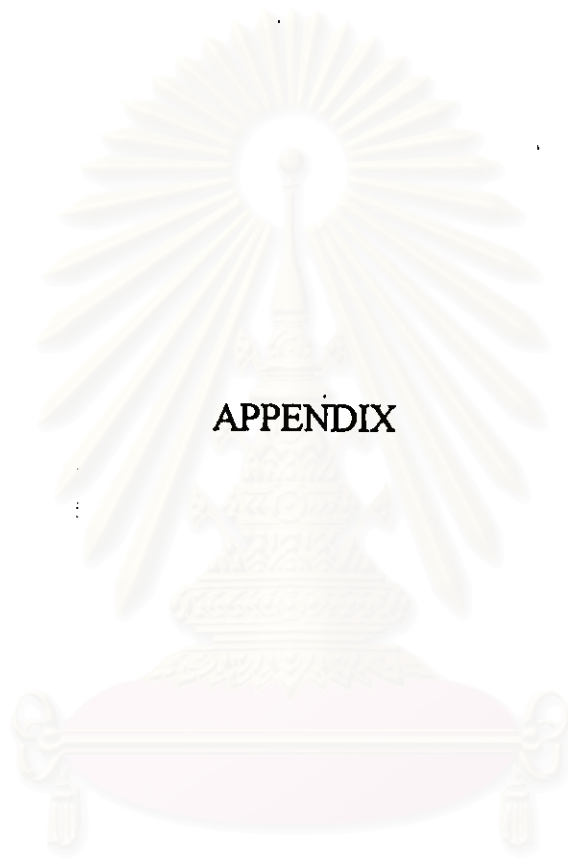


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APPENDIX

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## APPENDIX A

### RANDOM NUMBERS GENERATION

The effectiveness of the stochastic simulation is intimately connected with the quality of the random numbers being used. Appendix A gives listings of FORTRAN 77 subroutines employed for generation of random numbers.

#### Random number generators

##### A.1 Starting value

###### SUBROUTINE START

\*\*\*\*\*

Subroutine to starting value

These instructions yield a non-repetitive starting value for the random number generator for each run of the program.

\*\*\*\*\*

```
REAL*8 TI
INTEGER*4 IT
COMMON /RNG1/ IY,RANR
TI = IT*101.
120 IF (TI-24350542) 300,150,150
150 TI = TI/10
GOTO 120
300 IY = 42758321+INT(TI)
IY = (IY/2)*2+1
```

```
RETURN
```

```
END
```

## A.2 Uniform random number generator

Subroutine RANDOM was used to generate a uniform random number, whose values lie between 0 and 1.

```
SUBROUTINE RANDOM
```

```
*****
```

SUBROUTINE RANDOM generates a uniform random number with a mean of 0.5 and a range of 0.0 to 1.0

```
*****
```

```
REAL*8 YY,AA
```

```
COMMON /RNG1/ IY,RANR
```

```
YY = 3125.*IY
```

```
AA = INT(YY/67108864)*67108864.
```

```
IY = INT(YY - AA)
```

```
RANR = IY/67108864.
```

```
RETURN
```

```
END
```

### A.3 Normal random number generator

Subroutine NRG was used to generate a normal random number with a mean of 0.0 and a standard deviation of 1.0.

#### SUBROUTINE NRG

\*\*\*\*\*

SUBROUTINE NRG generates a standard normal random number using two uniform random numbers

\*\*\*\*\*

```

COMMON /RNG1/ IY,RANR
CALL RANDOM
XO = SQRT(-2.0 * ALOG(RANR))
CALL RANDOM
TR = 6.2831853072 * RANR
XT = XO * SIN(TR)
XO = XO * COS(TR)
RETURN
END

```

where

IY = STARTING VALUE  
RANR = UNIFORMLY DISTRIBUTED RANDOM NUMBER  
XO = NORMALLY DISTRIBUTED RANDOM NUMBER  
XT = NORMALLY DISTRIBUTED RANDOM NUMBER

## **APPENDIX B**

### **ALGORITHM AND FLOWCHART**

Appendix B gives algorithms and flowcharts for generation and analysis the dispersion of additives.

#### **B.1 Algorithm for generation and analysis the dispersion of additives.**

##### **B.1.1 Algorithm to generate dispersion patterns.**

1. Open file to write.
2. Enter concentration, particle size of A and B particles and adhesion probability.
3. Input a seed for random number.
4. Select the type of dispersion and generate A particles according to the selected type of dispersion (either uniform or normal random dispersion).
5. Check and eliminate A particles that overlap and keep the desired number of A particles.
6. Input a seed for random number.
7. Select the type of dispersion and generate B particles according to the selected type of dispersion (either uniform or normal random dispersion) and specified adhesion probability.
8. Check and eliminate B particles that overlap themselves.
9. Check and eliminate B particles that overlap any A particles.
10. Keep the wanted number of B particles
11. Identify those B particles adhering onto A particles.
12. write all simulated data to file.



### **B.1.2 Algorithm to analysis dispersion patterns.**

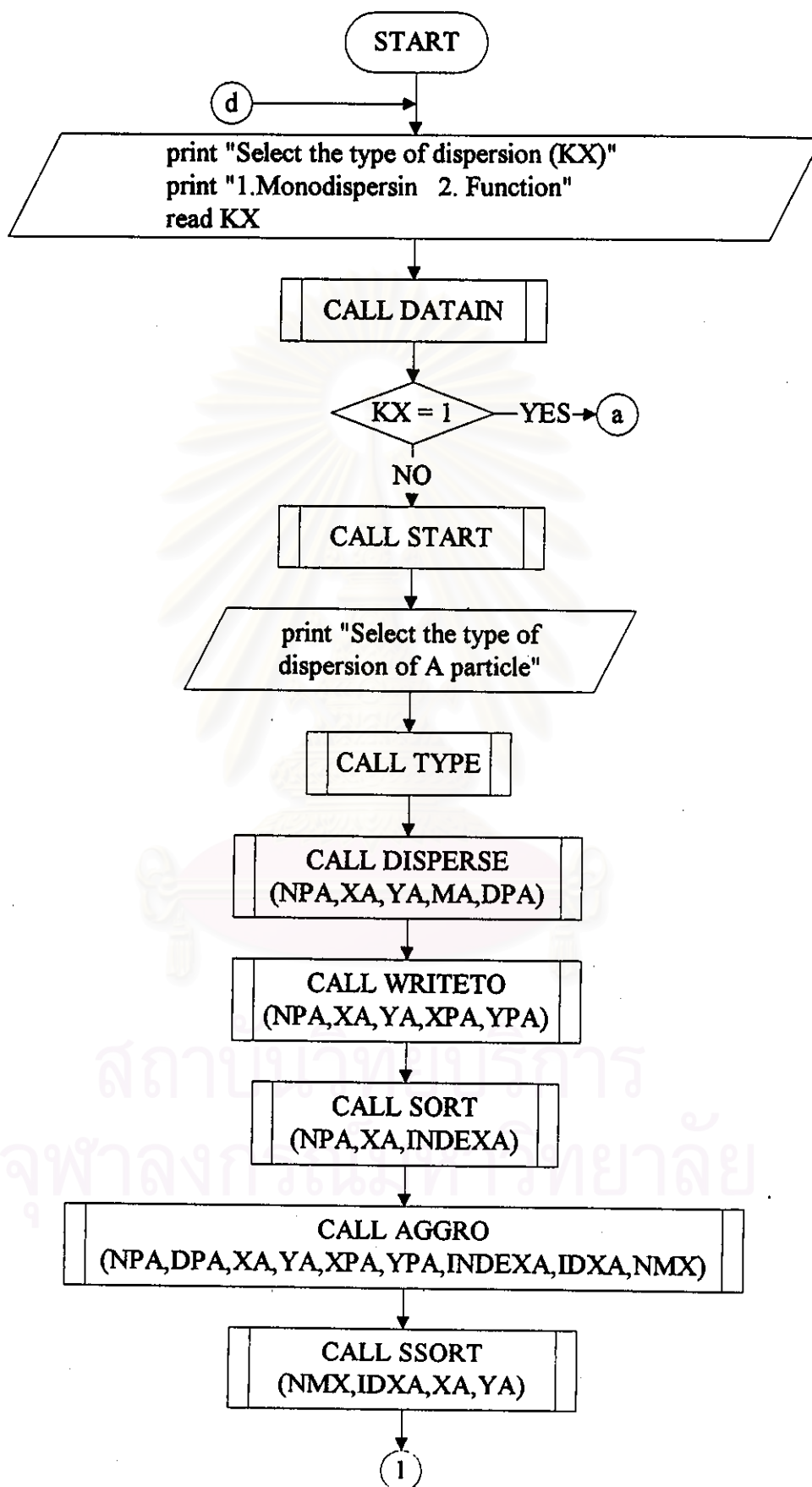
1. Open generated data file to read concentration and particle size of A and B particles, adhesion probability, identified B particles adhering on to A and position (X,Y) of A and B particles.
2. Input a seed for random number.
3. Count subsections  $N(n)$  occupied by A particles, B particles and A plus B particles.
4. Calculate the coefficient of variation  $D_s(n)$  given by equation (3.18) of A particles, B particles and A plus B particles.
5. Calculate the degree of mixedness (M) given by equation (3.8) of A particles and B particles.
6. Write  $N(n)$ ,  $D_s(n)$ , M, and number of identified B particles adhering onto A.

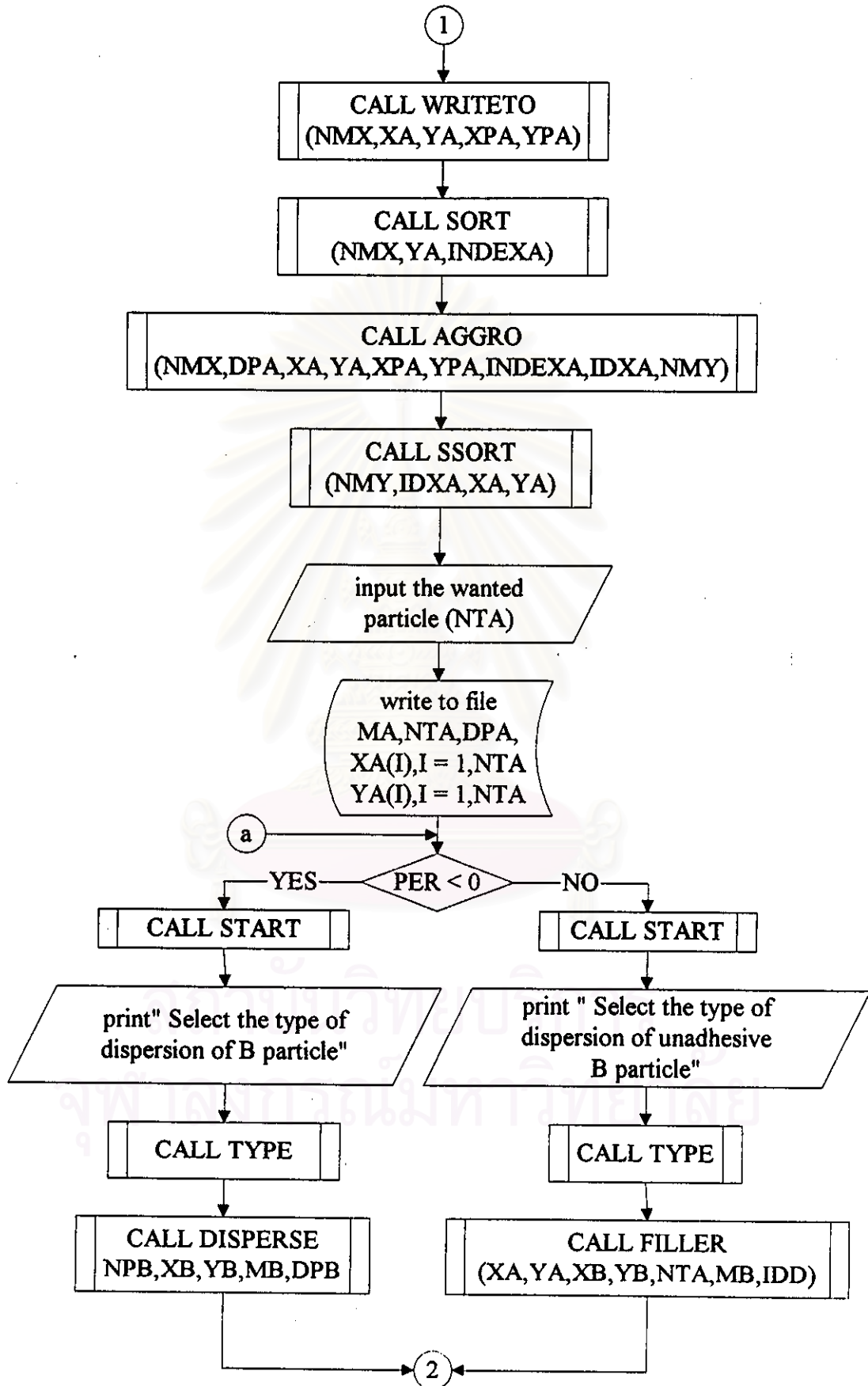
### **B.2 Flowchart for generation and analysis the dispersion of additives.**

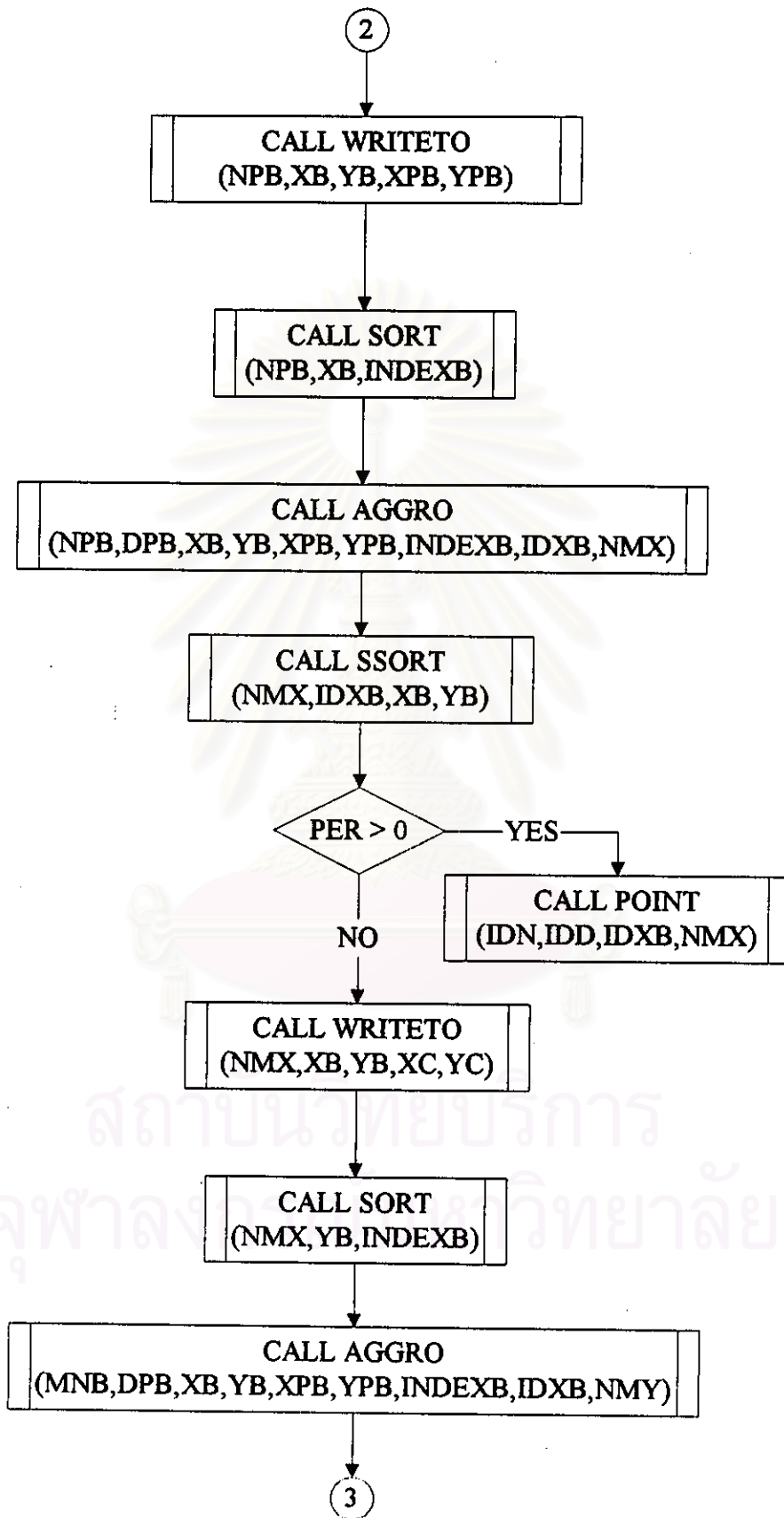
Here is the flowchart of main program for generation and analysis the dispersion of additive and flowchart of subroutines which are used in main programs.

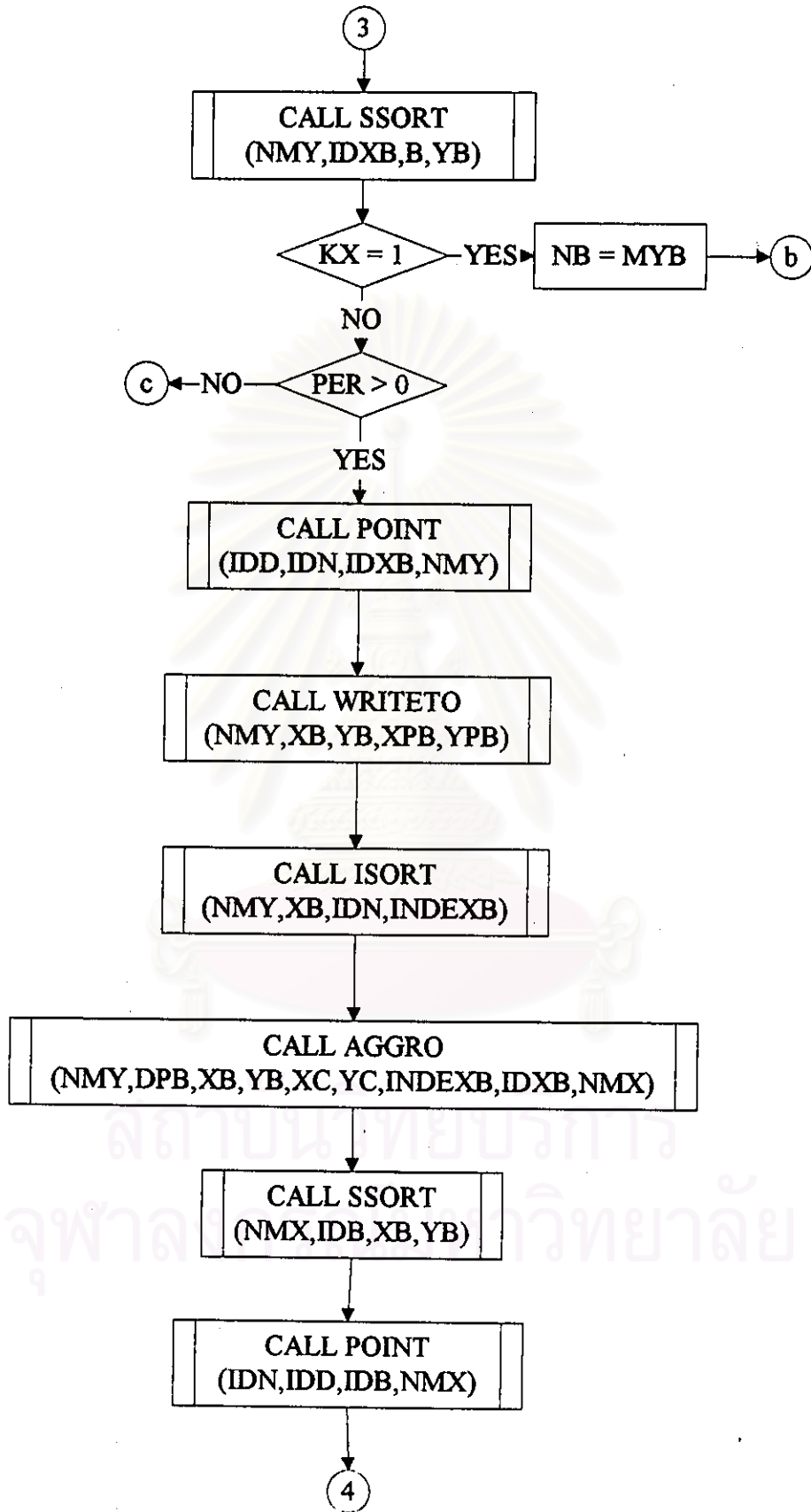
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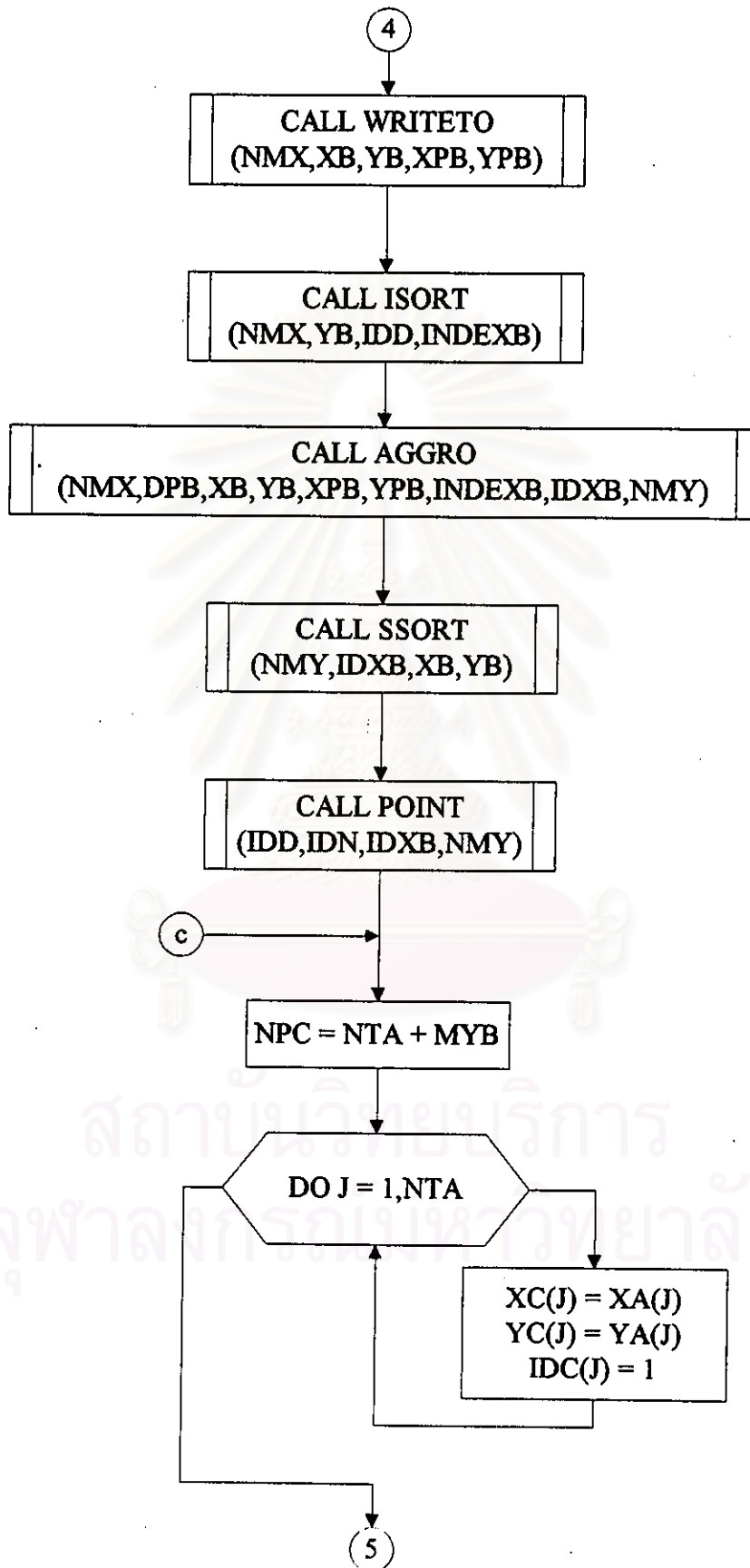
## GENERATION PROGRAM

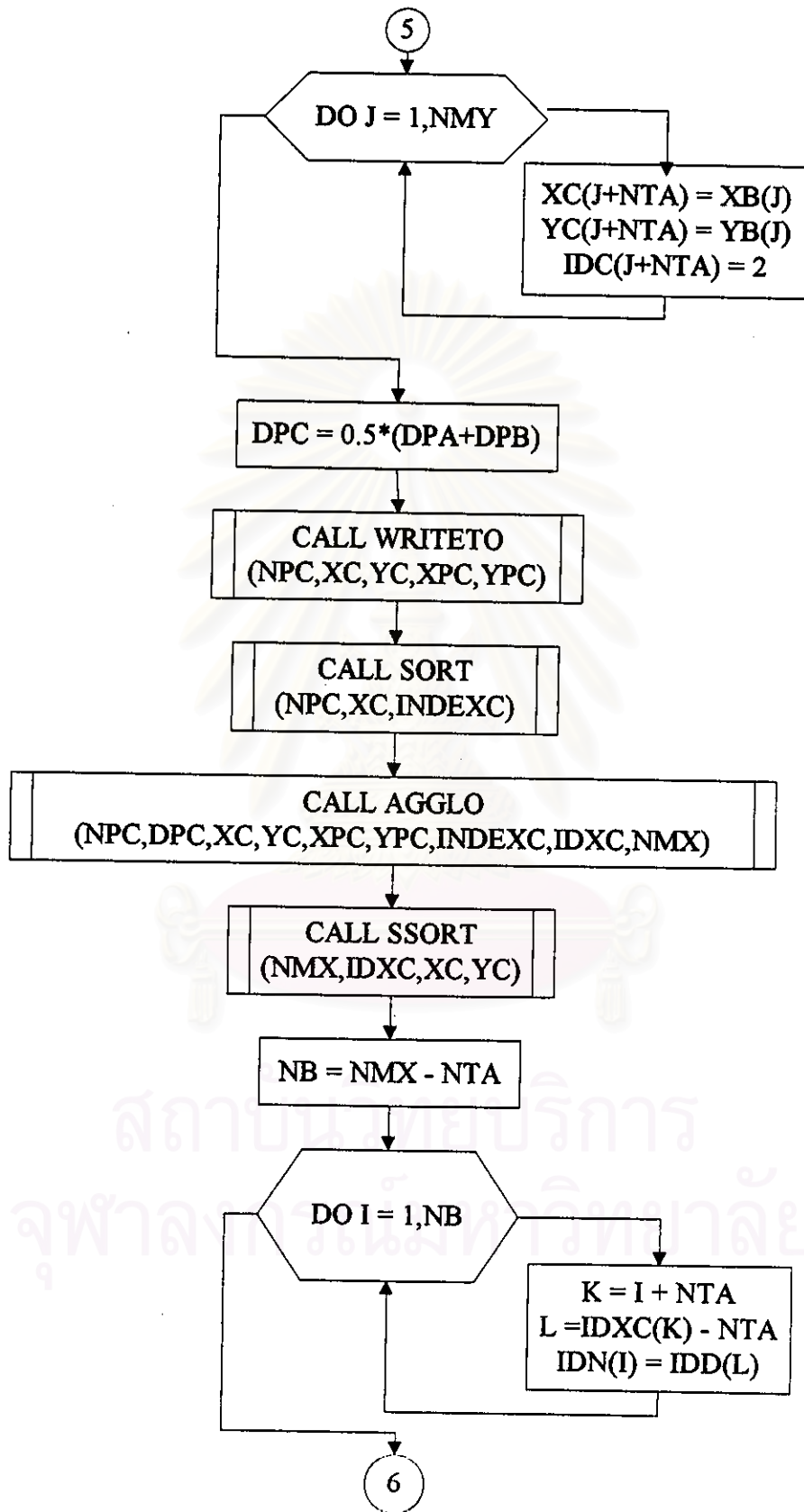


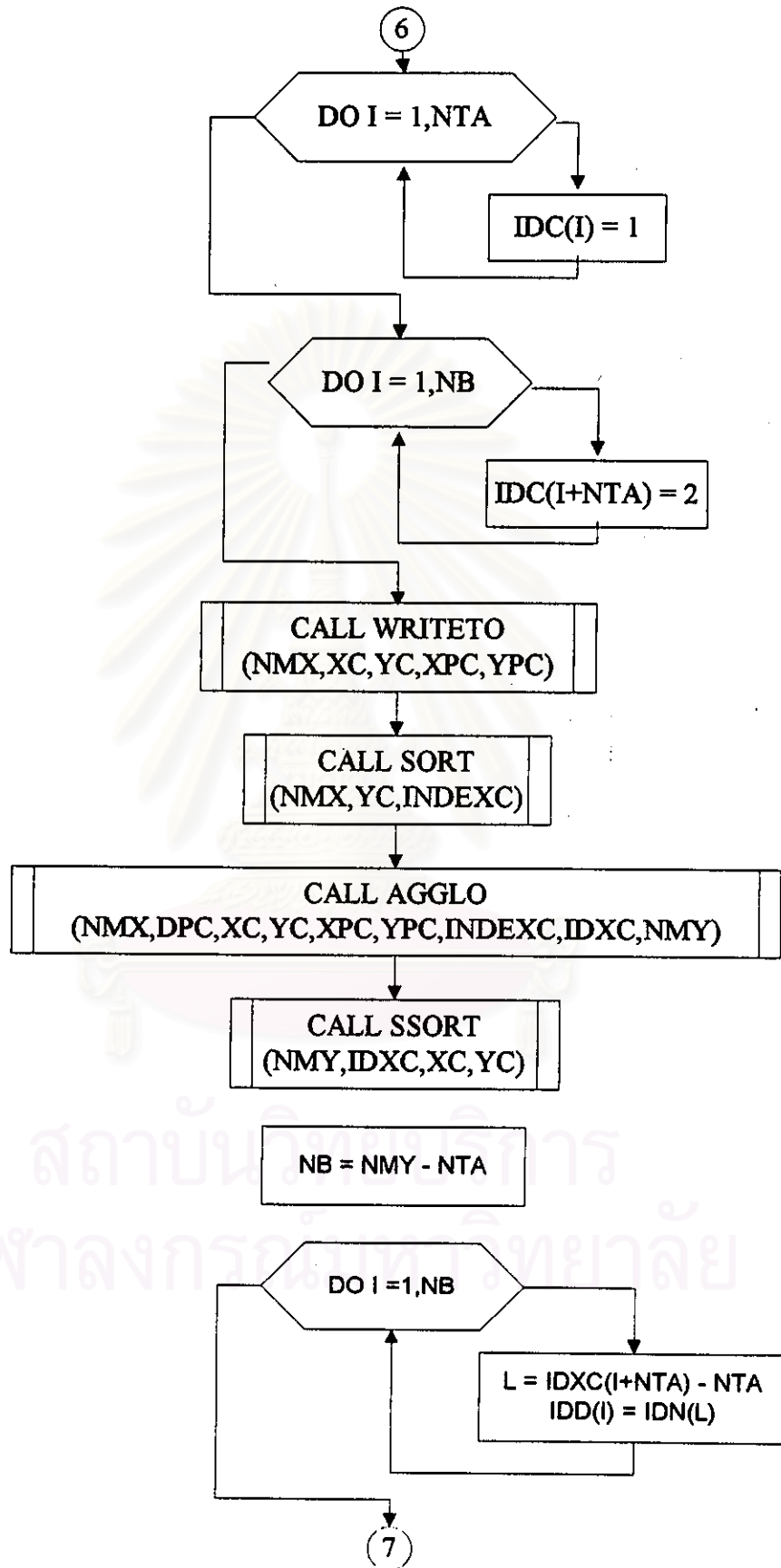




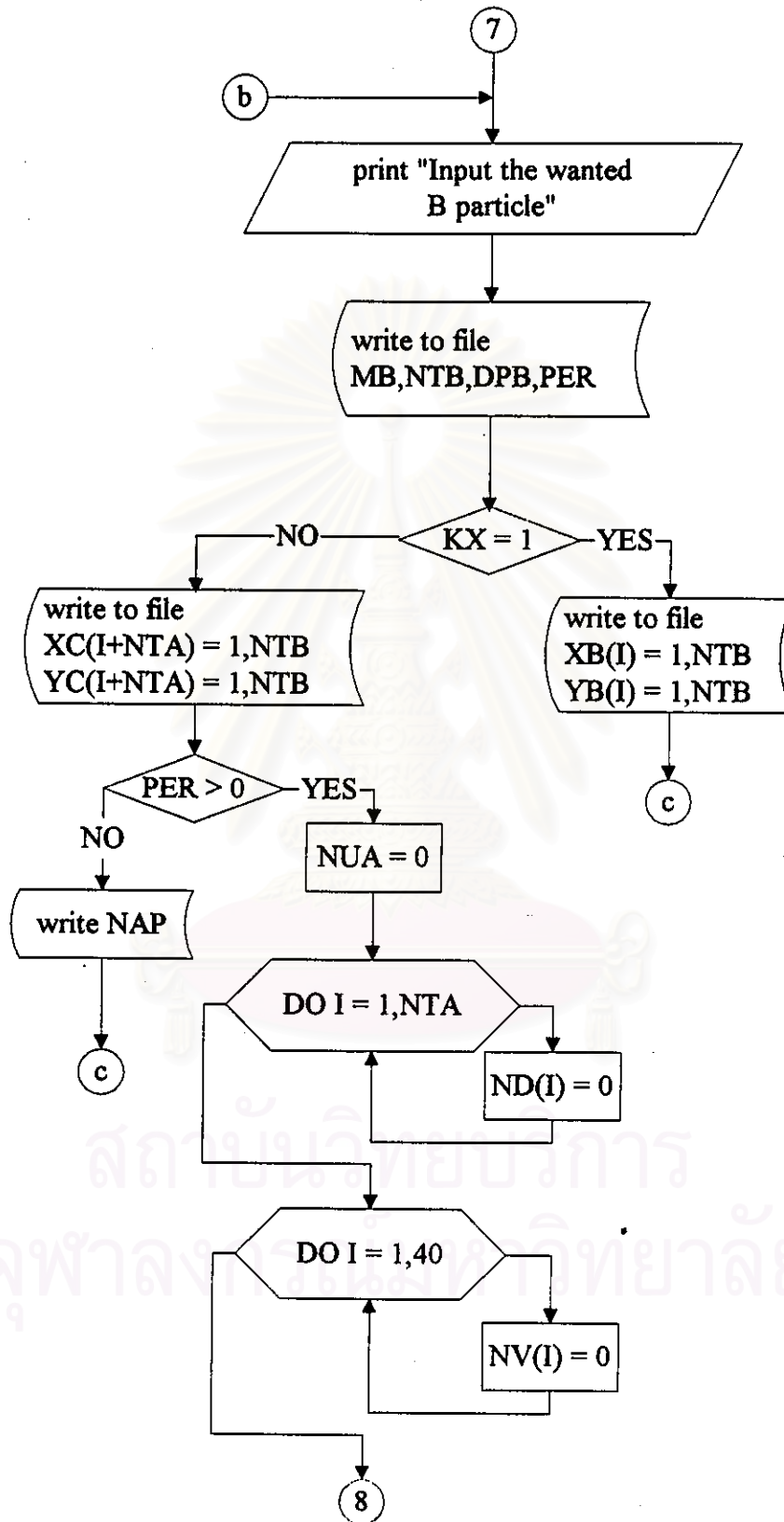


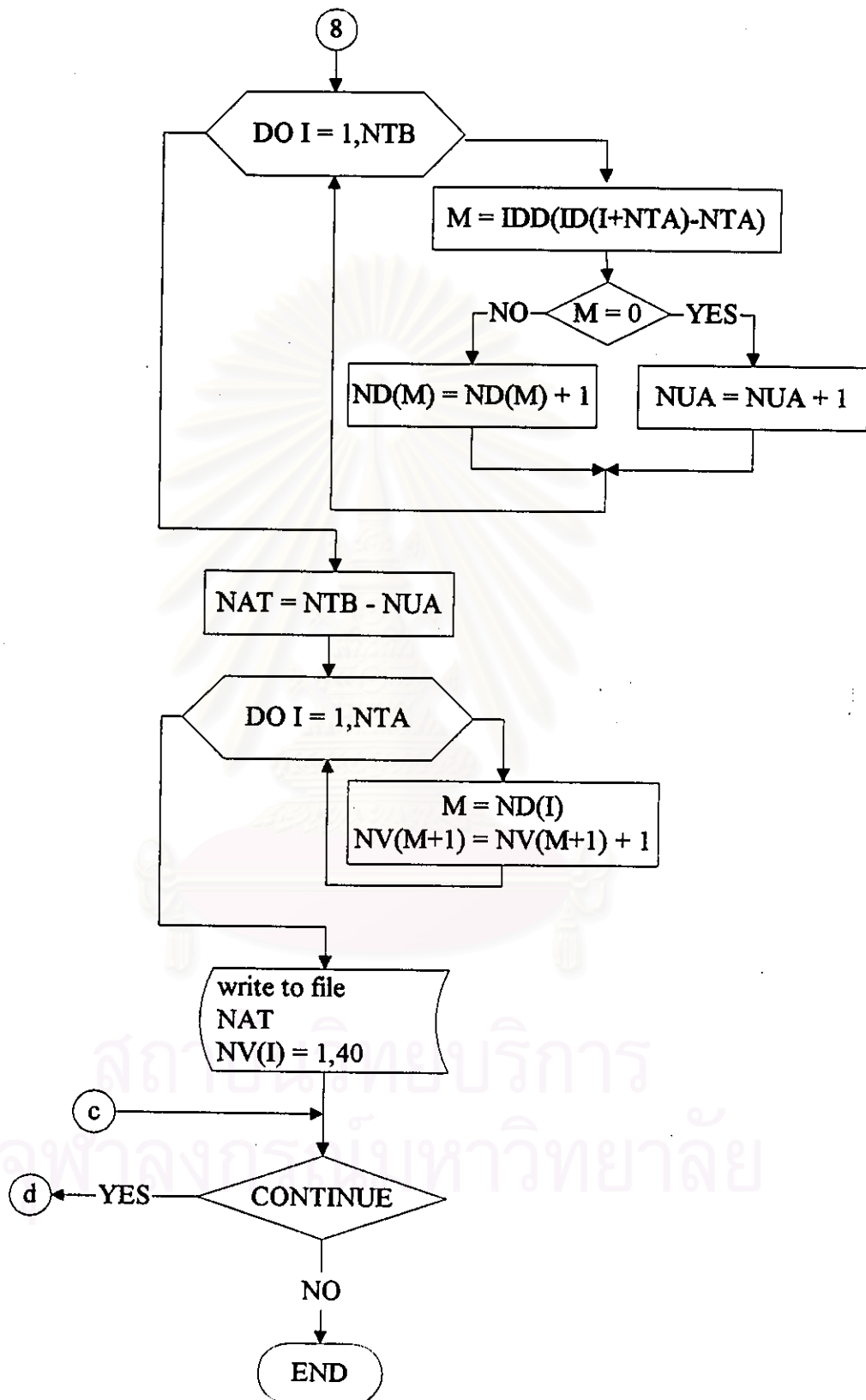




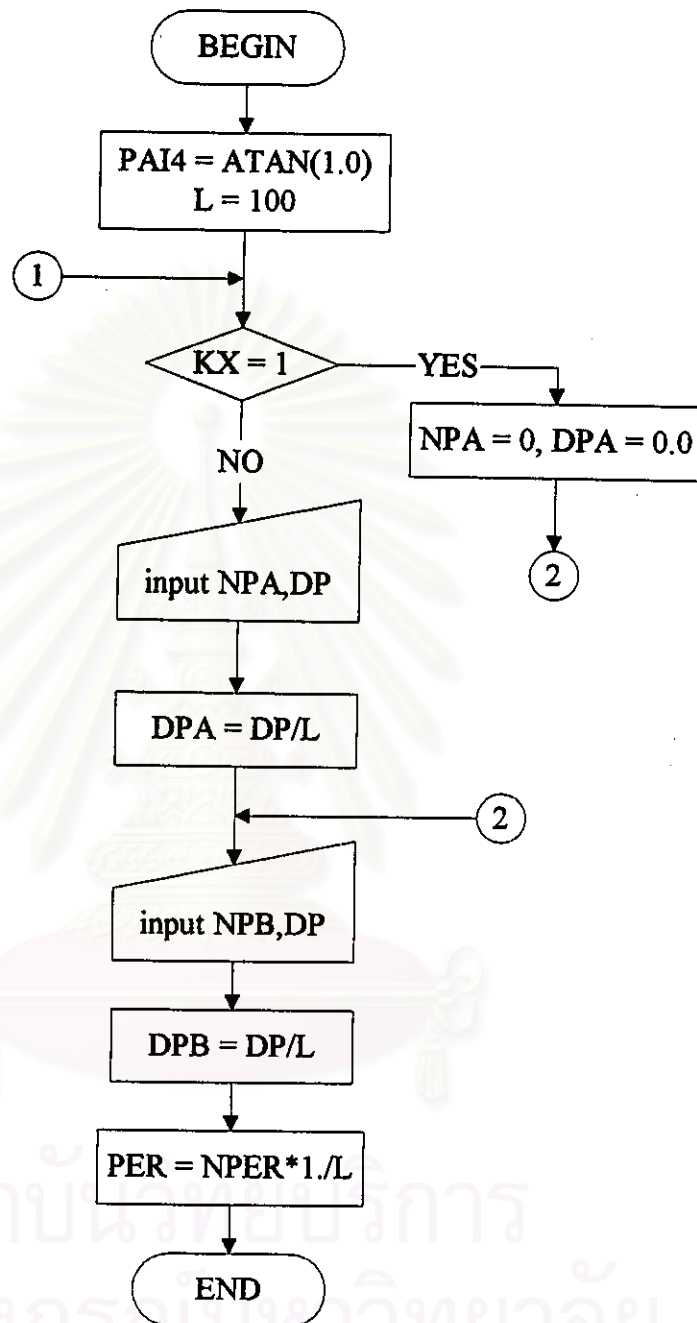




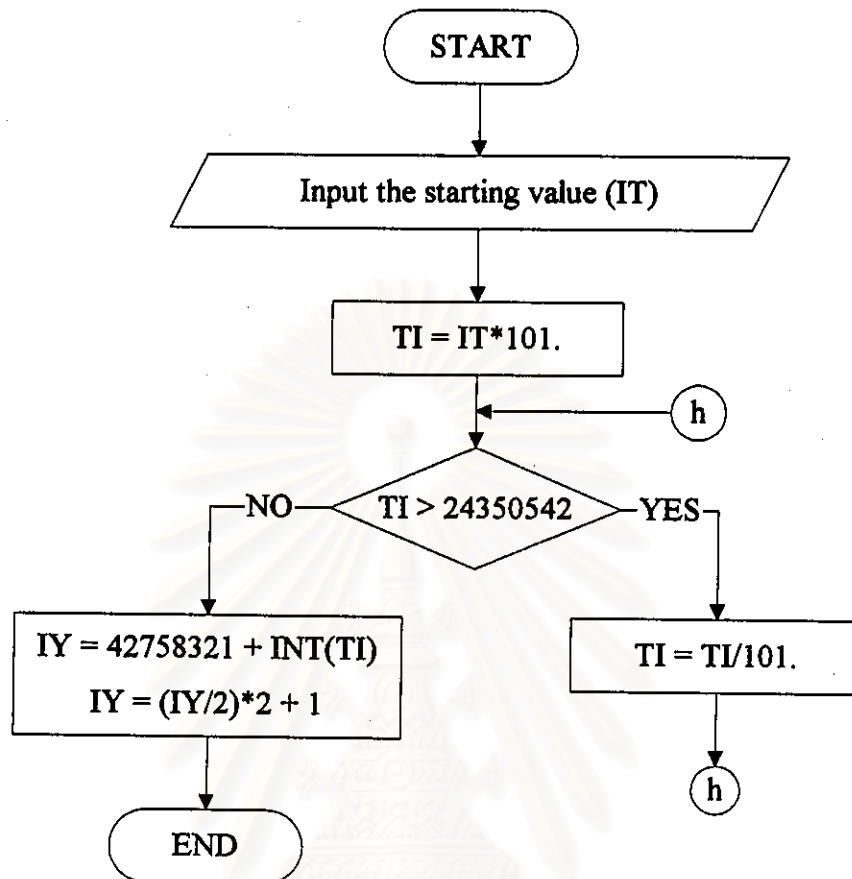




## SUBROUTINE DATAIN

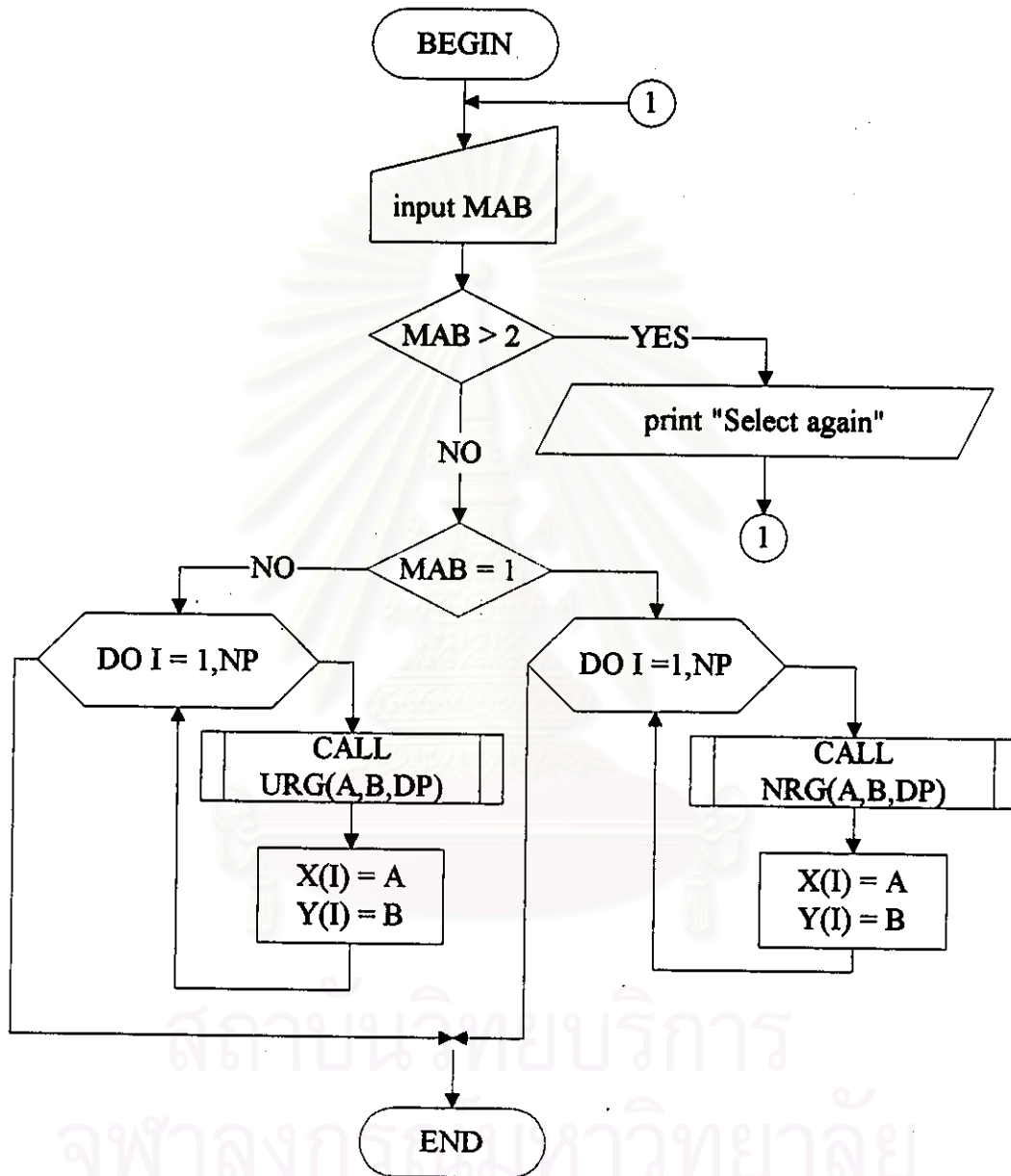


## SOUBROUTINE START

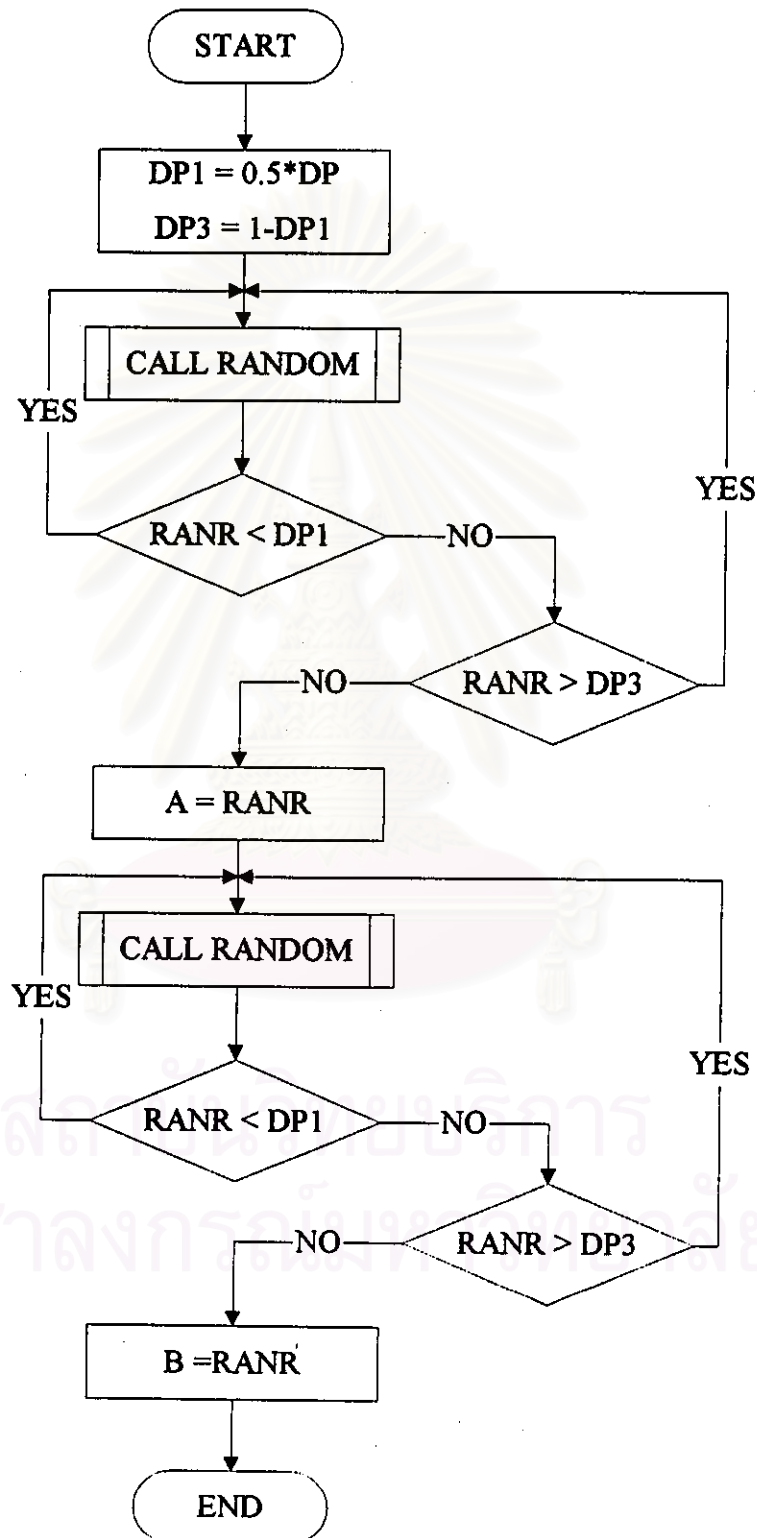


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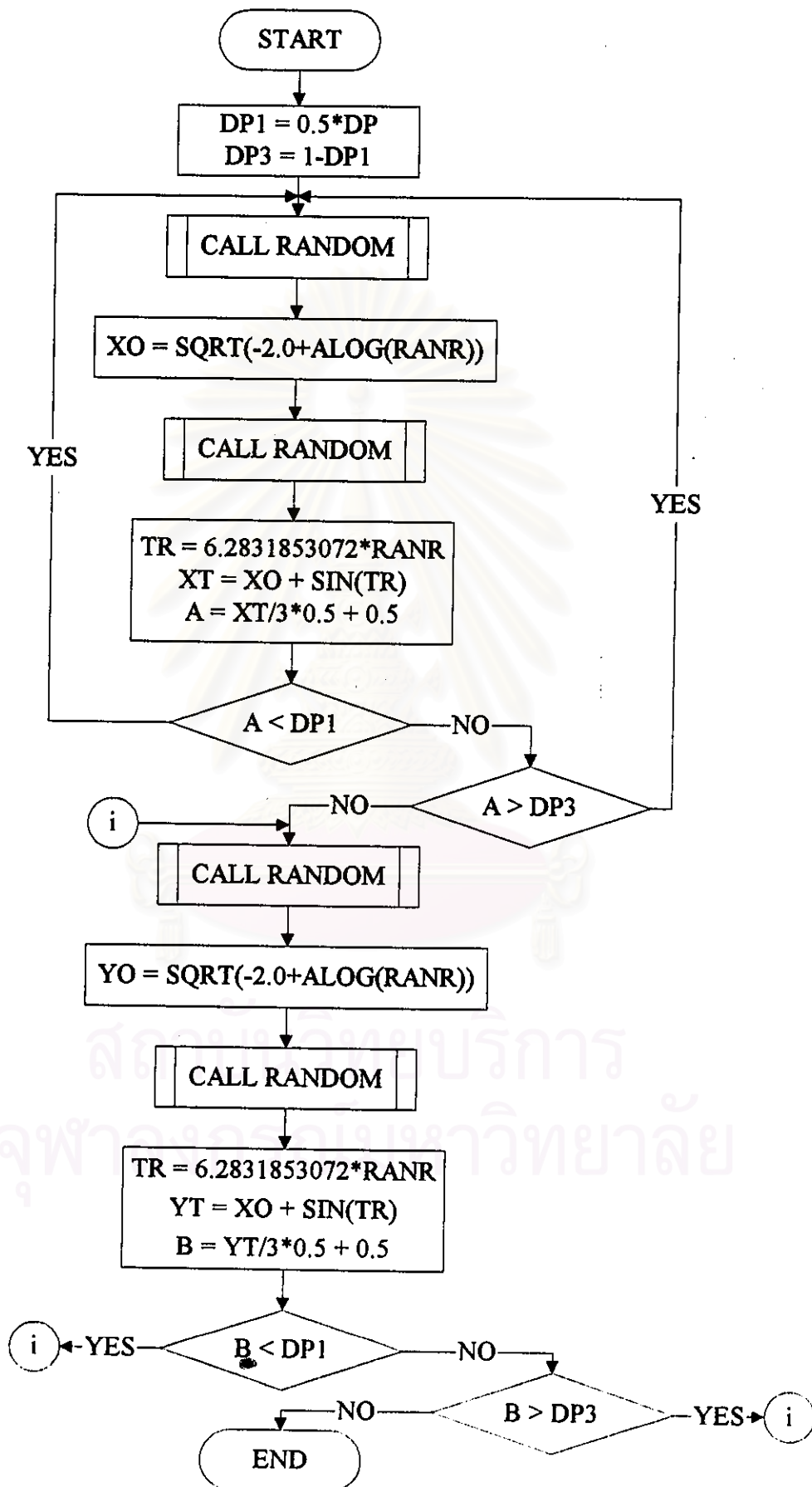
## SUBROUTINE DISPERSE (NP,X,Y,MAB,DP)



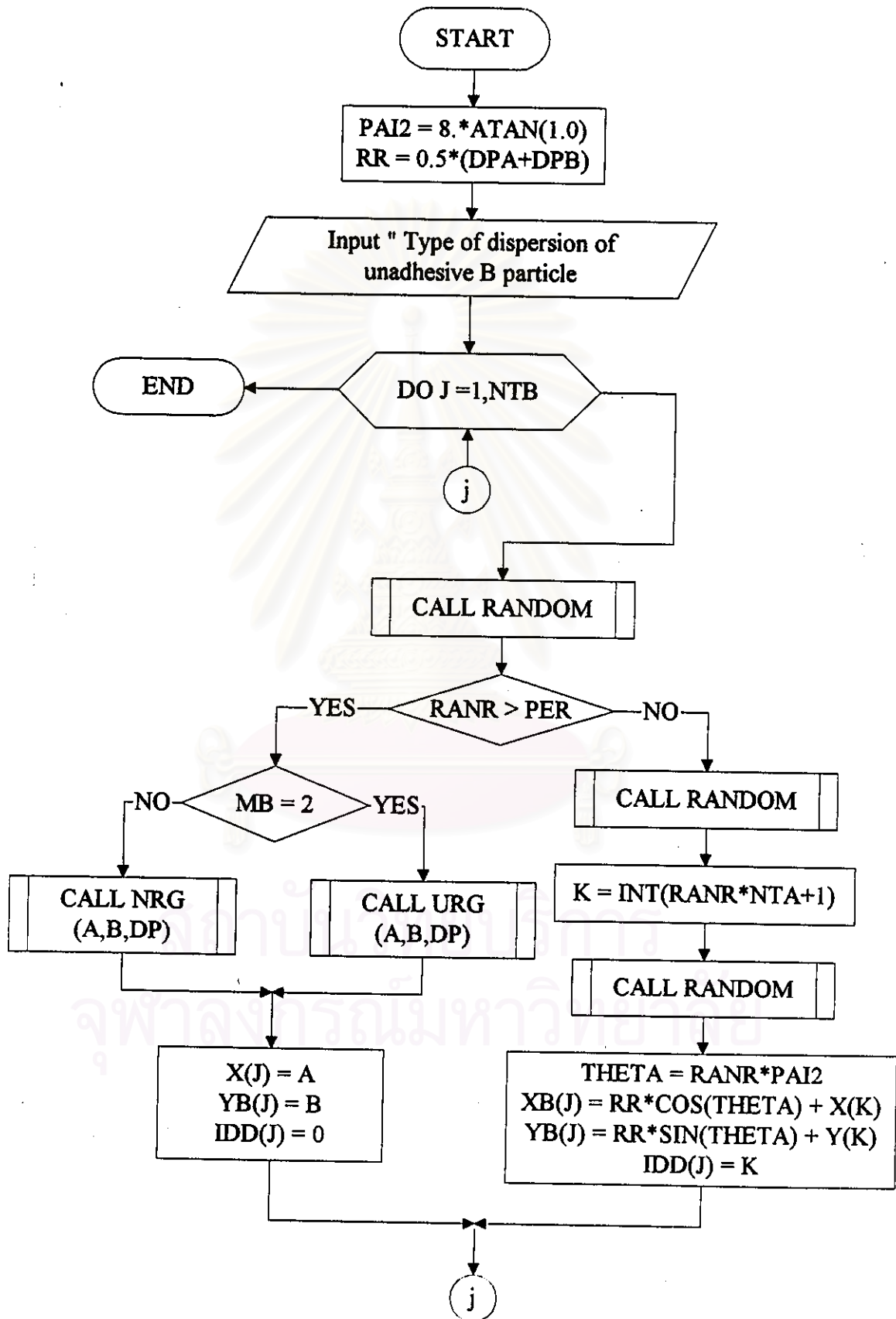
## SUBROUTINE URG (A,B,DP)



## SUBROUTINE NRG (A,B,DP)

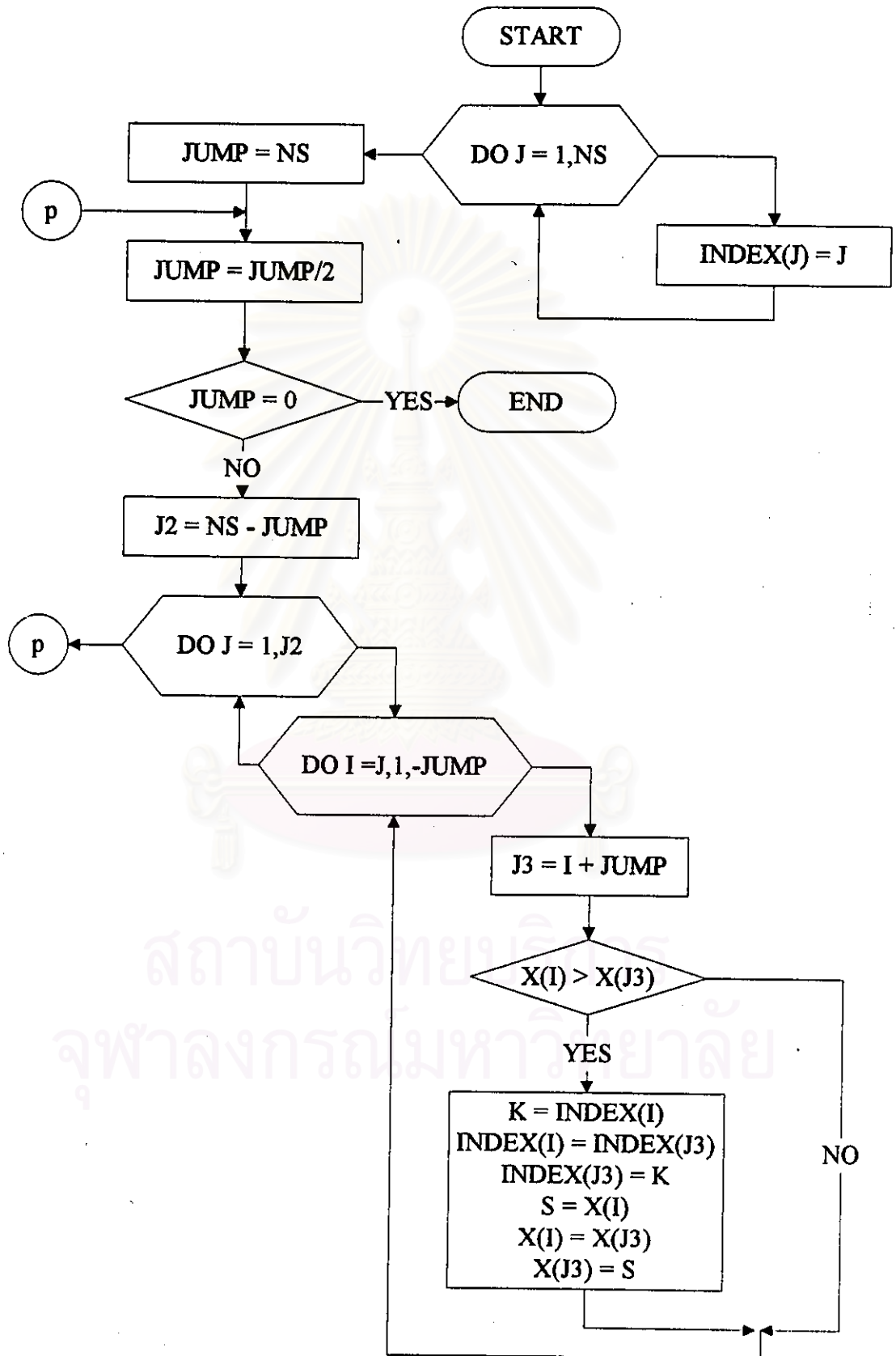


## SUBROUTINE FILLER (X,Y,XB,YB,NTA,NTB,IDD)

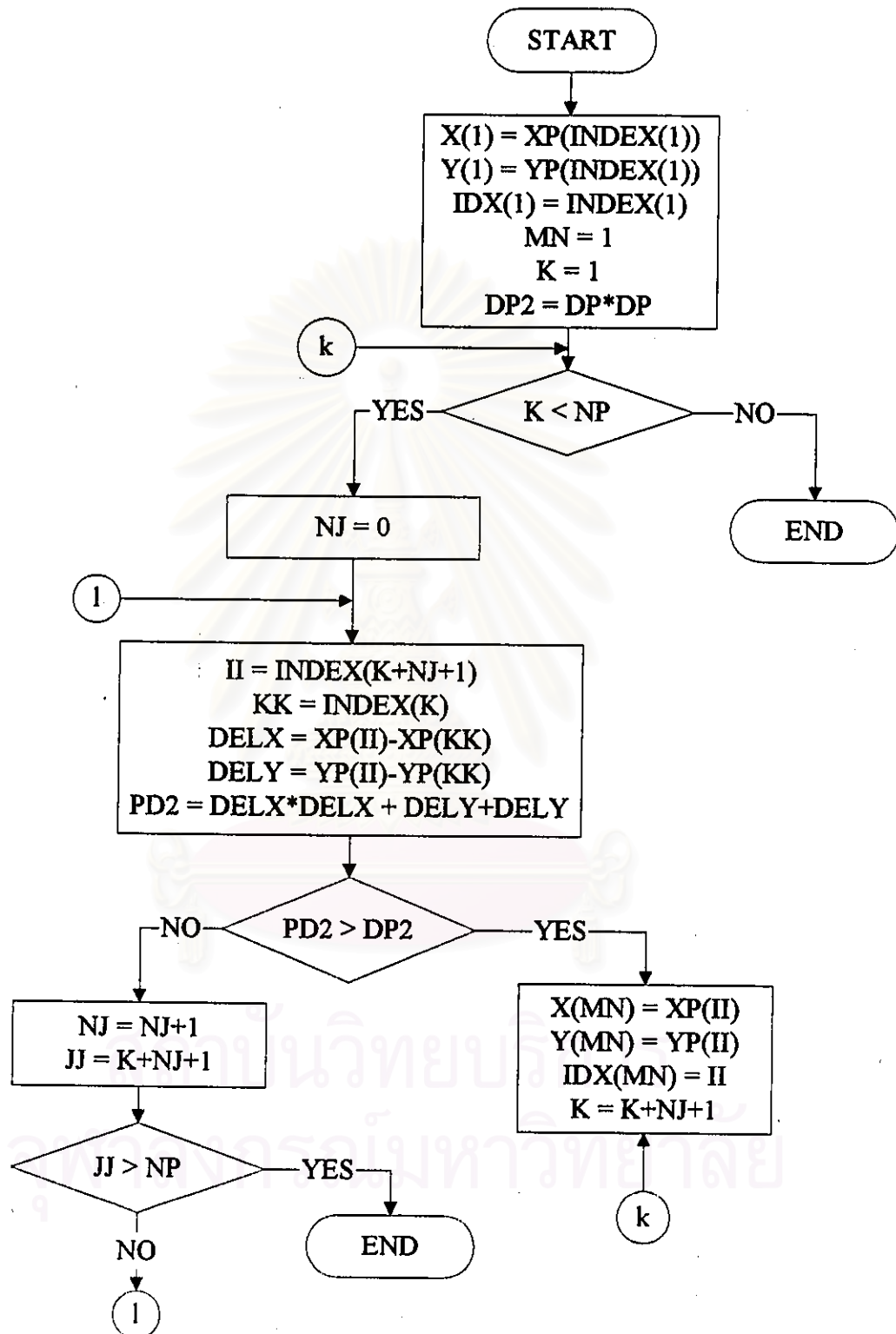




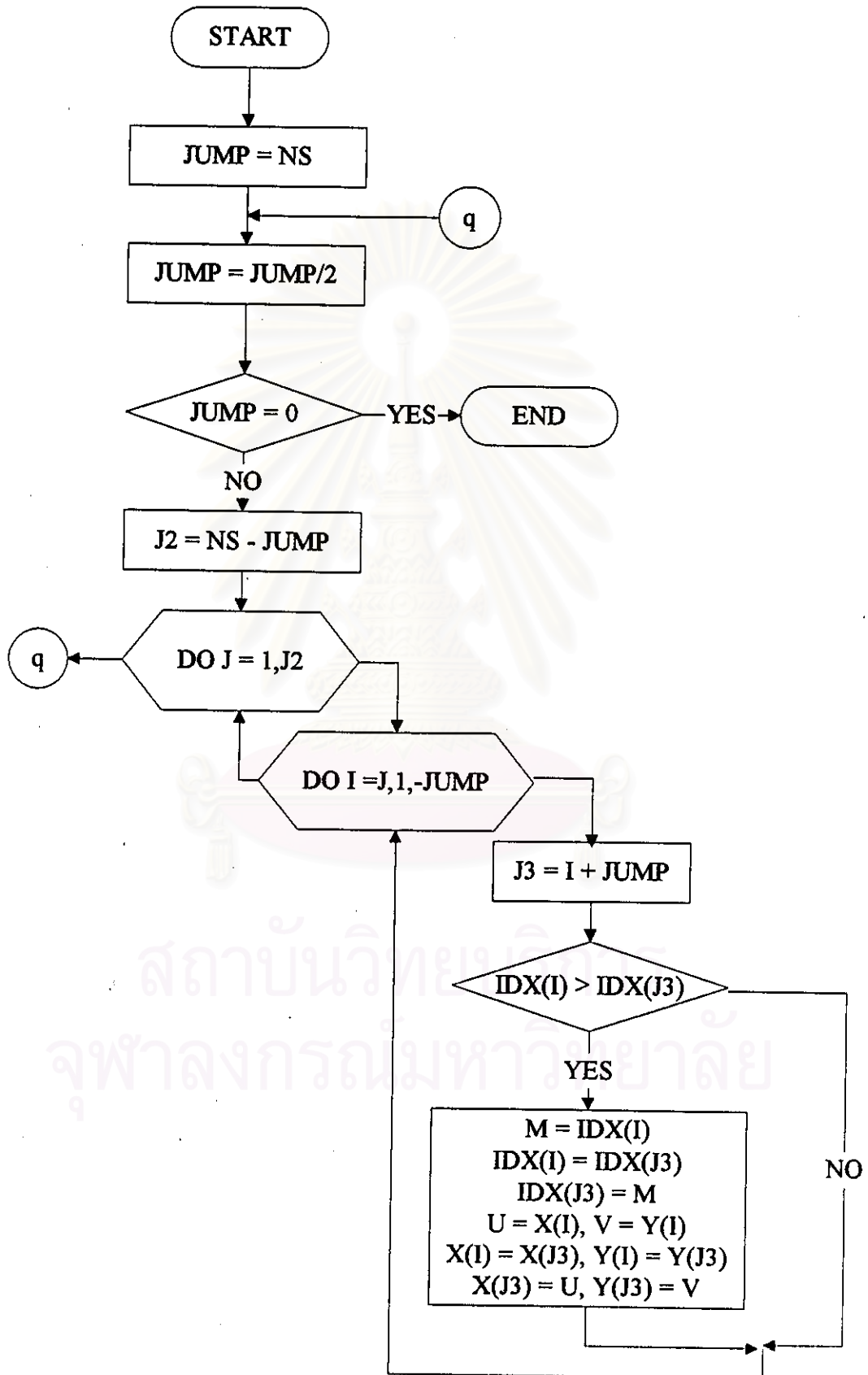
## SUBROUTINE SORT (NS,X,INDEX)



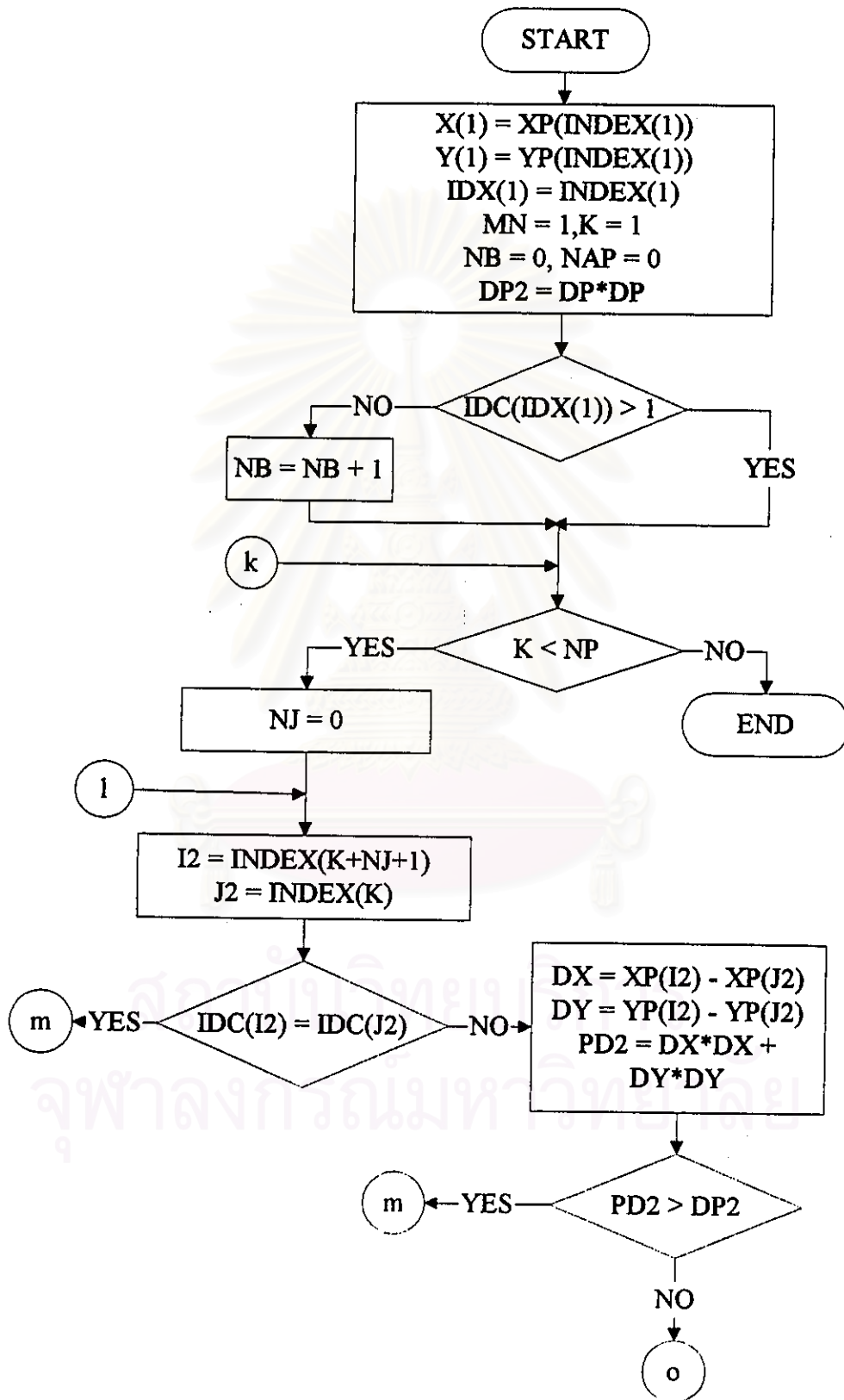
## SUBROUTINE AGGRO (NP,DP,X,Y,XP,YP,INDEX,IDX,MN)

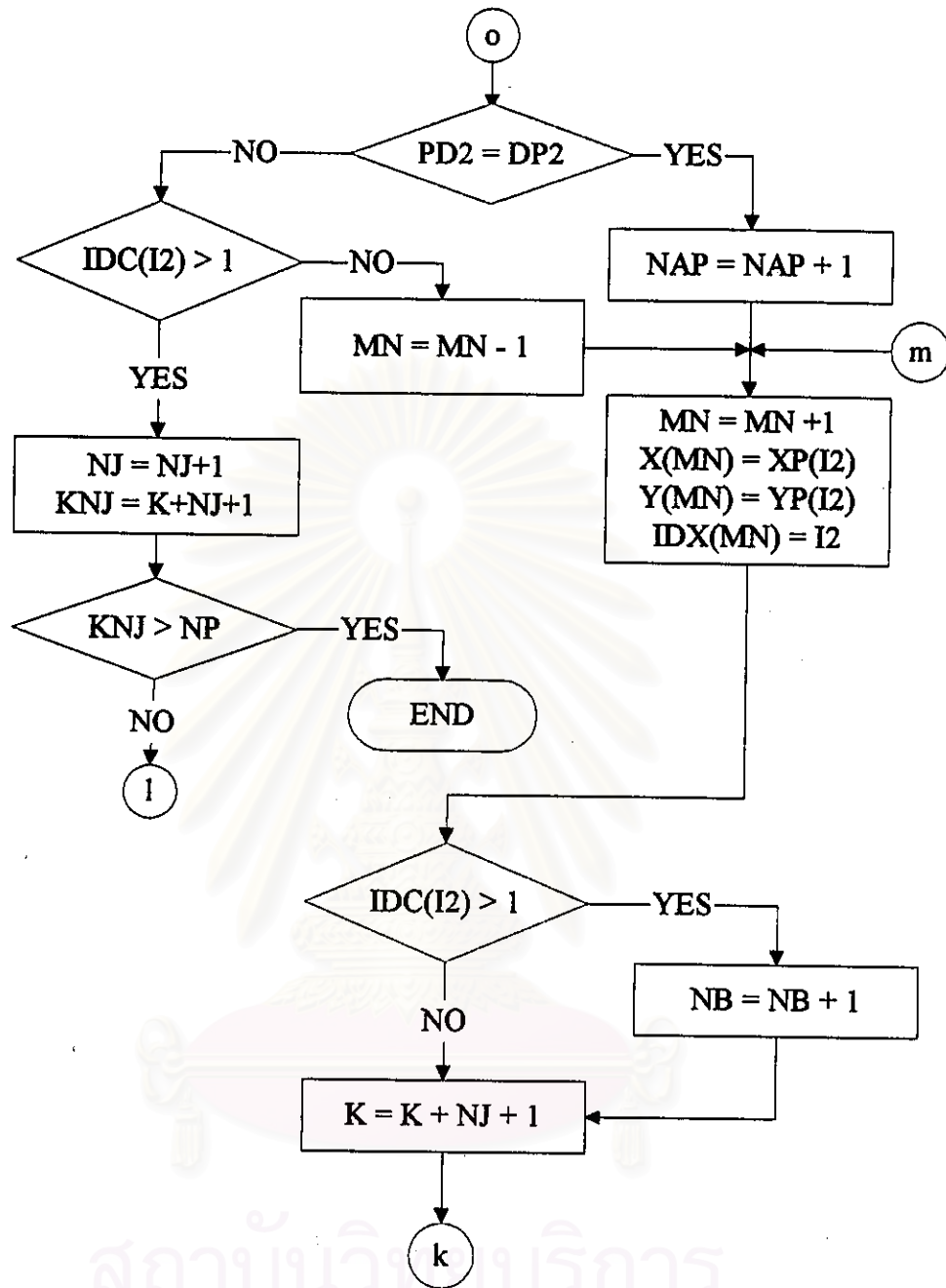


## SUBROUTINE SSORT (MN,IDX,X,Y)



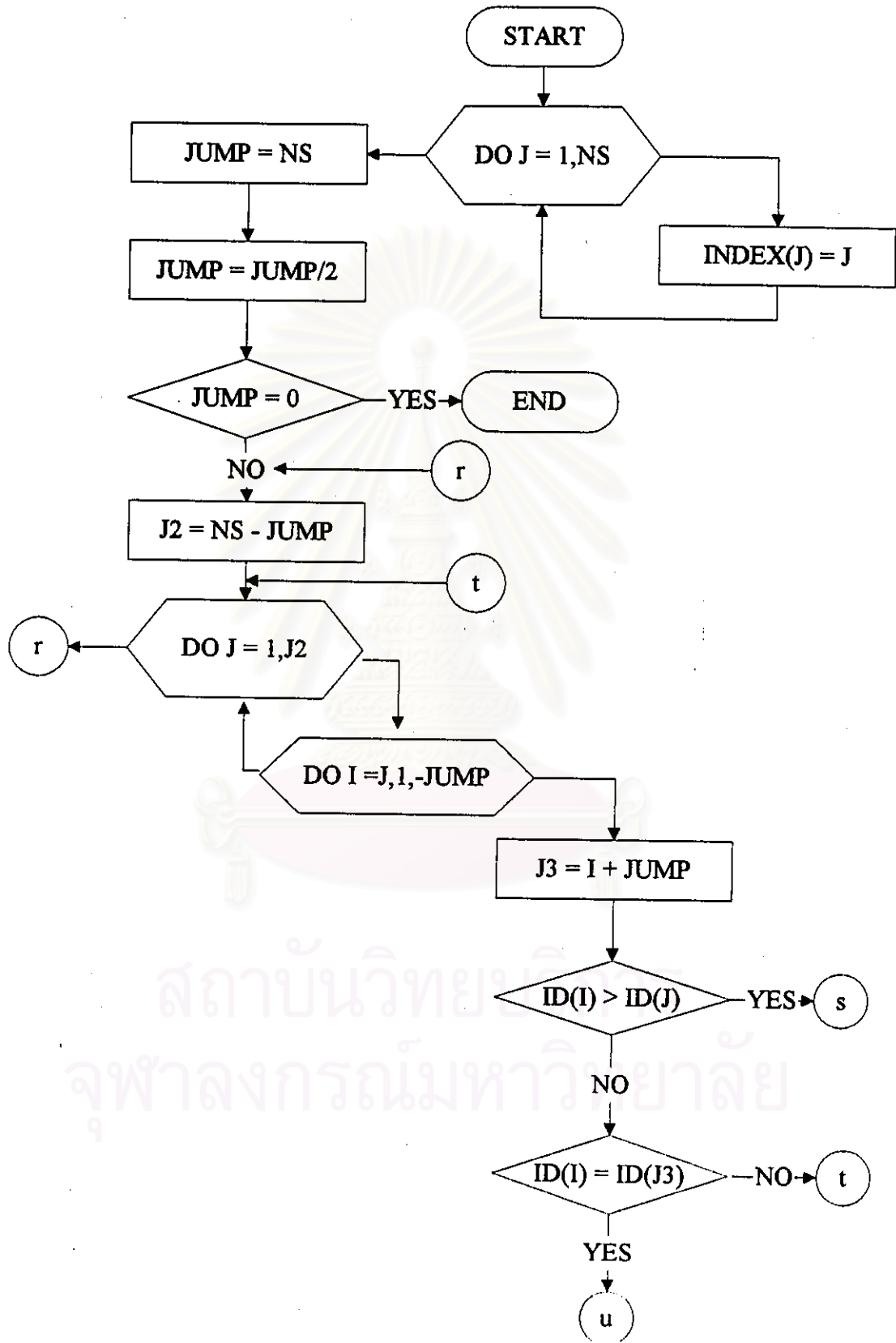
## SUBROUTINE AGGLO (NP,DP,X,Y,XP,YP,INDEX,IDX,MN)

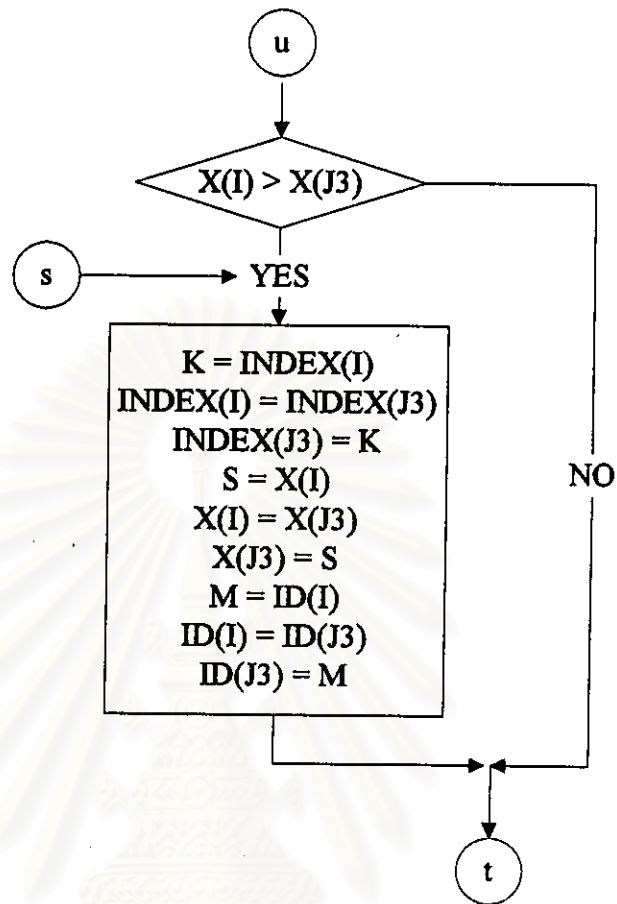




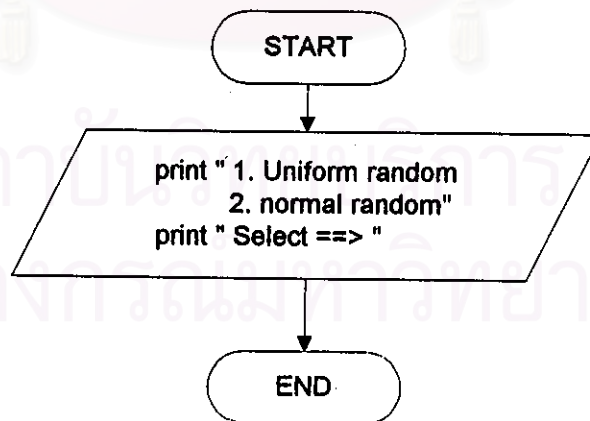
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## SUBROUTINE ISORT (NS,X,ID,INDEX)

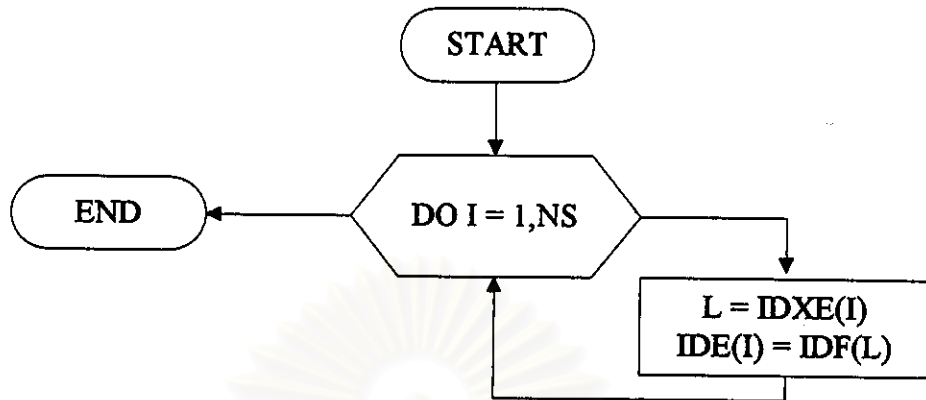




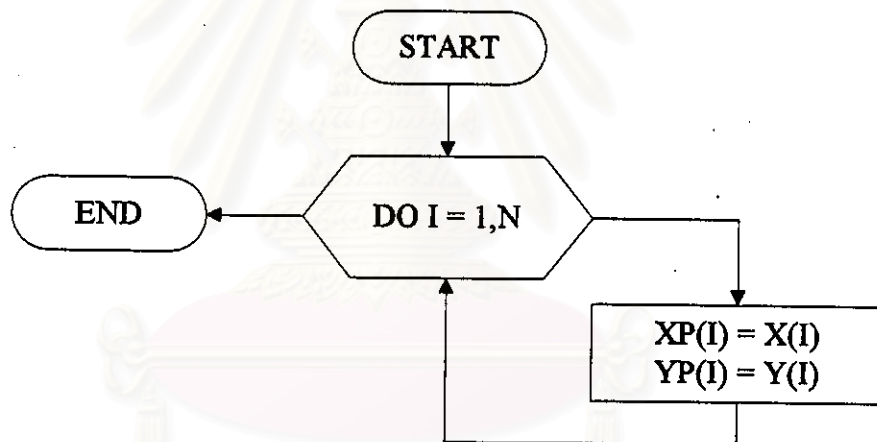
### SOURROUTINE TYPE



## SUBROUTINE POINT (IDE,IDF,IDX,NS)



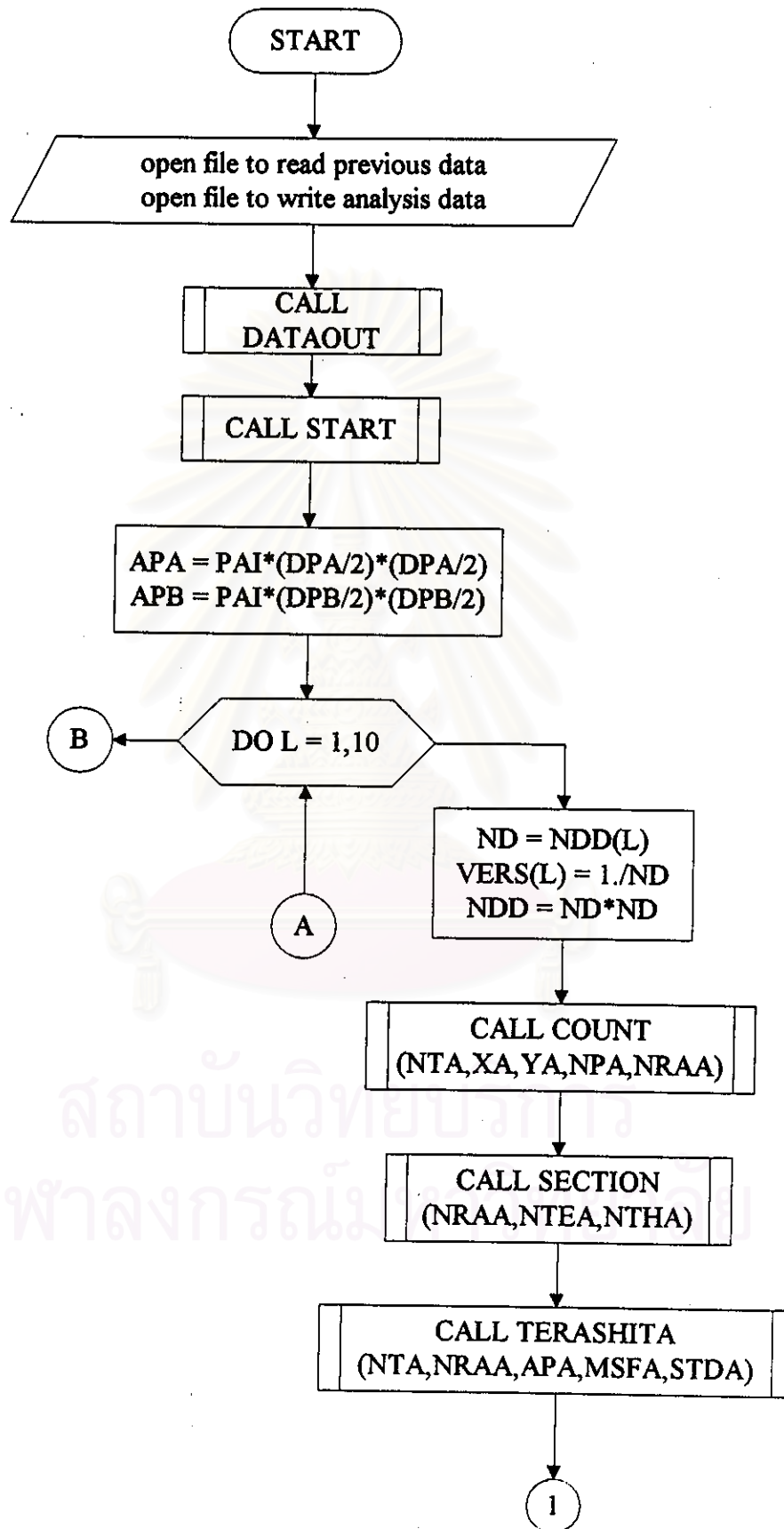
## SUBROUTINE WRITETO (N,X,Y,XP,YP)

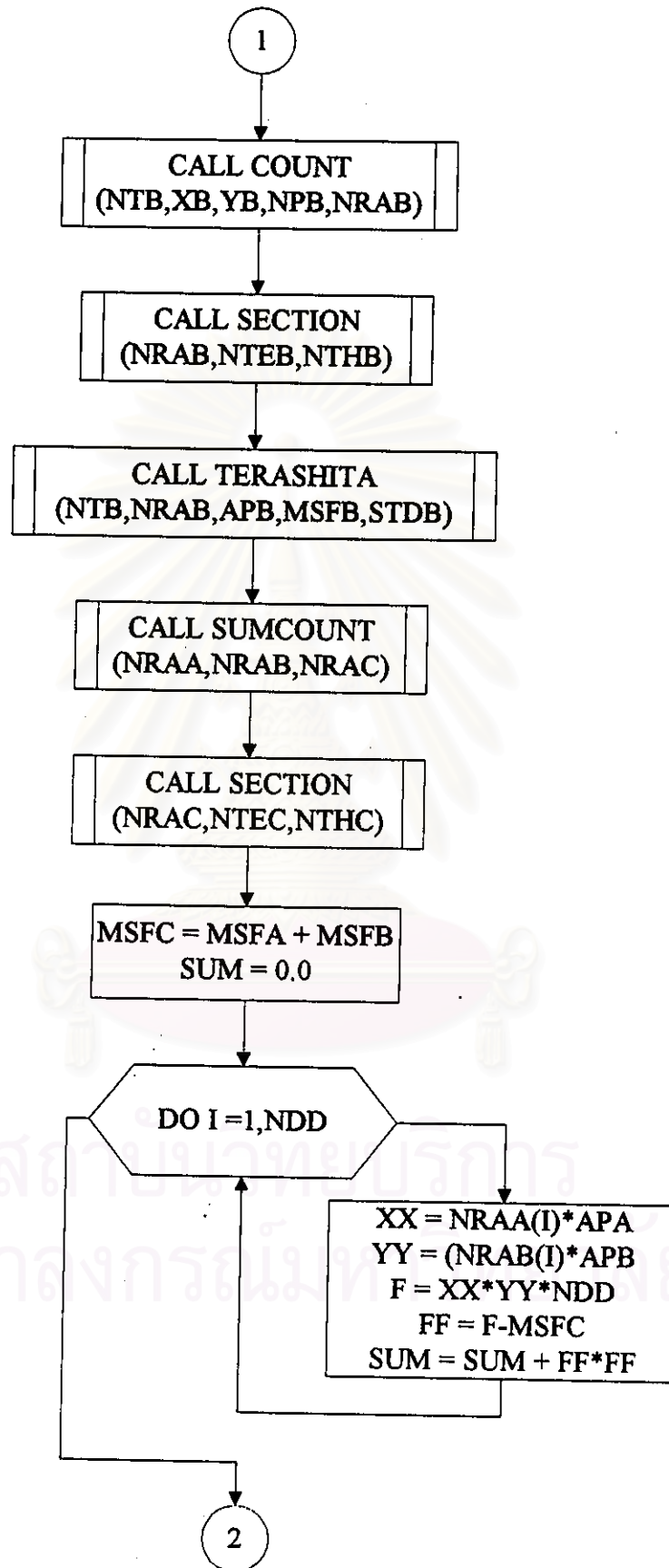


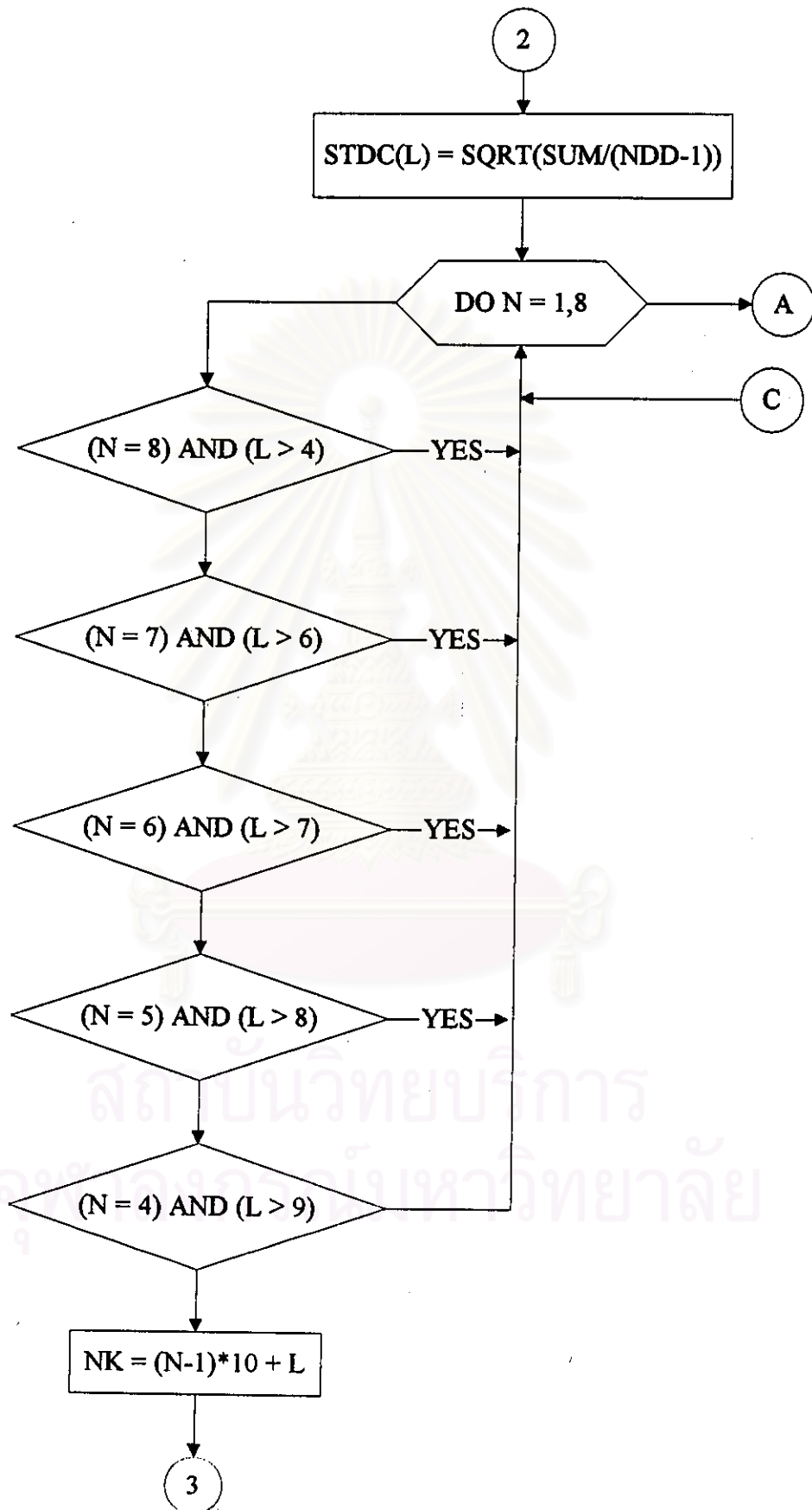
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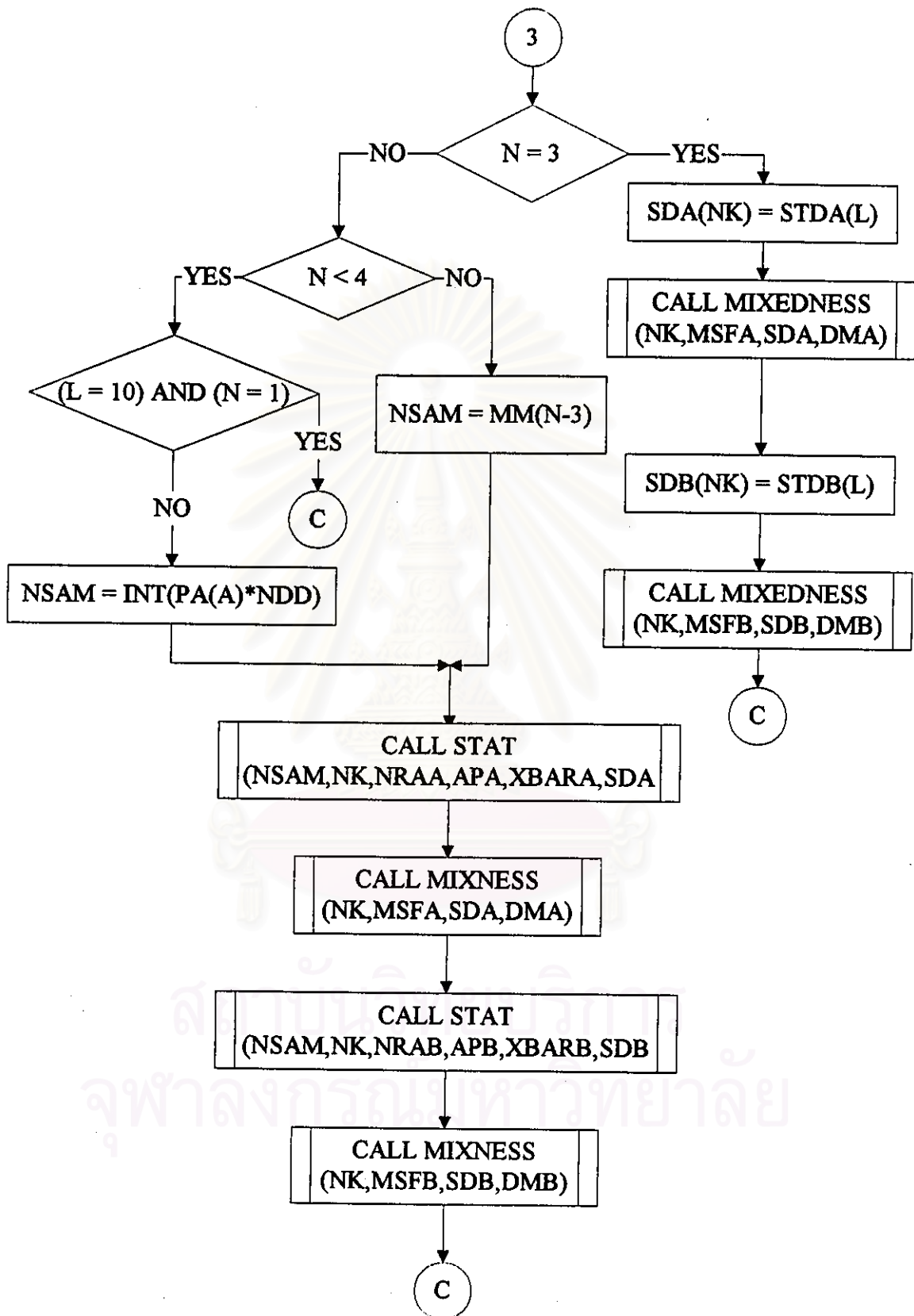


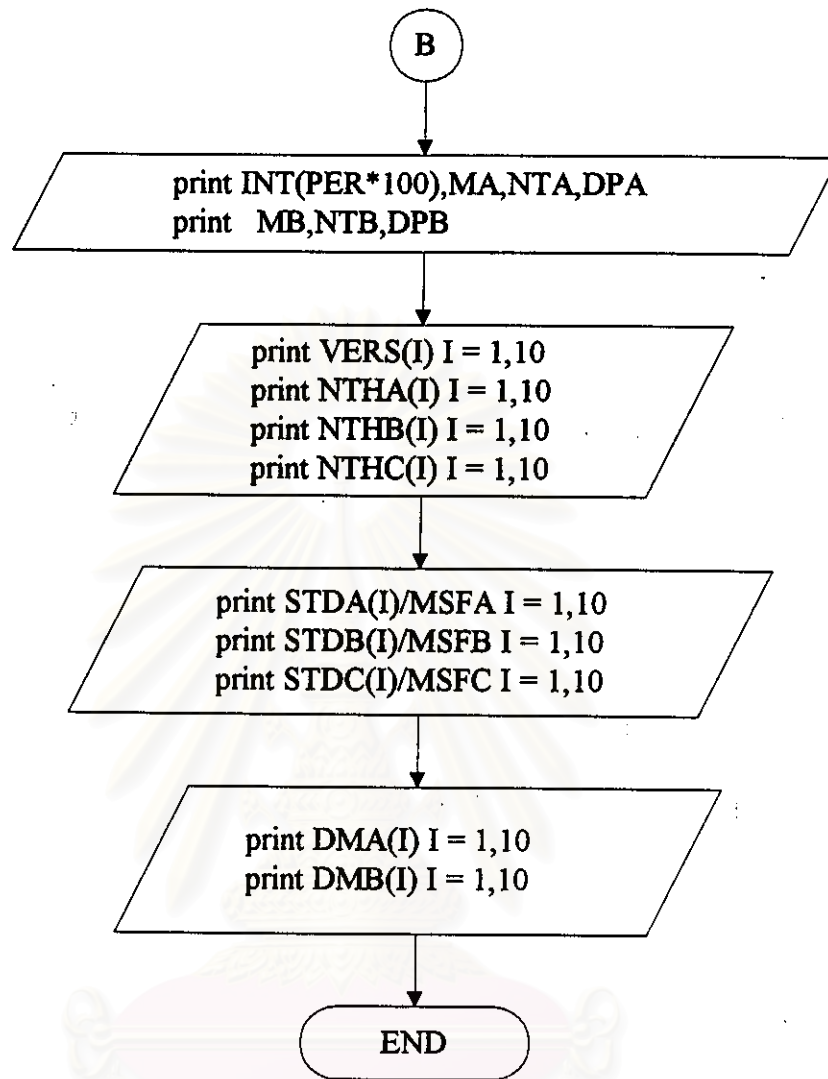
## ANALYSIS PROGRAM





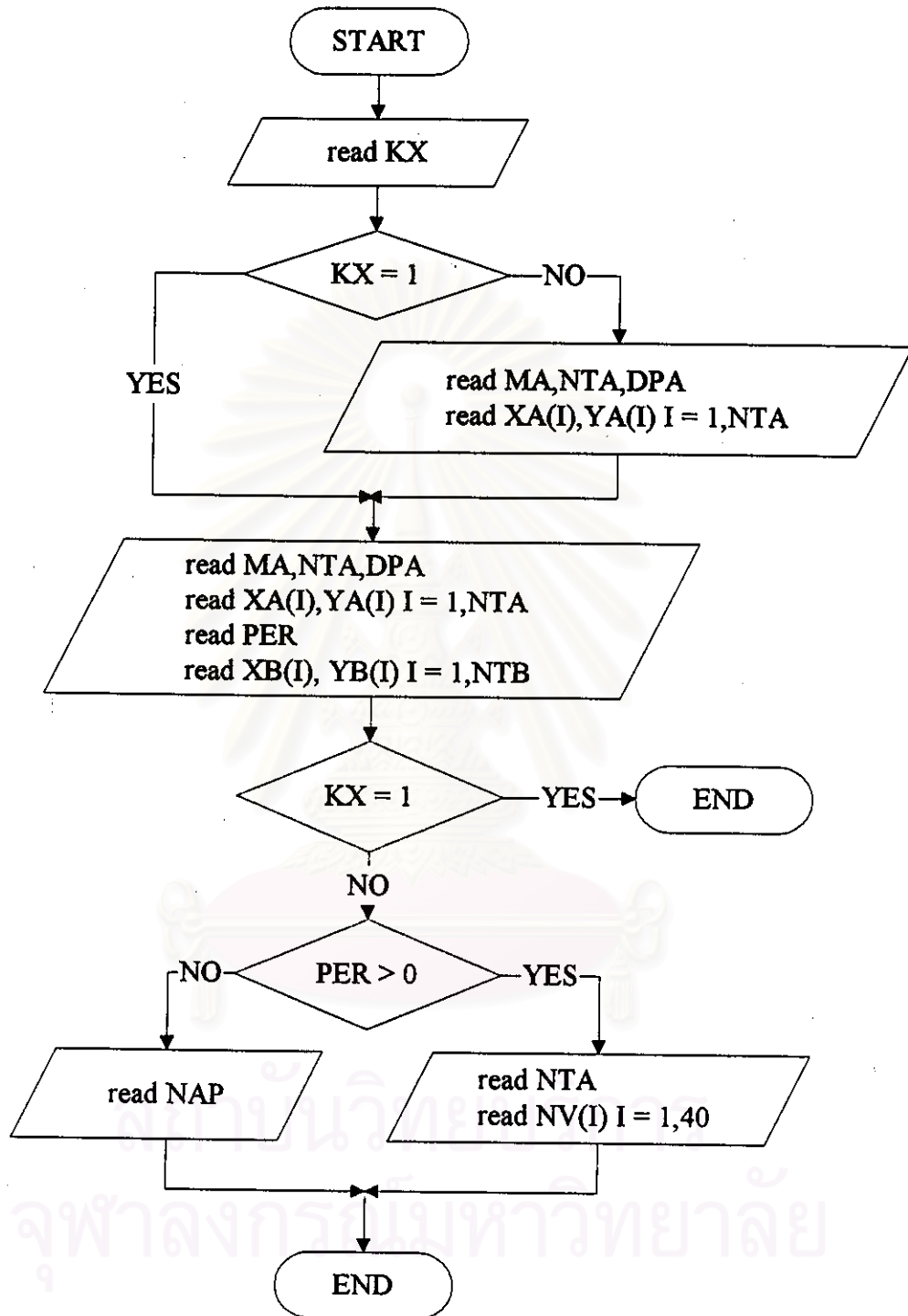




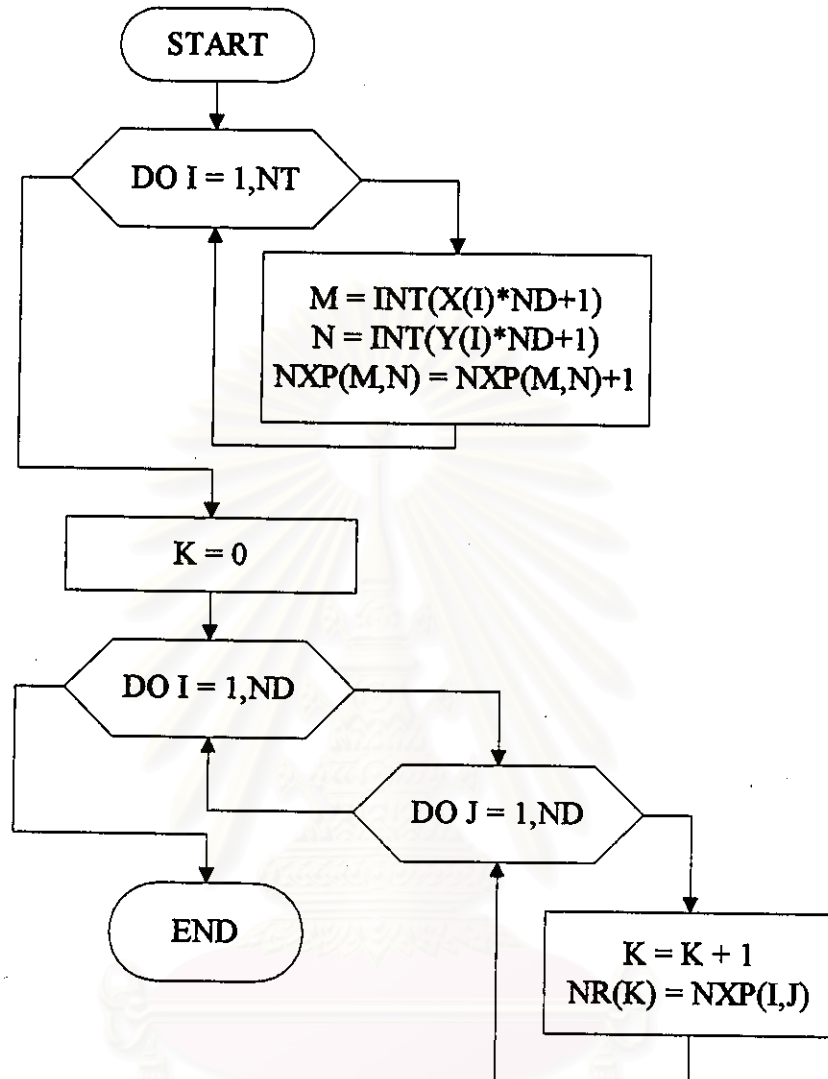


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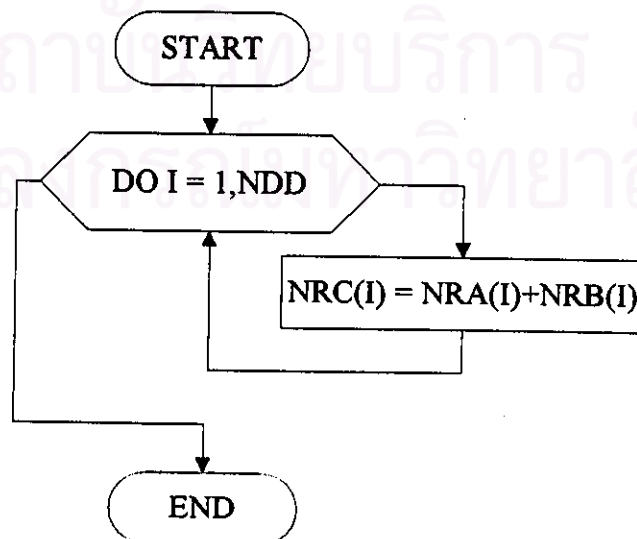
## SUBROUTINE DATAOUT



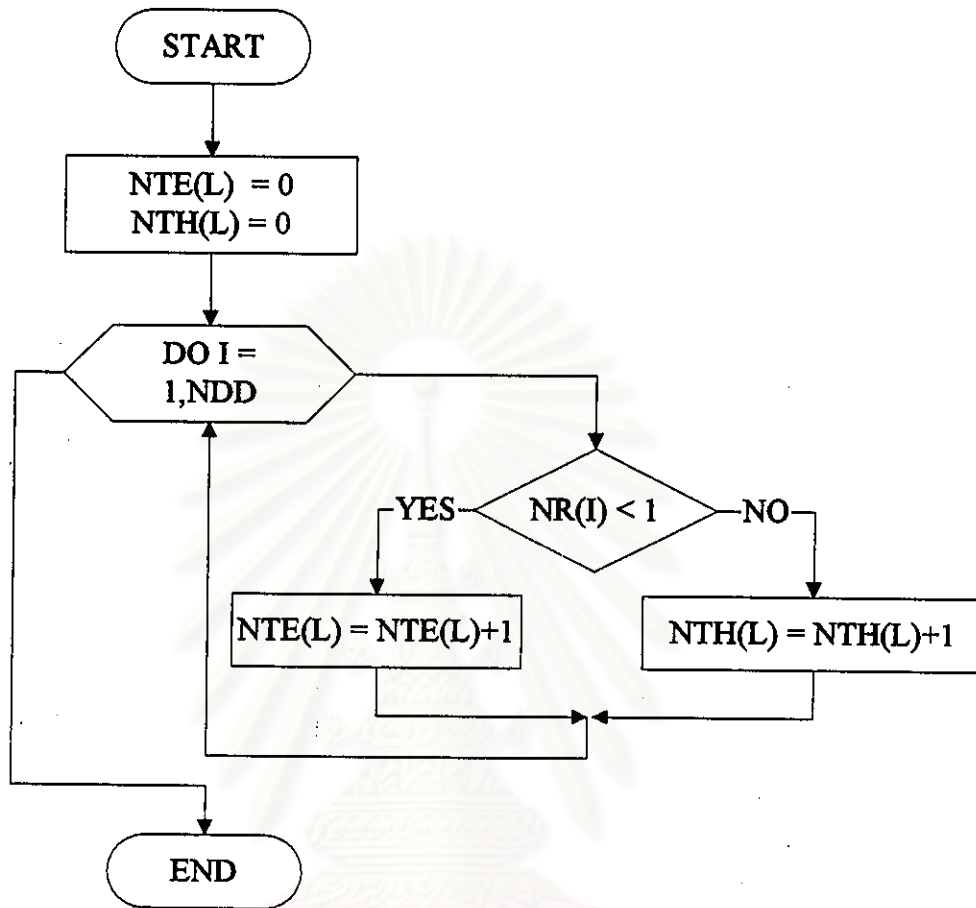
## SUBROUTINE COUNT (NT,X,Y,NXP,NR)



## SUBROUTINE SUMCOUNT(NRA,NRB,NRC)



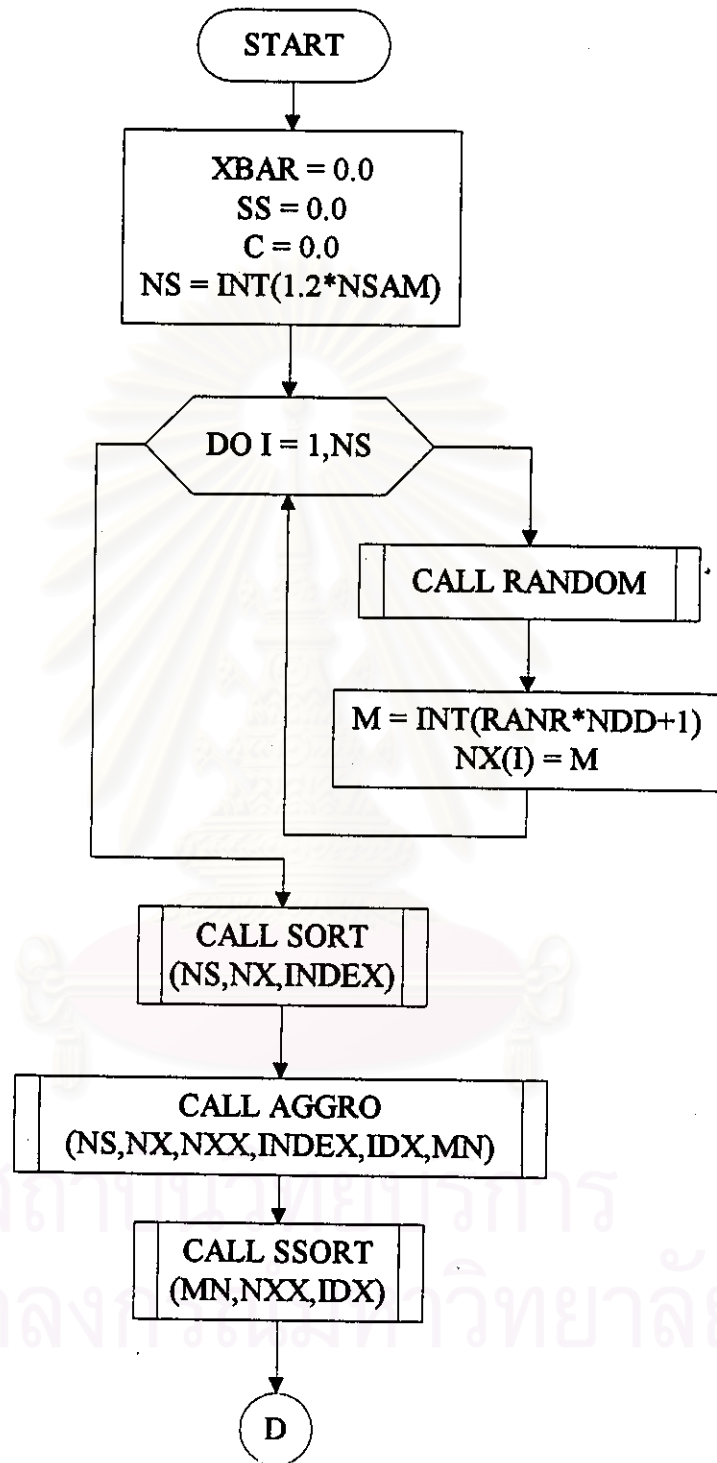
## SUBROUTINE SECTION (NR,NTE,NTH)

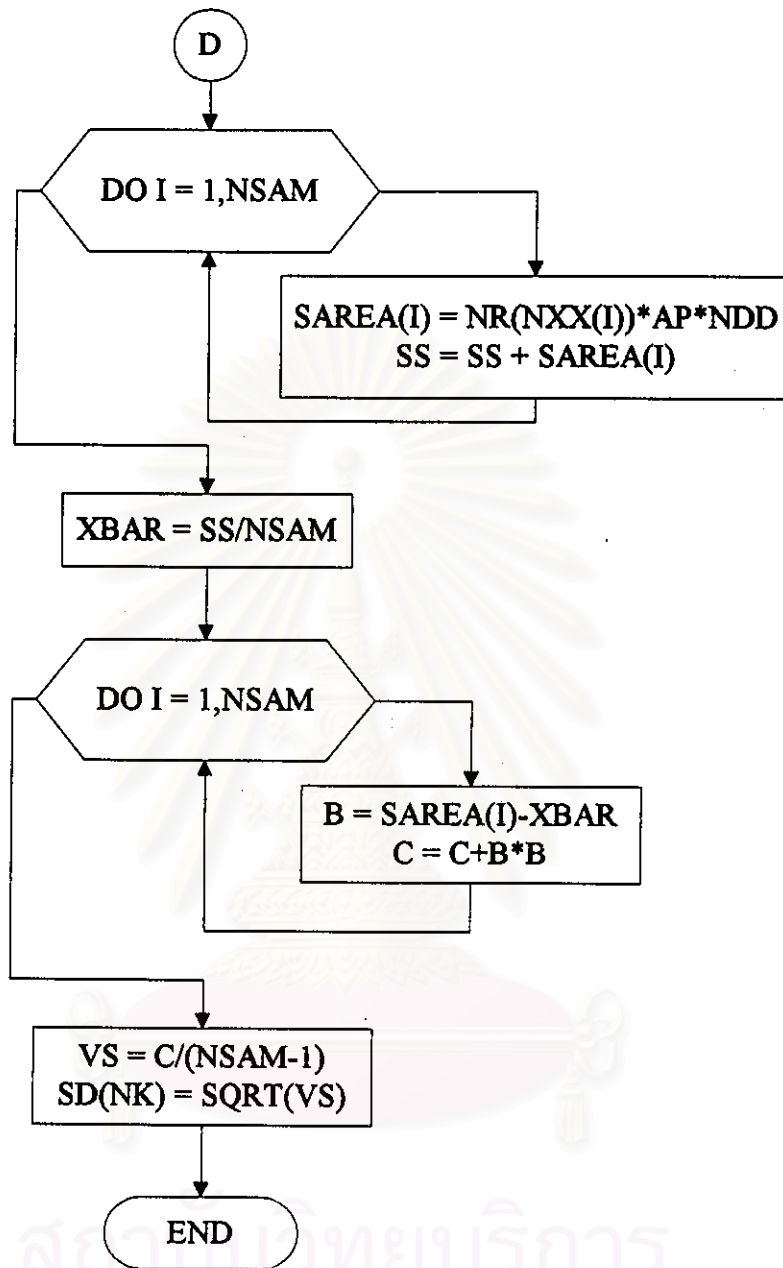


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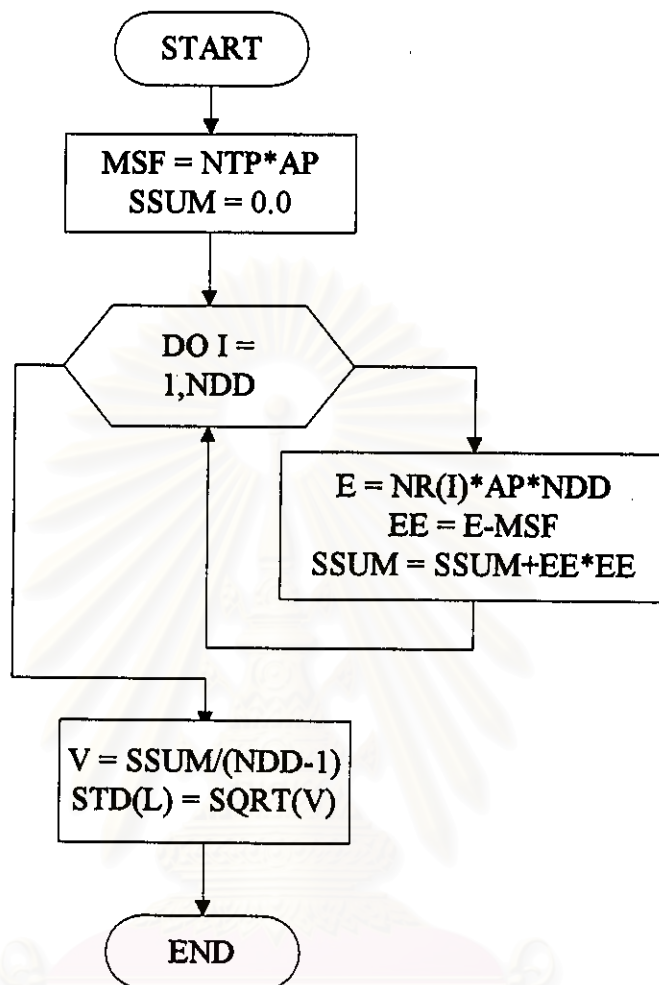


SUBROUTINE STAT (NSAM,NK,NR,AP,XBAR,SD)



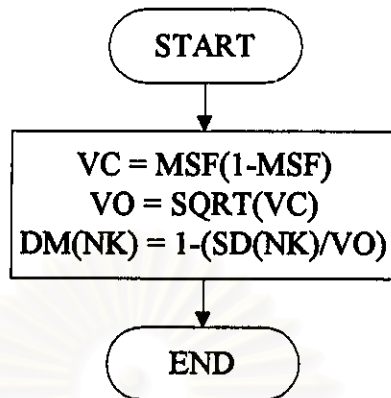


SUBROUTINE TERASHI (NTP,NR,AP,MSF,STD)

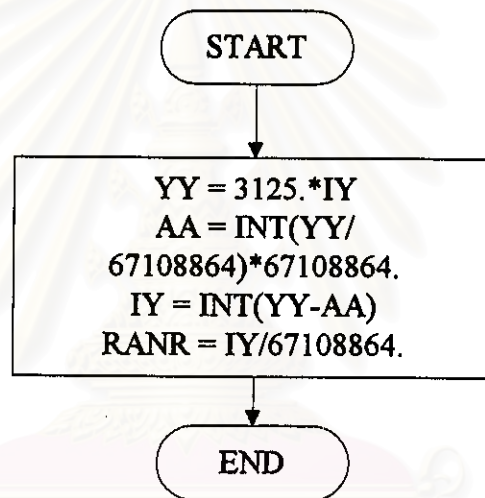


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## SUBROUTINE MIXNESS (NK,MSF,SD,DM)



## SUBROUTINE RANDOM



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## APPENDIX C

### COMPUTER -SIMULATED RESULTS

The relationship between the quantitative indices and the various conditions obtained from computer simulation gives the following table.



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Table C1 The degree of mixedness of B particles in the case of uniform - uniform dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Degree of mixedness of B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.9993	0.9992	0.9992	0.9991	0.9990
	2:1	0.9991	0.9991	0.9989	0.9986	0.9984
	5:1	0.9982	0.9980	0.9974	0.9966	0.9957
	10:1	0.9977	0.9974	0.9961	0.9945	0.9931
0.04:1	1:1	0.9985	0.9986	0.9984	0.9980	0.9979
	2:1	0.9983	0.9981	0.9979	0.9967	0.9969
	5:1	0.9963	0.9962	0.9951	0.9933	0.9917
	10:1	0.9956	0.9949	0.9924	0.9888	0.9862
0.10:1	1:1	0.9963	0.9966	0.9960	0.9955	0.9950
	2:1	0.9954	0.9954	0.9948	0.9939	0.9924
	5:1	0.9911	0.9905	0.9879	0.9833	0.9798
	10:1	0.9889	0.9873	0.9824	0.9744	0.9673
0.20:1	1:1	0.9933	0.9933	0.9927	0.9917	0.9887
	2:1	0.9914	0.9908	0.9895	0.9871	0.9856
	5:1	0.9826	0.9806	0.9767	0.9686	0.9608
	10:1	0.9780	0.9751	0.9664	0.9514	0.9341

Table C2 The degree of mixedness of B particles in the case of uniform - normal dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Degree of mixedness of B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.9973	0.9974	0.9982	0.9989	0.9990
	2:1	0.9959	0.9965	0.9974	0.9978	0.9975
	5:1	0.9937	0.9946	0.9959	0.9964	0.9958
	10:1	0.9911	0.9925	0.9939	0.9941	0.9930
0.04:1	1:1	0.9945	0.9953	0.9962	0.9978	0.9979
	2:1	0.9919	0.9927	0.9945	0.9953	0.9953
	5:1	0.9872	0.9882	0.9917	0.9924	0.9915
	10:1	0.9821	0.9848	0.9881	0.9885	0.9863
0.10:1	1:1	0.9865	0.9886	0.9915	0.9947	0.9951
	2:1	0.9796	0.9822	0.9864	0.9888	0.9885
	5:1	0.9685	0.9734	0.9791	0.9817	0.9794
	10:1	0.9556	0.9621	0.9700	0.9712	0.9673
0.20:1	1:1	0.9733	0.9760	0.9827	0.9889	0.9903
	2:1	0.9606	0.9656	0.9725	0.9775	0.9764
	5:1	0.9375	0.9467	0.9572	0.9644	0.9607
	10:1	0.9111	0.9239	0.9376	0.9438	0.9337

Table C3 The degree of mixedness of B particles in the case of normal - uniform dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Degree of mixedness of B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.9992	0.9992	0.9985	0.9977	0.9972
	2:1	0.9986	0.9983	0.9976	0.9963	0.9955
	5:1	0.9982	0.9978	0.9961	0.9940	0.9924
	10:1	0.9978	0.9970	0.9945	0.9909	0.9865
0.04:1	1:1	0.9985	0.9983	0.9972	0.9956	0.9943
	2:1	0.9968	0.9969	0.9951	0.9924	0.9908
	5:1	0.9965	0.9956	0.9925	0.9885	0.9852
	10:1	0.9956	0.9939	0.9888	0.9827	0.9778
0.10:1	1:1	0.9962	0.9958	0.9933	0.9887	0.9852
	2:1	0.9929	0.9918	0.9880	0.9816	0.9763
	5:1	0.9911	0.9892	0.9818	0.9711	0.9620
	10:1	0.9889	0.9854	0.9738	0.9596	0.9445
0.20:1	1:1	0.9930	0.9918	0.9854	0.9765	0.9715
	2:1	0.9860	0.9838	0.9761	0.9638	0.9554
	5:1	0.9827	0.9783	0.9645	0.9451	0.9250
	10:1	0.9781	0.9721	0.9513	0.9226	0.8906

Table C4 The degree of mixedness of B particles in the case of normal - normal dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Degree of mixedness of B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.9973	0.9972	0.9972	0.9970	0.9968
	2:1	0.9962	0.9960	0.9962	0.9958	0.9956
	5:1	0.9936	0.9935	0.9934	0.9928	0.9925
	10:1	0.9910	0.9910	0.9905	0.9896	0.9890
0.04:1	1:1	0.9943	0.9944	0.9945	0.9943	0.9942
	2:1	0.9923	0.9922	0.9921	0.9916	0.9911
	5:1	0.9873	0.9871	0.9868	0.9861	0.9852
	10:1	0.9823	0.9819	0.9810	0.9794	0.9779
0.10:1	1:1	0.9864	0.9867	0.9857	0.9854	0.9849
	2:1	0.9806	0.9801	0.9799	0.9798	0.9780
	5:1	0.9686	0.9678	0.9668	0.9652	0.9624
	10:1	0.9557	0.9553	0.9535	0.9496	0.9447
0.20:1	1:1	0.9727	0.9726	0.9721	0.9752	0.9720
	2:1	0.9610	0.9604	0.9603	0.9589	0.9593
	5:1	0.9365	0.9365	0.9344	0.9298	0.9285
	10:1	0.9116	0.9110	0.9078	0.9032	0.8952

Table C5 The normalized count-based fractal dimension of B particles  
in the case of uniform - uniform dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized count-based fractal dimension of B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	1.0029	1.0006	0.9857	0.9563	0.9102
	2:1	0.9994	0.9970	0.9801	0.9487	0.9350
	5:1	0.9999	0.9978	0.9856	0.9429	0.9396
	10:1	0.9991	0.9981	0.9876	0.9446	0.9358
0.04:1	1:1	0.9978	0.9969	0.9842	0.9559	0.9411
	2:1	1.0007	0.9966	0.9867	0.9483	0.9361
	5:1	0.9996	0.9978	0.9837	0.9499	0.9373
	10:1	1.0002	0.9980	0.9866	0.9566	0.9411
0.10:1	1:1	0.9981	0.9960	0.9939	0.9580	0.9159
	2:1	0.9977	0.9987	0.9825	0.9493	0.9360
	5:1	1.0001	0.9977	0.9918	0.9493	0.9369
	10:1	0.9999	0.9979	0.9894	0.9577	0.9385
0.20:1	1:1	1.0012	0.9953	0.9849	0.9644	0.9341
	2:1	0.9971	0.9961	0.9823	0.9527	0.9335
	5:1	1.0003	0.9977	0.9884	0.9564	0.9462
	10:1	1.0002	0.9983	0.9912	0.9665	0.9417

Table C6 The normalized count-based fractal dimension of B particles  
in the case of uniform - normal dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized count-based fractal dimension of B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.8288	0.8614	0.9064	0.9371	0.9170
	2:1	0.8460	0.8832	0.9209	0.9668	0.9364
	5:1	0.8670	0.9172	0.9289	0.9459	0.9390
	10:1	0.8933	0.9271	0.9274	0.9326	0.9368
0.04:1	1:1	0.8250	0.8715	0.9220	0.9448	0.9155
	2:1	0.8409	0.8799	0.9186	0.9645	0.9409
	5:1	0.8674	0.9146	0.9281	0.9485	0.9417
	10:1	0.8923	0.9236	0.9296	0.9333	0.9392
0.10:1	1:1	0.8333	0.8726	0.9232	0.9406	0.9211
	2:1	0.8344	0.8905	0.9256	0.9699	0.9449
	5:1	0.8687	0.9180	0.9333	0.9480	0.9467
	10:1	0.8936	0.9316	0.9298	0.9370	0.9425
0.20:1	1:1	0.8241	0.8638	0.9212	0.9345	0.9366
	2:1	0.8377	0.8956	0.9224	0.9349	0.9460
	5:1	0.8729	0.9198	0.9302	0.9230	0.9440
	10:1	0.8902	0.9315	0.9327	0.9421	0.9433



Table C7 The normalized count-based fractal dimension of B particles  
in the case of normal - uniform dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized count-based fractal dimension of B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.9963	0.9912	0.9483	0.8695	0.7883
	2:1	1.0000	0.9910	0.9636	0.8755	0.7828
	5:1	1.0000	0.9960	0.9766	0.9114	0.7759
	10:1	0.9993	0.9975	0.9838	0.9271	0.7871
0.04:1	1:1	0.9938	0.9888	0.9635	0.8641	0.7864
	2:1	1.0000	0.9954	0.9641	0.8774	0.7743
	5:1	0.9999	0.9971	0.9758	0.9119	0.7833
	10:1	0.9999	0.9979	0.9847	0.9296	0.7770
0.10:1	1:1	1.0051	0.9939	0.9602	0.8675	0.7725
	2:1	1.0000	0.9896	0.9663	0.8825	0.7906
	5:1	1.0006	0.9958	0.9795	0.9201	0.7805
	10:1	0.9998	0.9974	0.9868	0.9439	0.7852
0.20:1	1:1	0.9971	0.9927	0.9566	0.8604	0.7844
	2:1	1.0000	0.9907	0.9606	0.8874	0.8012
	5:1	0.9990	0.9969	0.9800	0.9252	0.7828
	10:1	1.0000	0.9987	0.9891	0.9573	0.7965

Table C8 The normalized count-based fractal dimension of B particles  
in the case of normal - normal dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized count-based fractal dimension of B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.8247	0.8199	0.8086	0.7912	0.7642
	2:1	0.8515	0.8332	0.8255	0.7965	0.7761
	5:1	0.8745	0.8645	0.8446	0.8058	0.7783
	10:1	0.8941	0.8862	0.8614	0.8154	0.7767
0.04:1	1:1	0.8275	0.8105	0.8020	0.7922	0.7817
	2:1	0.8430	0.8365	0.8282	0.7908	0.7795
	5:1	0.8733	0.8636	0.8486	0.8103	0.7817
	10:1	0.8964	0.8881	0.8662	0.8226	0.7897
0.10:1	1:1	0.8262	0.8183	0.8014	0.7956	0.7713
	2:1	0.8398	0.8335	0.8214	0.7979	0.7687
	5:1	0.8738	0.8657	0.8460	0.8113	0.7762
	10:1	0.8935	0.8867	0.8673	0.8260	0.7809
0.20:1	1:1	0.8256	0.8128	0.7975	0.7905	0.7865
	2:1	0.8411	0.8381	0.8239	0.8054	0.7938
	5:1	0.8690	0.8650	0.8501	0.8210	0.7956
	10:1	0.8922	0.8884	0.8714	0.8423	0.8002

Table C9 The normalized count-based fractal dimension of A plus B particles in the case of uniform - uniform dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized count-based fractal dimension of A plus B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	1.0747	1.0734	1.0603	1.0434	1.0111
	2:1	1.0278	1.0215	1.0042	0.9741	0.9643
	5:1	1.0063	1.0020	0.9875	0.9446	0.9413
	10:1	1.0008	0.9987	0.9878	0.9447	0.9358
0.04:1	1:1	1.0778	1.0726	1.0593	1.0333	1.0122
	2:1	1.0310	1.0239	1.0076	0.9730	0.9640
	5:1	1.0061	1.0016	0.9897	0.9468	0.9388
	10:1	1.0016	0.9984	0.9868	0.9466	0.9411
0.10:1	1:1	1.0751	1.0704	1.0611	1.0283	1.0096
	2:1	1.0294	1.0246	1.0059	0.9733	0.9640
	5:1	1.0051	1.0008	0.9886	0.9500	0.9362
	10:1	1.0014	0.9982	0.9895	0.9529	0.9404
0.20:1	1:1	1.0777	1.0679	1.0599	1.0274	1.0091
	2:1	1.0283	1.0228	1.0058	0.9740	0.9709
	5:1	1.0055	1.0014	0.9849	0.9576	0.9467
	10:1	1.0016	0.9988	0.9913	0.9665	0.9417

Table C10 The normalized count-based fractal dimension of A plus B particles in the case of uniform - normal dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized count-based fractal dimension of A plus B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	1.0488	1.0433	1.0420	1.0335	1.0066
	2:1	0.9968	0.9815	0.9781	0.9948	0.9624
	5:1	0.9465	0.9476	0.9372	0.9483	0.9400
	10:1	0.9404	0.9349	0.9284	0.9327	0.9368
0.04:1	1:1	1.0463	1.0463	1.0409	1.0346	1.0084
	2:1	0.9866	0.9796	0.9694	0.9888	0.9679
	5:1	0.9475	0.9461	0.9367	0.9503	0.9429
	10:1	0.9396	0.9388	0.9306	0.9336	0.9393
0.10:1	1:1	1.0438	1.0466	1.0444	1.0298	1.0112
	2:1	0.9871	0.9813	0.9761	0.9952	0.9675
	5:1	0.9486	0.9477	0.9400	0.9497	0.9468
	10:1	0.9404	0.9389	0.9304	0.9370	0.9425
0.20:1	1:1	1.0474	1.0468	1.0410	1.0338	1.0135
	2:1	0.9870	0.9855	0.9761	0.9615	0.9663
	5:1	0.9515	0.9497	0.9381	0.9245	0.9451
	10:1	0.9400	0.9398	0.9307	0.9422	0.9433

Table C11 The normalized count-based fractal dimension of A plus B particles in the case of normal - uniform dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized count-based fractal dimension of A plus B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	1.0465	1.0319	0.9929	0.9276	0.8327
	2:1	1.0065	1.0000	0.9758	0.8922	0.8020
	5:1	1.0046	0.9981	0.9778	0.9129	0.7808
	10:1	1.0008	0.9978	0.9838	0.9271	0.7871
0.04:1	1:1	1.0463	1.0329	1.0049	0.9175	0.8444
	2:1	1.0000	1.0098	0.9769	0.8952	0.8001
	5:1	1.0041	0.9990	0.9769	0.9131	0.7861
	10:1	1.0011	0.9982	0.9848	0.9297	0.7770
0.10:1	1:1	1.0517	1.0331	1.0000	0.9273	0.8355
	2:1	1.0000	1.0062	0.9778	0.8989	0.8160
	5:1	1.0043	0.9977	0.9804	0.9211	0.7809
	10:1	1.0009	0.9976	0.9868	0.9440	0.7711
0.20:1	1:1	1.0506	1.0340	0.9963	0.9172	0.8471
	2:1	1.0214	1.0052	0.9725	0.9010	0.8200
	5:1	1.0032	0.9982	0.9808	0.9259	0.7848
	10:1	1.0012	0.9980	0.9892	0.9574	0.7965

Table C12 The normalized count-based fractal dimension of A plus B particles in the case of normal - normal dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized count-based fractal dimension of A plus B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.8944	0.8866	0.8800	0.8555	0.8398
	2:1	0.8791	0.8659	0.8480	0.8132	0.8093
	5:1	0.8864	0.8717	0.8485	0.8082	0.7792
	10:1	0.9001	0.8882	0.8617	0.8157	0.7767
0.04:1	1:1	0.8978	0.8795	0.8789	0.8651	0.8450
	2:1	0.8758	0.8716	0.8549	0.8184	0.8000
	5:1	0.8845	0.8720	0.8519	0.8126	0.7870
	10:1	0.9016	0.8898	0.8665	0.8229	0.7900
0.10:1	1:1	0.8946	0.8860	0.8633	0.8589	0.8362
	2:1	0.8692	0.8646	0.8452	0.8244	0.7971
	5:1	0.8864	0.8744	0.8492	0.8147	0.7777
	10:1	0.8988	0.8888	0.8677	0.8257	0.7809
0.20:1	1:1	0.9012	0.8859	0.8773	0.8509	0.8344
	2:1	0.8753	0.8648	0.8490	0.8232	0.8159
	5:1	0.8830	0.8704	0.8540	0.8217	0.7967
	10:1	0.8989	0.8905	0.8717	0.8423	0.7851

Table C13 The normalized area-based fractal dimension of B particles in the case of uniform - uniform dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized area-based fractal dimension of B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.9974	0.9953	0.9845	0.9810	0.9718
	2:1	1.0035	0.9961	0.9759	0.9750	0.9587
	5:1	0.9998	0.9868	0.9650	0.9542	0.9463
	10:1	0.9977	0.9809	0.9627	0.9436	0.9309
0.04:1	1:1	0.9997	1.0097	0.9896	0.9817	0.9765
	2:1	1.0194	1.0044	0.9821	0.9684	0.9488
	5:1	1.0181	0.9956	0.9773	0.9544	0.9437
	10:1	1.0060	0.9879	0.9703	0.9391	0.9240
0.10:1	1:1	0.9992	1.0040	0.9870	0.9715	0.9655
	2:1	0.9979	0.9948	0.9696	0.9581	0.9491
	5:1	1.0099	0.9852	0.9745	0.9434	0.9310
	10:1	0.9954	0.9680	0.9474	0.9215	0.9023
0.20:1	1:1	1.0086	1.0009	0.9819	0.9738	0.9544
	2:1	1.0000	0.9880	0.9709	0.9562	0.9518
	5:1	1.0179	0.9709	0.9661	0.9536	0.9172
	10:1	1.0030	0.9693	0.9386	0.9106	0.9089

Table C14 The normalized area-based fractal dimension of B particles in the case of uniform - normal dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized area-based fractal dimension of B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.5926	0.6379	0.8007	0.9262	0.9767
	2:1	0.3897	0.4912	0.7466	0.9247	0.9402
	5:1	0.2245	0.3007	0.6091	0.8867	0.9458
	10:1	0.1289	0.2089	0.5220	0.8727	0.9606
0.04:1	1:1	0.5680	0.6558	0.7900	0.9636	0.9658
	2:1	0.4219	0.4820	0.7109	0.8865	0.9672
	5:1	0.2151	0.3016	0.5788	0.8640	0.9424
	10:1	0.1230	0.1989	0.5326	0.8806	0.9411
0.10:1	1:1	0.5681	0.6586	0.7991	0.9484	0.9685
	2:1	0.4157	0.4927	0.7230	0.9109	0.9641
	5:1	0.2185	0.3043	0.5814	0.8681	0.9510
	10:1	0.1252	0.1958	0.4793	0.8244	0.9491
0.20:1	1:1	0.5824	0.6526	0.8134	0.8979	0.9730
	2:1	0.3884	0.5110	0.6702	0.8926	0.9299
	5:1	0.2198	0.2993	0.5305	0.8676	0.9375
	10:1	0.1297	0.1899	0.4110	0.7769	0.9366

Table C15 The normalized area-based fractal dimension of B particles normal - uniform dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized area-based fractal dimension of B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.9929	0.9659	0.8471	0.7412	0.6602
	2:1	1.0144	0.8865	0.7876	0.6467	0.6020
	5:1	1.0023	0.8325	0.6566	0.5554	0.5361
	10:1	1.0019	0.7490	0.6123	0.5139	0.4894
0.04:1	1:1	0.9956	0.9681	0.8618	0.7464	0.6648
	2:1	0.9887	0.9435	0.7840	0.6474	0.5713
	5:1	0.9952	0.8347	0.6464	0.5683	0.5259
	10:1	0.9966	0.7150	0.5709	0.5162	0.4941
0.10:1	1:1	1.0088	0.9699	0.8757	0.6968	0.6412
	2:1	1.0041	0.9048	0.7854	0.6383	0.5653
	5:1	0.9986	0.8530	0.6650	0.5332	0.4970
	10:1	0.9957	0.7395	0.5849	0.5024	0.4650
0.20:1	1:1	1.0142	0.9560	0.8531	0.6824	0.6413
	2:1	1.0089	0.9133	0.7763	0.5914	0.5701
	5:1	1.0210	0.8342	0.6522	0.5306	0.4802
	10:1	1.0043	0.7817	0.5794	0.4828	0.4759

Table C16 The normalized area-based fractal dimension of B particles in the case of normal - normal dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized area-based fractal dimension of B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.5558	0.5644	0.5863	0.6352	0.6426
	2:1	0.4093	0.4213	0.4566	0.5272	0.5785
	5:1	0.2160	0.2311	0.3184	0.4463	0.5369
	10:1	0.1213	0.1533	0.2695	0.4092	0.4990
0.04:1	1:1	0.5684	0.5495	0.6099	0.6304	0.6605
	2:1	0.4119	0.4284	0.4567	0.5174	0.5779
	5:1	0.2195	0.2305	0.3119	0.4589	0.5408
	10:1	0.1317	0.1500	0.2640	0.3947	0.4943
0.10:1	1:1	0.5827	0.5884	0.5679	0.6058	0.6597
	2:1	0.3976	0.3991	0.4453	0.5359	0.5508
	5:1	0.2229	0.2260	0.3085	0.4558	0.4957
	10:1	0.1268	0.1424	0.2331	0.3735	0.4539
0.20:1	1:1	0.5733	0.5685	0.5762	0.6008	0.6394
	2:1	0.4148	0.4039	0.4269	0.5063	0.5690
	5:1	0.2168	0.2325	0.3023	0.3736	0.4996
	10:1	0.1287	0.1441	0.2170	0.3491	0.4650

Table C17 The normalized area-based fractal dimension of A plus B particles in the case of uniform - uniform dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized area-based fractal dimension of A plus B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	1.0161	1.0095	1.0149	0.9931	1.0153
	2:1	1.0047	0.9905	0.9906	1.0160	1.0081
	5:1	1.0032	1.0077	0.9974	1.0002	1.0010
	10:1	0.9990	0.9959	1.0046	0.9918	0.9832
0.04:1	1:1	1.0220	1.0186	1.0044	1.0205	1.0156
	2:1	0.9982	1.0096	0.9928	1.0066	1.0119
	5:1	1.0215	1.0062	1.0165	1.0045	1.0018
	10:1	1.0065	1.0047	0.9984	0.9877	0.9816
0.10:1	1:1	0.9982	1.0085	1.0054	0.9950	0.9931
	2:1	1.0094	1.0066	1.0072	0.9956	0.9971
	5:1	1.0056	1.0000	0.9967	0.9873	0.9858
	10:1	1.0016	0.9900	0.9843	0.9782	0.9770
0.20:1	1:1	1.0080	1.0047	1.0091	1.0000	0.9871
	2:1	1.0118	1.0150	0.9894	0.9969	0.9857
	5:1	1.0055	1.0026	0.9984	0.9940	0.9780
	10:1	1.0065	0.9903	0.9790	0.9720	0.9599

Table C18 The normalized area-based fractal dimension of A plus B particles in the case of uniform - normal dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized area-based fractal dimension of A plus B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.9975	0.9965	0.9926	1.0103	0.9851
	2:1	1.0058	1.0082	1.0188	1.0118	1.0017
	5:1	0.9997	1.0257	1.0176	1.0228	1.0158
	10:1	1.0181	1.0263	1.0210	0.9930	1.0257
0.04:1	1:1	0.9857	1.0011	1.0298	1.0051	1.0178
	2:1	1.0016	0.9882	0.9931	0.9842	1.0099
	5:1	1.0084	1.0143	1.0013	0.9962	1.0059
	10:1	0.9859	1.0128	1.0197	1.0226	0.9905
0.10:1	1:1	0.9788	0.9971	1.0364	1.0032	1.0044
	2:1	1.0130	1.0167	1.0070	1.0206	1.0188
	5:1	1.0093	1.0052	0.9997	1.0150	1.0216
	10:1	0.9920	0.9900	0.9817	0.9781	0.9921
0.20:1	1:1	0.9954	1.0038	0.9860	1.0112	1.0043
	2:1	0.9918	0.9771	0.9944	0.9918	1.0119
	5:1	0.9708	1.0076	0.9640	0.9881	0.9869
	10:1	0.8257	0.8550	0.9173	0.9684	0.9758

Table C19 The normalized area-based fractal dimension of A plus B particles in the case of normal - uniform dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized area-based fractal dimension of A plus B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.5733	0.5498	0.5356	0.5764	0.5893
	2:1	0.5520	0.5789	0.5816	0.5767	0.5717
	5:1	0.5421	0.5312	0.5600	0.5567	0.5586
	10:1	0.5837	0.5627	0.5875	0.5415	0.5696
0.04:1	1:1	0.5702	0.5861	0.5559	0.5689	0.5569
	2:1	0.5670	0.5722	0.5600	0.5562	0.5520
	5:1	0.5630	0.5723	0.5748	0.5673	0.5504
	10:1	0.5965	0.5598	0.5503	0.5581	0.5723
0.10:1	1:1	0.5484	0.5771	0.5826	0.5779	0.5684
	2:1	0.5611	0.5574	0.5640	0.5487	0.5587
	5:1	0.5837	0.5716	0.5591	0.5309	0.5319
	10:1	0.5445	0.5591	0.5444	0.5643	0.5438
0.20:1	1:1	0.5625	0.5677	0.5548	0.5586	0.5694
	2:1	0.5557	0.5391	0.5608	0.5478	0.5684
	5:1	0.5572	0.5676	0.5562	0.5597	0.5384
	10:1	0.5802	0.5780	0.5355	0.5172	0.5294

Table C20 The normalized area-based fractal dimension of A plus B particles in the case of normal - normal dispersion at various conditions.

Particle size ratio (B:A)	Concentration ratio (B:A)	Normalized area-based fractal dimension of A plus B particles				
		Adhesion probability				
		0%	20%	50%	80%	100%
0.02:1	1:1	0.5252	0.5622	0.5549	0.5736	0.5610
	2:1	0.5601	0.5596	0.5534	0.5675	0.5521
	5:1	0.5544	0.5440	0.5724	0.5637	0.5718
	10:1	0.5621	0.5266	0.5863	0.5619	0.5716
0.04:1	1:1	0.5481	0.5674	0.5570	0.5875	0.5370
	2:1	0.5522	0.5635	0.5668	0.5737	0.5656
	5:1	0.5767	0.5637	0.5679	0.5747	0.5831
	10:1	0.5655	0.5467	0.5520	0.5565	0.5581
0.10:1	1:1	0.5979	0.5593	0.5349	0.5610	0.5774
	2:1	0.5300	0.5524	0.5485	0.5532	0.5487
	5:1	0.5245	0.5540	0.5181	0.5439	0.5299
	10:1	0.5346	0.5203	0.5353	0.5419	0.5307
0.20:1	1:1	0.5669	0.5610	0.5660	0.5679	0.5644
	2:1	0.5240	0.5312	0.5457	0.5679	0.5636
	5:1	0.4908	0.5052	0.5288	0.5361	0.5598
	10:1	0.4193	0.4303	0.4520	0.5087	0.5457

## APPENDIX D

### EXAMPLE OF CALCULATION THE QUANTITATIVE INDICES

#### D.1 Degree of mixedness

Degree of mixedness for the ideal case of uniform random dispersion obtained from computer-simulated result for the concentration of 5000 particles is calculated as following.

$$\text{From } M = 1 - \frac{\sigma_s}{\sigma_o}$$

$$\text{Here } \sigma_s = 0.0432$$

$$\sigma_o^2 = \bar{x}(1 - \bar{x}) = 0.0982(1 - 0.0982)$$

$$\begin{aligned} \text{Thus } M &= 1 - (0.0432/0.2975) \\ &= 0.8549 \end{aligned}$$

#### D.2 Count-based fractal dimension

Here is an example of the calculation of count-based fractal dimension for the ideal case of uniform random dispersion. The table and plot below shows the relationship between  $N(n)$  and  $1/n$  obtained from simulation result for the concentration of 5000 particles.

$$\text{From } F_c = \frac{-\text{Log}N(n)}{\text{Log}(1/n)}$$

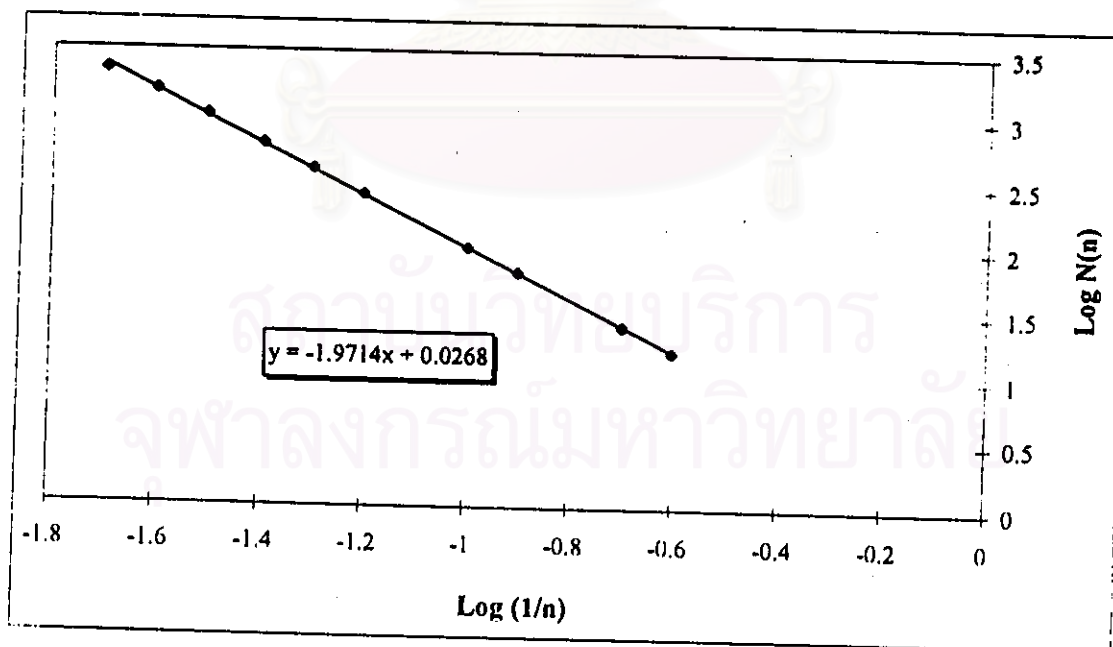
The count-based fractal dimension was obtained by linear regression from the portion of the most numerous observe data lying on the same straight line.



Thus  $F_c = 1.9714$

n	1/n	N(n)
4	0.25000	16
5	0.20000	25
8	0.12500	64
10	0.10000	100
16	0.06250	256
20	0.05000	400
25	0.04000	625
32	0.03125	1020
40	0.02500	1541
50	0.02000	2182

Plotting the relationship between  $\log(N(n))$  and  $\log(1/n)$



### D.3 Area-based fractal dimension

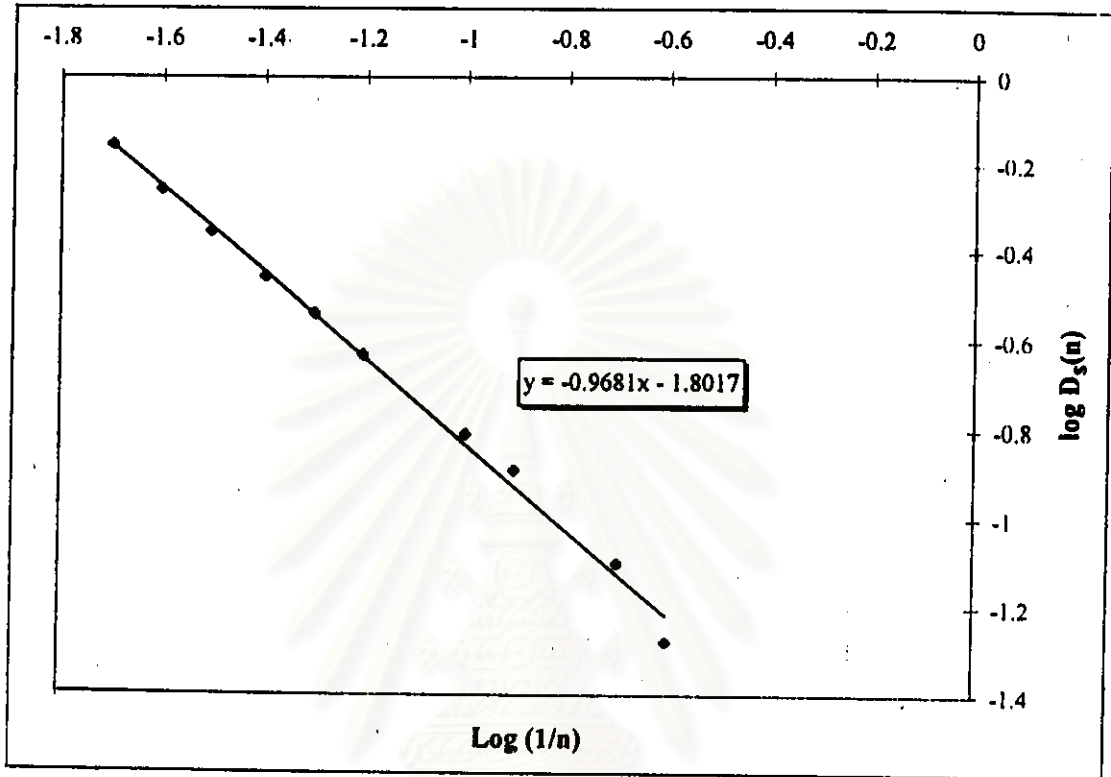
In the case of area-based fractal dimension for ideal case of the uniform random dispersion, plotting the relationship between coefficient of variation ( $D_s(n)$ ) and the similarity ratio ( $1/n$ ) (concentration of 5000 particles) gives the following table and figure.

n	1/n	$D_s(n)$
4	0.25000	0.0525
5	0.20000	0.0794
8	0.12500	0.1286
10	0.10000	0.1548
16	0.06250	0.2328
20	0.05000	0.2879
25	0.04000	0.3477
32	0.03125	0.4397
40	0.02500	0.5506
50	0.02000	0.6981

From chapter 3, 
$$F_A = \frac{-\text{Log}D_s(n)}{\text{Log}(1/n)}$$

In the same way, the area-based fractal dimension can be obtained by linear regression to be

$$F_A = 0.9681$$



#### D.4 Coordination number

##### D.4.1 Mean

In binary additive system, a number of adhering particles which adhere onto core particles can be calculated as follow.

Concentration ratio :	10:1
observe adhesion probability :	74.66%

From Mean = Concentration ratio x observed adhesion probability

$$= 10 \times 0.7466$$

$$= 7.466$$

Thus Coordination number = 7.466

#### D.4.2 Mode

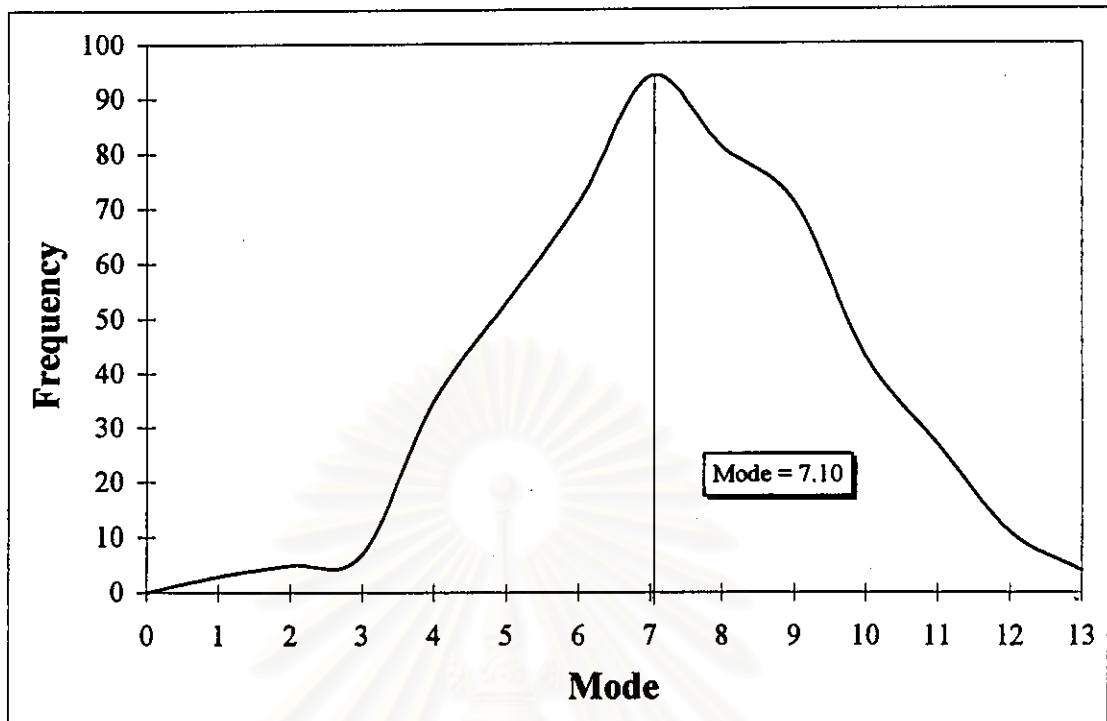
In the case of coordination number obtained by mode for binary additive system, The table and plot below show the relationship between mode and number of adhering particles obtained from the simulation result for the concentration of adhering particles of 5000 particles and 80% adhesion.

Mode	Number of adhering particles
0	0
1	3
2	5
3	7
4	35
5	53
6	71
7	94
8	81
9	71
10	43
11	27
12	11
13	4

The mode was obtained from the most number of adhering particles position.

Thus Mode = 7.10

Coordination number = 7.10



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## APPENDIX E

### CRITERIA USED IN SELECTING THE SUITABLE QUANTITATIVE INDICES

#### E.1 Single additive systems

The main interest here is the quantitative evaluation of the state of dispersion in single or binary additive systems so that samples obtained under different conditions and/or different processes can be compared. The criteria used in selecting the suitable quantitative indexes in the single additive systems are as follows:

1. The suitable index can clearly characterize the type of dispersion as ideal uniform, ideal normal or nonideal and show a large difference in values between the two ideal cases.
2. The suitable index should not be influenced by the particle size since the additive is often polydisperse in size. Ideally it should also be independent of the particle concentration as long as there is a sufficiently large number of particles for analysis.

The trends of the relationships between either factor (the concentration or particle size) and the quantitative indexes ( the degree of mixedness, the count-based and the area-based fractal dimensions) for both ideal uniform and normal random dispersions is described in the following table.

	Concentration		Particle size	
	Uniform	Normal	Uniform	Normal
M	**	**	—	—
F <sub>C</sub>	+	+	0	0
F <sub>A</sub>	0	—	0	0

The symbols in this table are defined as follows:

- \*\* It fails to distinguish between the ideal cases when the particle size is tiny.
- + The value of index tends to increase when the factor increases.
- The value of index tends to decrease when the factor increases.
- 0 The value of index is essentially constant when the factor changes.

It may be concluded that the degree of mixedness is not suitable at all when the particle size is tiny, though it is slightly affected by the concentration when the particle size is big.

The count-based and area-based fractal dimensions are suitable indexes because they do not depend on the particle size and are only affected somewhat by the concentration. The drawback can be minimized by using the normalized fractal dimensions. In fact, the area-based fractal dimension is the most suitable.

## **E.2 Binary additive systems**

The criteria used in selecting the suitable indexes for the A particles in the binary additive systems are the same as the case of the single additive systems. The criteria used in selecting the suitable quantitative indexes for the B particles or A plus B particles in the binary additive systems are as follows:

1. The suitable index can clearly characterize the type of dispersion as ideal uniform, ideal normal or nonideal and show a large difference in values between the two ideal cases.
2. The suitable index should not be influenced by the B : A particle size ratio. Ideally it should also independent of the B : A concentration ratio as long as a sufficiently large number of particles is present.

3. Furthermore, the index should contain as much information as possible on the adhesion probability of B on A.

The trends of the relationships between each factor (the adhesion probability, the B : A concentration ratio and the B : A particle size ratio) and the quantitative indexes ( the degree of mixedness of B particles, the normalized count-based and area-based fractal dimensions and the coordination number) for the four combinations of ideal dispersion are described in the following table.

		Adhesion probability				Concentration ratio				Particle size ratio			
		UU	UN	NU	NN	UU	UN	NU	NN	UU	UN	NU	NN
M	B	**	**	**	**	**	**	**	**	—	—	—	—
$F_C^*$	B	—	+	—	—	+	+	+	+	0	0	0	0
	A+B	—	■	—	—	—	—	—	—	0	0	0	0
$F_A^*$	B	—	+	—	—	—	—	—	—	0	0	0	0
	A+B	*	*	*	*	*	*	*	*	*	*	*	*
CO.	Mean	+	+	+	+	×	×	×	×	×	×	×	×
	Mode	+	+	+	+	×	×	×	×	×	×	×	×

The symbols in this table are defined as follows:

UU Uniform A - uniform B random dispersion

UN Uniform A - normal B random dispersion

NU Normal A - uniform B random dispersion

NN Normal A - normal B random dispersion

■ It is rather confusing to estimate the adhesion probability from the index.



- \* It fails to distinguish between the dispersion type when both the B : A particle size ratio is small and the B : A concentration ratio low.
- \*\* It fails to distinguish between the dispersion type when the B : A particle size ratio is small.
- x It fails to distinguish between types of dispersions.
- + The value of index trends to increase when the factor increases.
- The value of index trends to decrease when the factor increases.
- 0 The value of index remains essentially constant when the factor changes.

As expected from its definition, coordination number can not characterize the type of dispersion of A and/or B particles nor evaluate the degree of dispersion. It is however used to double check the estimate of the adhesion probability when the A particles follow an ideal random dispersion and is needed to estimate the adhesion probability when the A particles follow some non-ideal random dispersion.

The normalized area-based fractal dimension of A plus B particles is not suitable for evaluating the degree of dispersion and characterizing the type of dispersion of the mixture. This is because each A particle has a much greater area than the B particles, so the A particles camouflage the effect shown by the B particles.

The normalized count-based fractal dimension of A plus B particles is also not the suitable index. It is found that the effect of the adhesion probability is rather confusing when A and B are of different dispersion types and different concentrations.

The degree of mixedness can not be used for evaluating the dispersion state and characterizing the dispersion type and the adhesion probability in a binary system. This is because it is a poor indicator of the adhesion probability at low B : A concentration ratio and/or small B : A particle size ratio.

Both the count-based and area-based fractal dimensions do not change when the particle size ratio increases, so they are suitable quantitative indexes for evaluating the degree of dispersion of binary additive systems. These indexes can be used together to characterize the type of dispersion and to estimate adhesion probability for the four combinations of ideal dispersions.



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