left[\frac{V_{DGZ\tau(n-1)} + \Delta Vn - V\max}{(\tau_n - \tau_{n-1})} \right] \qquad (3.6)$$

$$F\max_n = \left[\frac{V_{DGZ\tau(n-1)} - V\min}{(\tau_n - \tau_{n-1})} \right] \qquad (3.7)$$

Where:

V_{MIN}: Minimum stock level constraint (10 m^3)
V_{MAX}: Maximum stock level constraint (150 m^3)

F min is the minimum flow rate of slurry out off DGZ in order to allow enough space volume in DGZ for new coming batch discharge to DGZ without any waiting time.

F max is the maximum flow rate of slurry out off DGZ, but it is not impacted to line shut down because volume in DGZ below V_{MIN} before new coming batch will arrive in DGZ.

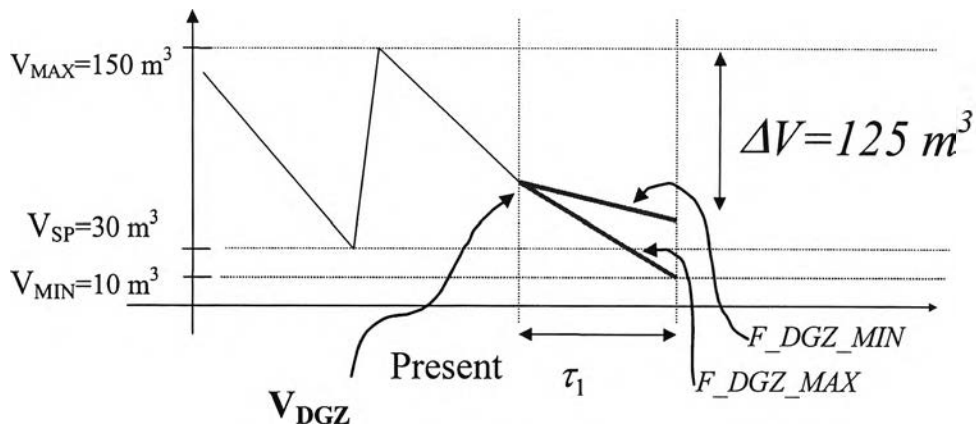These formulas can be understood by consideration at Fig.3.9.

Figure 3.9 Simple diagrams for understanding cost function (J) and constrained.

The feed rate, F is calculated and selected following diagram in Fig. 3.10 following dot blue point of diagram in the same figure.
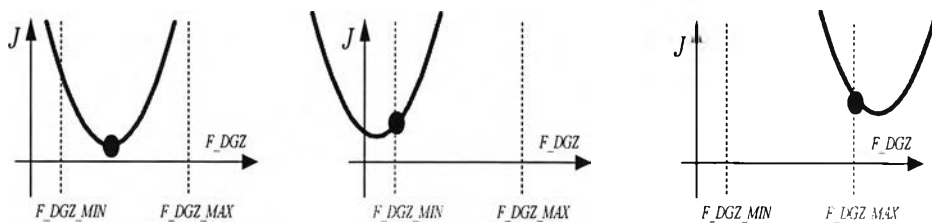

Figure 3.10 Feed rate calculation selection

3.7 Verify formula of slurry feeding and production input in model simulation

Refer to section 3.4, it need to be derived each equation in for finding the repeated formula and use it in simulation. The derived equation can be understood by consideration in Fig 3.11.
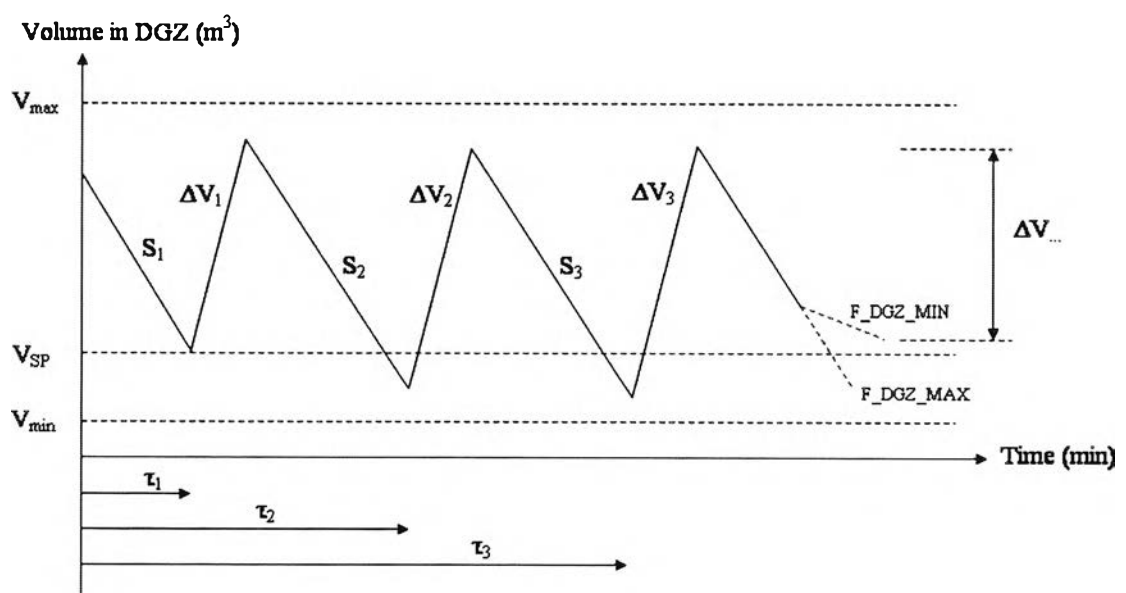

Figure 3.11 Simple diagram for described derive equation

Where

V_{max}: 150 m^3
V_{sp}: 30m^3
V_{min}: 10m^3
V_{DGZ}: Current volume in DGZ (m^3)
S: Slope of graph which is slurry flow out of DGZ (S = V_{DGZ} / time (m^3/min))
τ: Absolute time which batch arrive in DGZ
ΔV: Volume increase in DGZ from discharge autoclave

Refer to data in table 3.7 and 3.8 Discharge flow rate from autoclave 1 and 2, we can assume that one discharge from batch reactor from both autoclave become constant by.

$\Delta V_1 = V_2 - V_1 = 107\text{m}^3$; Volume increase in DGZ from discharge AC1.
$\Delta V_2 = V_3 - V_2 = 125\text{m}^3$; Volume increase in DGZ from discharge AC2.

These values are repeated like as formula below

$$\Delta V_n = \begin{cases} 107 \ m^3; & n = 1, \ 3 \ ,5 \ ,7,... \\ 125 \ m^3; & n = 2 \ ,4 \ ,6 \ ,8,... \end{cases}$$

3.7.1 Principle to find slurry flow out DGZ

We derive formula for finding slurry flow out off DGZ (F_DGZ) in order to find set point of slurry flow rate out off DGZ and find the repeated system for set up in model. The formula is described base on Fig 3.11 following here below.

$$S_1 = \frac{V - V_{sp}}{\tau_1} \tag{3.8}$$

$$S_2 = \frac{V_{DGZ\tau1} + \Delta V_1 - F_2(\tau_2 - \tau_1)}{\tau_2 - \tau_1} \tag{3.9}$$

$$S_3 = \frac{V_{DGZ\tau2} + \Delta V_2 - F_3(\tau_3 - \tau_2)}{\tau_3 - \tau_2} \tag{3.10}$$

$$S_4 = \frac{V_{DGZ\tau3} + \Delta V_3 - F_4(\tau_4 - \tau_3)}{\tau_4 - \tau_3} \tag{3.11}$$

It can be created the repeated formula following here below in equation 3.12

$$S_n = \frac{V_{DGZm-1} + \Delta V_{n-1} - F_n(\tau_n - \tau_{n-1})}{\tau_n - \tau_{n-1}} \tag{3.12}$$

3.7.2 Principle to find minimum slurry flow out DGZ

F min is the minimum flow rate of slurry out off DGZ in order to allow enough space volume in DGZ for new coming batch discharge to DGZ without waiting time. We derive formula for finding minimum slurry flow out from DGZ (F_DGZ_MIN) in order to find the minimum set point of slurry flow rate out of DGZ in each batch. It is also finding the repeated system for set up in model. The formula is described base on Fig 3.11 following here below.

$$F_{min} = \frac{V_{DGZ} + \Delta V - V_{max}}{\tau} \qquad (3.13)$$

F_{min} = Need not to compare with S_1

$$F_{min2} = \frac{(V_{DGZ@(\tau1)} + \Delta V_1) - (V_{max} - \Delta V_2)}{\tau_2 - \tau_1} \qquad (3.14)$$

$$F_{min2} = \frac{(V_{DGZ@(\tau1)} + 107) - (150 - 125)}{\tau_2 - \tau_1} \qquad (3.15)$$

$$F_{min2} = \frac{(V_{DGZ@(\tau1)} + 82)}{\tau_2 - \tau_1} \qquad (3.16)$$

$$F_{min3} = \frac{(V_{DGZ@(\tau2)} + \Delta V_2) - (V_{max} - \Delta V_3)}{\tau_3 - \tau_2} \qquad (3.17)$$

$$F_{min3} = \frac{(V_{DGZ@(\tau2)} + 125) - (150 - 107)}{\tau_3 - \tau_2} \qquad (3.18)$$

$$F_{min3} = \frac{(V_{DGZ@(\tau2)} + 82)}{\tau_3 - \tau_2} \qquad (3.19)$$

It can be created the repeated formula following here below in equation 3.20.

$$F_{min\,n} = \frac{(V_{DGZ@(n-1)} + 82)}{\tau_n - \tau_{n-1}} \qquad (3.20)$$

3.7.3 Principle to find maximum slurry flow out DGZ

F max is the maximum flow rate of slurry out off DGZ, but it is not impacted to production line shut down because Volume in DGZ below V_{min} before new coming batch will arrive in DGZ. We derive formula for finding maximum slurry flow out from DGZ (F_DGZ_MAX) in order to find the maximum set point of slurry flow rate out in each batch, and find the repeated system for set up in model. The formula is described base on Fig 3.11 following here below.

$$F_{\max} = \frac{V_{DGZ} - V_{\min}}{\tau}$$ (3.21)

F_{max} = Need not to compare with S_1

$$F_{\max 2} = \frac{(V_{DGZ@(\tau 1)} + \Delta V_1) - V_{\min}}{\tau_2 - \tau_1}$$ (3.22)

$$F_{\max 2} = \frac{(V_{DGZ@(\tau 1)} + 107) - 10}{\tau_2 - \tau_1}$$ (3.23)

$$F_{\max 2} = \frac{(V_{DGZ@(\tau 1)} + 97)}{\tau_2 - \tau_1}$$ (3.24)

$$F_{\max 3} = \frac{(V_{DGZ@(\tau 1)} + \Delta V_2) - V_{\min}}{\tau_3 - \tau_2}$$ (3.25)

$$F_{\max 3} = \frac{(V_{DGZ@(\tau 1)} + 125) - 10}{\tau_3 - \tau_2}$$ (3.26)

$$F_{\max 3} = \frac{(V_{DGZ@(\tau 1)} + 115)}{\tau_3 - \tau_2}$$ (3.27)

It can be created the repeated formula for F_{max} in 2 cases as equation 3.28 below. Therefore, it is observed the formulas for AC1 and AC2 are not the same because they are different in slurry discharge volume from both reactors.

$$F_{max} = \begin{cases} F_{\max 2} = \dfrac{(V_{DGZ@(\tau 1)} + 97)}{\tau_2 - \tau_1}; & n = 2, 4, 6, 8 ,... \\[4mm] F_{\max 3} = \dfrac{(V_{DGZ@(\tau 1)} + 115)}{\tau_3 - \tau_2}; & n = 3, 5, 7 ,9 ,... \end{cases}$$ (3.28)

3.7.4 Production calculation

F_DGZ_SP (m3/min) will be selected following principle in Fig 3.10; Feed rate calculation selection via SORT program in model. Production in term of volume in each period can be calculated by formula.

$$Production_n \ (m^3) = F\_DGZ\_SP_n \times (\tau_n - \tau_{n-1})$$ (3.29)

Production in term of volume in time horizon example one day can be calculated following here below.

$$Production_{one\ day}\ (m^3) = \sum Production_n \qquad\qquad (3.30)$$

Where n is in period one day

Therefore, final product of plant is PVC resin which is counted by weight (ton). So, the production that is considered in objective function model shall be production in term of weight. It is easily to convert in term of weight production by multiply it with density of slurry which is assumed constant value following formula below.

$$Production_{one\ day}\ (ton) = \sum Production_n\ (m^3) \times (Slurry\ density\ (ton/m^3)) \qquad (3.31)$$

Where

n is in period one day

3.8 Engineering optimization

Engineering optimization problems usually contain multi-modal objective functions, and involve highly nonlinear inequality and/or equality constraints. Therefore, solving these problems consists of exploring very complex search spaces.

Recently, evolutionary algorithms (EAs) are receiving increasing attention, because of their potential to effectively explore a wide range of complex optimization problems. A number of evolutionary algorithm based approaches have been proposed during last decades. A comprehensive description of EA can be found in many literatures.

Differential evolutionary algorithm (DE) is a novel evolutionary optimization algorithm being capable of handling non-differentiable, nonlinear and multi-modal objective functions. The basic idea of DE is to use vector differences for perturbing the vector population. DE is a very simple population based optimization technique which is at the same time very powerful and robust. However, multiple nonlinear constraints handling in DE has been found rather difficult. Moreover, it is one of the major drawbacks when applying DE to solve constrained optimization problems. Thus, and efficient constraint handling technique is considered necessary.

This technique was compared with a traditional constraint handling techniques both in terms of solution quality and the number of function evaluations required in studying of Kheawhom in 2009. In his summary, the performance of his developed scheme compares favorably with traditional penalty function method. His developed algorithm can effectively handle constraints encountered in chemical engineering optimization problems.

This study was selected differential evolutionary algorithm (DE) technique for optimization module.

3.8.1 Constrained optimization problem

A constrained optimization problem is generally expressed as:

Min F(x),

s.t. $g_l(x) \leq 0; l = 1, 2,..., L,$
$h_m(x) = 0; m = 1, 2,..., M,$
$x_n^{(L)} \leq x_n \leq x_n^{(U)}; n = 1, 2,..., N.$ (3.32)

Where, x_n is an optimization variable varying in the range $[x_n^{(L)}, x_n^{(U)}]$. The function F(x) is the objective function with $g_l(x)$ inequality constraint and $h_m(x)$ equality constraint.

3.8.2 Differential evolutionary algorithm

DE was first introduced as it is typical for EAs, DE does not require any prior cognition of the search space, nor of the derivative information. It is a very simple population based, stochastic optimization algorithm, which is very powerful and also robust. Figure 3.12 shows the flowchart of DE. The algorithm starts by generating an initial population of N vectors. In this work, we used Hammersley sequence sampling technique introduced by Preechakul and Kheawhom to generate an initial population. Mutation and recombination are then performed on each vector X_i of the generated population to create a trial vector U_i. Various mutation schemes have been proposed [20]. In this work, we deliberate using basic De/rand/1/bin scheme starts by randomly selecting three vectors in the populations. The perturbed vector V_i is then generated based on the three previously selected vectors as follows:

$$V_i = X_{r3} + F(X_{r2} - X_{r1})$$ (3.33)

Where,

X_{r1}, X_{r2} and X_{r3} are randomly selected vectors, and r1 ≠ r2 ≠ r3 ≠ i are satisfied. F ε [0, 1+] is a control parameter of the algorithm.

The trigonometric mutation scheme also starts by randomly selecting three vectors in the populations as in the DE/rand/1/bin scheme. But, the perturbed variable is calculated using the center point of the hypergeometric triangle of three earlier selected vectors. The perturbed vector V_i is then generated by perturbing the center point a sum of three weighted vector differentials, as described by the following formulation:

$$V_i = \frac{X_{r1} + X_{r2} + X_{r3}}{3} + (p_2 - p_1)(X_{r1} - X_{r2}) + (p_3 - p_2)(X_{r2} - X_{r3}) + (p_1 - p_3)(X_{r3} - X_{r1}),$$

$$p_1 = \frac{|F(X_{r1})|}{|F(X_{r1})| + |F(X_{r2})| + |F(X_{r3})|},$$

$$p_2 = \frac{|F(X_{r2})|}{|F(X_{r1})| + |F(X_{r2})| + |F(X_{r3})|},$$

$$p_3 = \frac{|F(X_{r3})|}{|F(X_{r1})| + |F(X_{r2})| + |F(X_{r3})|}, \qquad (3.34)$$

Where, X_{r1}, X_{r2} and X_{r3} are randomly selected vectors, and $r1 \neq r2 \neq r3 \neq i$ are satisfied. $F(X_{r1})$, $F(X_{r2})$ and $F(X_{r3})$ are the objective functions evaluated at X_{r1}, X_{r2} and X_{r3} vectors, respectively.

The perturbed vector $V_i(v_{i,1}, v_{i,2}, ..., v_{i,n})$ and its parent vector $X_i(x_{i,1}, x_{i,2}, ..., x_{i,n})$ are subjected to the crossover operation, that finally generates the trial vector $U_i(u_{i,1}, u_{i,2}, ..., u_{i,n})$ as follows:

$$u_{i,j} = \begin{cases} v_{i,j} & \text{if random}[0,1) \leq CR \ \lor \ j = \text{random}[1,n); \\ x_{i,j} & \text{otherwise} \end{cases}$$

Where $CR \ \varepsilon \ [0,1]$ is a crossover factor. At each generation i, the created trial vector U_i is then compared with its parent vector X_i. If the trial vector is better than the parent vector, the trial vector replaces its parent vector in the population, as expressed in the following formulation:

$$X_{i+j} = \begin{cases} U_i & \text{if } f(U_i) \leq f(X_i) \\ X_i & \text{otherwise} \end{cases}$$

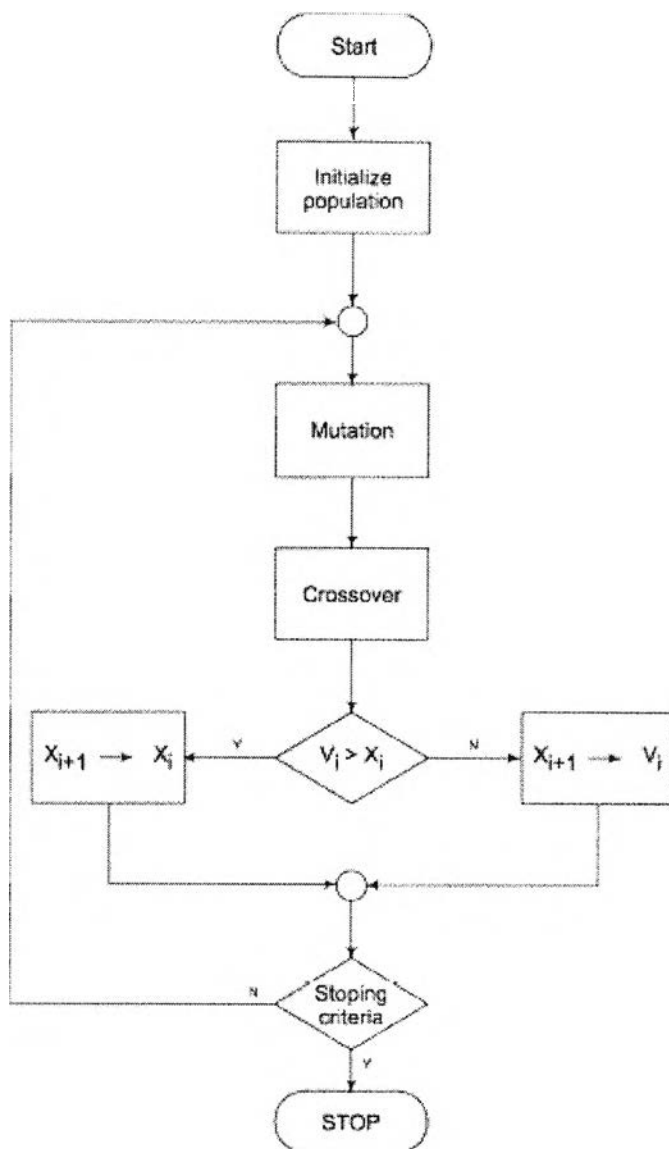The evolutionary process repeats until the stopping criteria is satisfied.

```
                          ╭──────────╮
                          │   Start  │
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                               ┊
                          ┌──────────┐
                          │ Initialize│
                          │ population│
                          └────┬─────┘
                               │
                 ┌─────────────◯
                 │             │
                 │        ┌──────────┐
                 │        │ Mutation │
                 │        └────┬─────┘
                 │             │
                 │        ┌──────────┐
                 │        │ Crossover│
                 │        └────┬─────┘
                 │             │
   ┌──────────┐  Y      ◇─────────◇   N   ┌──────────┐
   │Xᵢ₊₁ → Xᵢ │◄────────│ Vⱼ > Xᵢ │──────►│Xᵢ₊₁ → Vⱼ │
   └────┬─────┘         ◇─────────◇       └────┬─────┘
        │                                      │
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                       │
              N    ◇────────◇
        ┌─────────│ Stoping │
        │         │ criteria│
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        │              │ Y
        │         ╭──────────╮
        │         │   STOP   │
        │         ╰──────────╯
        └────────────
```

Figure 3.12 Flowchart of the differential evolutionary algorithm.