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Appendix A

Details of Programs of Physico-Chemical Mathematical Models

• Program of Physico-Chemical Mathematical Model for Brimblecombe and Spedding (1974)'s Reaction Rate, Freiberg (1974)'s Reaction Rate and Ibusuki, Ohsawa and Takeuchi (1990)'s Reaction Rate in Ammonia-Rich Environment

```
#include <stdio.h>
#include <math.h>
#include <time.h>
#include <memory.h>
#define XMAX 107
#define YMAX 80
#define ZMAX 35
#define RAND_MAX 32767 /* (2^15)-1 */
main (ac,av)
int ac;
char **av;
{
int     c1[XMAX][YMAX][ZMAX],c2[XMAX][YMAX][ZMAX],
        c3[XMAX][YMAX][ZMAX],c4[XMAX][YMAX][ZMAX],
        c5[XMAX][YMAX][ZMAX],c6[XMAX][YMAX][ZMAX],
        i,j,k,i0,j0,k0,ii,jj,kk,n,N,T,no_of_row,no_of_col,no_of_height,
        opt,no_of_quanta,no_of_time,no_of_printing,max_of_printing,sum;
float   x,x0,y,y0,z,z0,t,w,l,h,dummx,dummy,dummz,y_coeff,z_coeff,rnd,
        W,L,H,K,K_time_step,u,Hs,Vs,d,delta_h,x1,Ts,Ta,dummh,
        delta_h0,delta_h1,delta_h2,delta_h3,delta_h4,delta_h5;
FILE    *fp,*parafp;
char    fname[50],name[50];

        if ( ac != 2)
        {
                printf("No parameter file name\n");
                exit(1);
        }
        parafp = fopen(av[1],"r");
        fscanf (parafp,"%s",fname);
        fp = fopen(fname,"w");
        fprintf (fp,"The output file name is %s\n",fname);
        fscanf (parafp,"%s",name);
        fprintf (fp,"The condition of the reaction is %s\n",name);
        fscanf (parafp,"%f",&W);
        fprintf (fp,"The width of interested area (m) = %.2f\n",W);
```

```
fscanf (parafp,"%f",&L);
fprintf (fp,"The length of interested area (m) = %.2f\n",L);
fscanf (parafp,"%f",&H);
fprintf (fp,"The height of interested area (m) = %.2f\n",H);
fscanf (parafp,"%f",&w);
fprintf (fp,"The width of each cell (m) = %.2f\n",w);
fscanf (parafp,"%f",&l);
fprintf (fp,"The length of each cell (m) = %.2f\n",l);
fscanf (parafp,"%f",&h);
fprintf (fp,"The height of each cell (m) = %.2f\n",h);
fscanf (parafp,"%f",&x0);
fprintf (fp,"The location of each point source in the x-axis (m) = %.2f\n",x0);
fscanf (parafp,"%f",&y0);
fprintf (fp,"The location of each point source in the y-axis (m) = %.2f\n",y0);
fscanf (parafp,"%d",&N);
fprintf (fp,"The number of SO2 quanta in each point source = %d\n",N);
fscanf (parafp,"%f",&u);
fprintf (fp,"The velocity of wind at the stack height (m/sec) = %.2f\n",u);
fscanf (parafp,"%f",&Hs);
fprintf (fp,"The height of stack (m) = %.2f\n",Hs);
fscanf (parafp,"%f",&Vs);
fprintf (fp,"The velocity of gas (m/s) = %.3f\n",Vs);
fscanf (parafp,"%f",&d);
fprintf (fp,"The diameter of stack (m) = %.2f\n",d);
fscanf (parafp,"%f",&x1);
fprintf (fp,"The downwind distance from source (m) = %.2f\n",x1);
fscanf (parafp,"%f",&Ts);
fprintf (fp,"The temperature of stack (K) = %.2f\n",Ts);
fscanf (parafp,"%f",&Ta);
fprintf (fp,"The atmosphere temperature (K) = %.3f\n",Ta);
fscanf (parafp,"%d",&T);
fprintf (fp,"The number of time step = %d\n",T);
fscanf (parafp,"%f",&t);
fprintf (fp,"The time step (sec) = %.2f\n",t);
fscanf (parafp,"%f",&y_coeff);
fprintf (fp,"The coeff. of dispersion in the y-axis (m) = %.2f\n",y_coeff);
fscanf (parafp,"%f",&z_coeff);
fprintf (fp,"The coeff. of dispersion in the z-axis (m) = %.2f\n",z_coeff);
fscanf (parafp,"%f",&K);
fprintf (fp,"The rate constant (sec^-1 or cell/q-sec) = %.20f\n",K);
fprintf (fp,"%32s\n","Menu selection");
fprintf (fp,"\n");
fprintf (fp," 1. Brimblecombe and Spedding (1974)'s reaction rate\n");
fprintf (fp," 2. Freiberg (1974)'s reaction rate in ammonia-rich environment\n");
fprintf (fp," 3. Ibusuki et al. (1990)'s reaction rate in ammonia-rich
environment\n");
fprintf (fp,"\n");
fscanf (parafp,"%d",&opt);
fprintf (fp,"        Selection ====> %d\n",opt);
```

```
fscanf (parafp,"%2d",&max_of_printing);
fprintf (fp,"The number of printed outputs =%d\n",max_of_printing);
printf("parameters ok\n");

no_of_col     = W/w;
no_of_row     = L/l;
no_of_height  = H/h;

if ( no_of_col > XMAX || no_of_row > YMAX || no_of_height > ZMAX)
{
        fprintf(fp,"\n Range of cell error\n");
        exit(1);
}

memset(c2,'\0',sizeof(c2));
memset(c3,'\0',sizeof(c3));
memset(c5,'\0',sizeof(c5));
memset(c6,'\0',sizeof(c6));

        delta_h0        = 1.6/u;
        delta_h1        = 9.81*Vs*d*d/4;
        delta_h2        = (Ts-Ta)/Ts;
        delta_h3        = delta_h1*delta_h2;
        delta_h4        = pow(delta_h3,0.3333);
        delta_h5        = pow(x1,0.6667);
        delta_h         = delta_h0*delta_h4*delta_h5;
        fprintf(fp,"The plume rise (m) = %.3f\n",delta_h);
        z0      = Hs+delta_h;
        fprintf(fp,"The effective height (m) = %.3f\n",z0);

        i0      = (int)floor(x0/w);
        j0      = (int)floor(y0/l);
        z0      = z0/h;
        dummh           = fmod(z0,1.0);
        rnd     = 1.0*rand()/RAND_MAX;
        if (rnd >= dummh)
                k0 = (int)floor(z0);
        else
                k0 = (int)ceil(z0);

        c2[i0][j0][k0] = N;
        fprintf(fp,"c2[%d][%d][%d] = %d\n",i0,j0,k0,c2[i0][j0][k0]);

for(no_of_time=1;no_of_time<=T;no_of_time++)
{
        for(i=0;i<=no_of_col;i++)
                for (j=0;j<=no_of_row;j++)
                        for (k=0;k<=no_of_height;k++)
                {
```

```
                if(c2[i][j][k] != 0)
                c3[i][j][k] += c2[i][j][k];
                if (c5[i][j][k] !=0)
                c6[i][j][k] += c5[i][j][k];
            }

        memcpy(c1,c2,sizeof(c2));
        memset(c2,'\0',sizeof(c2));
        memcpy(c4,c5,sizeof(c5));
        memset(c5,'\0',sizeof(c5));

        /*SO2 advection and dispersions*/

        for(i=0;i<=no_of_col;i++)
            for(j=0;j<=no_of_row;j++)
                for (k=0;k<=no_of_height;k++)
    {
            for(n=1;n<=c1[i][j][k];n++)
        {
            /* SO2 point source location */
            x = i;
            y = j;
            z = k;

            /*SO2 advection*/
            x = x + (u*t)/w;
            dummx = fmod(x,1.0);
            rnd = 1.0 * rand()/RAND_MAX;
            if (rnd >= dummx)
                x = floor(x);
            else
                x = ceil(x);

            /*SO2 dispersion in the y-axis*/
loop1:      rnd = 1.0 * rand()/RAND_MAX;
            if (rnd < 0.5)
                y = y - (y_coeff/l);
            else
                if (rnd > 0.5)
                y = y + (y_coeff/l);
                else
                goto loop1;
            dummy = fmod(y,1.0);
            rnd = 1.0 * rand()/RAND_MAX;
            if (rnd >= dummy)
                y = floor(y);
            else
                y = ceil(y);
```

```
            /*SO2 dispersion in the z-axis*/
loop2:      rnd = 1.0 * rand()/RAND_MAX;
            if (rnd < 0.5)
                    z = z - (z_coeff/h);
            else
                    if (rnd > 0.5)
                    z = z + (z_coeff/h);
                    else
                    goto loop2;
            if (z < 0.0)
                    z = -z;
            dummz = fmod(z,1.0);
            rnd = 1.0 * rand()/RAND_MAX;
            if (rnd >= dummz)
                    z = floor(z);
            else
                    z = ceil(z);

            ii      =  (int)floor(x);
            jj      =  (int)floor(y);
            kk      =  (int)floor(z);

            /*SO2 to SO4 transformation*/
            switch (opt)
            {
            case 1 : /*Brimblecombe and Spedding (1974)*/
                    K_time_step = K*t;
                    rnd = 1.0 * rand()/RAND_MAX;
                    if (rnd <= K_time_step)
                    c5[ii][jj][kk] += 1 ;
                    else
                    c2[ii][jj][kk] += 1 ;
                    break;

            case 2 : /*Freiberg (1974) in ammonia-rich environment*/
                    no_of_quanta = (n*n)-((n-1)*(n-1));
                    K_time_step = K*t*no_of_quanta;
                    rnd = 1.0 * rand()/RAND_MAX;
                    if (rnd <= K_time_step)
                    c5[ii][jj][kk] += 1 ;
                    else
                    c2[ii][jj][kk] += 1 ;
                    break;

            case 3 : /*Ibusuki et al. (1990) in ammonia-rich environment*/
                    no_of_quanta = (n*n)-((n-1)*(n-1));
                    K_time_step = K*t*no_of_quanta;
                    rnd = 1.0 * rand()/RAND_MAX;
                    if (rnd <= K_time_step)
```

```
                        c5[ii][jj][kk] += 1 ;
                        else
                        c2[ii][jj][kk] += 1 ;
                        break;

                default :
                        fprintf (fp,"Out of menu\n");
                }
        }
}


        for(i=0;i<=no_of_col;i++)
                for(j=0;j<=no_of_row;j++)
                        for (k=0;k<=no_of_height;k++)
{
                for(n=1;n<=c4[i][j][k];n++)
        {

                /*SO4 Point source location */
                x = i;
                y = j;
                z = k;

                /*SO4 advection*/
                x = x + (u*t)/w;
                dummx = fmod(x,1.0);
                rnd = 1.0 * rand()/RAND_MAX;
                if (rnd >= dummx)
                        x = floor(x);
                else
                        x = ceil(x);

                /*SO4 dispersion in the y-axis*/
loop3:          rnd = 1.0 * rand()/RAND_MAX;
                if (rnd < 0.5)
                        y = y - (y_coeff/l);
                else
                        if (rnd > 0.5)
                        y = y + (y_coeff/l);
                        else
                        goto loop3;
                dummy = fmod(y,1.0);
                rnd = 1.0 * rand()/RAND_MAX;
                if (rnd >= dummy)
                        y = floor(y);
                else
                        y = ceil(y);
```

```
                    /*SO4 dispersion in the z-axis*/
    loop4:          rnd = 1.0 * rand()/RAND_MAX;
                    if (rnd < 0.5)
                            z = z - (z_coeff/h);
                    else
                            if (rnd > 0.5)
                            z = z + (z_coeff/h);
                            else
                            goto loop4;
                            if (z < 0.0)
                            z = -z;
                    dummz = fmod(z,1.0);
                    rnd = 1.0 * rand()/RAND_MAX;
                    if (rnd >= dummz)
                            z = floor(z);
                    else
                            z = ceil(z);

                    ii      =  (int)floor(x);
                    jj      =  (int)floor(y);
                    kk      =  (int)floor(z);
    if (ii >= 0 && ii < no_of_col && jj < no_of_row && kk < no_of_height)
                            c5[ii][jj][kk] += 1;
            }
    }
}

            for(i=0;i<=no_of_col;i++)
                    for (j=0;j<=no_of_row;j++)
                            for (k=0;k<=no_of_height;k++)
                    {
                            if(c2[i][j][k] != 0)
                            c3[i][j][k] += c2[i][j][k];
                            if (c5[i][j][k] !=0)
                            c6[i][j][k] += c5[i][j][k];
                    }

    /*print output data*/
  for(no_of_printing=1;no_of_printing<=max_of_printing;no_of_printing++)
{
    fscanf (parafp,"%f",&x0);
    fprintf (fp,"\nThe location in the x-axis (m) = %.2f\n",x0);
    i0 = (int)floor(x0/w);
    fprintf(fp,"\nThe number of SO2 quanta in each cell is : ");
    sum = 0;
    for(kk=no_of_height;kk>=0;kk--)
    {
                    fprintf(fp,"\n");
                    for(jj=0;jj<=no_of_row;jj++)
```

```
                {
                        fprintf(fp,"%3d ",c3[i0][jj][kk]);
                        sum += c3[i0][jj][kk];
                }
    }
    fprintf(fp,"\nThe total of  SO2 quanta are =%d\n",sum);

    sum = 0;
    fprintf(fp,"\nThe number of SO4 quanta in each cell is : ");
    for(kk=no_of_height;kk>=0;kk--)
    {
                fprintf(fp,"\n");
                for(jj=0;jj<=no_of_row;jj++)
                        {
                        fprintf(fp,"%3d ",c6[i0][jj][kk]);
                        sum += c6[i0][jj][kk];
                }
    }
    fprintf(fp,"\nThe total of  SO4 quanta is =%d\n",sum);
}
    fprintf(fp,"\n");
    fclose(fp);
    fclose(parafp);
}
```

- **Program of Physico-Chemical Mathematical Model for Freiberg (1974)'s Reaction Rate in Ammonia-Deficient Environment**

```
#include <stdio.h>
#include <math.h>
#include <time.h>
#include <memory.h>
#define XMAX 107
#define YMAX 85
#define ZMAX 35
#define RAND_MAX 32767 /* (2^15)-1 */
main (ac,av)
int ac;
char **av;
{
int     c1[XMAX][YMAX][ZMAX],c2[XMAX][YMAX][ZMAX],
        c3[XMAX][YMAX][ZMAX],c4[XMAX][YMAX][ZMAX],
        c5[XMAX][YMAX][ZMAX],c6[XMAX][YMAX][ZMAX],
        i,j,k,i0,j0,k0,ii,jj,kk,n,N,T,no_of_row,no_of_col,no_of_height,
        opt,no_of_quanta,no_of_time,no_of_printing,max_of_printing,sum;
float   x,x0,y,y0,z,z0,t,w,l,h,dummx,dummy,dummz,y_coeff,z_coeff,rnd,
        W,L,H,K,K_time_step,u,Hs,Vs,d,delta_h,x1,Ts,Ta,dummh,
        delta_h0,delta_h1,delta_h2,delta_h3,delta_h4,delta_h5,Q,NH3,sum1,
        c7[XMAX][YMAX][ZMAX],c8[XMAX][YMAX][ZMAX];
FILE    *fp,*parafp;
char    fname[50],name[50];
        if ( ac != 2)
        {
                printf("No parameter file name\n");
                exit(1);
        }
        parafp = fopen(av[1],"r");
        fscanf (parafp,"%s",fname);
        fp = fopen(fname,"w");
        fprintf (fp,"The output file name is %s\n",fname);
        fscanf (parafp,"%s",name);
        fprintf (fp,"The condition of the reaction is %s\n",name);
        fscanf (parafp,"%f",&W);
        fprintf (fp,"The width of interested area (m) = %.2f\n",W);
        fscanf (parafp,"%f",&L);
        fprintf (fp,"The length of interested area (m) = %.2f\n",L);
        fscanf (parafp,"%f",&H);
        fprintf (fp,"The height of interested area (m) = %.2f\n",H);
        fscanf (parafp,"%f",&w);
        fprintf (fp,"The width of each cell (m) = %.2f\n",w);
        fscanf (parafp,"%f",&l);
        fprintf (fp,"The length of each cell (m) = %.2f\n",l);
```

```
fscanf (parafp,"%f",&h);
fprintf (fp,"The height of each cell (m) = %.2f\n",h);
fscanf (parafp,"%f",&x0);
fprintf (fp,"The location of each point source in the x-axis (m) = %.2f\n",x0);
fscanf (parafp,"%f",&y0);
fprintf (fp,"The location of each point source in the y-axis (m) = %.2f\n",y0);
fscanf (parafp,"%d",&N);
fprintf (fp,"The number of SO2 quanta in each point source = %d\n",N);
fscanf (parafp,"%f",&Q);
fprintf (fp,"The SO2 emission rate (g/sec) = %.2f\n",Q);
fscanf (parafp,"%f",&u);
fprintf (fp,"The velocity of wind at the stack height (m/sec) = %.2f\n",u);
fscanf (parafp,"%f",&Hs);
fprintf (fp,"The height of stack (m) = %.2f\n",Hs);
fscanf (parafp,"%f",&Vs);
fprintf (fp,"The velocity of gas (m/s) = %.3f\n",Vs);
fscanf (parafp,"%f",&d);
fprintf (fp,"The diameter of stack (m) = %.2f\n",d);
fscanf (parafp,"%f",&x1);
fprintf (fp,"The downwind distance from source (m) = %.2f\n",x1);
fscanf (parafp,"%f",&Ts);
fprintf (fp,"The temperature of stack (K) = %.2f\n",Ts);
fscanf (parafp,"%f",&Ta);
fprintf (fp,"The atmosphere temperature (K) = %.3f\n",Ta);
fscanf (parafp,"%d",&T);
fprintf (fp,"The number of time step = %d\n",T);
fscanf (parafp,"%f",&t);
fprintf (fp,"The time step (sec) = %.2f\n",t);
fscanf (parafp,"%f",&y_coeff);
fprintf (fp,"The coeff. of dispersion in the y-axis (m) = %.2f\n",y_coeff);
fscanf (parafp,"%f",&z_coeff);
fprintf (fp,"The coeff. of dispersion in the z-axis (m) = %.2f\n",z_coeff);
fscanf (parafp,"%f",&NH3);
fprintf (fp,"The initial concentration of NH3 in each cell (ppb) = %.2f\n",NH3);
fscanf (parafp,"%f",&K);
fprintf (fp,"The rate constant (m^12/mol^4-sec) = %.2f\n",K);
fprintf (fp,"%32s\n","Menu selection");
fprintf (fp,"\n");
fprintf (fp," 1. Freiberg(1974)'s reaction rate in ammonia-deficient
environment\n");
fprintf (fp,"\n");
fscanf (parafp,"%d",&opt);
fprintf (fp,"          Selection ====> %d\n",opt);
fscanf (parafp,"%2d",&max_of_printing);
fprintf (fp,"The number of printed outputs =%d\n",max_of_printing);
printf("parameters ok\n");

no_of_col    = W/w;
no_of_row    = L/l;
```

```
no_of_height = H/h;

if ( no_of_col > XMAX || no_of_row > YMAX || no_of_height > ZMAX)
{
        fprintf(fp,"\n Range of cell error\n");
        exit(1);
}

memset(c2,'\0',sizeof(c2));
memset(c3,'\0',sizeof(c3));
memset(c5,'\0',sizeof(c5));
memset(c6,'\0',sizeof(c6));
memset(c7,'\0',sizeof(c7));
memset(c8,'\0',sizeof(c8));

        delta_h0        = 1.6/u;
        delta_h1        = 9.81*Vs*d*d/4;
        delta_h2        = (Ts-Ta)/Ts;
        delta_h3        = delta_h1*delta_h2;
        delta_h4        = pow(delta_h3,0.3333);
        delta_h5        = pow(x1,0.6667);
        delta_h         = delta_h0*delta_h4*delta_h5;
        fprintf(fp,"The plume rise (m) = %.3f\n",delta_h);
        z0 = Hs+delta_h;
        fprintf(fp,"The effective height (m) = %.3f\n",z0);

        i0      = (int)floor(x0/w);
        j0      = (int)floor(y0/l);
        z0      = z0/h;
        dummh           = fmod(z0,1.0);
        rnd     = 1.0*rand()/RAND_MAX;
        if (rnd >= dummh)
                k0 = (int)floor(z0);
        else
                k0 = (int)ceil(z0);

        c2[i0][j0][k0] = N;
        fprintf(fp,"c2[%d][%d][%d] = %d\n",i0,j0,k0,c2[i0][j0][k0]);

for(no_of_time=1;no_of_time<=T;no_of_time++)
{

        for(i=0;i<=no_of_col;i++)
                for (j=0;j<=no_of_row;j++)
                        for (k=0;k<=no_of_height;k++)
                {
                        if(c2[i][j][k] != 0)
                        c3[i][j][k] += c2[i][j][k];
                        if (c5[i][j][k] !=0)
```

```
                c6[i][j][k] += c5[i][j][k];
            }

    memcpy(c1,c2,sizeof(c2));
    memset(c2,'\0',sizeof(c2));
    memcpy(c4,c5,sizeof(c5));
    memset(c5,'\0',sizeof(c5));

    /*SO4 advection and dispersions*/
    for(i=0;i<=no_of_col;i++)
            for(j=0;j<=no_of_row;j++)
                    for (k=0;k<=no_of_height;k++)
{
            for(n=1;n<=c4[i][j][k];n++)
    {
            /*SO4 Point source location */
            x = i;
            y = j;
            z = k;

            /*SO4 advection*/
            x = x + (u*t)/w;
            dummx = fmod(x,1.0);
            rnd = 1.0 * rand()/RAND_MAX;
            if (rnd >= dummx)
                    x = floor(x);
            else
                    x = ceil(x);

            /*SO4 dispersion in the y-axis*/
loop3:      rnd = 1.0 * rand()/RAND_MAX;
            if (rnd < 0.5)
                    y = y - (y_coeff/l);
            else
                    if (rnd > 0.5)
                    y = y + (y_coeff/l);
                    else
                    goto loop3;

            dummy = fmod(y,1.0);
            rnd = 1.0 * rand()/RAND_MAX;
            if (rnd >= dummy)
                    y = floor(y);
            else
                    y = ceil(y);

            /*SO4 dispersion in the z-axis*/
loop4:      rnd = 1.0 * rand()/RAND_MAX;
            if (rnd < 0.5)
```

```
                        z = z - (z_coeff/h);
                else
                        if (rnd > 0.5)
                        z = z + (z_coeff/h);
                        else
                        goto loop4;
                        if (z < 0.0)
                        z = -z;
                dummz = fmod(z,1.0);
                rnd = 1.0 * rand()/RAND_MAX;
                if (rnd >= dummz)
                        z = floor(z);
                else
                        z = ceil(z);

                ii      = (int)floor(x);
                jj      = (int)floor(y);
                kk      = (int)floor(z);

if (ii >= 0 && ii < no_of_col && jj < no_of_row && kk < no_of_height)
        {
        c5[ii][jj][kk] += 1;
        if ((2*c5[ii][jj][kk]*Q*t*0.000001)/(N*64) > (NH3*0.000001)/24.5)
                {
                c5[ii][jj][kk] -= 1;
                goto loop3;
                }
        }
                c8[ii][jj][kk] = NH3-(2*c5[ii][jj][kk]*Q*t*24.5)/(N*64);
        }
}


        /*SO2 advection and dispersions*/
        for(i=0;i<=no_of_col;i++)
                for(j=0;j<=no_of_row;j++)
                        for (k=0;k<=no_of_height;k++)
{
                for(n=1;n<=c1[i][j][k];n++)
        {
                /*SO2 Point source location */
                x = i;
                y = j;
                z = k;

                /*SO2 advection*/
                x = x + (u*t)/w;
                dummx = fmod(x,1.0);
                rnd = 1.0 * rand()/RAND_MAX;
```

```
            if (rnd >= dummx)
                    x = floor(x);
            else
                    x = ceil(x);

            /*SO2 dispersion in the y-axis*/
loop1:      rnd = 1.0 * rand()/RAND_MAX;
            if (rnd < 0.5)
                    y = y - (y_coeff/l);
            else
                    if (rnd > 0.5)
                    y = y + (y_coeff/l);
                    eise
                    goto loop1;
            dummy = fmod(y,1.0);
            rnd = 1.0 * rand()/RAND_MAX;
            if (rnd >= dummy)
                    y = floor(y);
            else
                    y = ceil(y);

            /*SO2 dispersion in the z-axis*/
loop2:      rnd = 1.0 * rand()/RAND_MAX;
            if (rnd < 0.5)
                    z = z - (z_coeff/h);
            else
                    if (rnd > 0.5)
                    z = z + (z_coeff/h);
                    else
                    goto loop2;

            if (z < 0.0)
                    z = -z;
            dummz = fmod(z,1.0);
            rnd = 1.0 * rand()/RAND_MAX;
            if (rnd >= dummz)
                    z = floor(z);
            else
                    z = ceil(z);

            ii      = (int)floor(x);
            jj      = (int)floor(y);
            kk      = (int)floor(z);

            /*SO2 to SO4 transformation*/

            switch (opt)
            {
            case 1 : /*Freiberg  (1974) in ammonia-deficient environment */
```

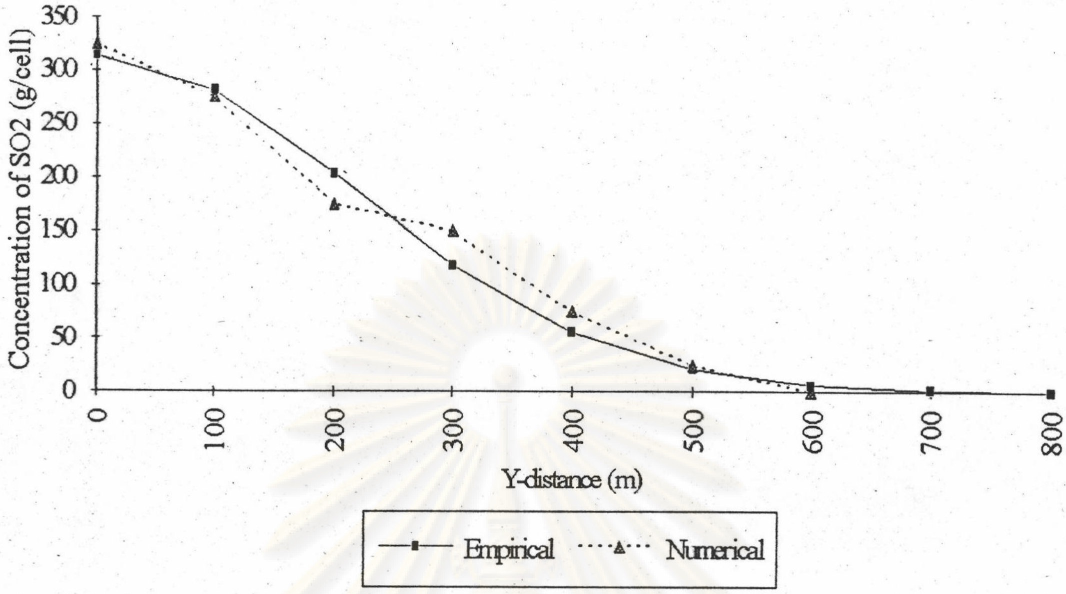
```
                              /*[NH3]t = [NH3]o - 2[SO4]*/
c7[ii][jj][kk] = ((NH3*0.000001)/24.5)-((2*c5[ii][jj][kk]*Q*t*0.000001)/(N*64));
                    if (c7[ii][jj][kk] >= ((2*c5[ii][jj][kk]*Q*t*0.000001)/(N*64)))
                              {
                              no_of_quanta = (n*n)-((n-1)*(n-1));
                              K_time_step =
(K*t*no_of_quanta*c7[ii][jj][kk]*c7[ii][jj][kk]*c7[ii][jj][kk]*Q*t*0.000001)/(64*N);
                              rnd = 1.0 * rand()/RAND_MAX;
                                        if (rnd <= K_time_step)
                                        {
                                        c5[ii][jj][kk] += 1 ;
                                        }
                                        else
                                        c2[ii][jj][kk] += 1;
                              }
                    else
                              {
          /*fprintf(fp,"\nNH3 insufficiency in c7[%d][%d][%d]\n",ii,jj,kk);*/
                              c2[ii][jj][kk] += 1 ;
                              }
                    c8[ii][jj][kk] = NH3-(2*c5[ii][jj][kk]*Q*t*24.5)/(N*64);
                              break;

                              default :
                              fprintf (fp,"Out of menu\n");
                    }
          }
     }
}


          for(i=0;i<=no_of_col;i++)
                    for (j=0;j<=no_of_row;j++)
                              for (k=0;k<=no_of_height;k++)
                    {
                              if(c2[i][j][k] != 0)
                              c3[i][j][k] += c2[i][j][k];
                              if (c5[i][j][k] !=0)
                              c6[i][j][k] += c5[i][j][k];
                    }


     /*print output data*/
   for(no_of_printing=1;no_of_printing<=max_of_printing;no_of_printing++)
{
     fscanf (parafp,"%f",&x0);
     fprintf (fp,"\nThe location in the x-axis (m) = %.2f\n",x0);
     i0 = (int)floor(x0/w);
     fprintf(fp,"\nThe number of SO2 quanta in each cell is : ");
```

```
        sum = 0;
        for(kk=no_of_height;kk>=0;kk--)
        {
                fprintf(fp,"\n");
                for(jj=0;jj<=no_of_row;jj++)
                {
                fprintf(fp,"%3d ",c3[i0][jj][kk]);
                sum += c3[i0][jj][kk];
                }
        }
        fprintf(fp,"\nThe total number of SO2 quanta is =%d\n",sum);

        sum1 = 0;
        fprintf(fp,"\nThe concentration of remaining NH3 (ppb) in each cell is : ");
        for(kk=no_of_height;kk>=0;kk--)
        {
                fprintf(fp,"\n");
                for(jj=0;jj<=no_of_row;jj++)
                {
                if(c8[i0][jj][kk] != 0)
                {
                fprintf(fp,"%7.2f ",c8[i0][jj][kk]);
                sum1 += c8[i0][jj][kk];
                }
                else
                fprintf(fp,"%7.2f ",NH3);
                }
        }
        fprintf(fp,"\nThe total concentration of remaining NH3 that reacts with SO4
(ppb) is =%.2f\n",sum1);

        sum = 0;
        fprintf(fp,"\nThe number of SO4 quanta in each cell is : ");
        for(kk=no_of_height;kk>=0;kk--)
        {
                fprintf(fp,"\n");
                for(jj=0;jj<=no_of_row;jj++)
                {
                fprintf(fp,"%3d ",c6[i0][jj][kk]);
                sum += c6[i0][jj][kk];
                }
        }
        fprintf(fp,"\nThe total number of SO4 quanta is =%d\n",sum);
}
        fprintf(fp,"\n");
        fclose(fp);
        fclose(parafp);
}
```

Appendix B

Results of Simulations

a)



b)

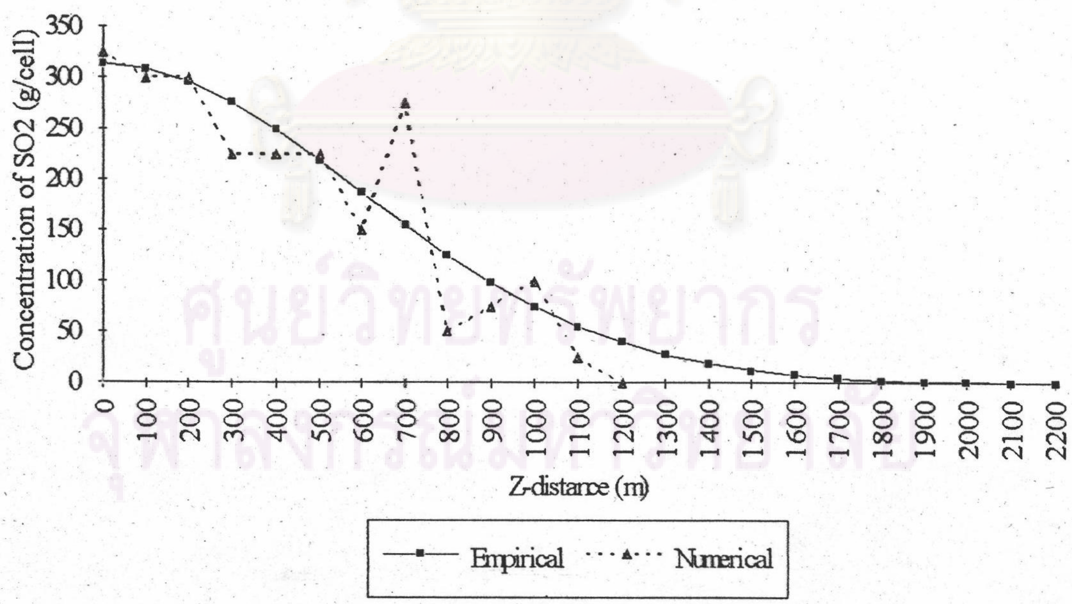
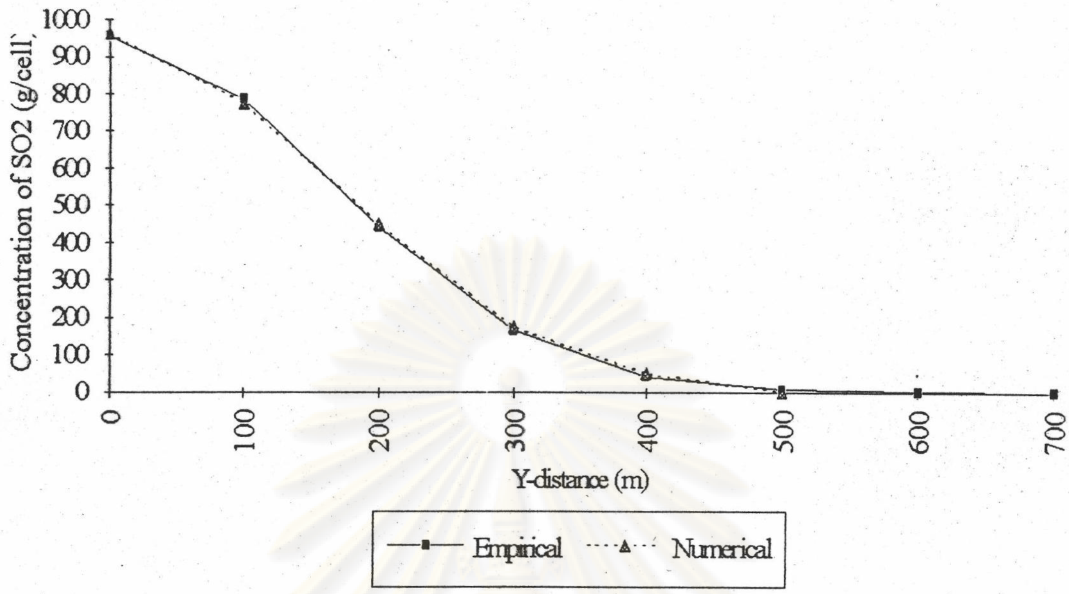


Figure 4.1 Comparison of the Empirical and Numerical Concentrations of SO_2 for Atmospheric Stability Class A at 1 km Downwind from the Source

a) Varying Y-Distance (Fixed z=0) b) Varying Z-Distance (Fixed y=0)

a)



b)

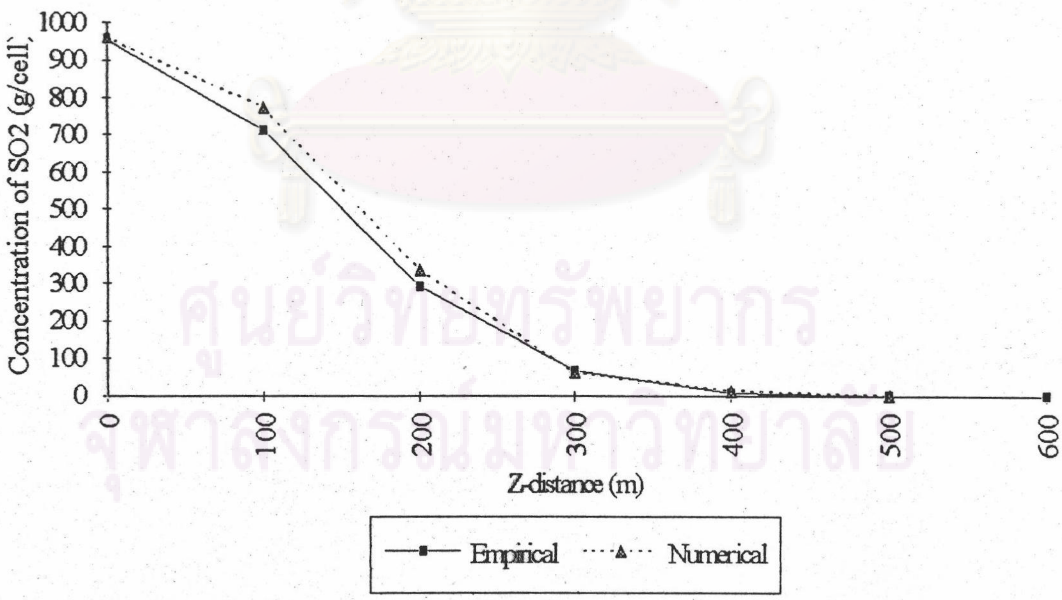
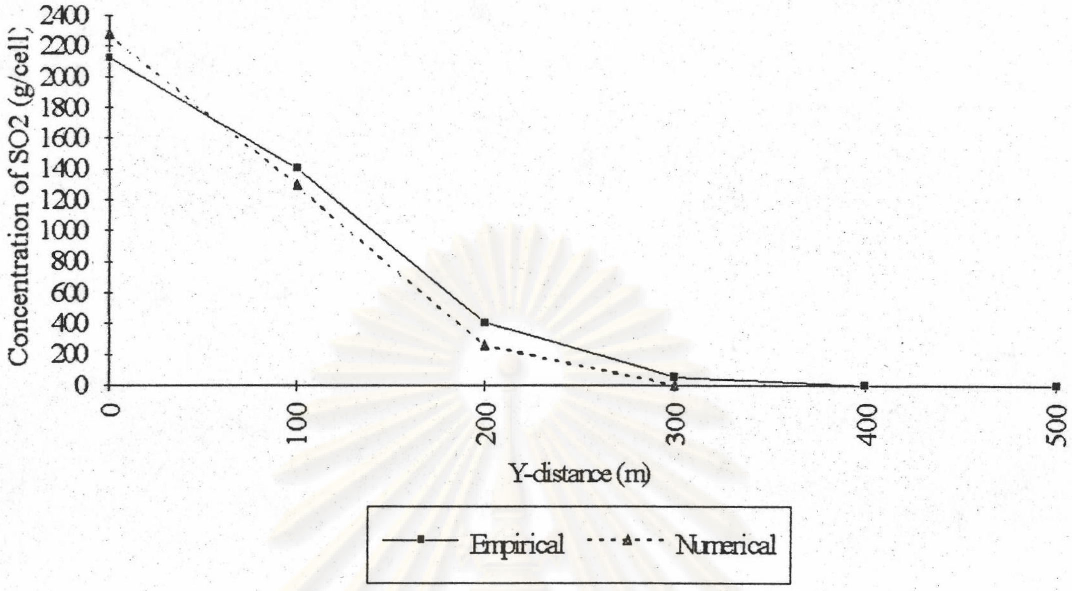


Figure 4.2 Comparison of the Empirical and Numerical Concentrations of SO_2 for Atmospheric Stability Class B at 1 km Downwind from the Source

a) Varying Y-Distance (Fixed z=0) b) Varying Z-Distance (Fixed y=0)

a)



b)

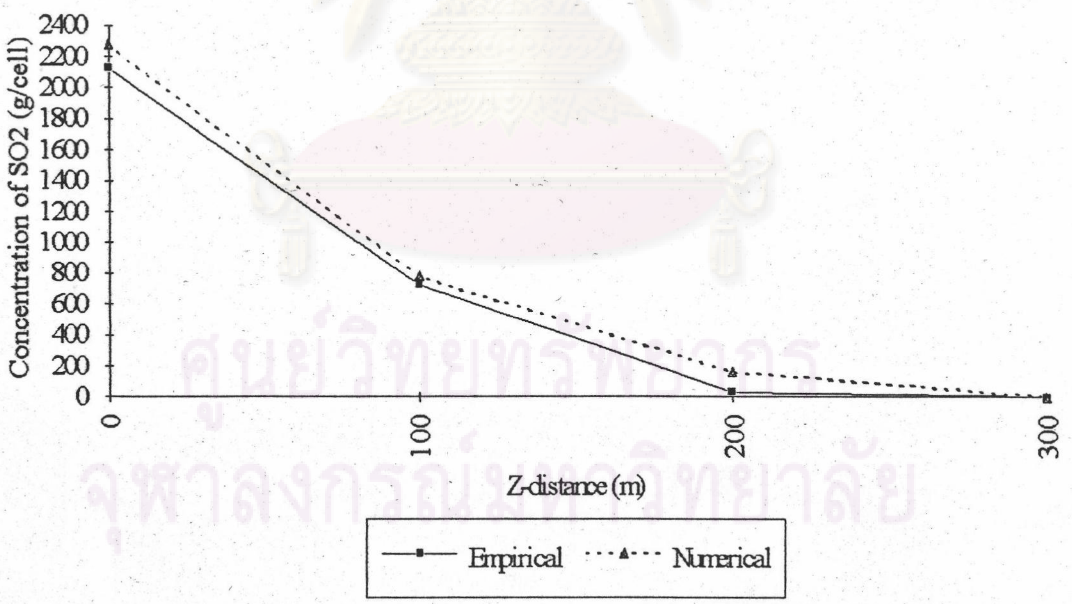
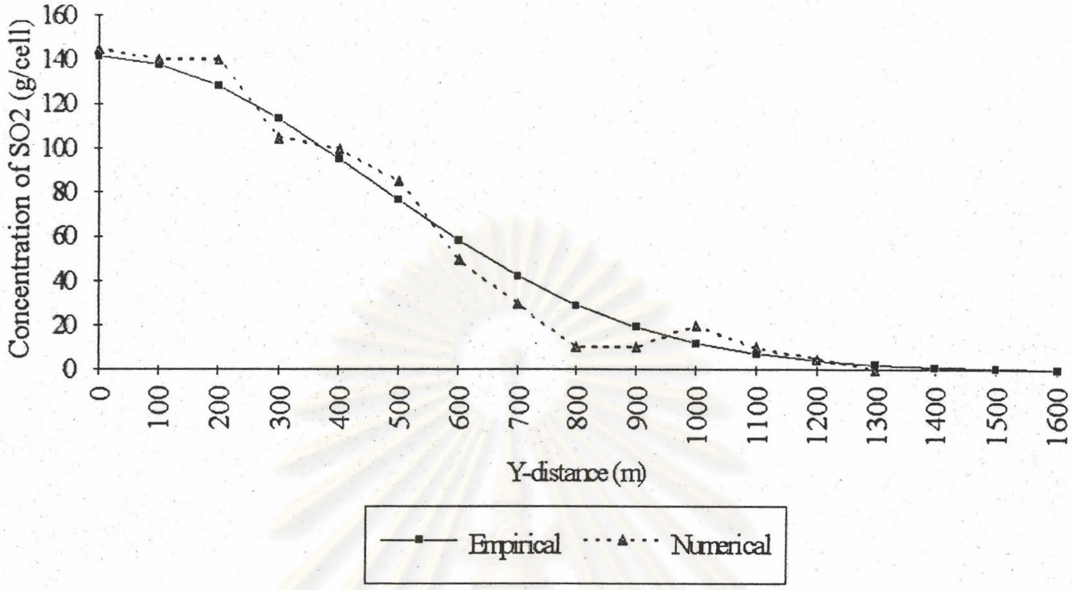


Figure 4.3 Comparison of the Empirical and Numerical Concentrations of SO_2 for Atmospheric Stability Class C at 1 km Downwind from the Source

a) Varying Y-Distance (Fixed z=0) **b) Varying Z-Distance (Fixed y=0)**

a)



b)

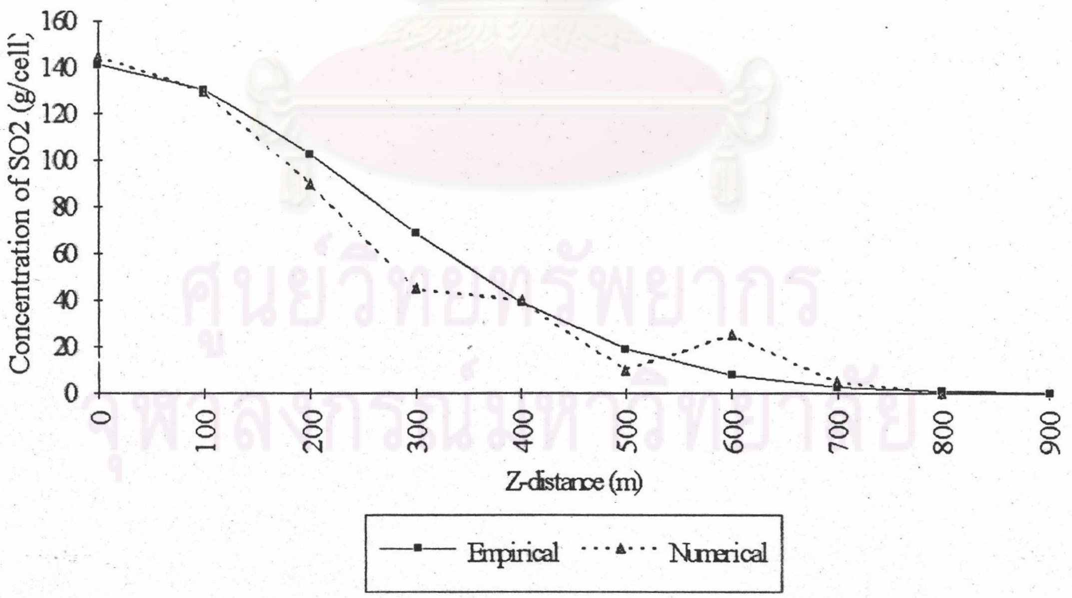


Figure 4.4 Comparison of the Empirical and Numerical Concentrations of SO_2 for Atmospheric Stability Class C at 5 km Downwind from the Source

a) Varying Y-Distance (Fixed z=0) b) Varying Z-Distance (Fixed y=0)

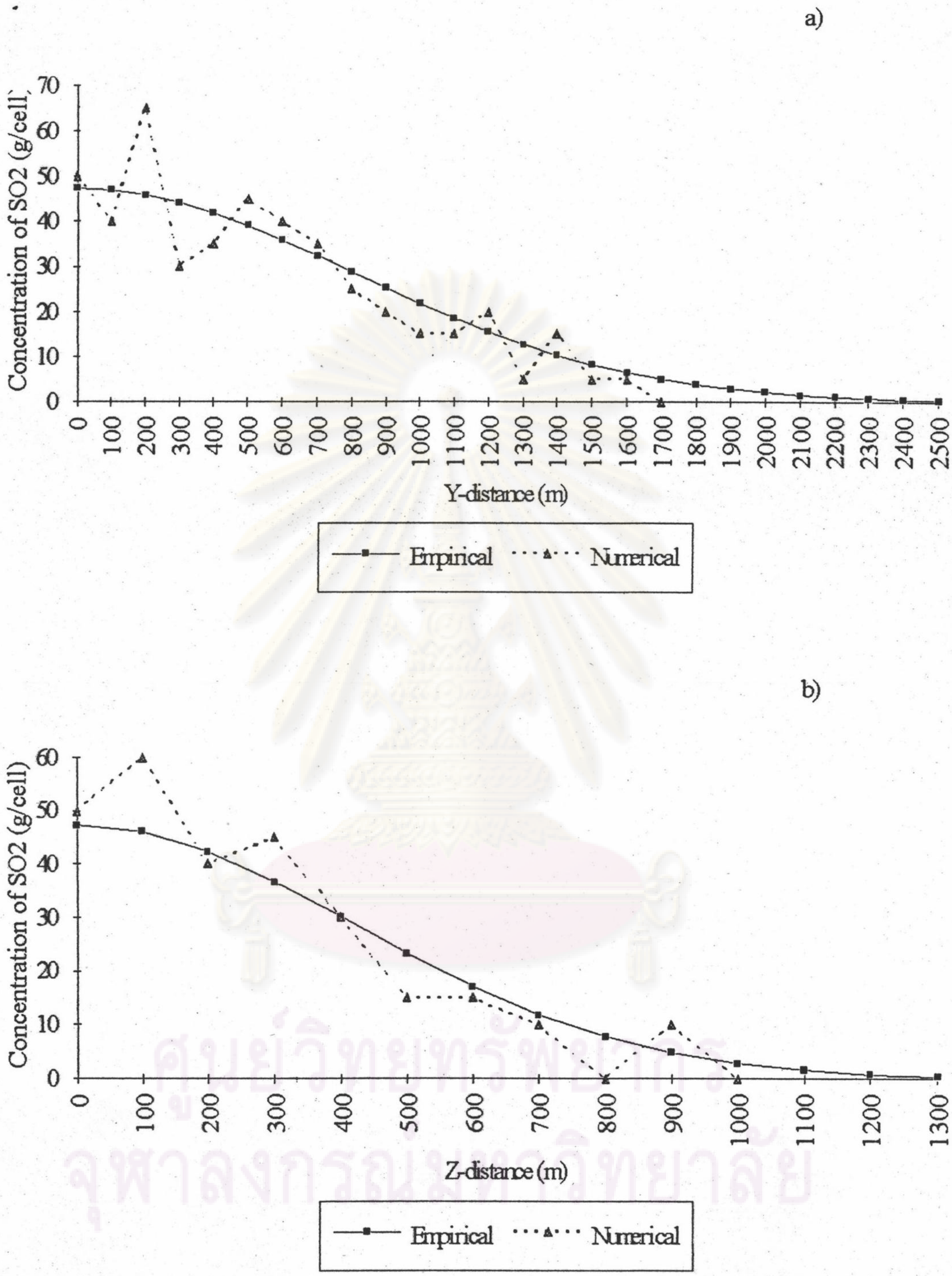
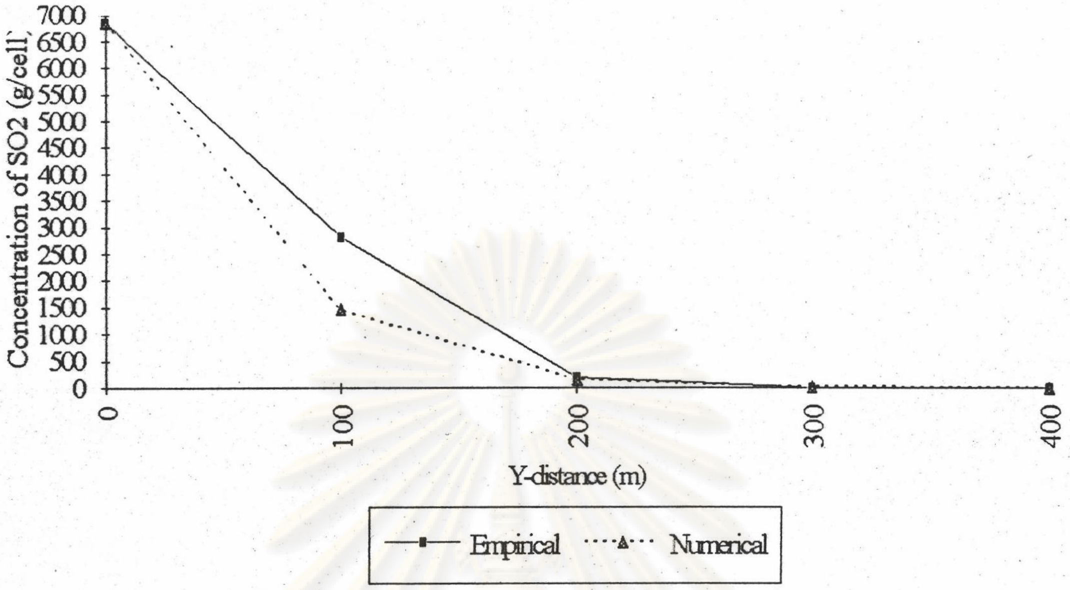


Figure 4.5 Comparison of the Empirical and Numerical Concentrations of SO_2 for Atmospheric Stability Class C at 10 km Downwind from the Source

a) Varying Y-Distance (Fixed z=0) **b) Varying Z-Distance (Fixed y=0)**

a)



b)

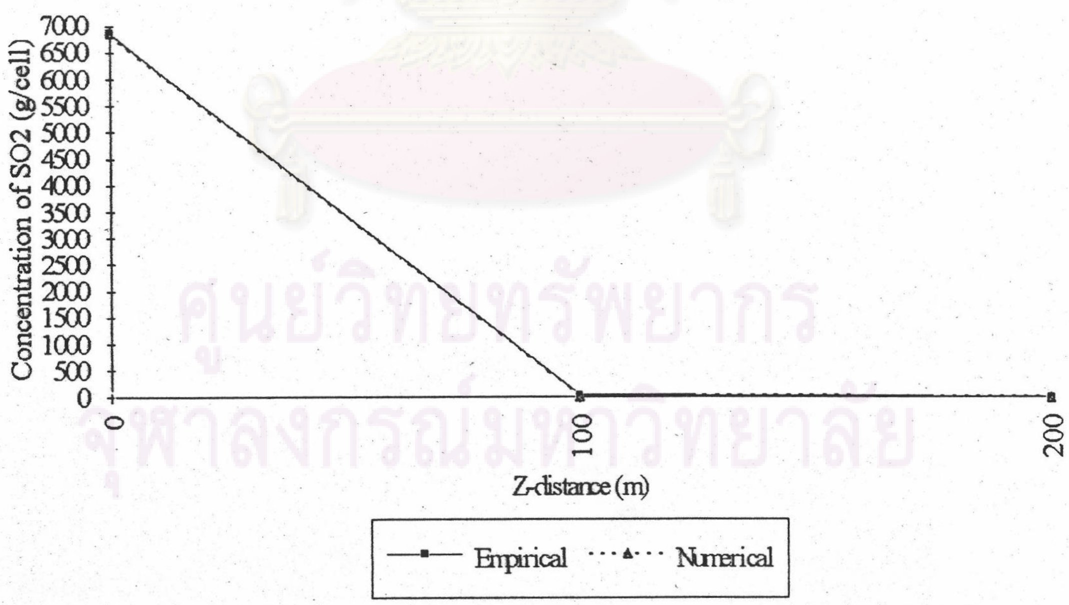
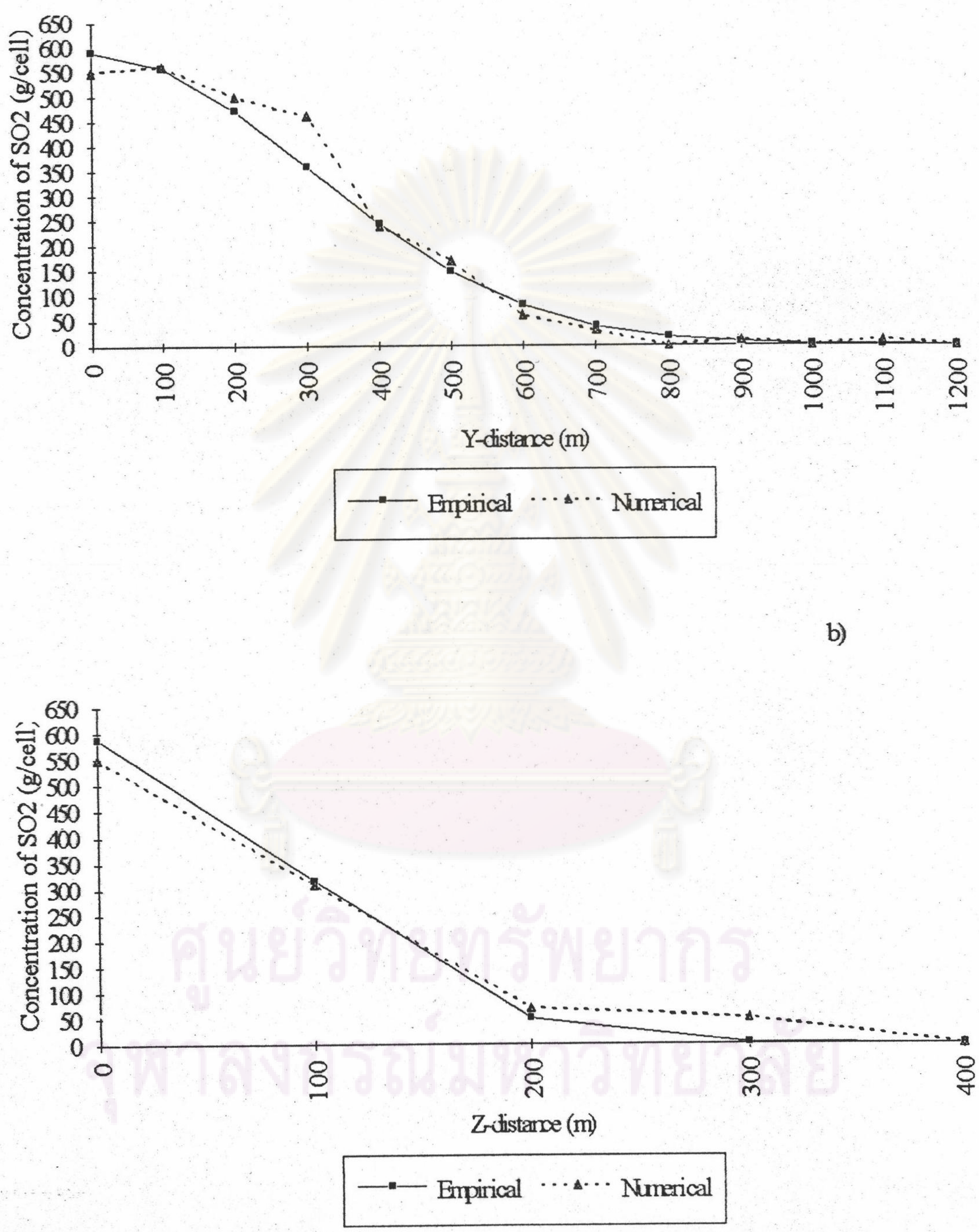


Figure 4.6 Comparison of the Empirical and Numerical Concentrations of SO_2 for Atmospheric Stability Class D at 1 km Downwind from the Source

a) Varying Y-Distance (Fixed z=0) **b) Varying Z-Distance (Fixed y=0)**

a)

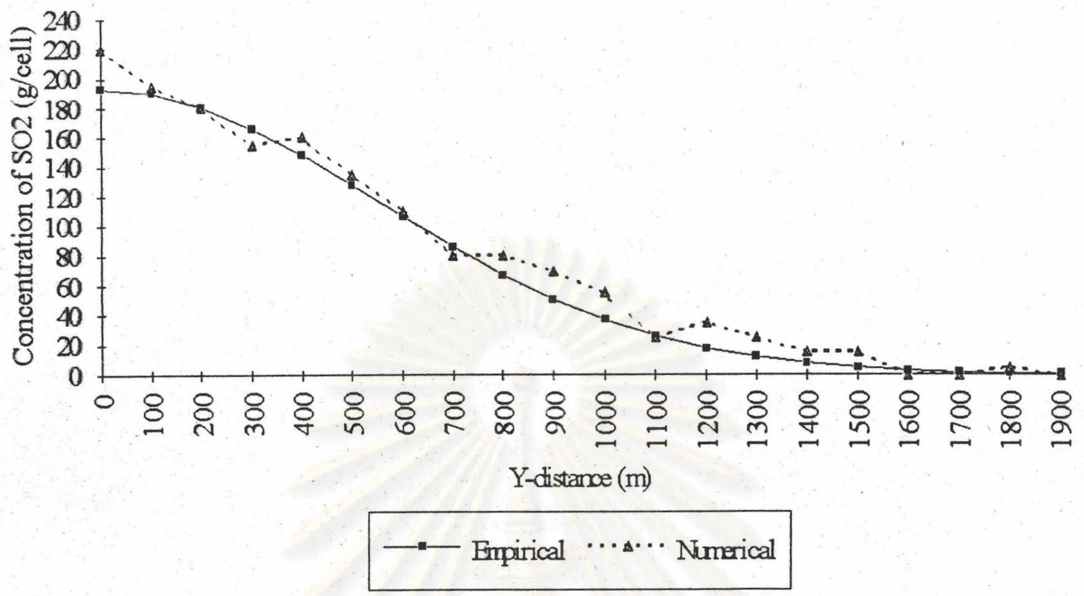


b)

Figure 4.7 Comparison of the Empirical and Numerical Concentrations of SO_2 for Atmospheric Stability Class D at 5 km Downwind from the Source

a) Varying Y-Distance (Fixed z=0) **b) Varying Z-Distance (Fixed y=0)**

a)



b)

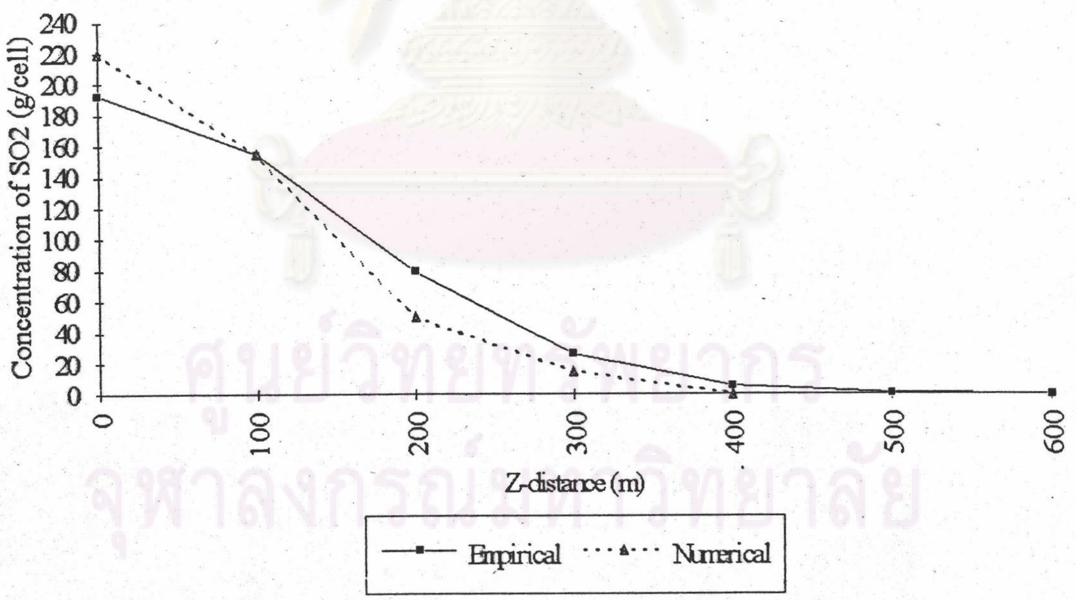


Figure 4.8 Comparison of the Empirical and Numerical Concentrations of SO_2 for Atmospheric Stability Class D at 10 km Downwind from the Source

a) Varying Y-Distance (Fixed z=0) **b) Varying Z-Distance (Fixed y=0)**

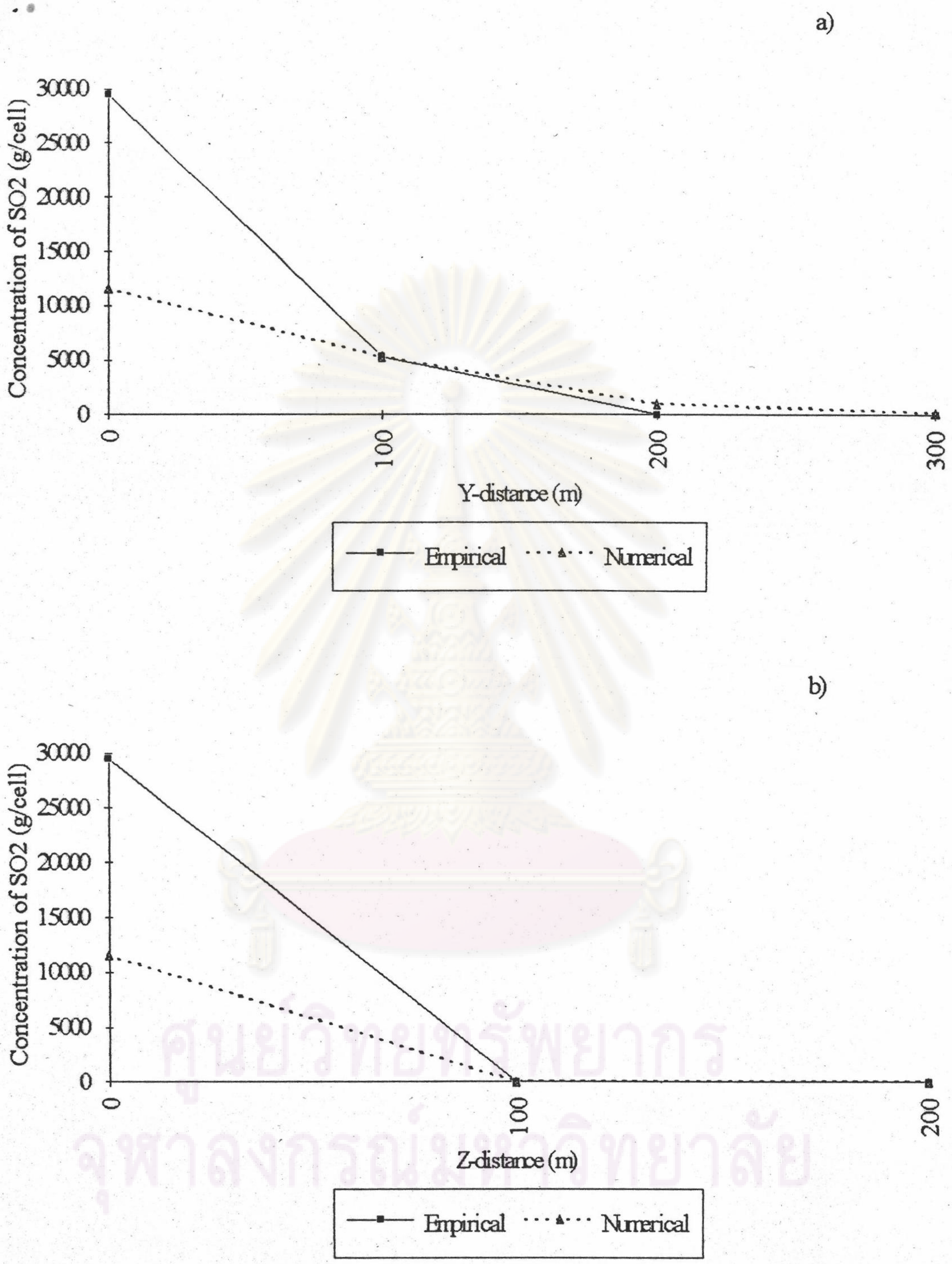
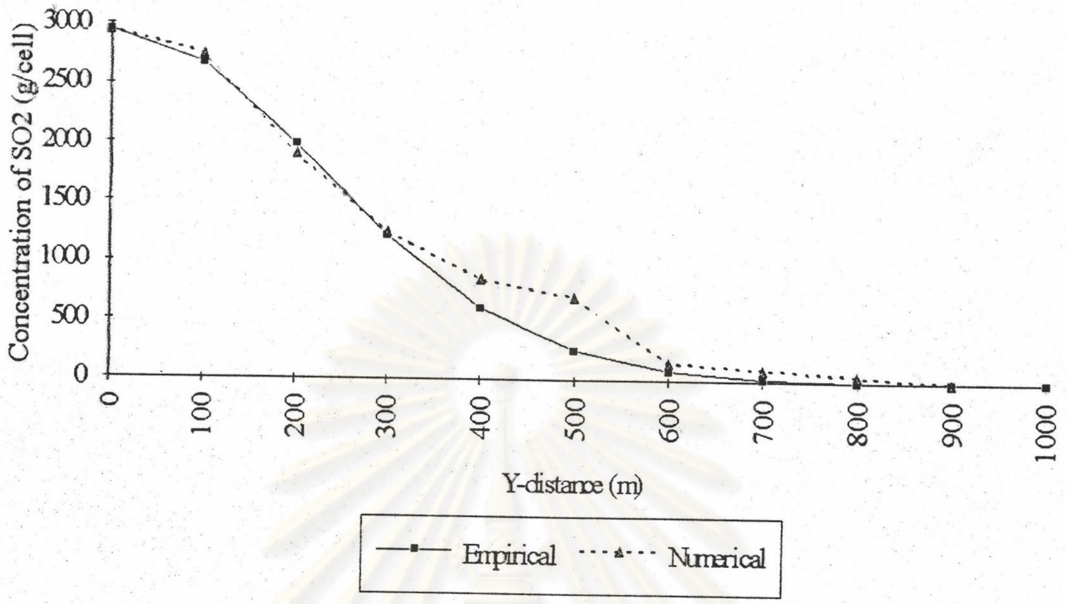


Figure 4.9 Comparison of the Empirical and Numerical Concentrations of SO_2 for Atmospheric Stability Class E at 1 km Downwind from the Source

a) Varying Y-Distance (Fixed z=0) **b) Varying Z-Distance (Fixed y=0)**

a)



b)

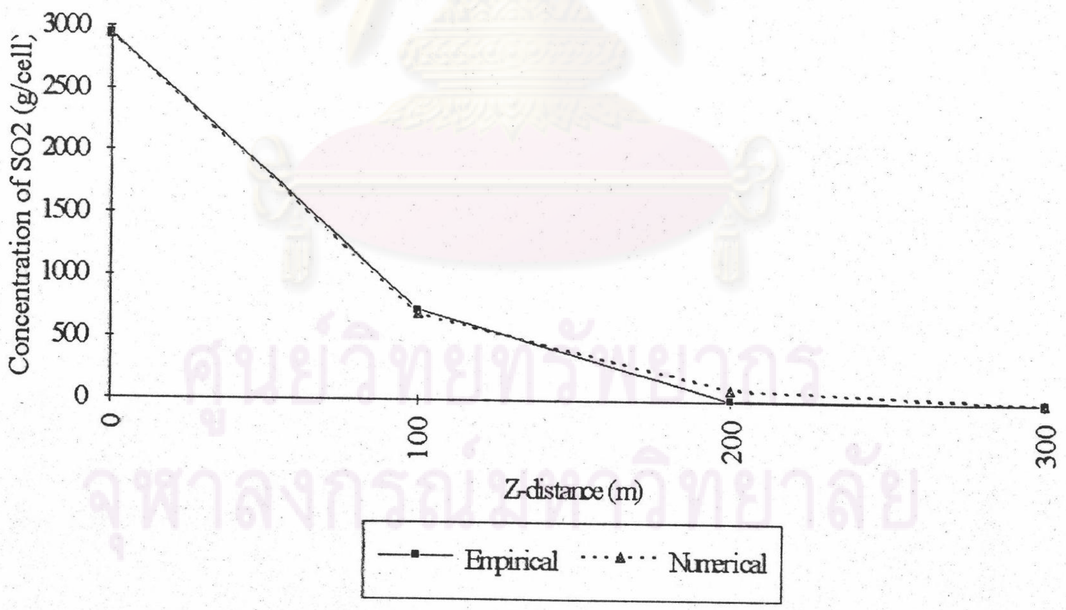
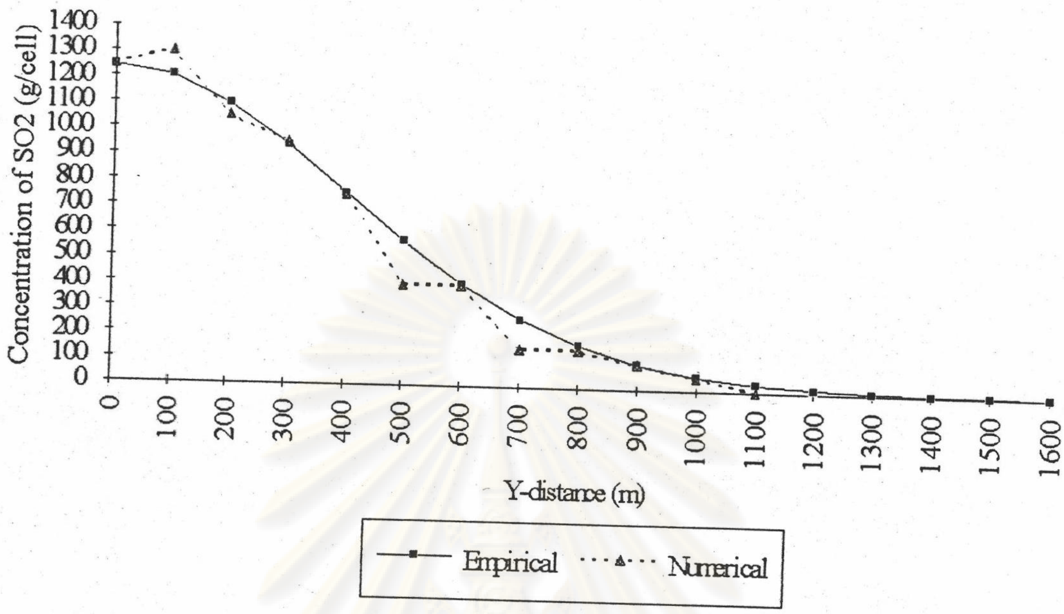


Figure 4.10 Comparison of the Empirical and Numerical Concentrations of SO_2 for Atmospheric Stability Class E at 5 km Downwind from the Source

a) Varying Y-Distance (Fixed z=0) **b) Varying Z-Distance (Fixed y=0)**

a)



b)

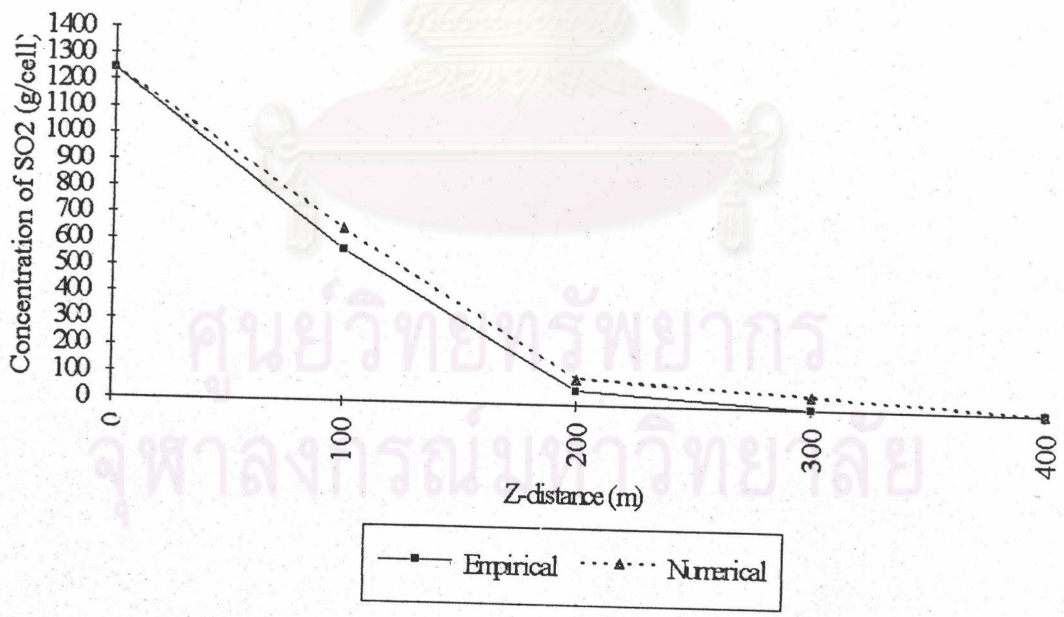
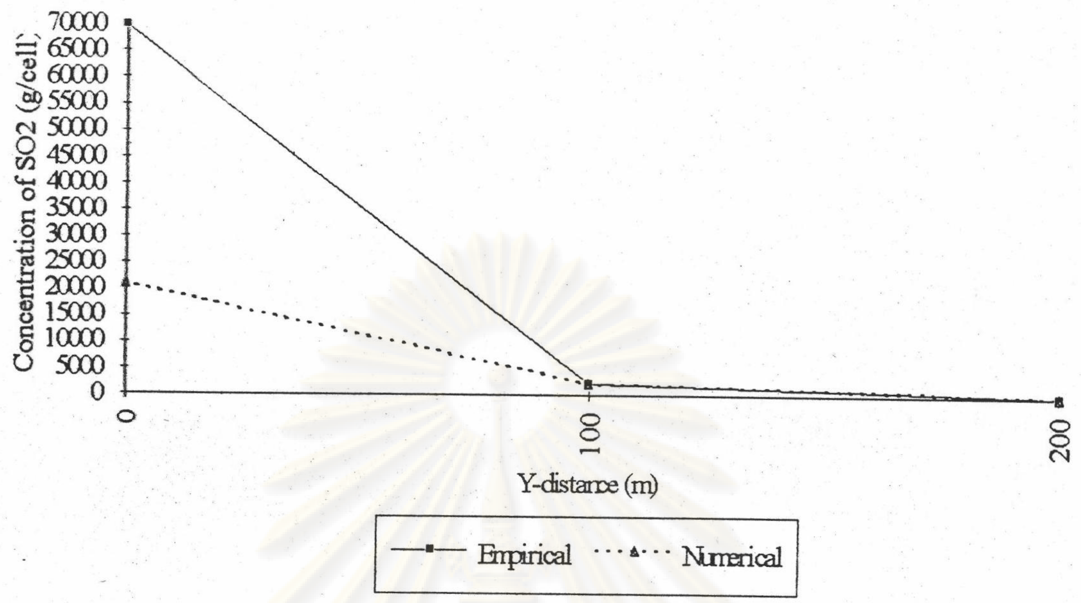


Figure 4.11 Comparison of the Empirical and Numerical Concentrations of SO_2 for Atmospheric Stability Class E at 10 km Downwind from the Source

a) Varying Y-Distance (Fixed z=0) **b) Varying Z-Distance (Fixed y=0)**

a)



b)

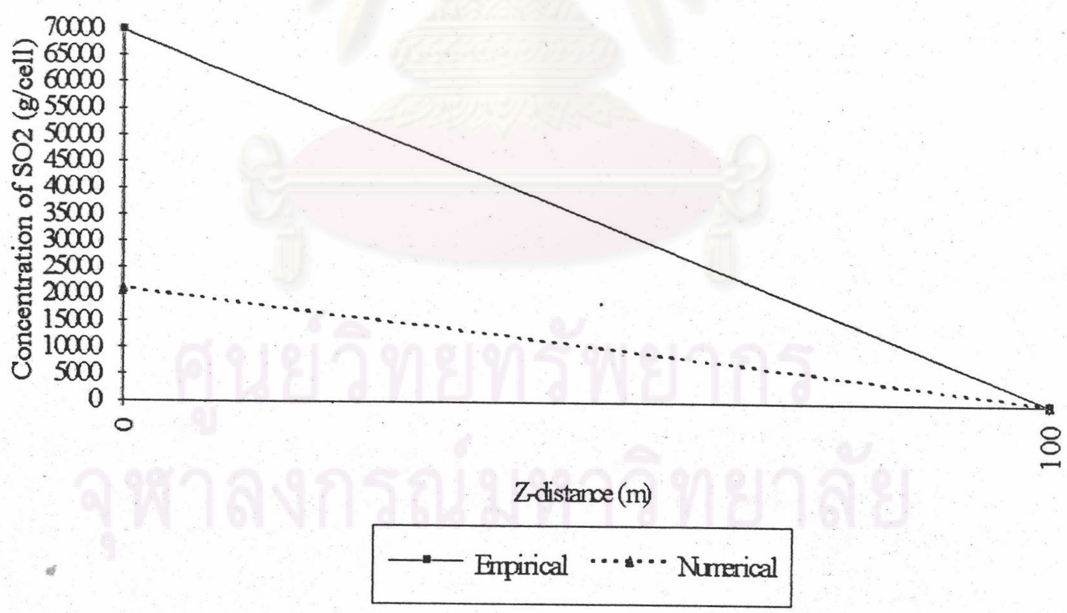
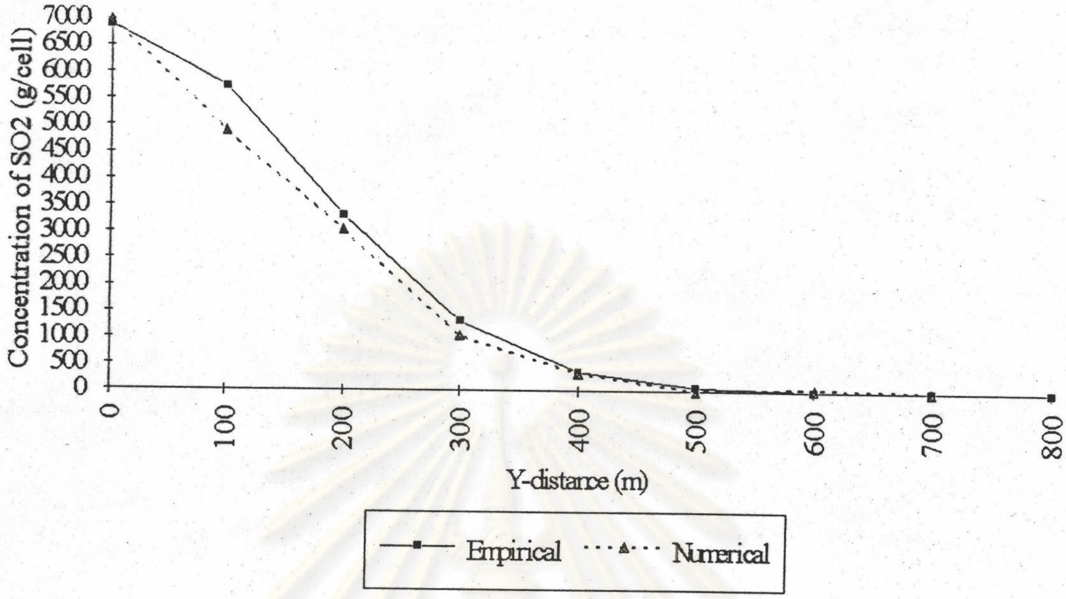


Figure 4.12 Comparison of the Empirical and Numerical Concentrations of SO_2 for Atmospheric Stability Class F at 1 km Downwind from the Source

a) Varying Y-Distance (Fixed z=0) **b) Varying Z-Distance (Fixed y=0)**

a)



b)

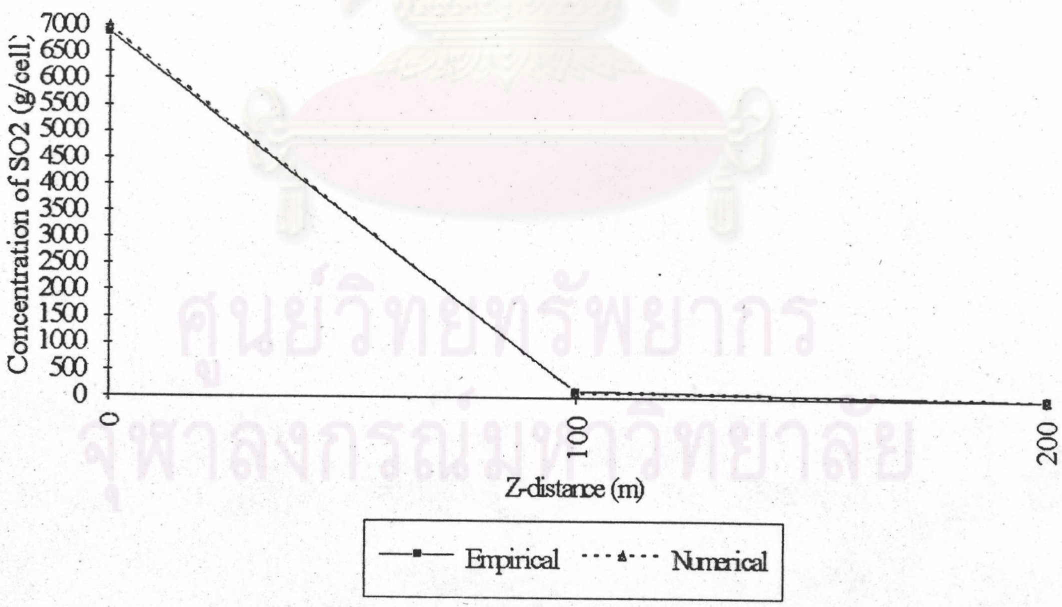


Figure 4.13 Comparison of the Empirical and Numerical Concentrations of SO_2 for Atmospheric Stability Class F at 5 km Downwind from the Source

a) Varying Y-Distance (Fixed z=0) **b) Varying Z-Distance (Fixed y=0)**

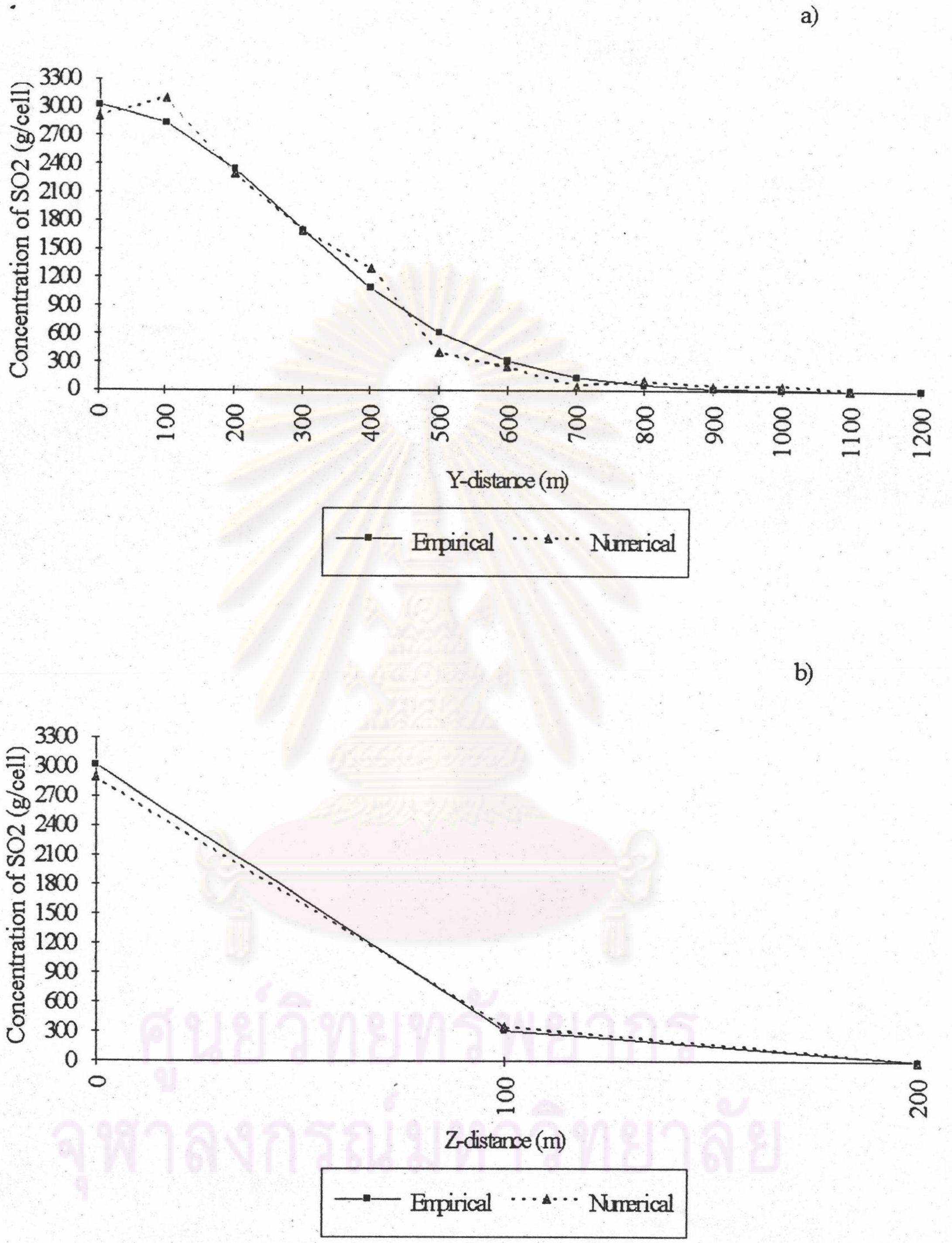


Figure 4.14 Comparison of the Empirical and Numerical Concentrations of SO_2 for Atmospheric Stability Class F at 10 km Downwind from the Source

a) Varying Y-Distance (Fixed z=0) **b) Varying Z-Distance (Fixed y=0)**

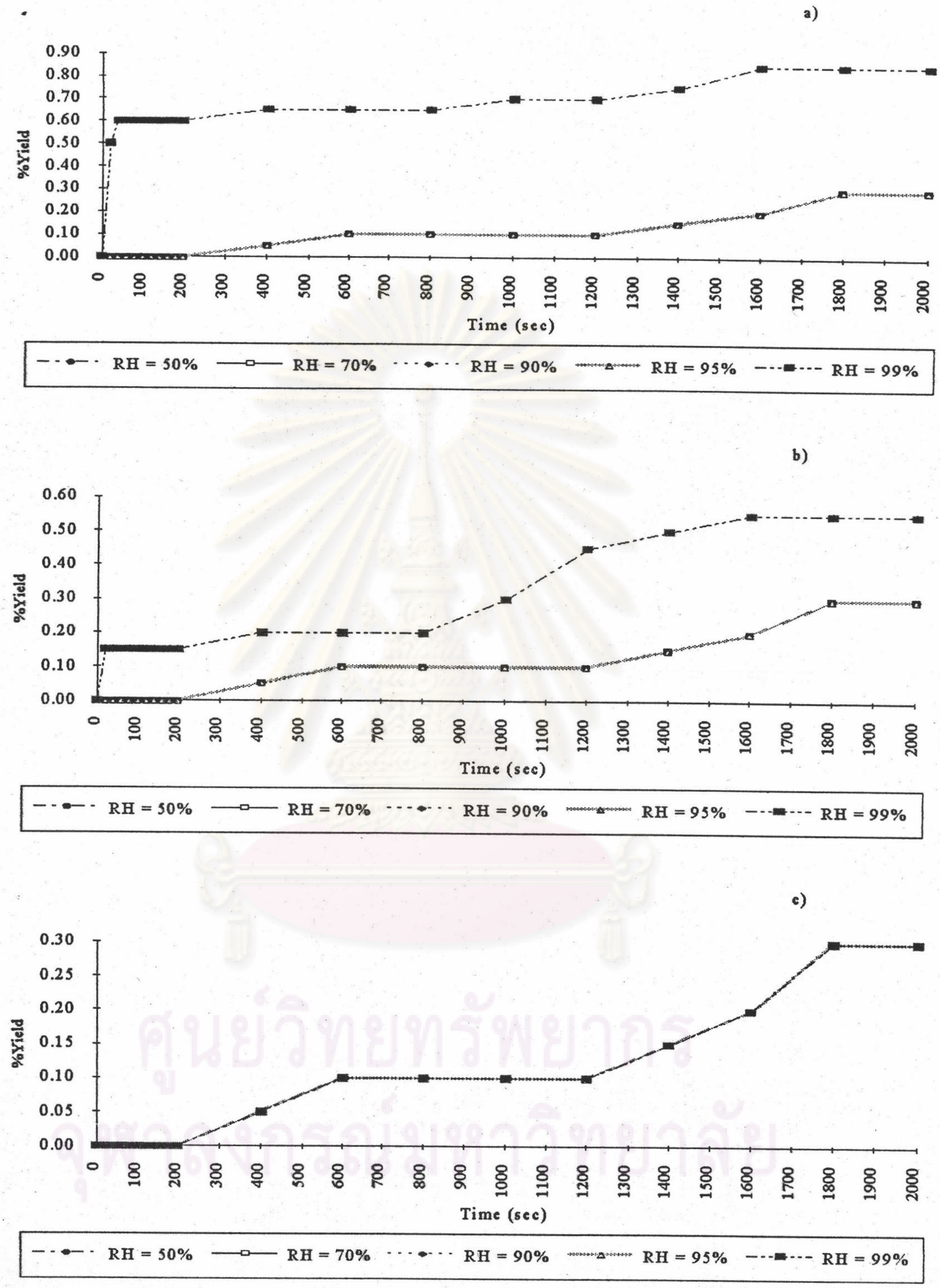


Figure 4.15 **%Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class C at [Fe] = 1201 ng/m³ and [NH_3] = 50 ppb**

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

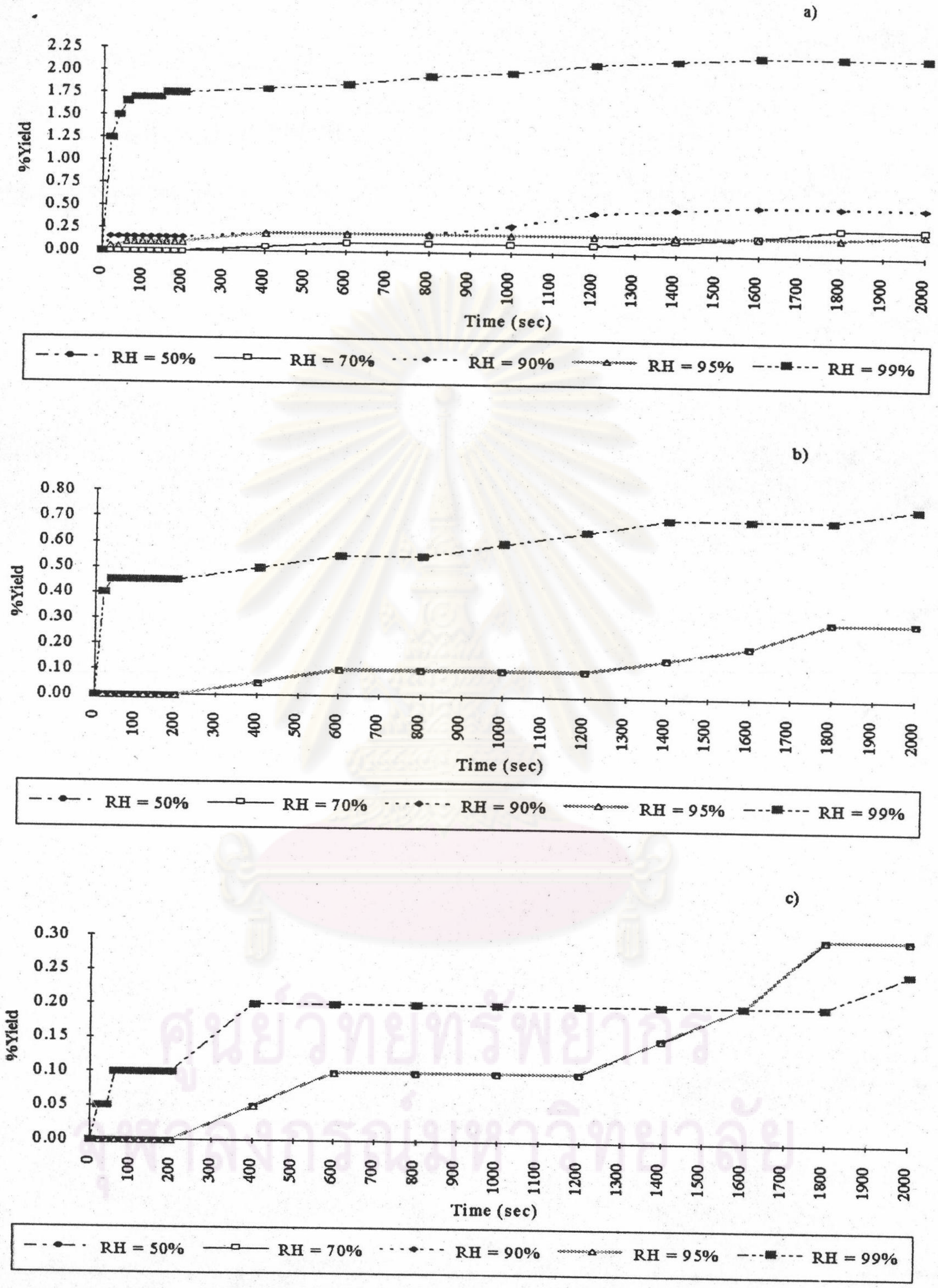


Figure 4.16 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class C at [Fe] = 1201 ng/m^3 and [NH_3] = 80 ppb

a) T = 20 ^{o}C **b) T = 25 ^{o}C** **c) T = 30 ^{o}C**

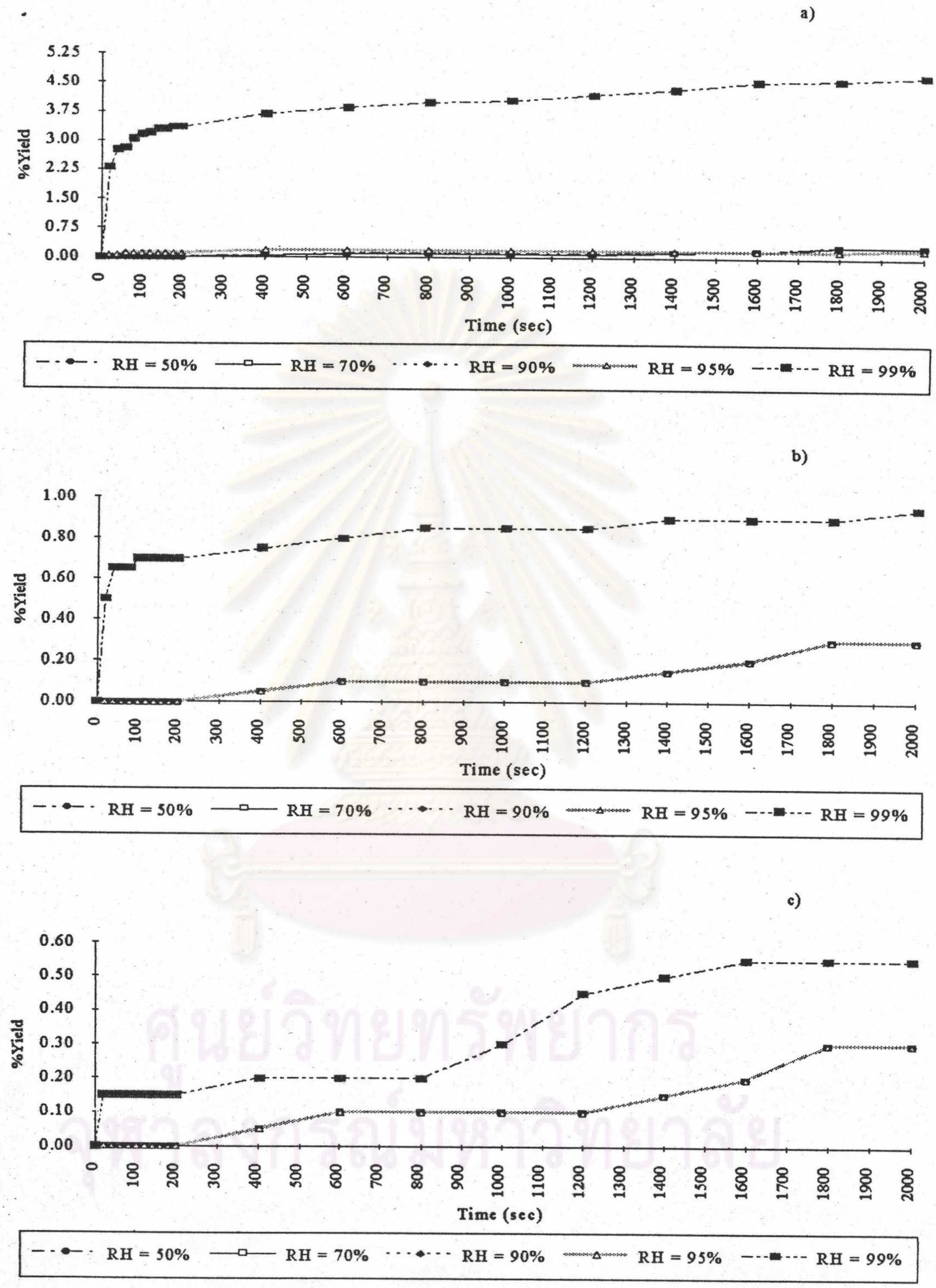


Figure 4.17 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class C at [Fe] = 1201 ng/m³ and $[NH_3]$ = 100 ppb

a) T = 20 °C b) T = 25 °C c) T = 30 °C

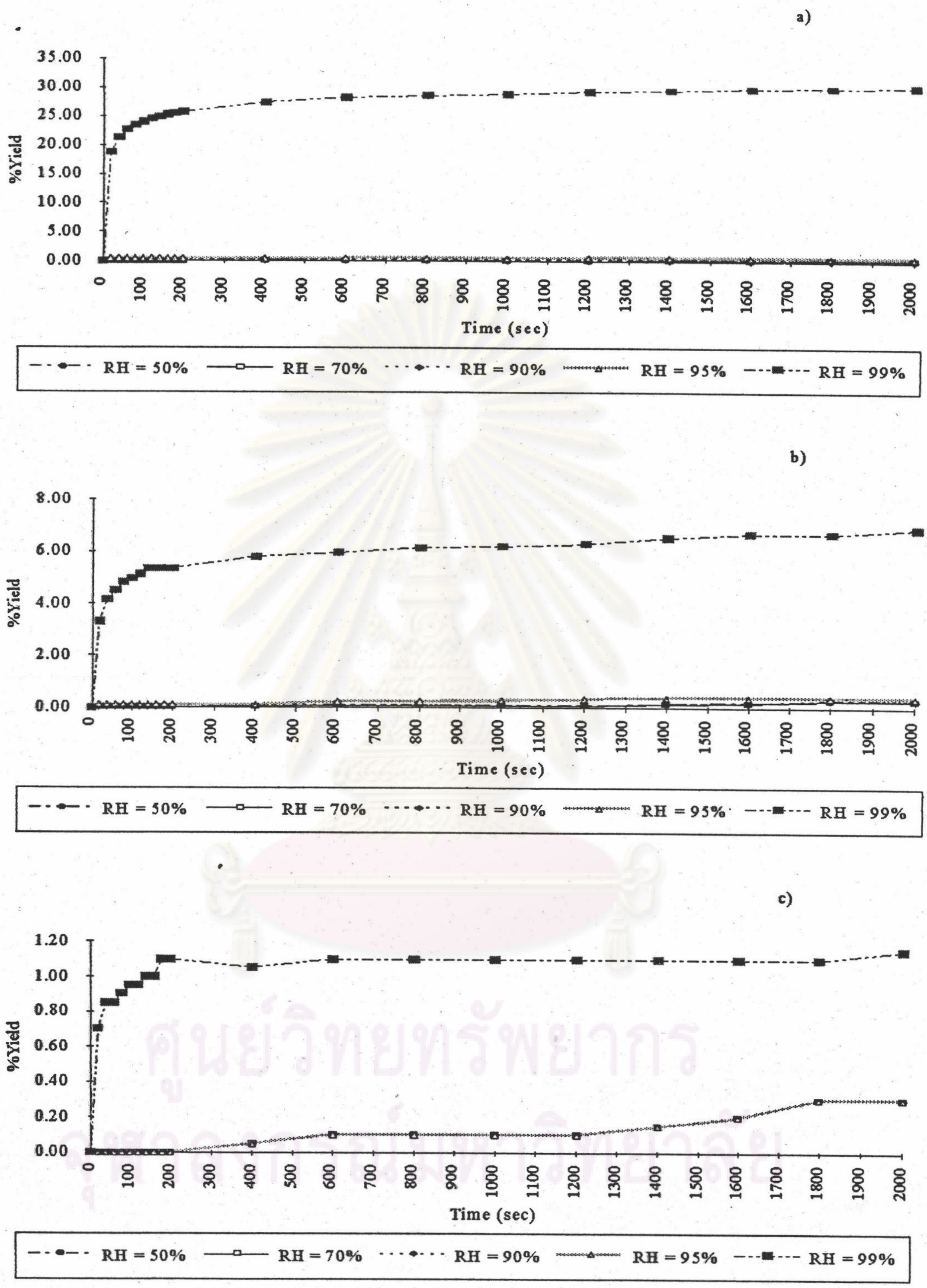


Figure 4.18 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class C at [Fe] = 0.1 mg/m^3 and [NH_3] = 50 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

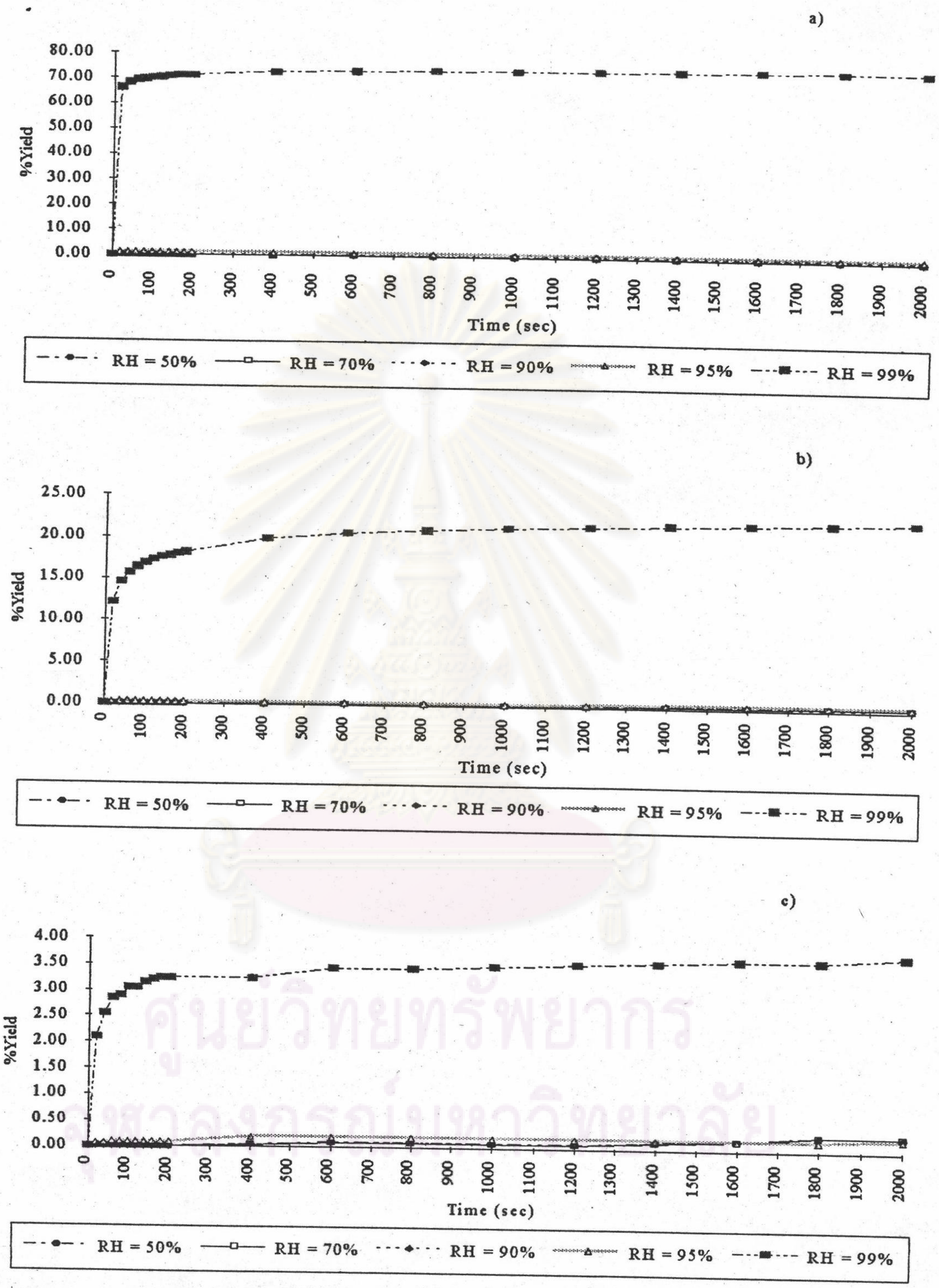


Figure 4.19 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class C at [Fe] = 0.1 mg/m³ and $[NH_3]$ = 80 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

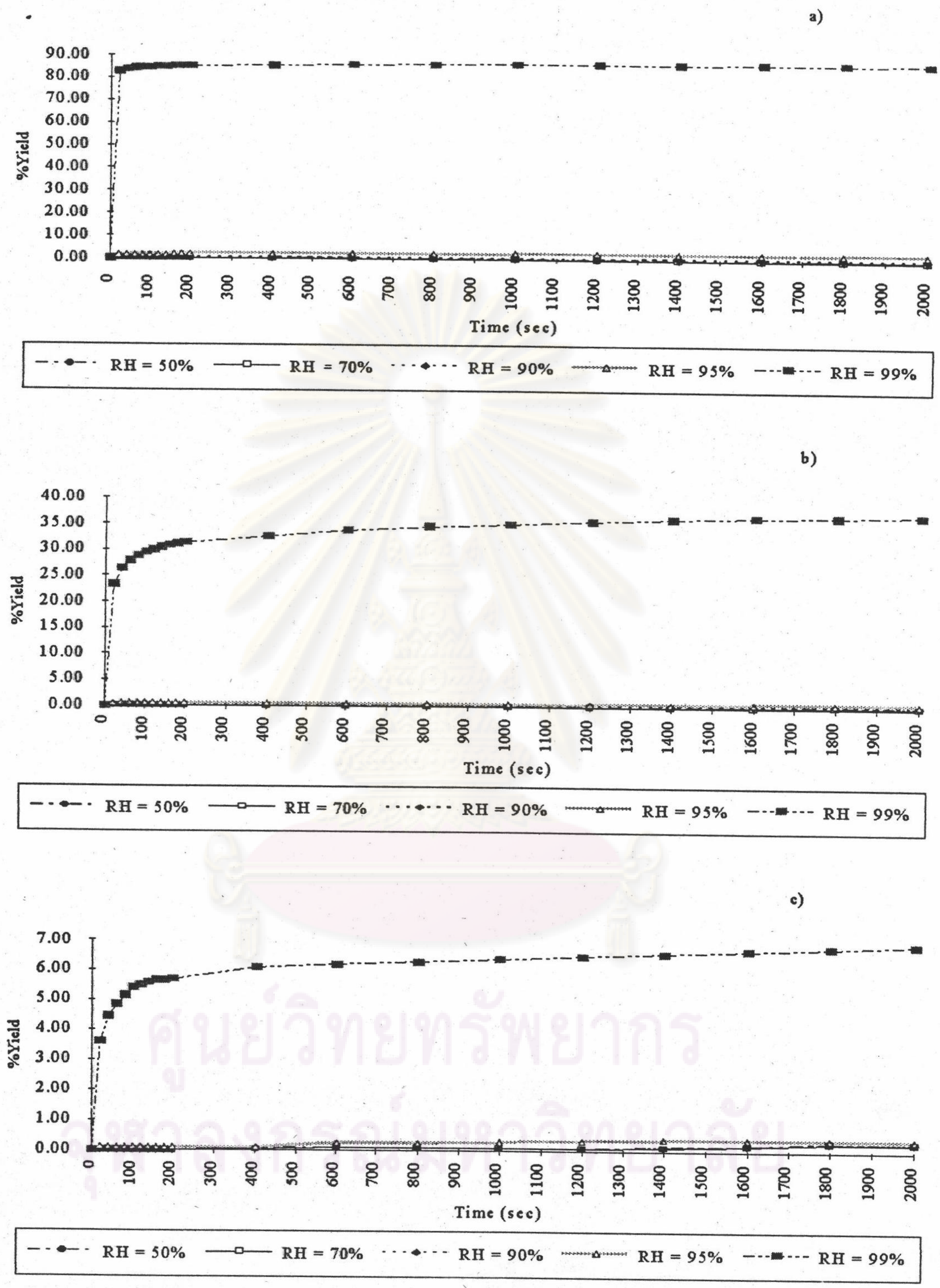


Figure 4.20 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class C at [Fe] = 0.1 mg/m^3 and $[NH_3]$ = 100 ppb

a) T = 20 °C b) T = 25 °C c) T = 30 °C

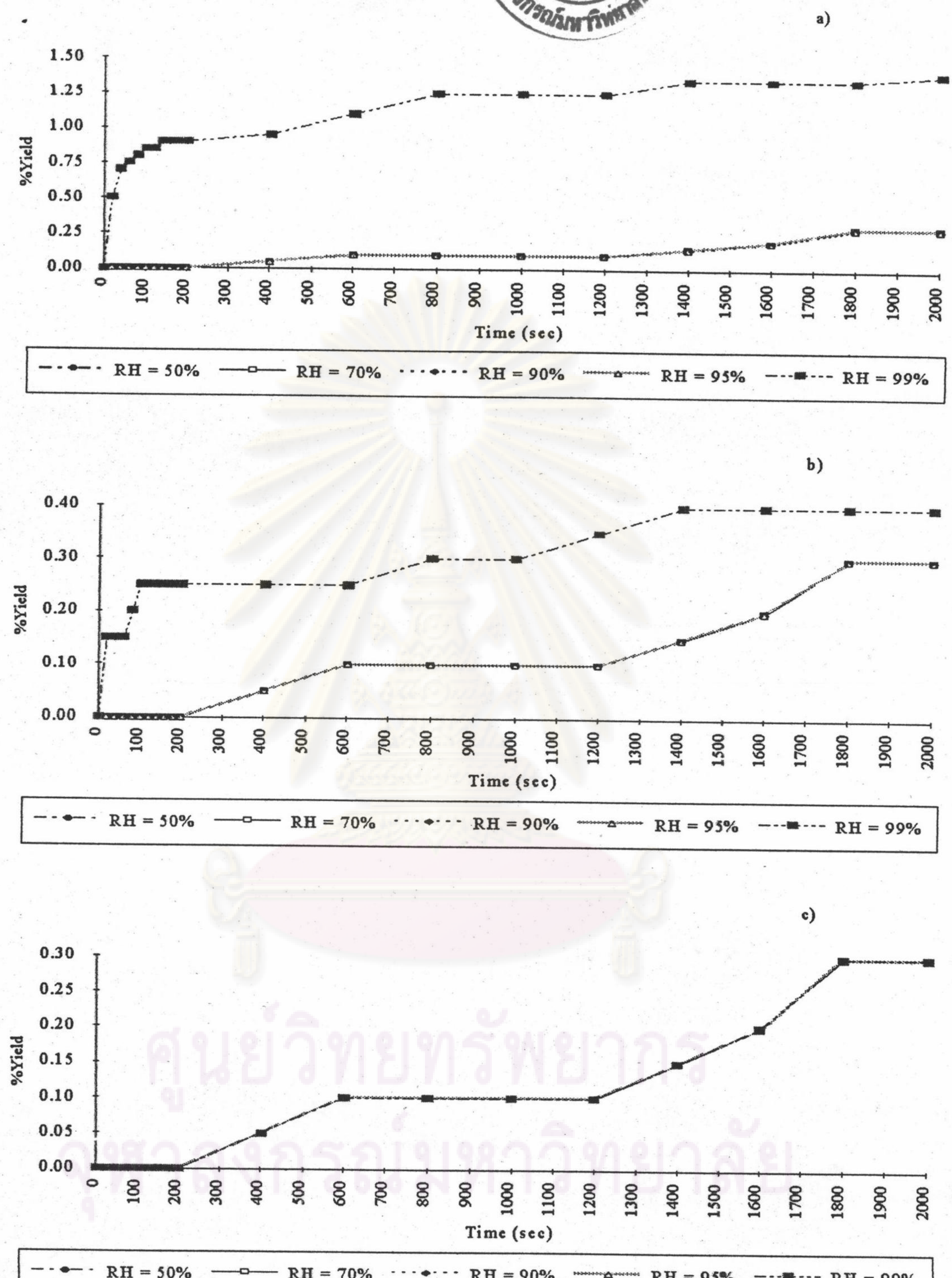


Figure 4.21 **%Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class D at [Fe] = 1201 ng/m³ and [NH_3] = 50 ppb**

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

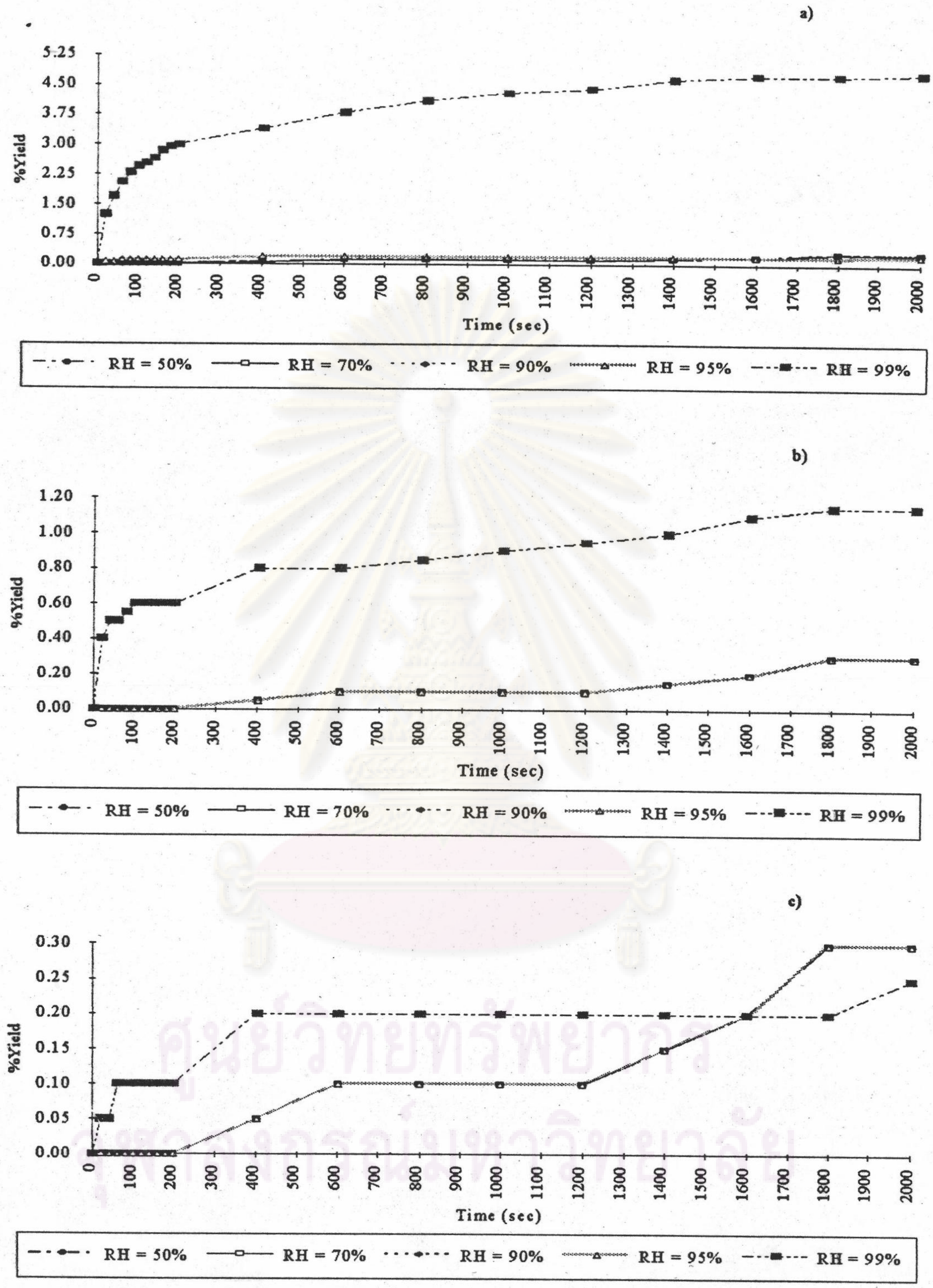


Figure 4.22 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class D at [Fe] = 1201 ng/m³ and $[NH_3]$ = 80 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

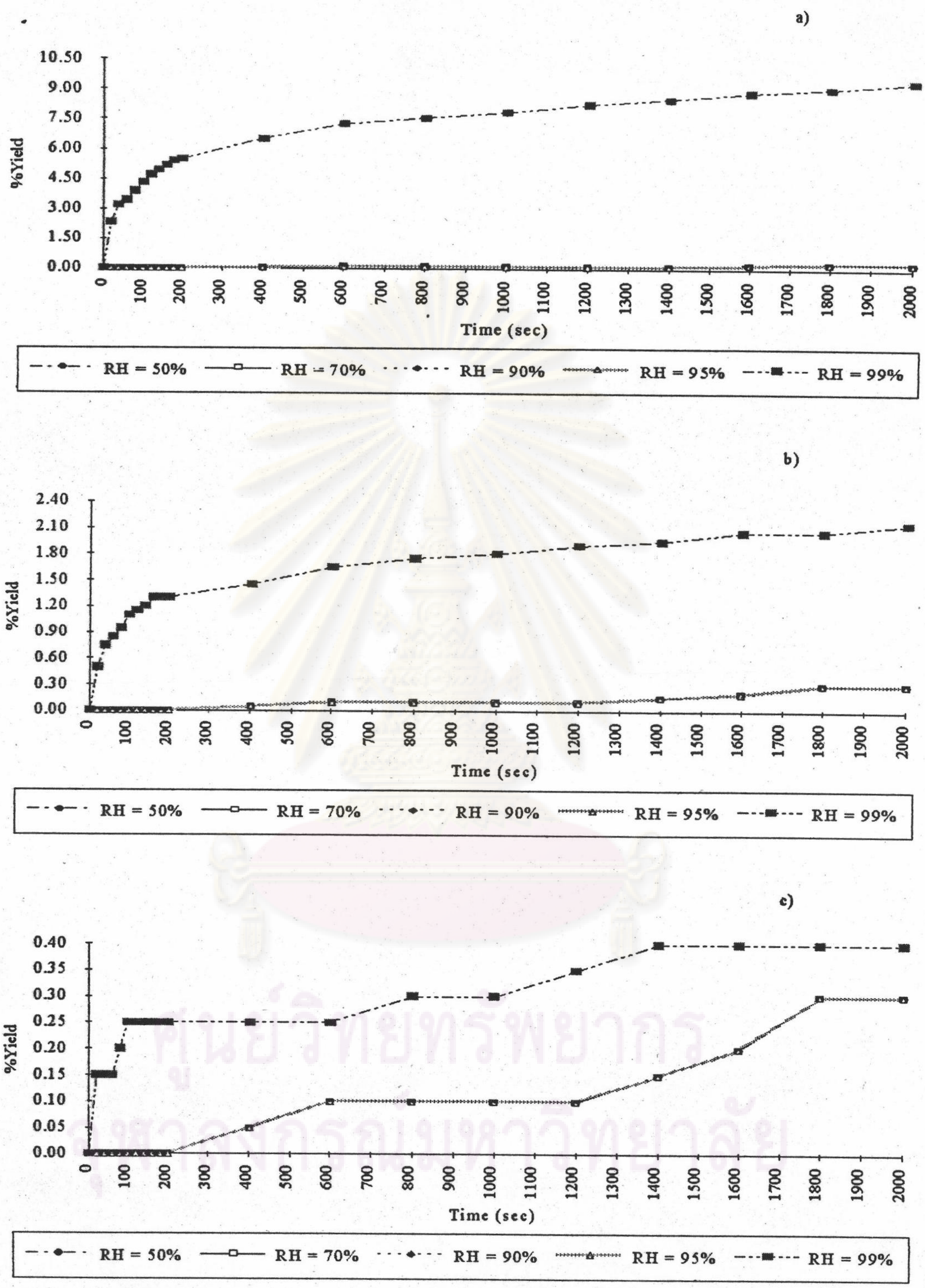


Figure 4.23 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class D at [Fe] = 1201 ng/m^3 and [NH_3] = 100 ppb

a) T = 20 °C b) T = 25 °C c) T = 30 °C

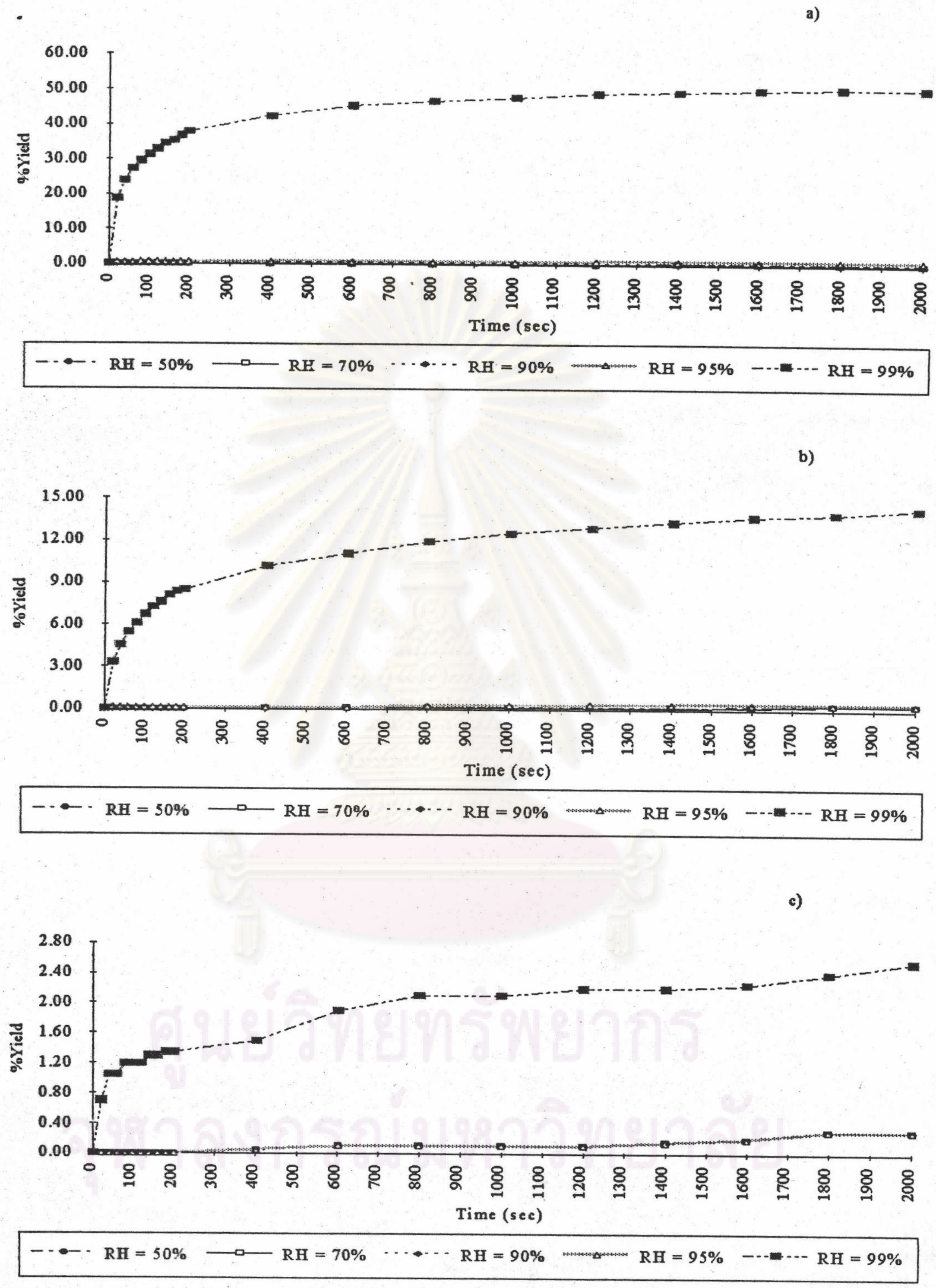
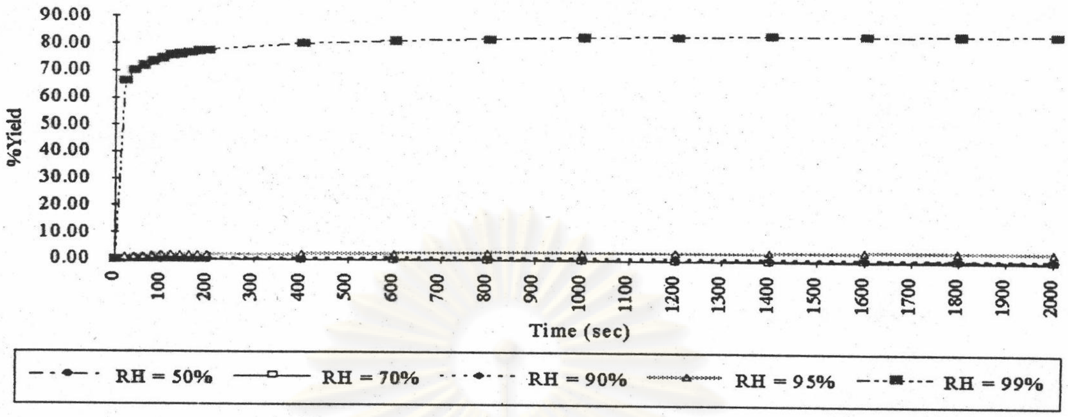


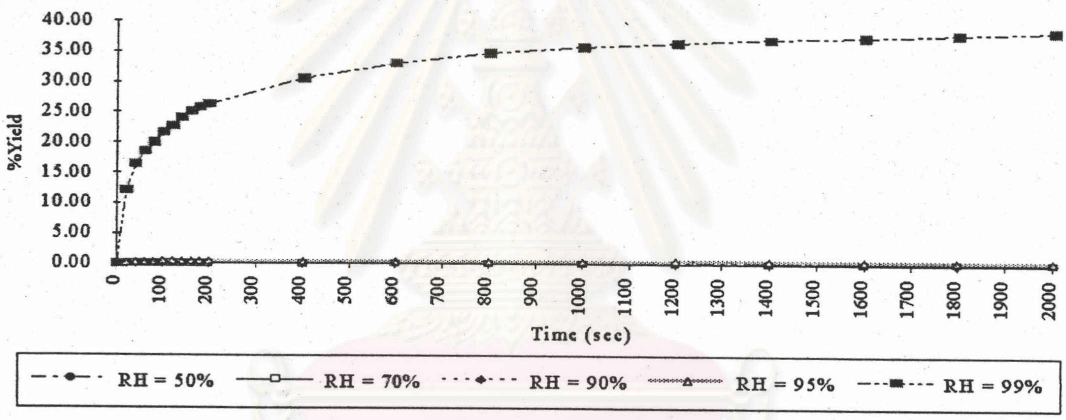
Figure 4.24 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class D at [Fe] = 0.1 mg/m³ and [NH_3] = 50 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

a)



b)



c)

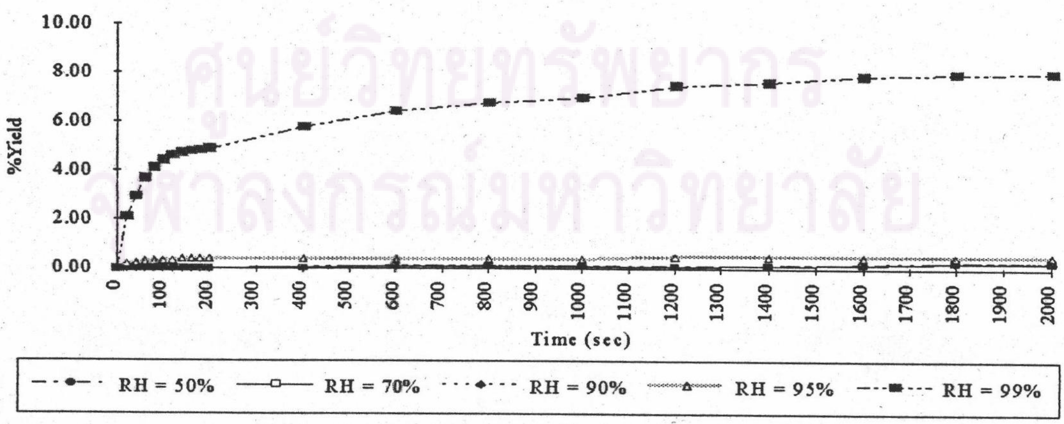
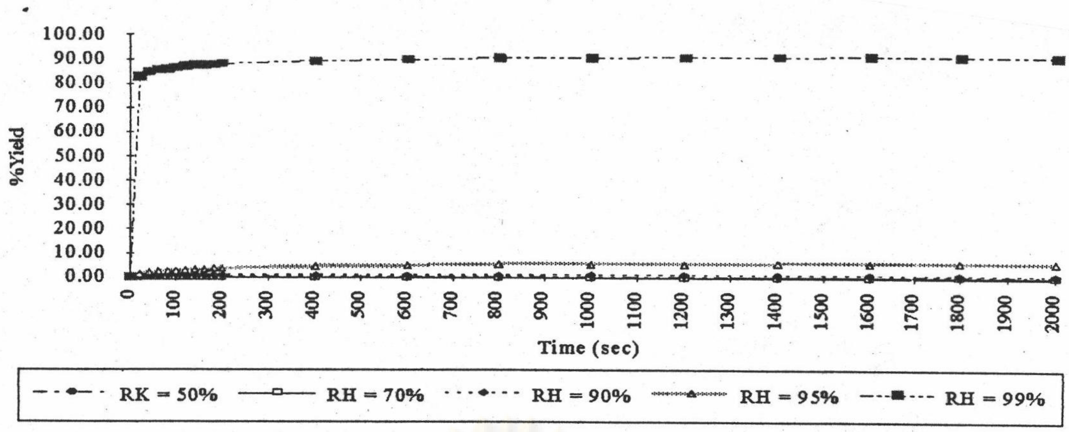
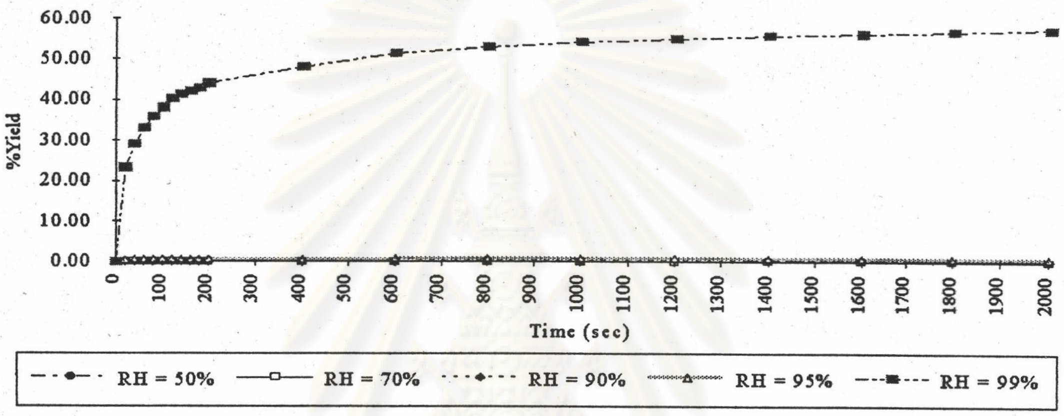


Figure 4.25 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class D at [Fe] = 0.1 mg/m^3 and [NH_3] = 80 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**



b)



c)

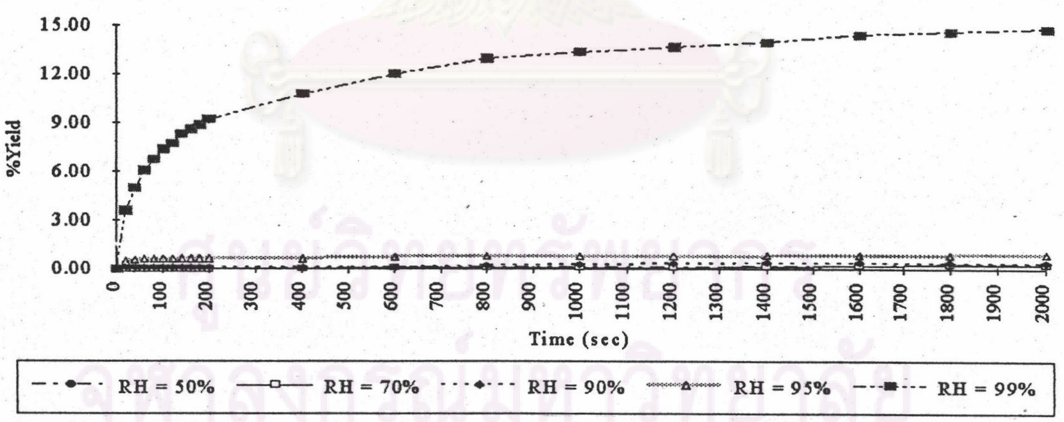


Figure 4.26 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class D at [Fe] = 0.1 mg/m³ and [NH_3] = 100 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

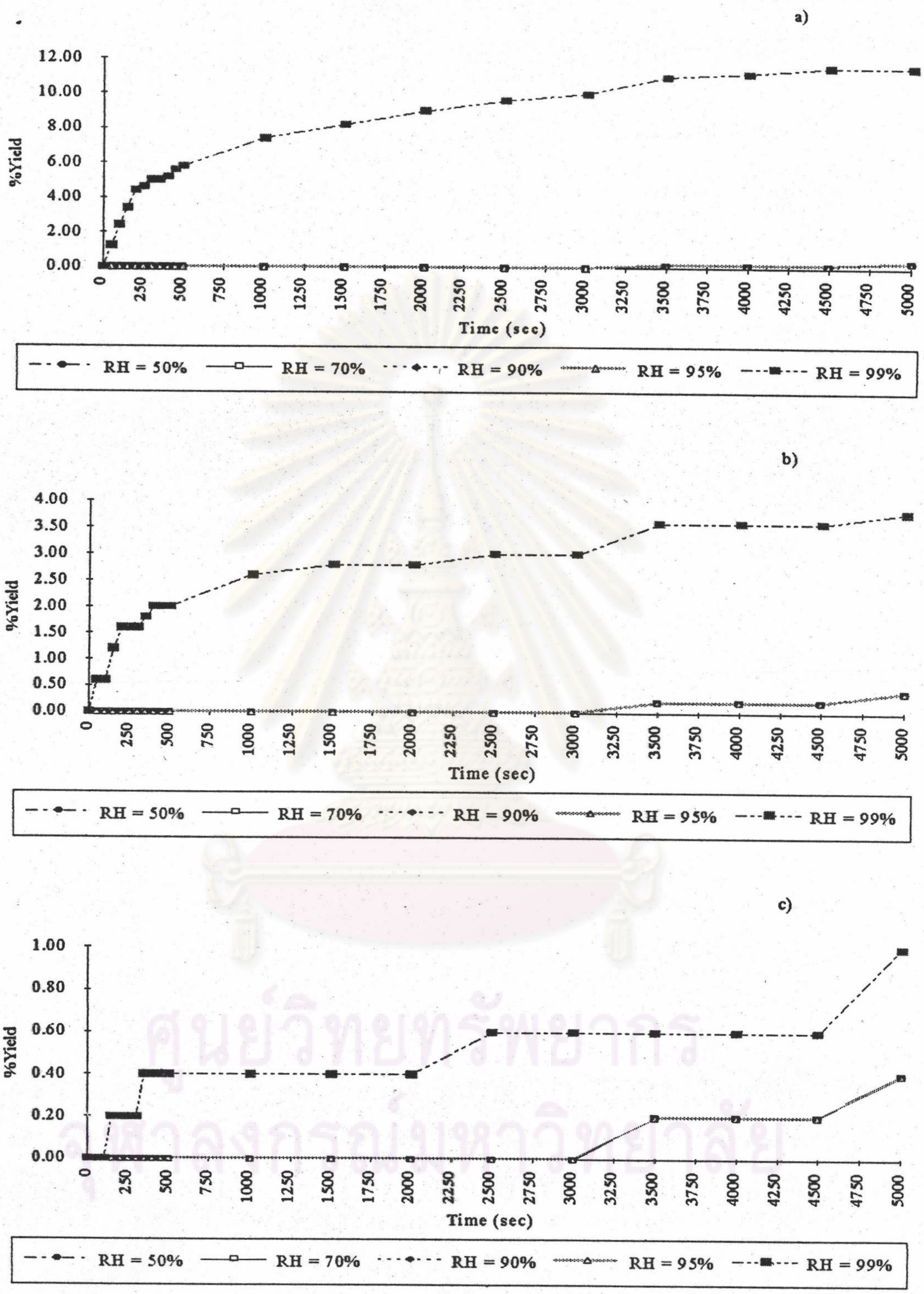


Figure 4.27 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class E at [Fe] = 1201 ng/m^3 and [NH_3] = 50 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

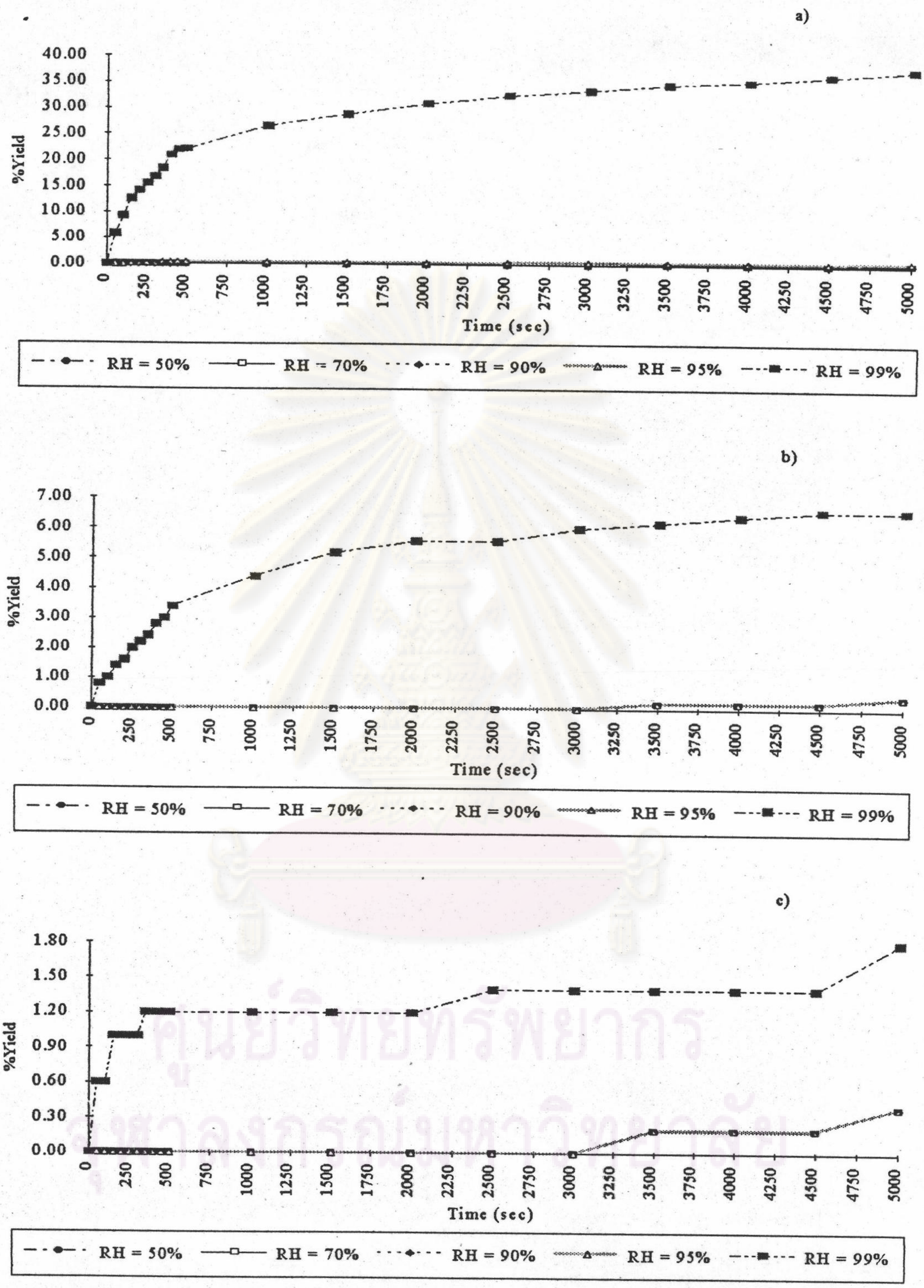


Figure 4.28 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class E at [Fe] = 1201 ng/m³ and [NH_3] = 80 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

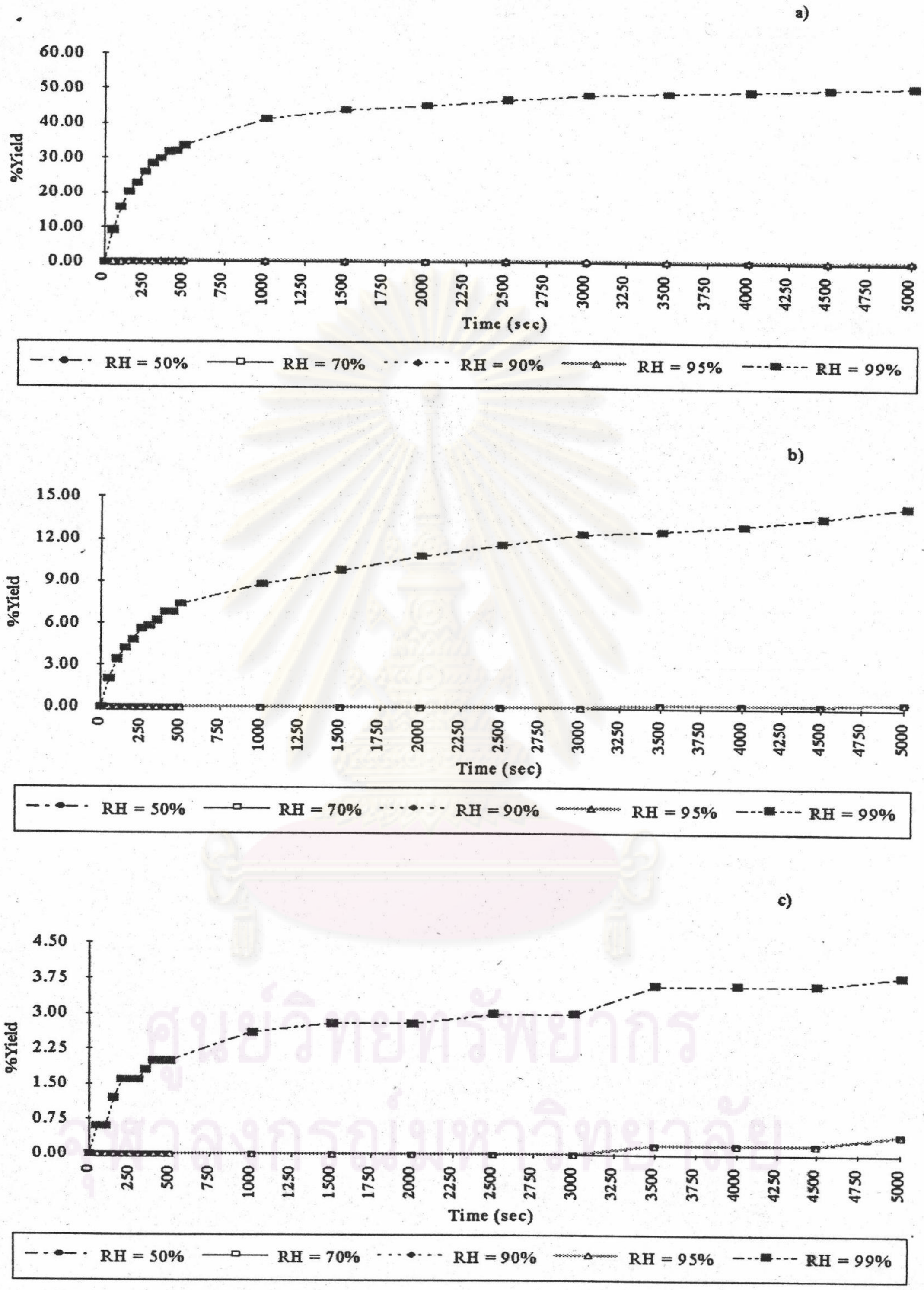


Figure 4.29 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class E at [Fe] = 1201 ng/m³ and [NH_3] = 100 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

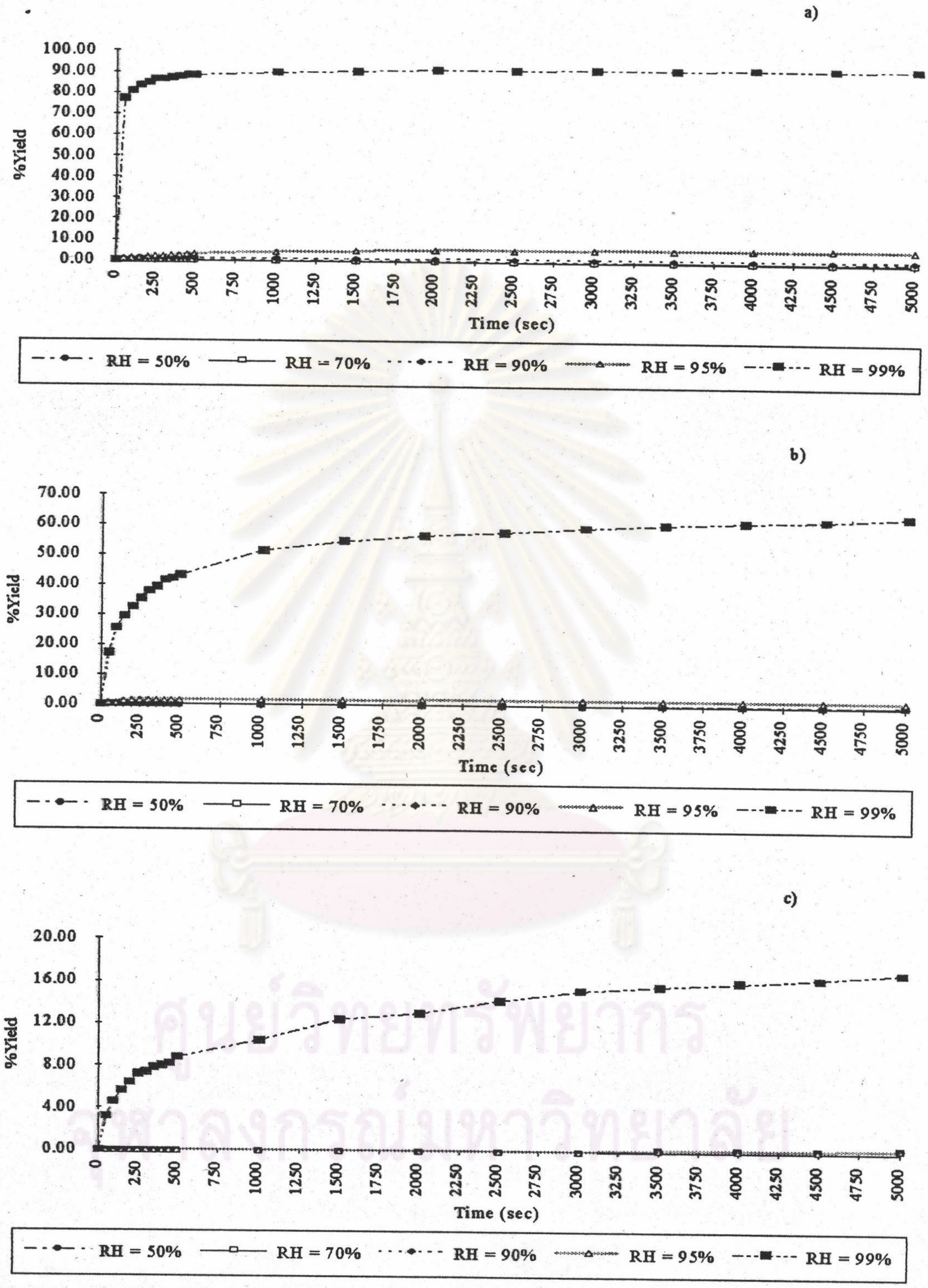


Figure 4.30 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class E at [Fe] = 0.1 mg/m^3 and [NH_3] = 50 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

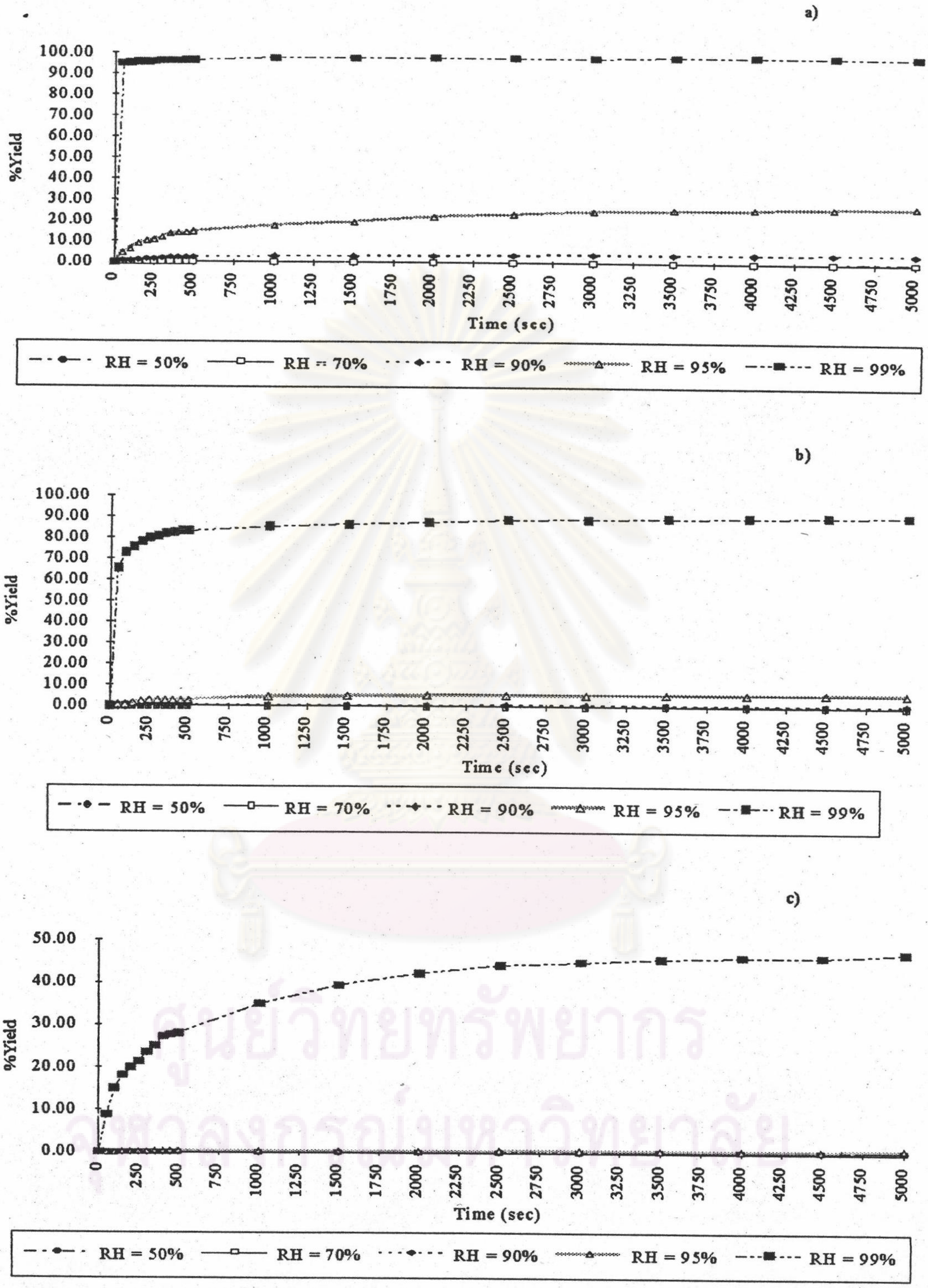


Figure 4.31 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class E at [Fe] = 0.1 mg/m^3 and [NH_3] = 80 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

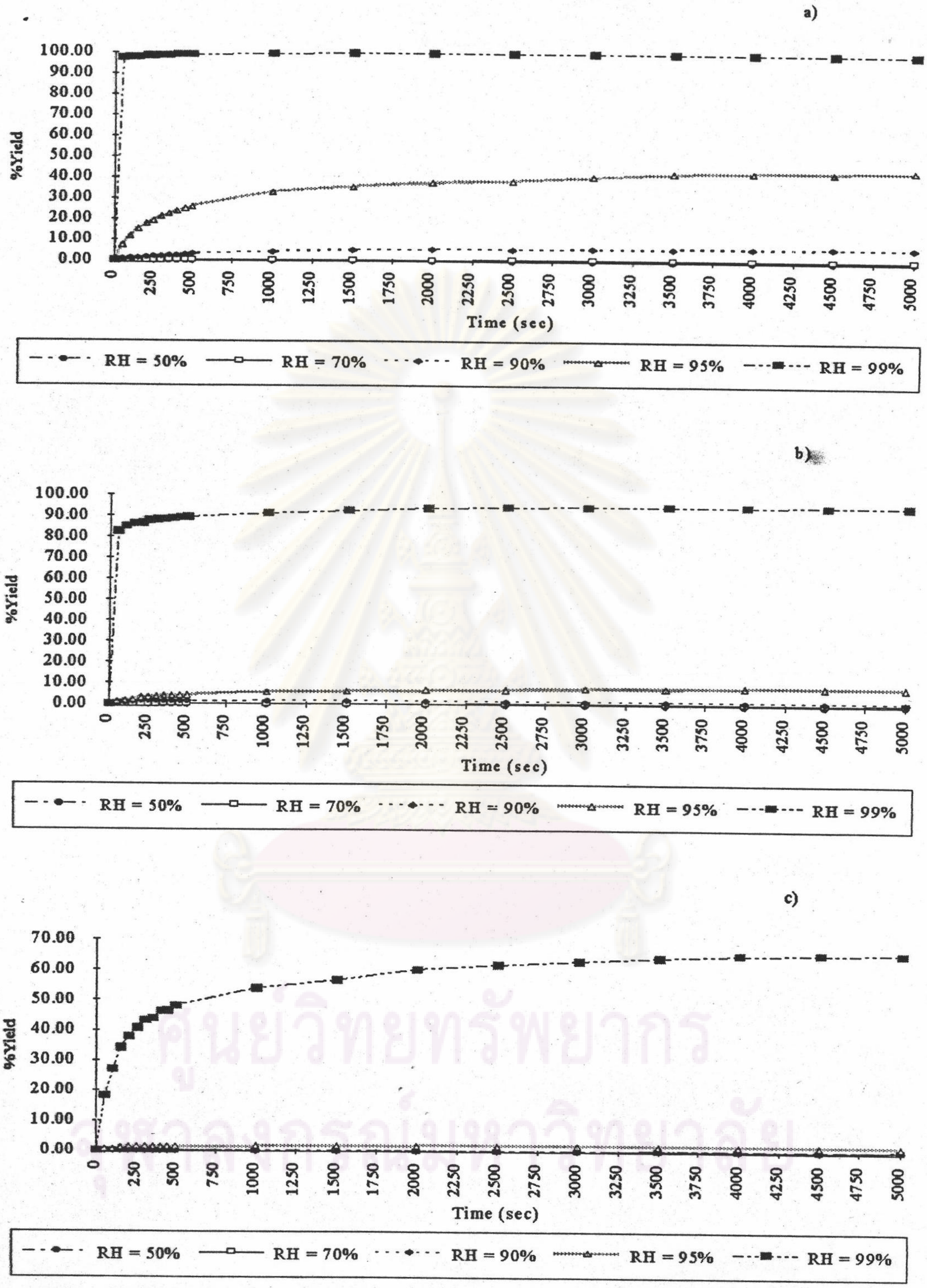


Figure 4.32 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class E at [Fe] = 0.1 mg/m³ and $[NH_3]$ = 100 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

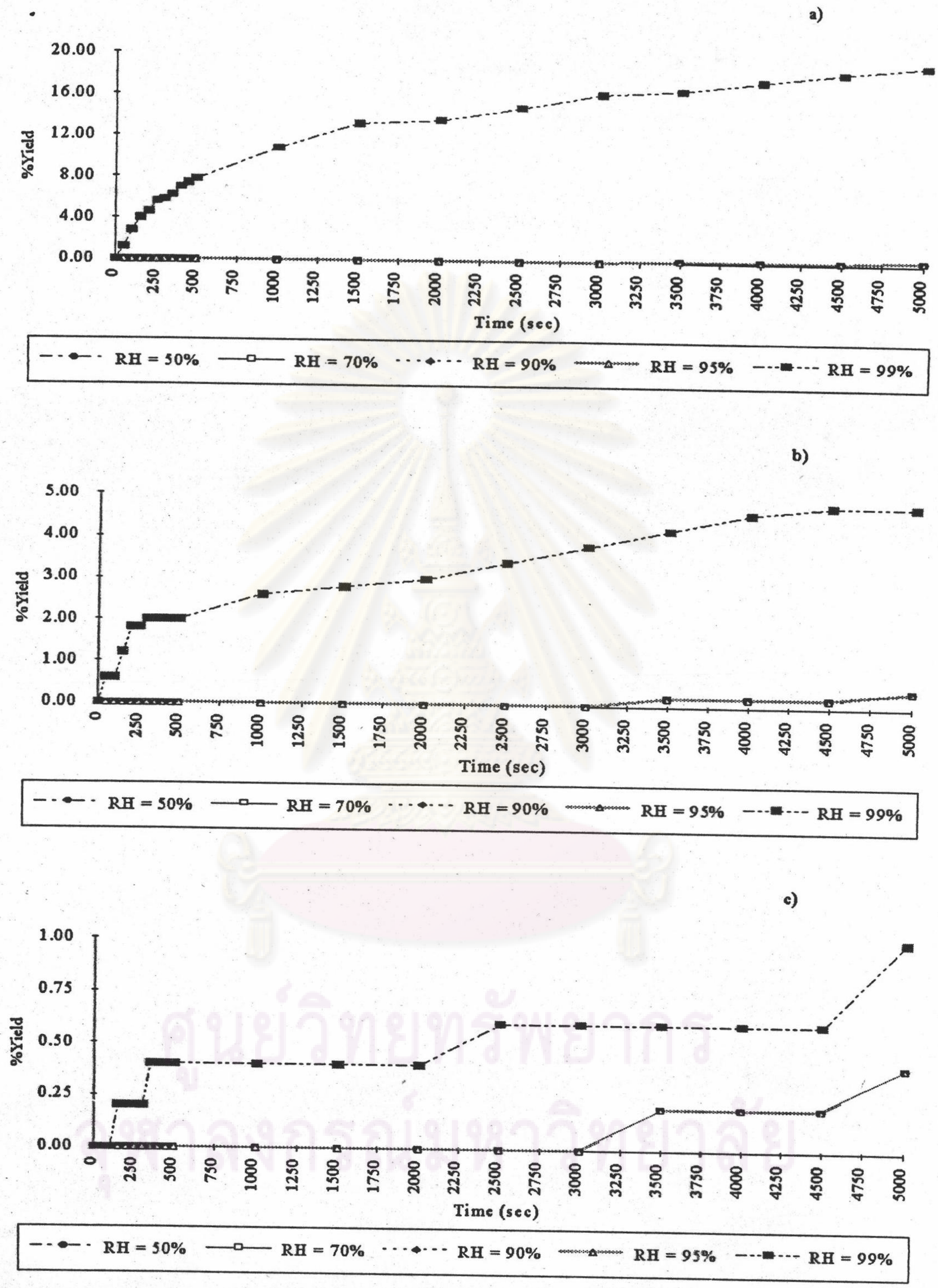


Figure 4.33 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class F at [Fe] = 1201 ng/m^3 and [NH_3] = 50 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

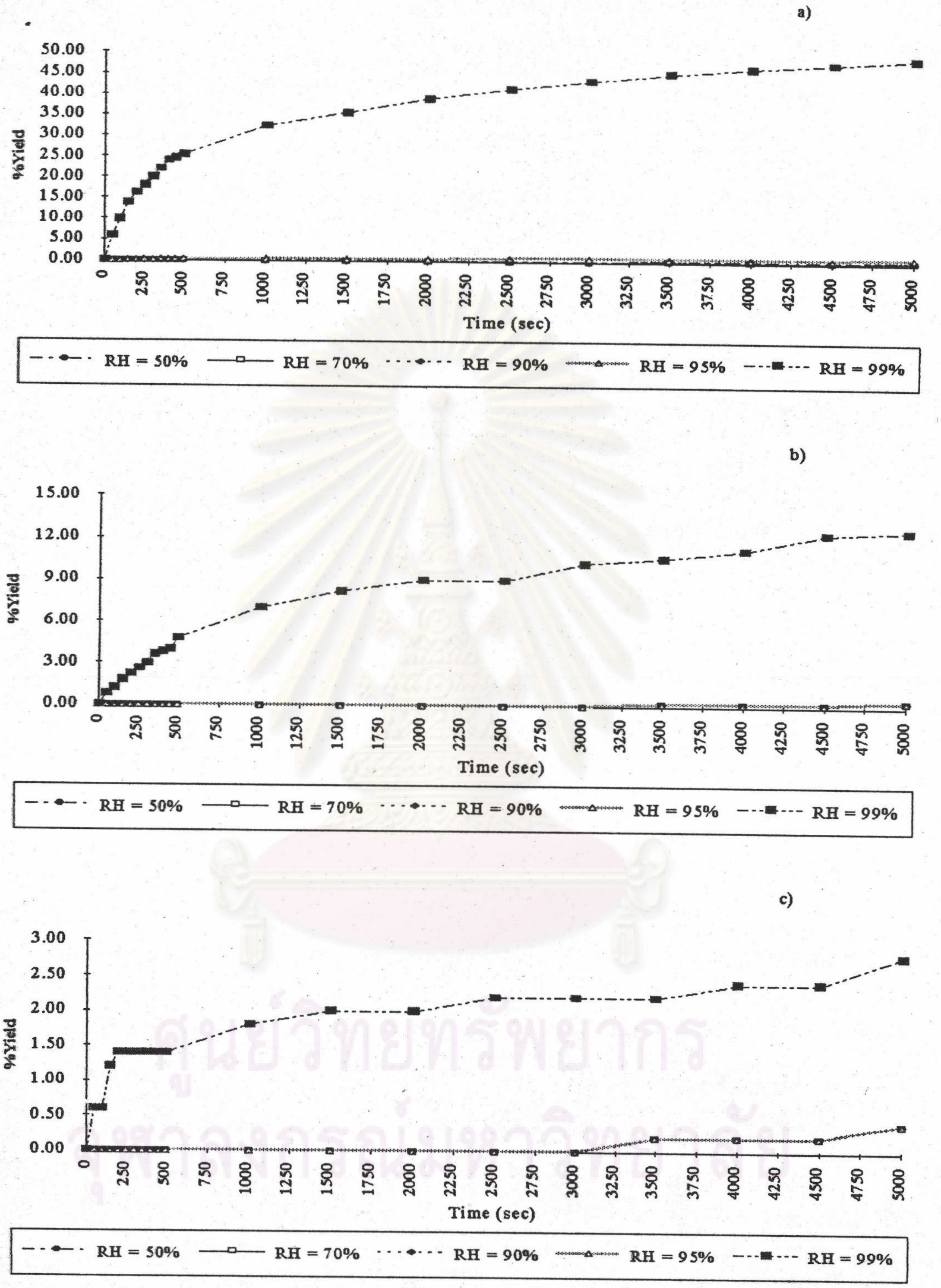


Figure 4.34 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class F at [Fe] = 1201 ng/m^3 and [NH_3] = 80 ppb

a) T = 20 °C b) T = 25 °C c) T = 30 °C

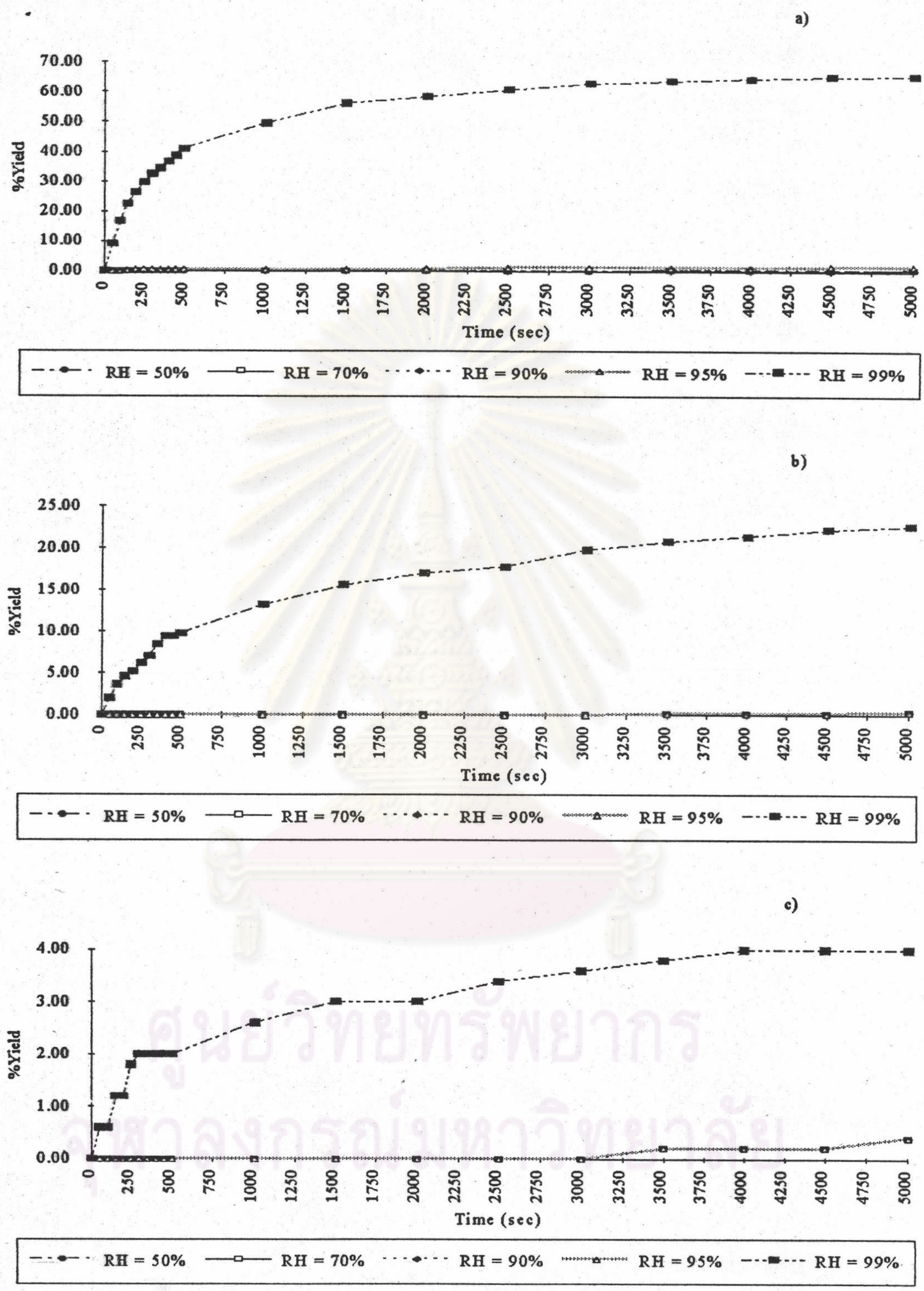


Figure 4.35 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class F at [Fe] = 1201 ng/m³ and [NH_3] = 100 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

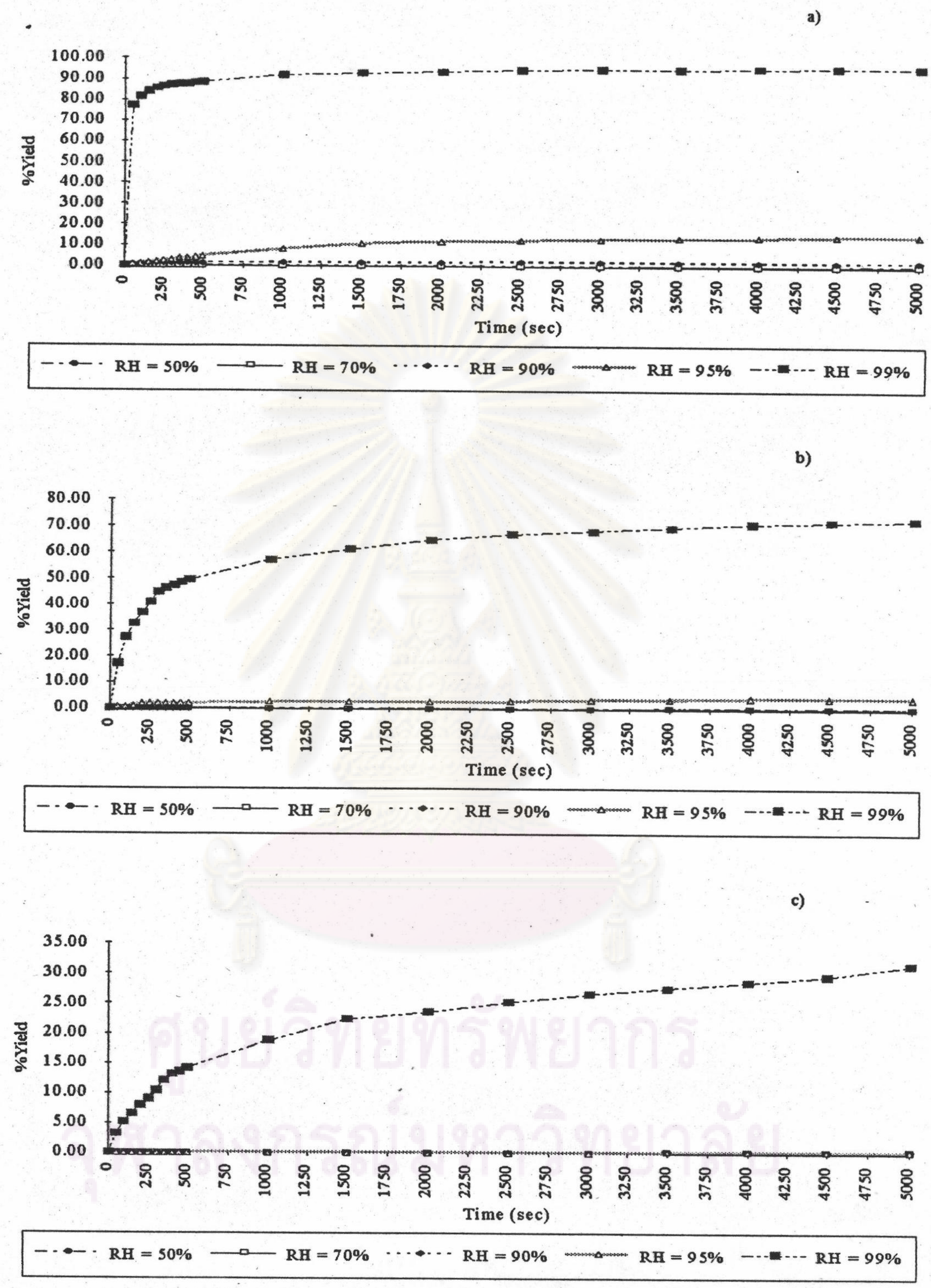


Figure 4.36 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class F at [Fe] = 0.1 mg/m³ and [NH_3] = 50 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

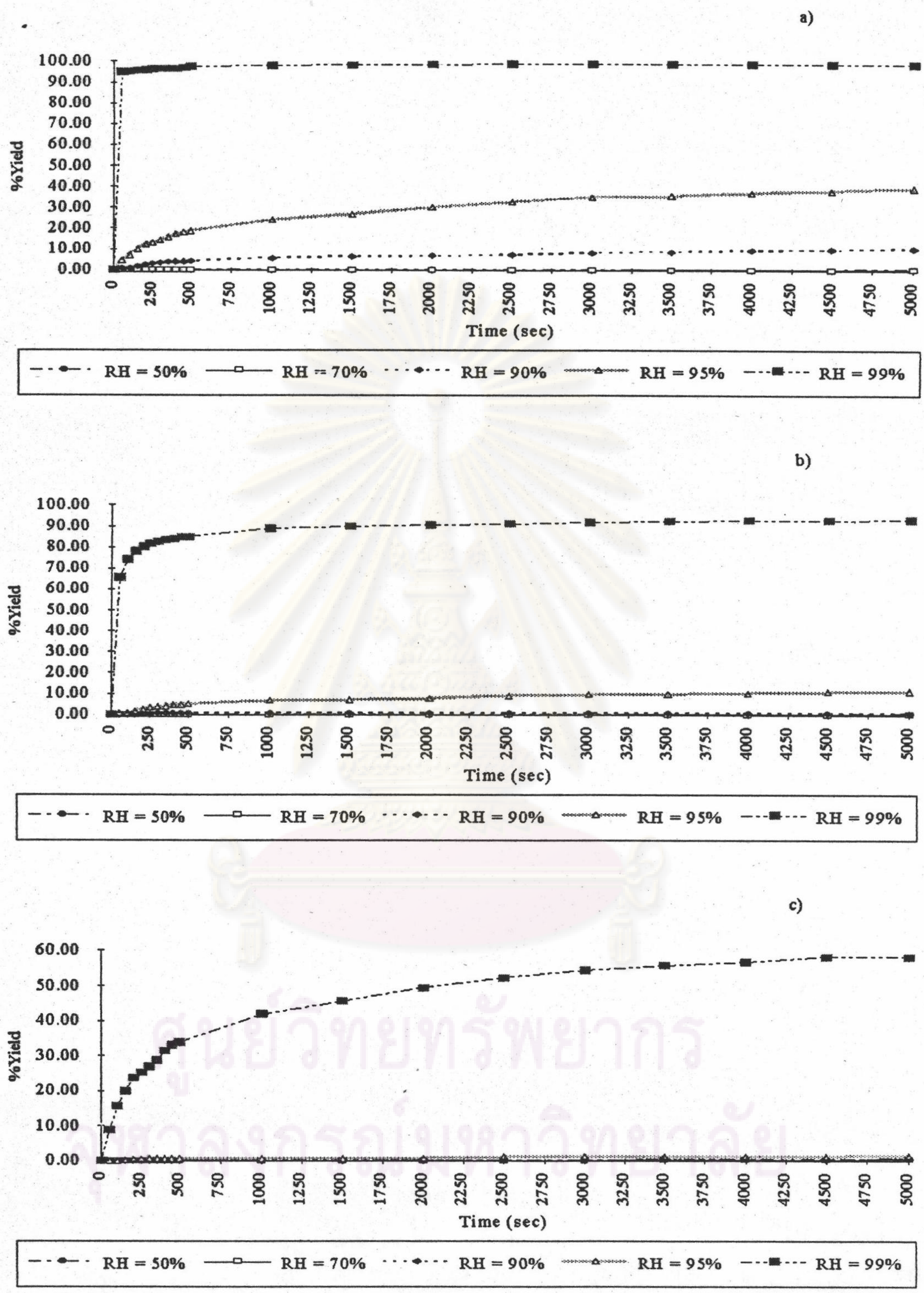


Figure 4.37 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class F at [Fe] = 0.1 mg/m³ and $[NH_3]$ = 80 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

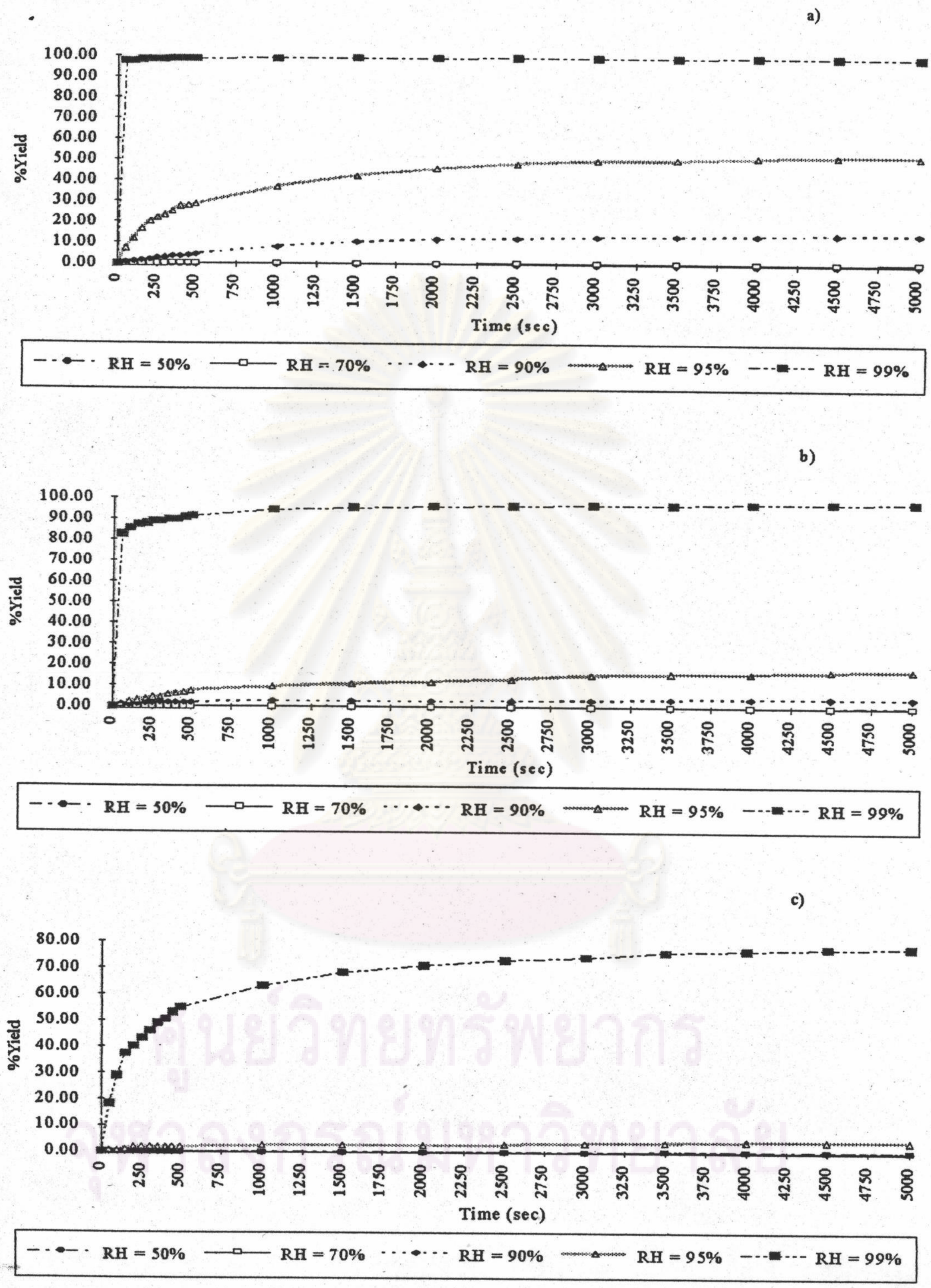


Figure 4.38 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Rich Environment for Atmospheric Stability Class F at [Fe] = 0.1 mg/m³ and [NH_3] = 100 ppb

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

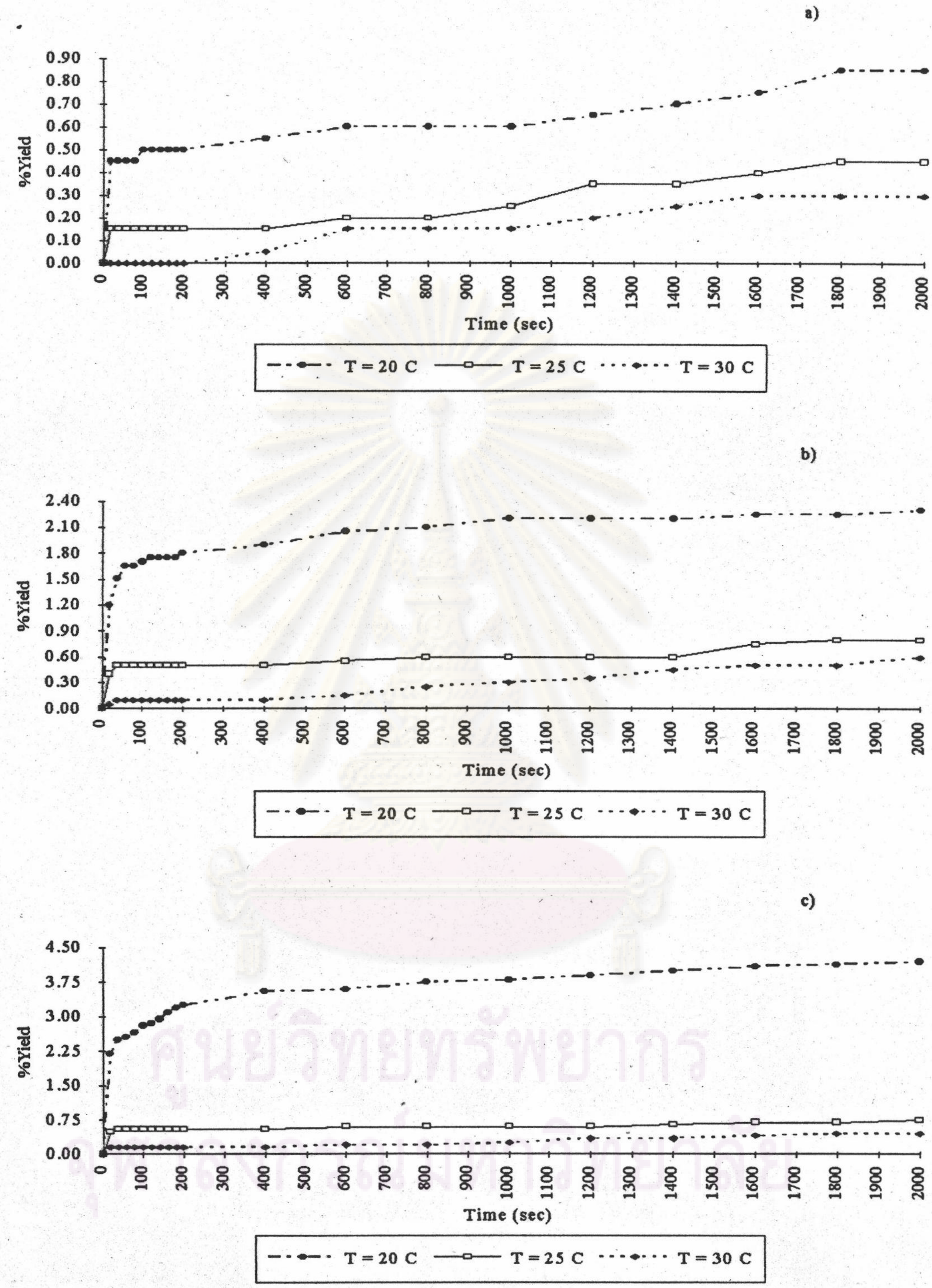


Figure 4.39 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Deficient Environment for Atmospheric Stability Class C at Relative Humidity = 99% and [Fe] = 1201 ng/m^3

a) [NH_3] = 50 ppb b) [NH_3] = 80 ppb c) [NH_3] =100 ppb

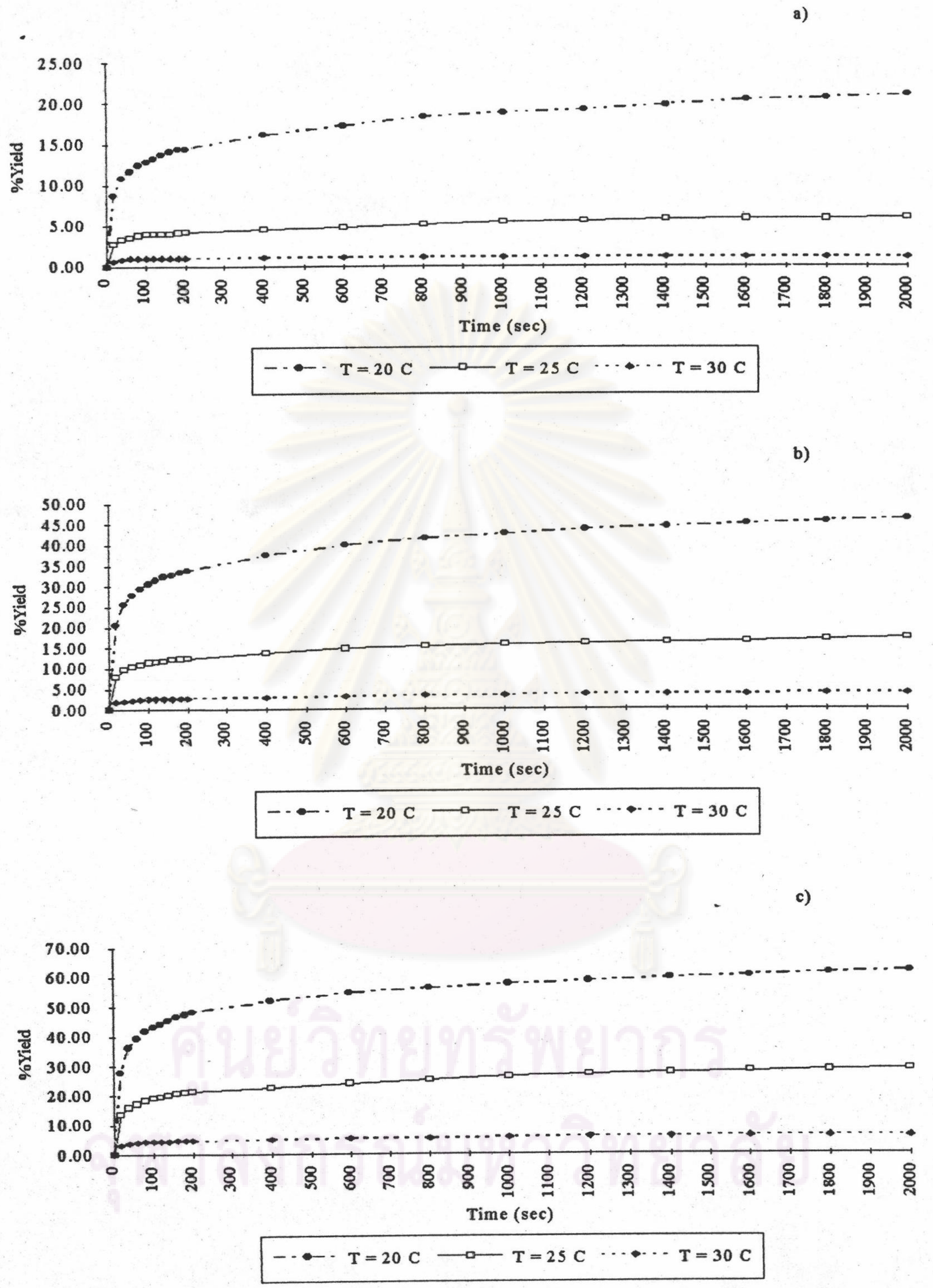


Figure 4.40 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Deficient Environment for Atmospheric Stability Class C at Relative Humidity = 99% and [Fe] = 0.1 mg/m^3

a) [NH_3] = 50 ppb b) [NH_3] = 80 ppb c) [NH_3] =100 ppb

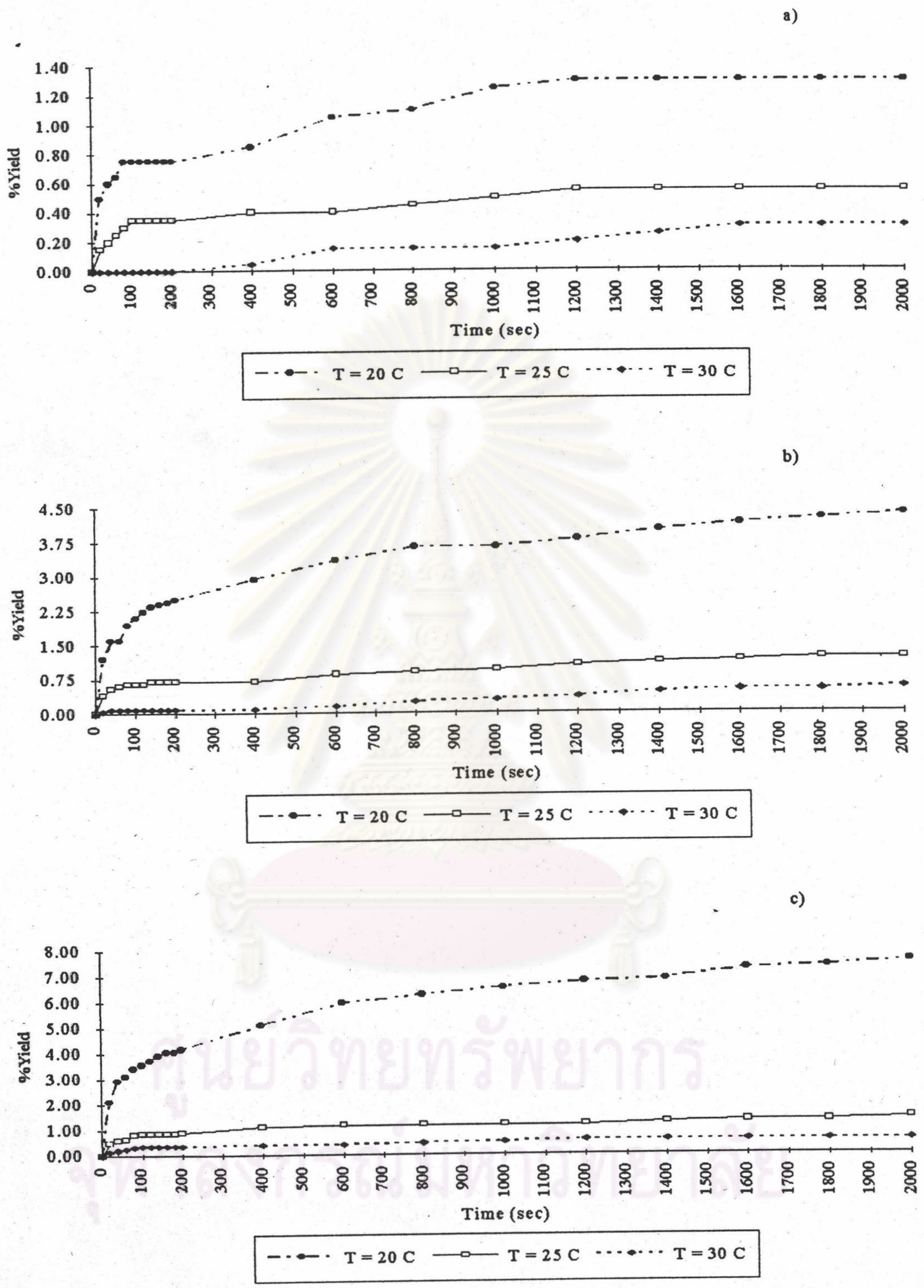


Figure 4.41 **%Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Deficient Environment for Atmospheric Stability Class D at Relative Humidity = 99% and [Fe] = 1201 ng/m^3**

a) [NH_3] = 50 ppb **b) [NH_3] = 80 ppb** **c) [NH_3] =100 ppb**

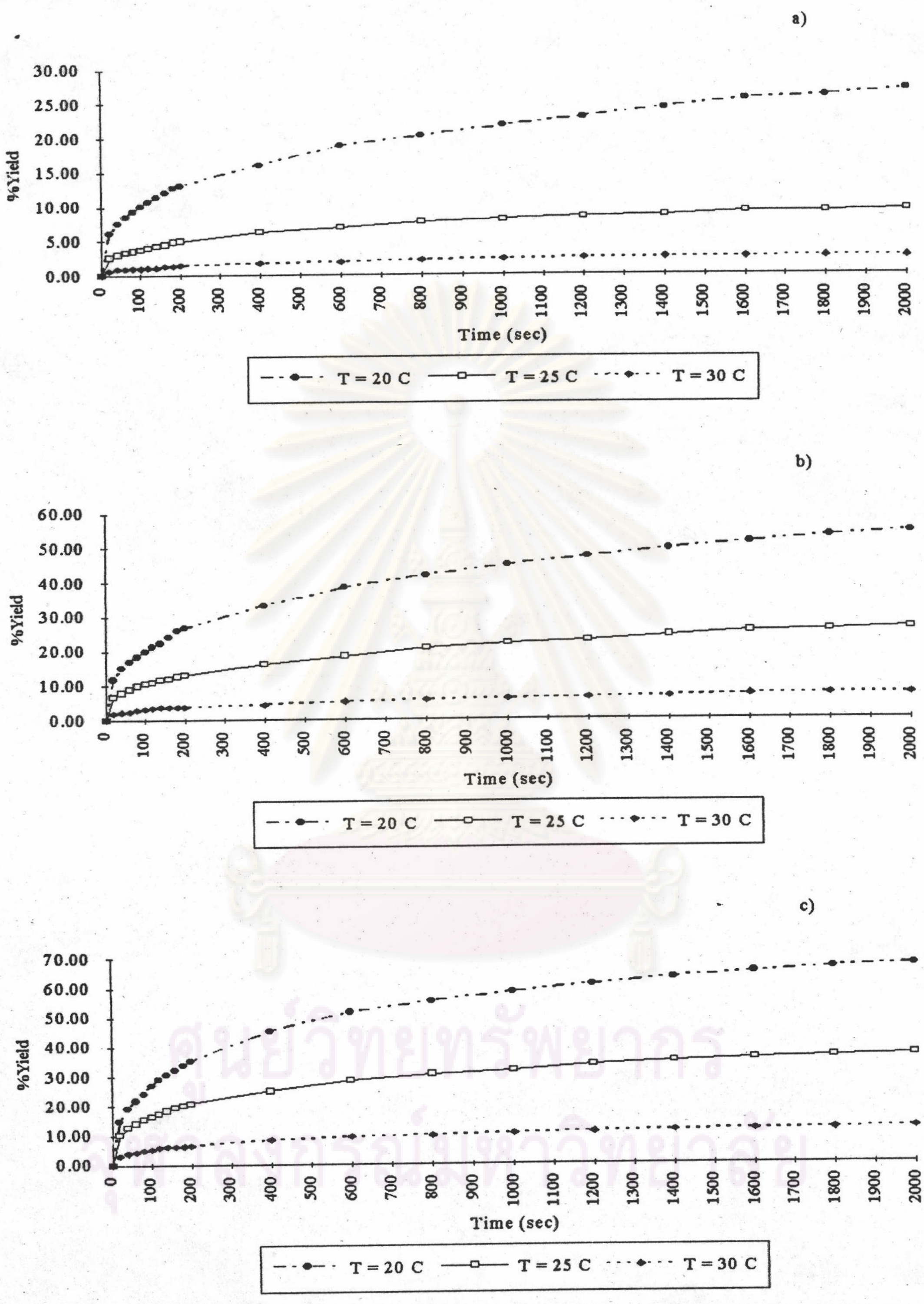


Figure 4.42 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Deficient Environment for Atmospheric Stability Class D at Relative Humidity = 99% and [Fe] = 0.1 mg/m^3

a) [NH_3] = 50 ppb **b) [NH_3] = 80 ppb** **c) [NH_3] =100 ppb**

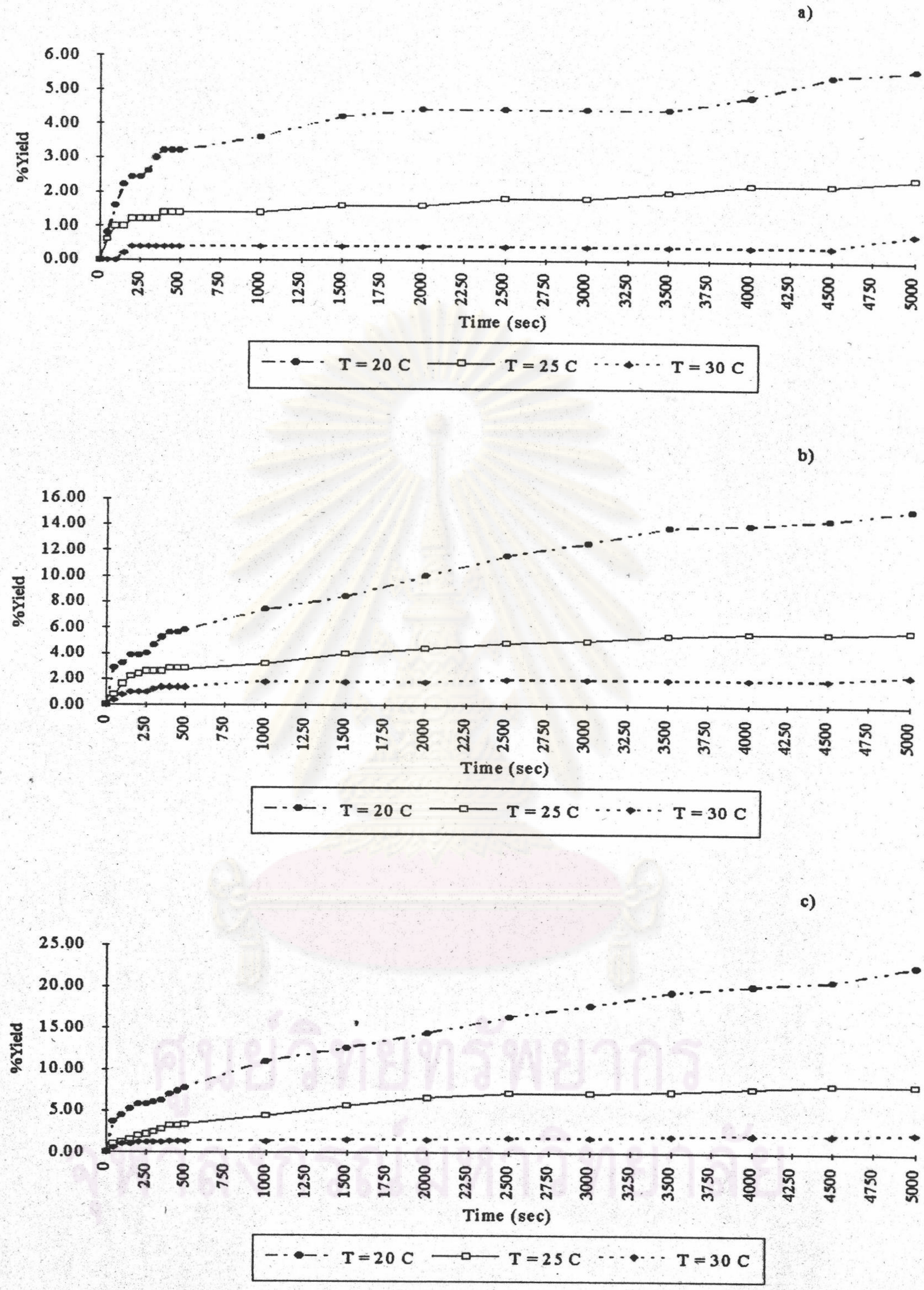


Figure 4.43 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Deficient Environment for Atmospheric Stability Class E at Relative Humidity = 99% and [Fe] = 1201 ng/m³

a) $[NH_3]$ = 50 ppb **b) $[NH_3]$ = 80 ppb** **c) $[NH_3]$ =100 ppb**

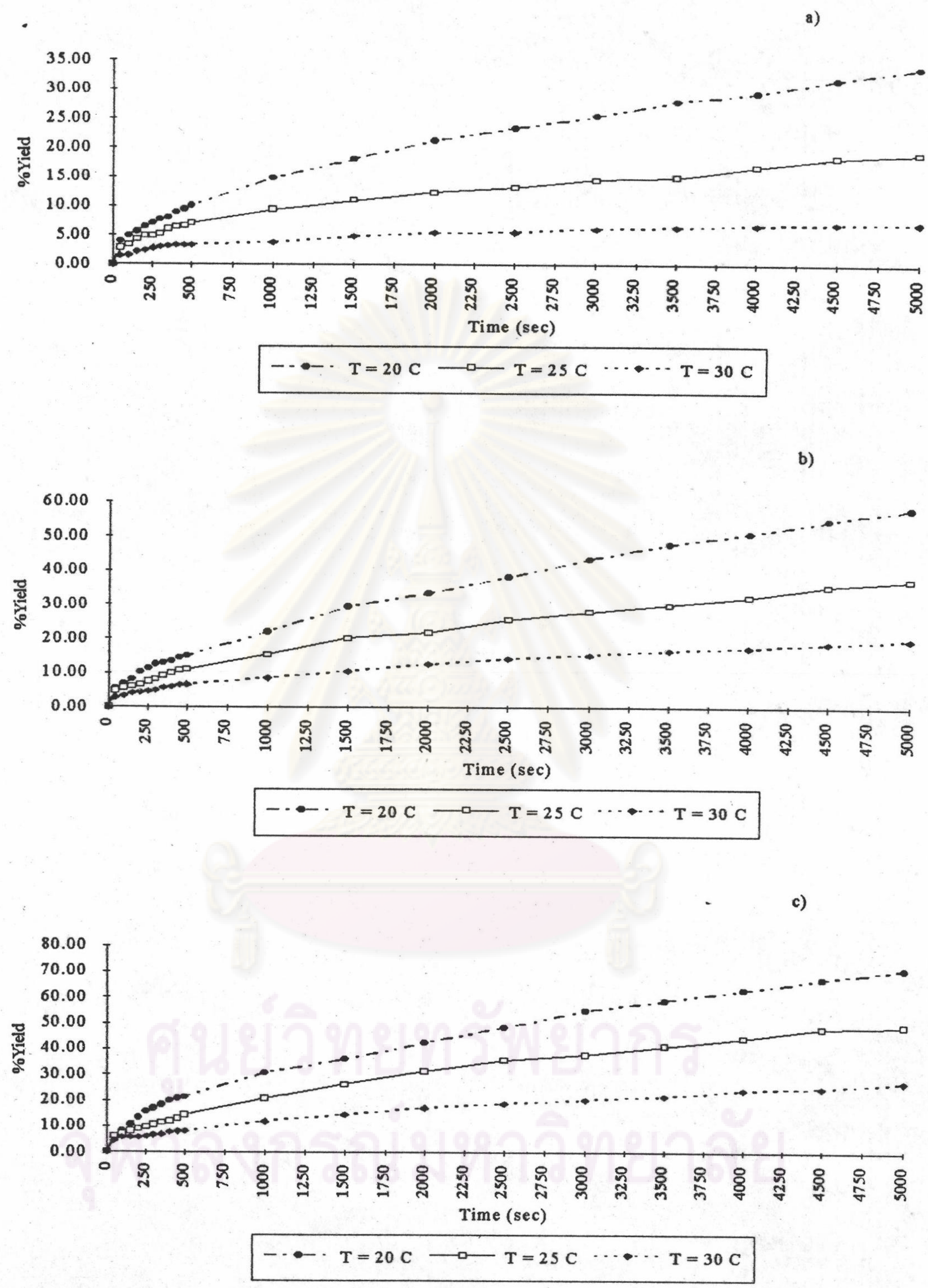


Figure 4.44 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Deficient Environment for Atmospheric Stability Class E at Relative Humidity = 99% and [Fe] = 0.1 mg/m³

a) [NH_3] = 50 ppb   b) [NH_3] = 80 ppb   c) [NH_3] =100 ppb

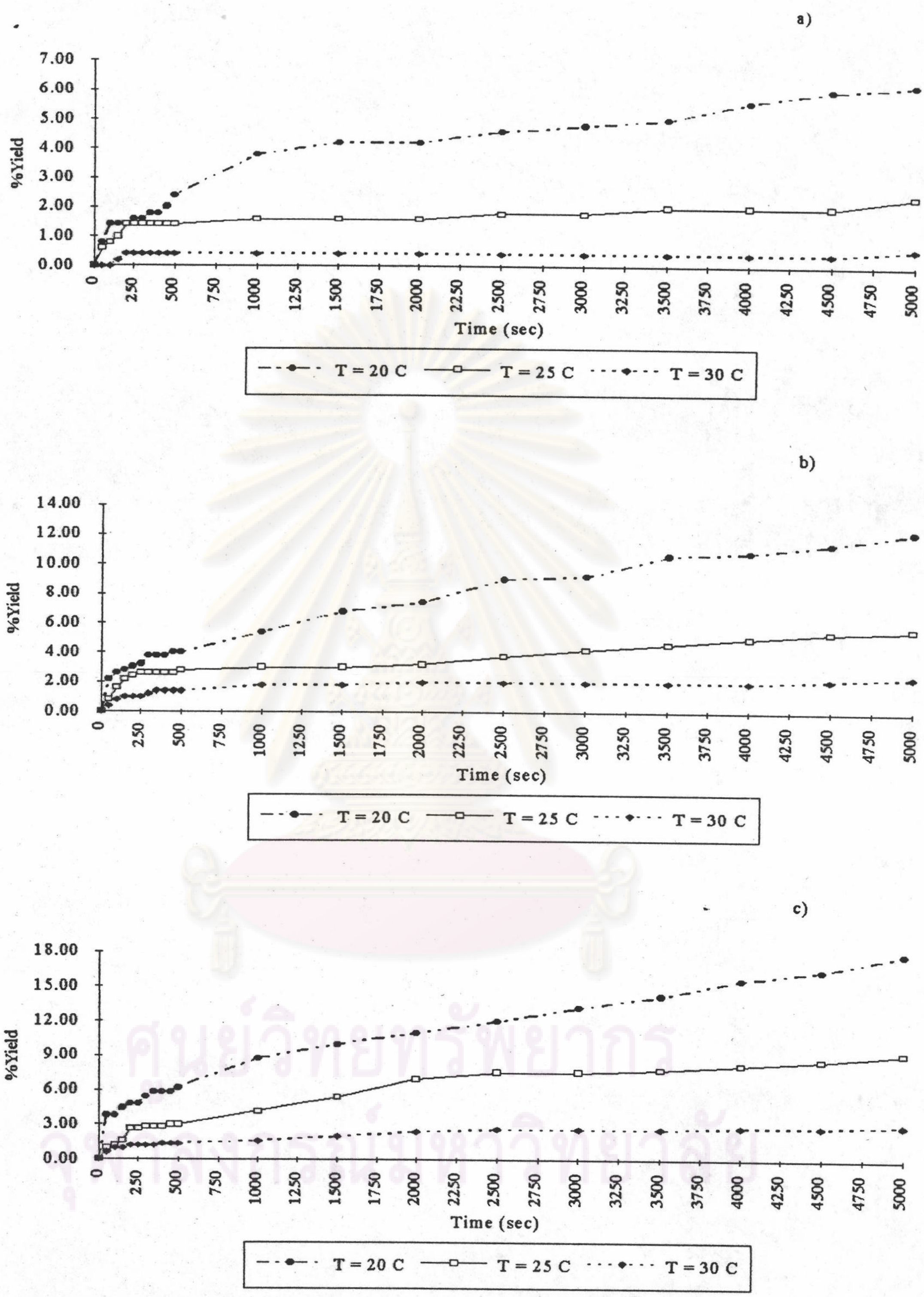


Figure 4.45 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Deficient Environment for Atmospheric Stability Class F at Relative Humidity = 99% and [Fe] = 1201 ng/m^3

a) [NH_3] = 50 ppb **b) [NH_3] = 80 ppb** **c) [NH_3] =100 ppb**

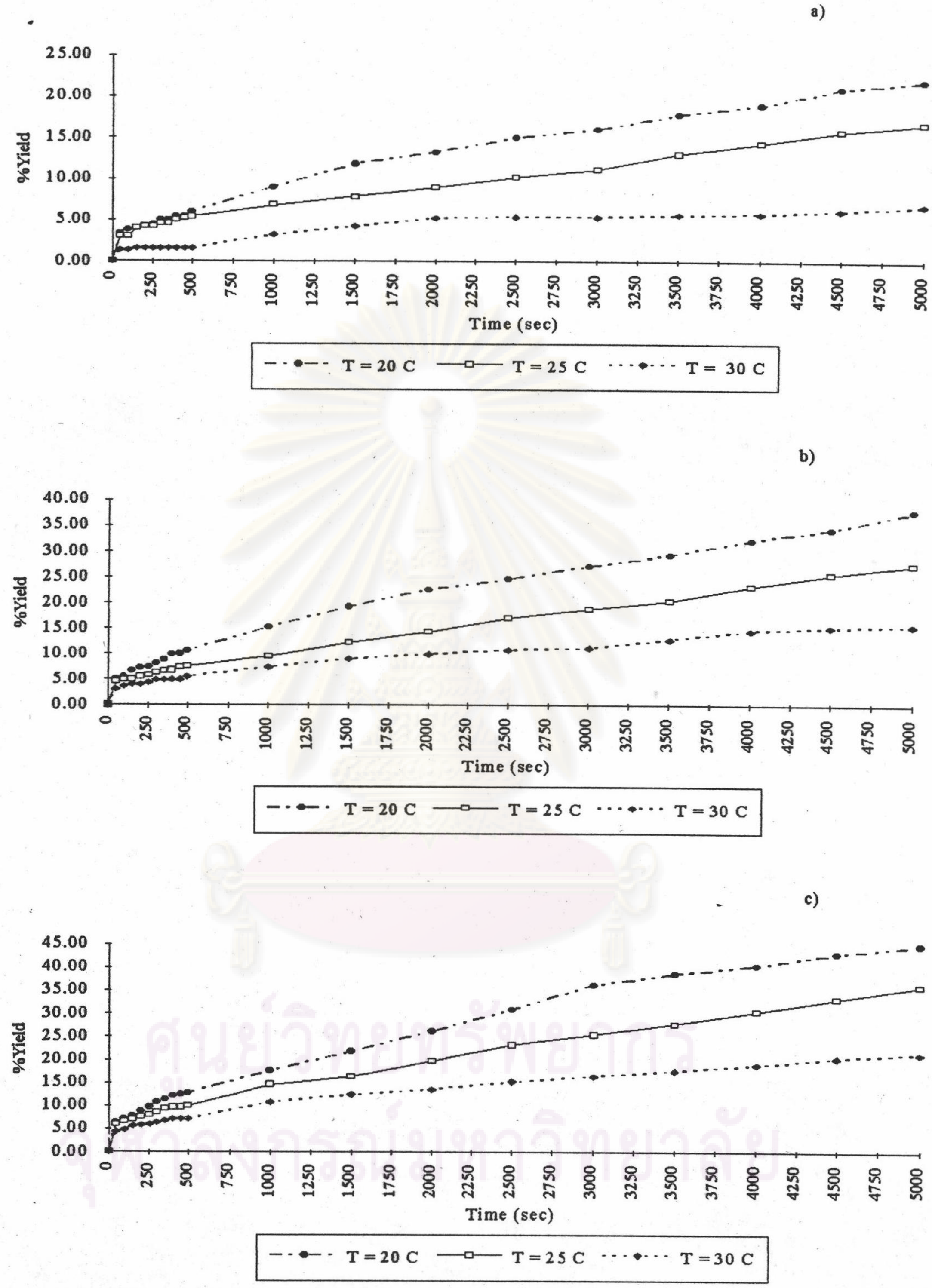


Figure 4.46 %Yield VS Time of Freiberg(1974)'s Reaction Rate in Ammonia-Deficient Environment for Atmospheric Stability Class F at Relative Humidity = 99% and [Fe] = 0.1 mg/m³

a) [NH_3] = 50 ppb **b) [NH_3] = 80 ppb** **c) [NH_3] =100 ppb**

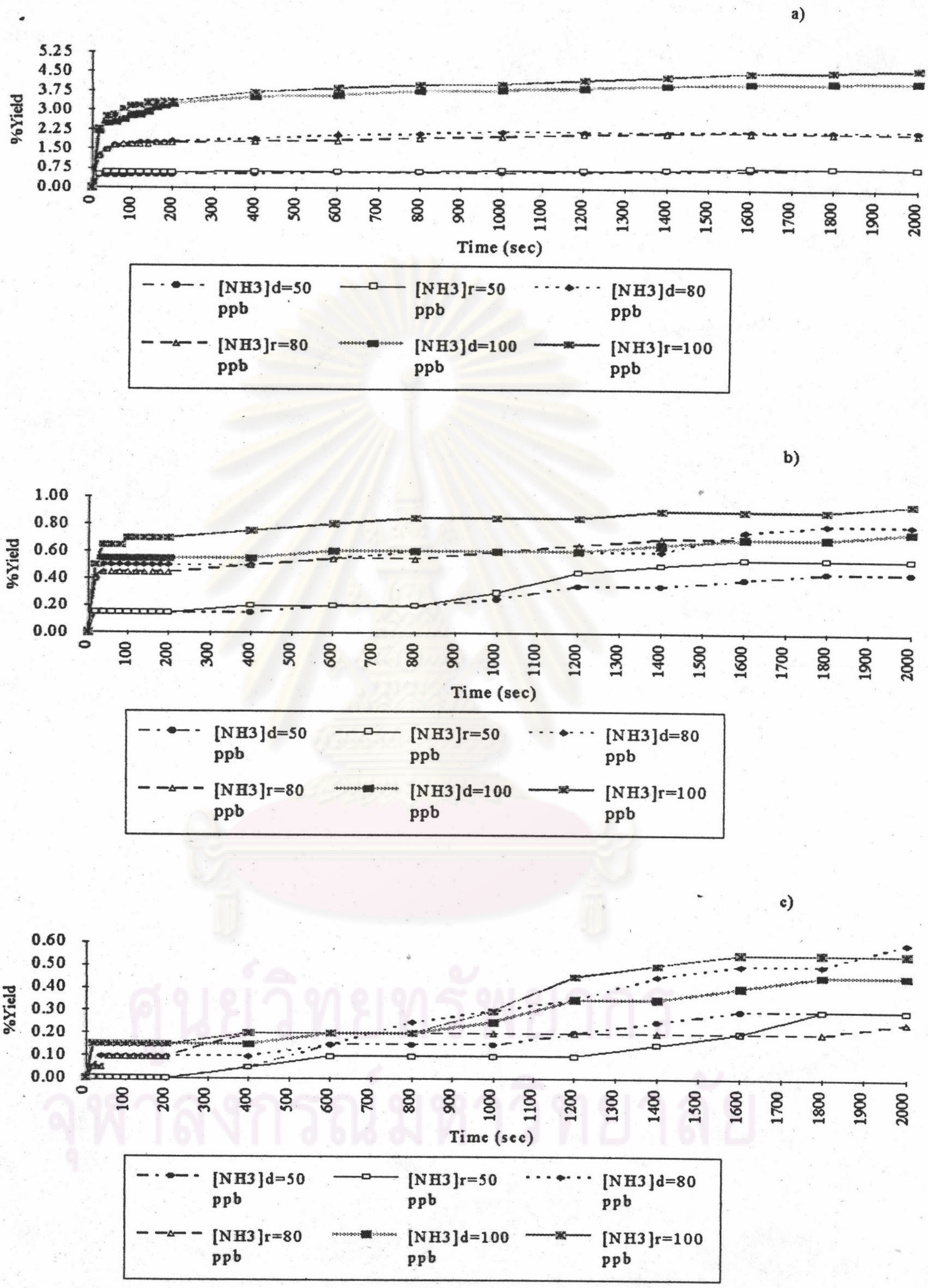
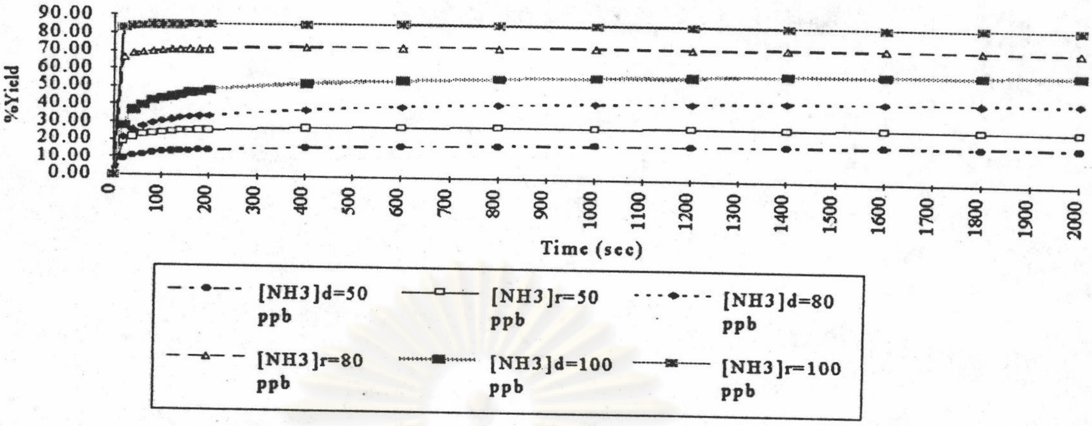


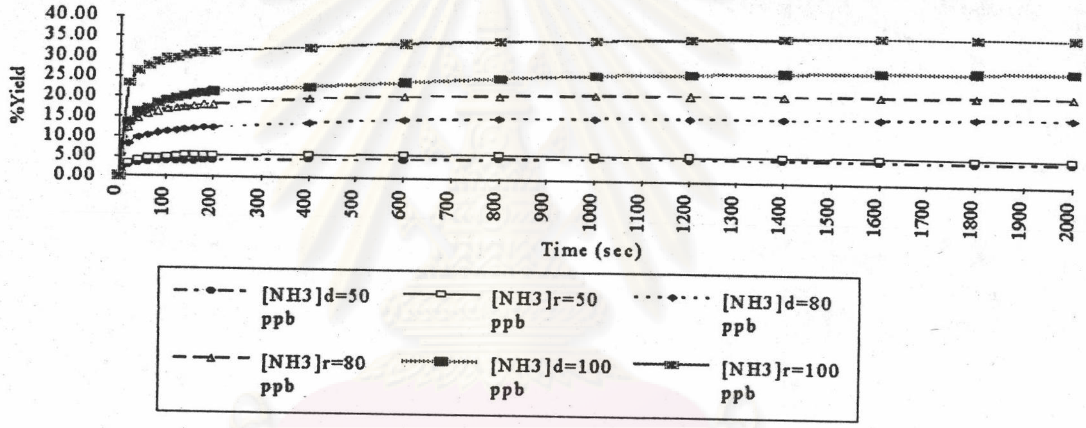
Figure 4.47 Comparison of Freiberg(1974)'s Yield between in Ammonia-Rich Environment and in Ammonia-Deficient Environment for Atmospheric Stability Class C at Relative Humidity = 99% and [Fe] = 1201 ng/m³

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

a)



b)



c)

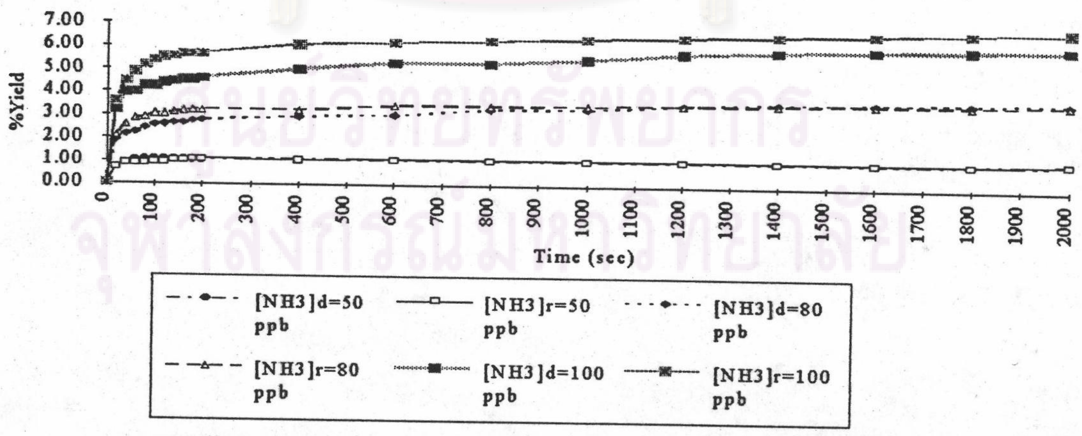


Figure 4.48 Comparison of Freiberg(1974)'s Yield between in Ammonia-Rich Environment and in Ammonia-Deficient Environment for Atmospheric Stability Class C at Relative Humidity = 99% and [Fe] = 0.1 mg/m³

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

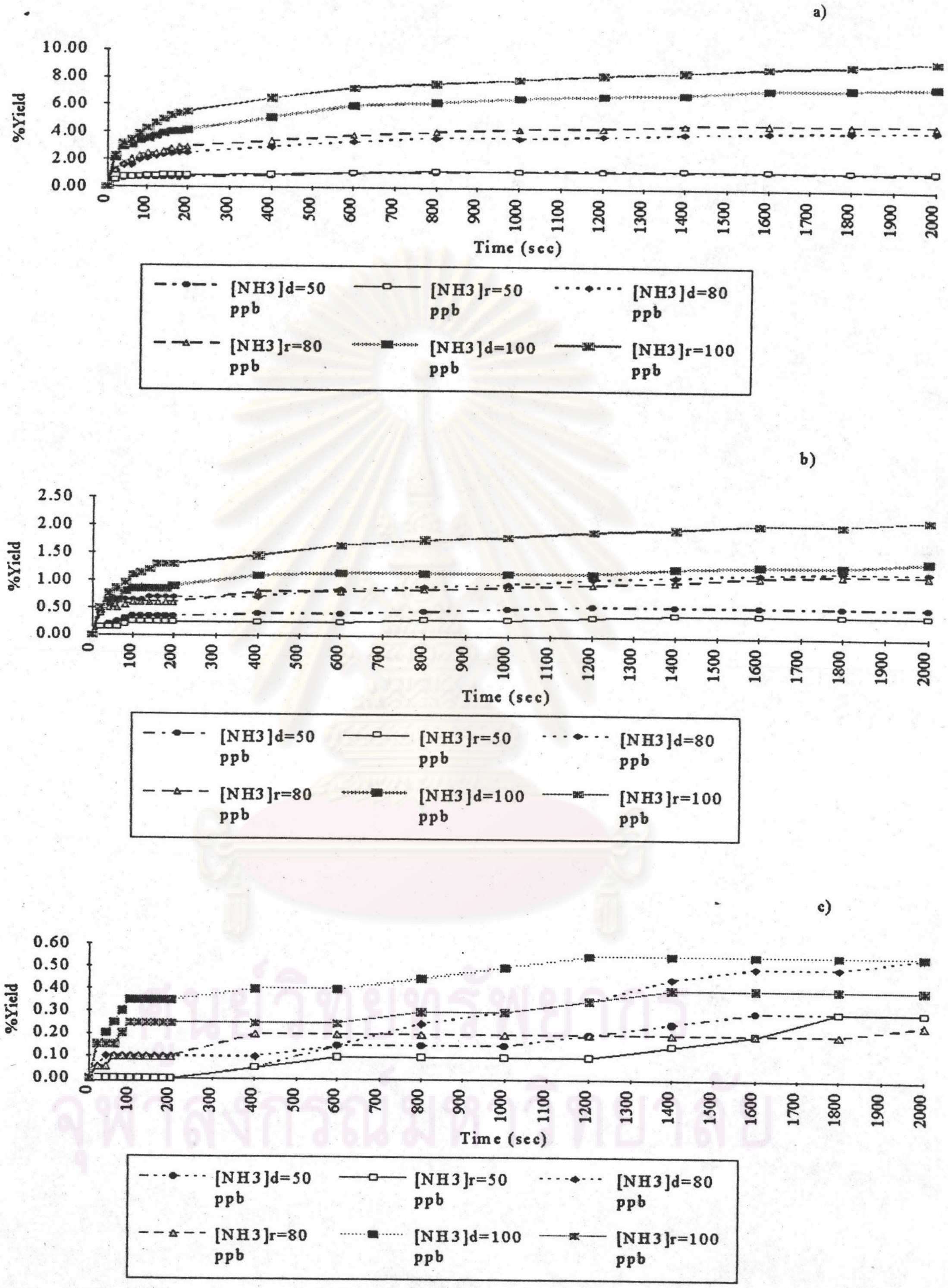


Figure 4.49 Comparison of Freiberg(1974)'s Yield between in Ammonia-Rich Environment and in Ammonia-Deficient Environment for Atmospheric Stability Class D at Relative Humidity = 99% and [Fe] = 1201 ng/m³

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

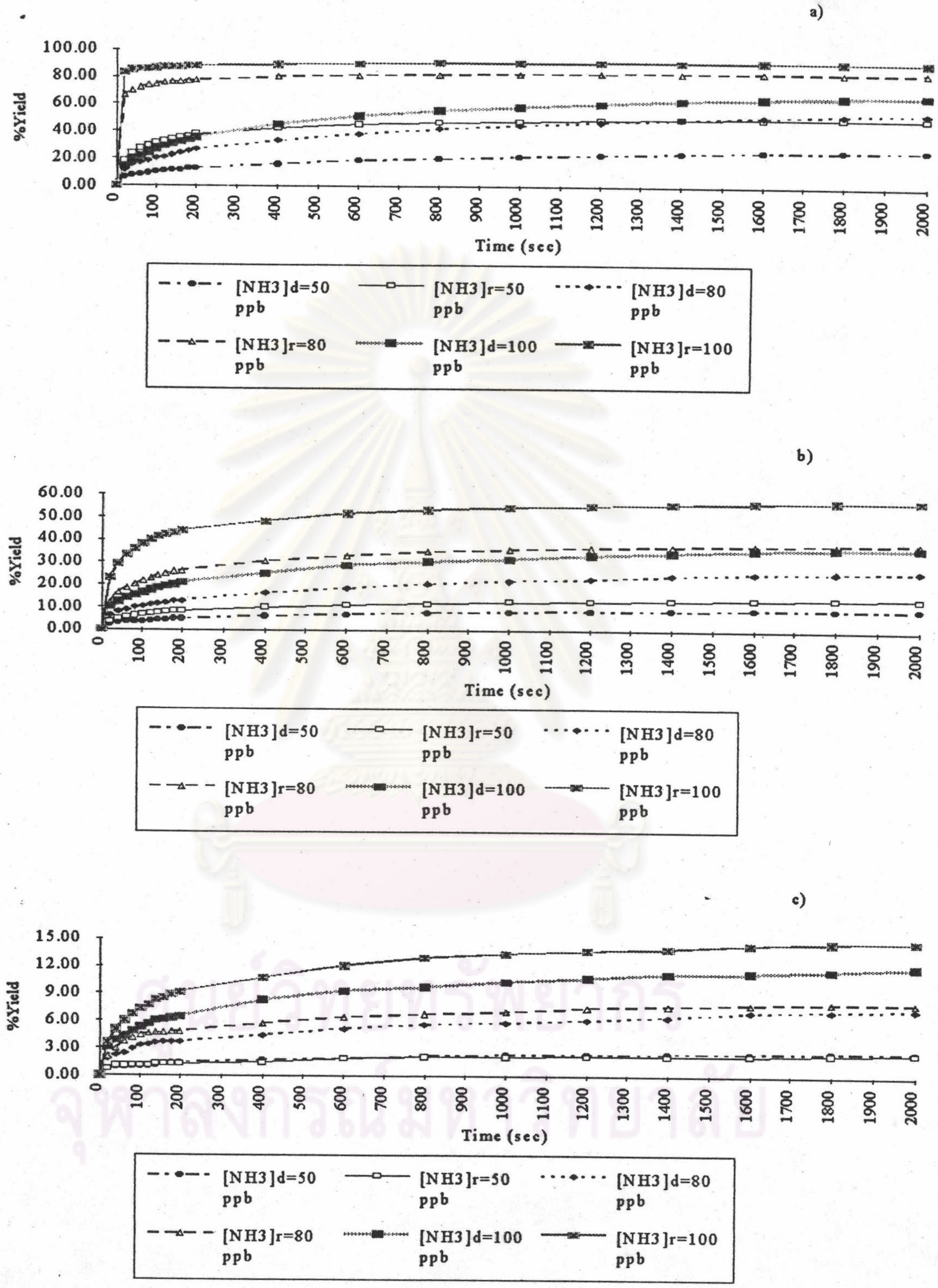


Figure 4.50 Comparison of Freiberg(1974)'s Yield between in Ammonia-Rich Environment and in Ammonia-Deficient Environment for Atmospheric Stability Class D at Relative Humidity = 99% and [Fe] = 0.1 mg/m³

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

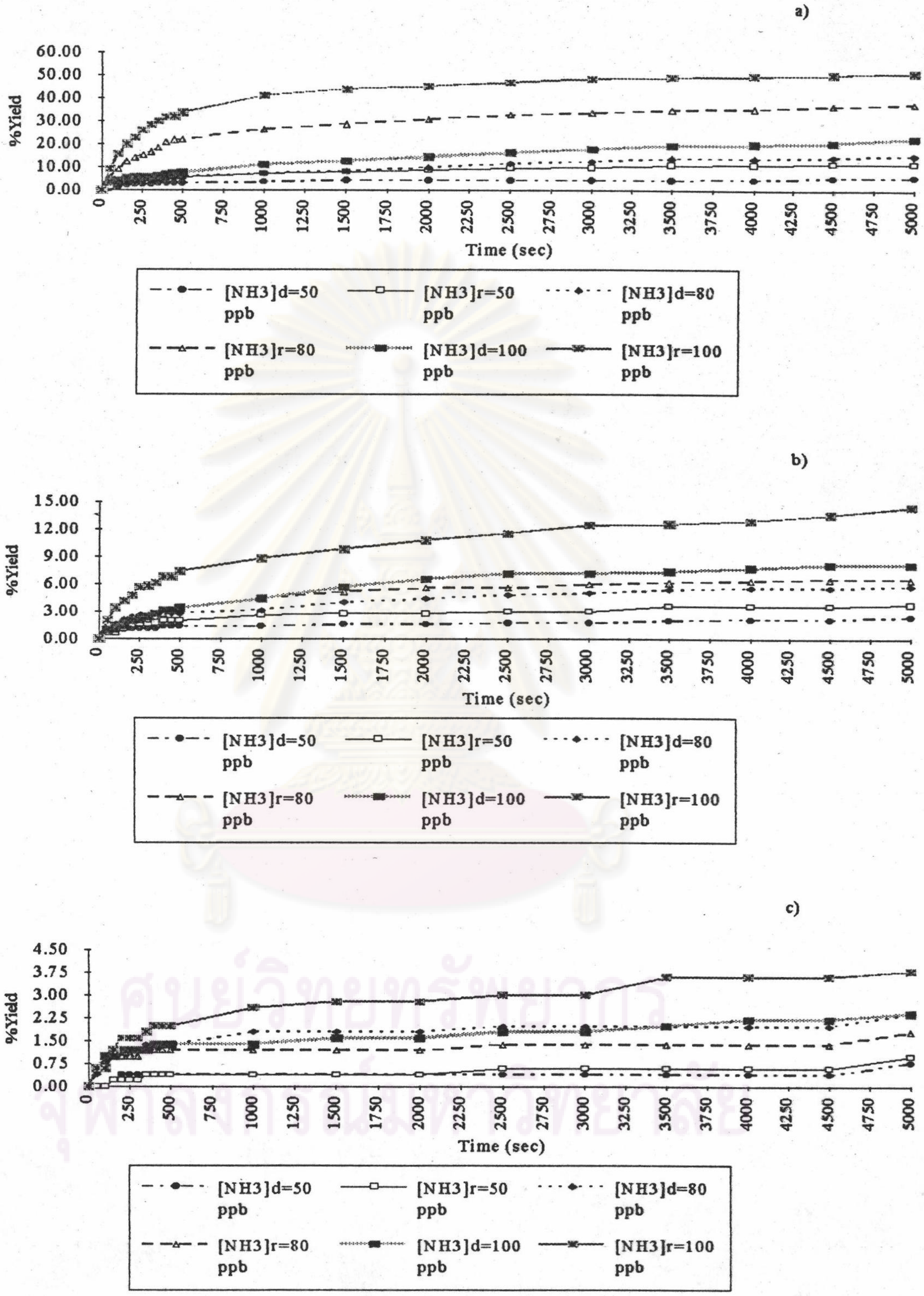


Figure 4.51 Comparison of Freiberg(1974)'s Yield between in Ammonia-Rich Environment and in Ammonia-Deficient Environment for Atmospheric Stability Class E at Relative Humidity = 99% and [Fe] = 1201 ng/m³

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

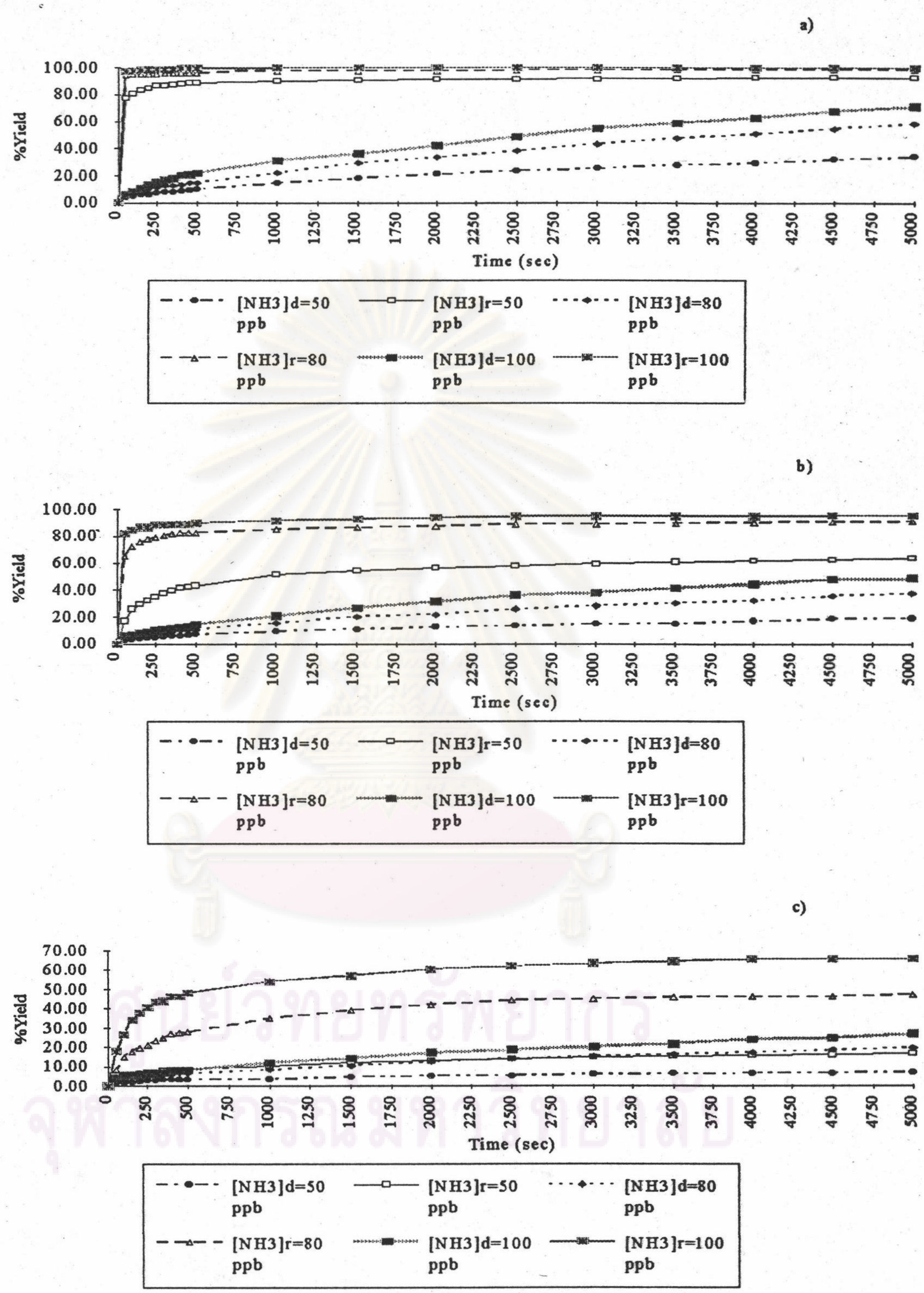


Figure 4.52 Comparison of Freiberg(1974)'s Yield between in Ammonia-Rich Environment and in Ammonia-Deficient Environment for Atmospheric Stability Class E at Relative Humidity = 99% and [Fe] = 0.1 mg/m³

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

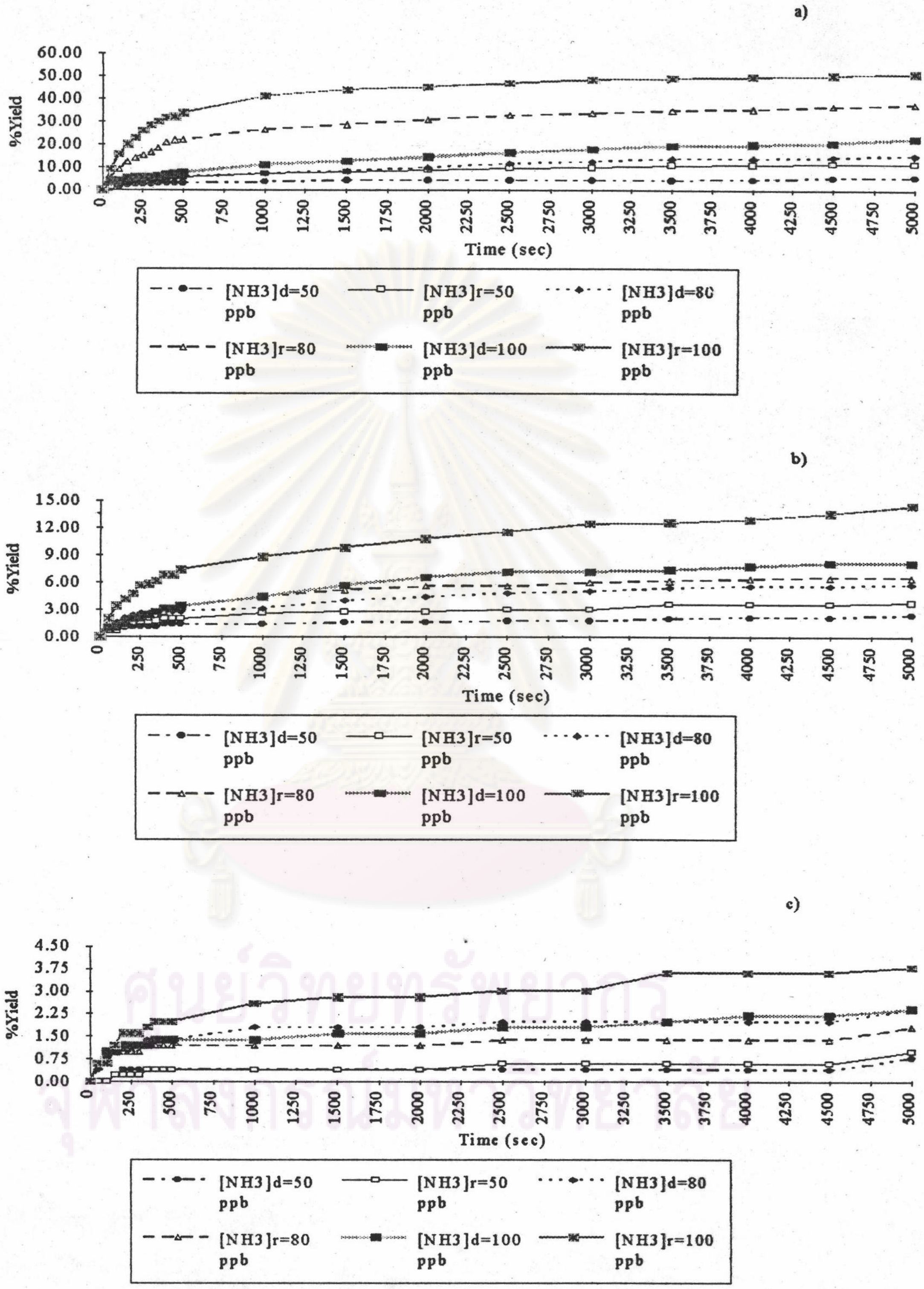
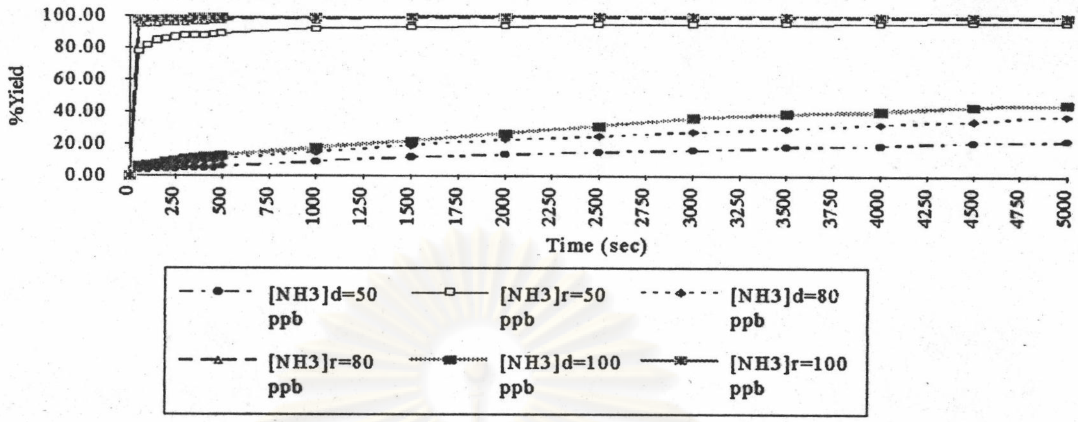


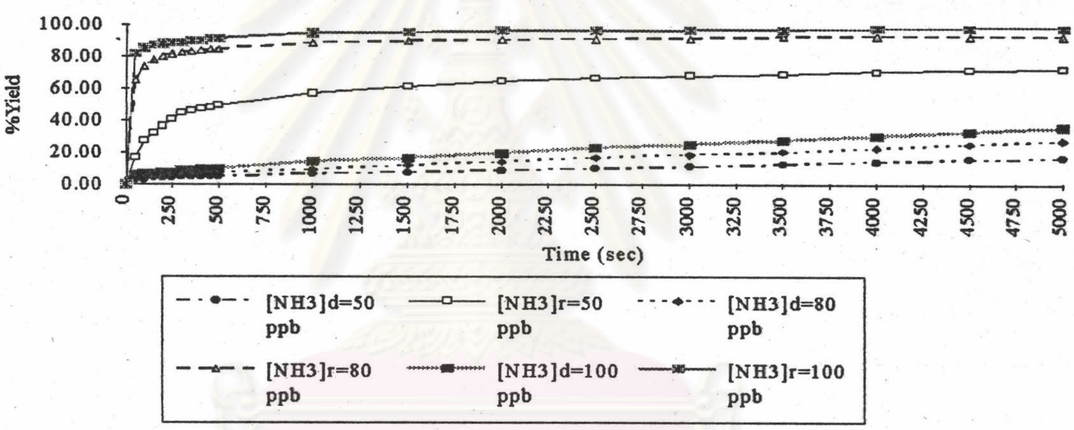
Figure 4.53 Comparison of Freiberg(1974)'s Yield between in Ammonia-Rich Environment and in Ammonia-Deficient Environment for Atmospheric Stability Class F at Relative Humidity = 99% and [Fe] = 1201 ng/m³

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

a)



b)



c)

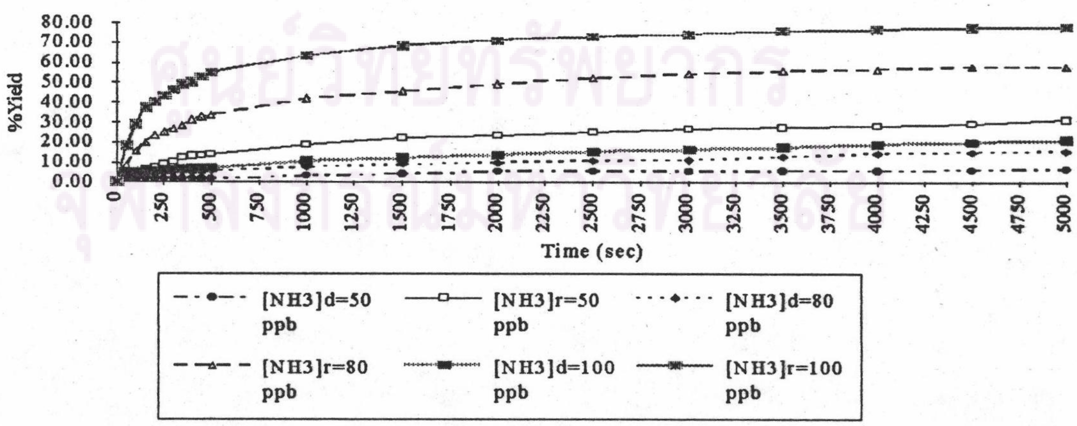
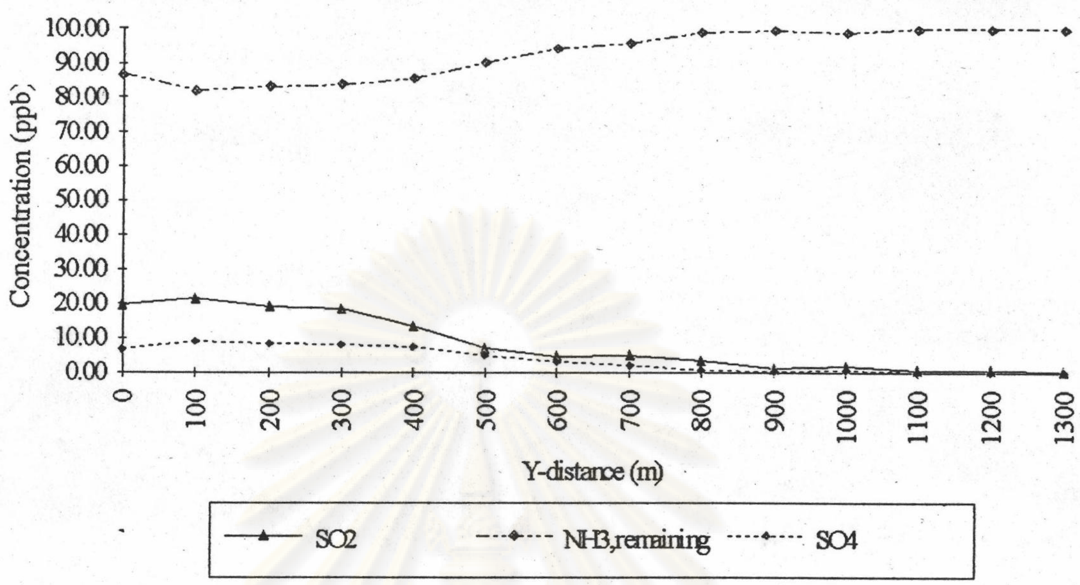


Figure 4.54 Comparison of Freiberg(1974)'s Yield between in Ammonia-Rich Environment and in Ammonia-Deficient Environment for Atmospheric Stability Class F at Relative Humidity = 99% and [Fe] = 0.1 mg/m³

a) T = 20 °C **b) T = 25 °C** **c) T = 30 °C**

a)



b)

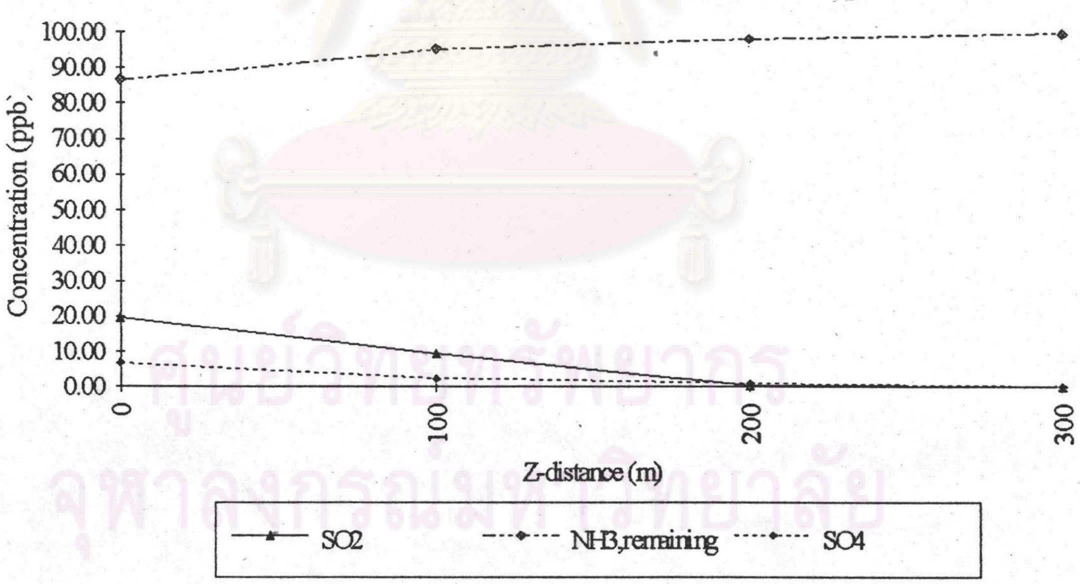
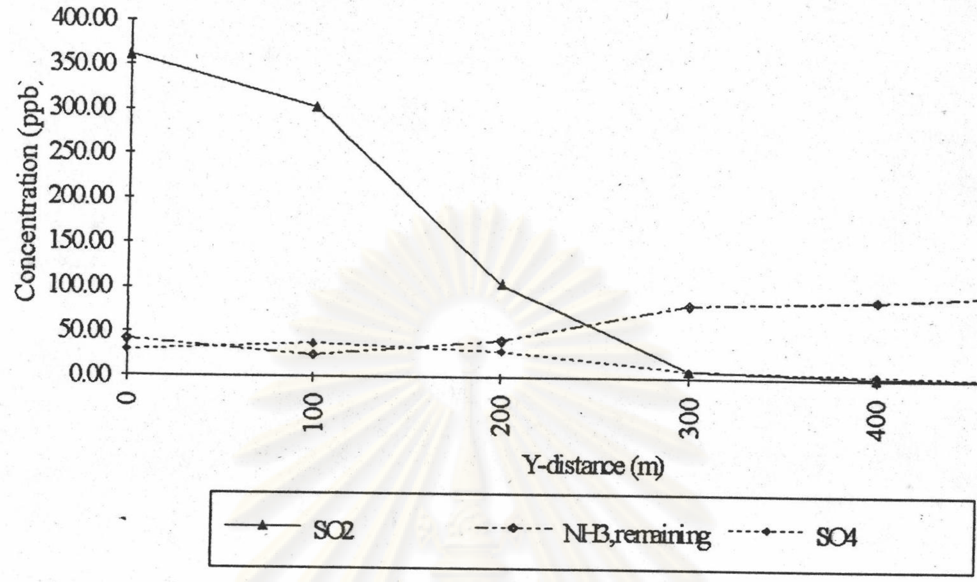


Figure 4.55 Sulfur Dioxide, Remaining Ammonia and Sulfate Concentration Profiles of Freiberg (1974)'s Reaction Rate in Ammonia-Deficient Environment for Atmospheric Stability Class D at 4 km Downwind from the Source, Relative Humidity = 99%, T = 25 °C, [Fé] = 0.1 mg/m^3 and [NH_3] = 100 ppb

a) Varying Y-Distance (Fixed z=0) **b) Varing Z-Distance (Fixed y=0)**

a)



b)

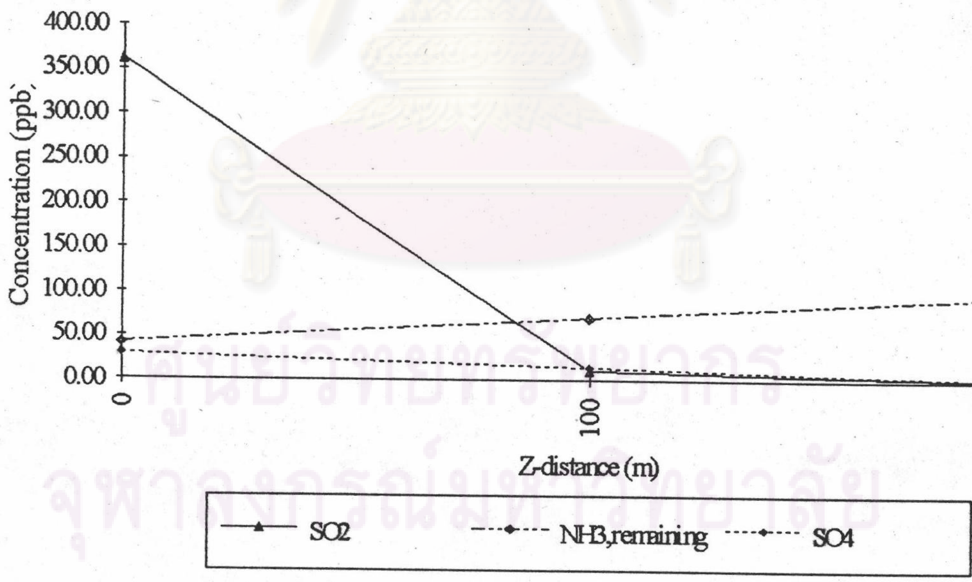


Figure 4.56 Sulfur Dioxide, Remaining Ammonia and Sulfate Concentration Profiles of Freiberg (1974)'s Reaction Rate in Ammonia-Deficient Environment for Atmospheric Stability Class F at 2 km Downwind from the Source, Relative Humidity = 99%, T = 20 °C, [Fé] = 0.1 mg/m³ and [NH_3] = 100 ppb

a) Varying Y-Distance (Fixed z=0) **b) Varing Z-Distance (Fixed y=0)**

Vita

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