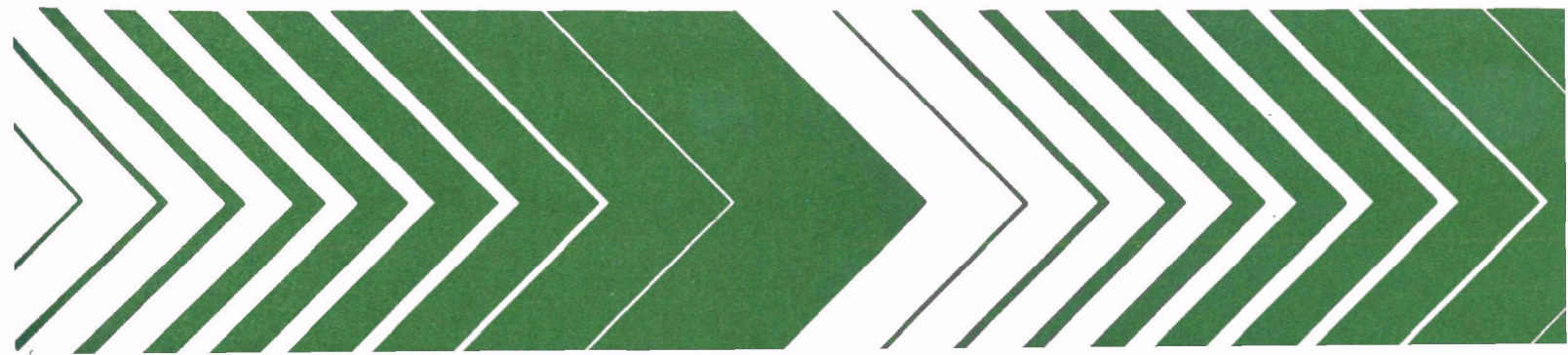




Modeling of Simulated Photochemical Smog with Kinetic Mechanisms

Volume 2.
Interim Report
Appendix



RESEARCH REPORTING SERIES

Research reports of the Office of Research and Development, U.S. Environmental Protection Agency, have been grouped into nine series. These nine broad categories were established to facilitate further development and application of environmental technology. Elimination of traditional grouping was consciously planned to foster technology transfer and a maximum interface in related fields. The nine series are:

1. Environmental Health Effects Research
2. Environmental Protection Technology
3. Ecological Research
4. Environmental Monitoring
5. Socioeconomic Environmental Studies
6. Scientific and Technical Assessment Reports (STAR)
7. Interagency Energy-Environment Research and Development
8. "Special" Reports
9. Miscellaneous Reports

This report has been assigned to the ECOLOGICAL RESEARCH series. This series describes research on the effects of pollution on humans, plant and animal species, and materials. Problems are assessed for their long- and short-term influences. Investigations include formation, transport, and pathway studies to determine the fate of pollutants and their effects. This work provides the technical basis for setting standards to minimize undesirable changes in living organisms in the aquatic, terrestrial, and atmospheric environments.

MODELING OF SIMULATED PHOTOCHEMICAL
SMOG WITH KINETIC MECHANISMS

Volume 2. Interim Report Appendix

by

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DISCLAIMER

This report has been reviewed by the Environmental Sciences Research Laboratory, U.S. Environmental Protection Agency, and approved for publication. Approval does not signify that the contents necessarily reflect the views and policies of the U.S. Environmental Protection Agency, nor does mention of trade names or commercial products constitute endorsement or recommendation for use.

ABSTRACT

Computer modeling of smog chamber data is discussed in three parts. First, a series of detailed chemical mechanisms were developed to describe the photochemical formation of ozone from nitrogen oxides and the following compounds (alone and in various combinations): formaldehyde, acetaldehyde, ethylene, propylene, butane, 1-butene, trans-2-butene, and 2,3-dimethylbutane. The aldehyde mechanisms were verified independently using data from experiments containing only nitrogen oxides and the appropriate aldehyde. The hydrocarbon mechanisms were then developed by adding the chemical reactions detailing the photooxidation steps of the particular hydrocarbon to the aldehyde mechanisms. Second, a generalized kinetic scheme intended for use in models simulating the formation of ozone in urban atmospheres was refined. The generalized mechanism includes a condensed version of the explicit mechanisms developed in the first part plus a semi-empirical scheme to describe the oxidation of aromatic hydrocarbons. Third, the effects of smog chambers on ozone formation were examined. For this part of the study, similar experiments using propylene and nitrogen oxides in eight different smog chambers were simulated. The main chamber effects identified thus far are apparently due to nitrogen oxides degassing from the walls during experiments and differences between chambers in the spectral distribution of ultraviolet irradiation.

Volume 1 contains all textual material; this volume contains graphs of measured and simulated pollutant concentrations for many smog chamber experiments. The two-volume report was submitted to the U.S. Environmental Protection Agency in fulfillment of Contract No. 68-02-2428 by Systems Applications, Incorporated. This report covers the period 23 August 1976 to 23 August 1978, and work was completed as of 18 August 1978.

CONTENTS

ABSTRACT	iii
ABBREVIATIONS	vii
APPENDIX: SIMULATION RESULTS	1
Part A: Simulation Results with Explicit Mechanisms	2
1. Formaldehyde Experiments by Bufalini, Gay, and Brubaker (1972). Simulated with explicit formaldehyde mechanism	3
2. Experiments by Bufalini, Gay, and Brubaker (1972). Simulated with explicit formaldehyde mechanism with added reactions for peroxyxynitric acid (HOONO_2) . . .	8
3. UCR Formaldehyde Experiments	11
4. UNC Formaldehyde Experiment	21
5. UCR Acetaldehyde Experiments	23
6. UCR Ethylene Experiments	31
7. UCR Propylene Experiments	49
8. UCR Butane Experiments	114
9. UCR 1-Butane Experiments	153
10. UCR Trans-2-Butene Experiments	160
11. UCR 2,3-Dimethylbutane Experiments	168
12. UCR Ethylene/Propylene Experiments	179
13. UCR Propylene/Butane Experiments	190
14. UCR Propylene/Trans-2-Butene Experiment	225
15. UCR Multiolefin Experiments	230
Part B: Simulation Results with the Carbon-Bond Mechanism . . .	250
1. UCR Formaldehyde Experiments	251
2. UCR Acetaldehyde Experiments	260
3. UCR Ethylene Experiments	265
4. UCR Propylene Experiments	269
5. UCR Butane Experiments	280
6. UCR 1-Butene Experiments	285
7. UCR Trans-2-Butene Experiments (with trans-2-butene treated as an olefin)	288

8.	UCR Trans-2-Butene Experiments (with trans-2-butene treated as a carbonyl)	291
9.	UCR 2,3-Dimethylbutane Experiments	293
10.	UCR Toluene Experiments	296
11.	UCR Propylene/Butane Experiments	316
12.	UCR Multiolefin Experiments	321
13.	UCR Seven-Hydrocarbon Experiments	326
Part C.	Simulation Results of Propylene Experiments Performed at Various Chambers	371
1.	UNC Chamber Experiments	372
2.	RTI Chamber Experiments	378
3.	Battelle Chamber Experiments	382
4.	NAPCA Chamber Experiments	386
5.	UCR-AGC Chamber Experiments	394
6.	CALSPAN Chamber Experiments	397
7.	Lockheed Chamber Experiments	401

ABBREVIATIONS

ALD2	Acetaldehyde	O3	Ozone
ALD3	Propionaldehyde	OLE	Olefins
ALD4	Butyraldehyde	PAN	Peroxyacetyl nitrate
AONE	Acetone	PAR	Paraffins
ARO	Aromatics	PPN	Peroxypropionyl nitrate
BLA	Blacklamp irradiation	PROP	Propylene
BUT	n-Butane	SCN3	Sec-butyl nitrate
BUT1	1-Butene	SPN3	Isopropyl nitrate
BUT2	Trans-2-butene	SUN	Sunlamp irradiation
CO	Carbon monoxide	SUNLAMP	Sunlamp irradiation
C2N3	Ethyl nitrate	UCR	University of California at Riverside
C4N3	n-Butyl nitrate	UNCB	University of North Carolina ("blue" side of chamber)
C6N3	2,3-Dimethylbutyl nitrate	UNCR	University of North Carolina ("red" side of chamber)
DBUT	2,3-Dimethylbutane		
EC	Evacuable chamber (at UCR)		
ETH	Ethylene		
FORM	Formaldehyde		
HCHO	Formaldehyde		
H2O2	Hydrogen peroxide		
MEK	Methylethylketone		
MEN3	Methyl nitrate		
NO	Nitrogen oxide		
NOX	Oxides of nitrogen (NO + NO ₂)		
NO2	Nitrogen dioxide		

APPENDIX

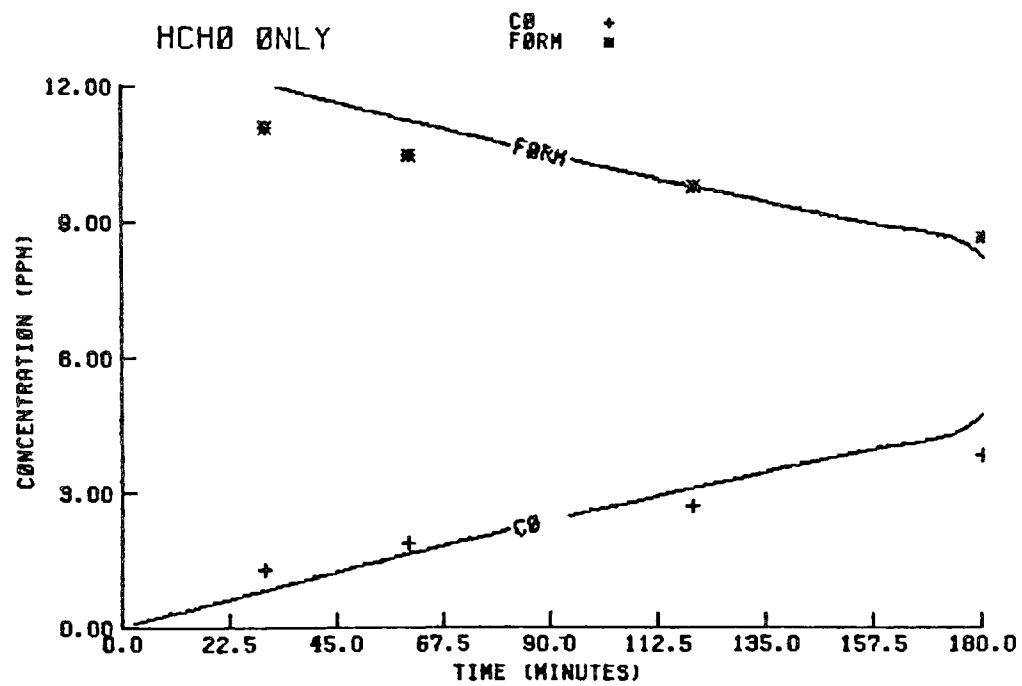
SIMULATION RESULTS

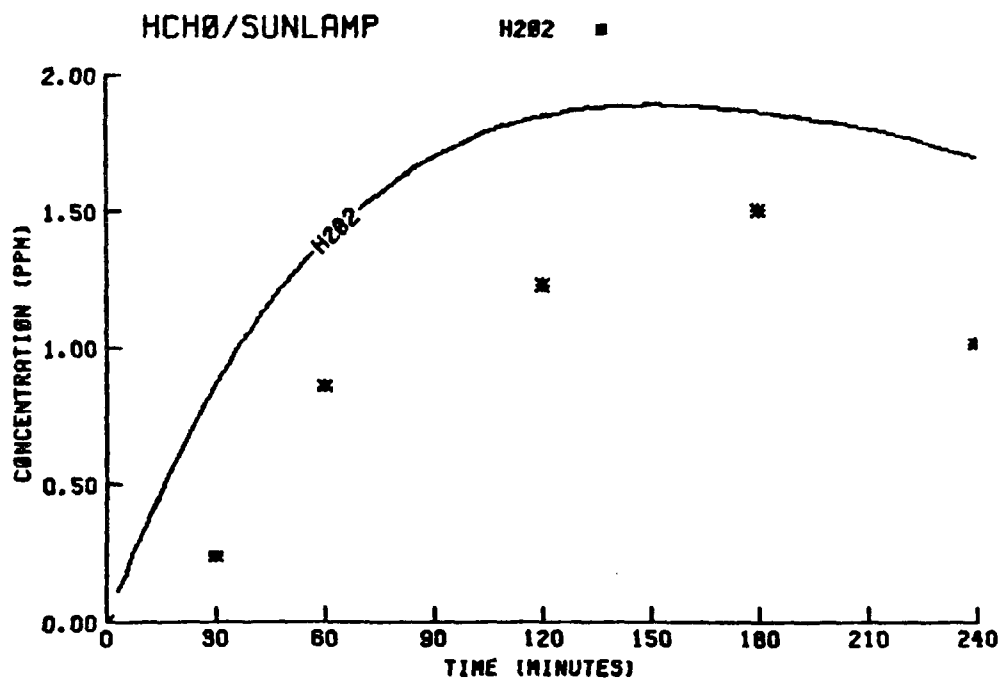
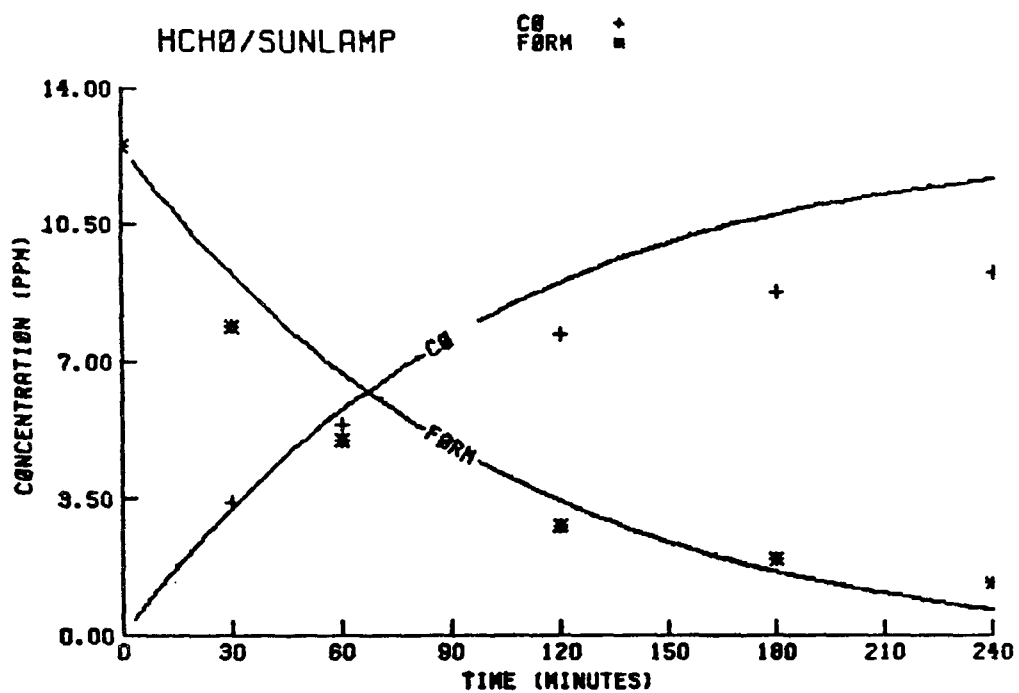
Volume I of this two-volume report discusses the results of this study. This volume (II) is the data volume: It presents graphs of simulated and measured pollutant concentrations in smog chamber experiments. In all figures, the symbols represent measured concentrations and the solid lines represent simulation concentrations. The pollutants are identified in the graphs by two- to four-space codes, which are given in the list of abbreviations. Simulations with explicit mechanisms (Part A) are presented first, followed by simulations with the Carbon-Bond Mechanism (Part B), and simulations with the explicit propylene mechanism in the study of chamber effects (Part C).

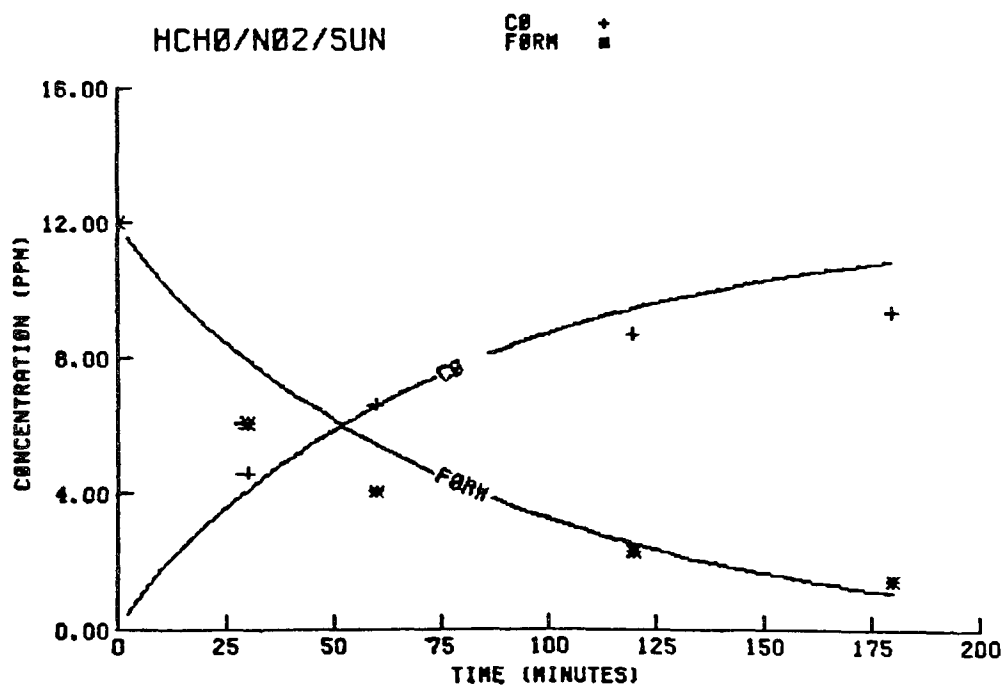
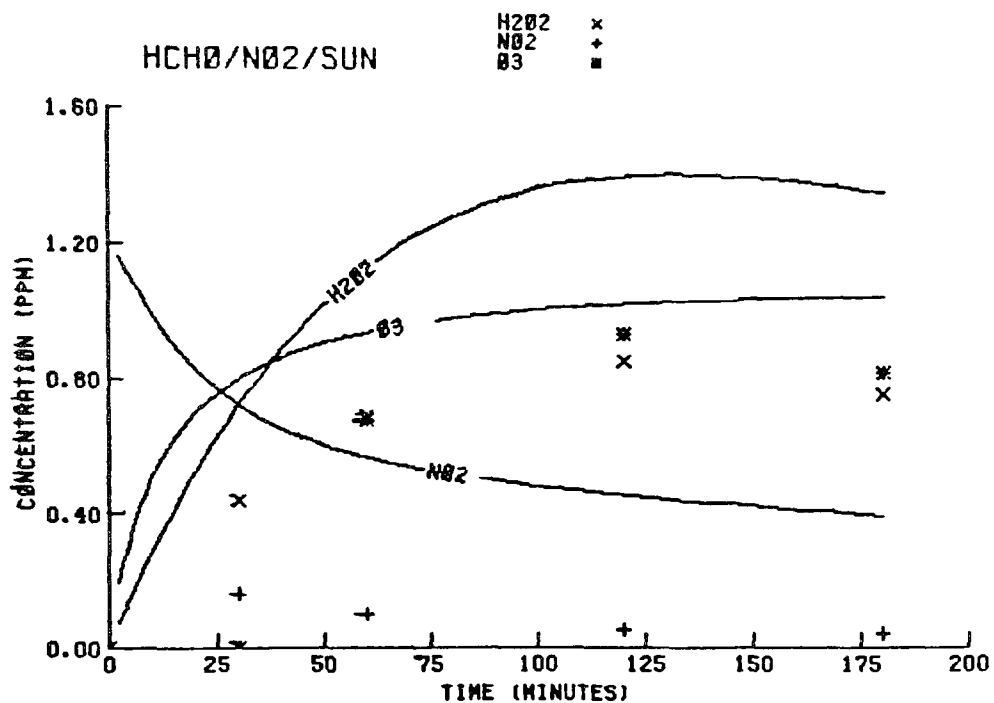
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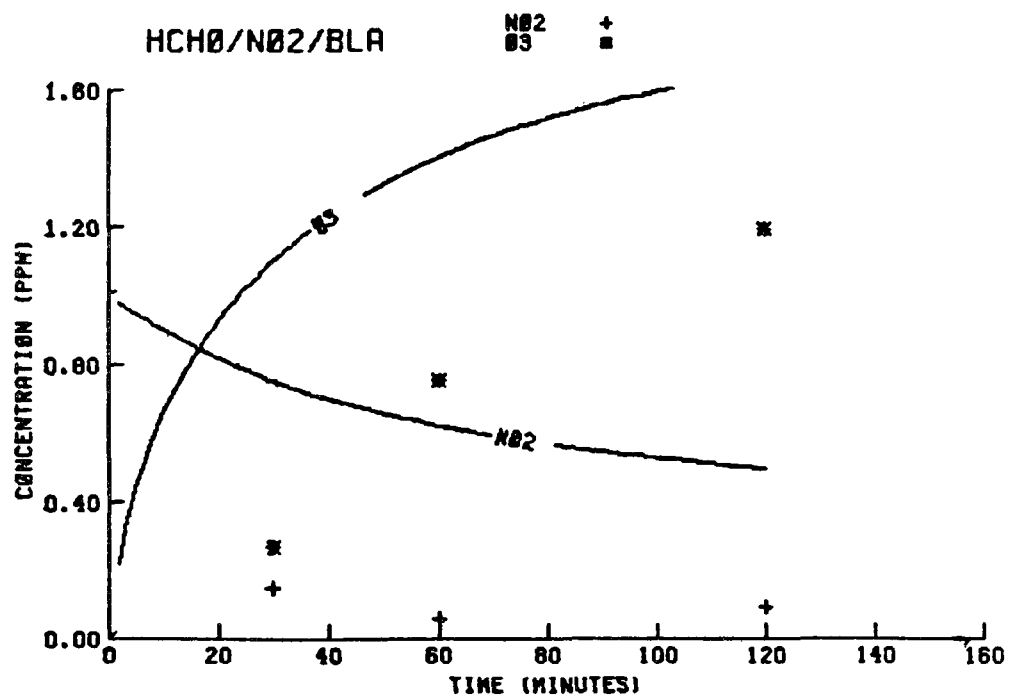
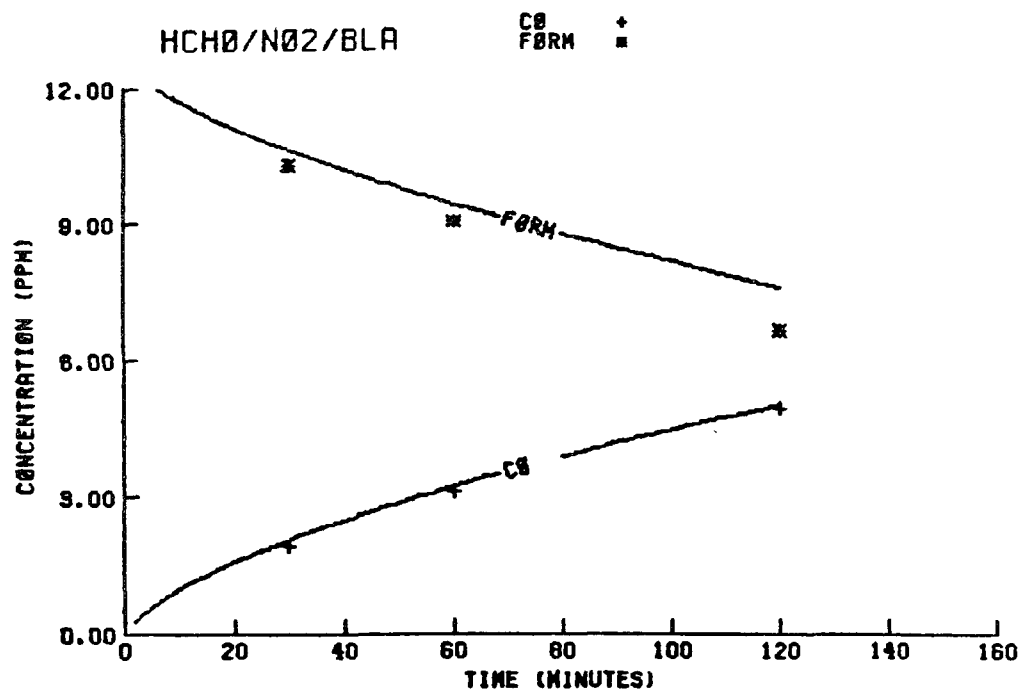
Simulation Results with Explicit Mechanisms

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Simulated with explicit formaldehyde mechanism.

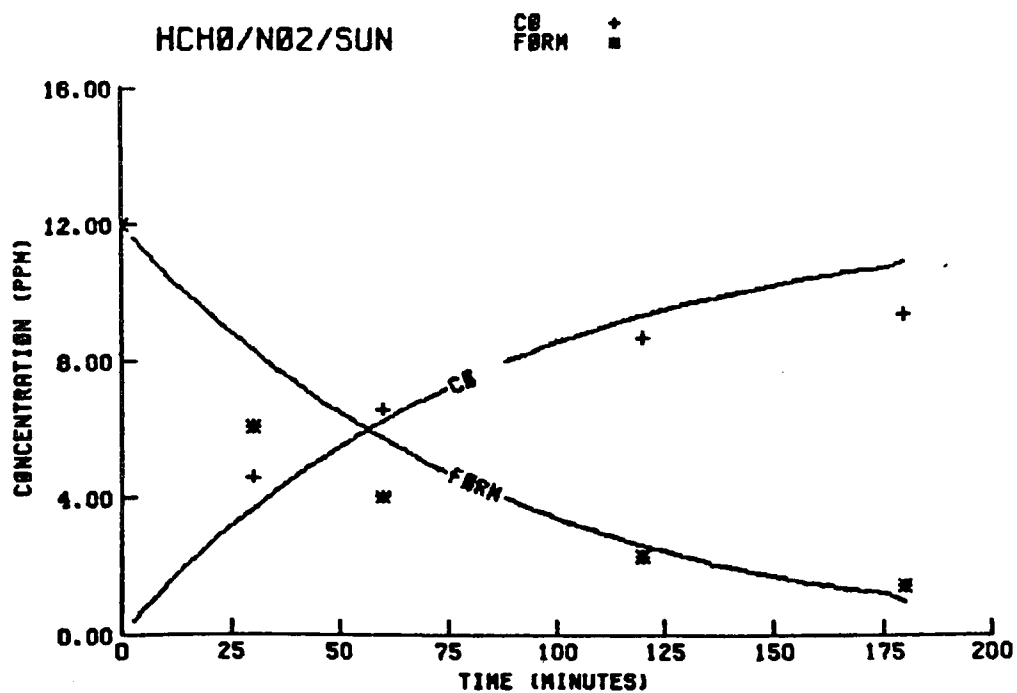
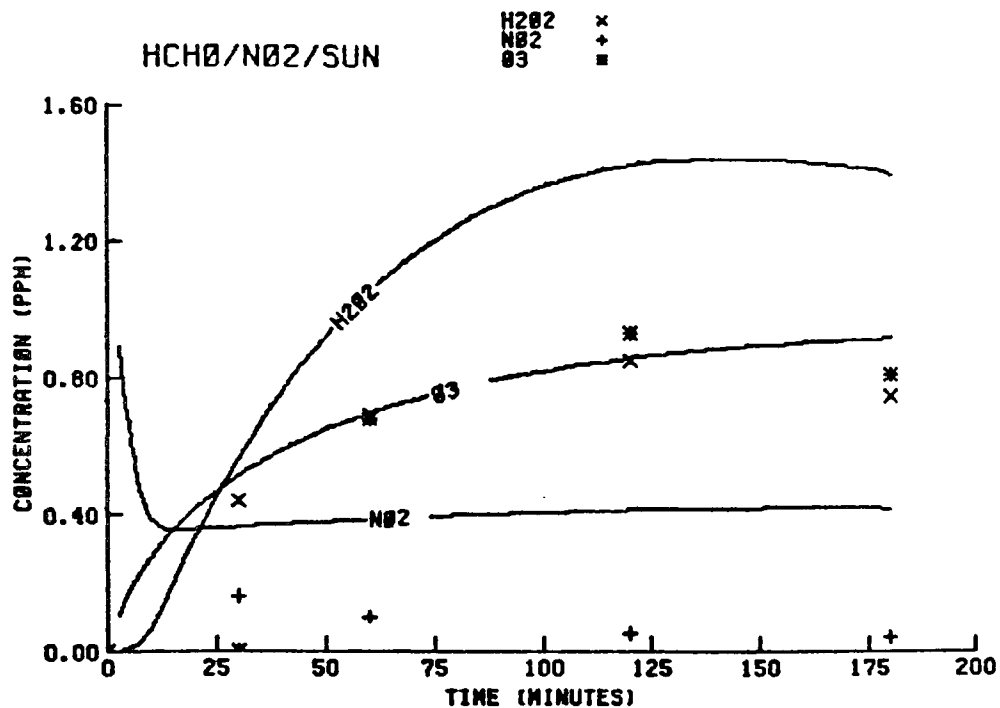


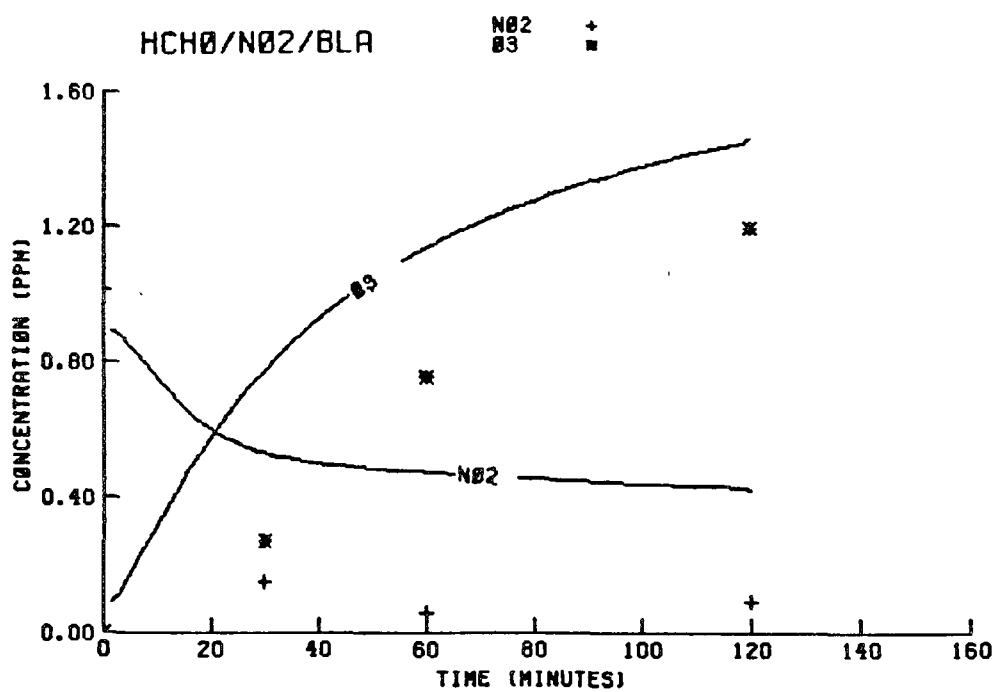
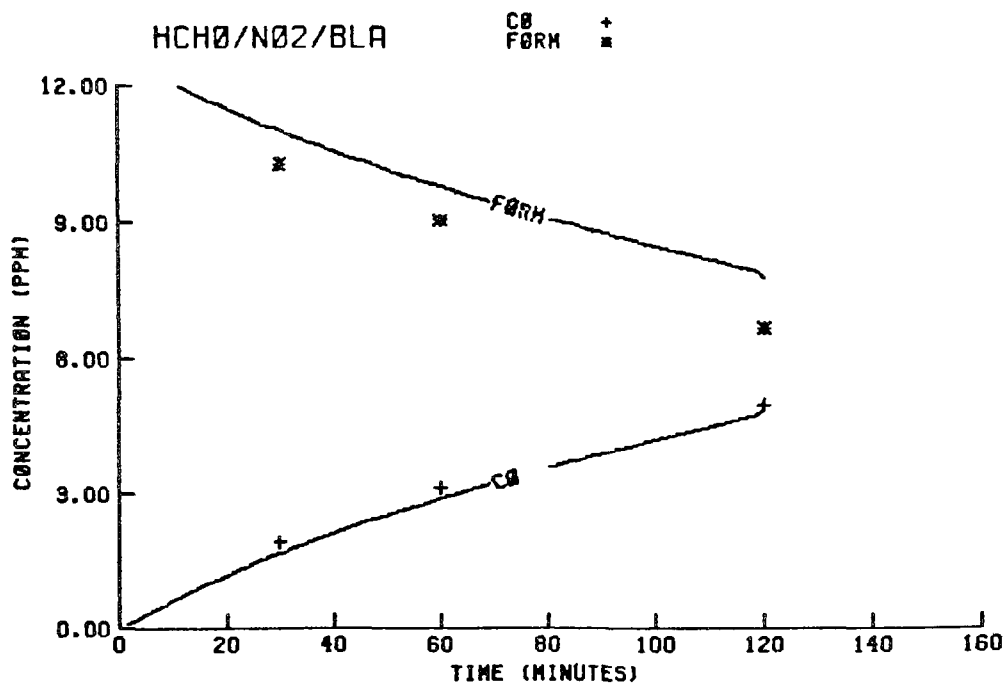




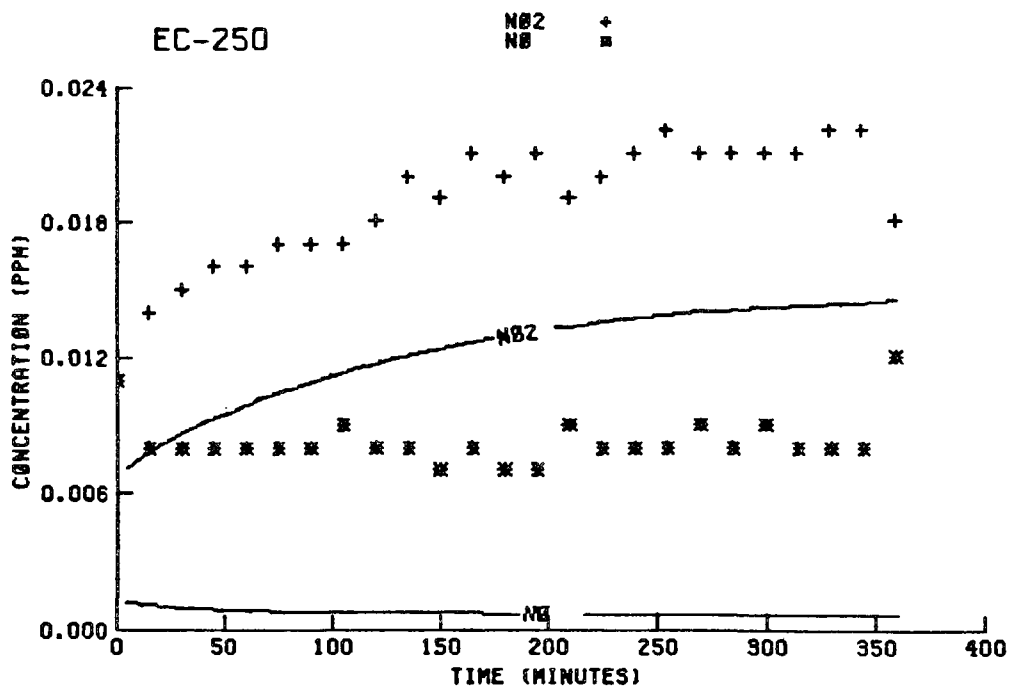
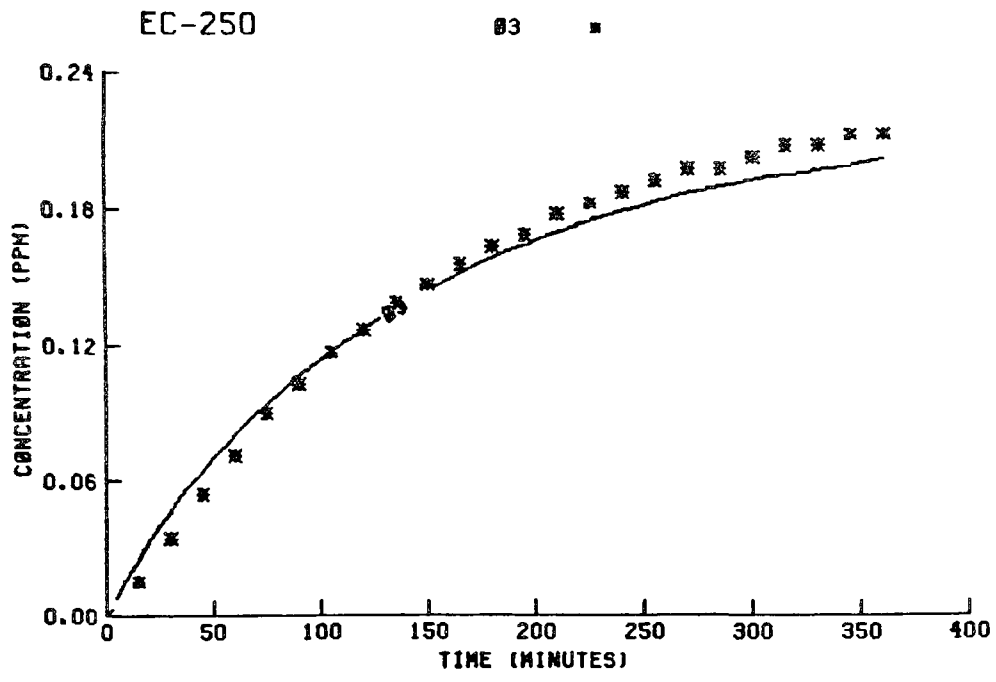


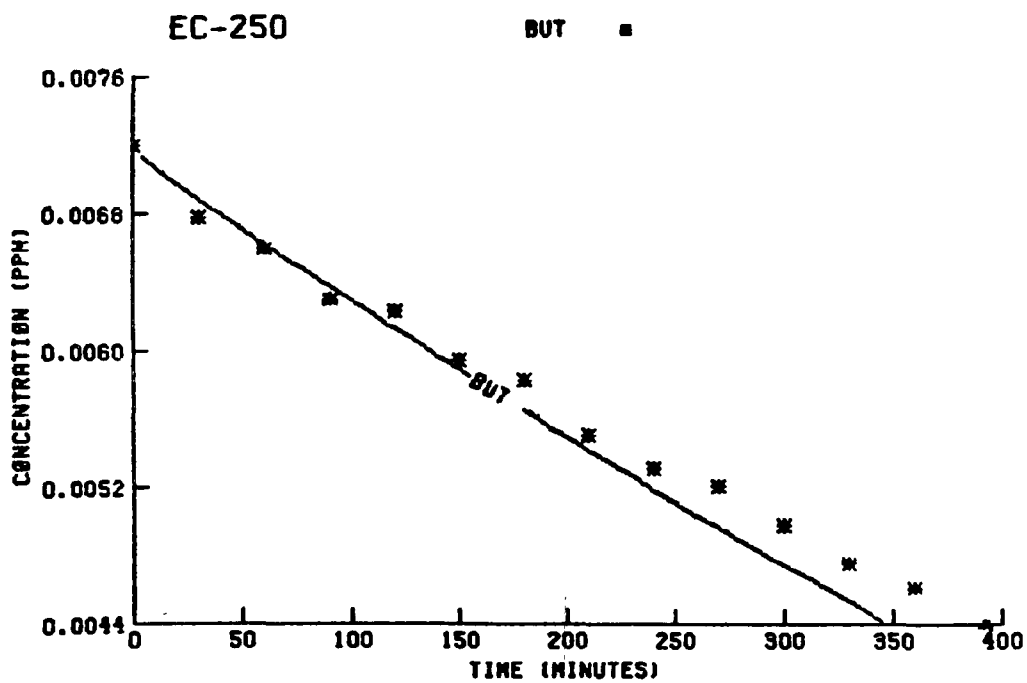
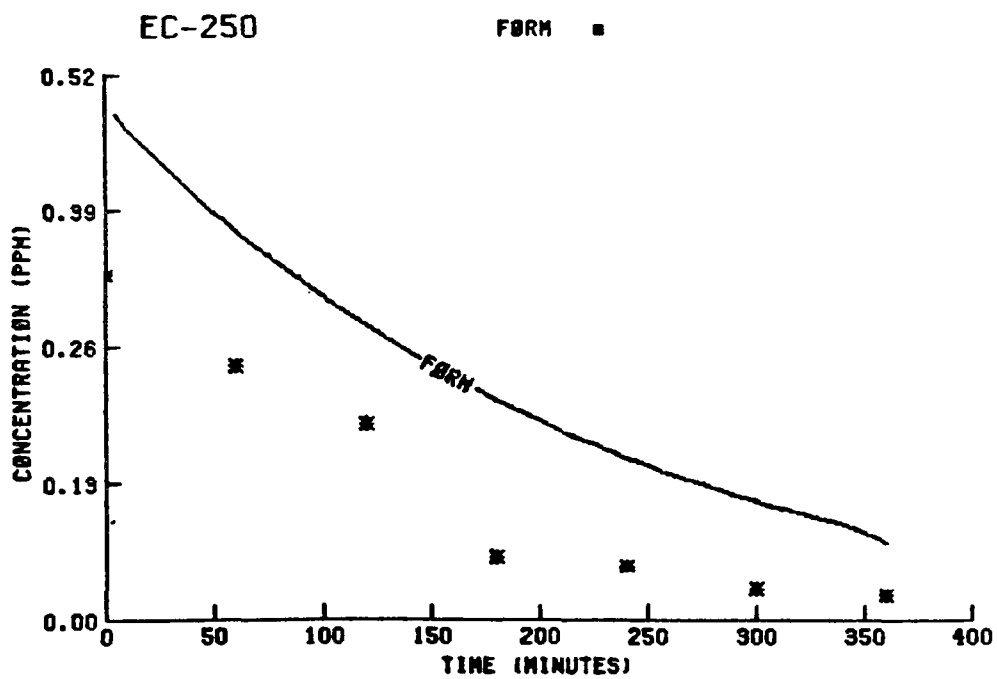
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Simulated with explicit formaldehyde mechanism with added
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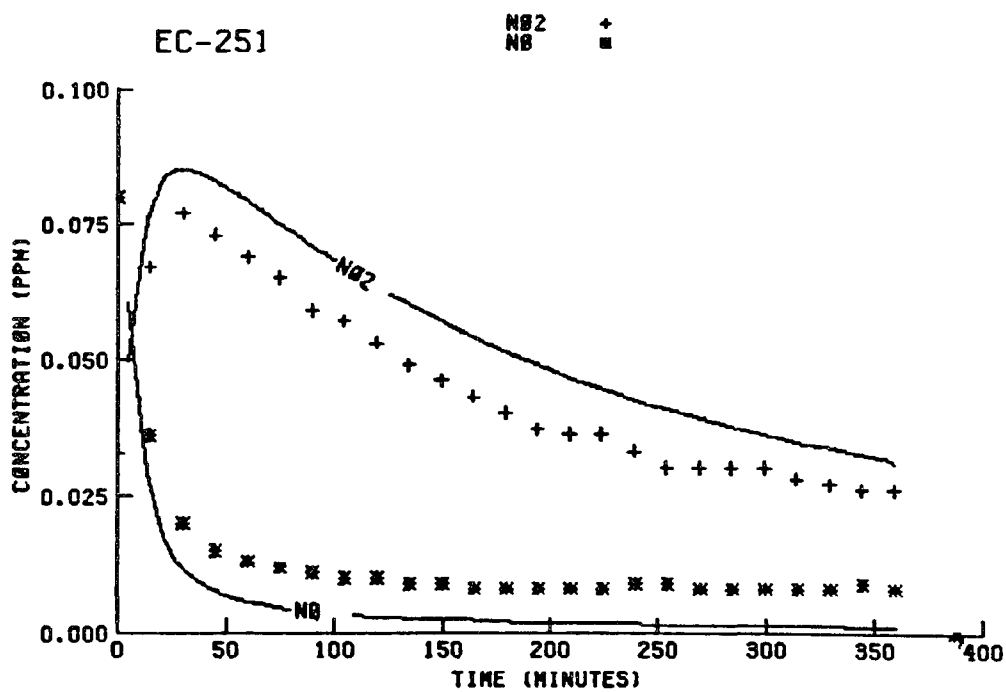
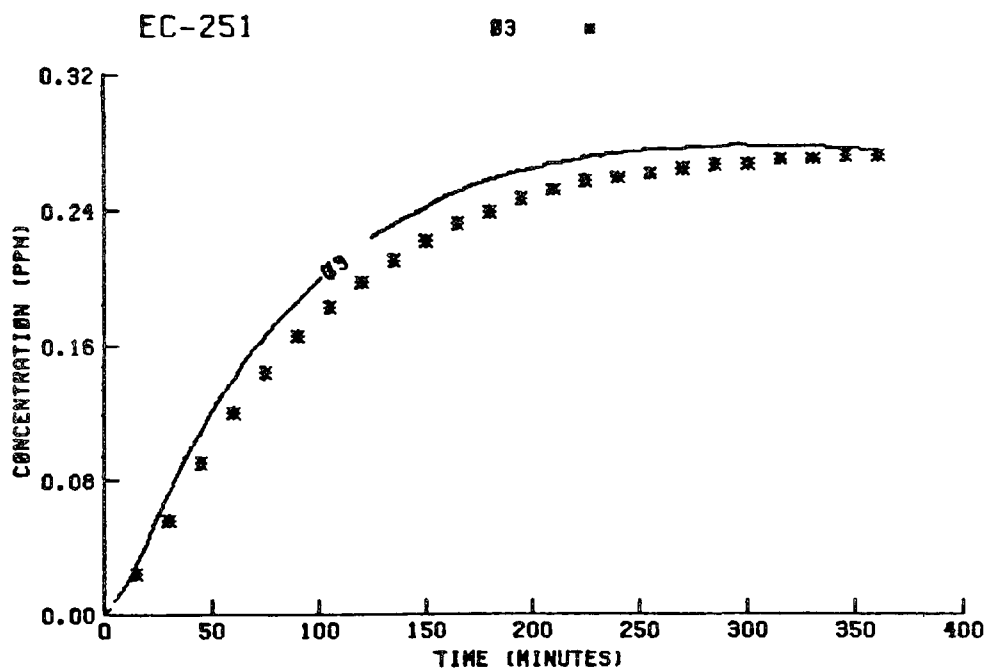


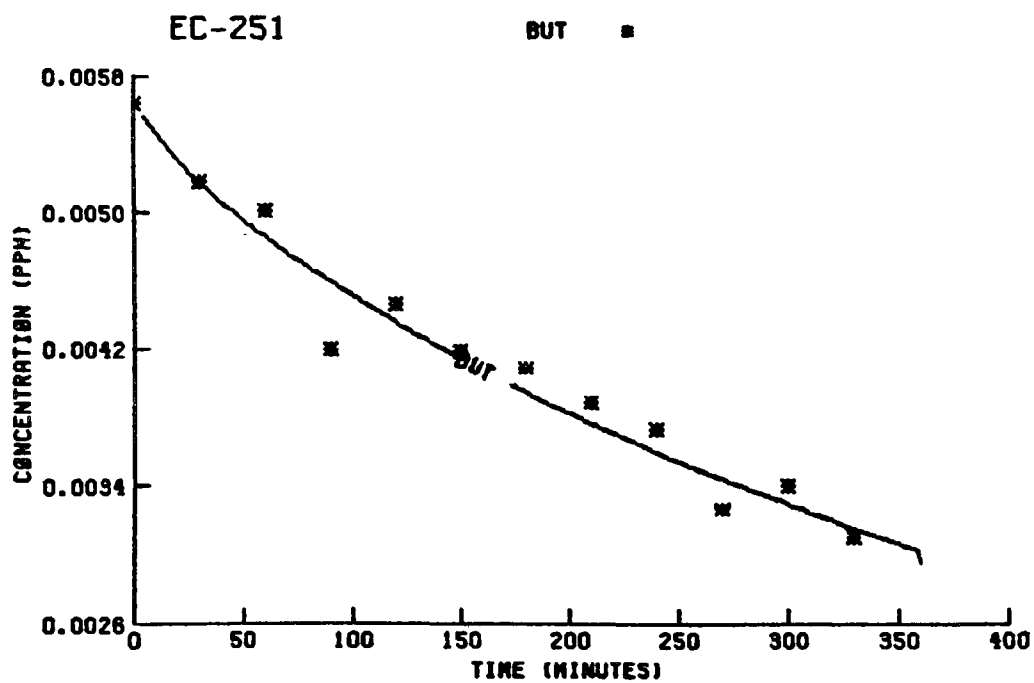
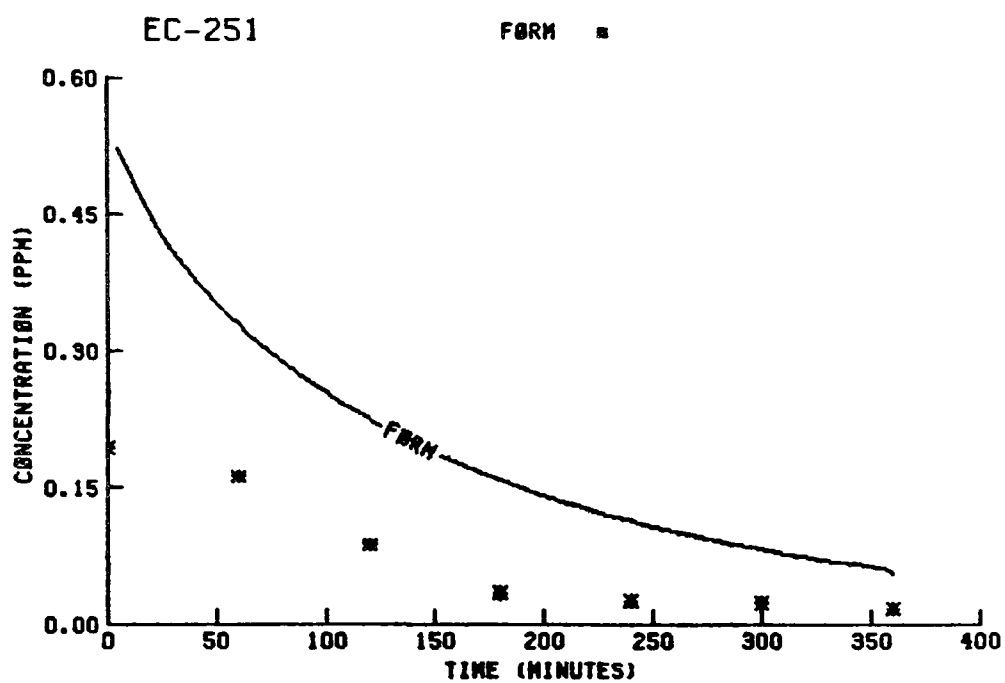


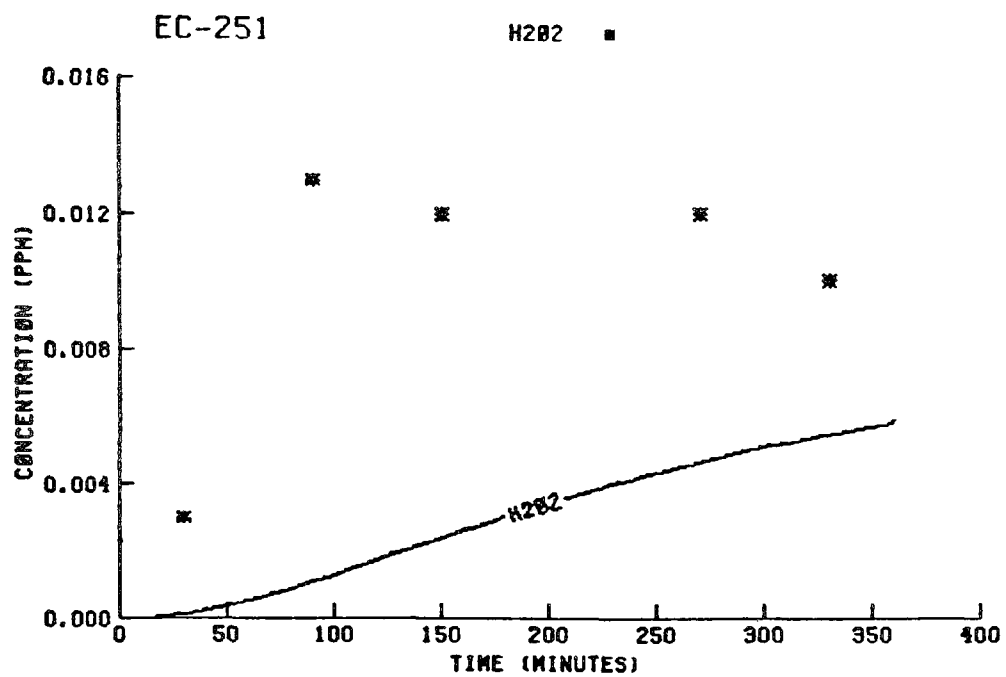
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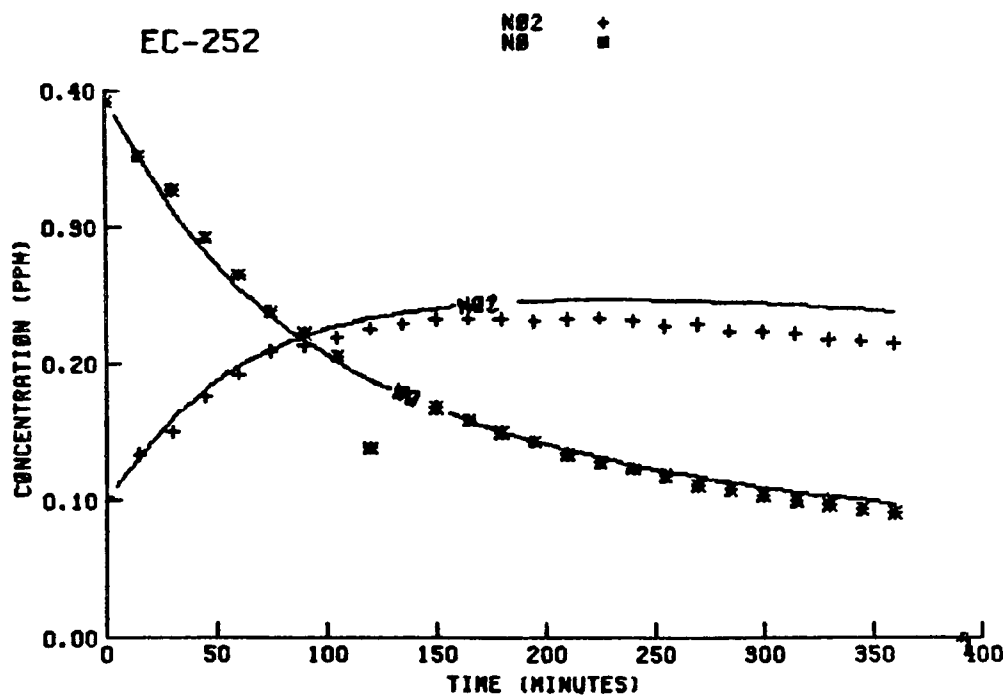
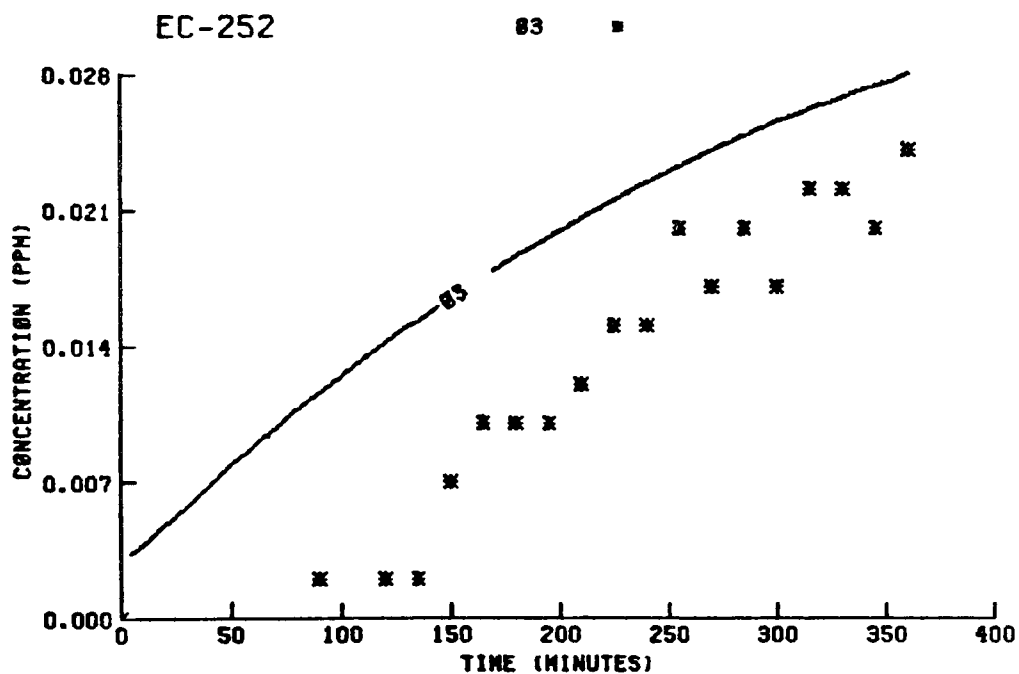


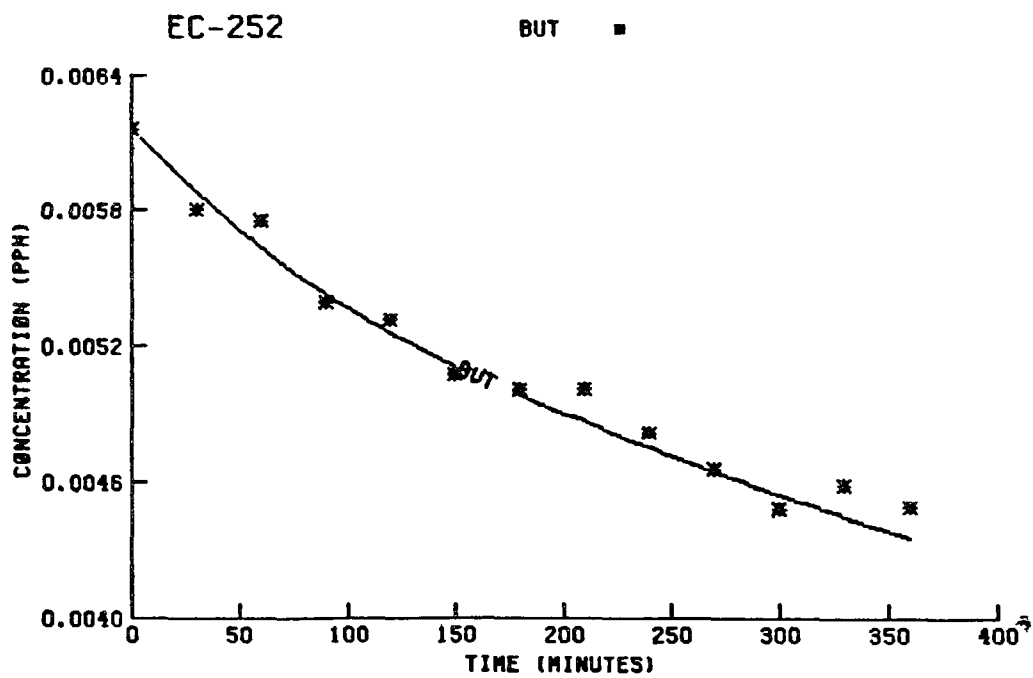
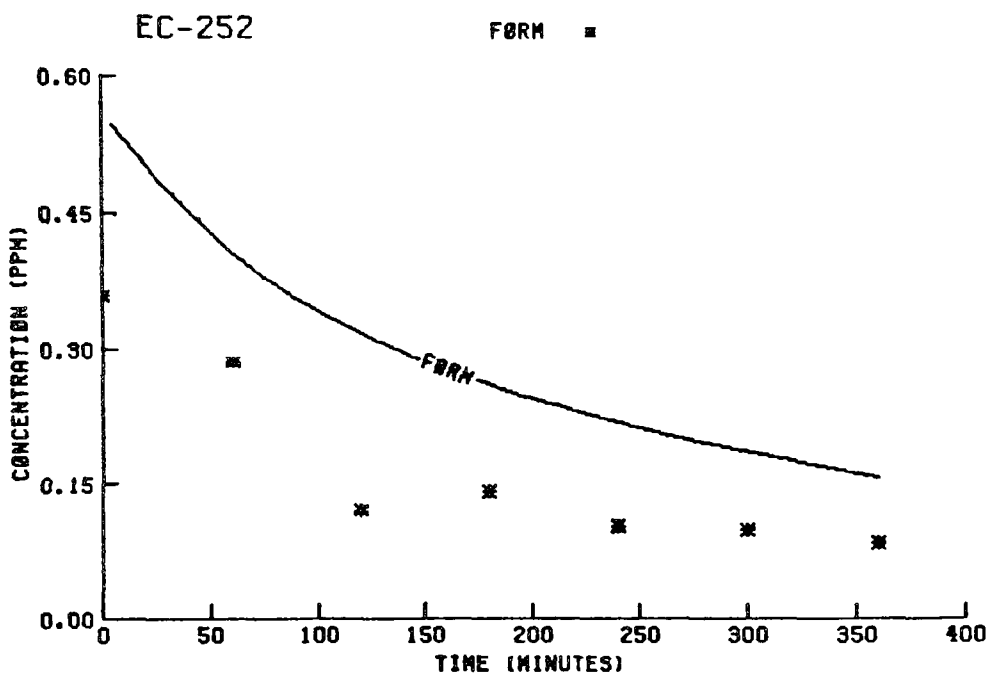


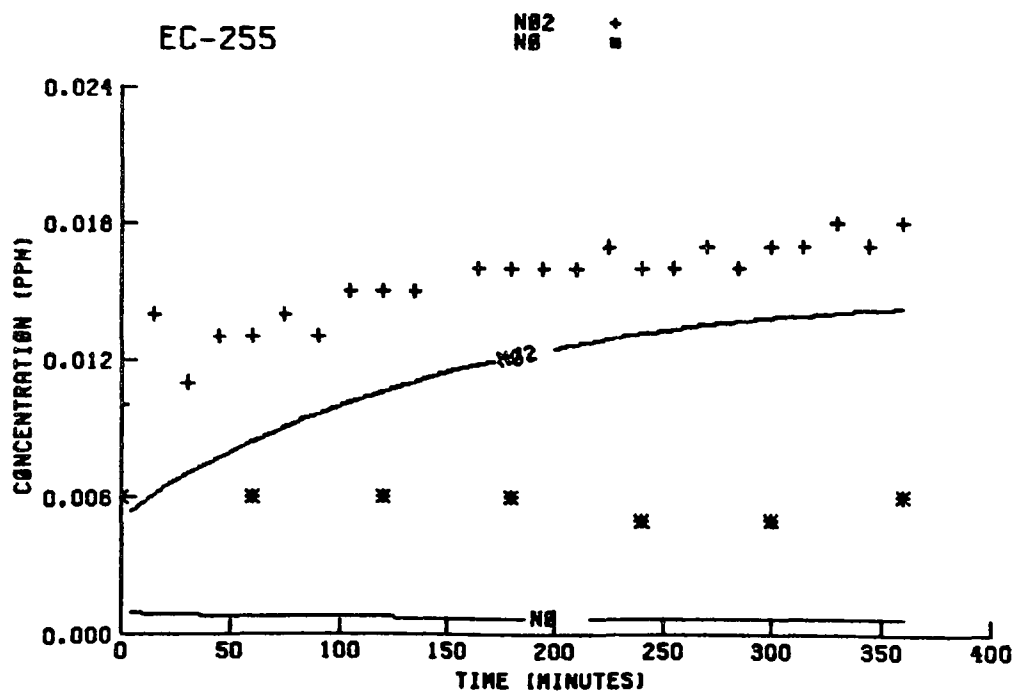
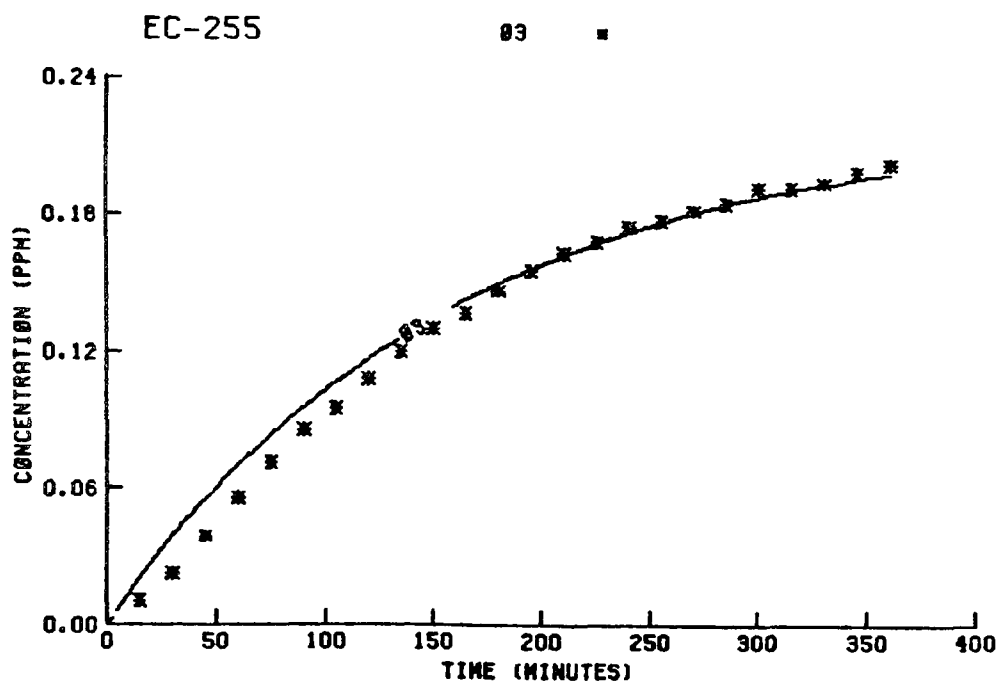


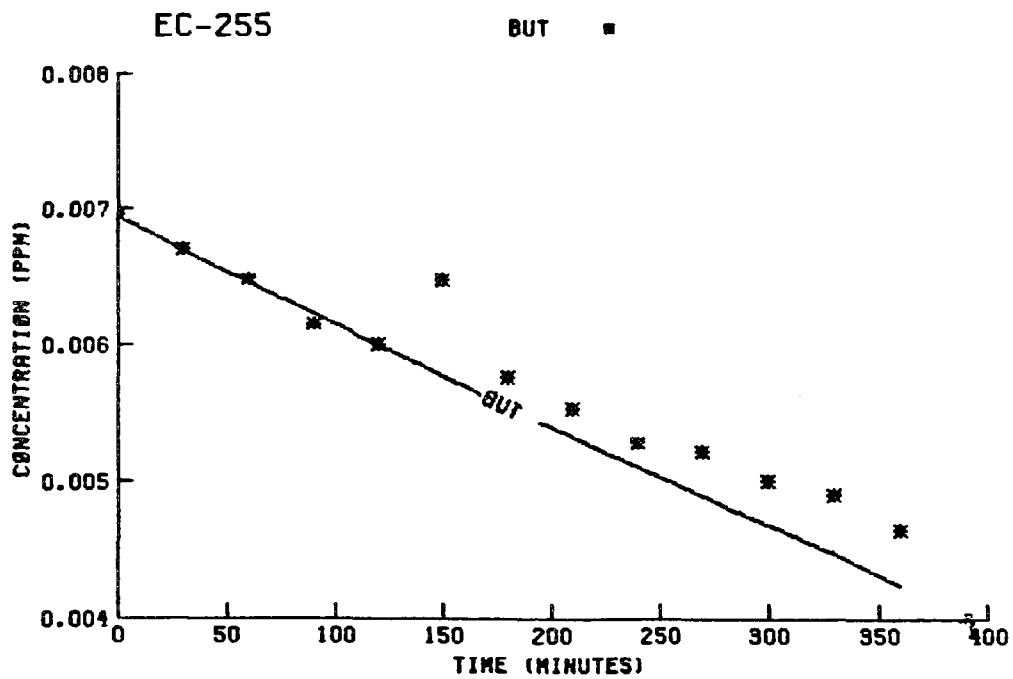
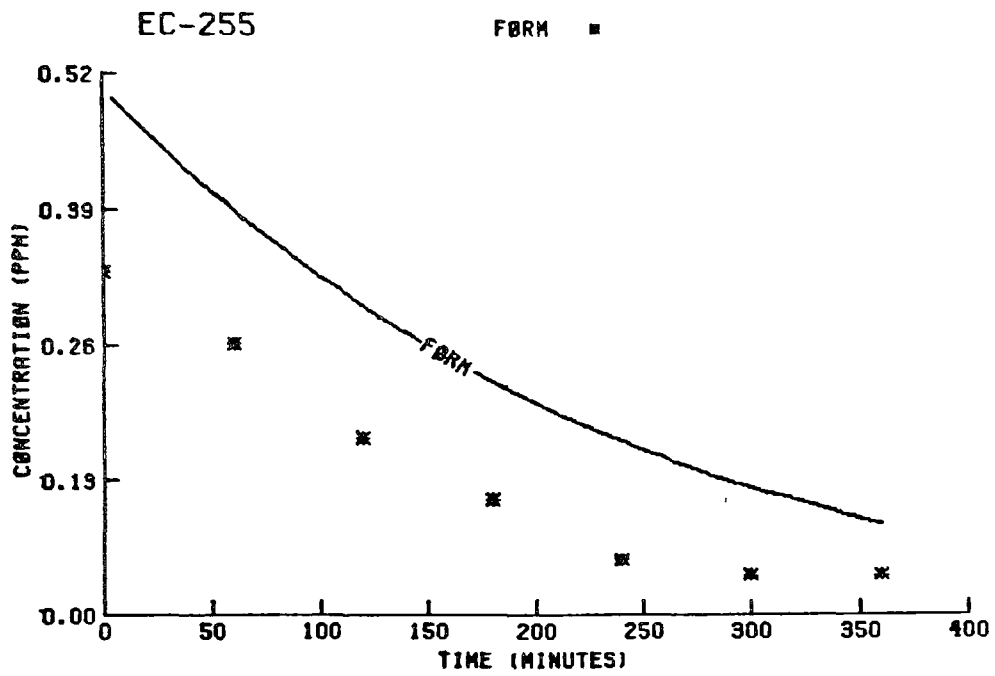




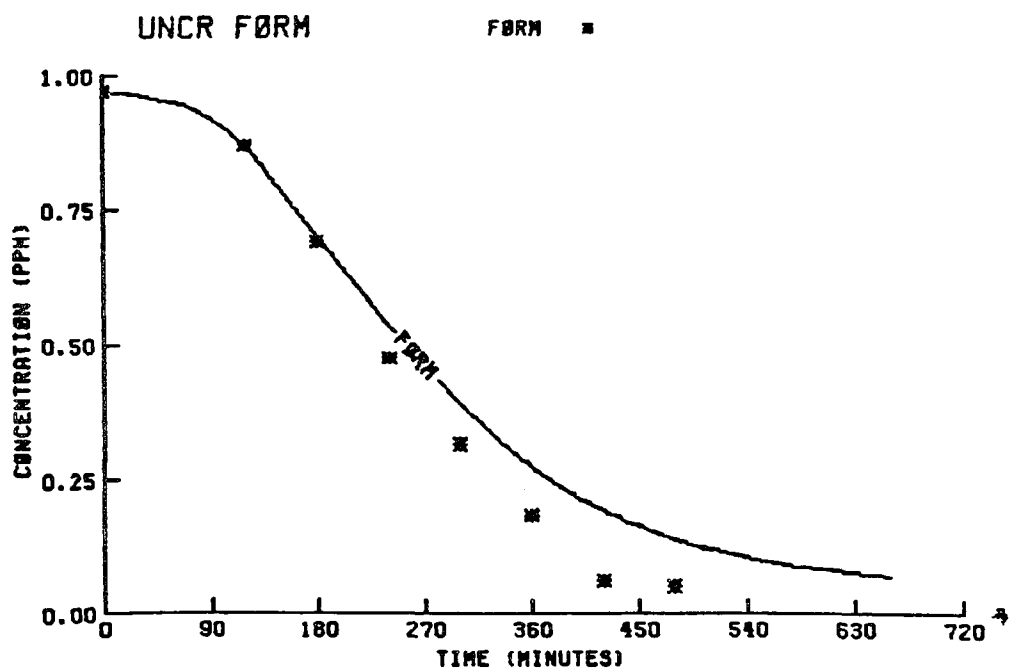
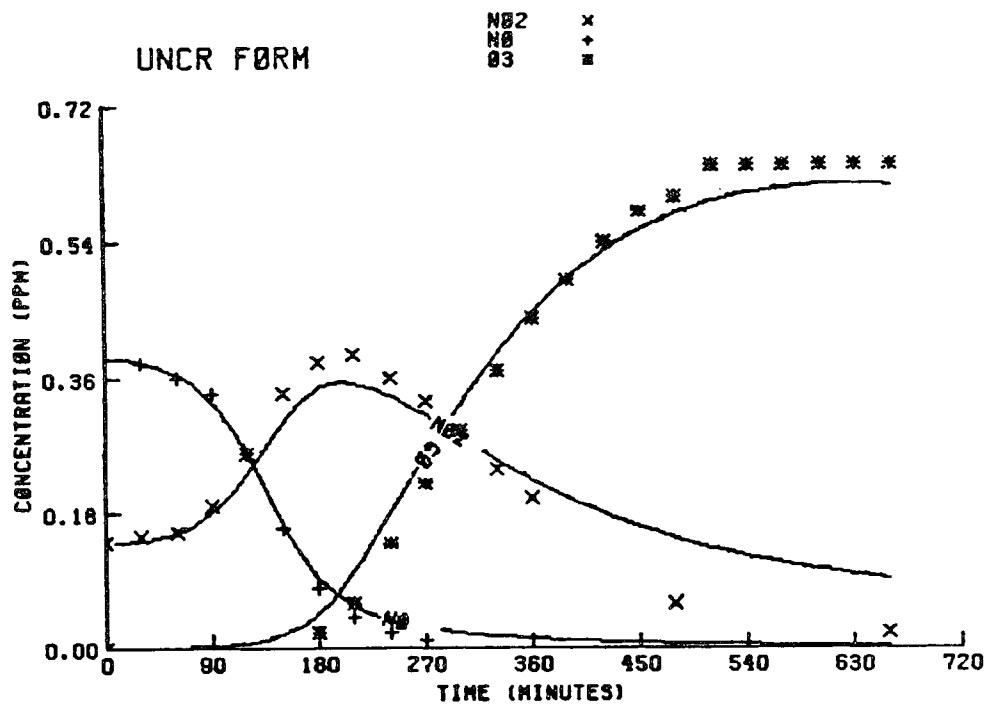








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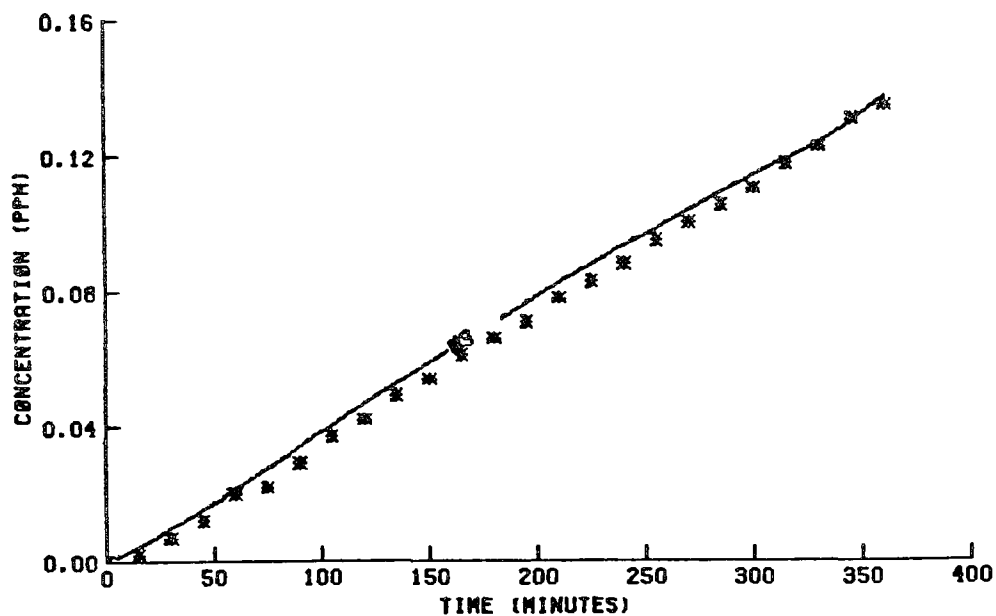


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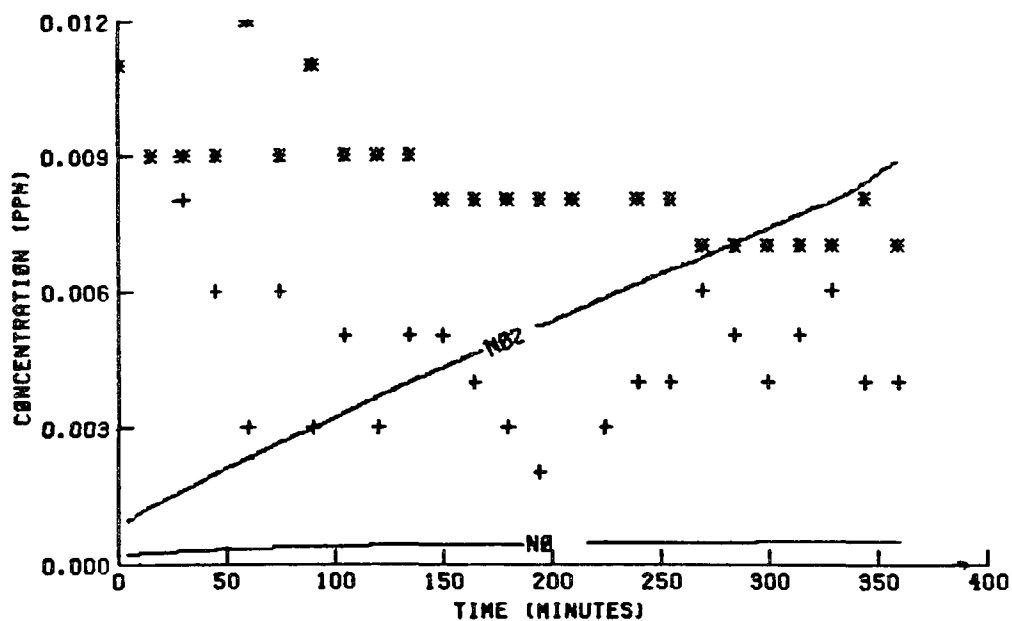
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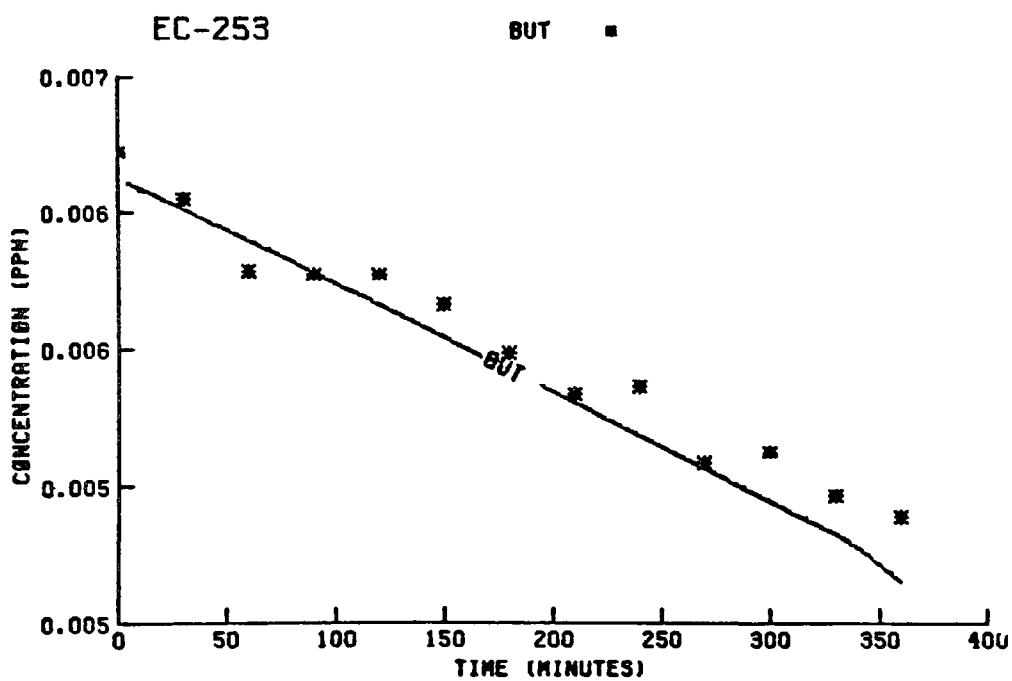
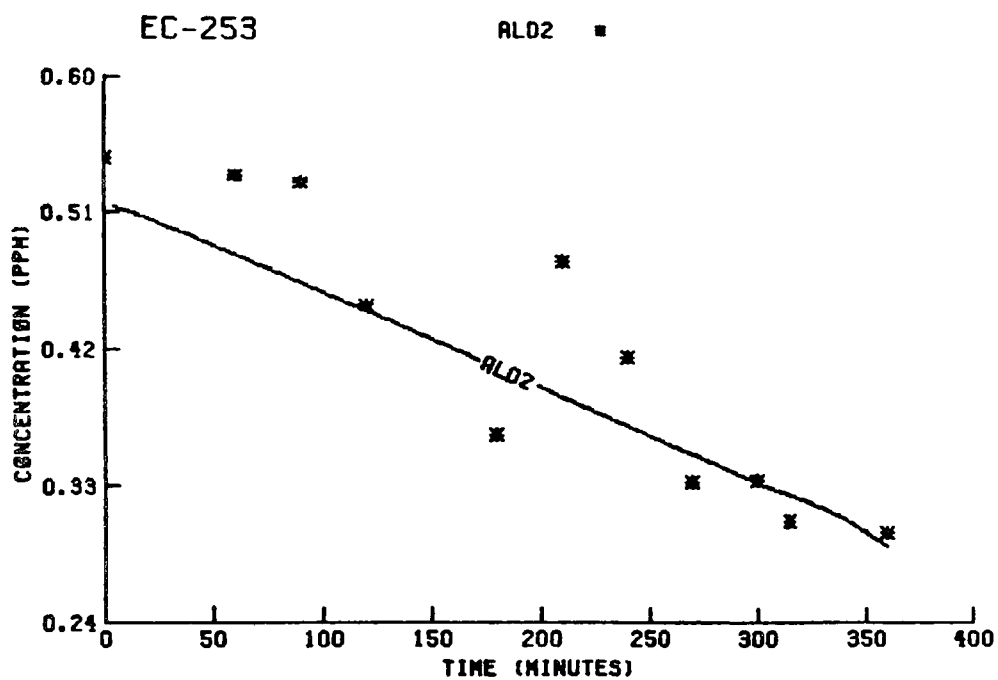


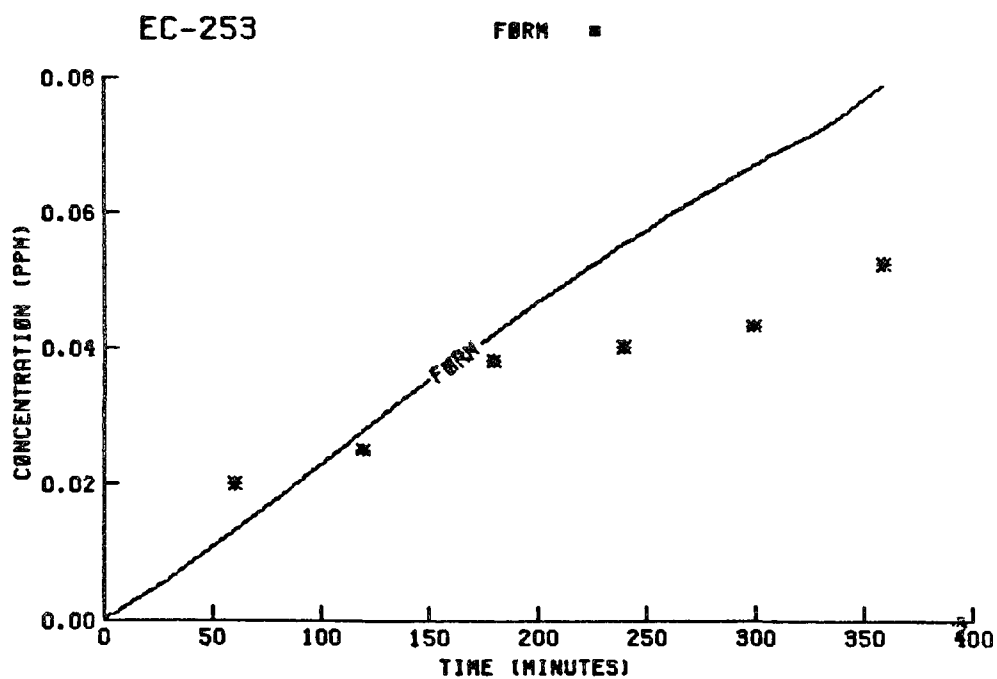
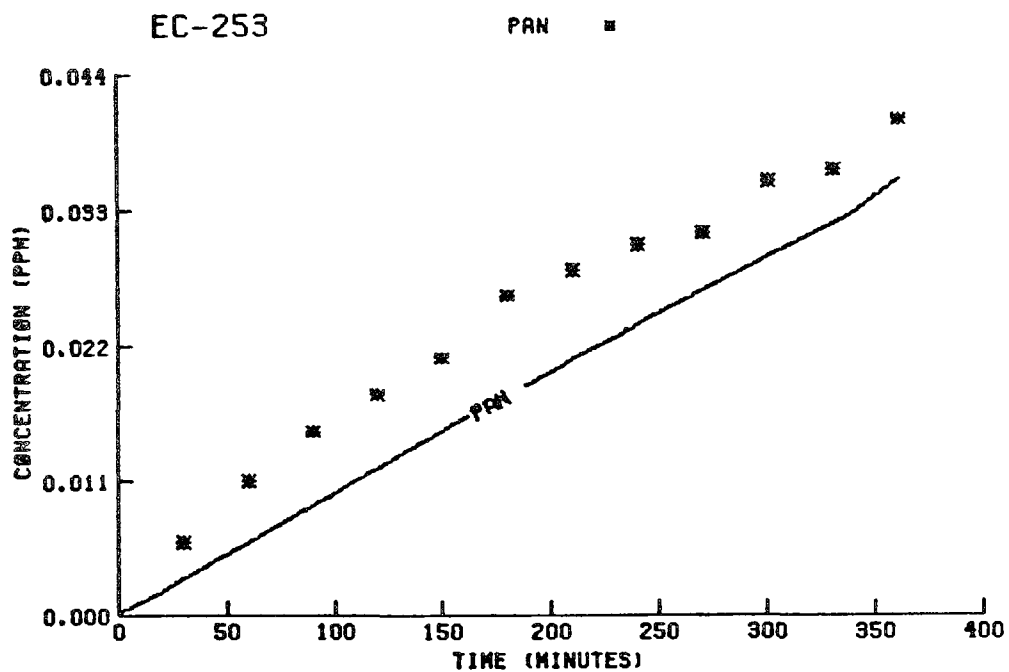
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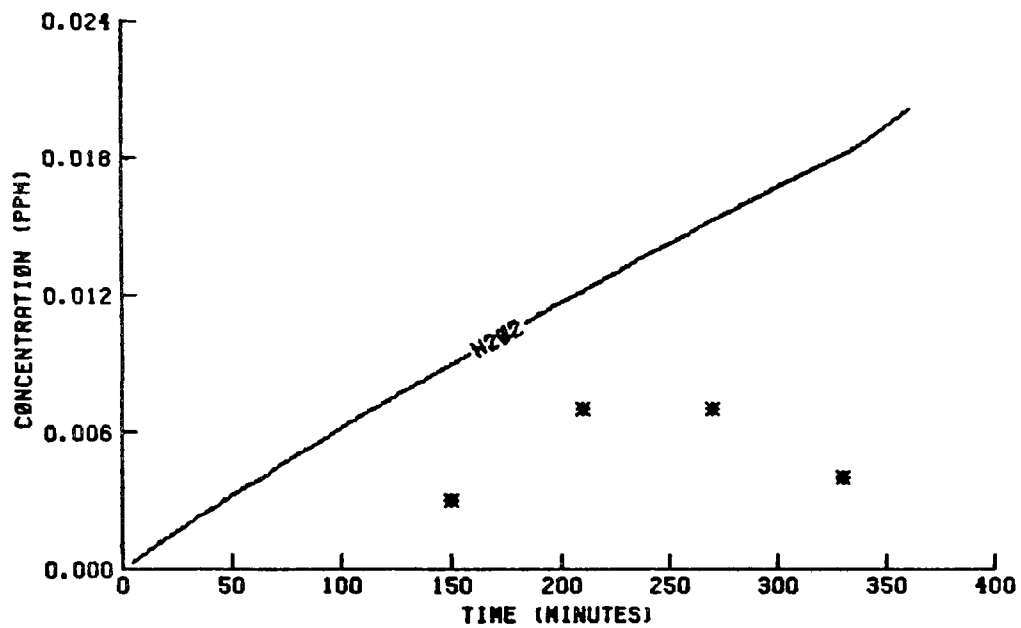


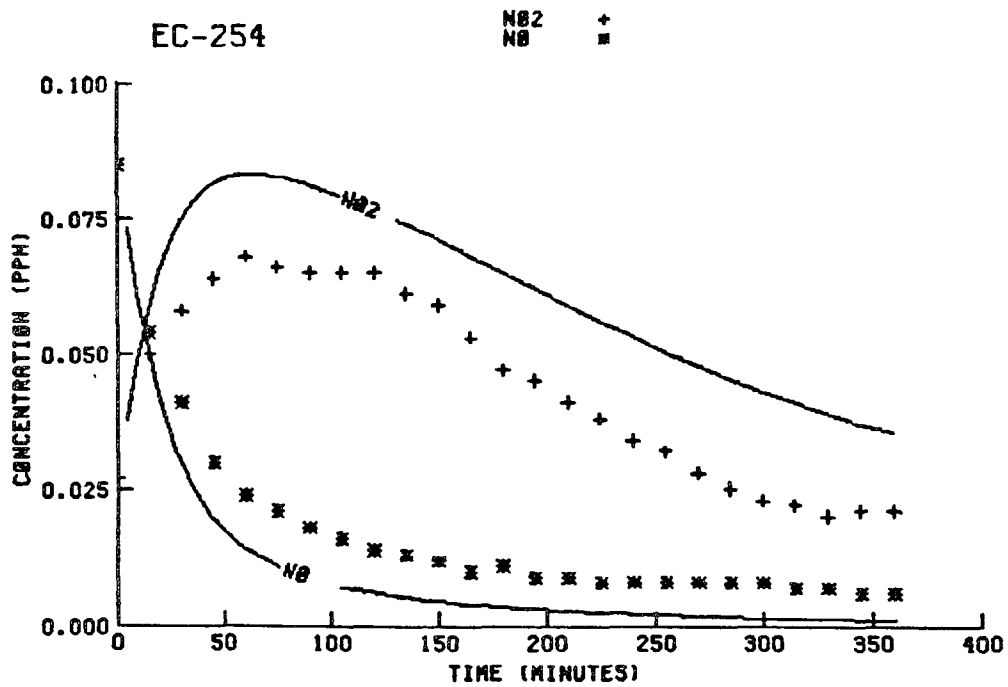
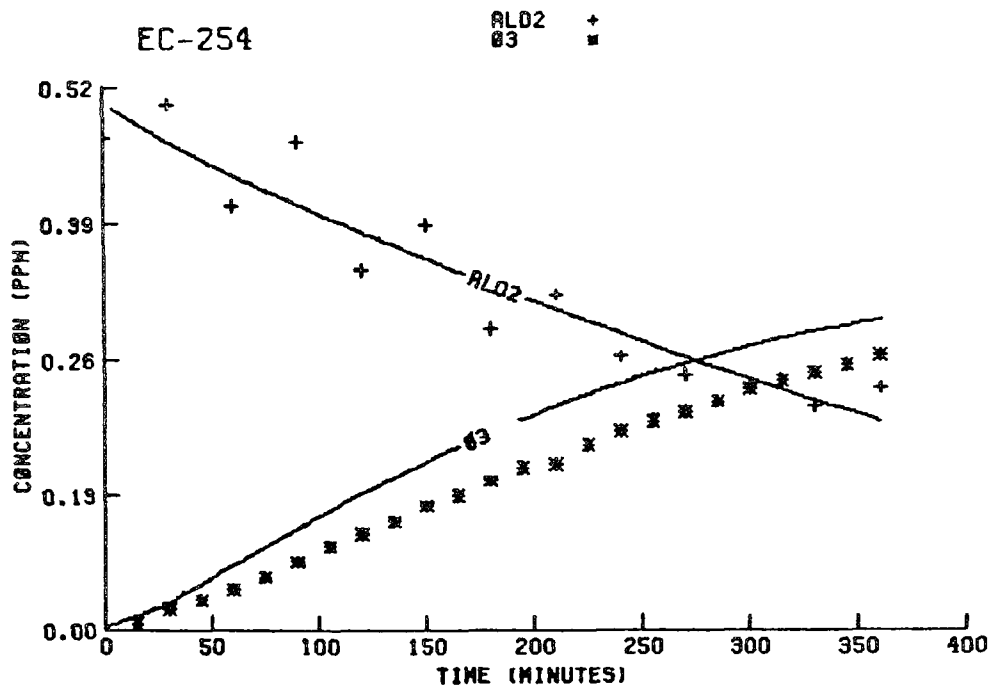


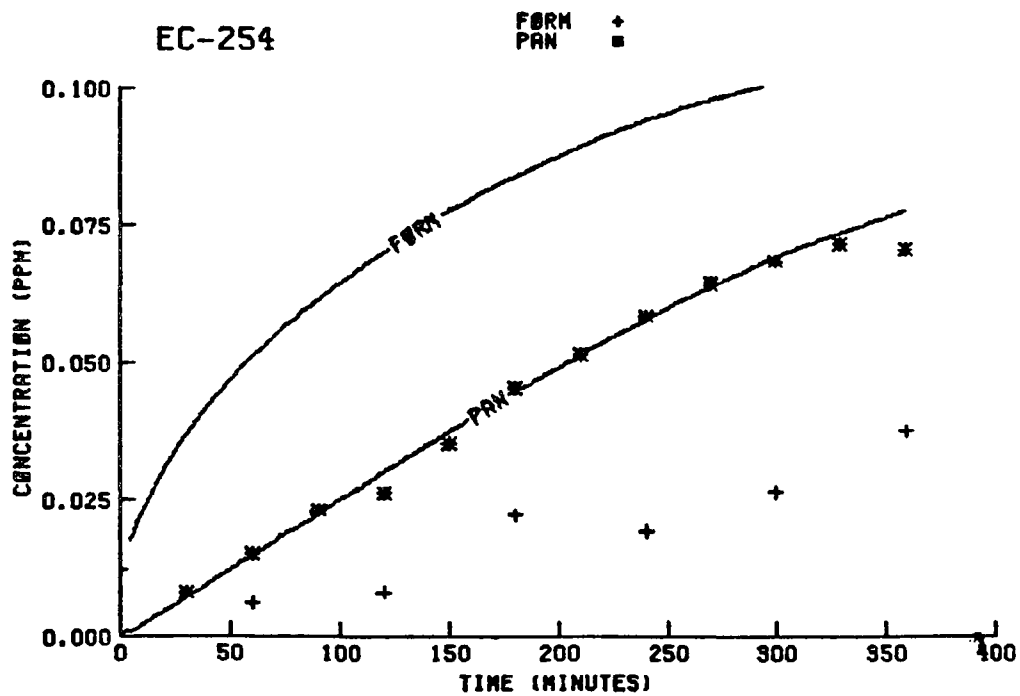
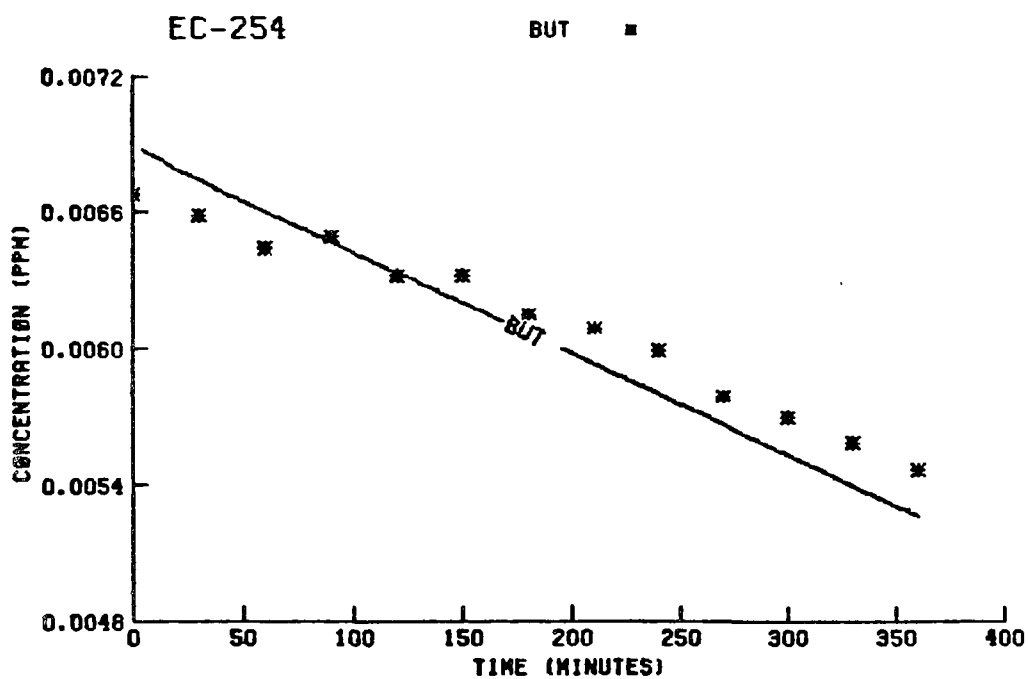


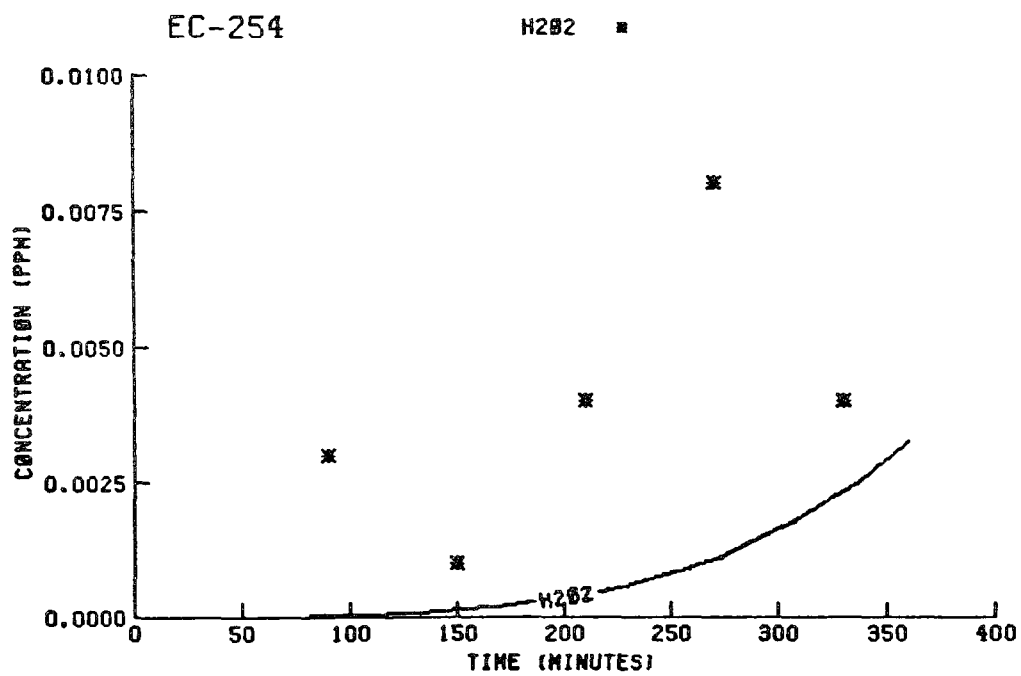
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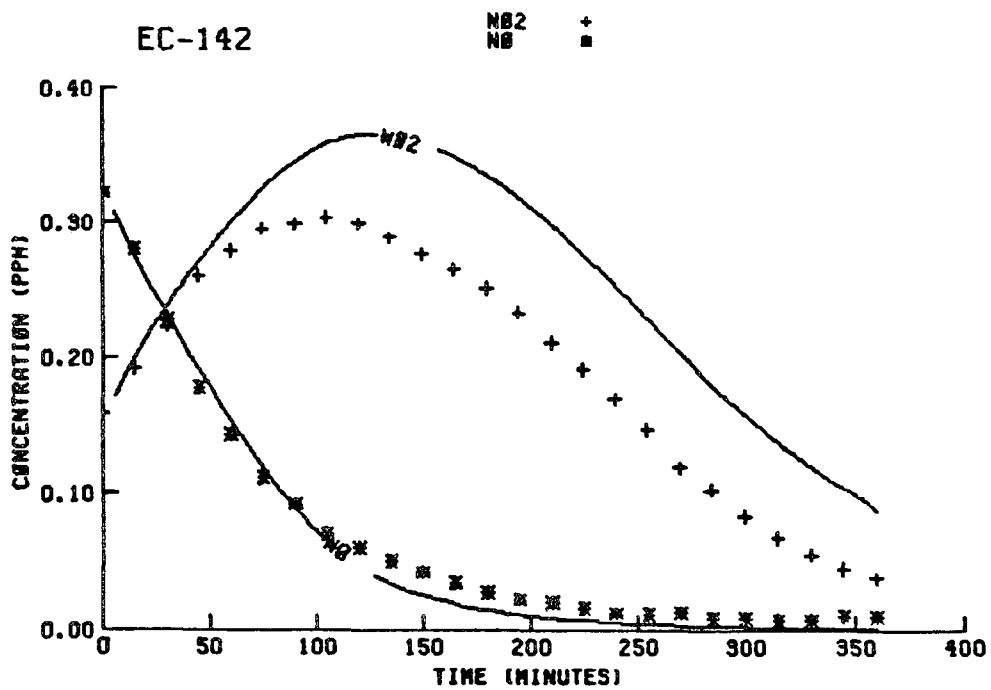
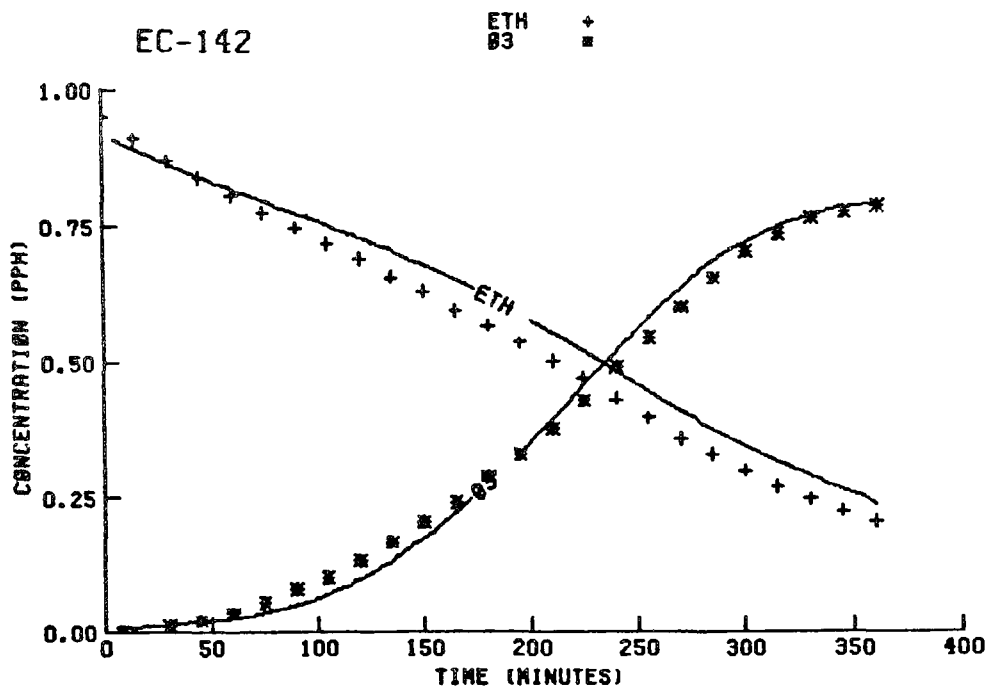


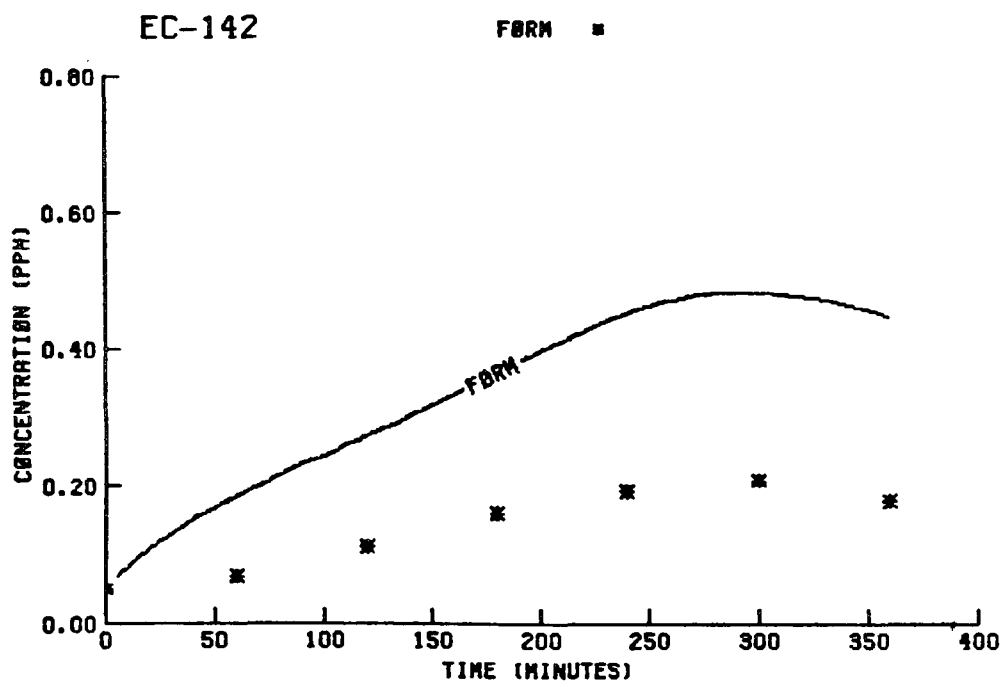
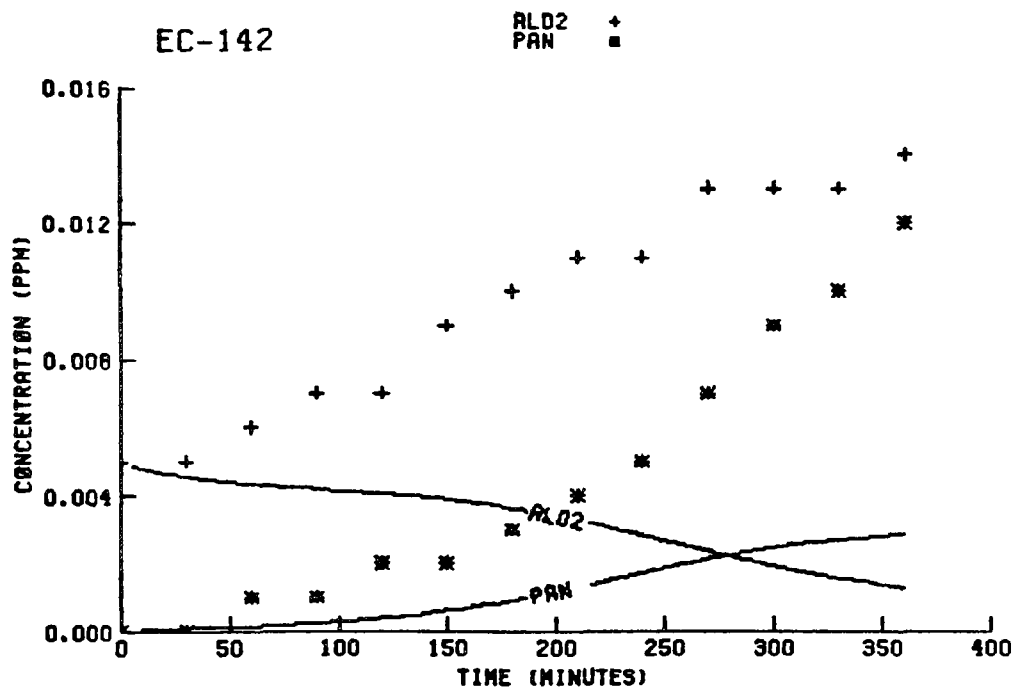






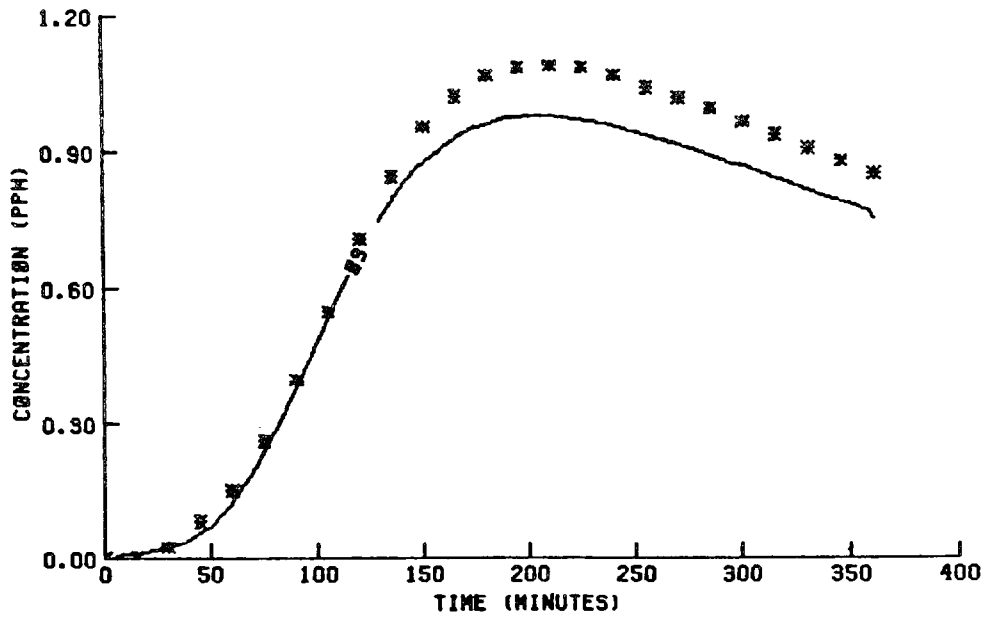
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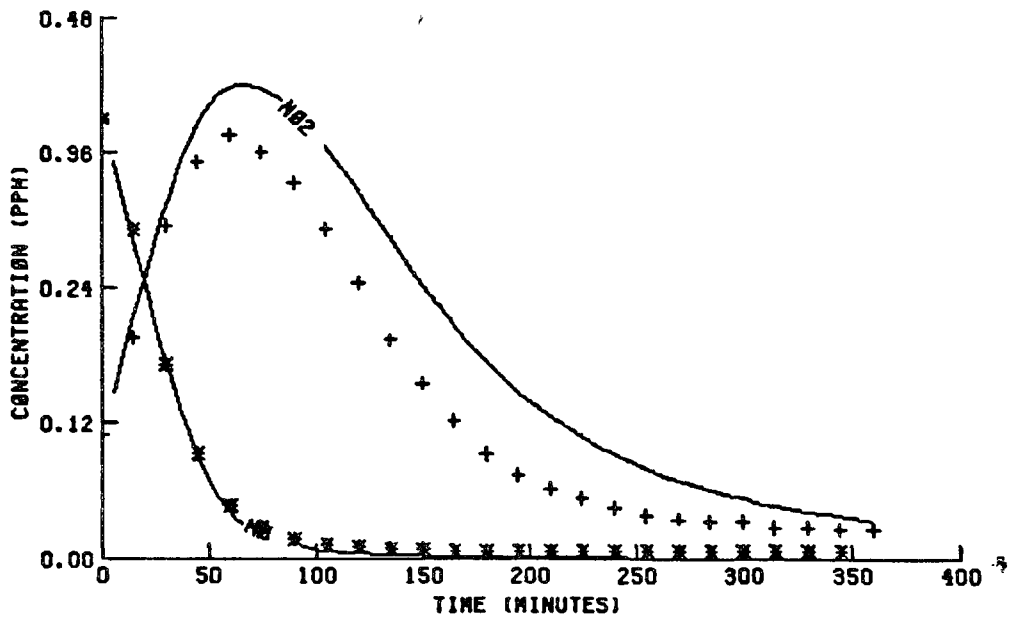
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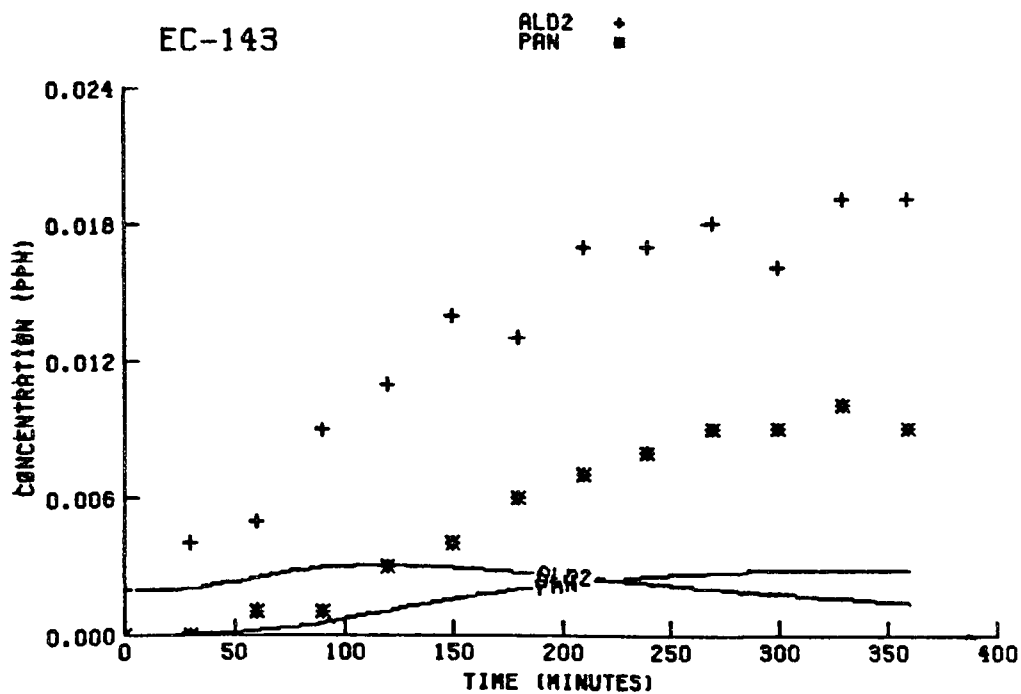
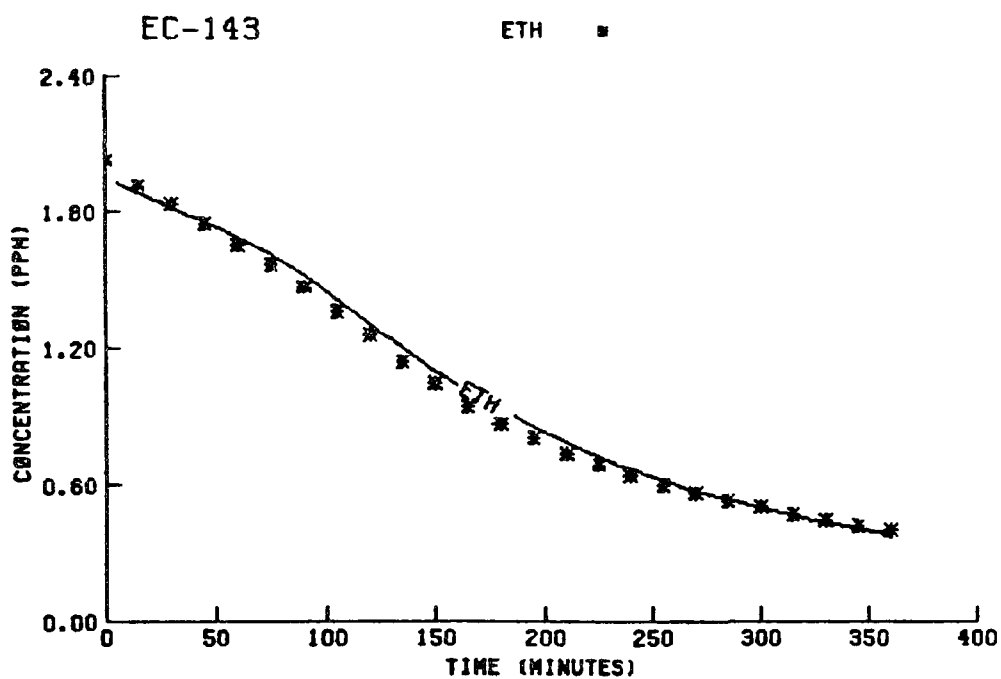
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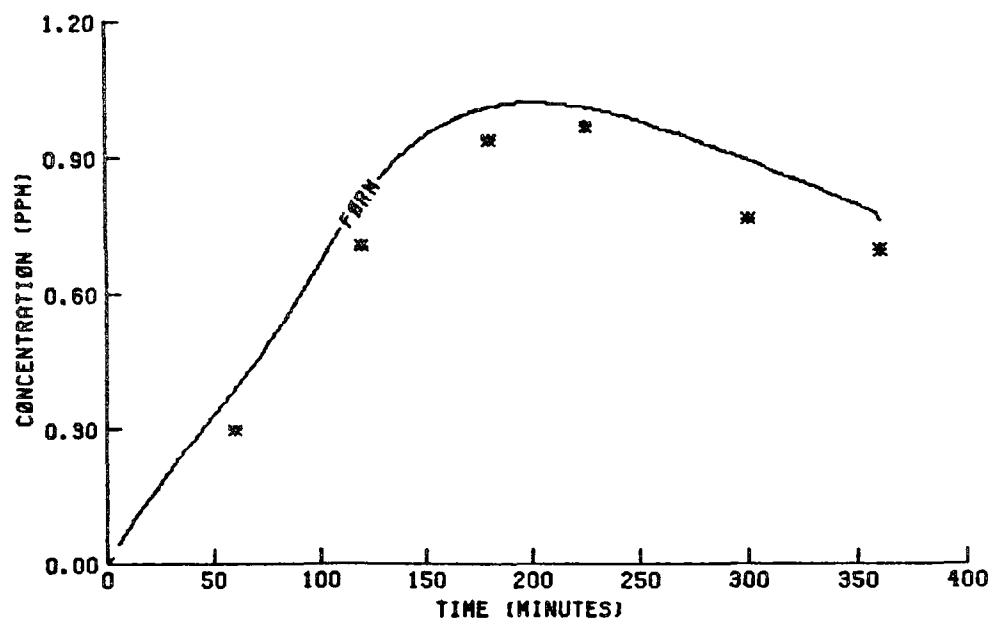
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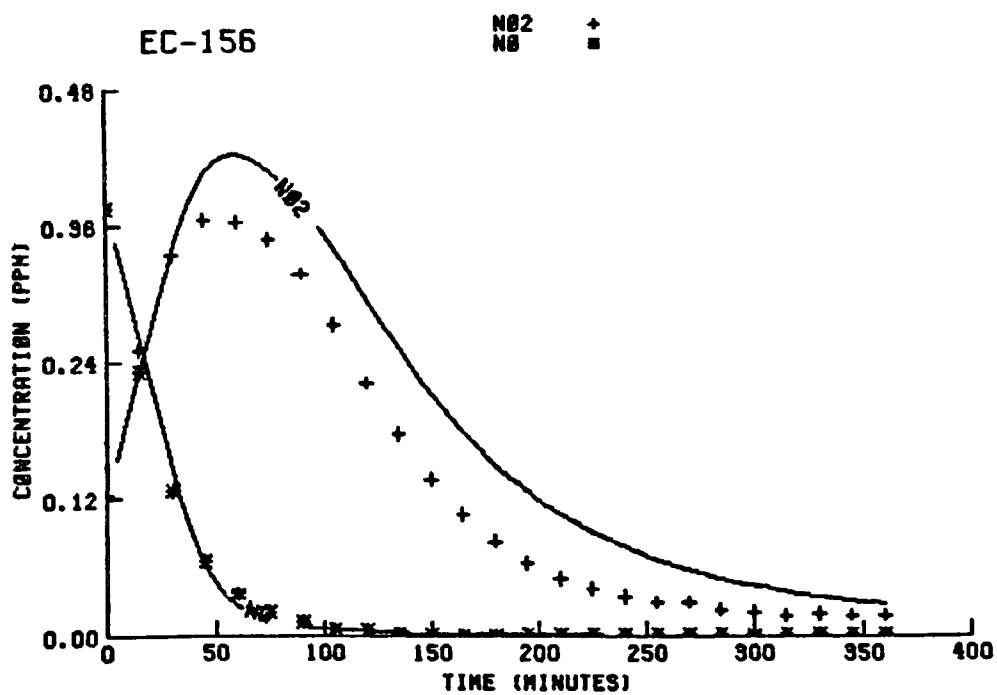
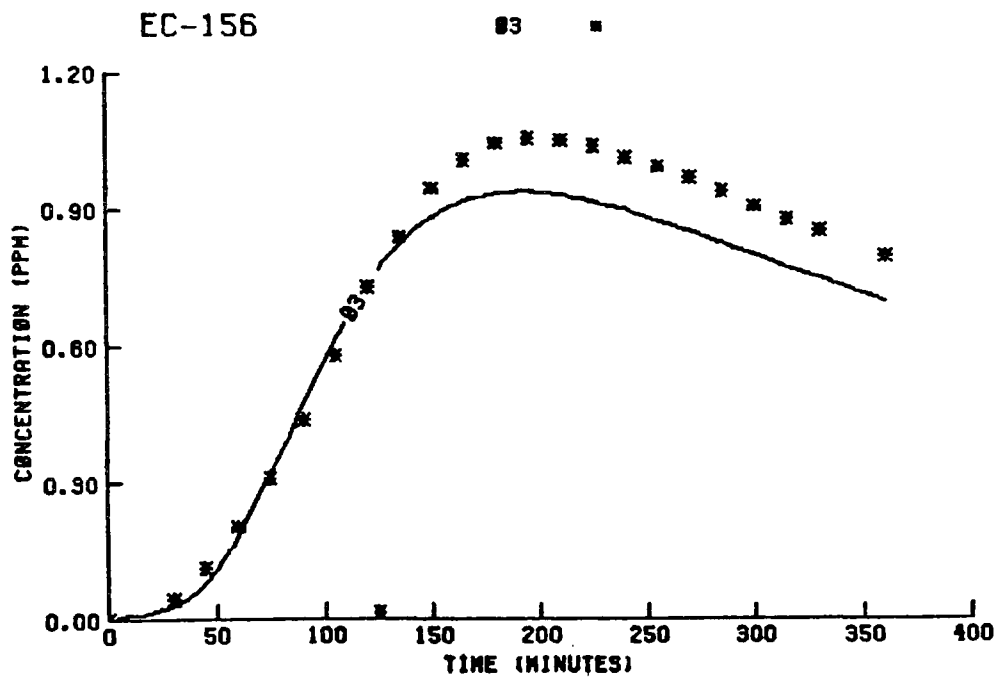


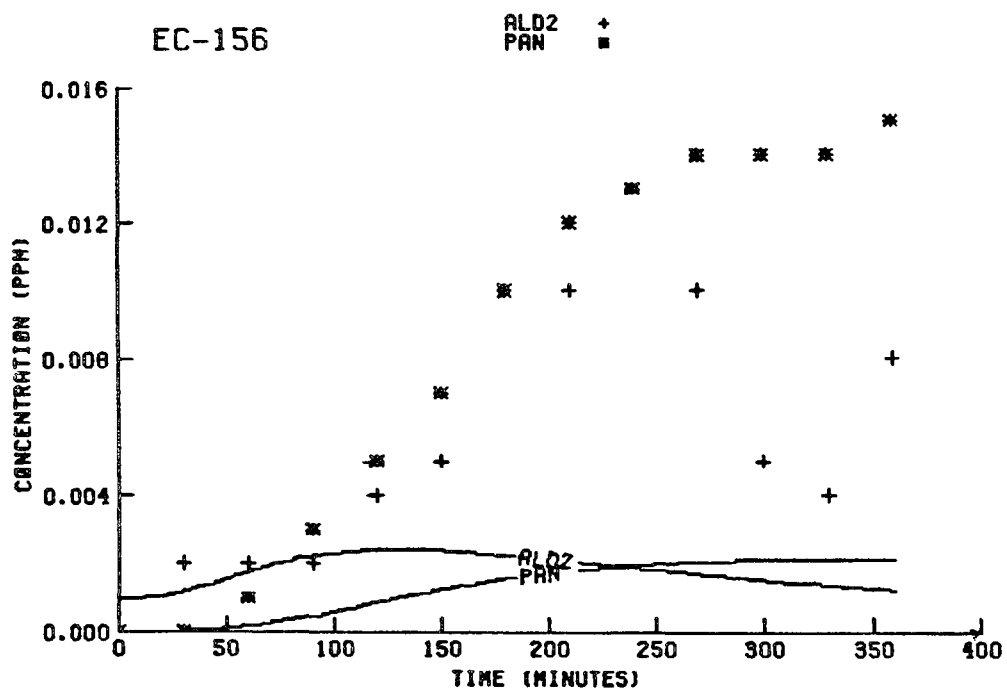
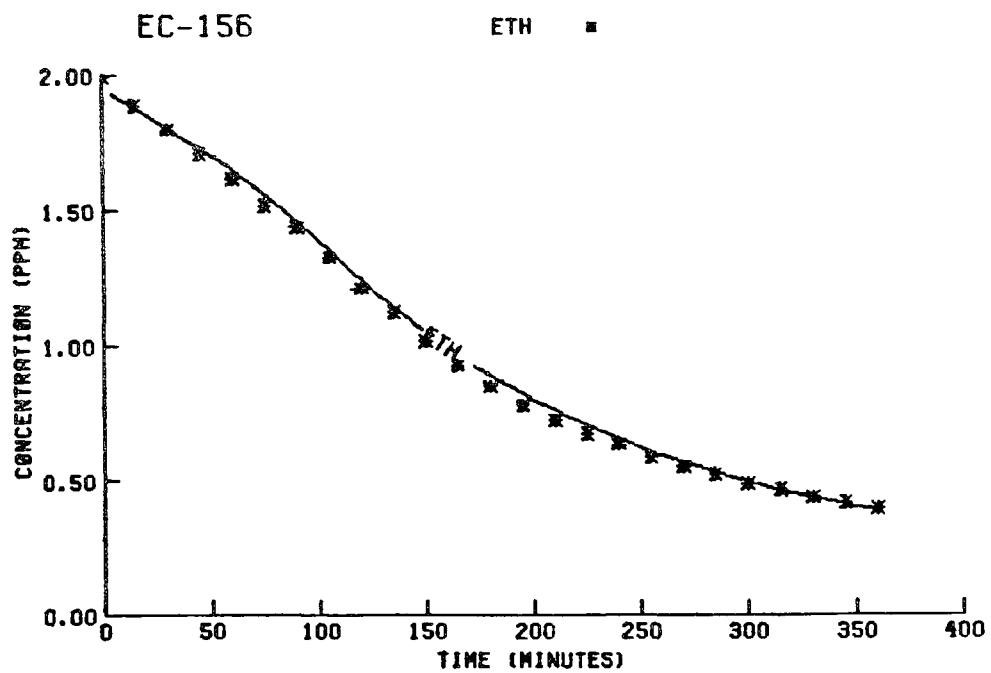


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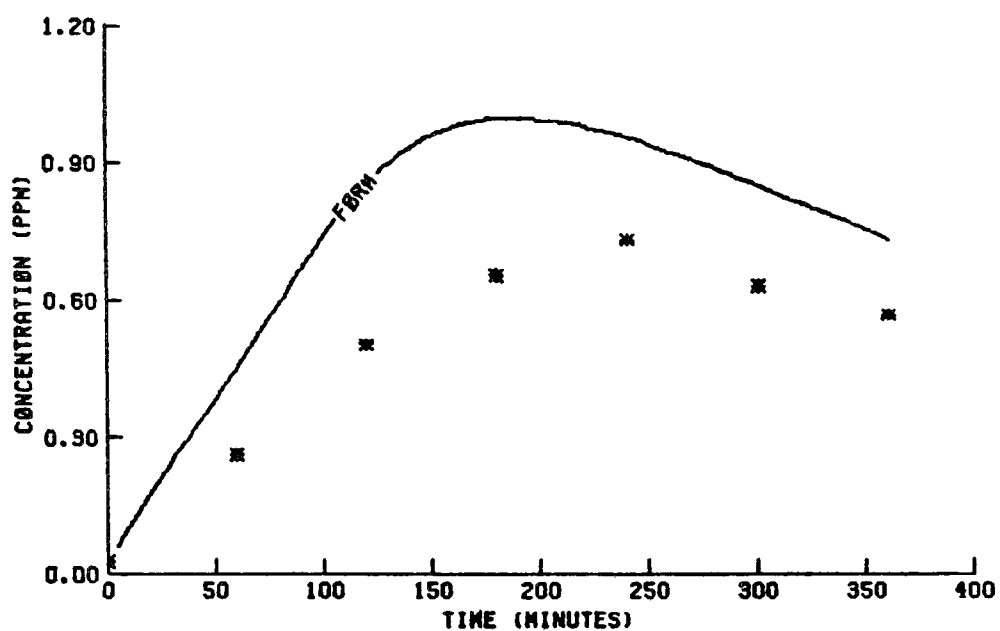






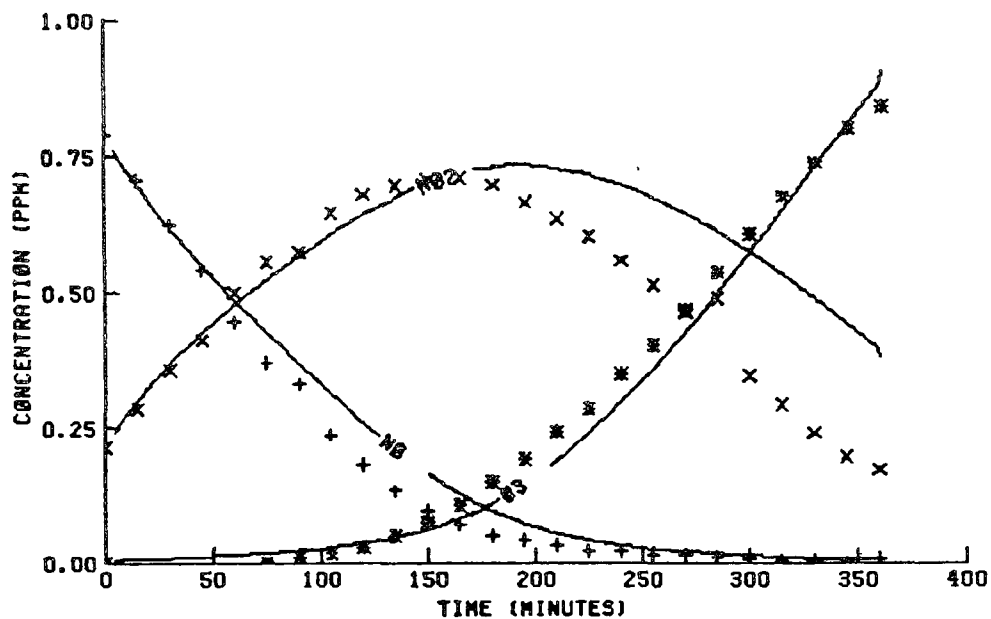
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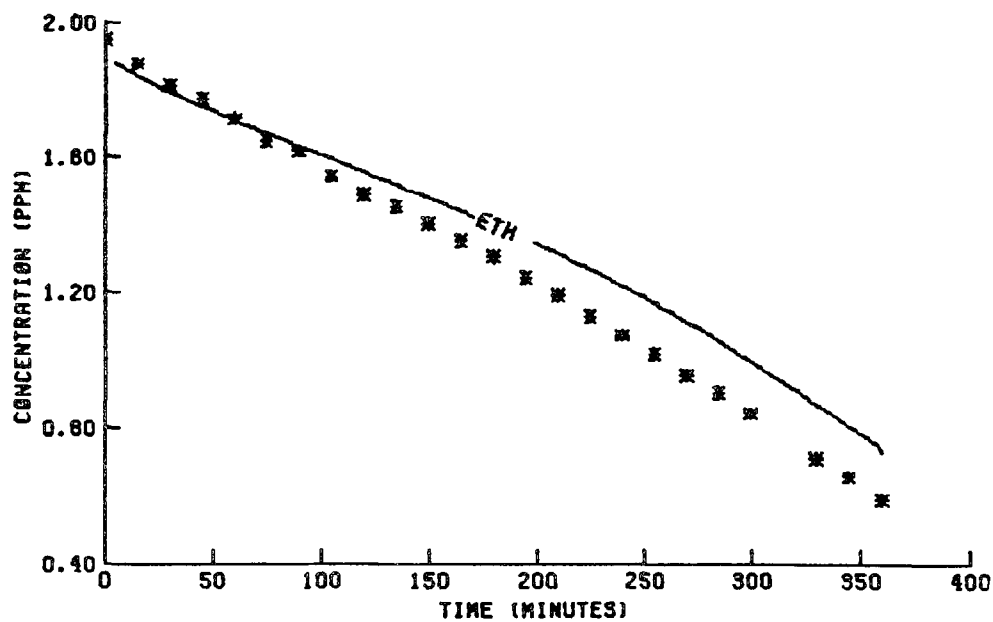
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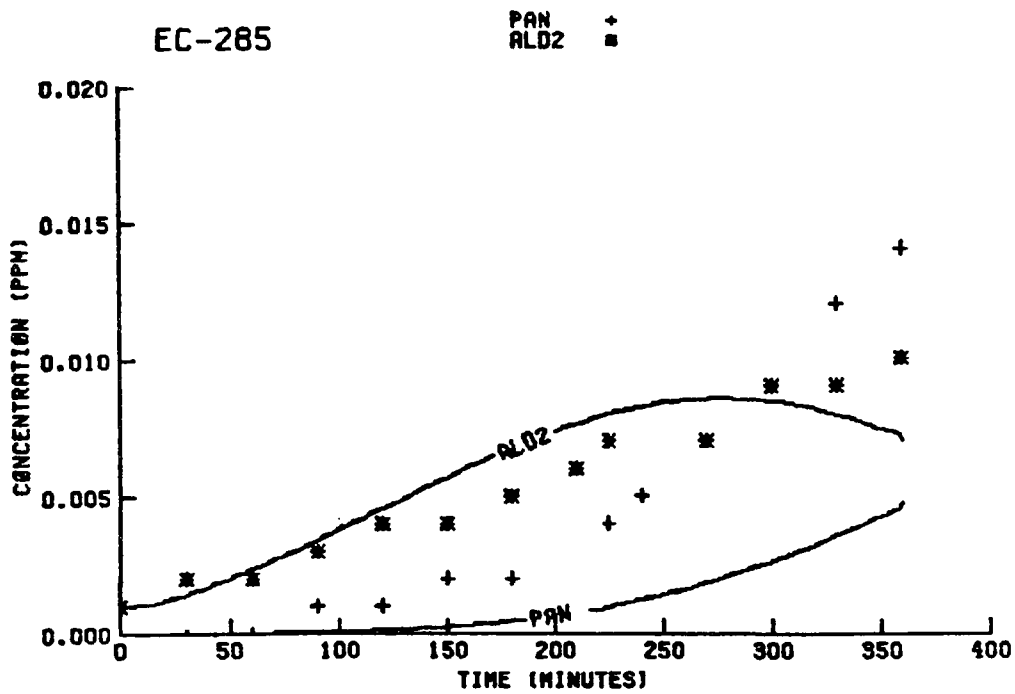
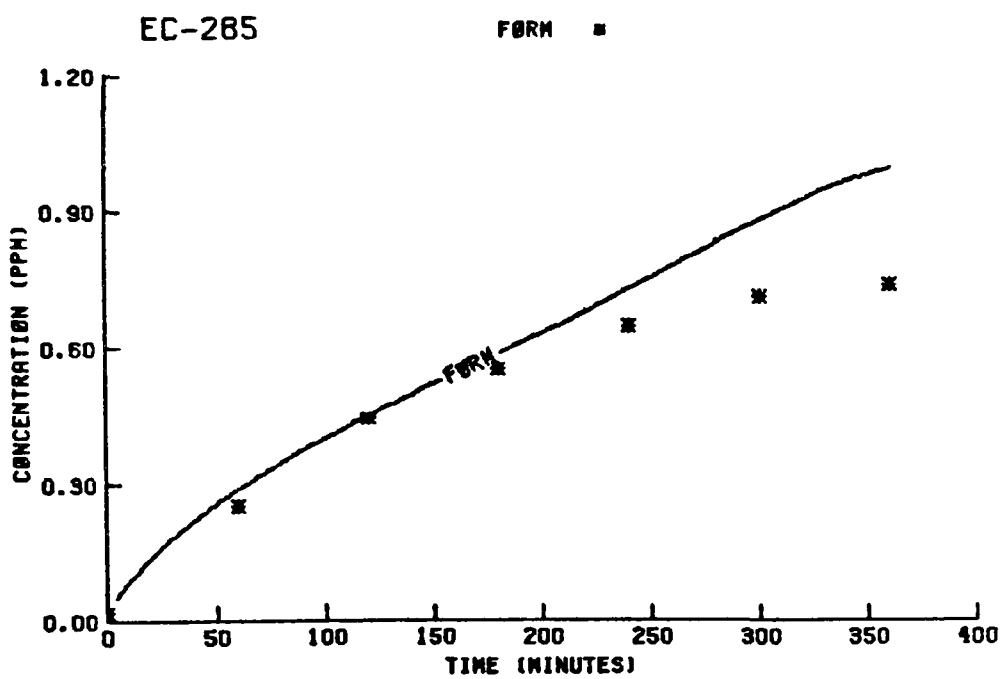
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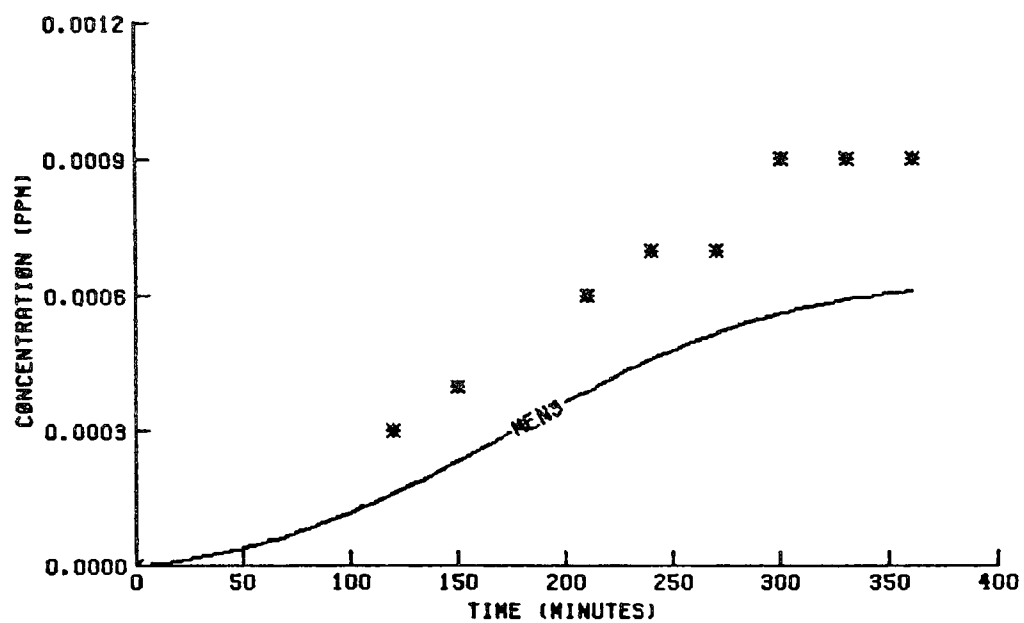
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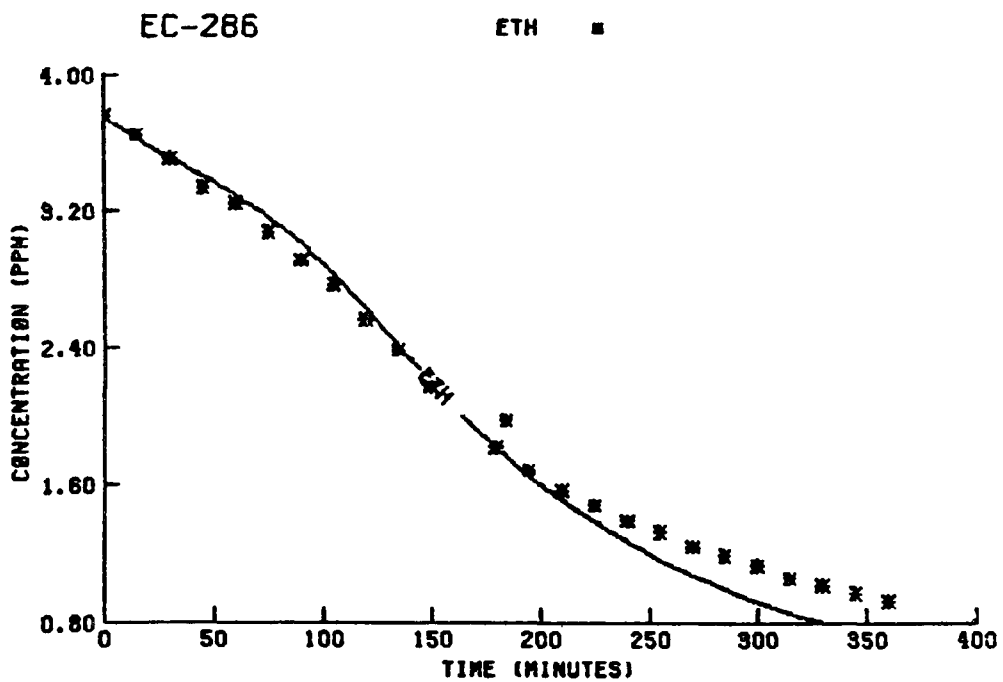
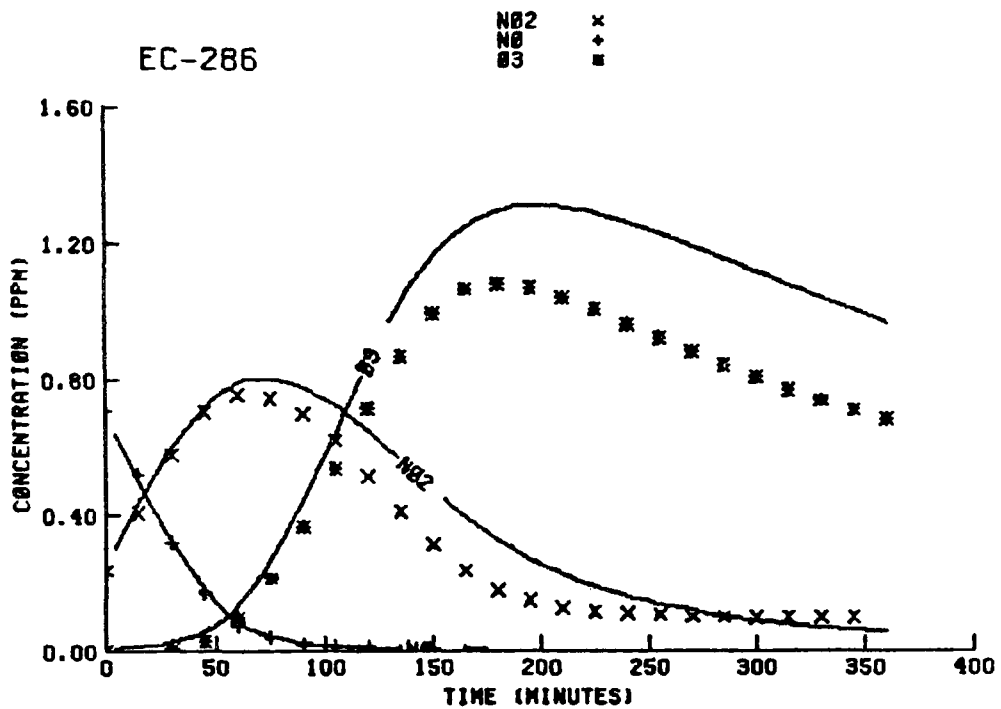


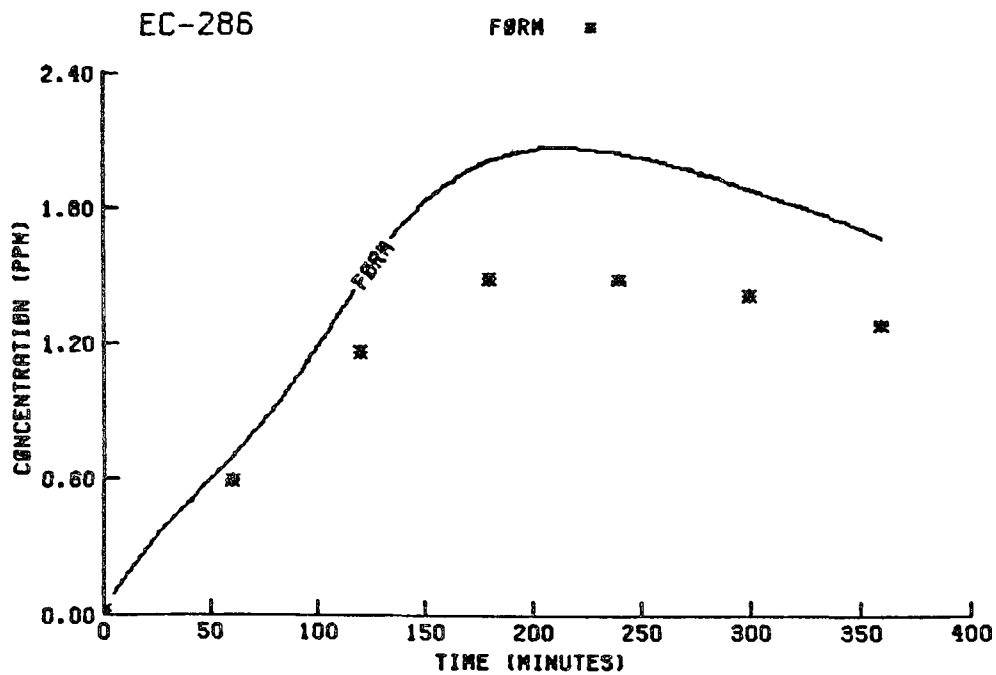
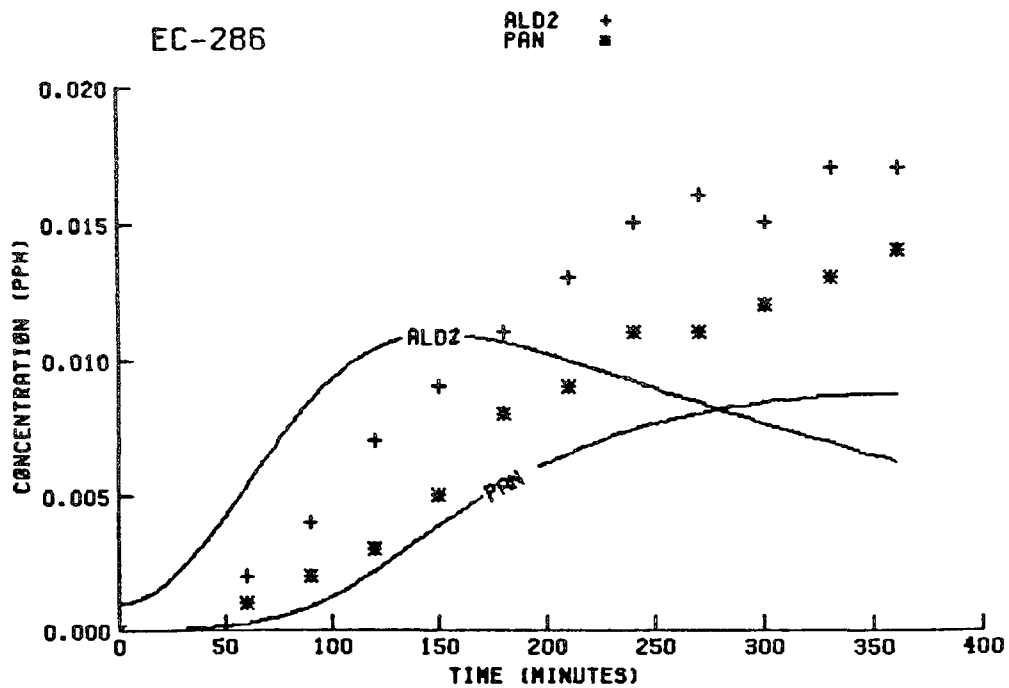


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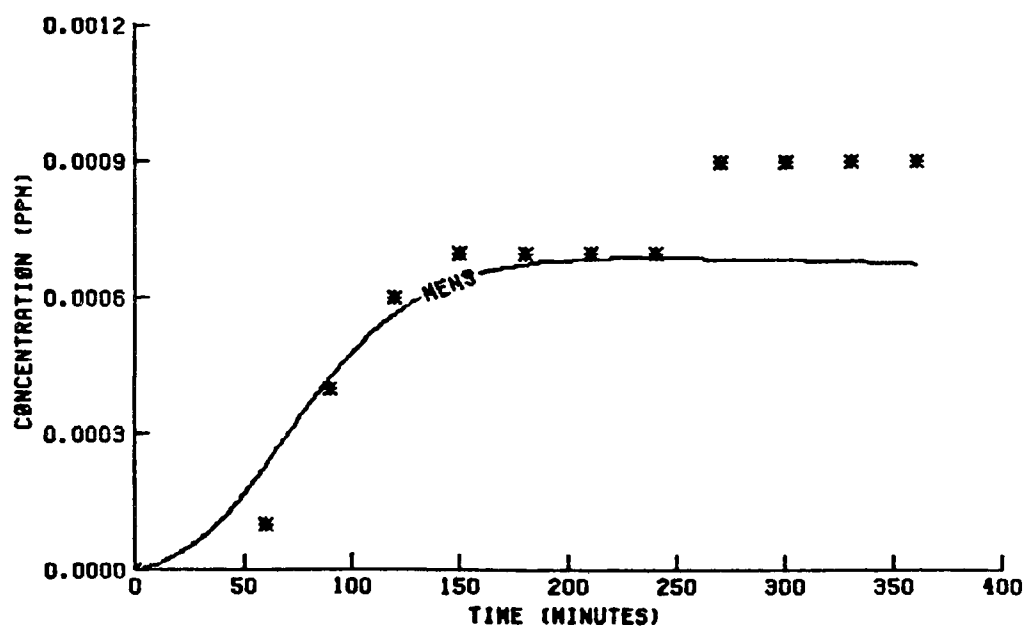






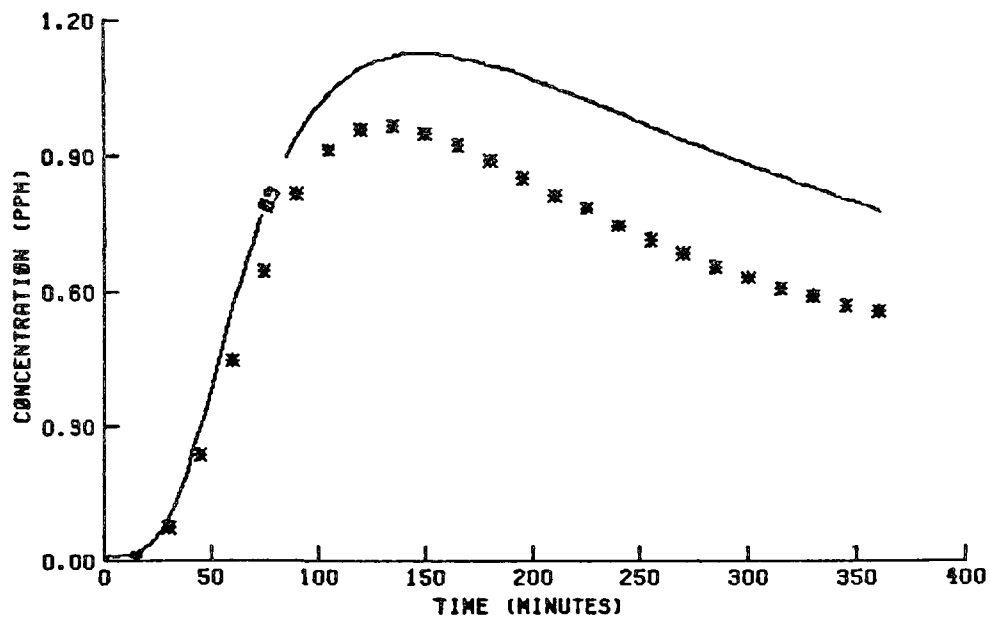
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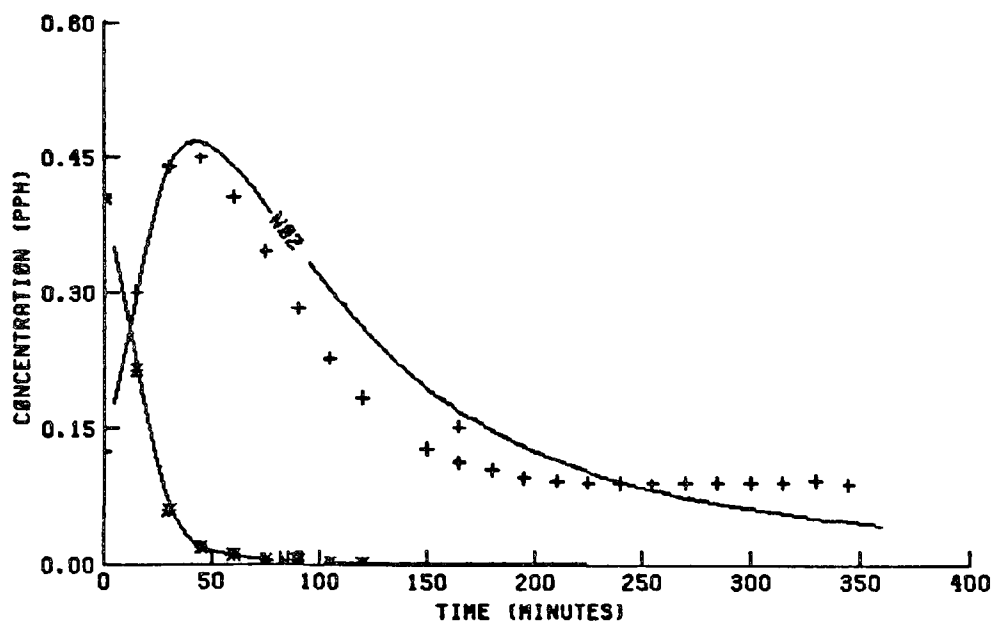
EC-287

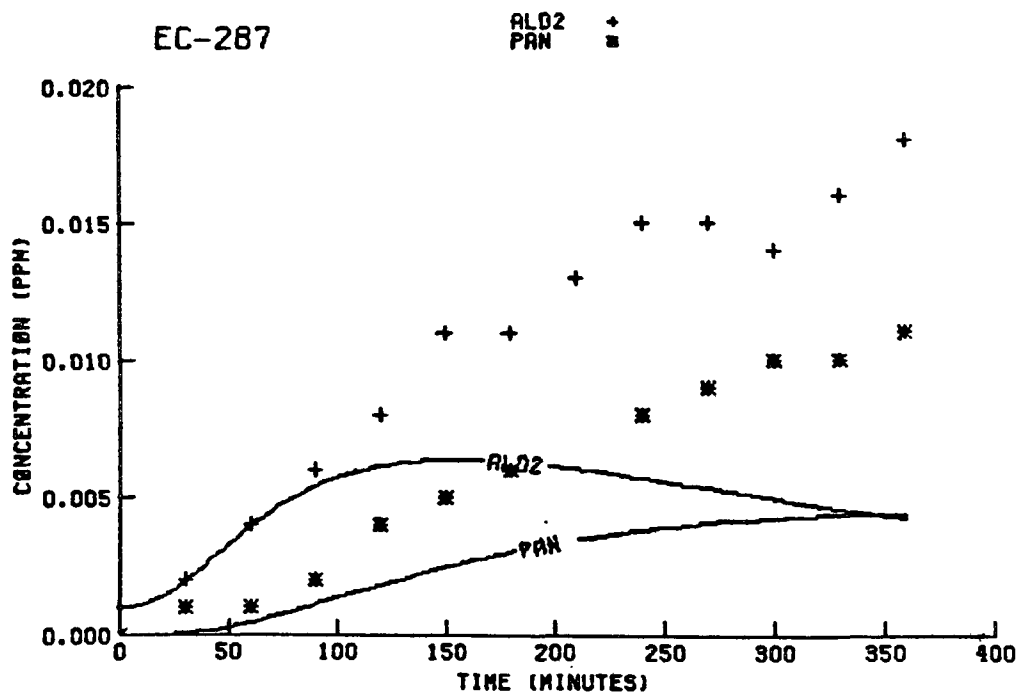
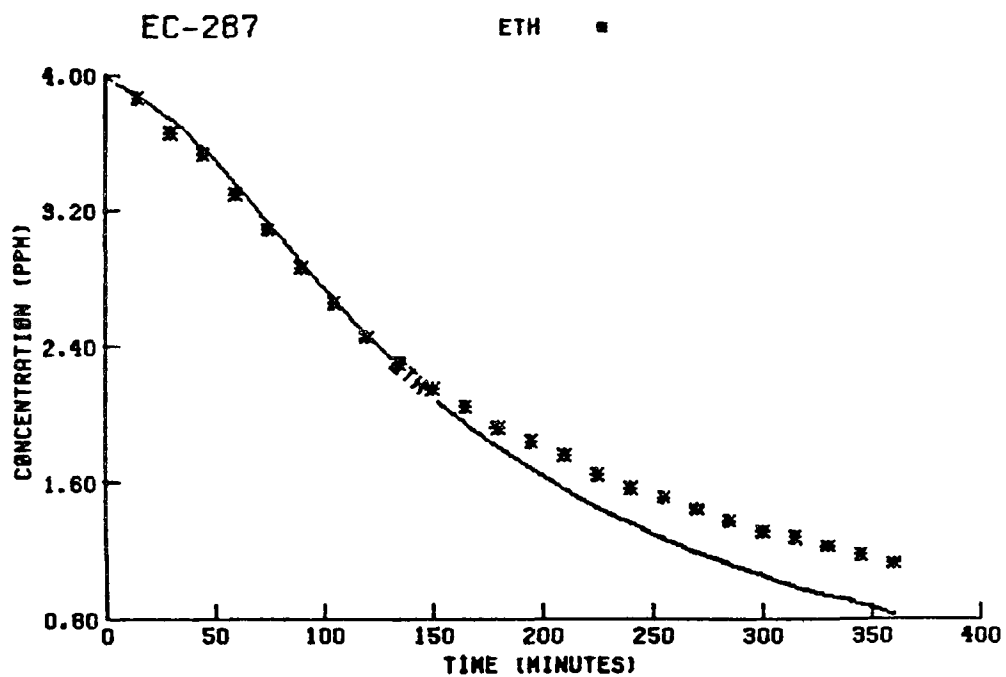
03 ■



EC-287

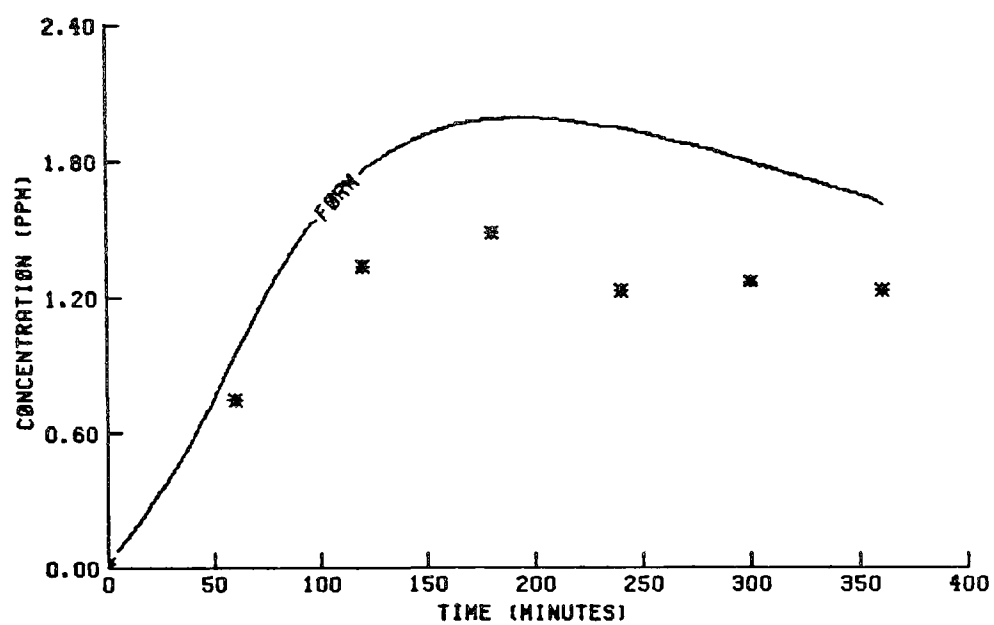
N02 +
N0 ■



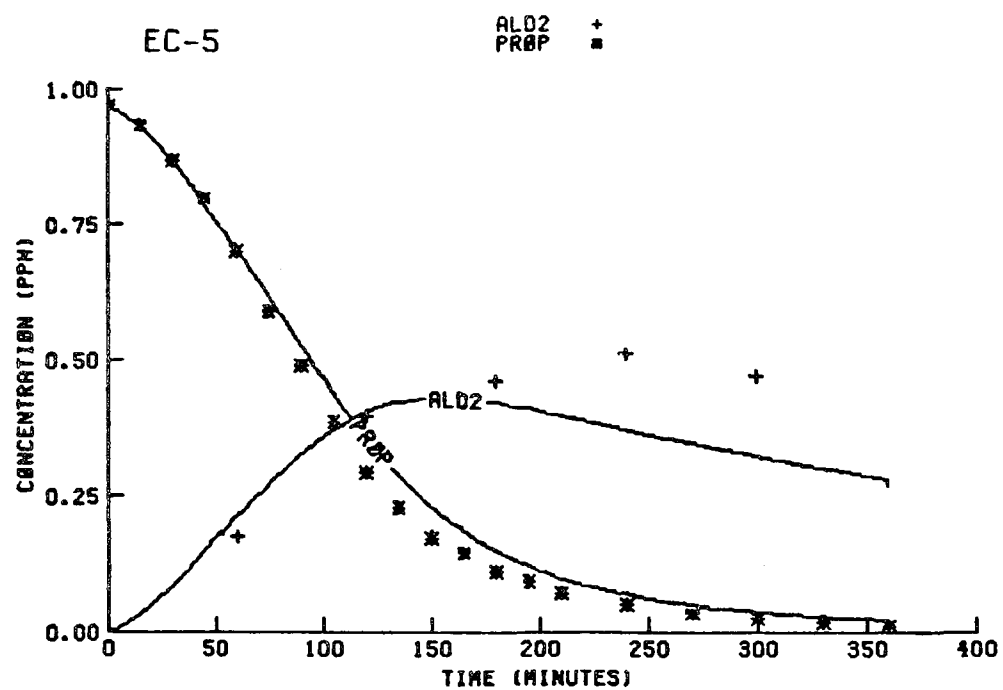
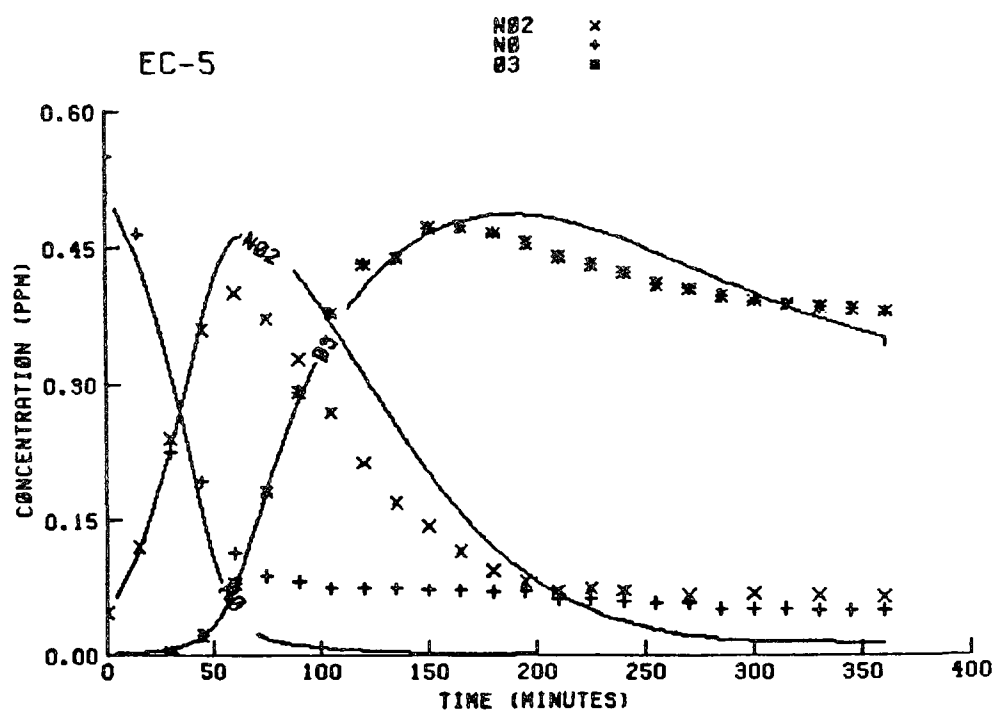


EC-267

F0RM ■

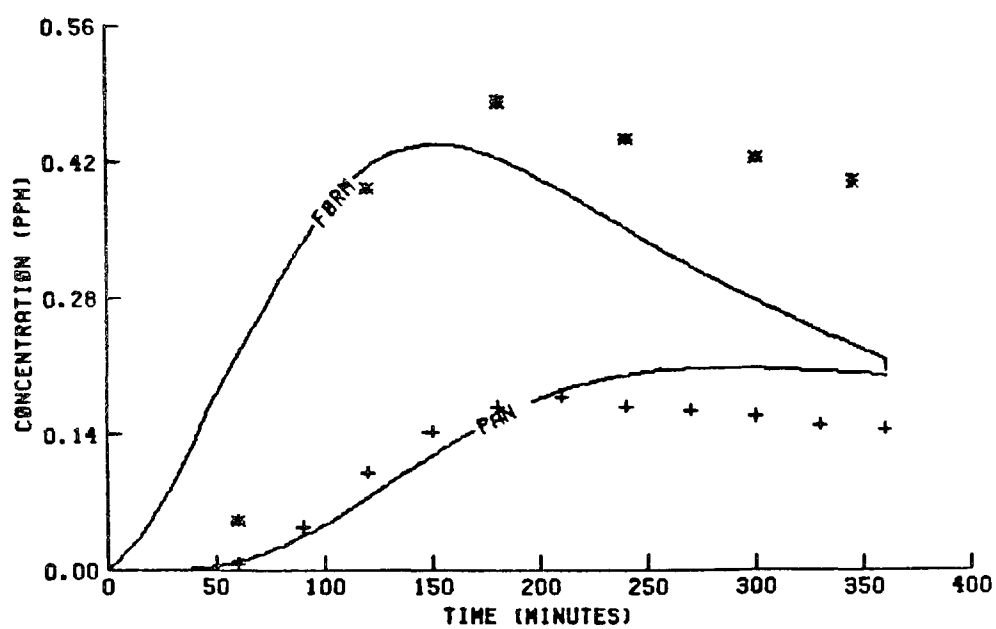


UCR PROPYLENE EXPERIMENTS



EC-5

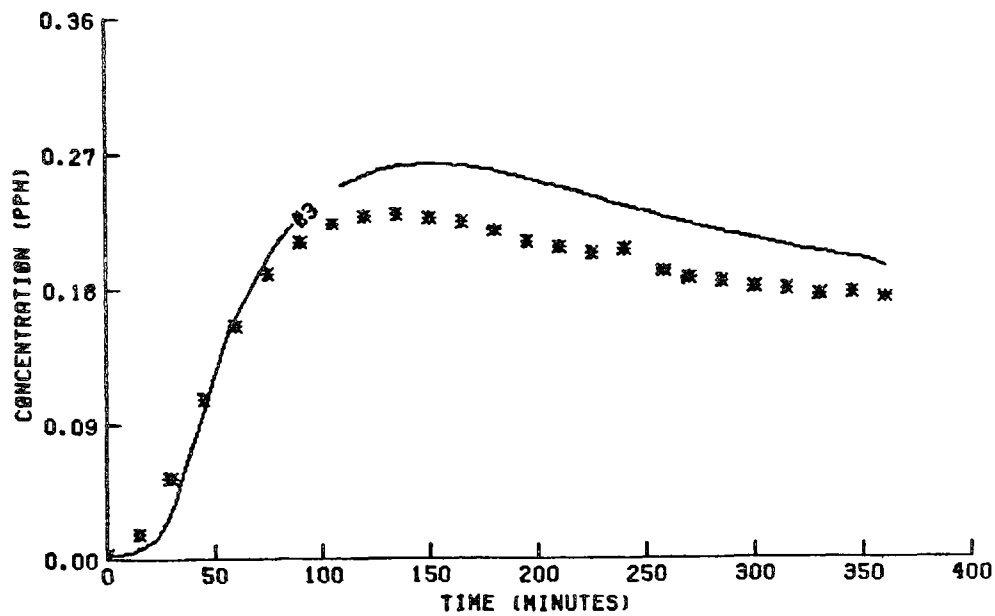
PAN +
FORM ■



EC-11

83

■



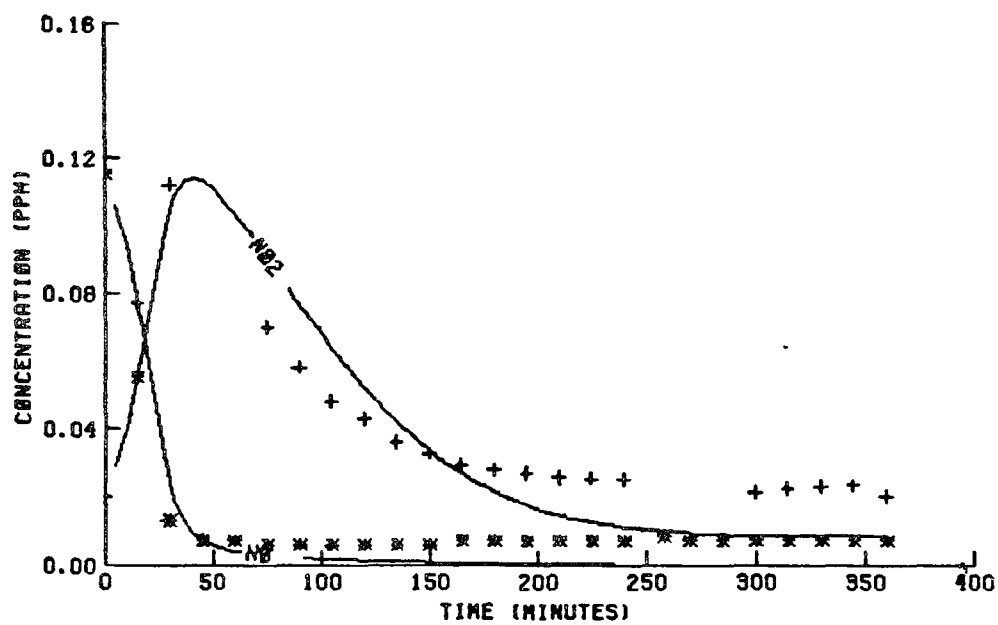
EC-11

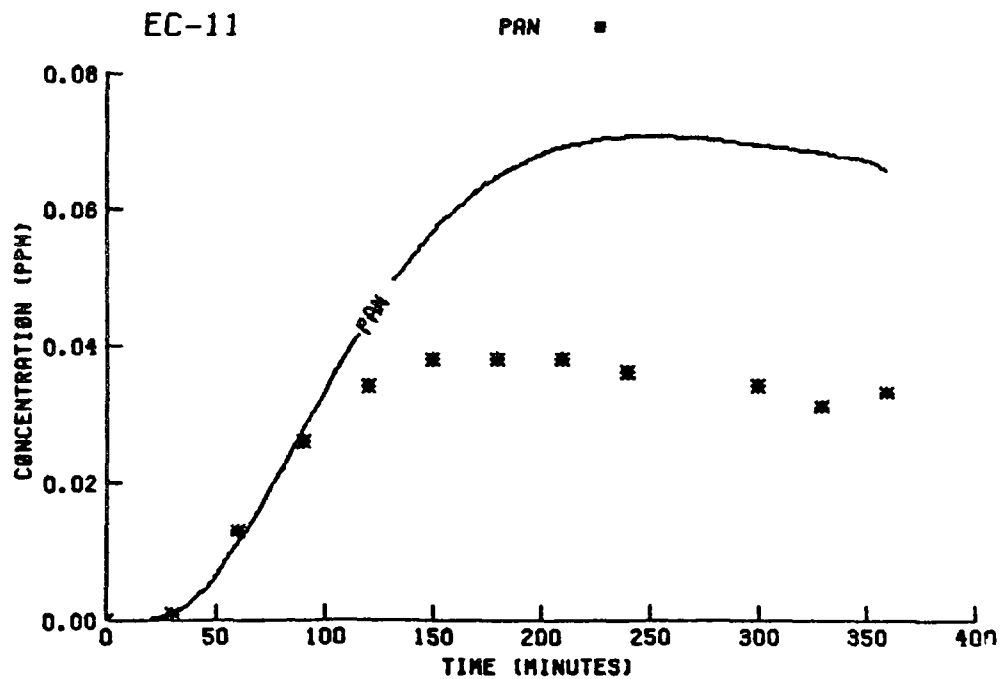
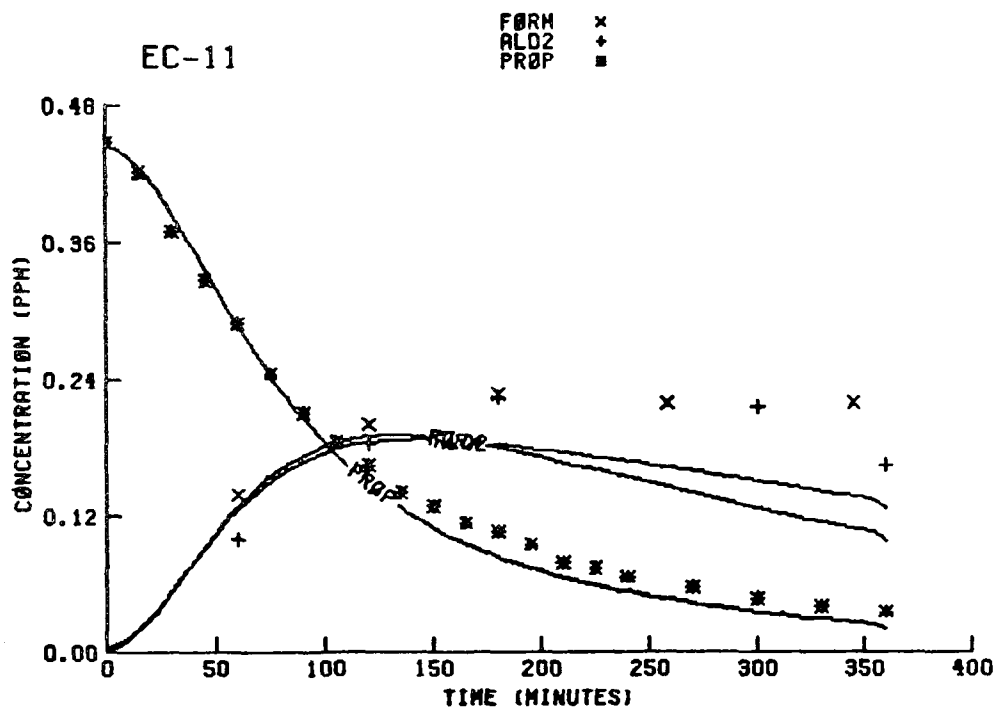
NB2

+

NB

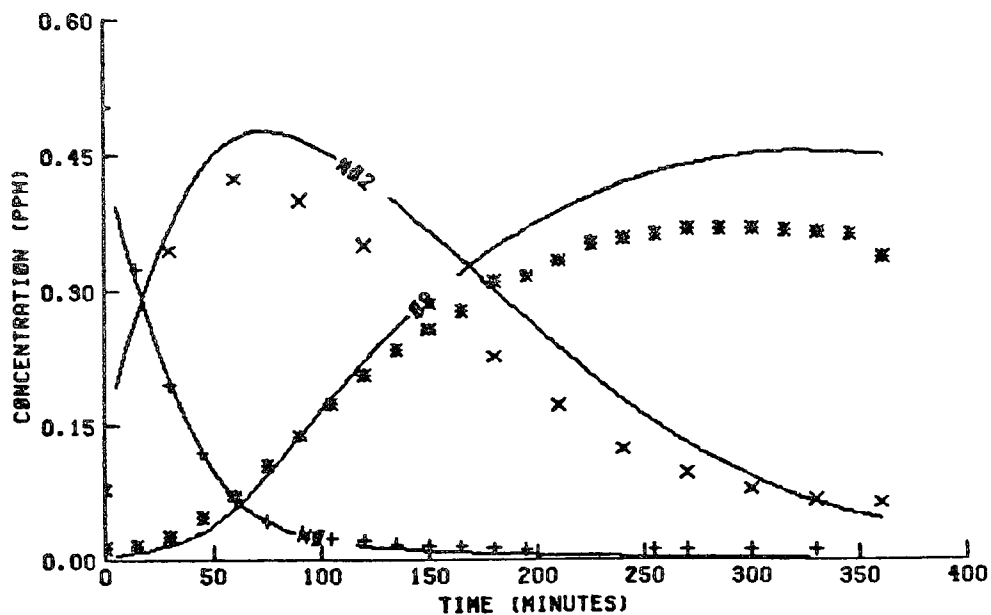
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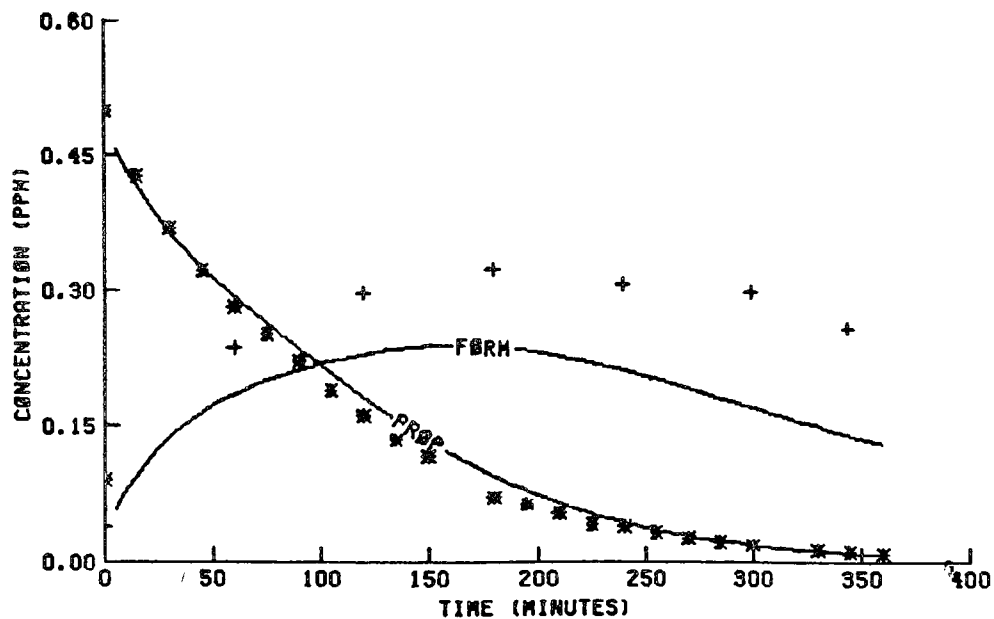
EC-13

NO2 x
NO +
O3 ■



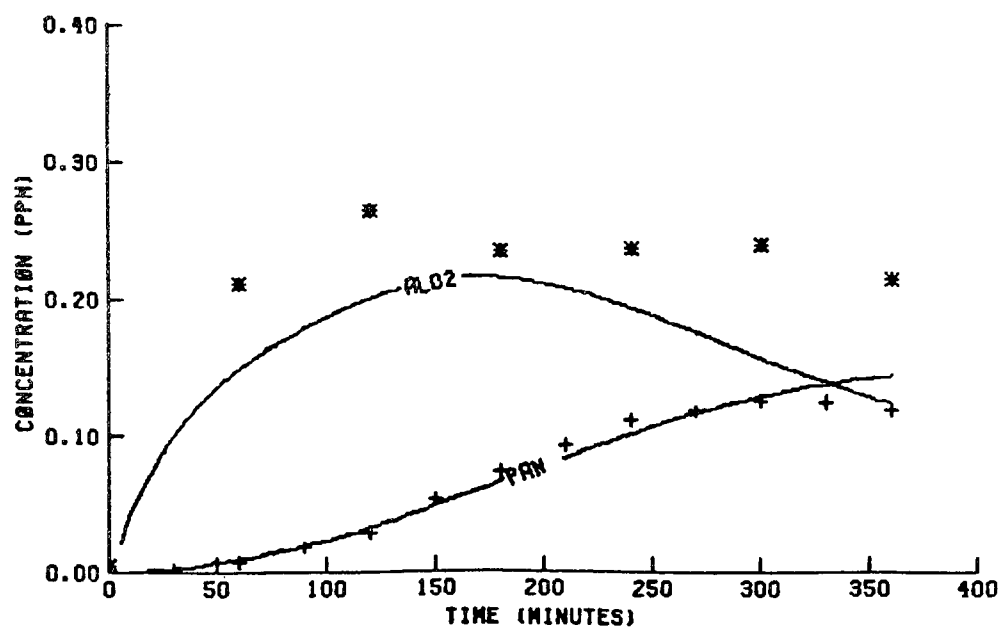
EC-13

FORM +
PROP ■



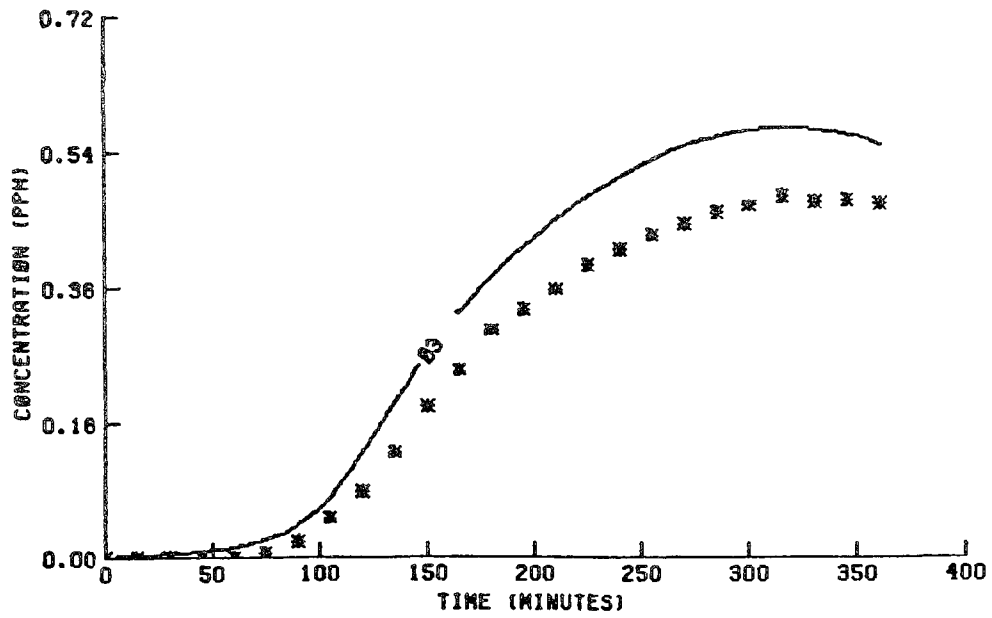
EC-13

PAN +
ALD2 ■



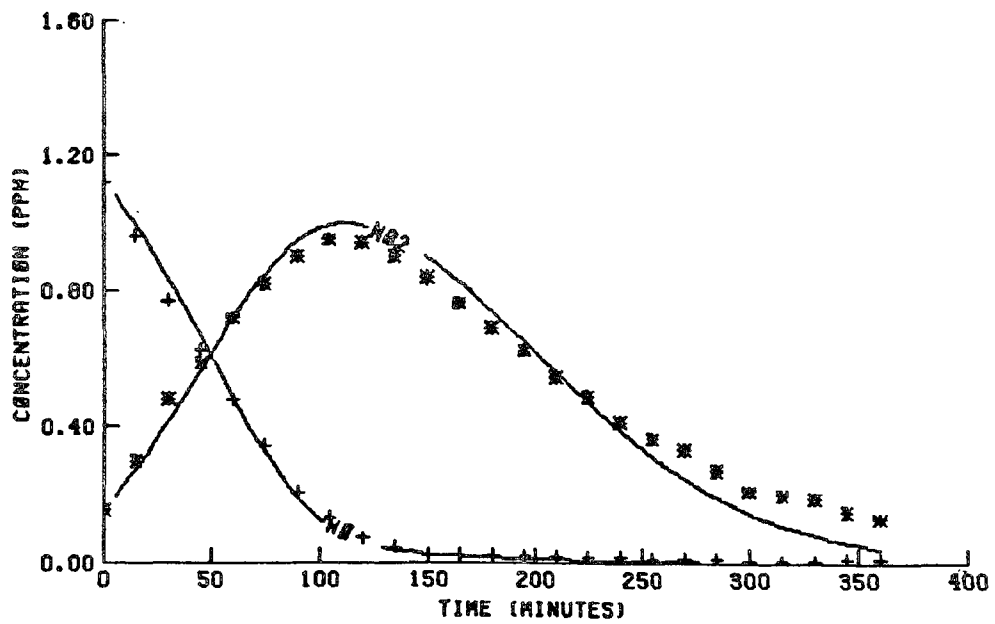
EC-16

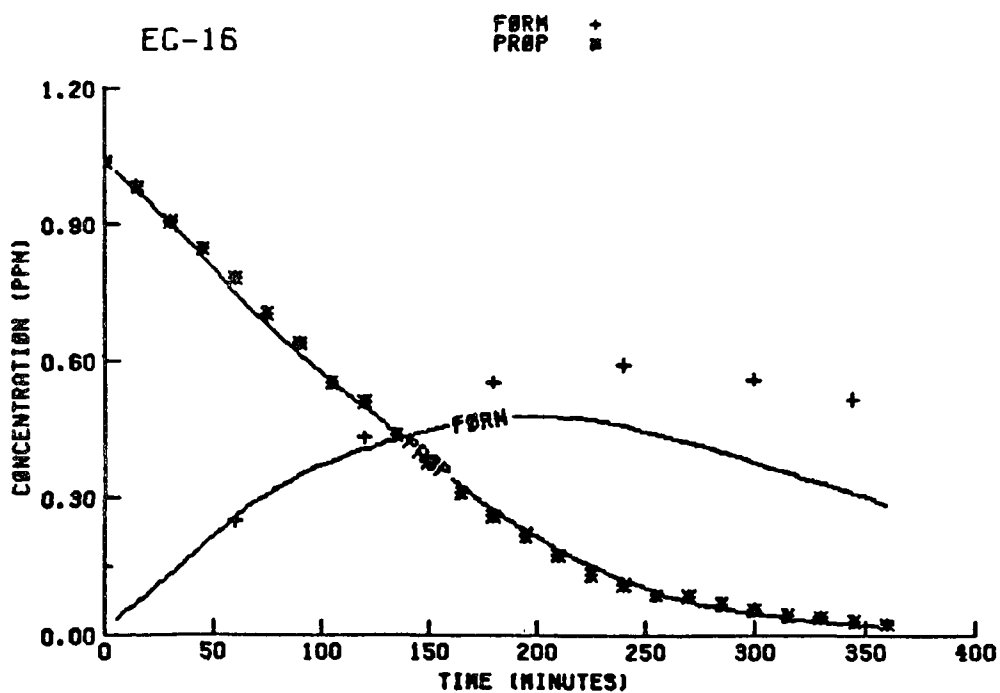
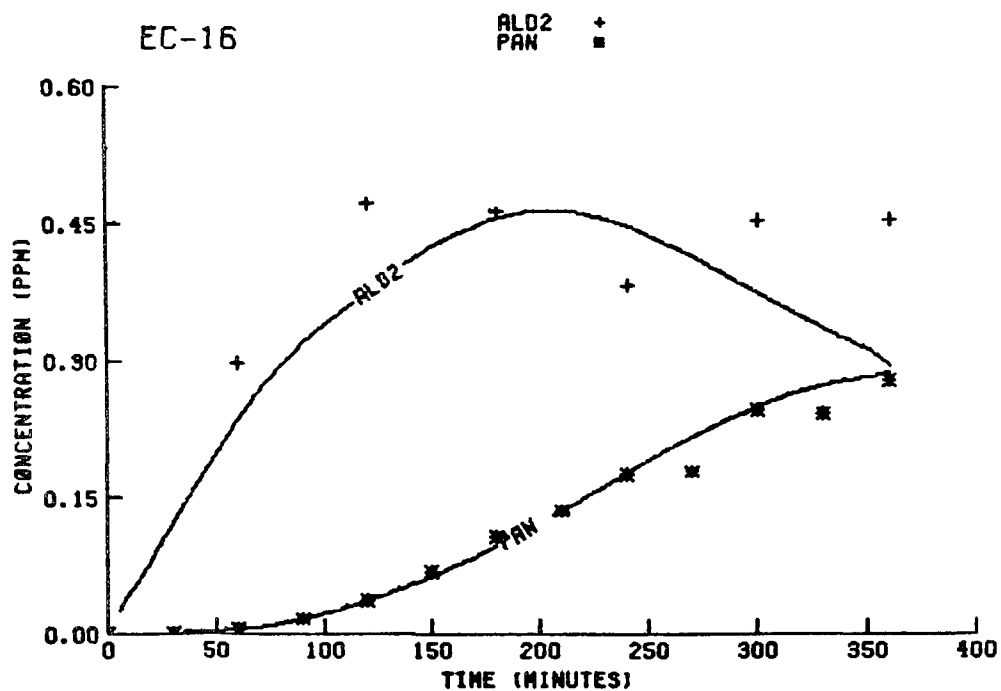
03

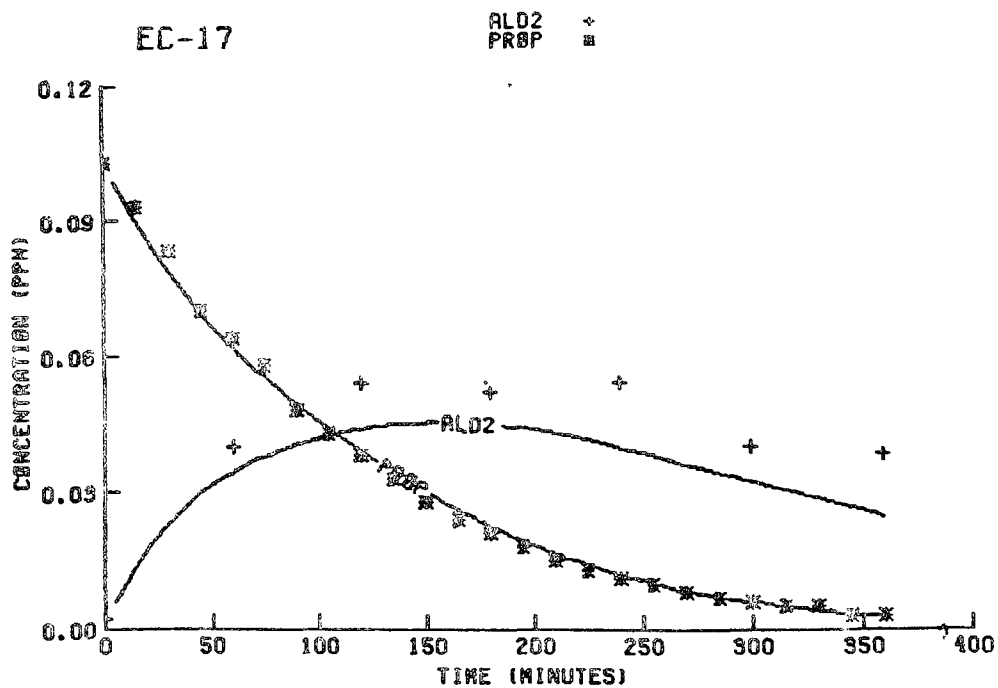
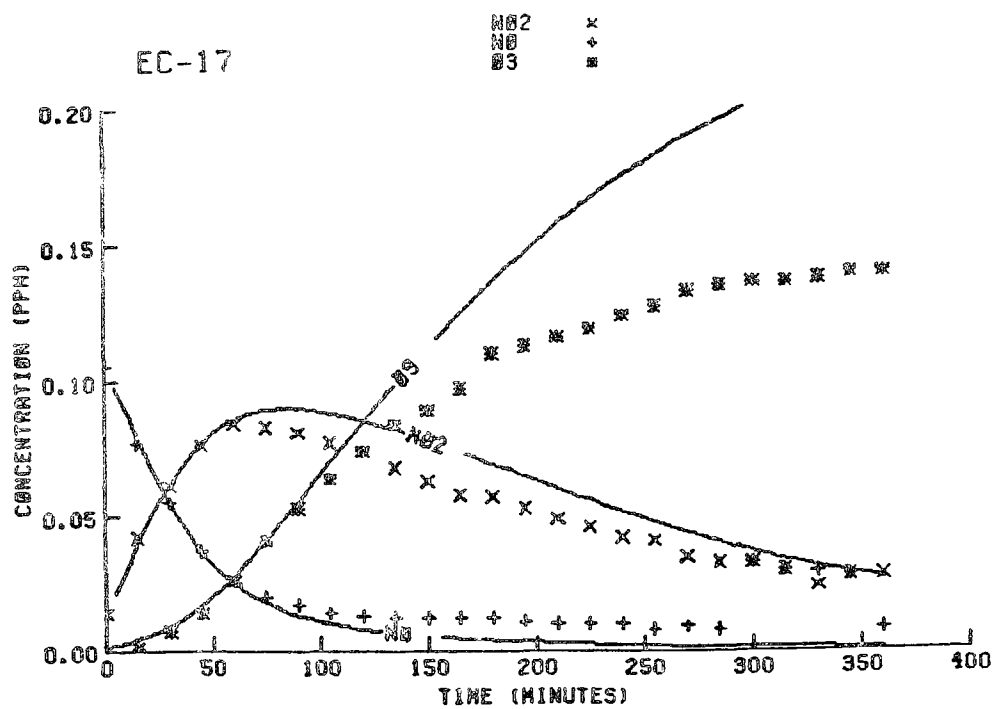


EC-16

NB +
NB2

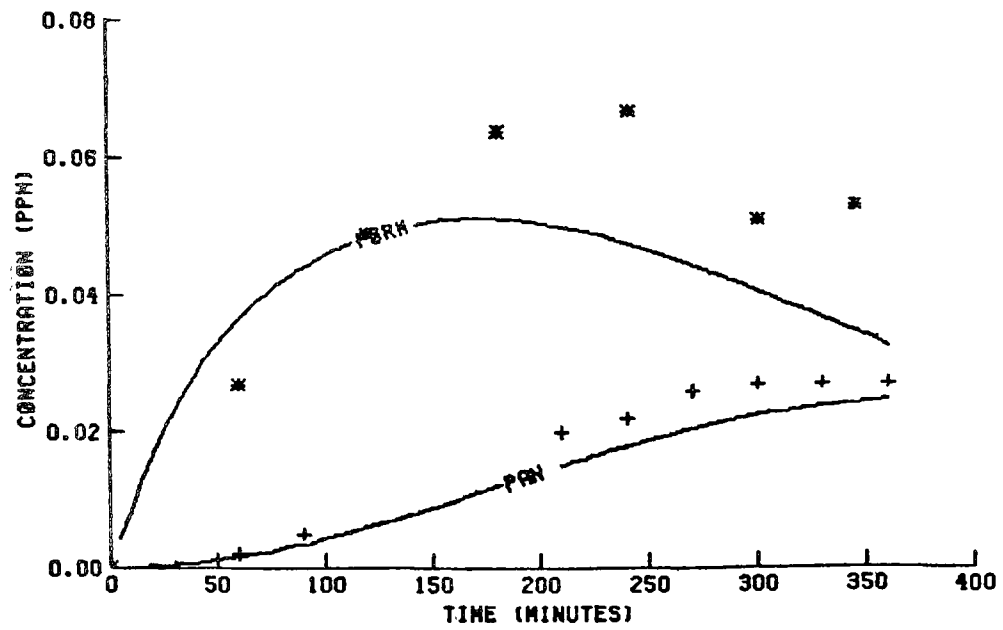






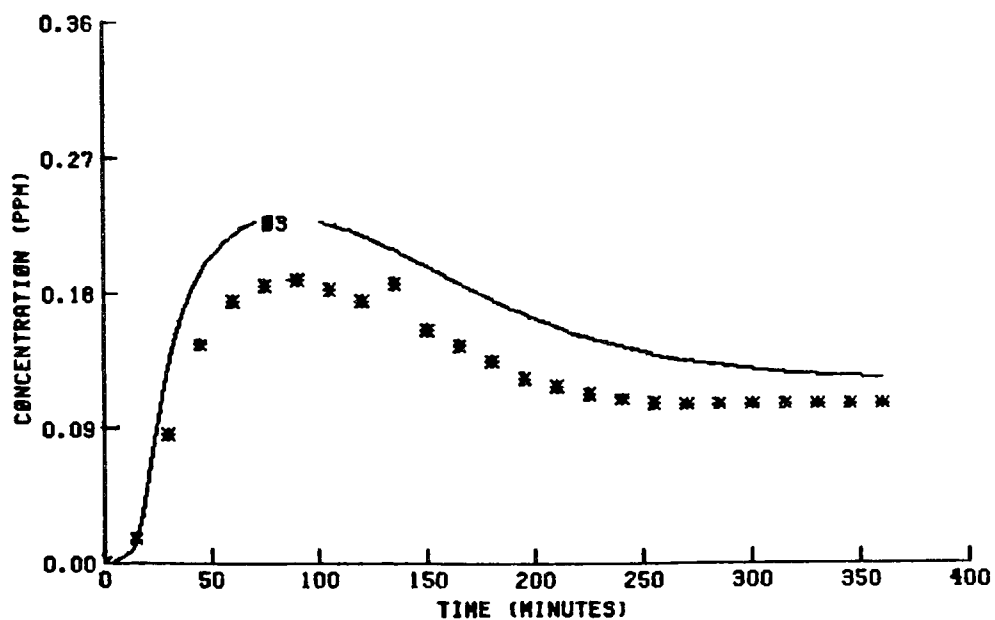
EC-17

PAN +
FORM *



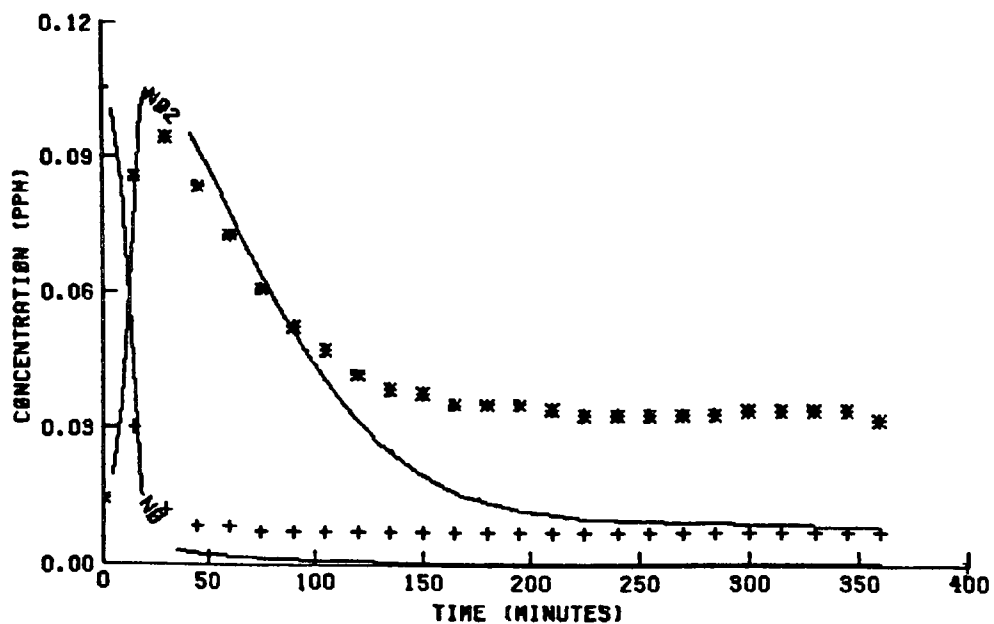
EC-18

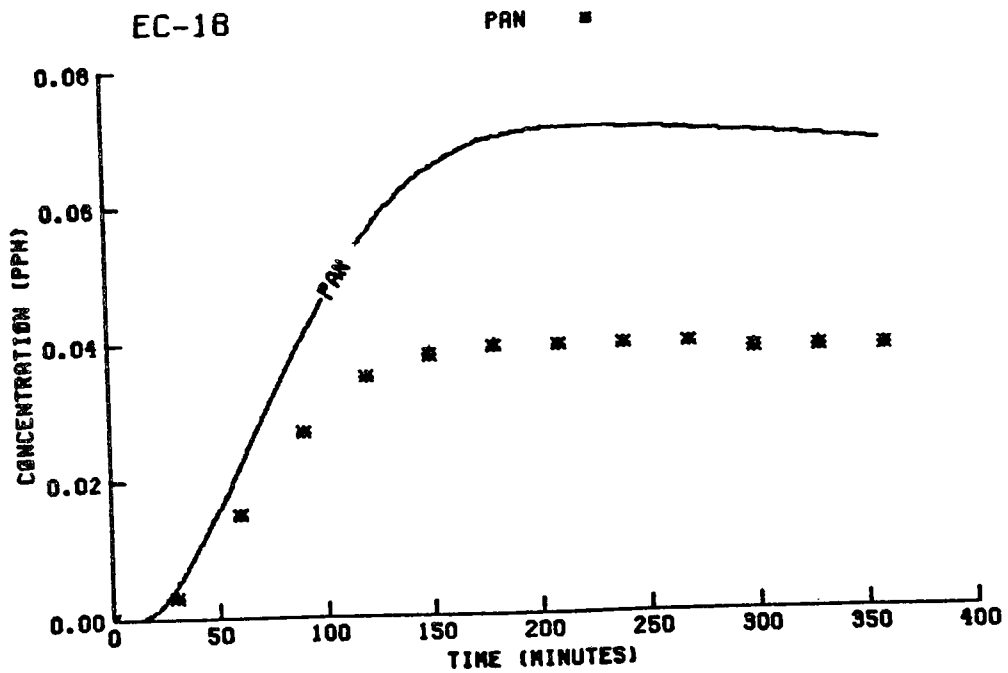
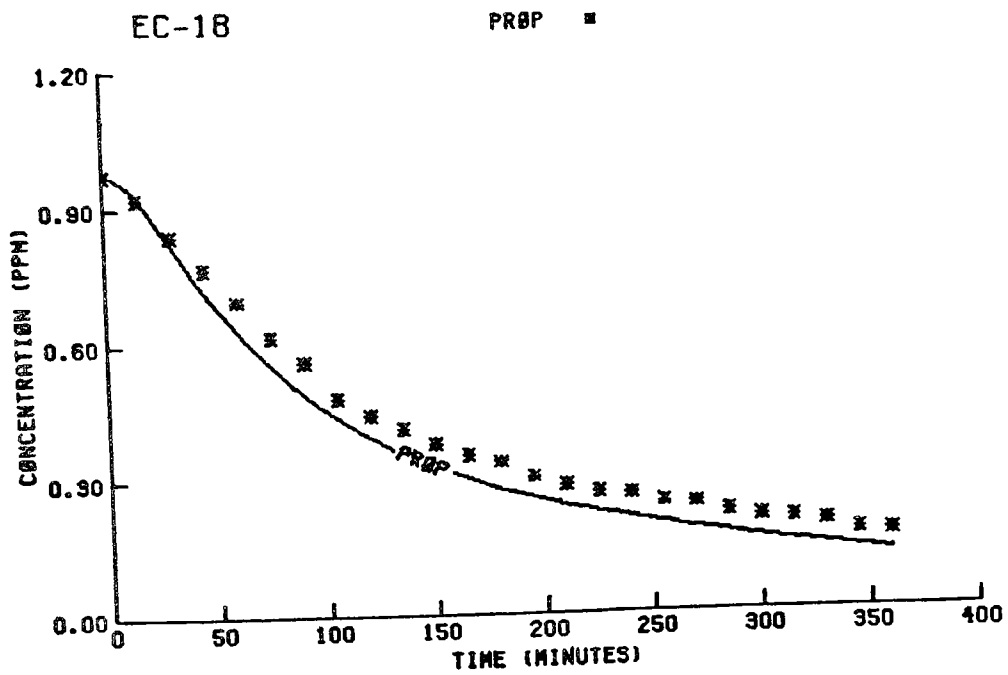
83 ■



EC-18

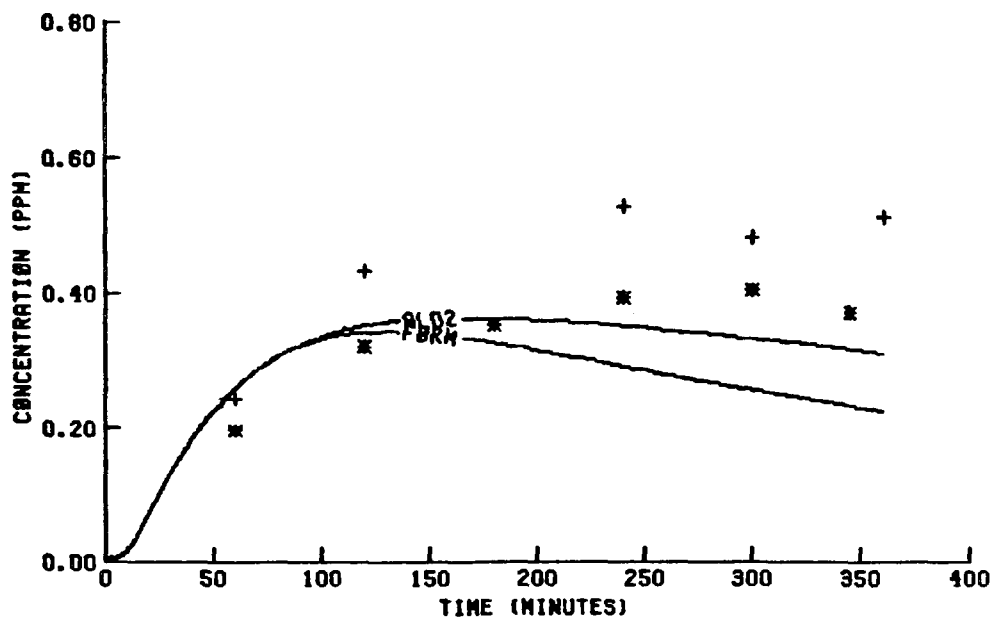
N8 +
N82 ■

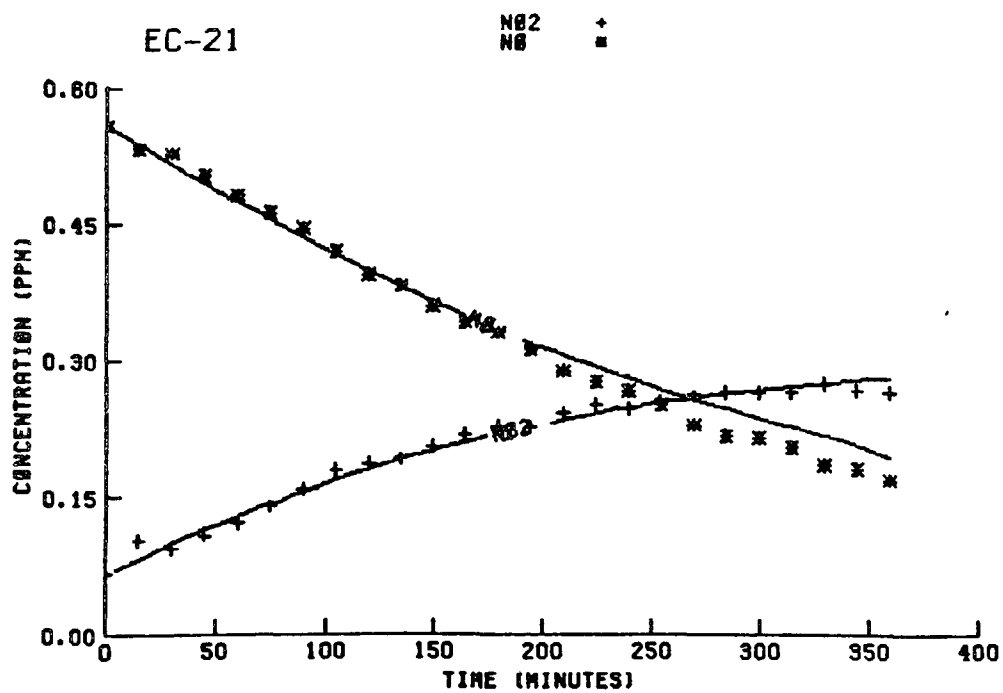
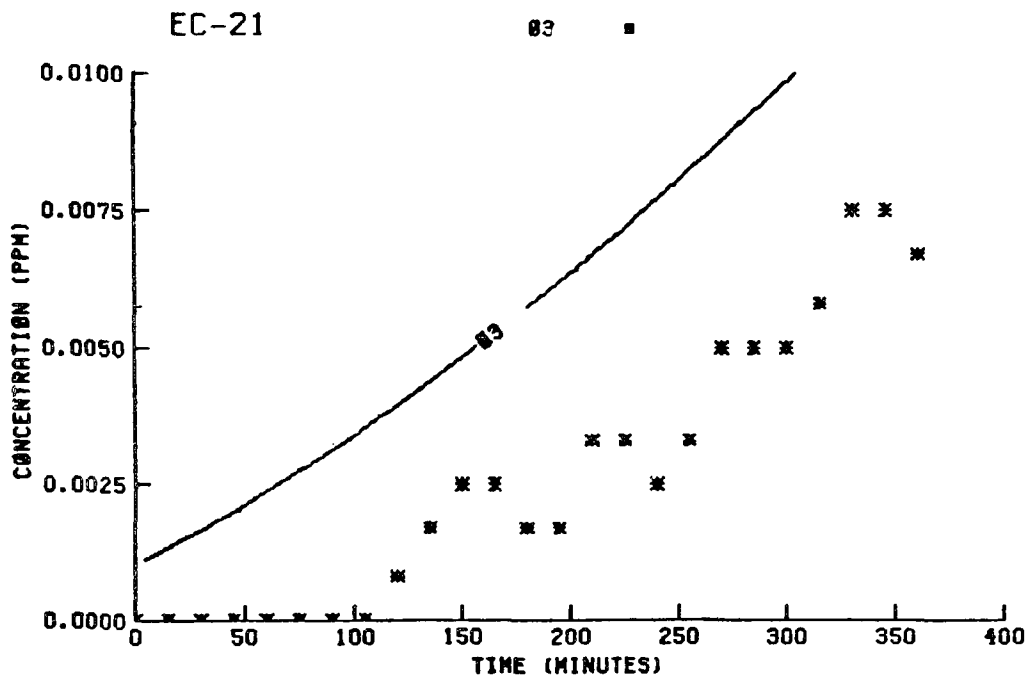


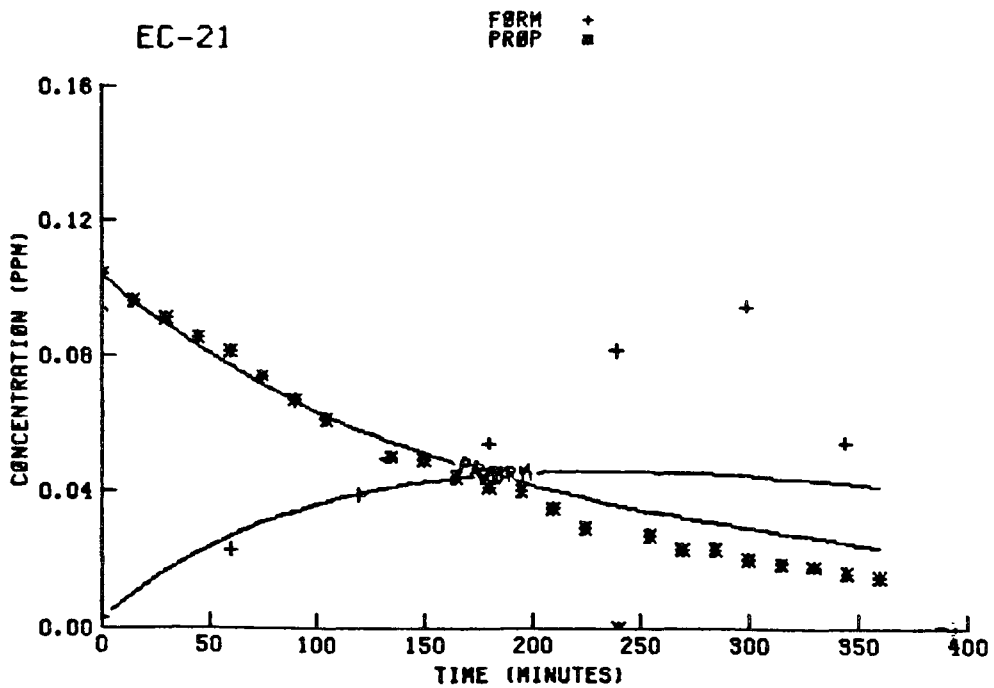
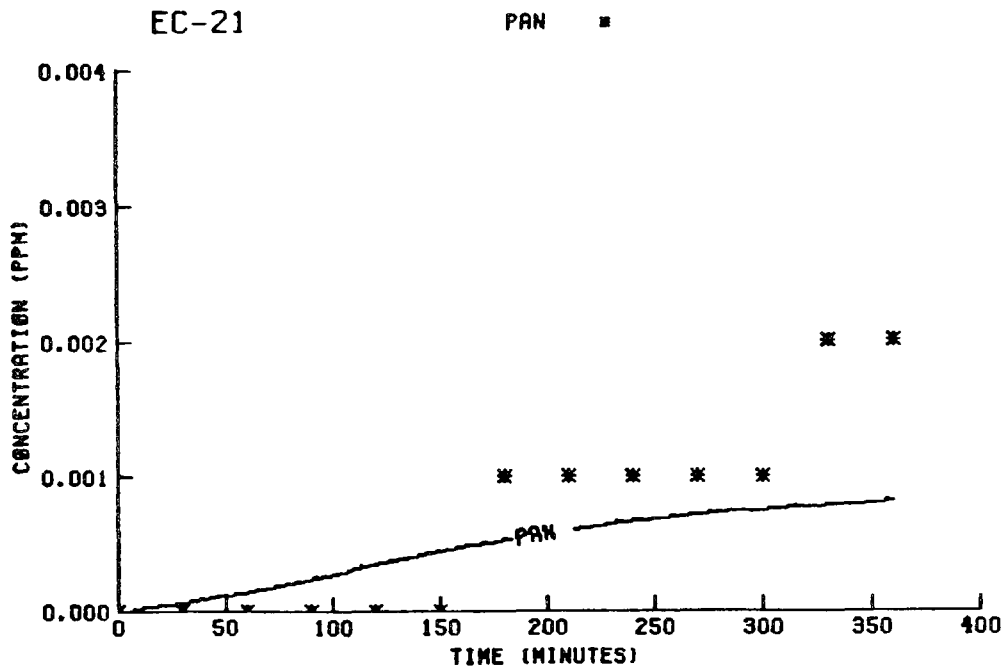


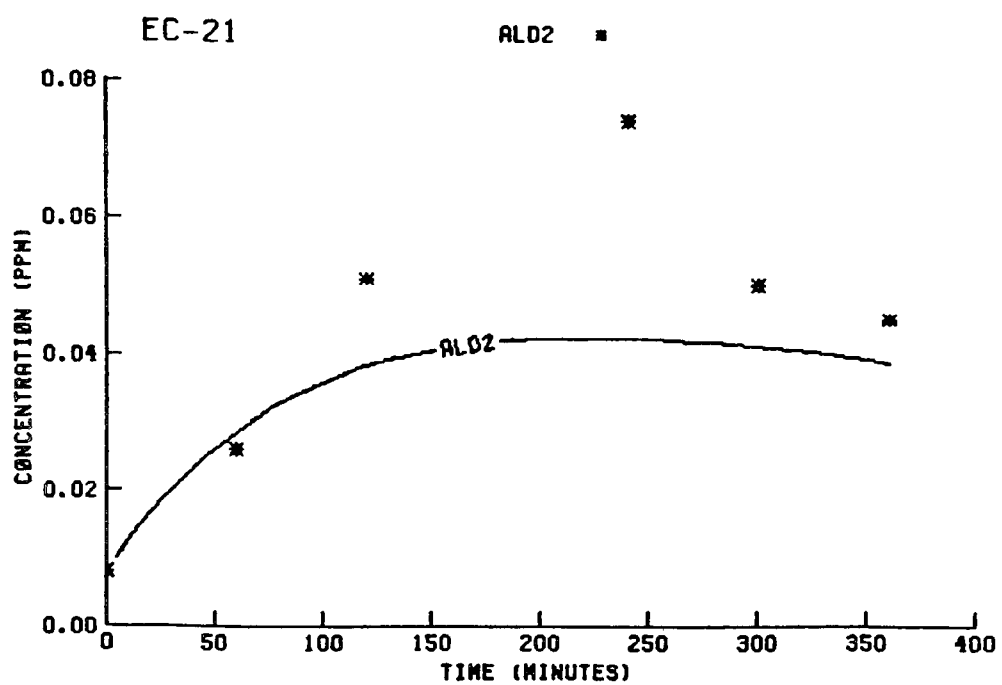
EC-18

ALD2 +
FBRH ■



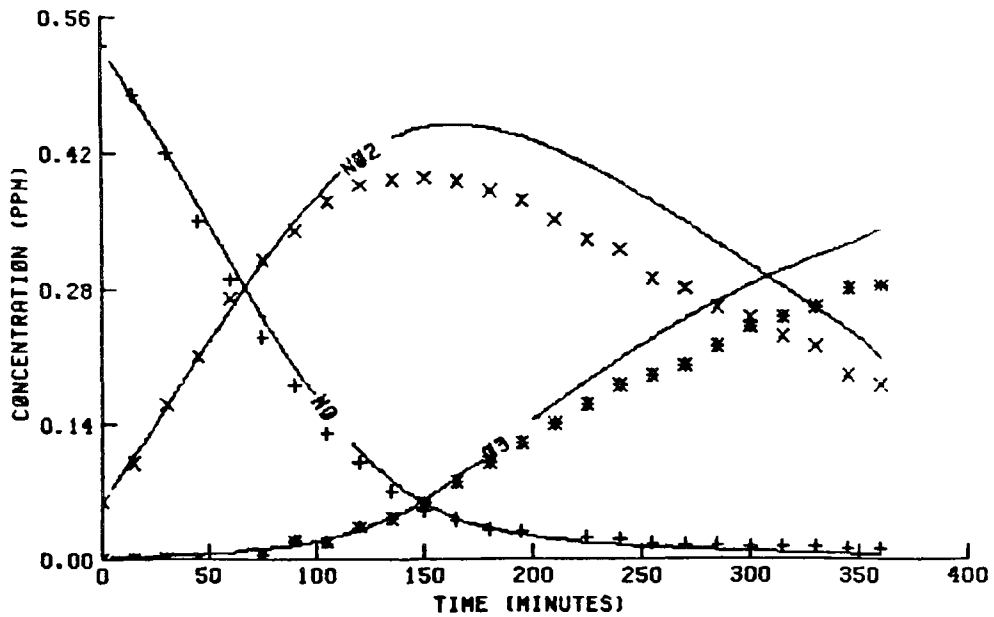






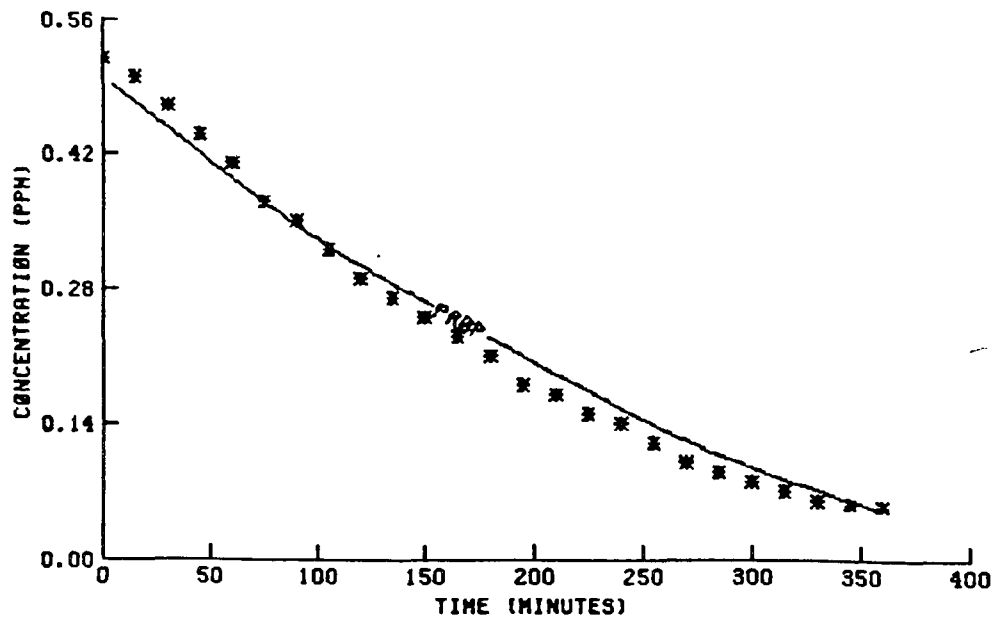
EC-5127

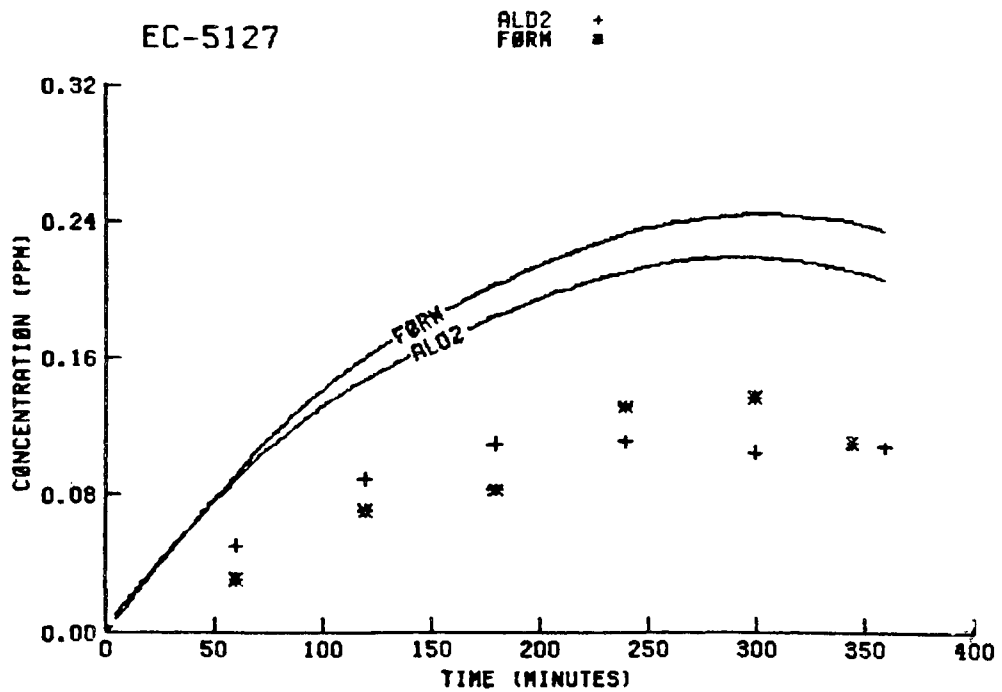
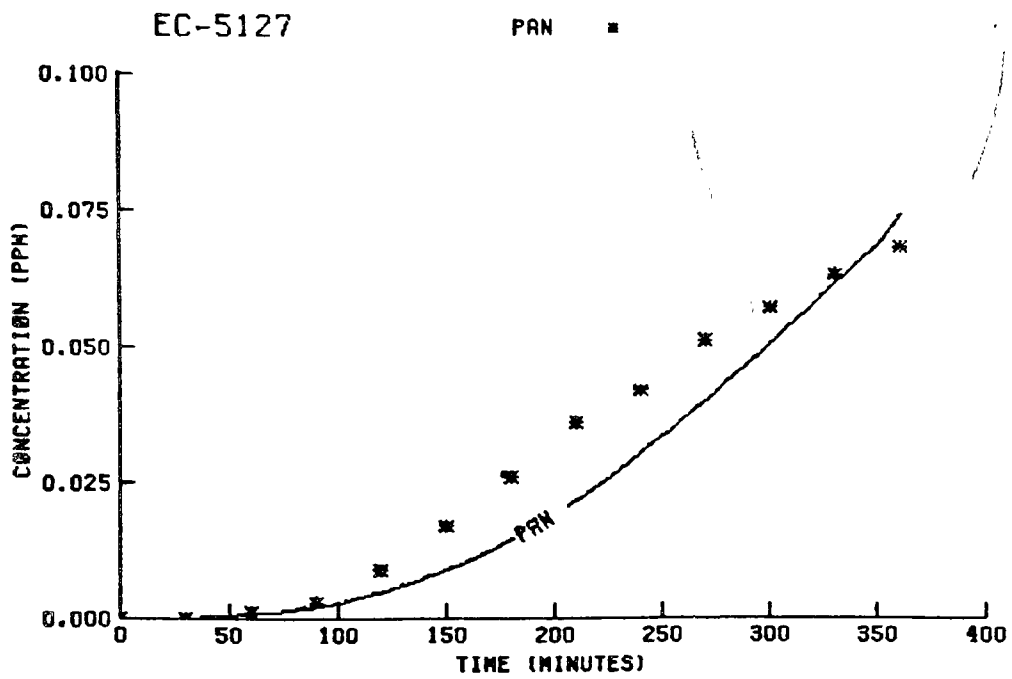
NO₂ x
NO +
O₃ ■

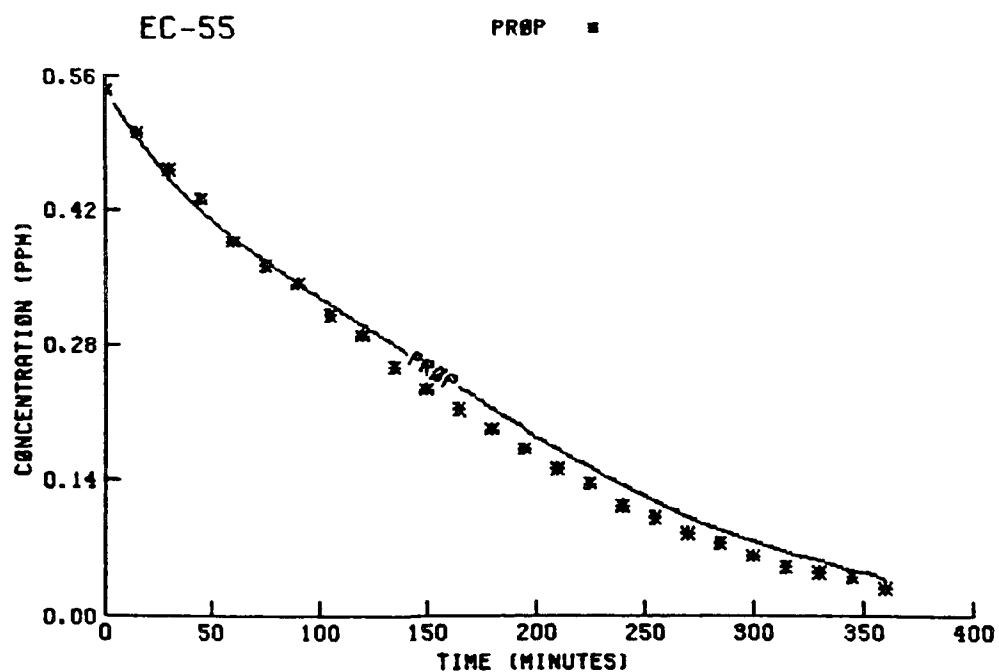
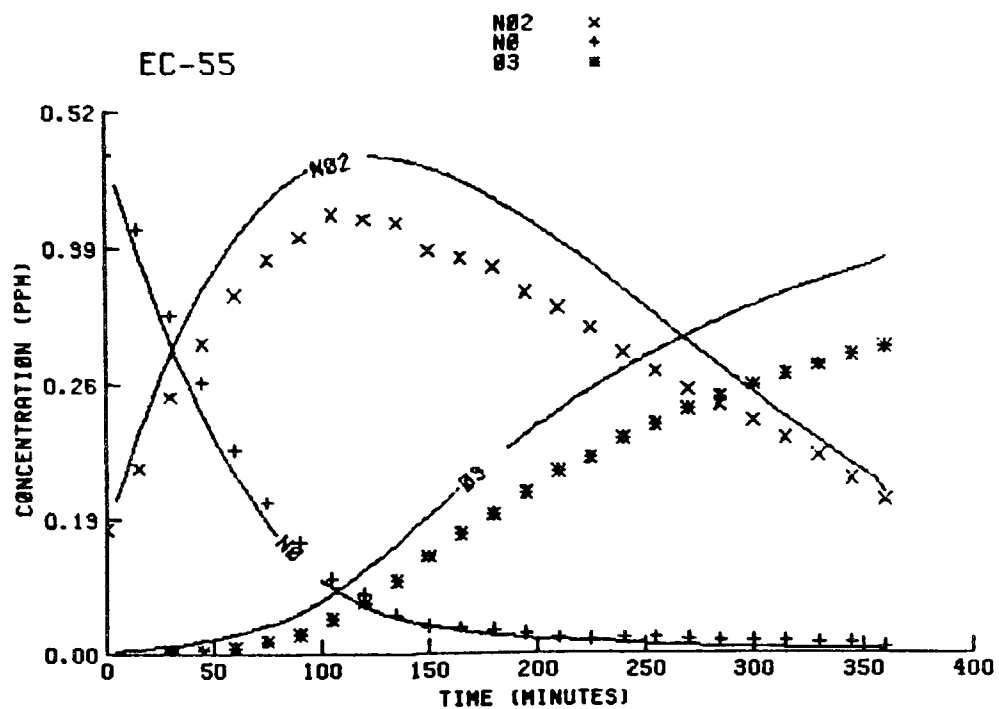


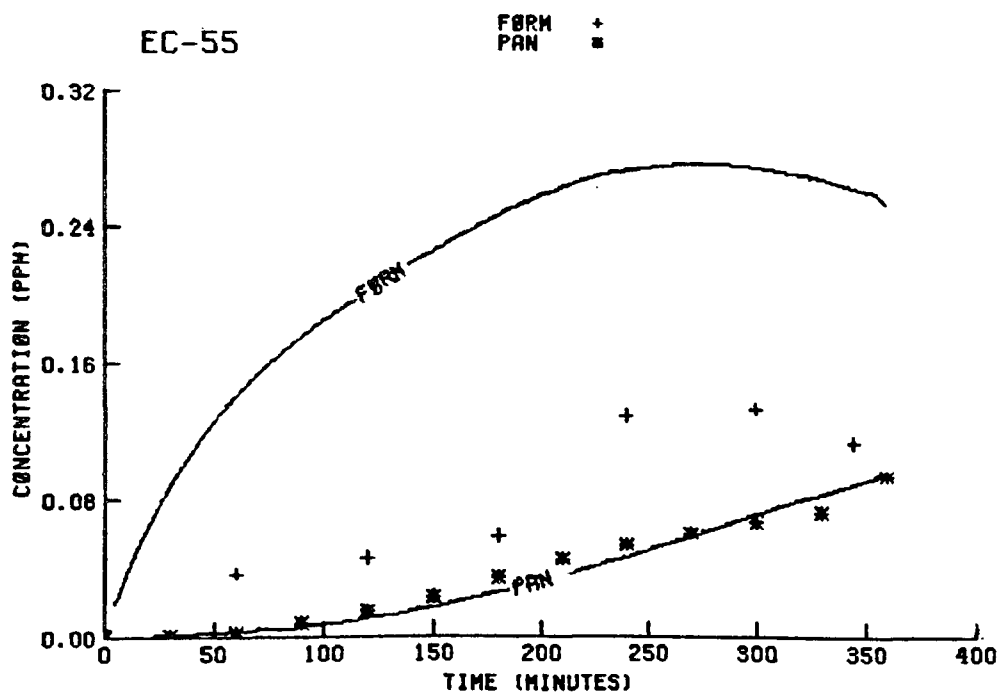
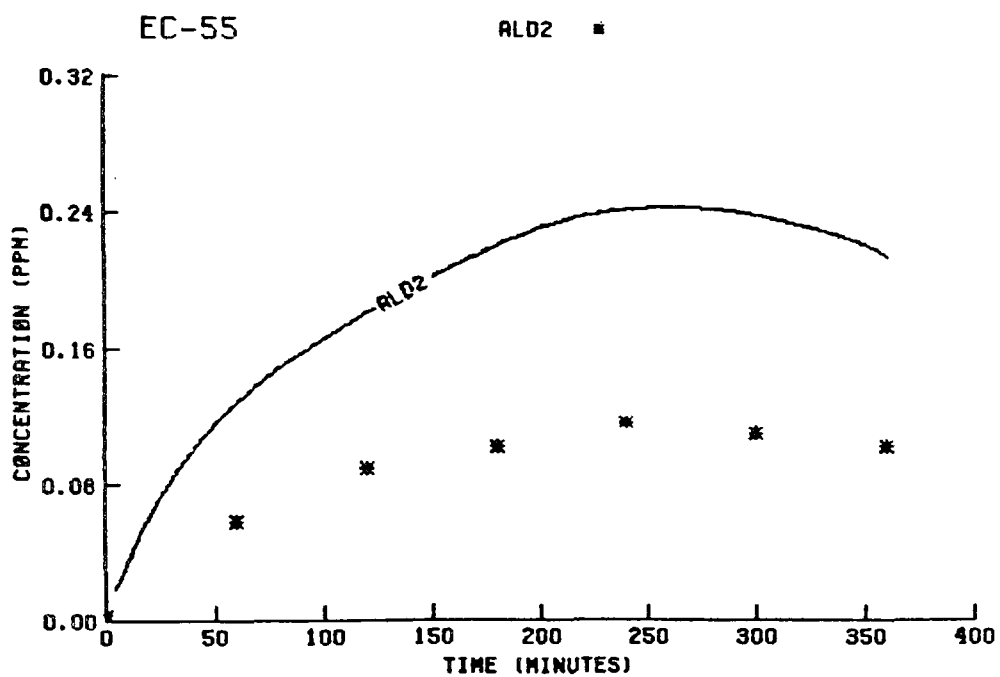
EC-5127

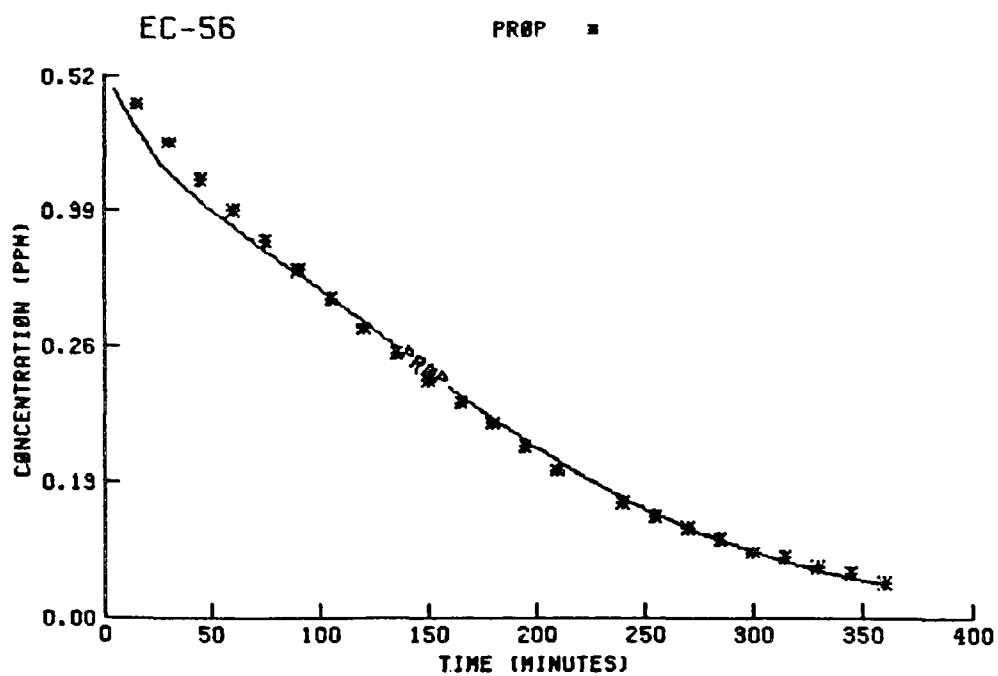
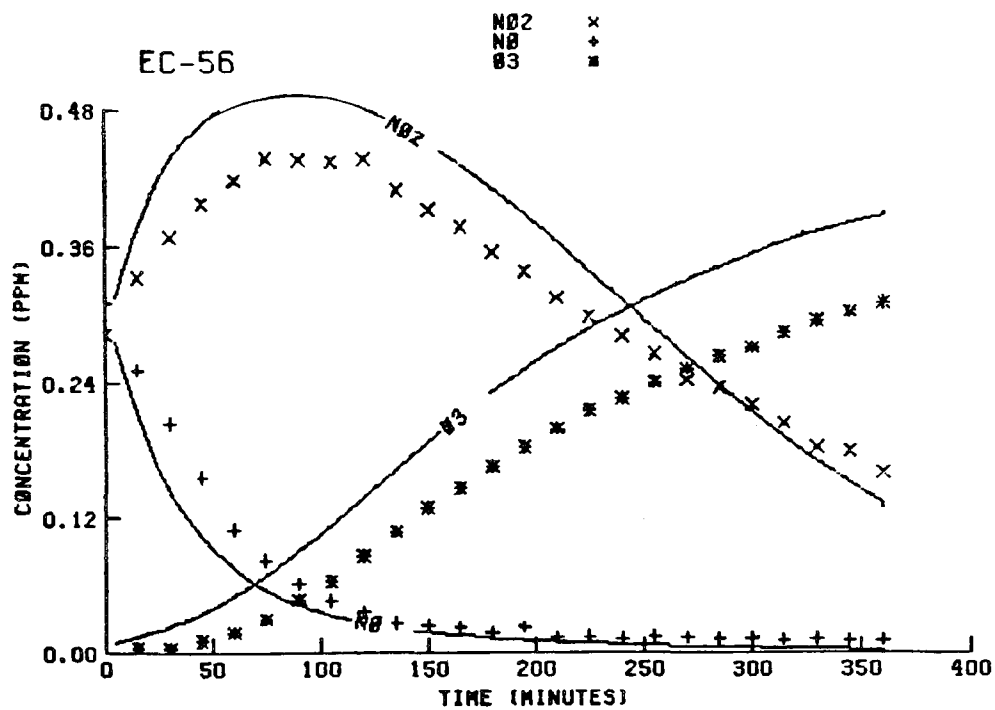
PRBP ■

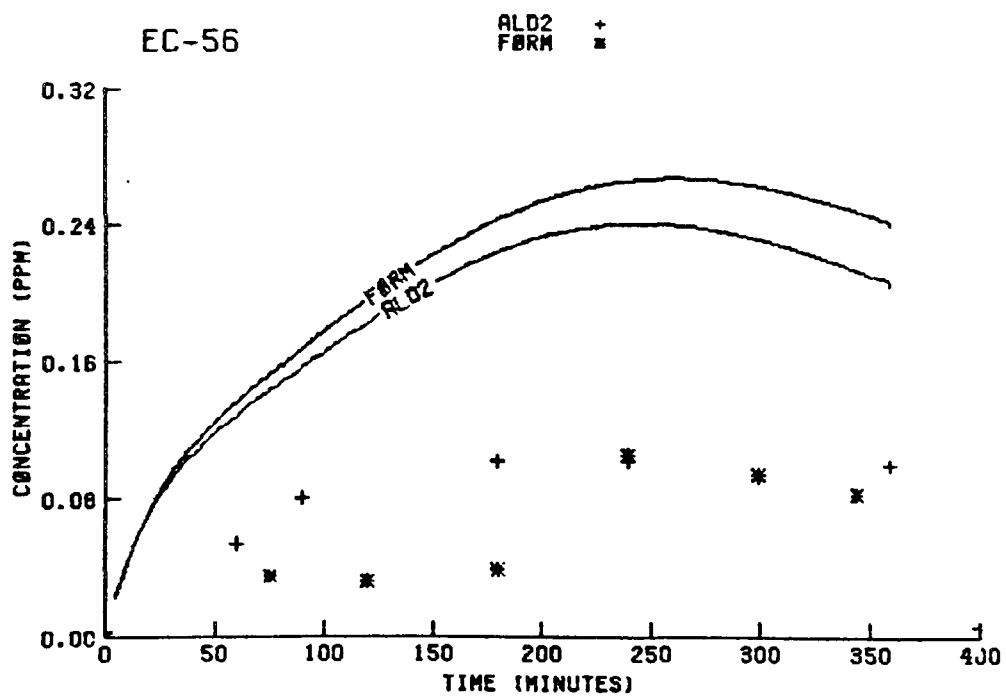
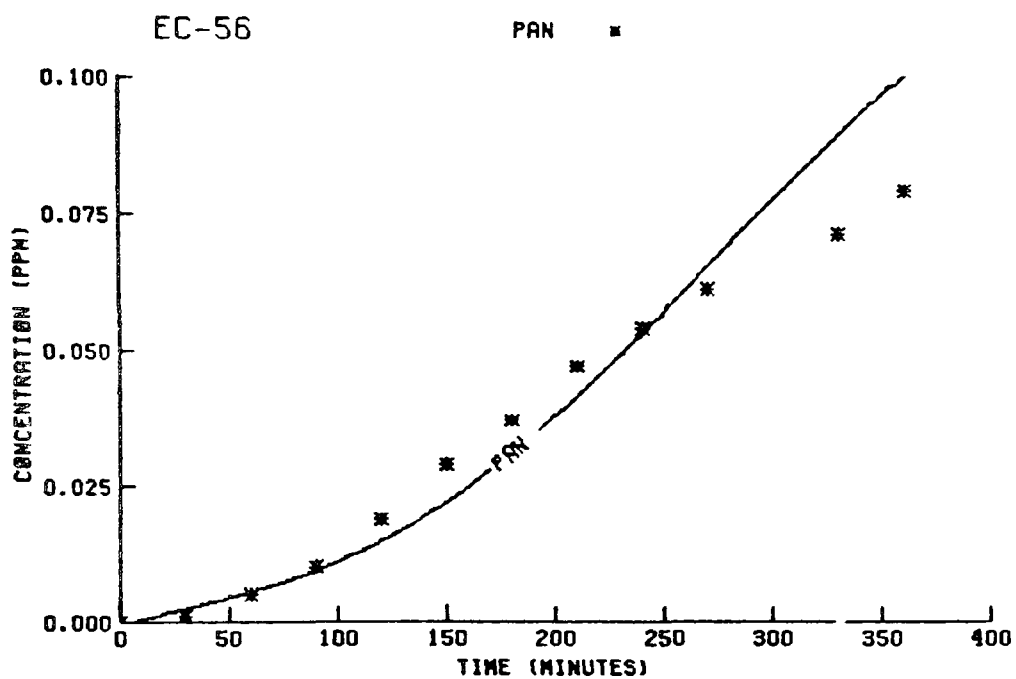


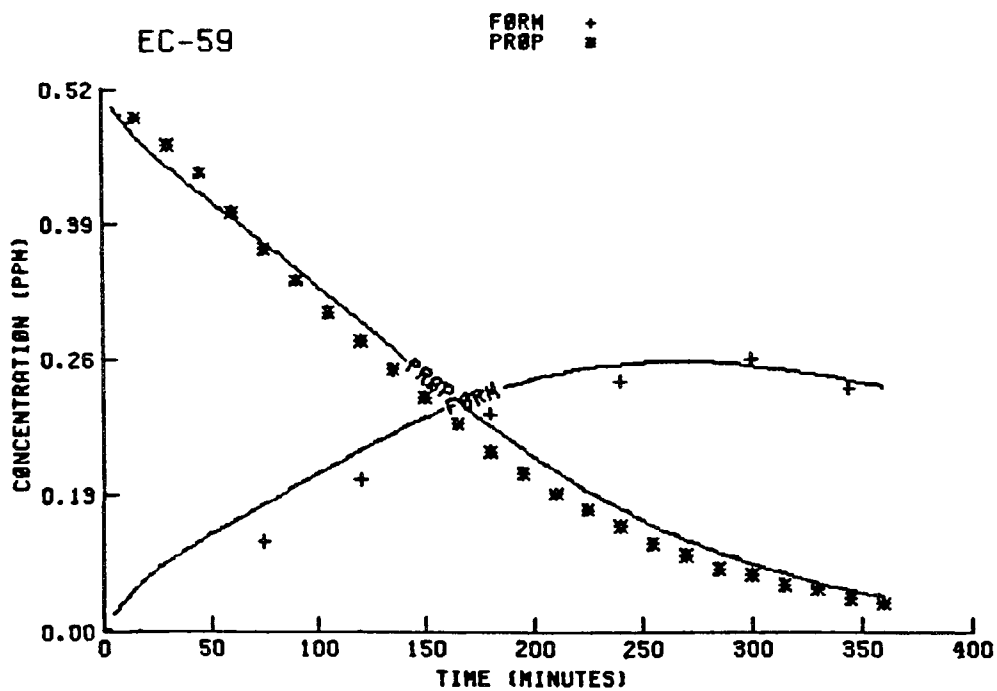
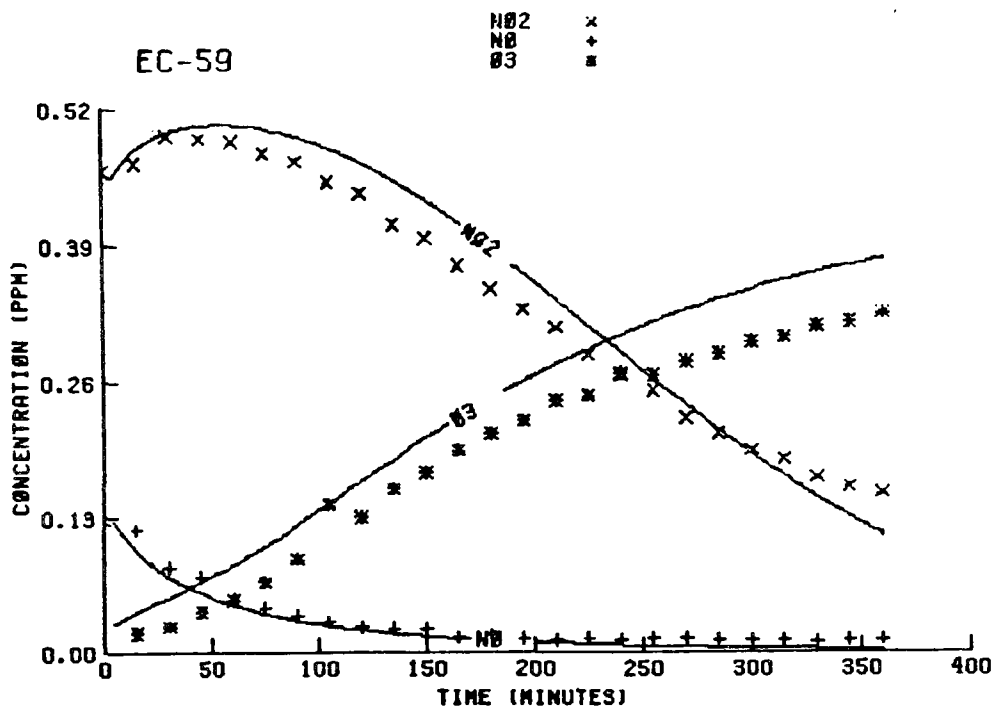


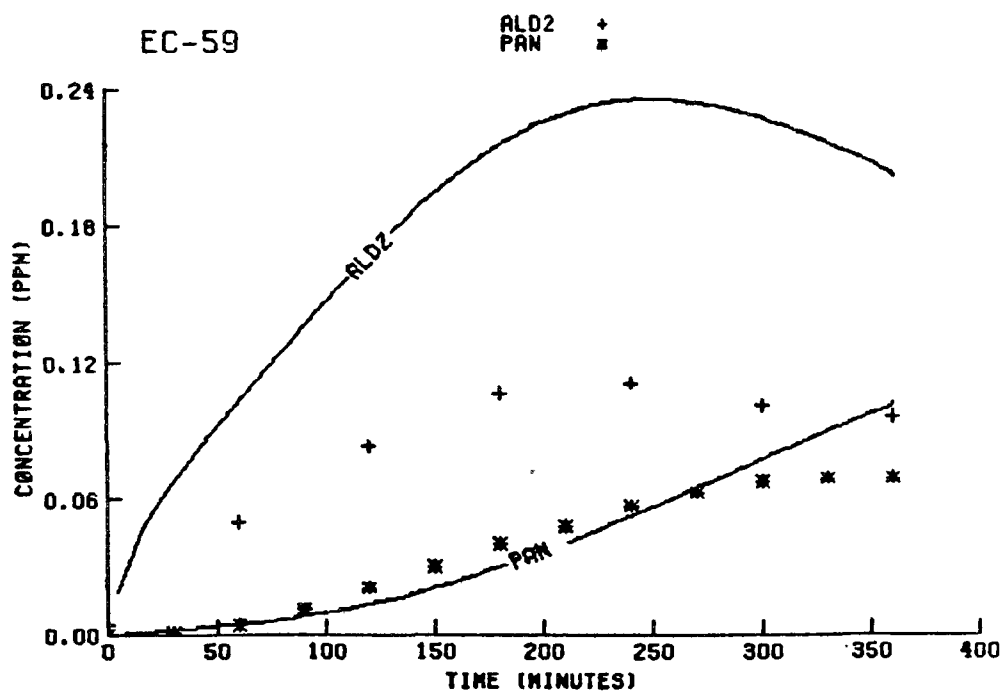








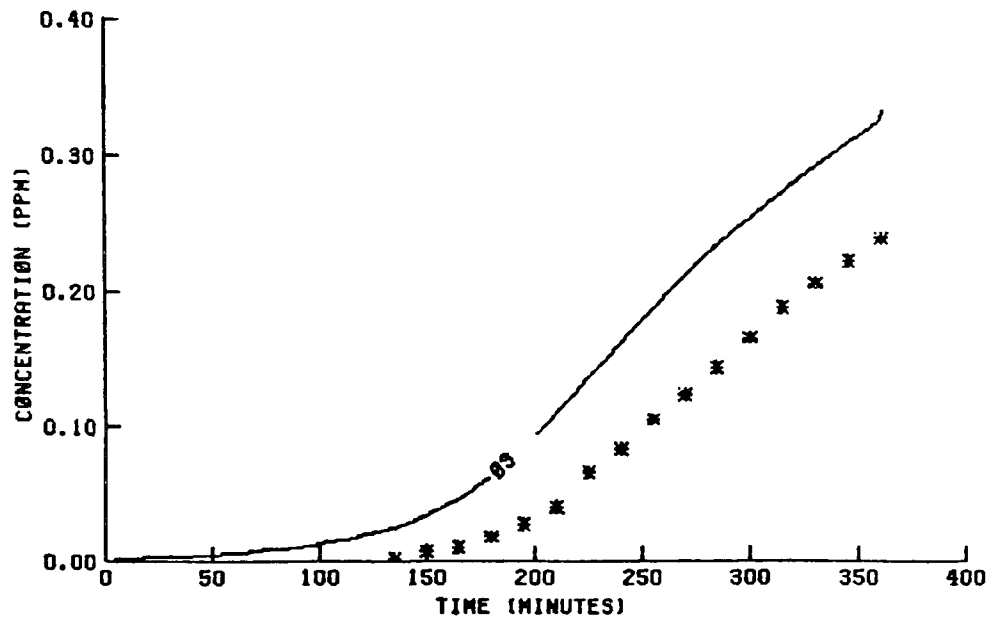




EC-60

03

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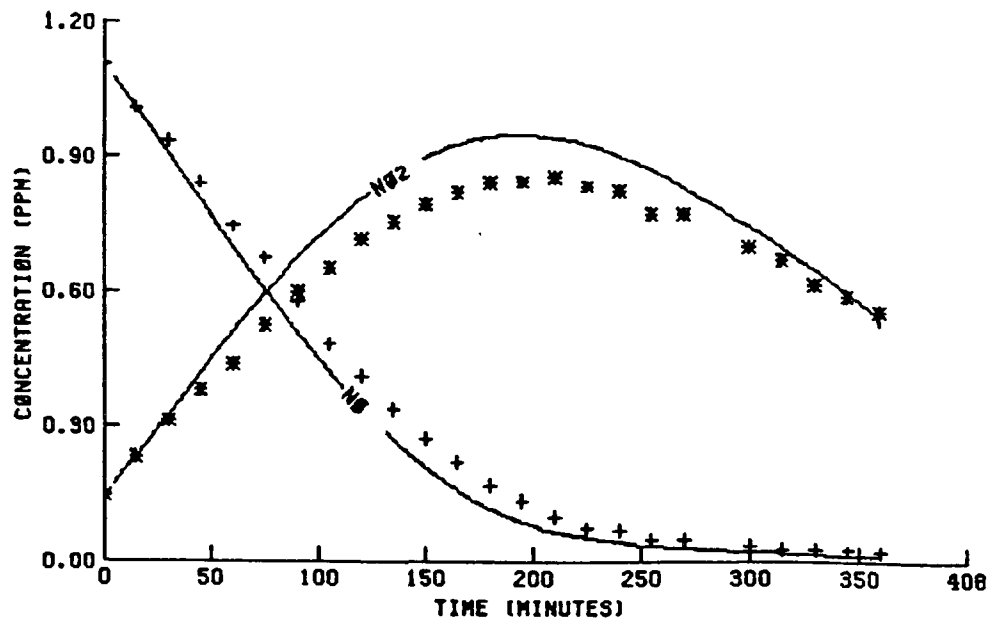
EC-60

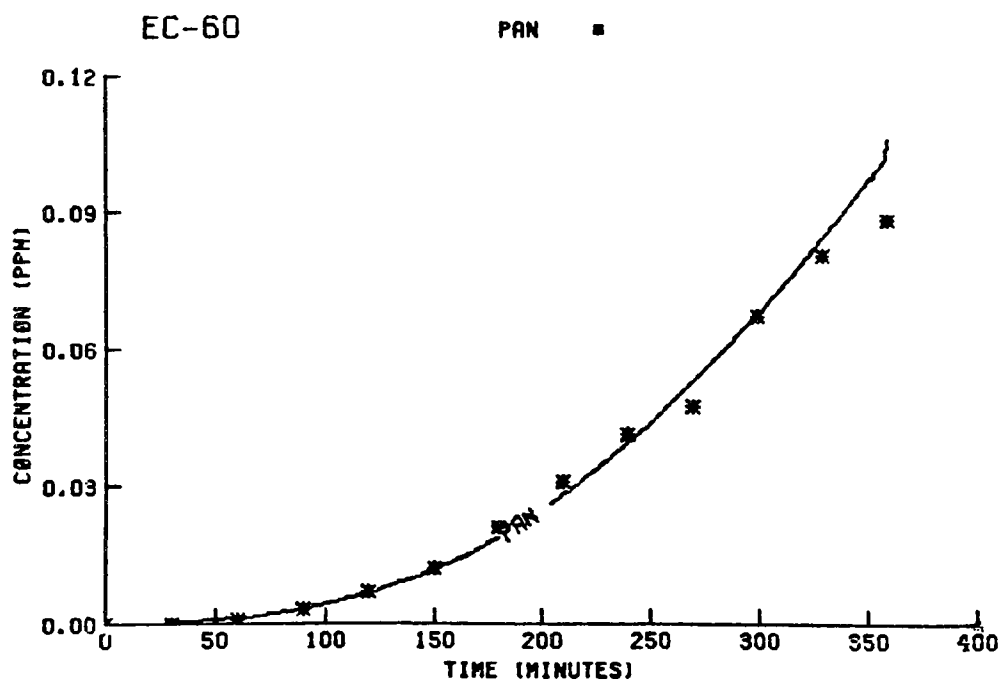
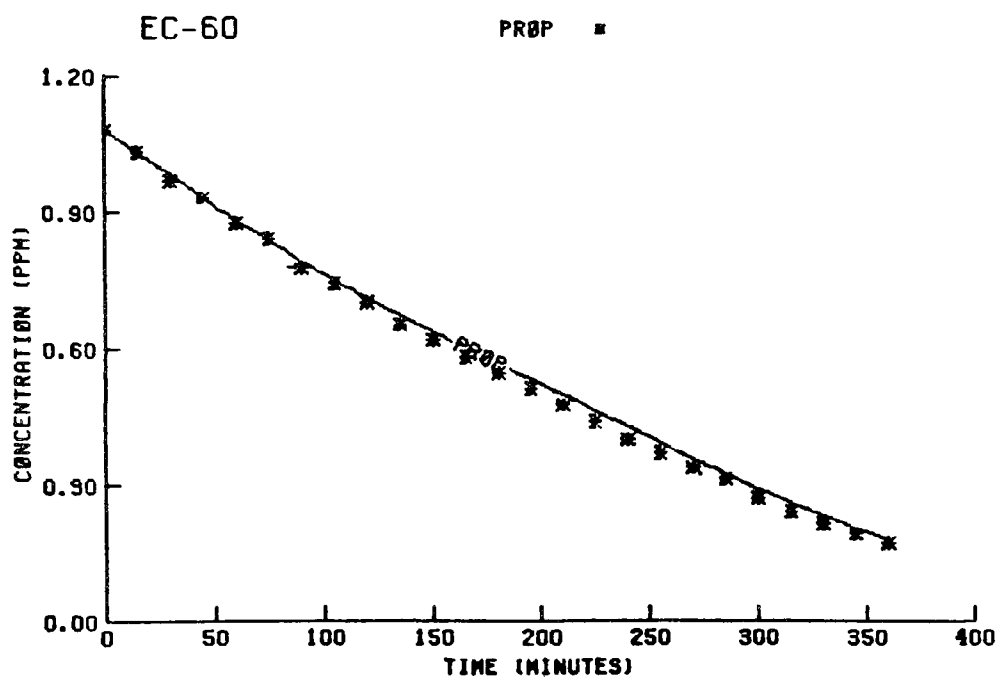
N0

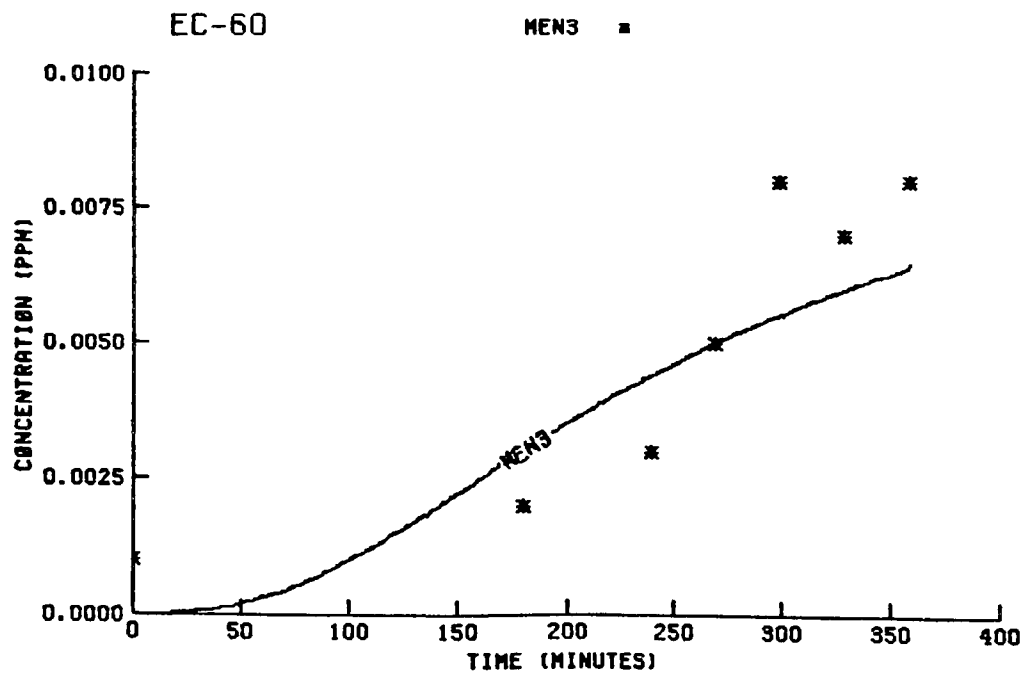
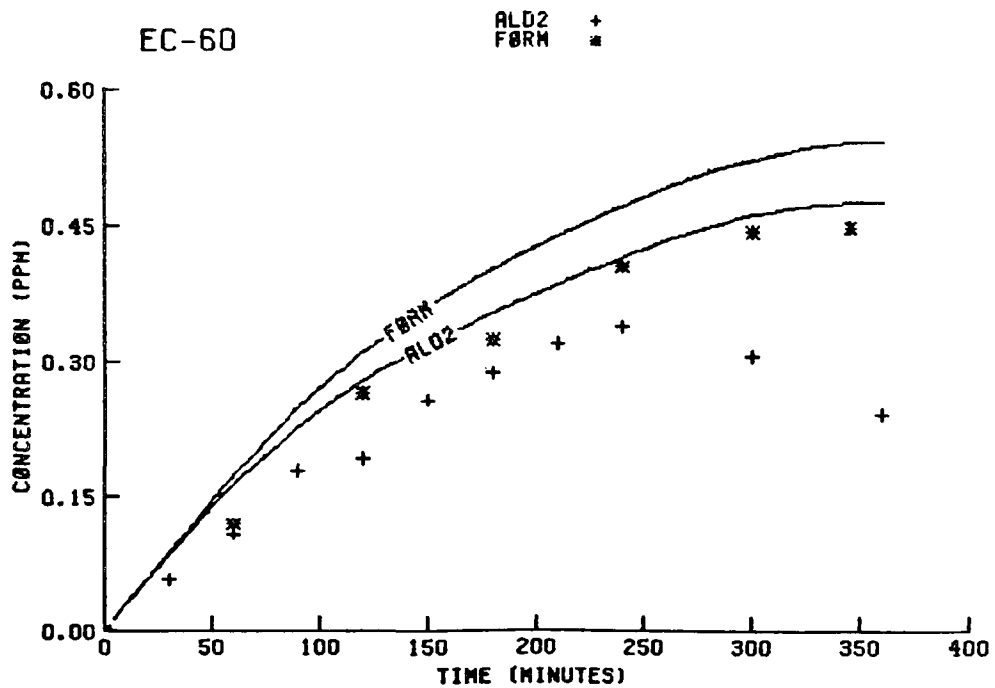
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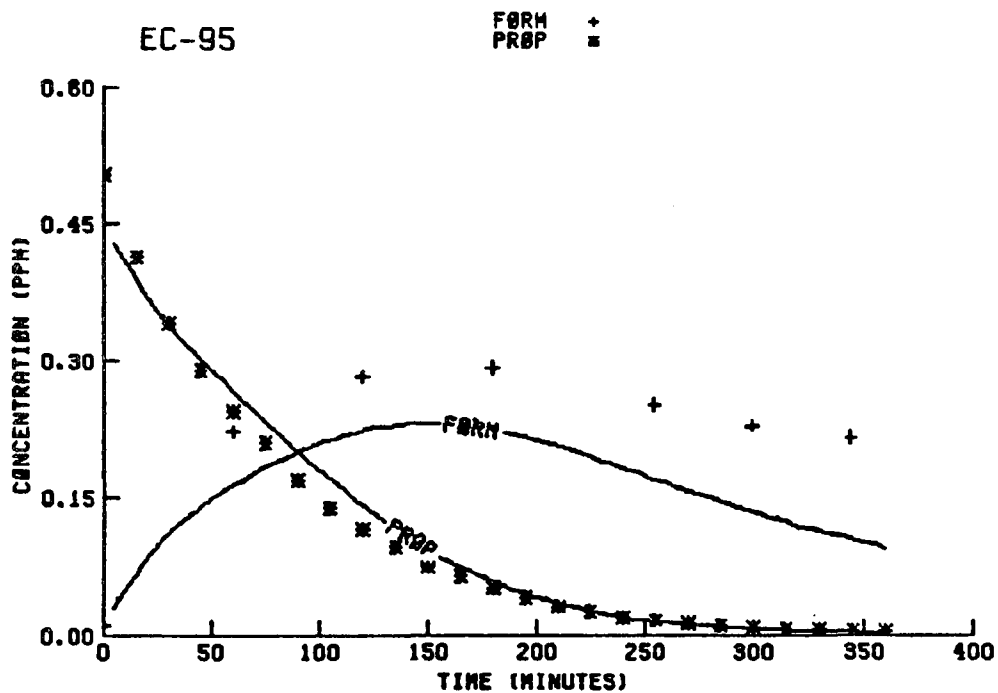
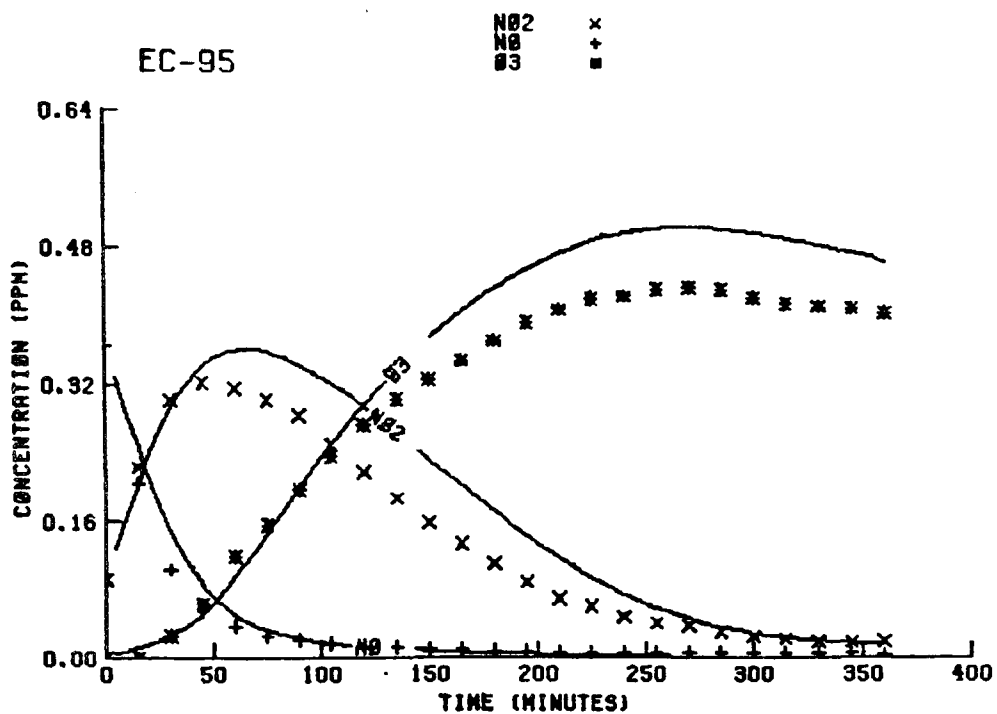
N02

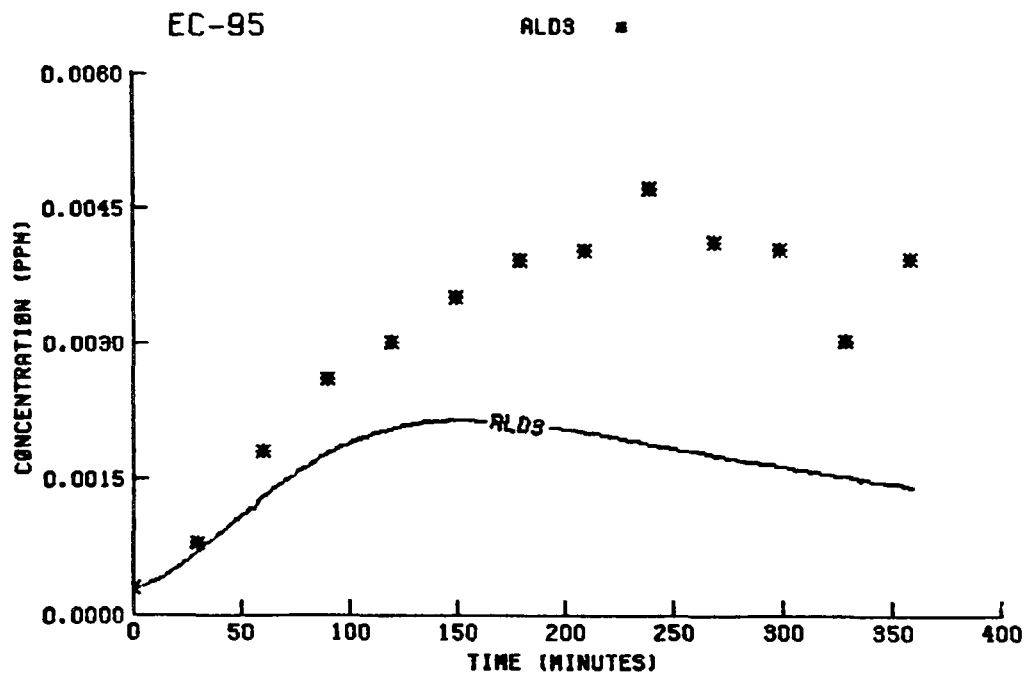
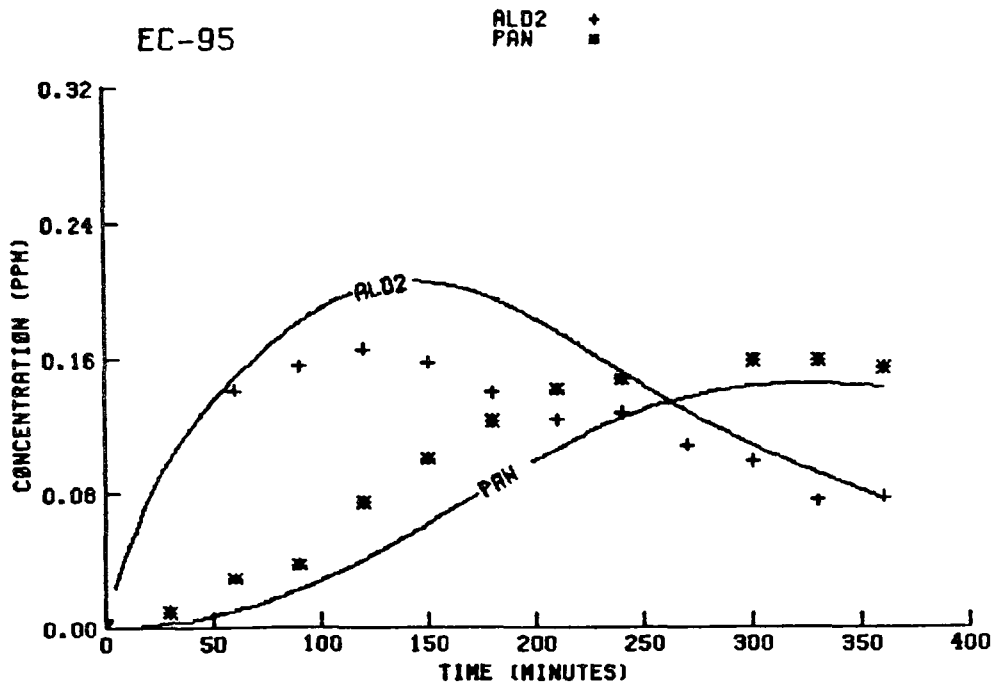
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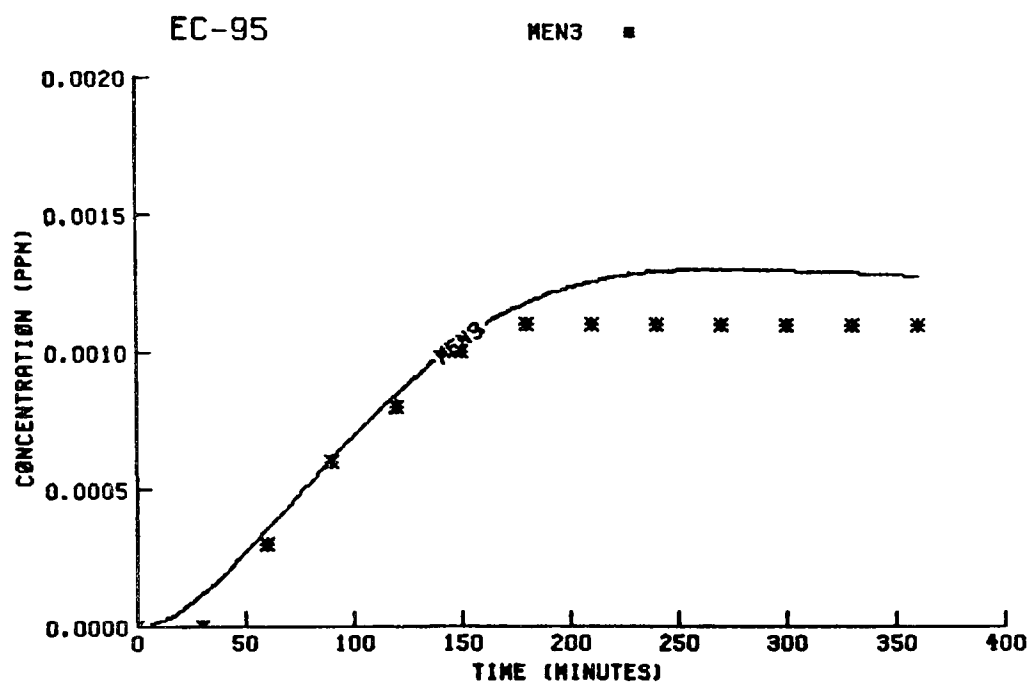


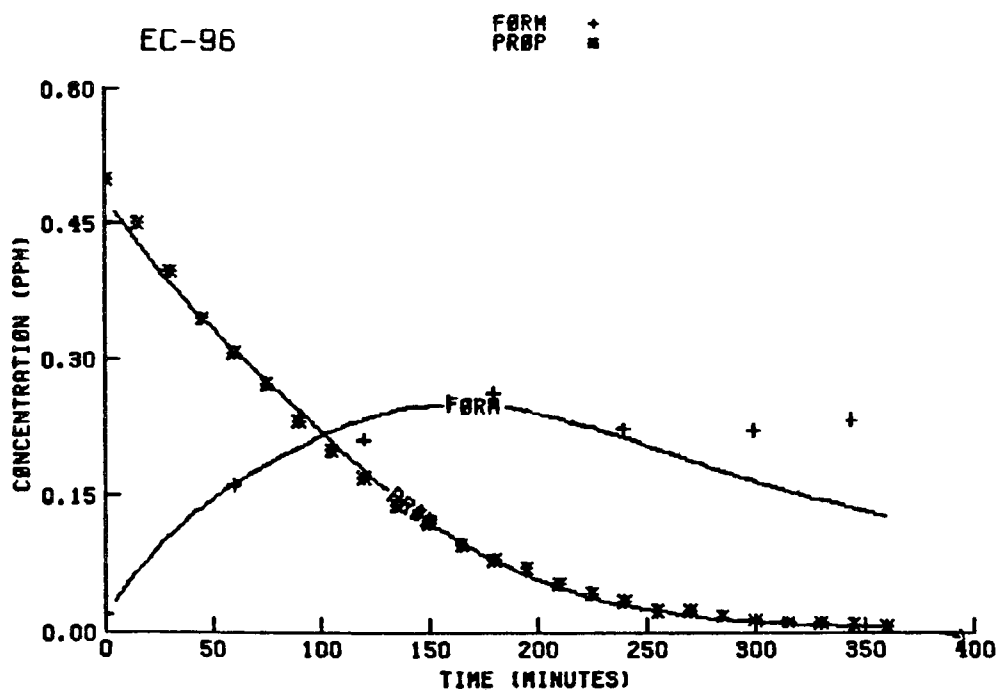
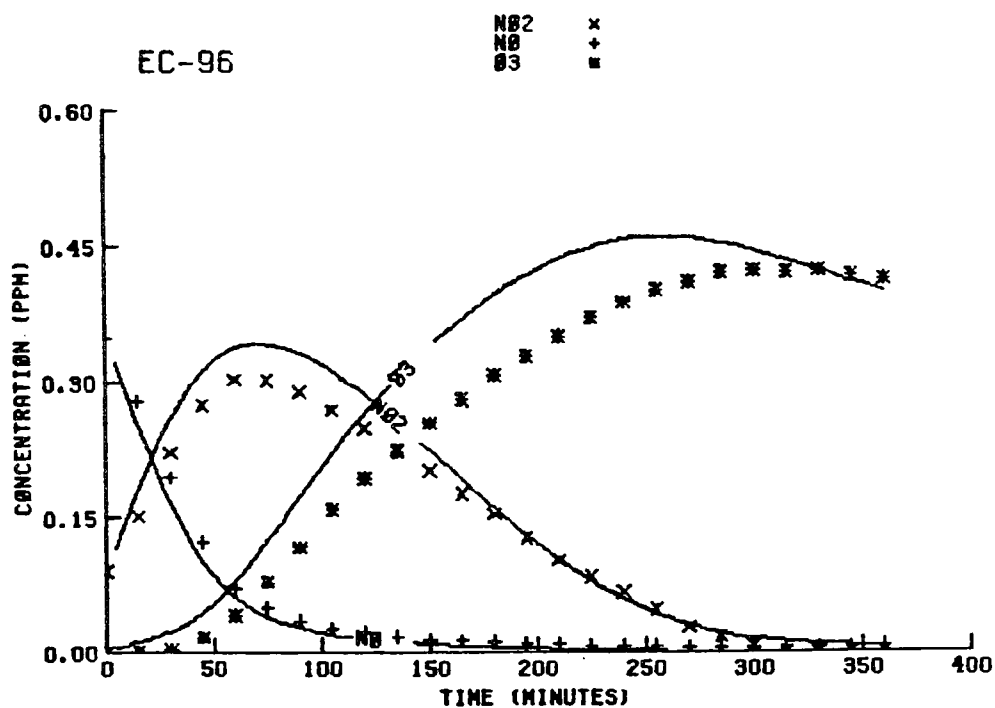


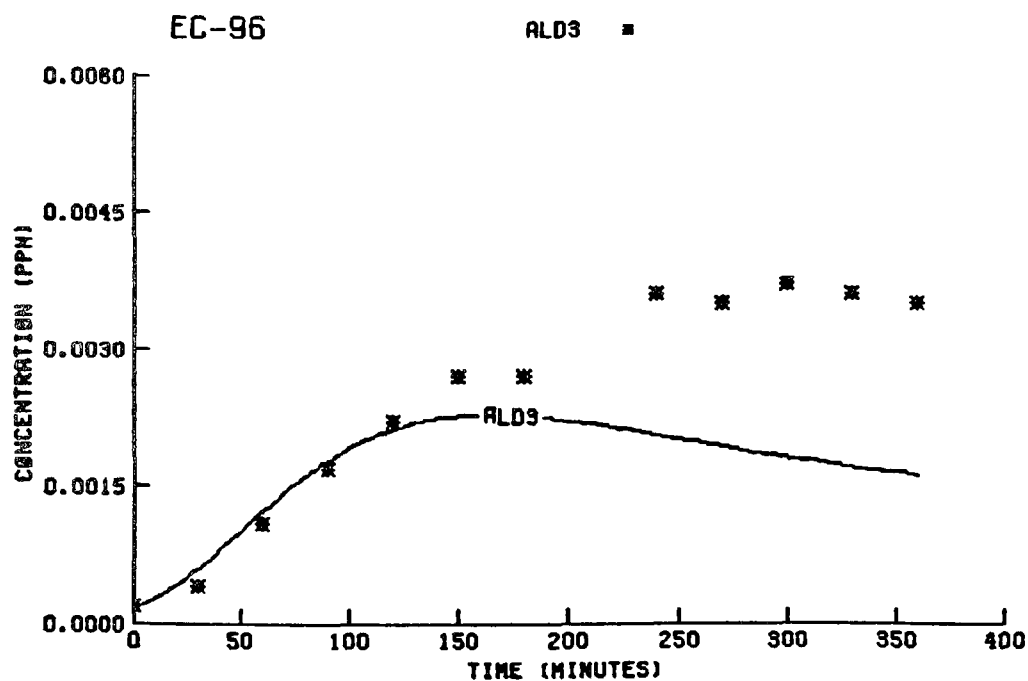
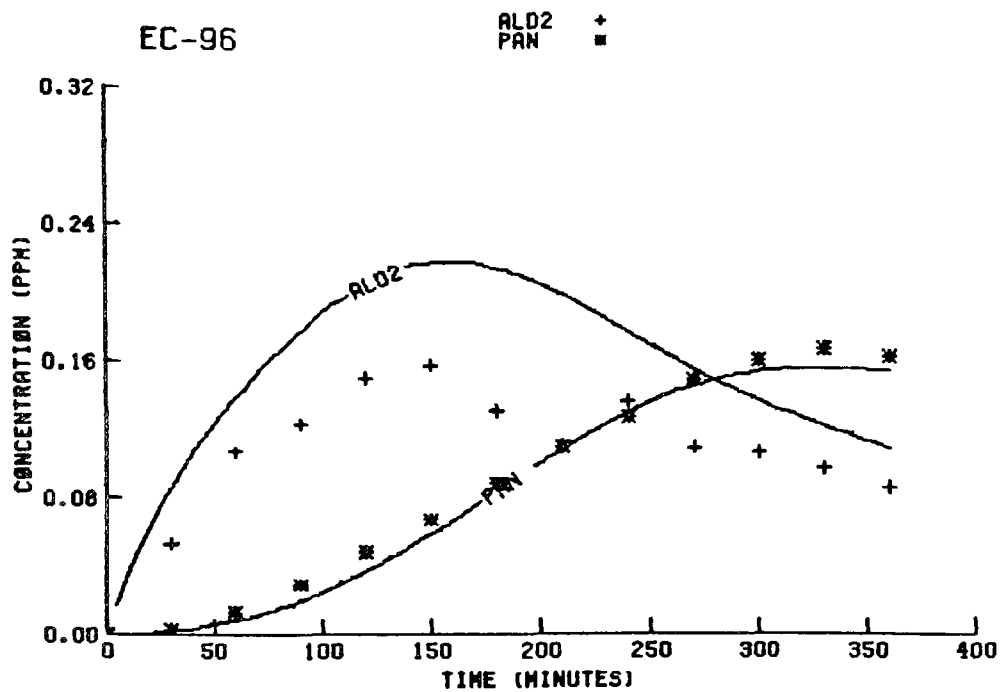


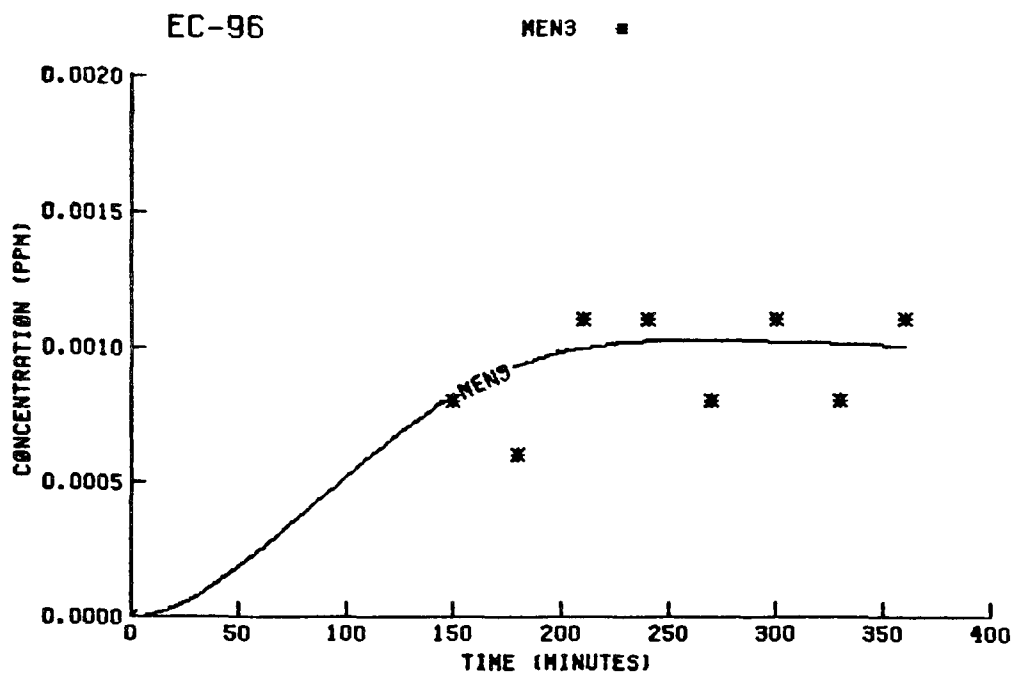


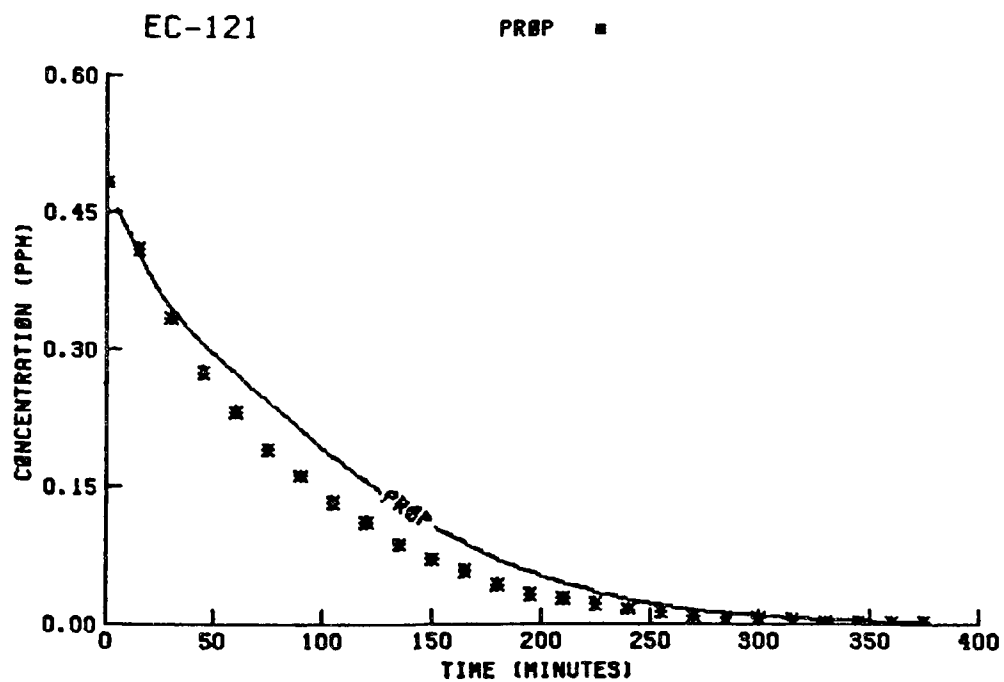
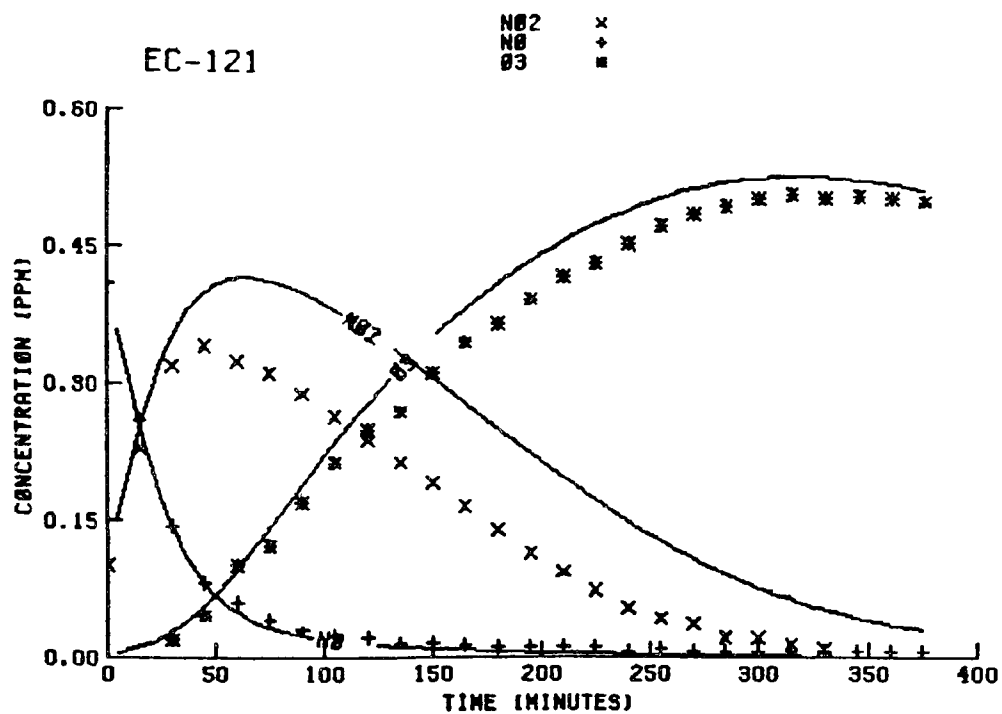


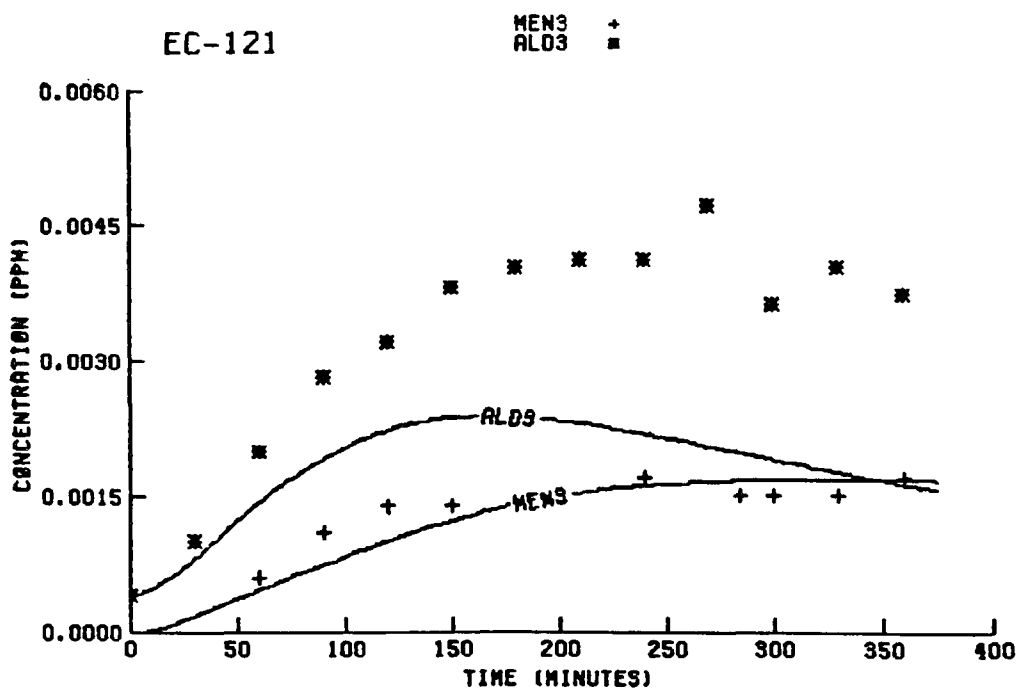
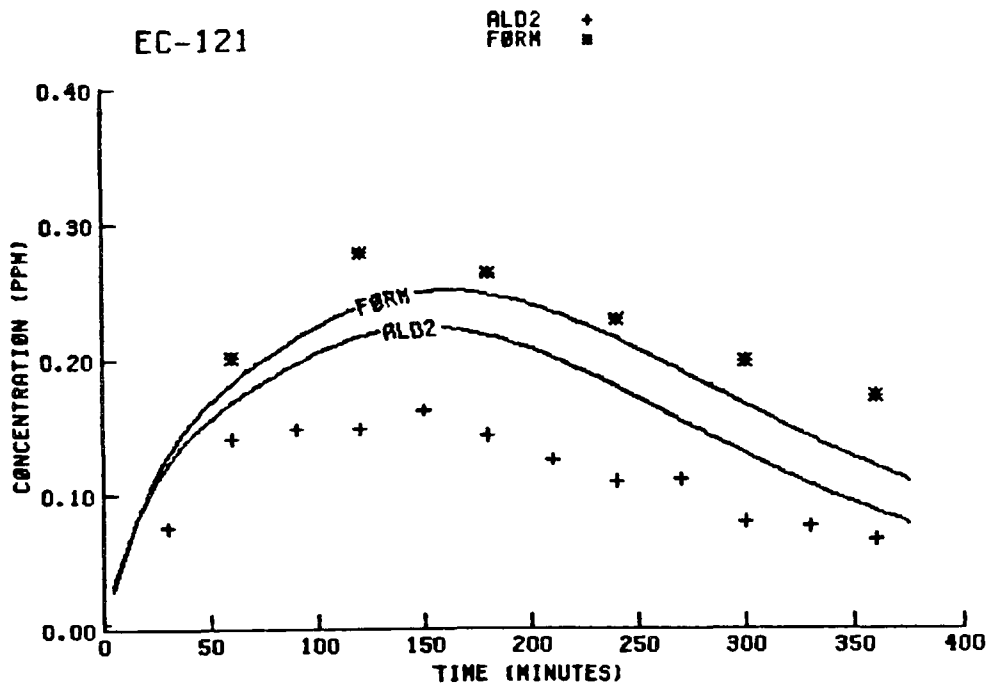






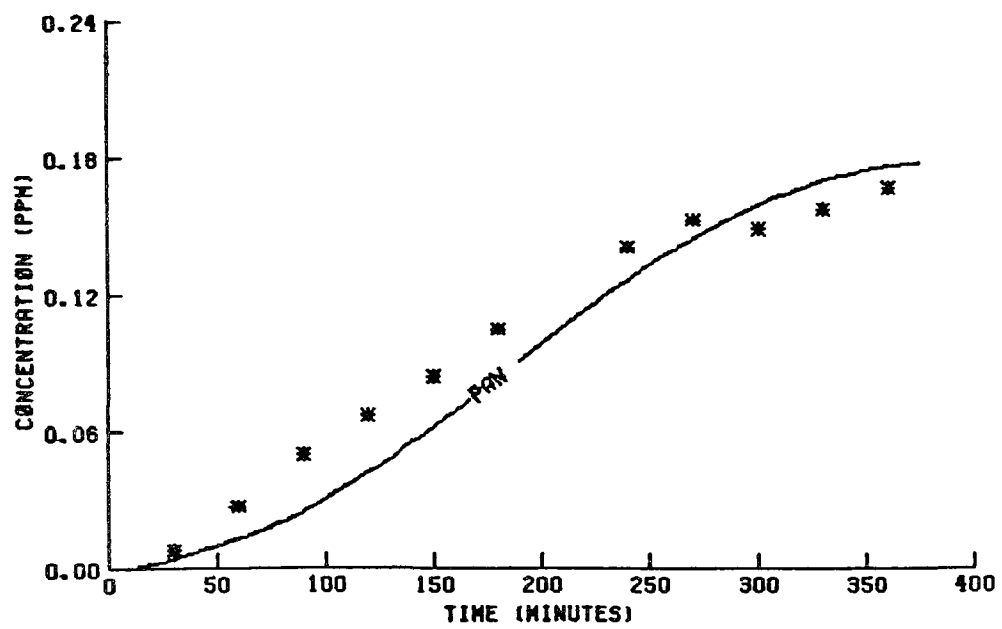


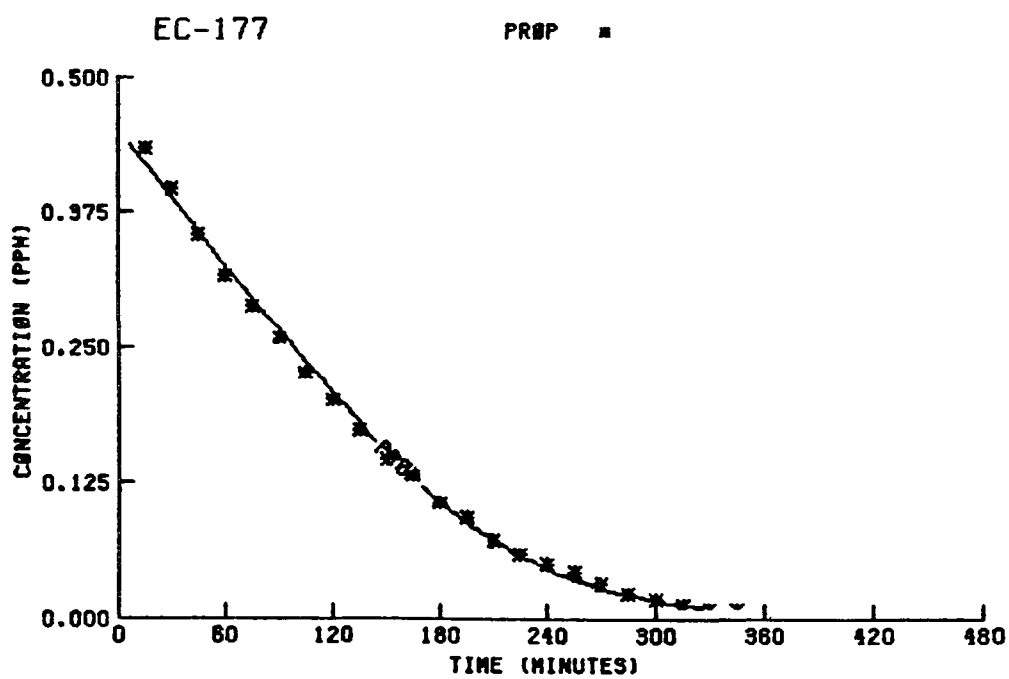
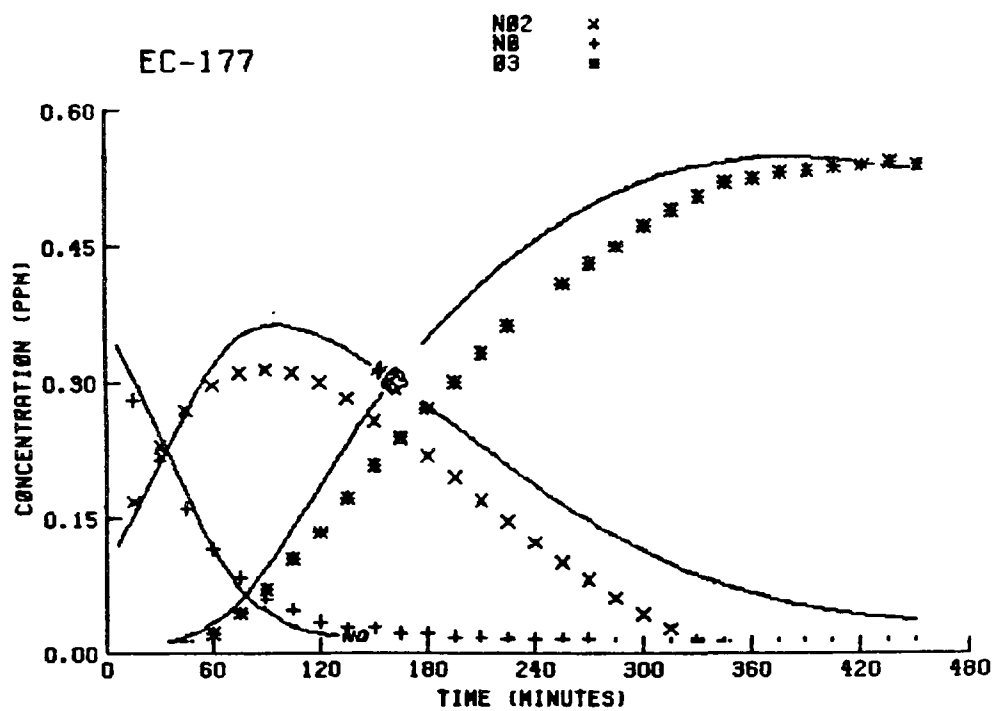


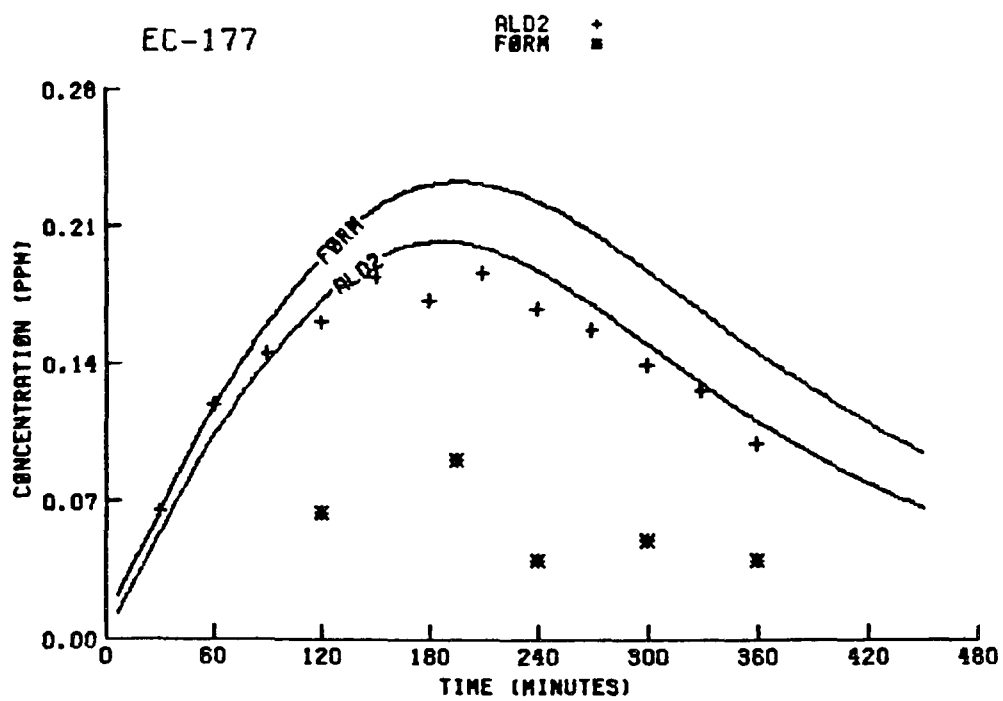
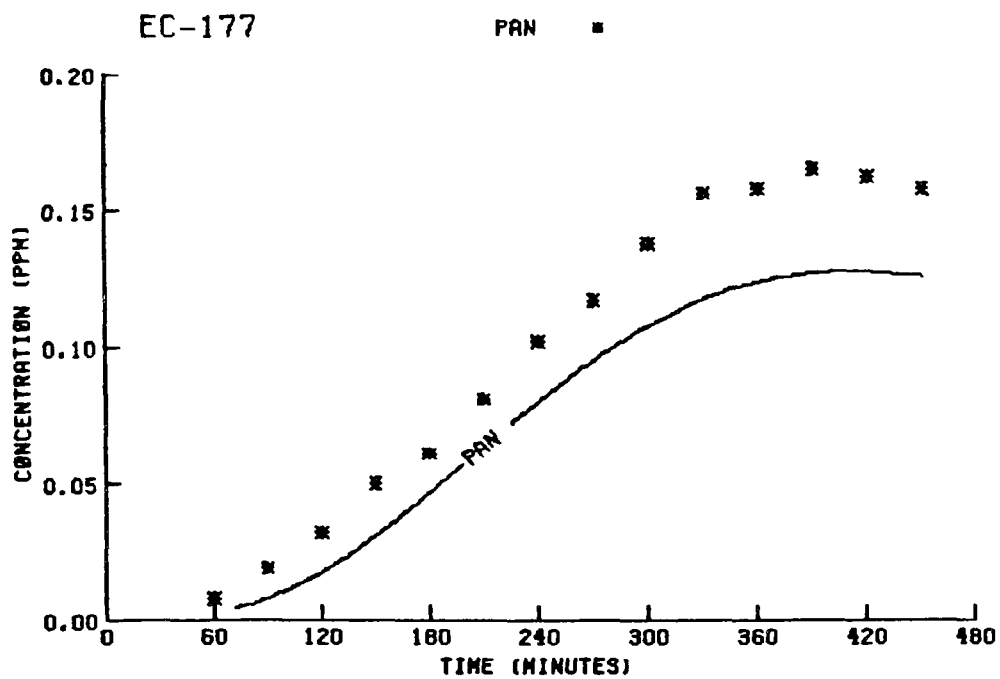


EC-121

PRN ■

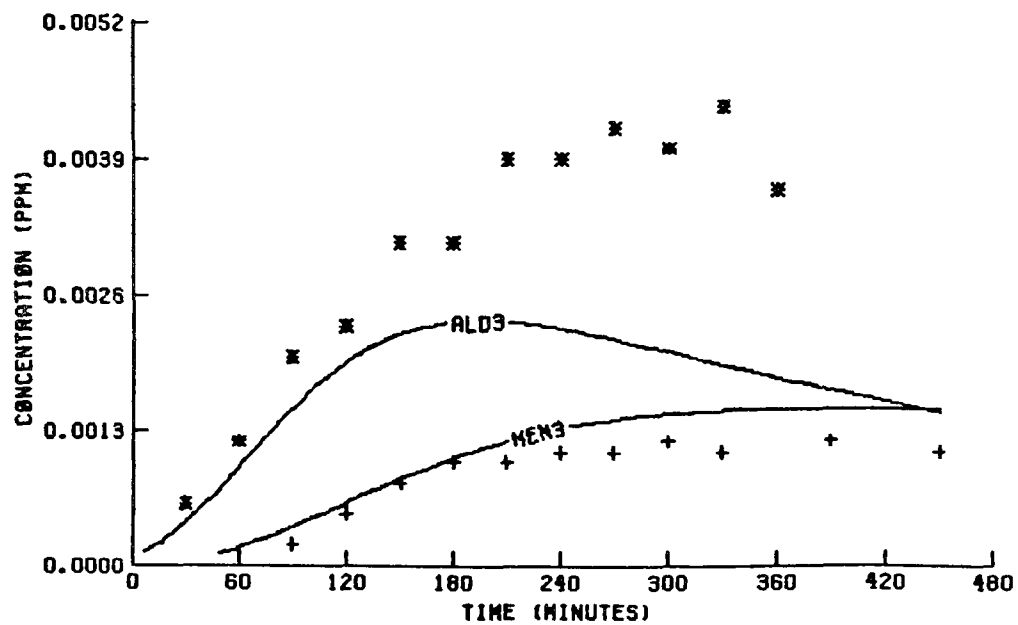


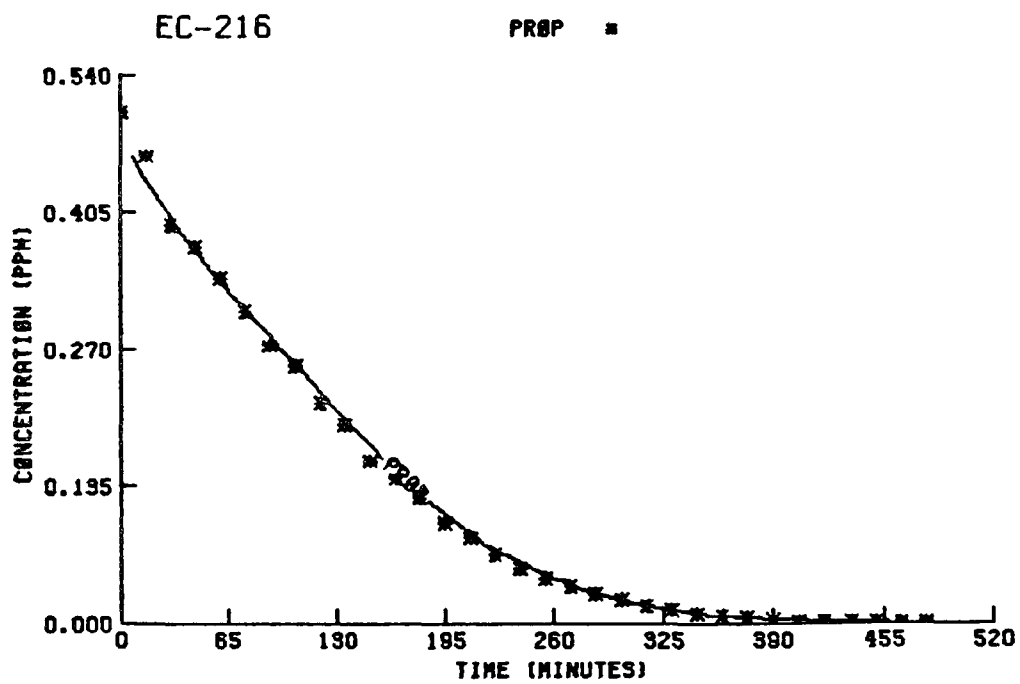
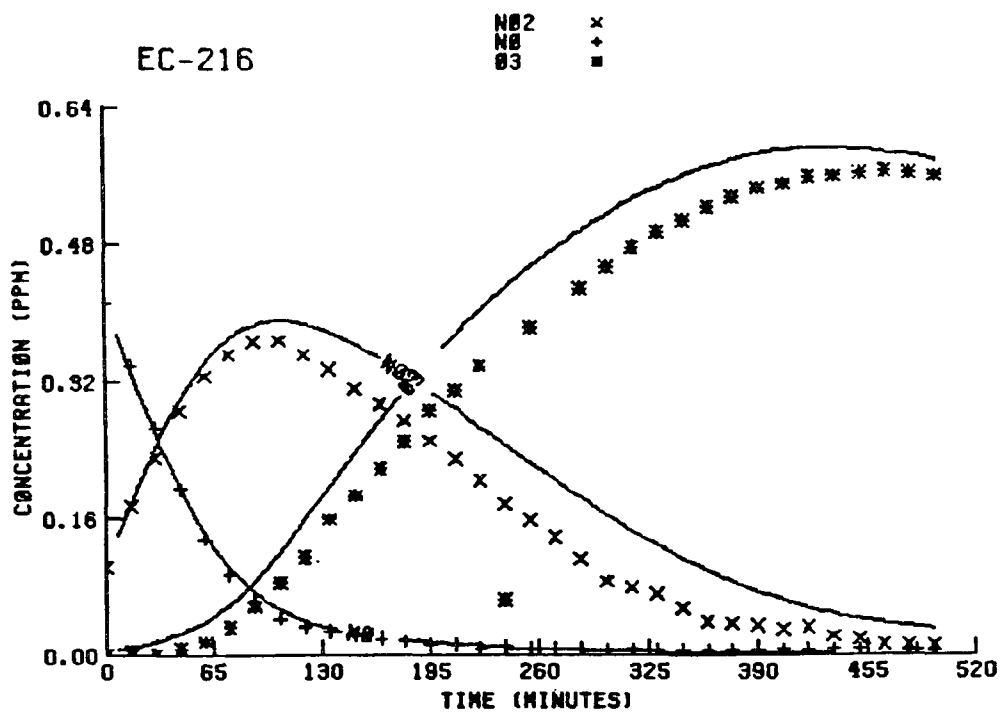


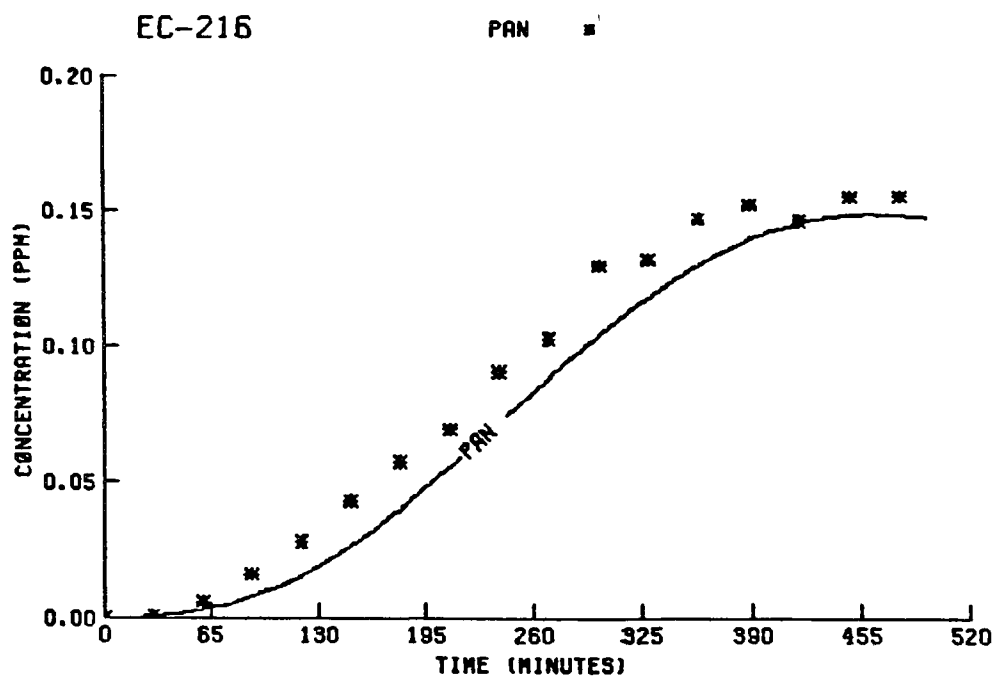
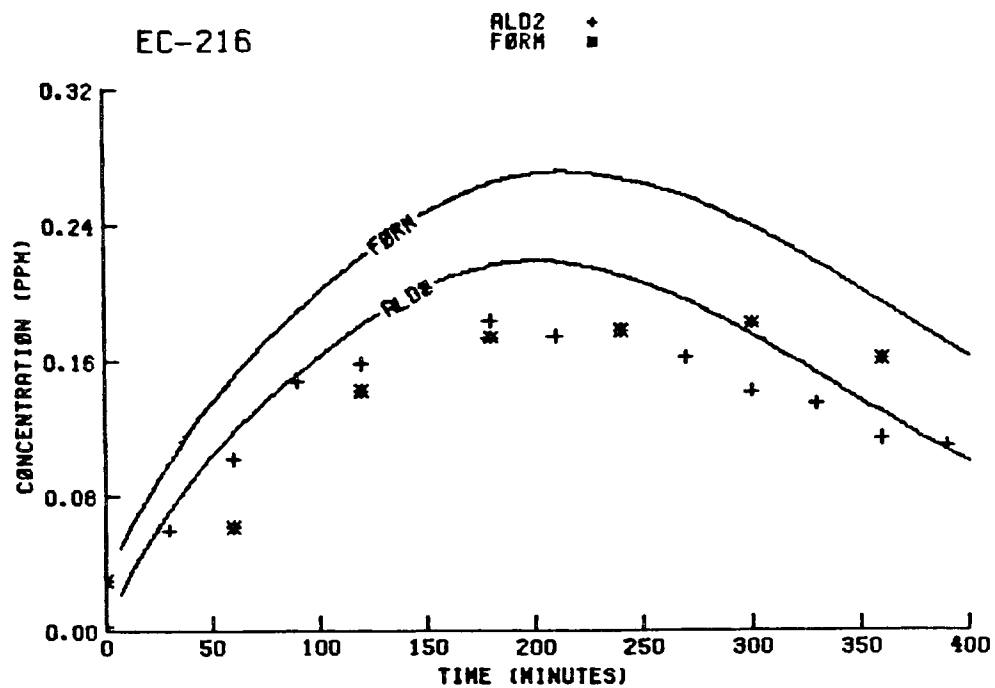


EC-177

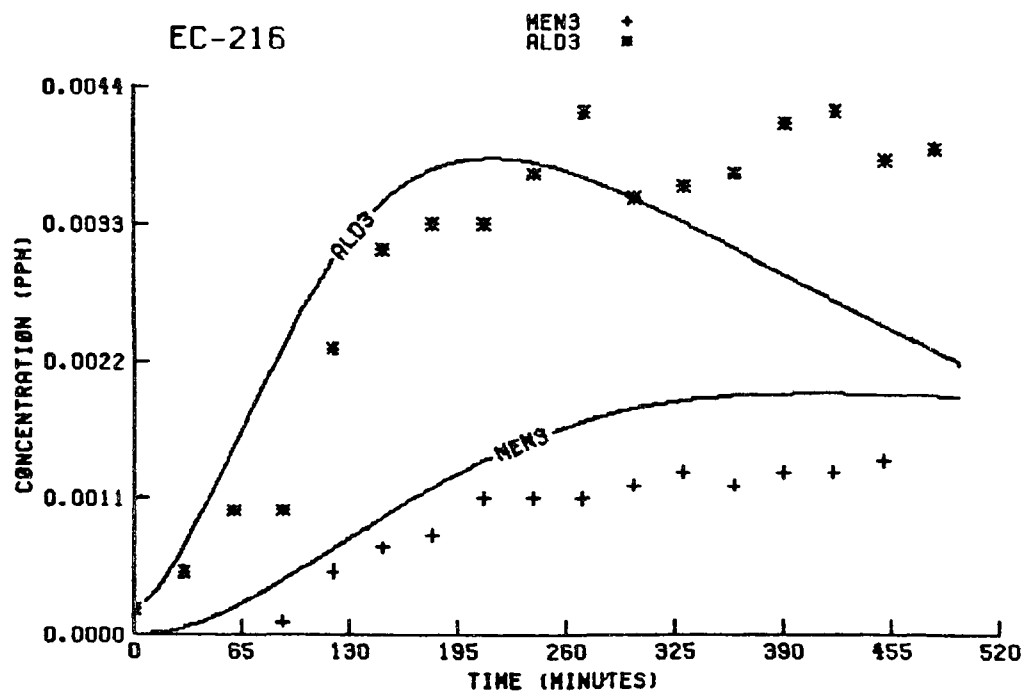
MEN3 +
ALD3 ■

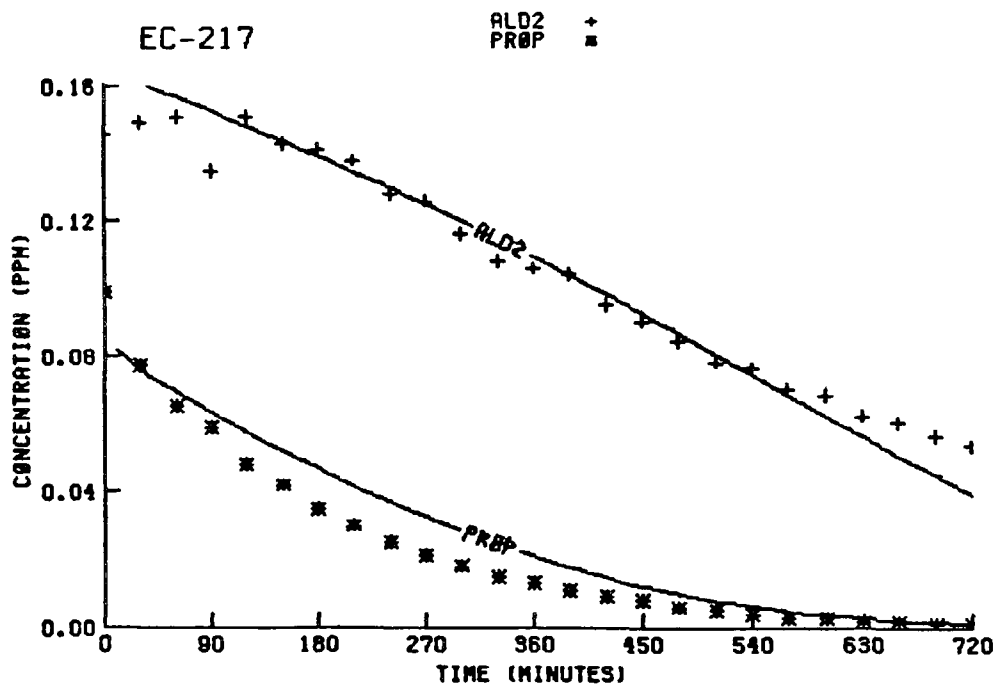
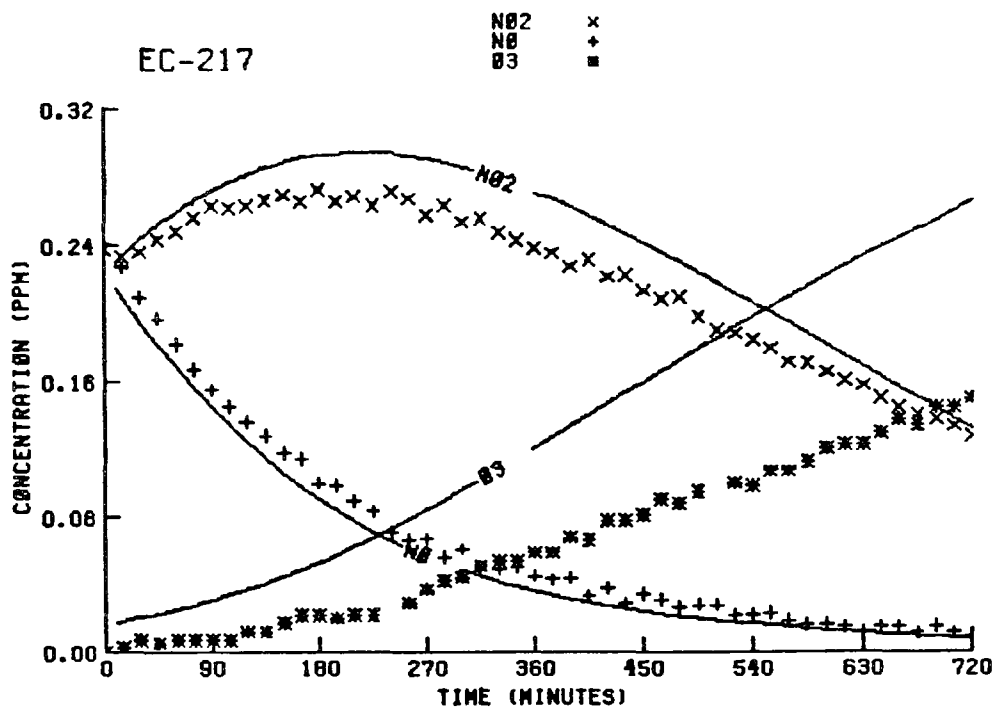


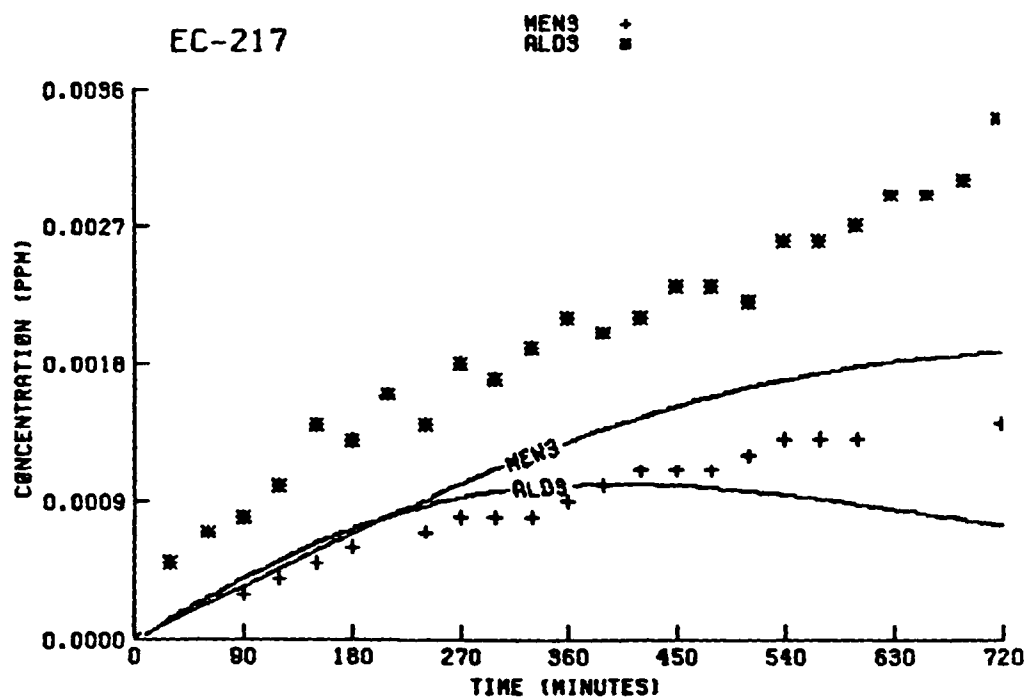
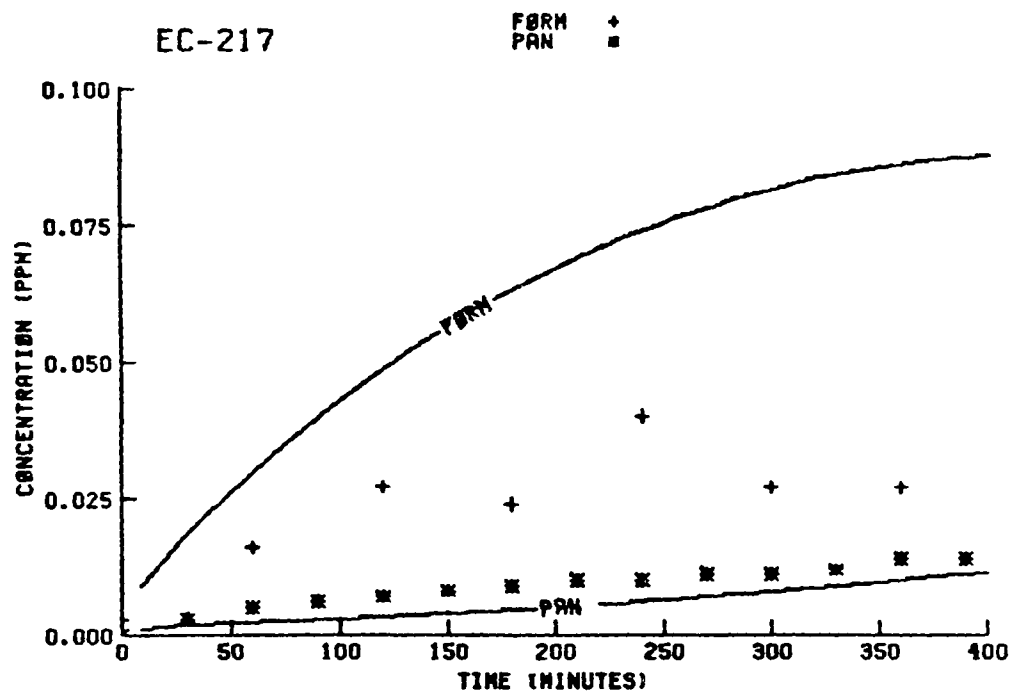


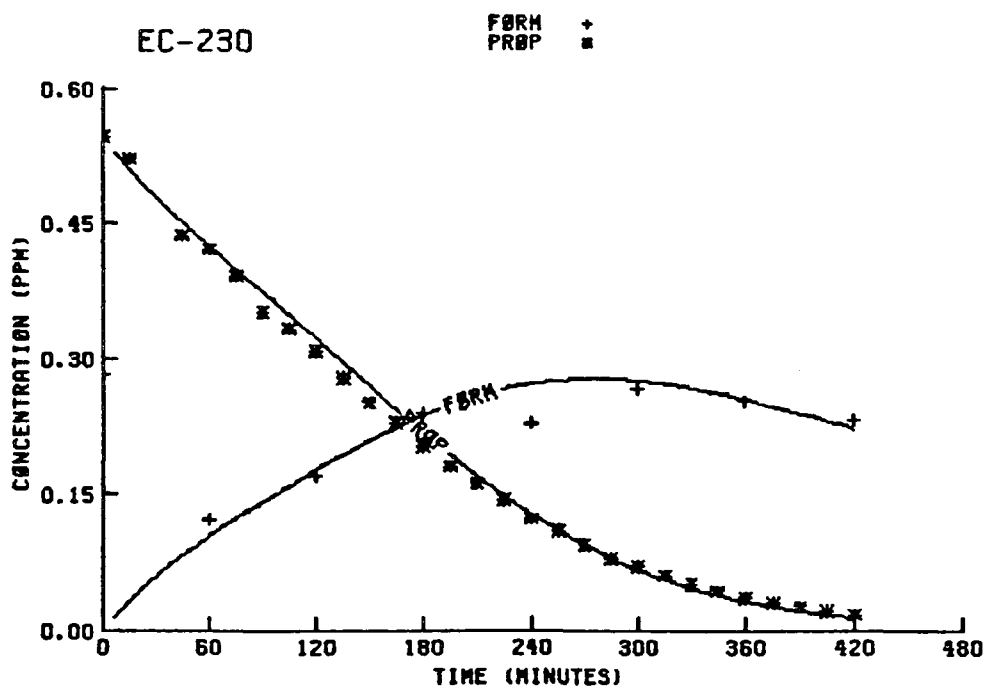
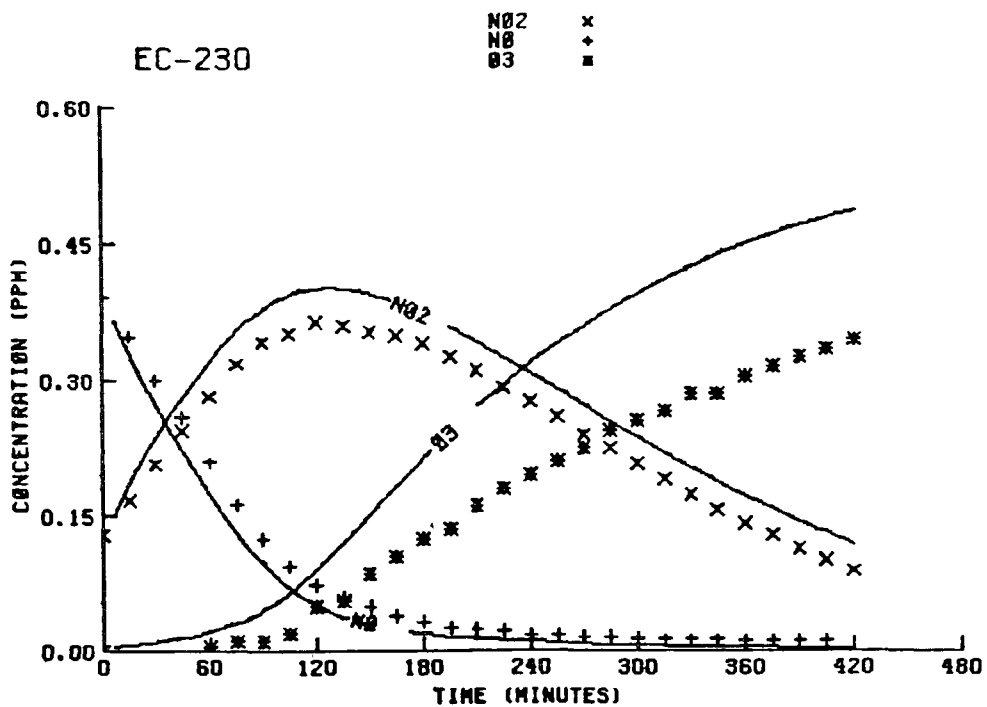


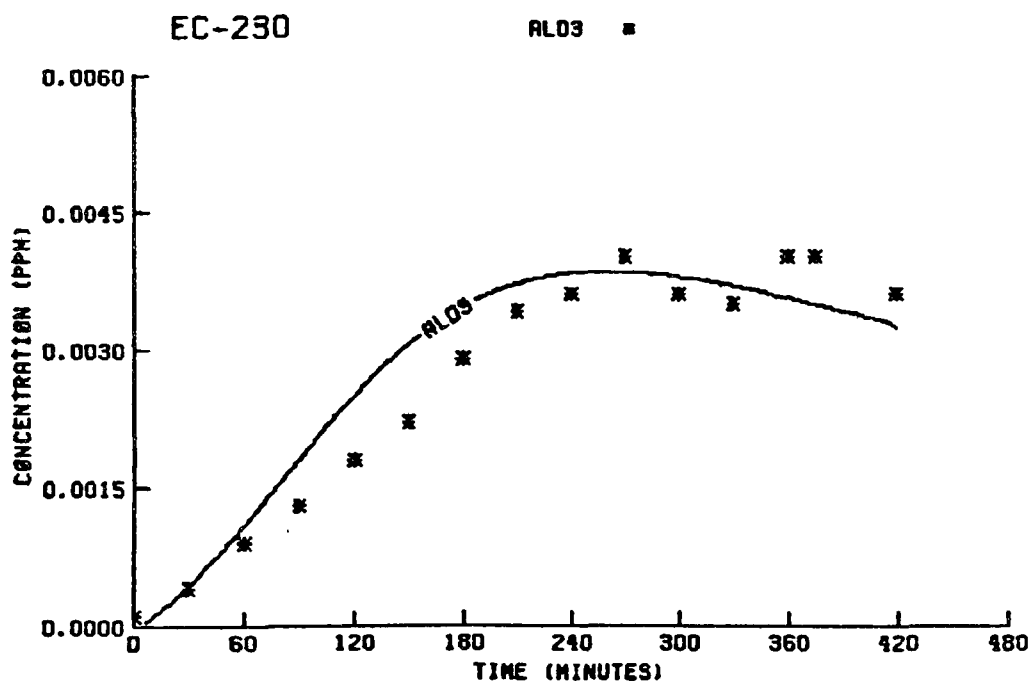
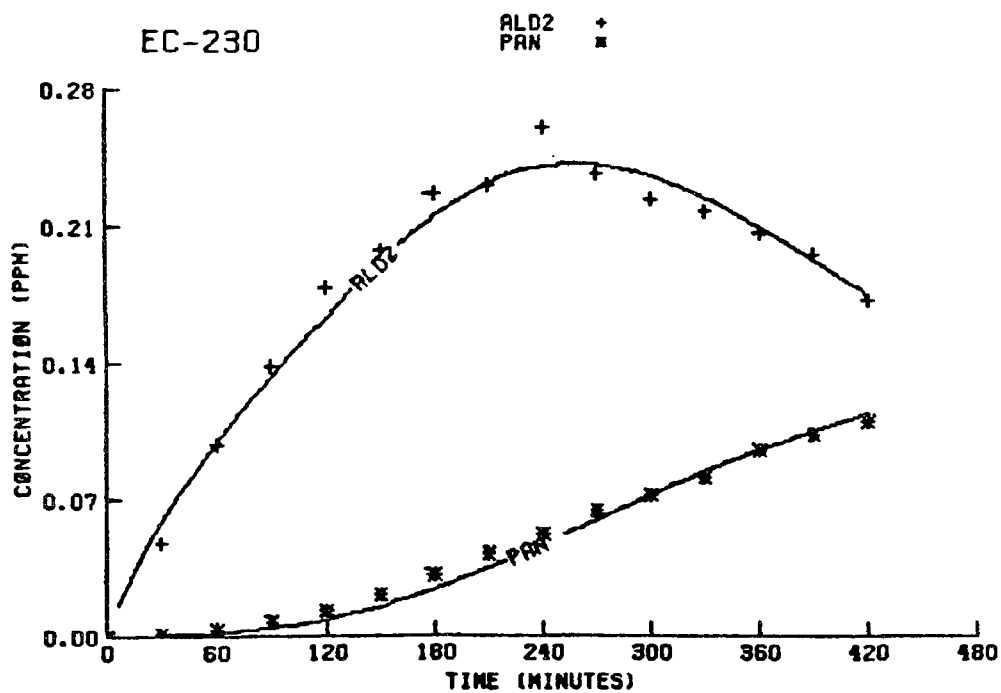
EC-216





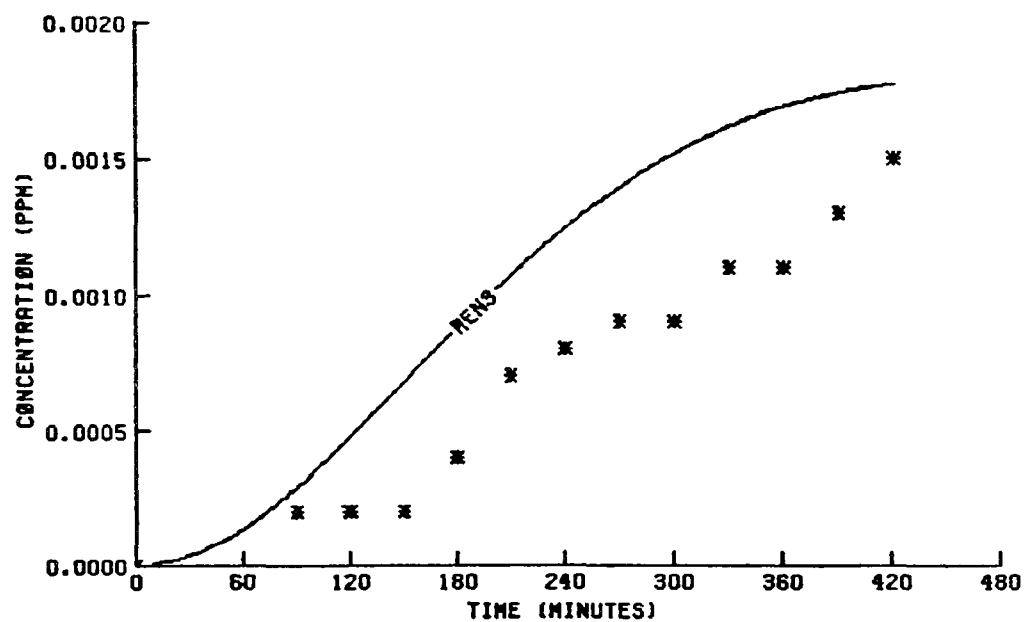






EC-230

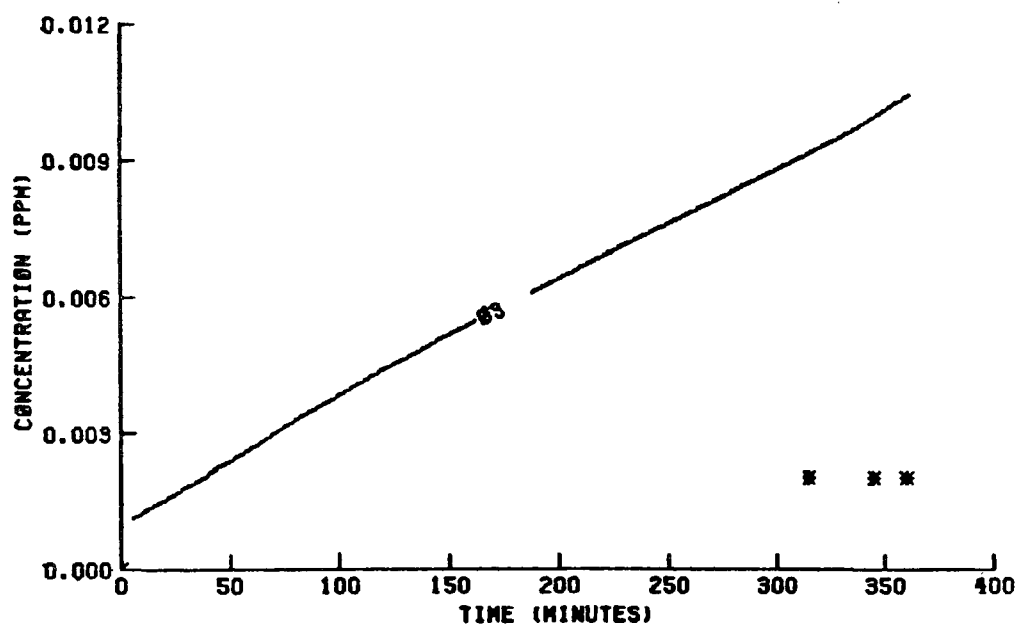
MEN3 ■



EC-256

83

■



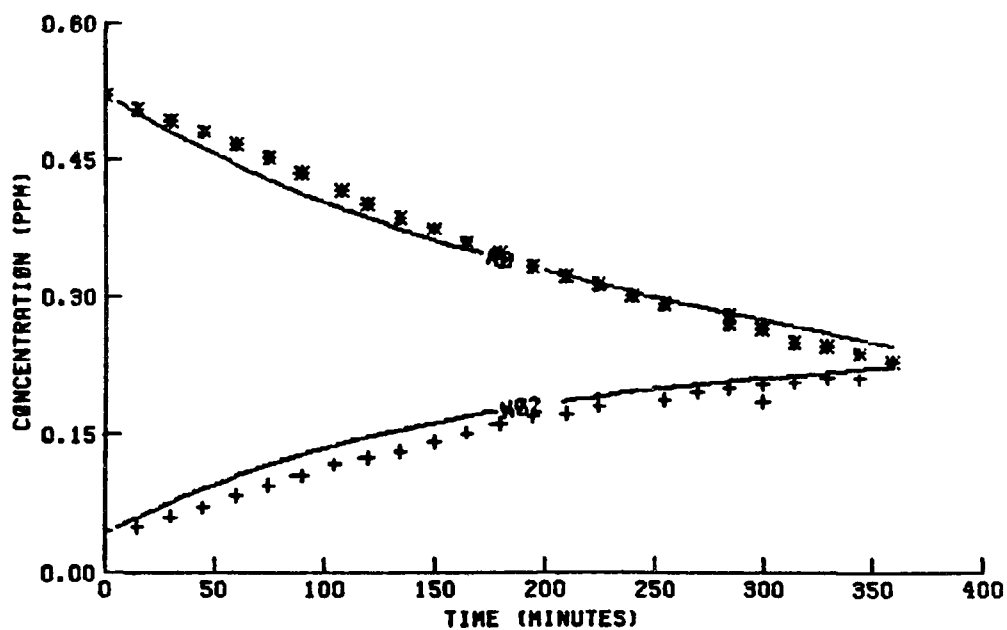
EC-256

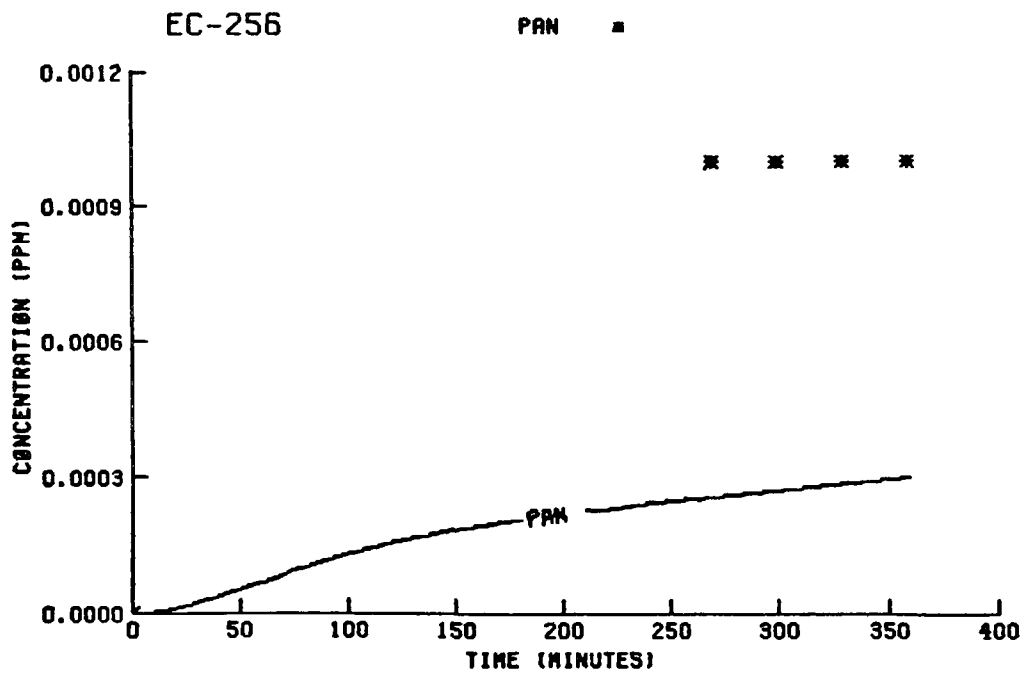
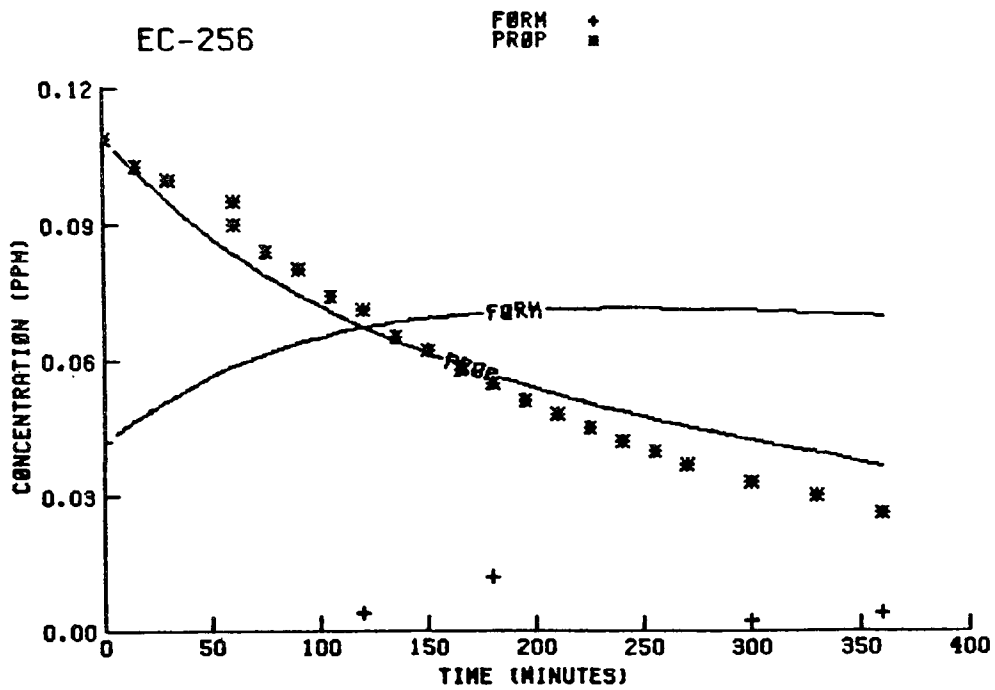
N82

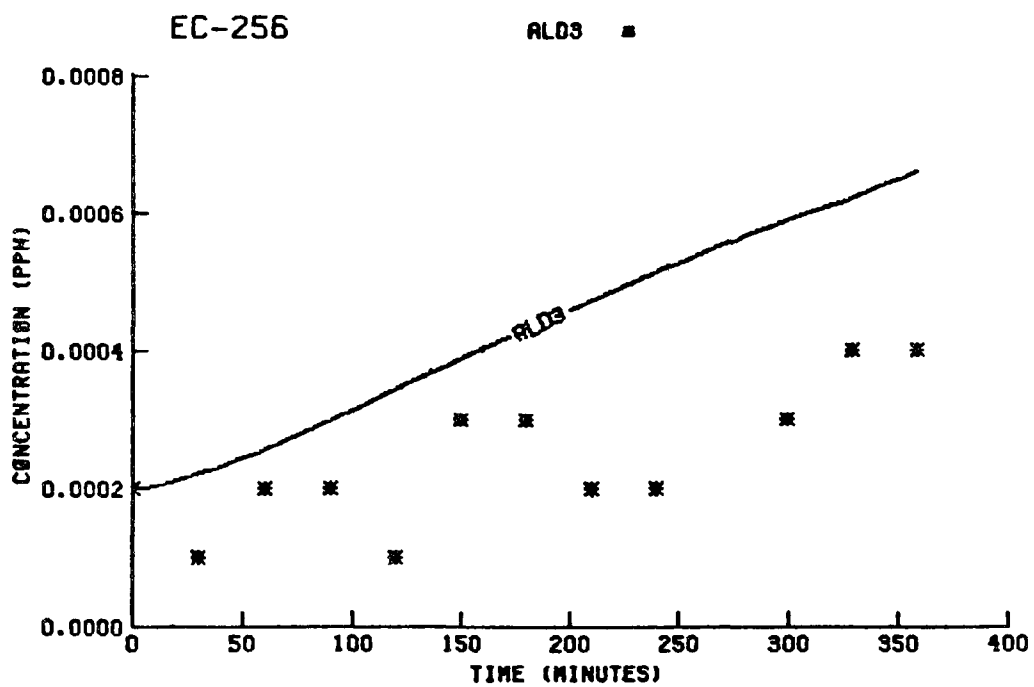
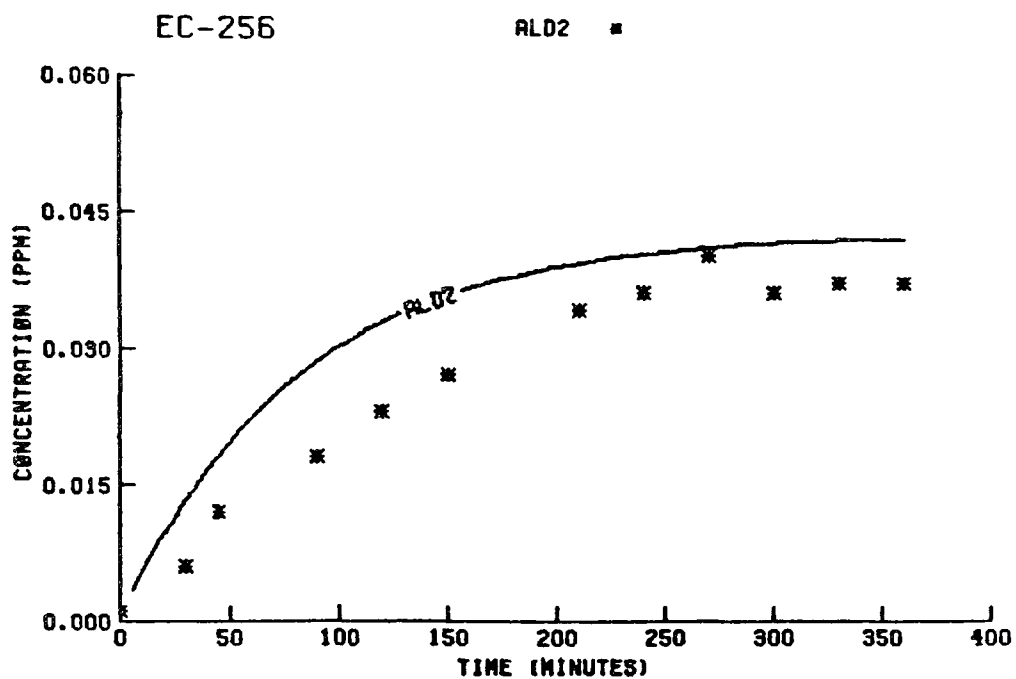
+

N8

■

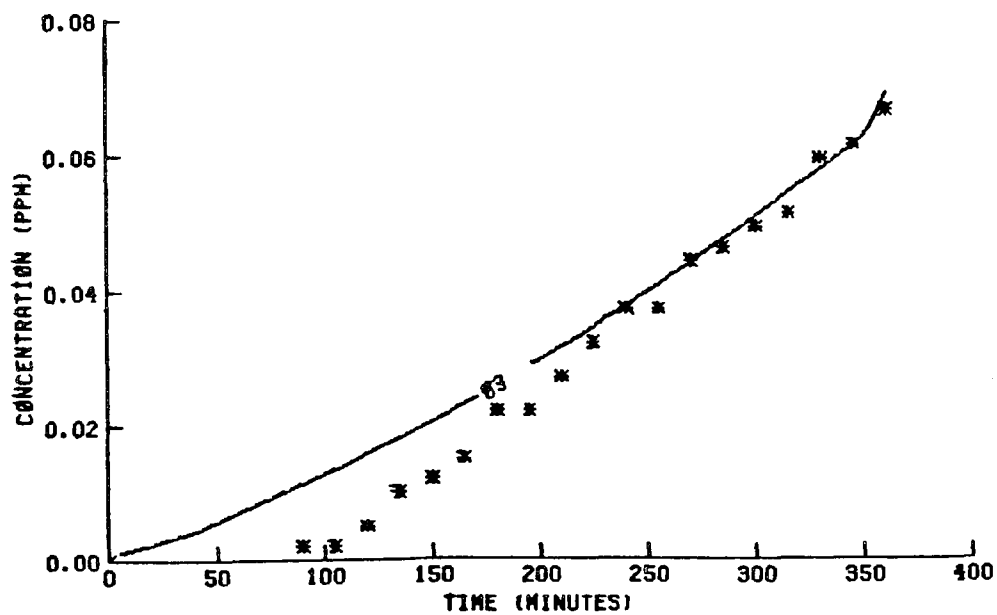






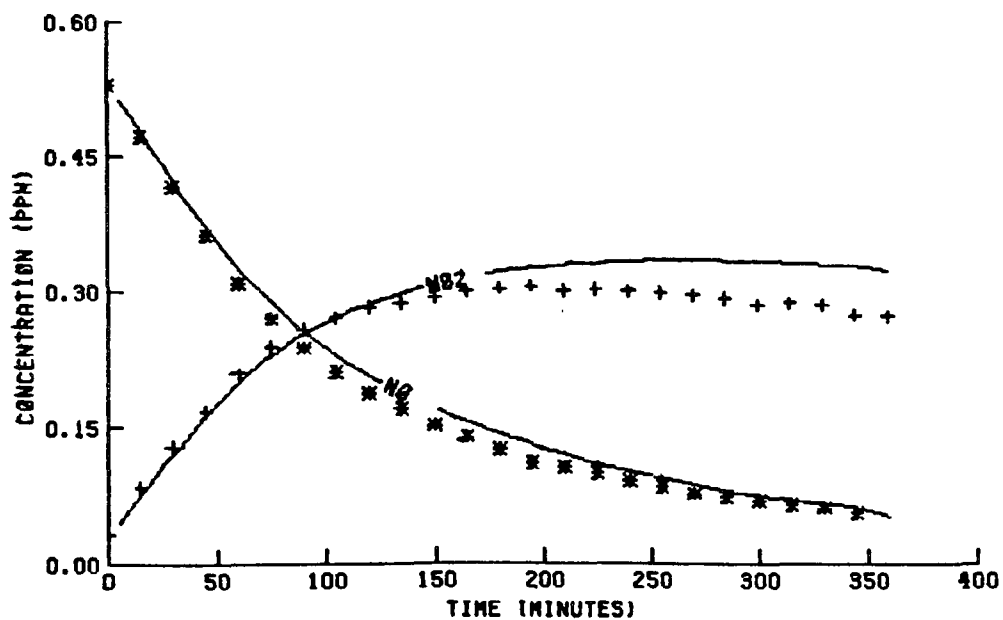
EC-257

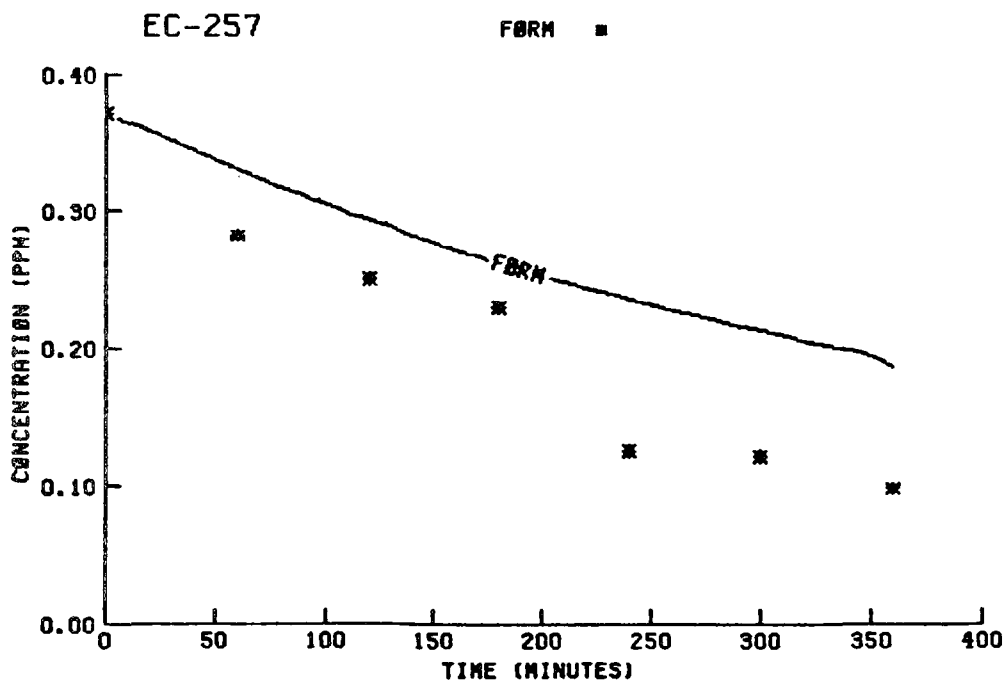
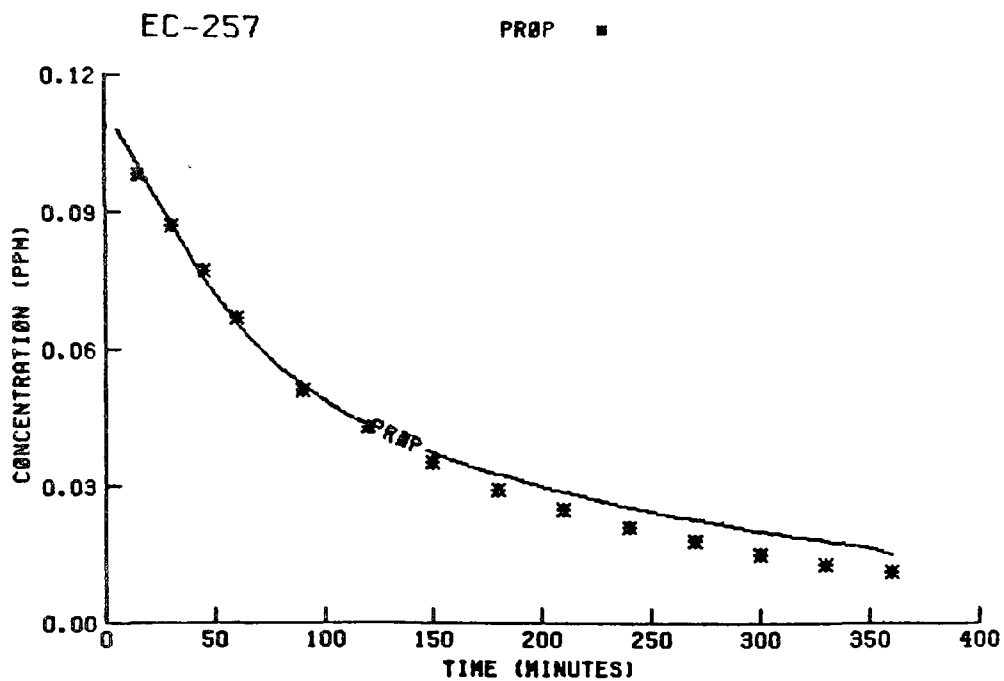
83

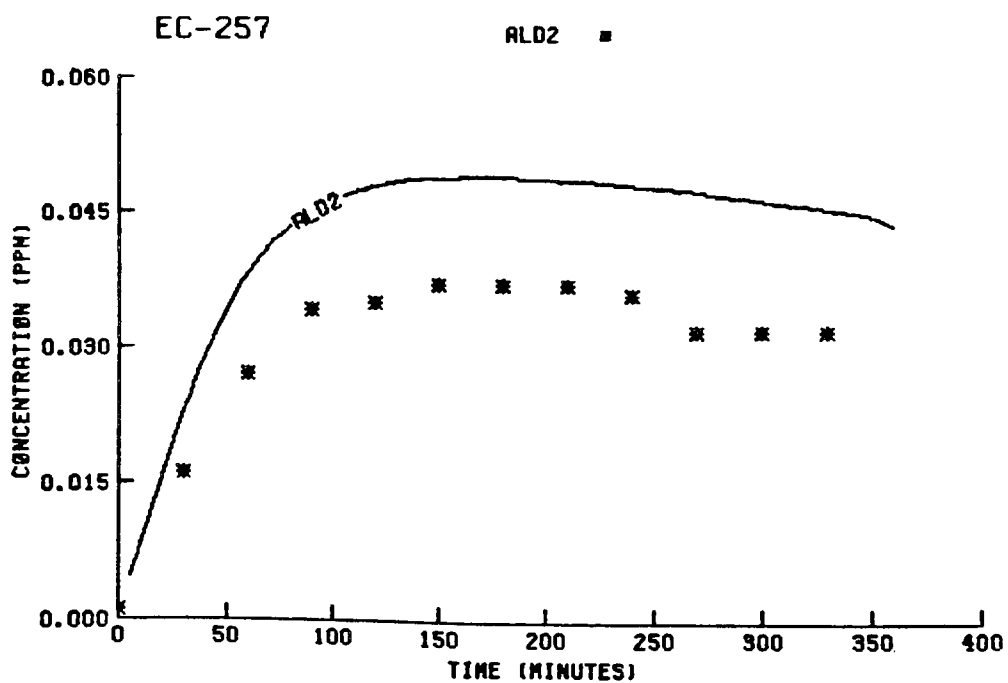
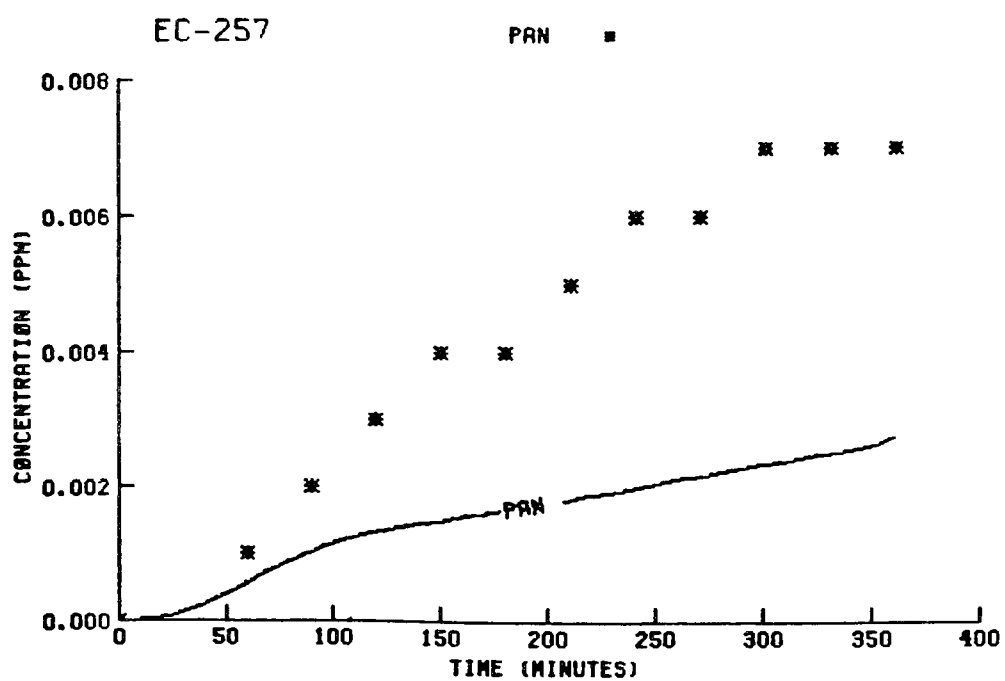


EC-257

N82
N8

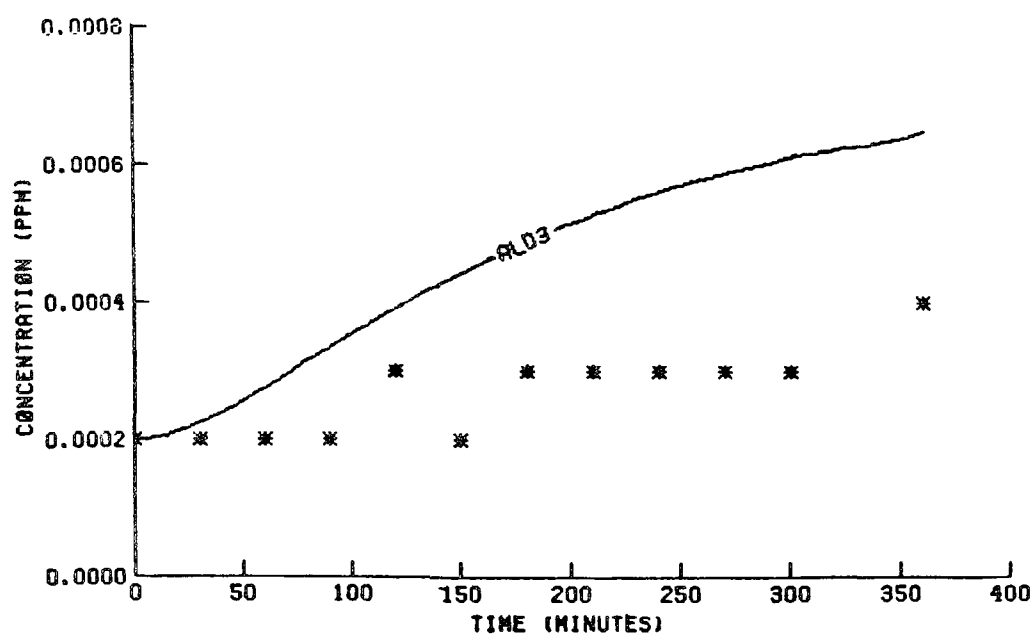






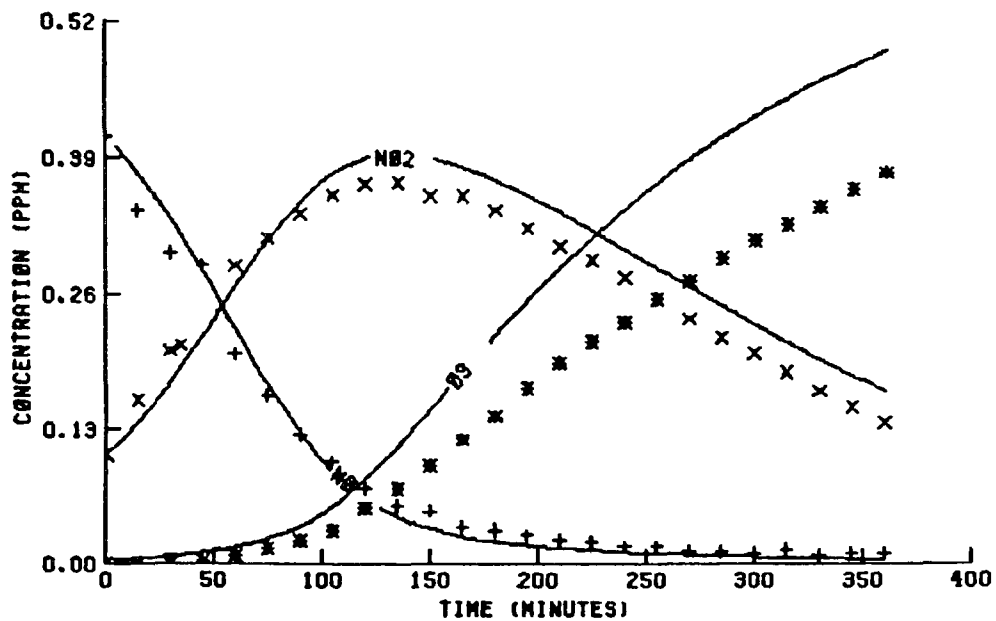
EC-257

ALD3 ■



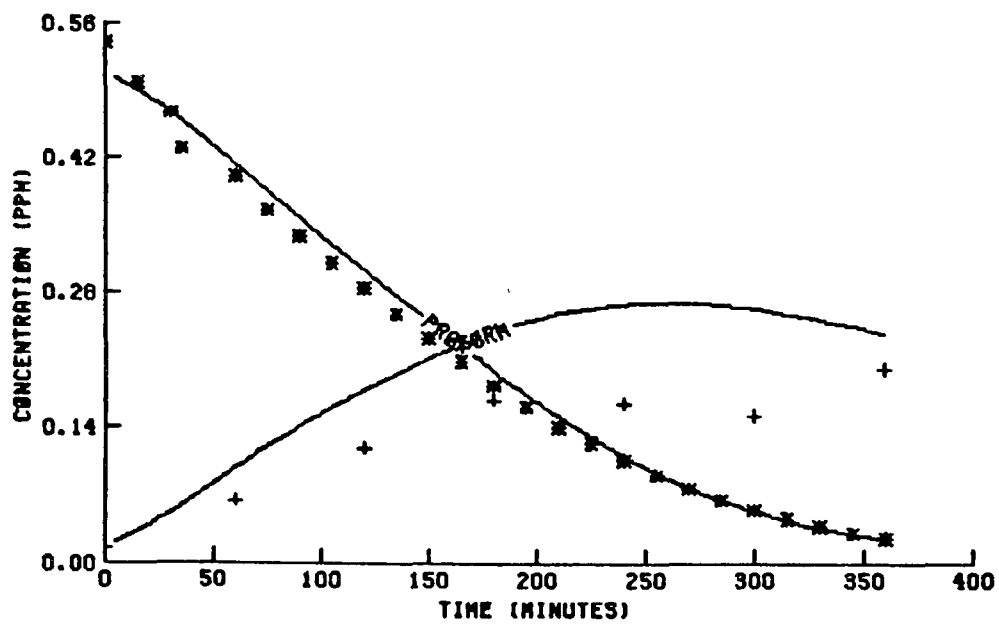
EC-276

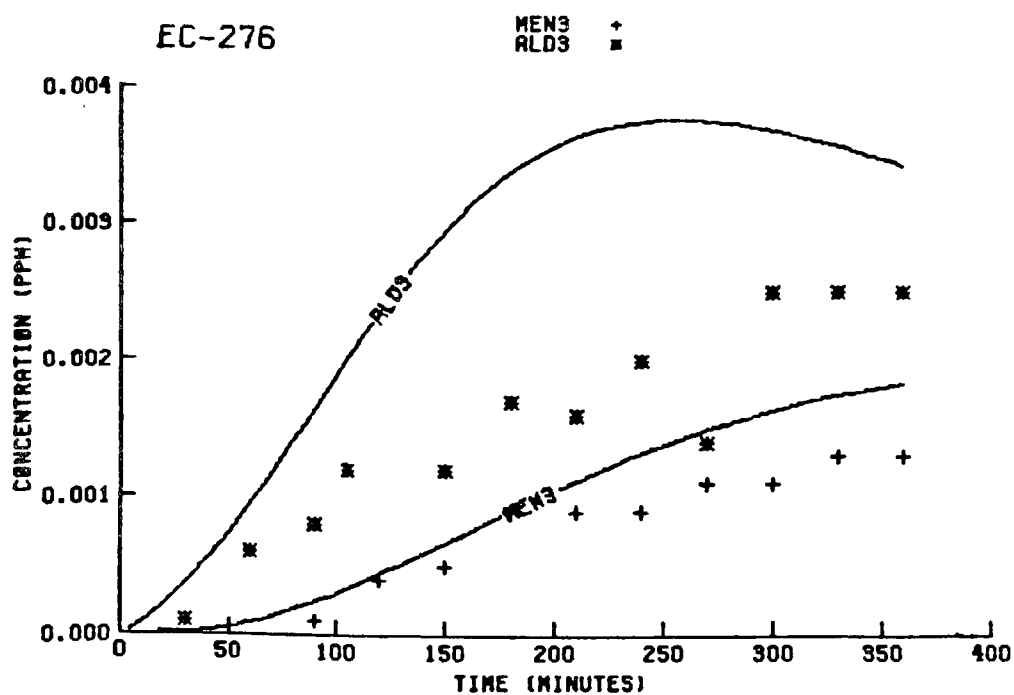
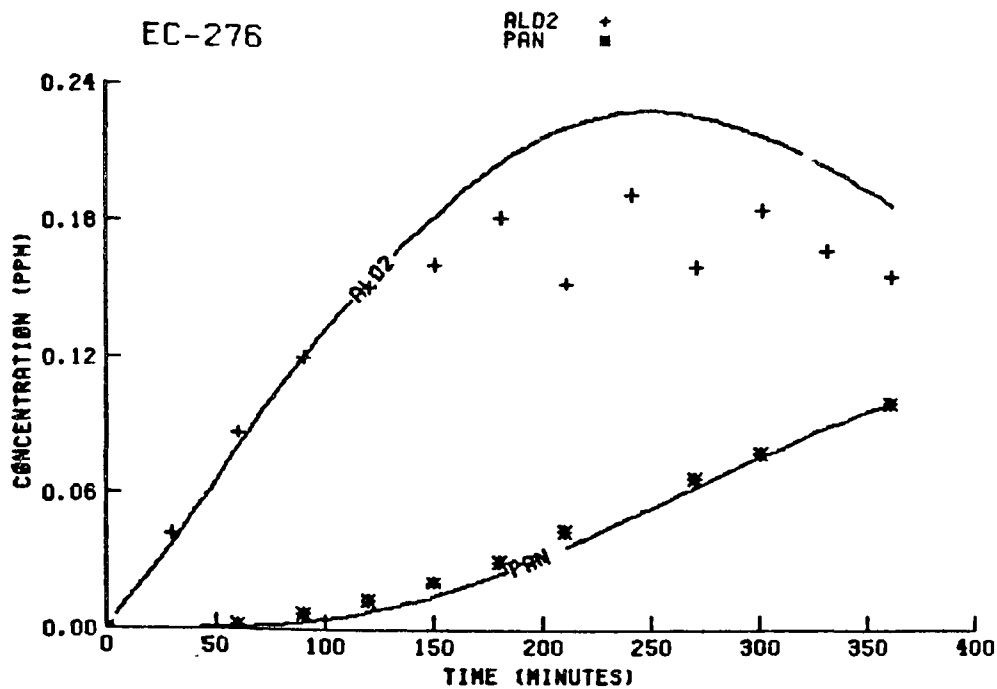
NB2 x
NB +
B3 ■



EC-276

FORM +
PROP ■

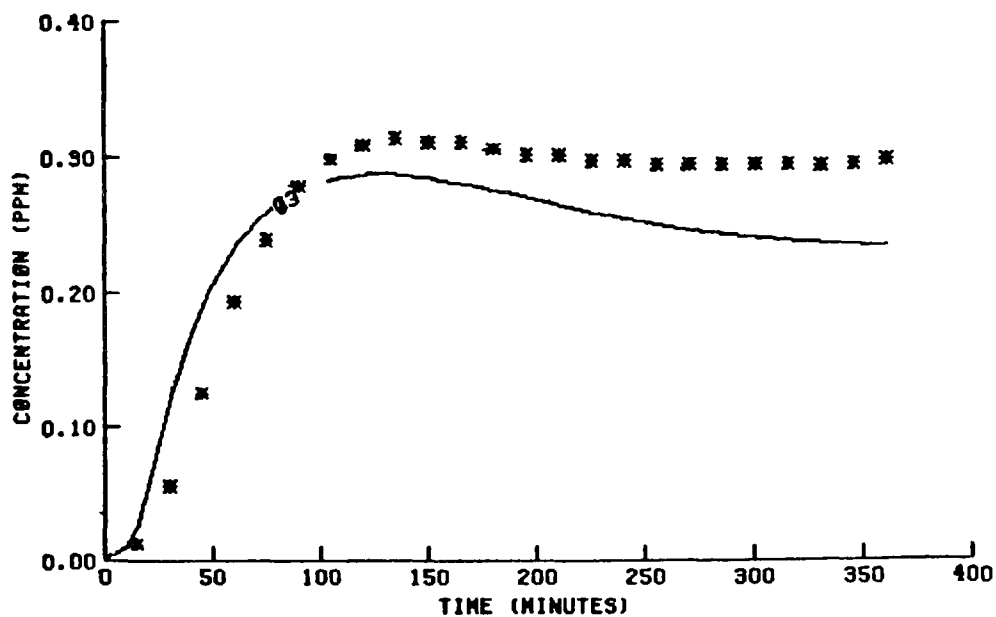




EC-277

03

■

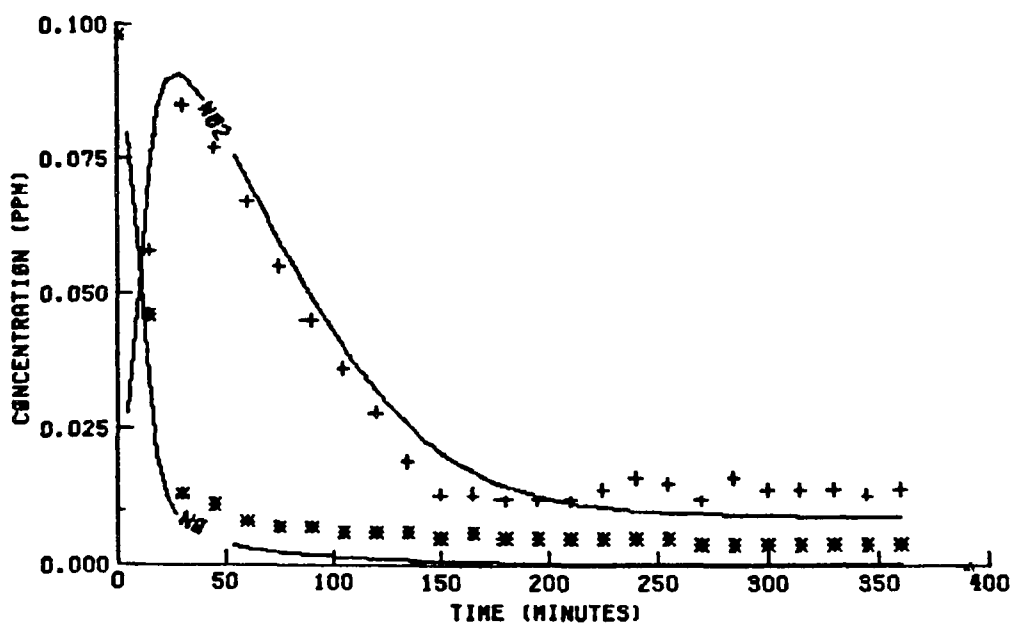


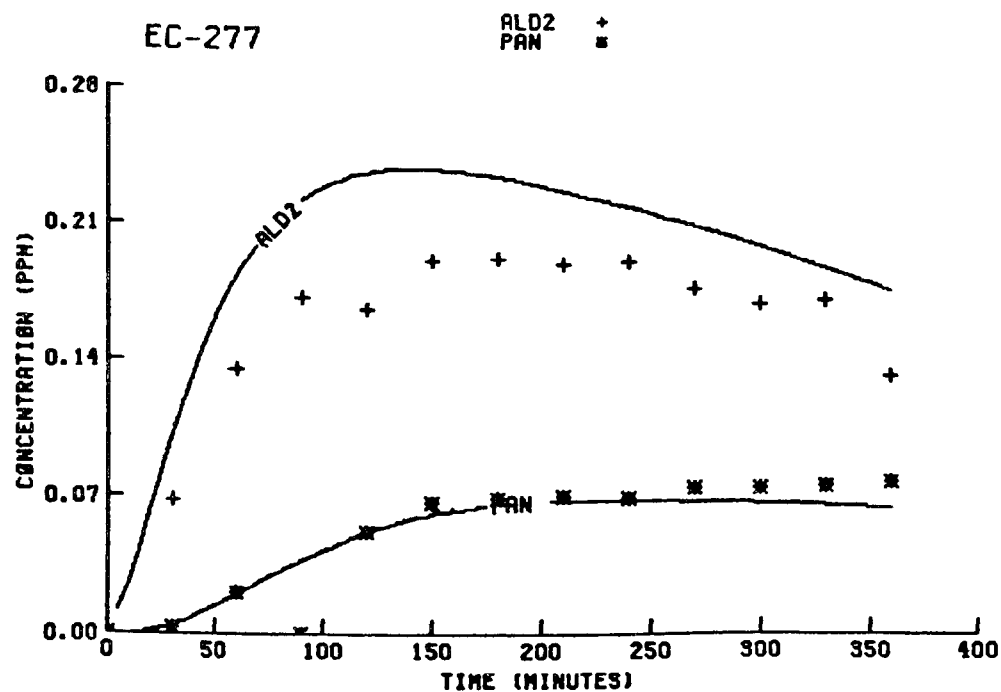
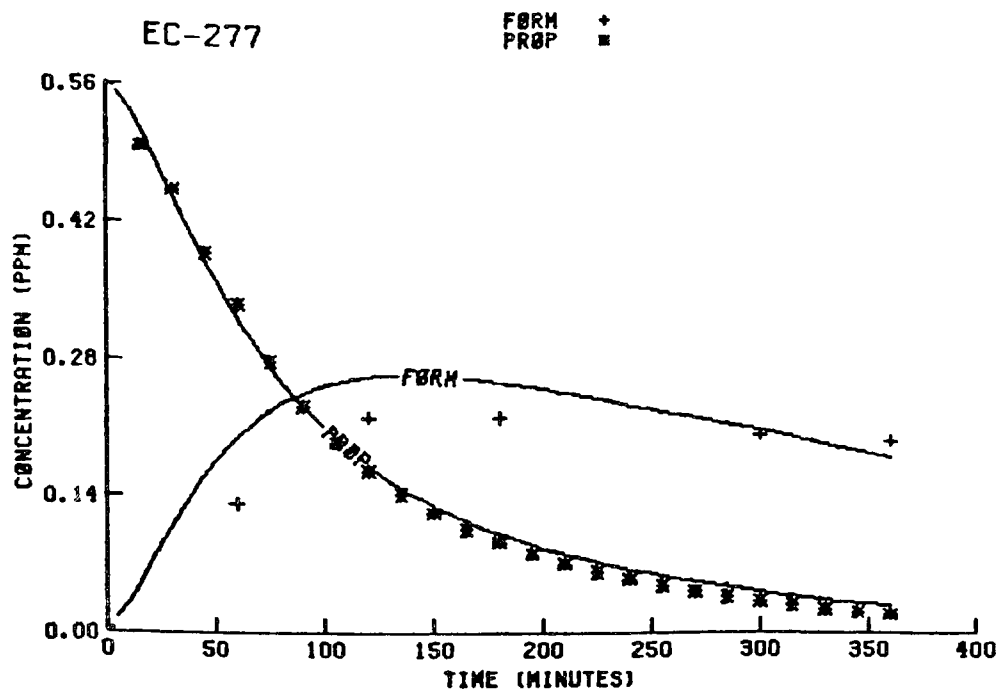
EC-277

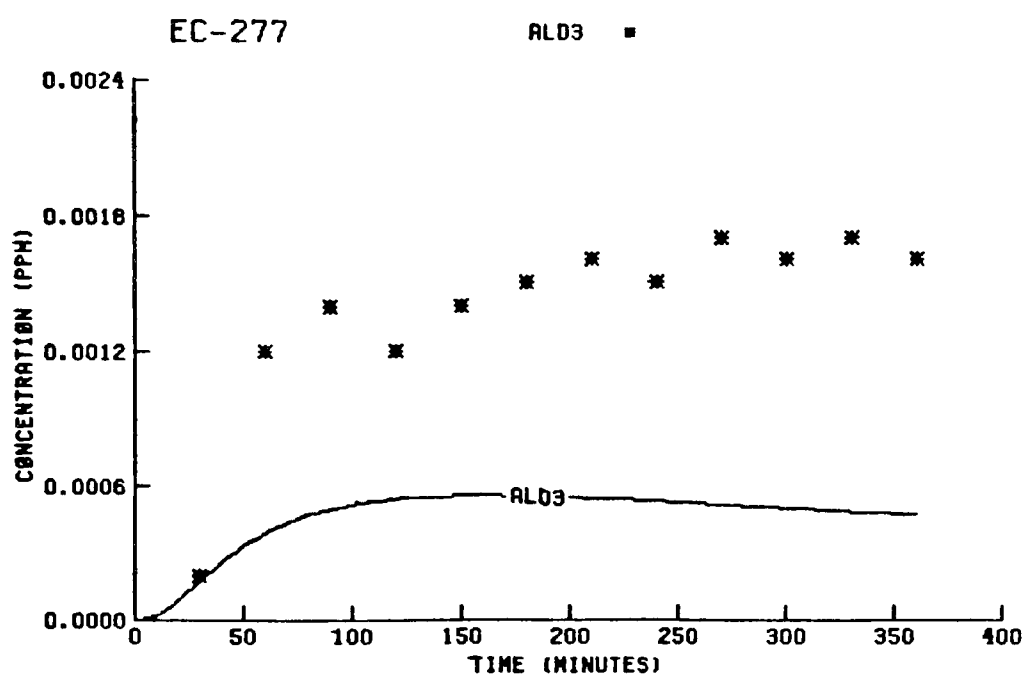
N02

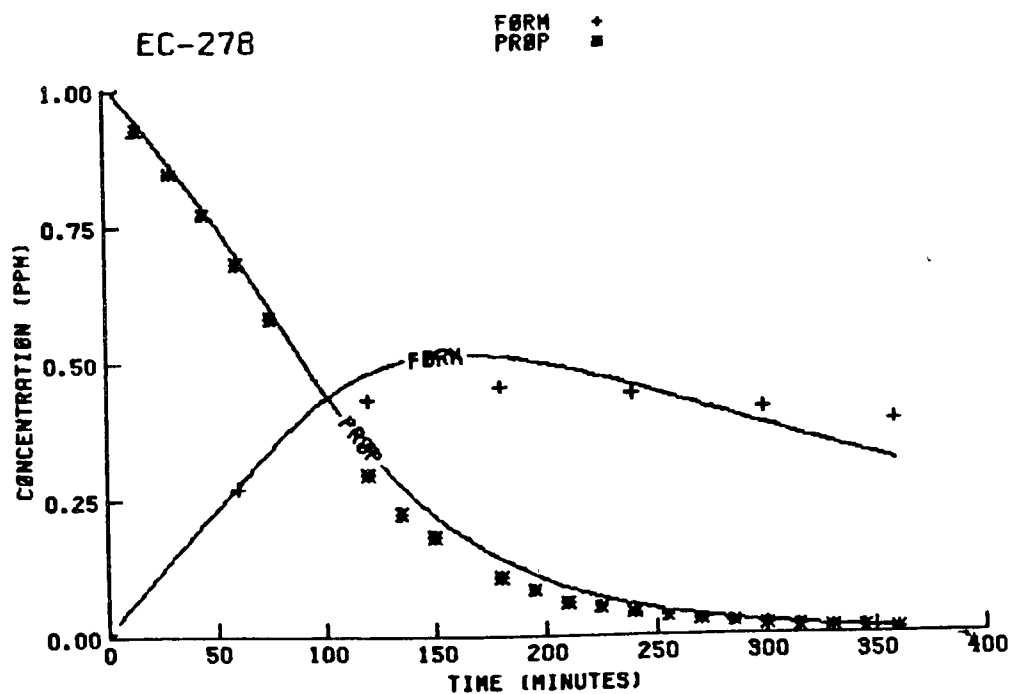
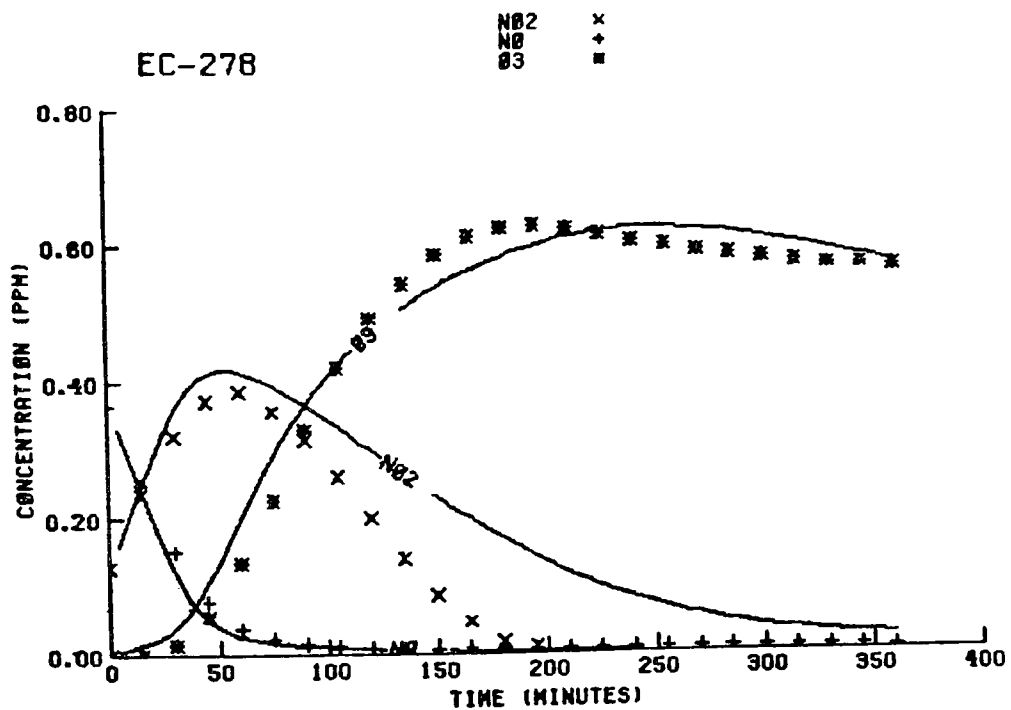
N0

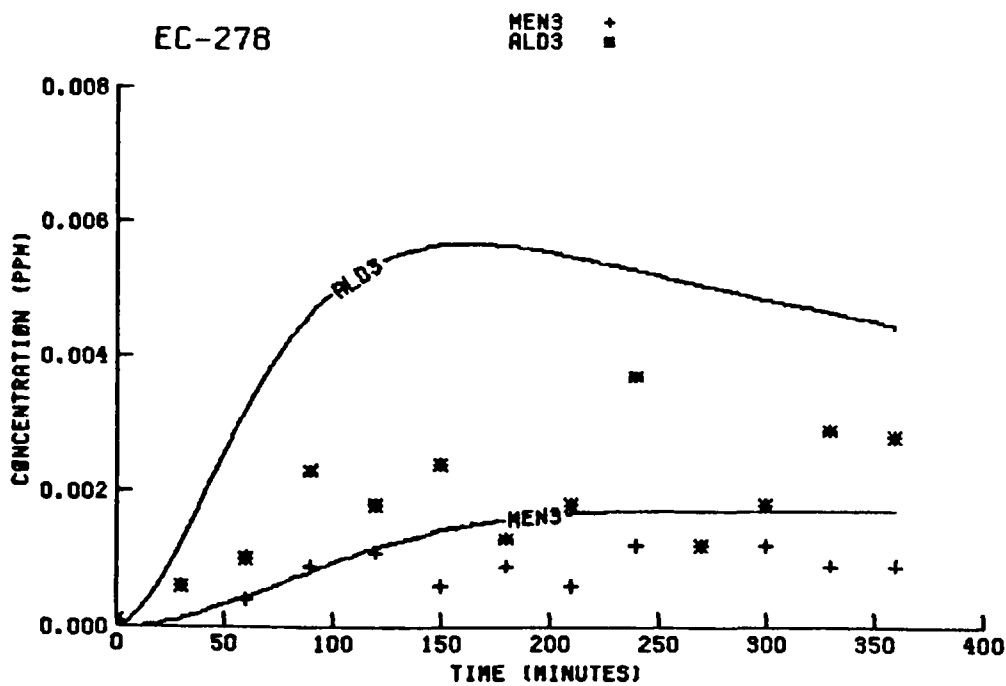
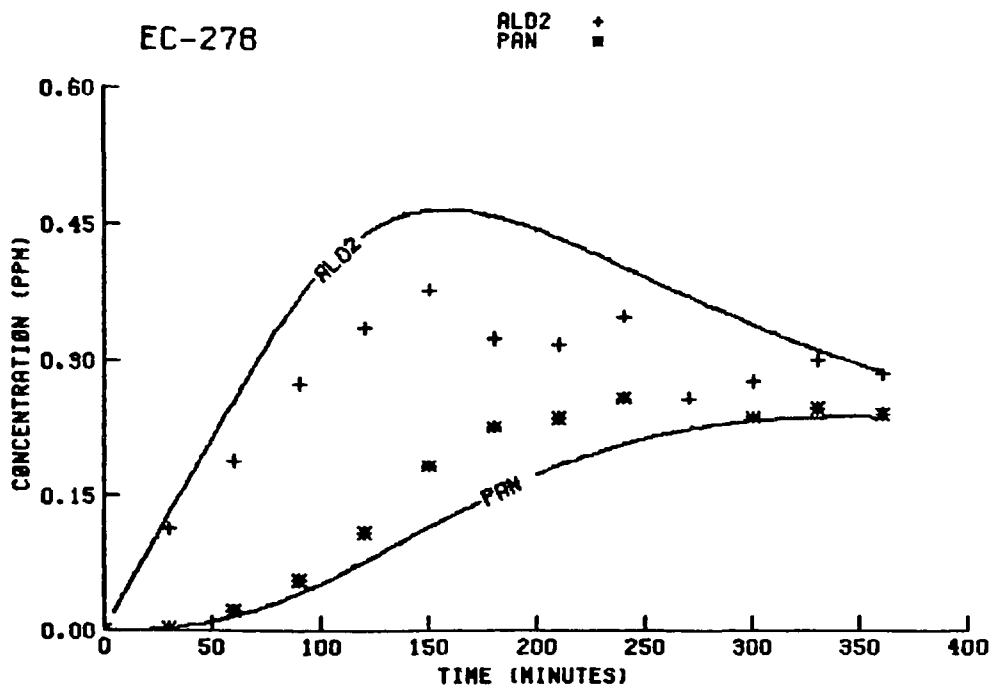
+

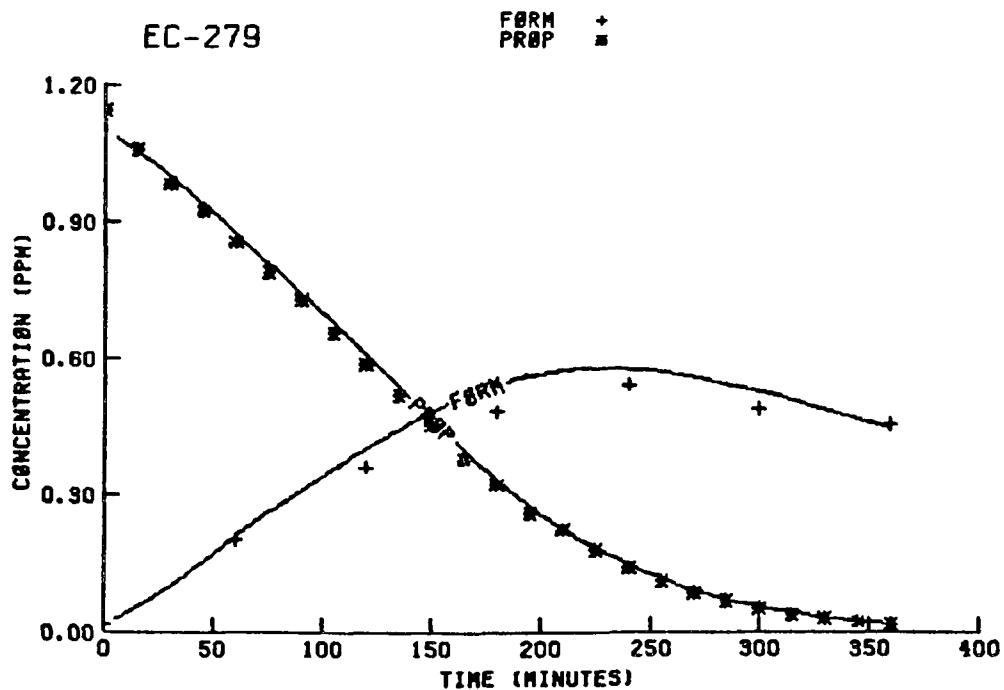
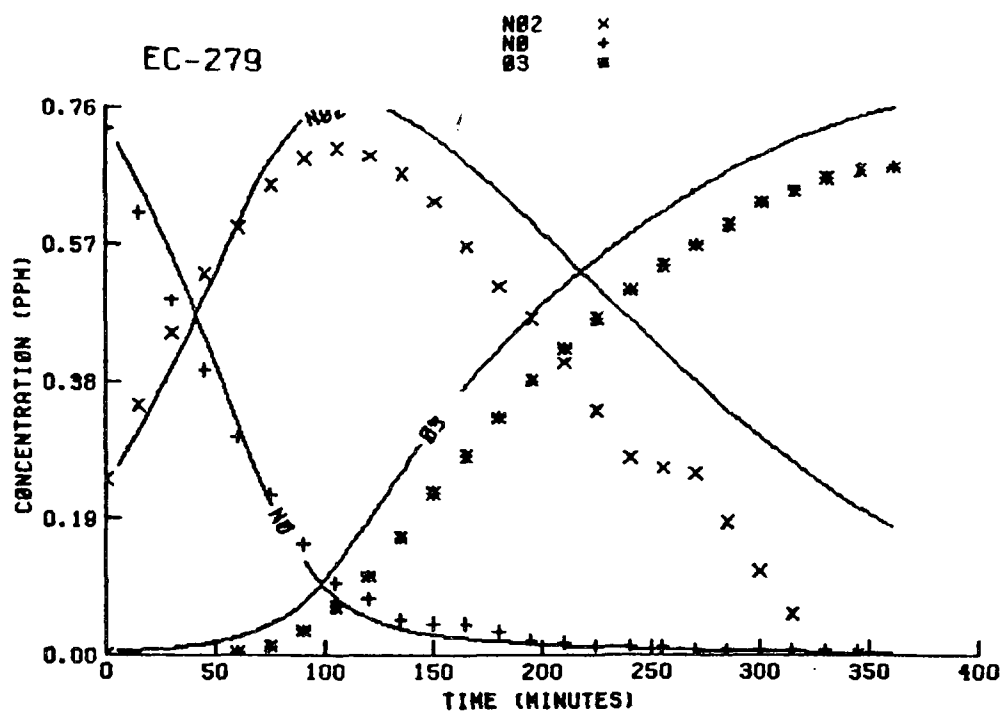


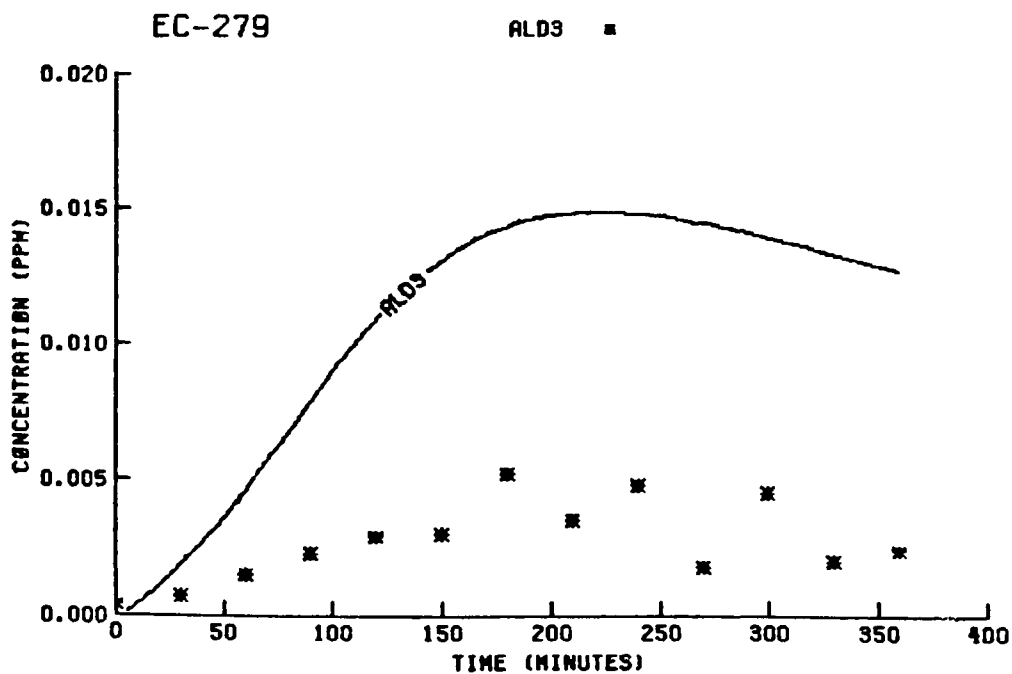
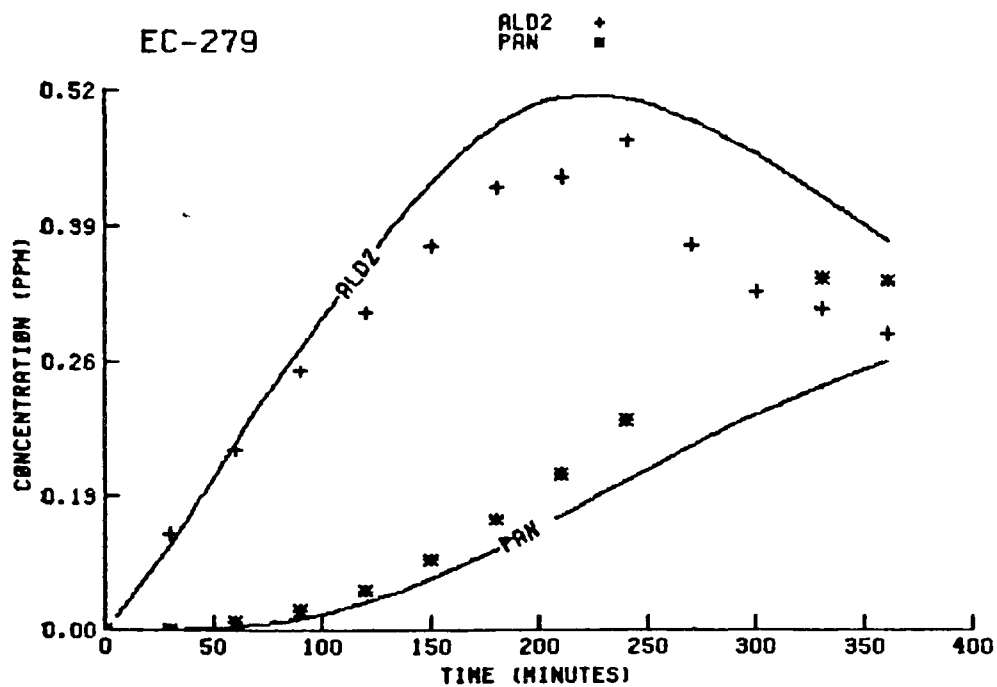






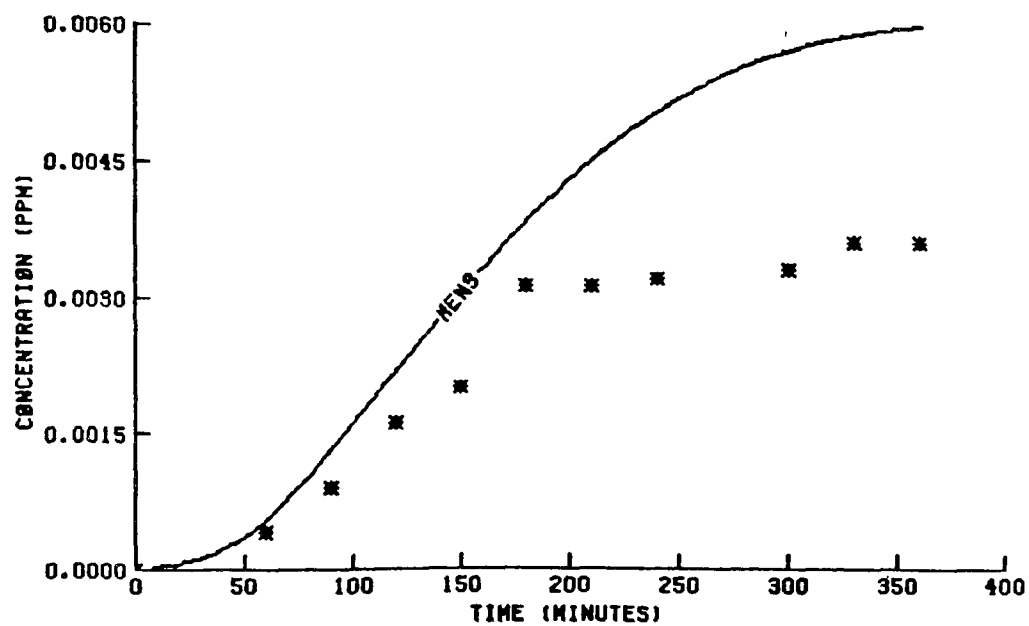






EC-279

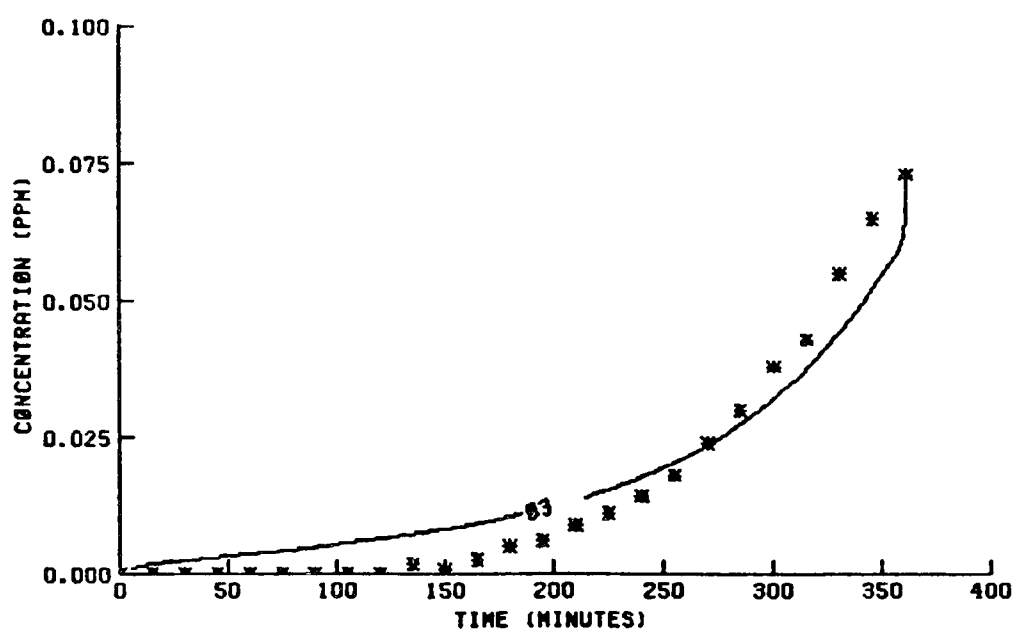
MEN3 ■



UCR BUTANE EXPERIMENTS

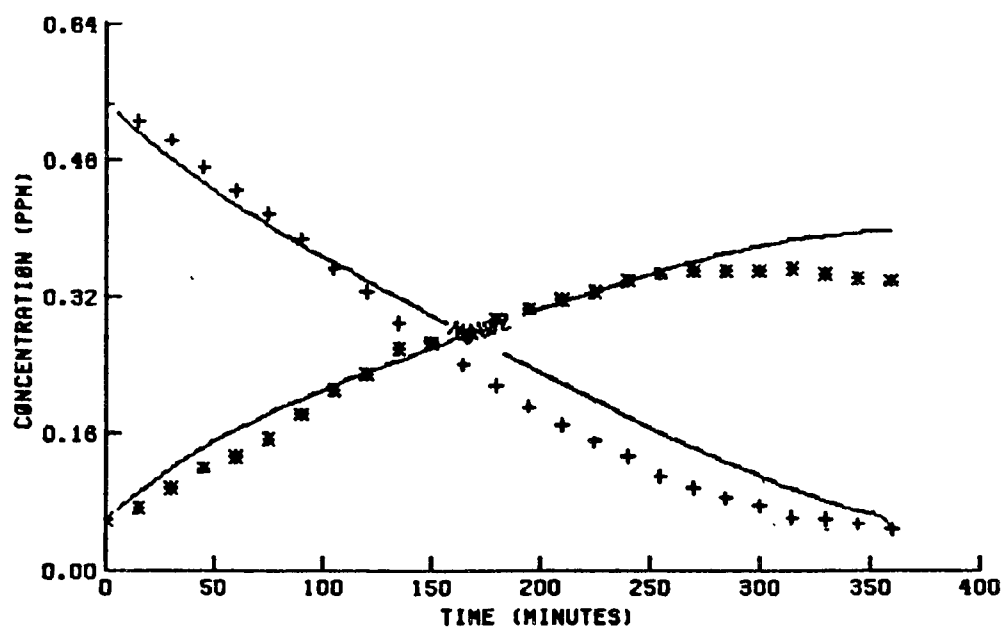
EC-39

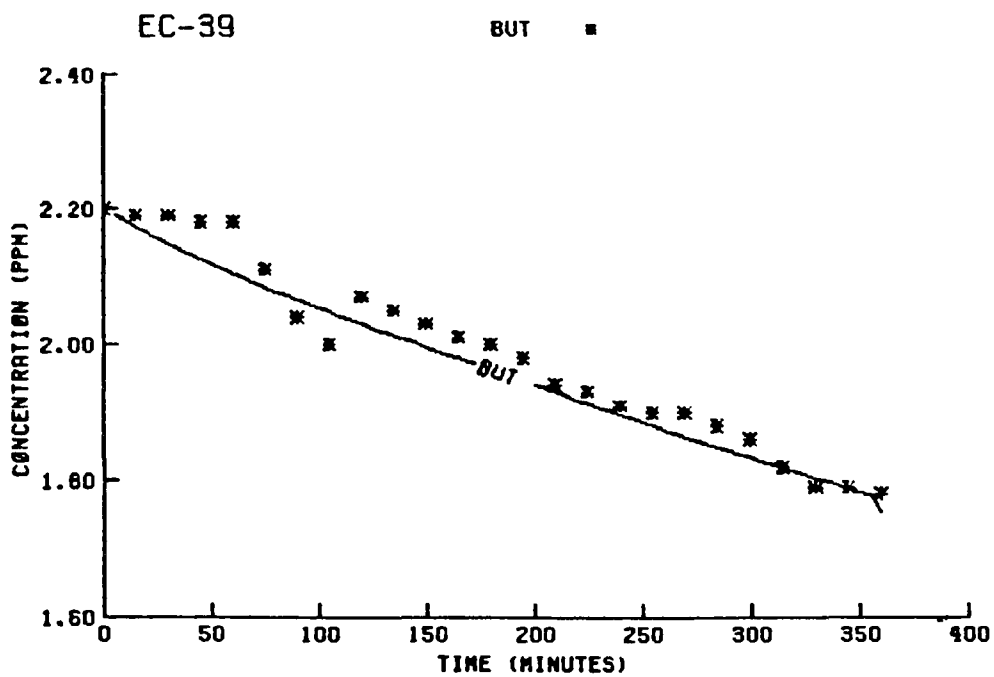
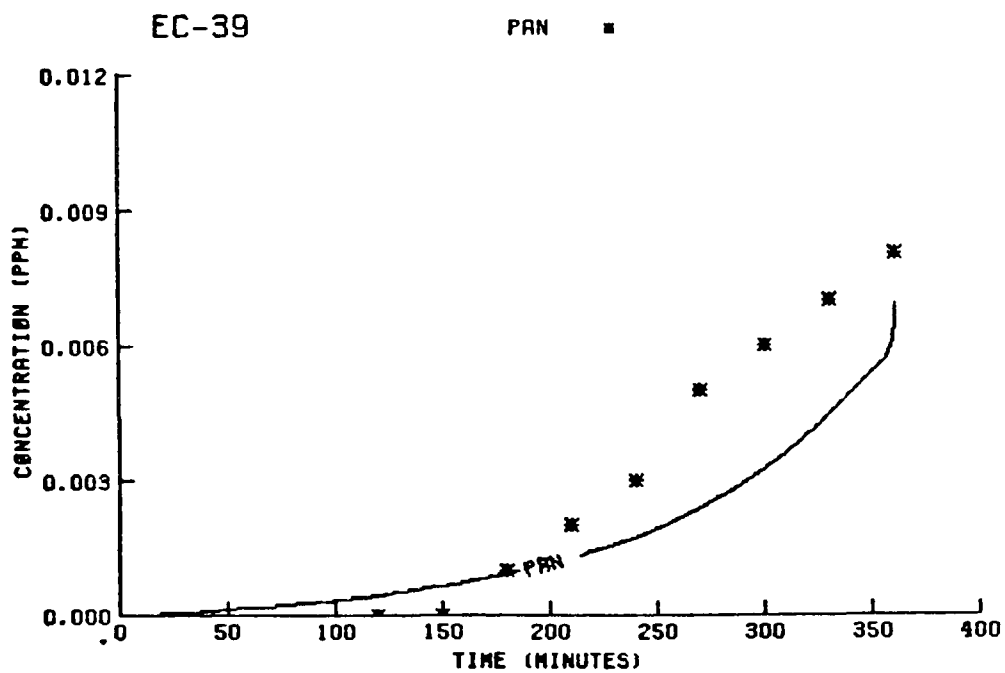
83

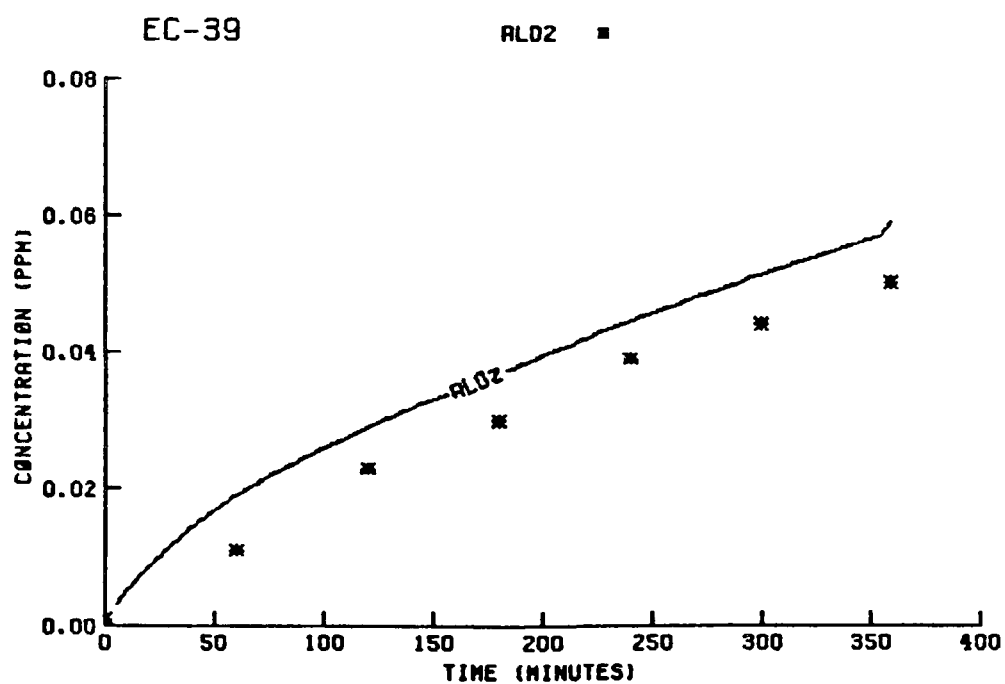
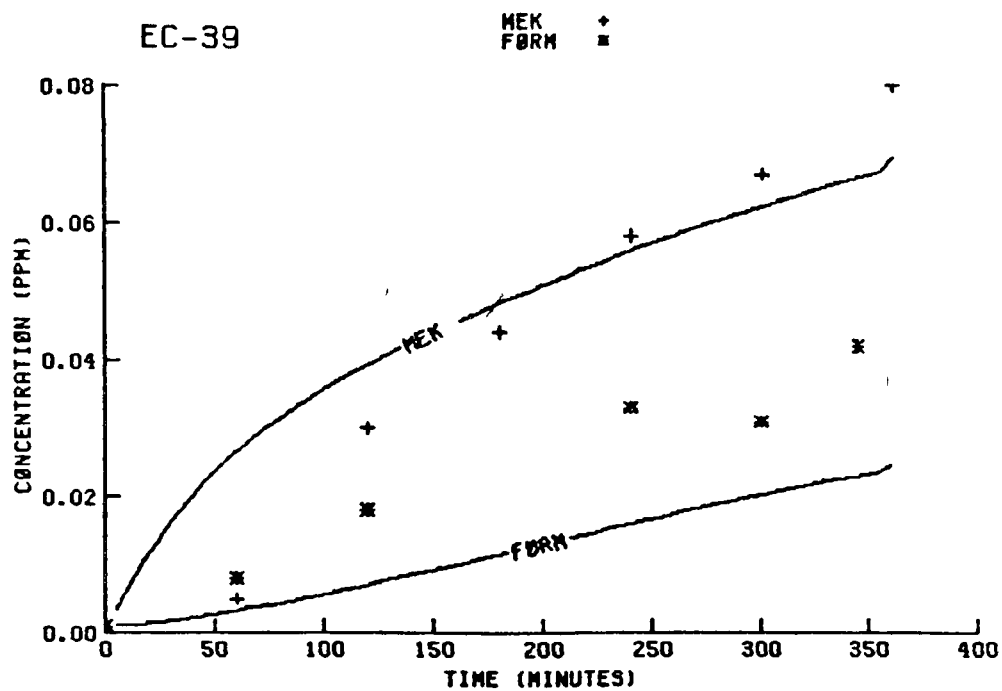


EC-39

N8
N82

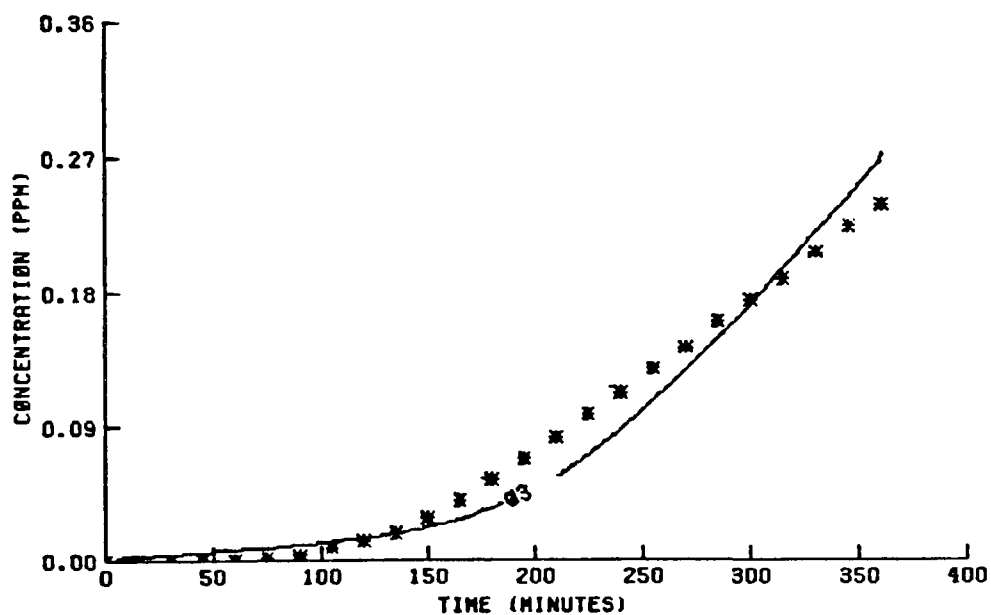






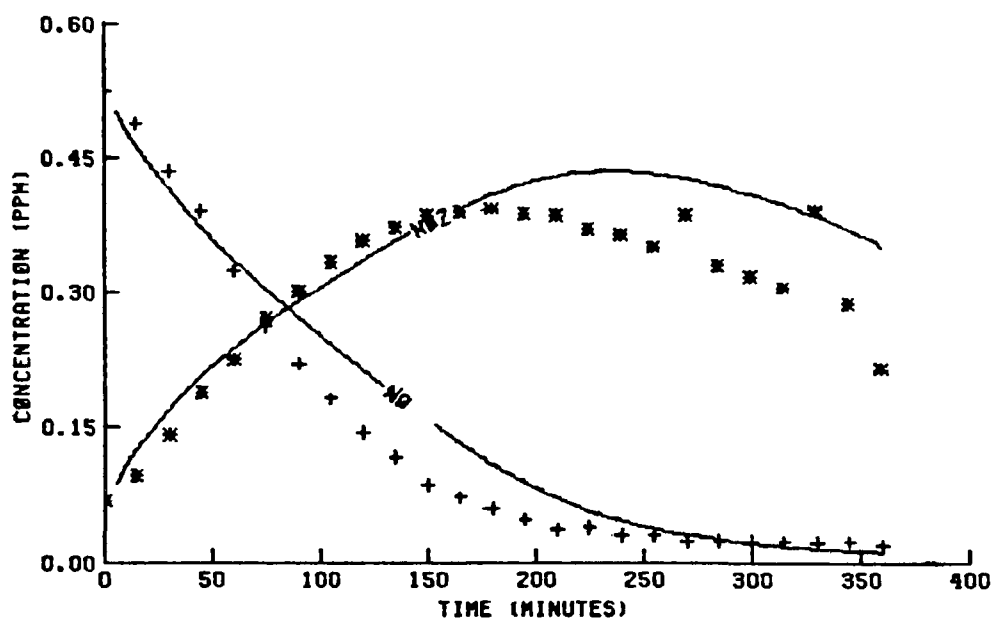
EC-41

03 *



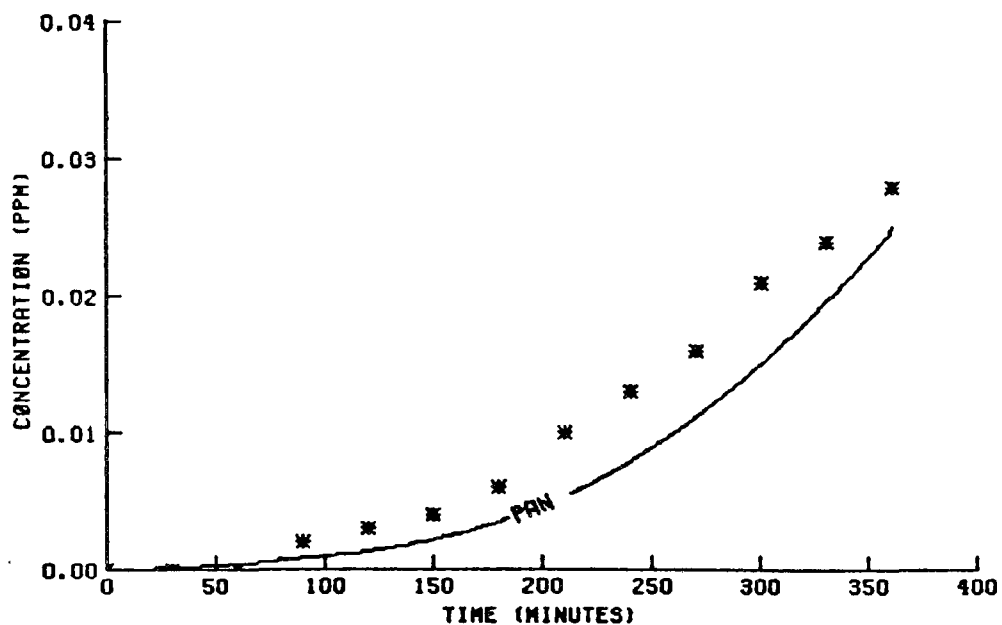
EC-41

N0 +
N02 *



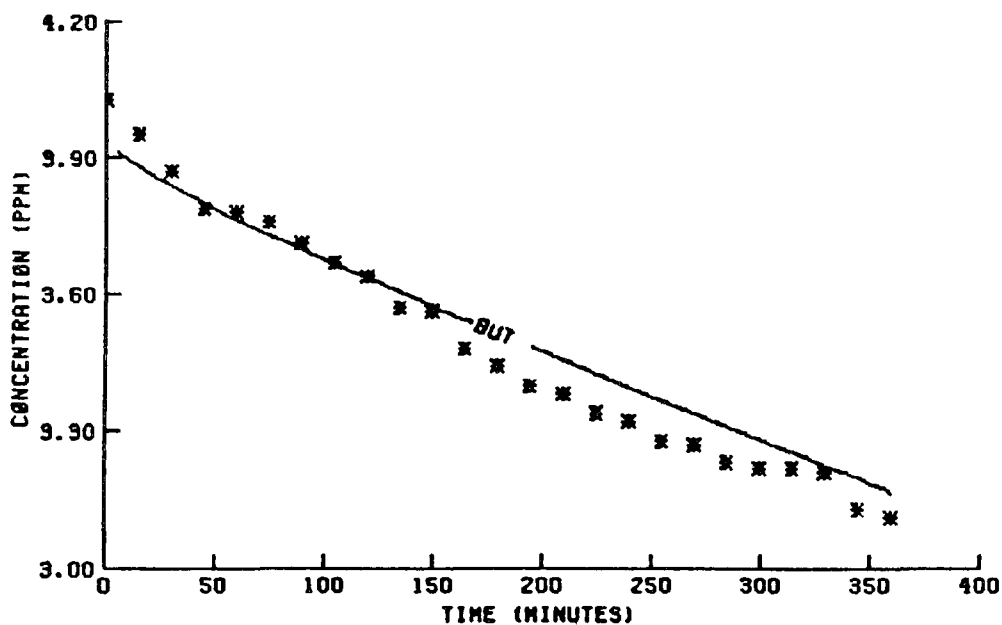
EC-41

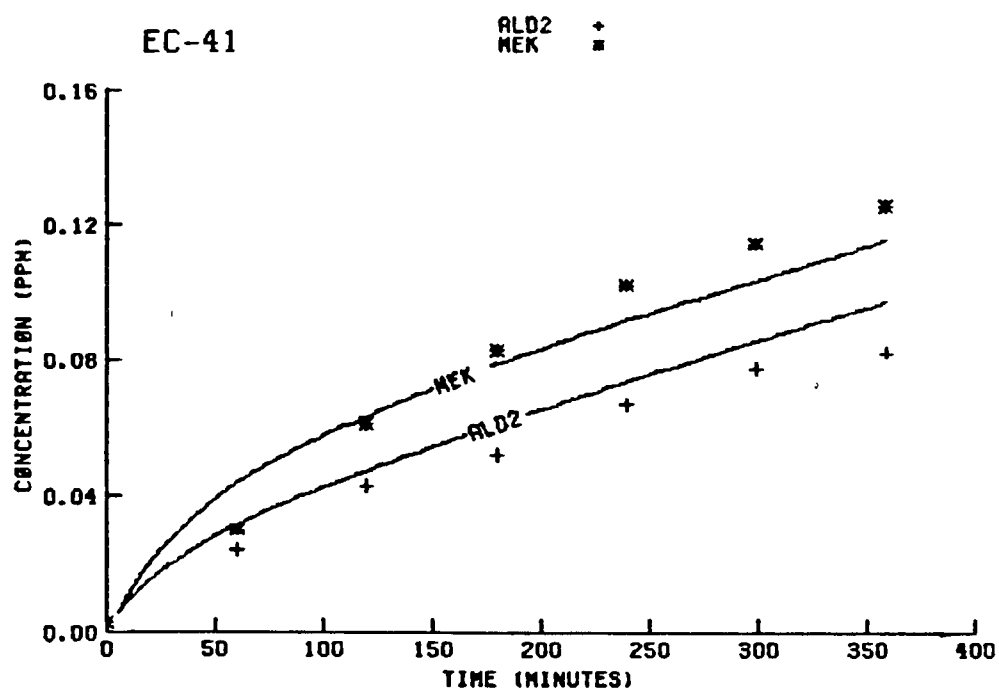
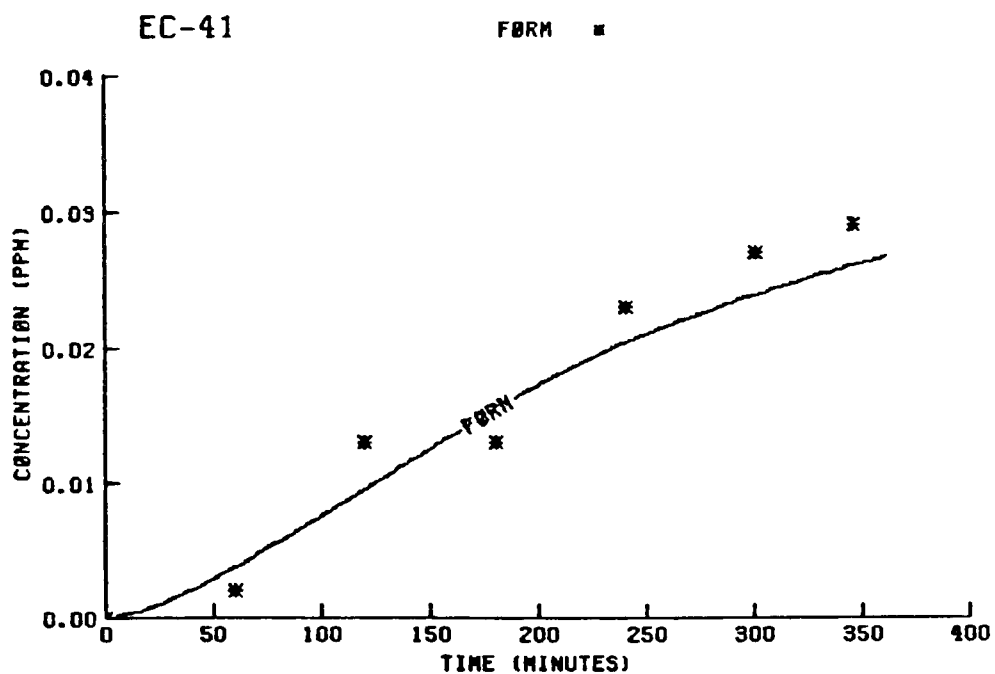
PAN ■

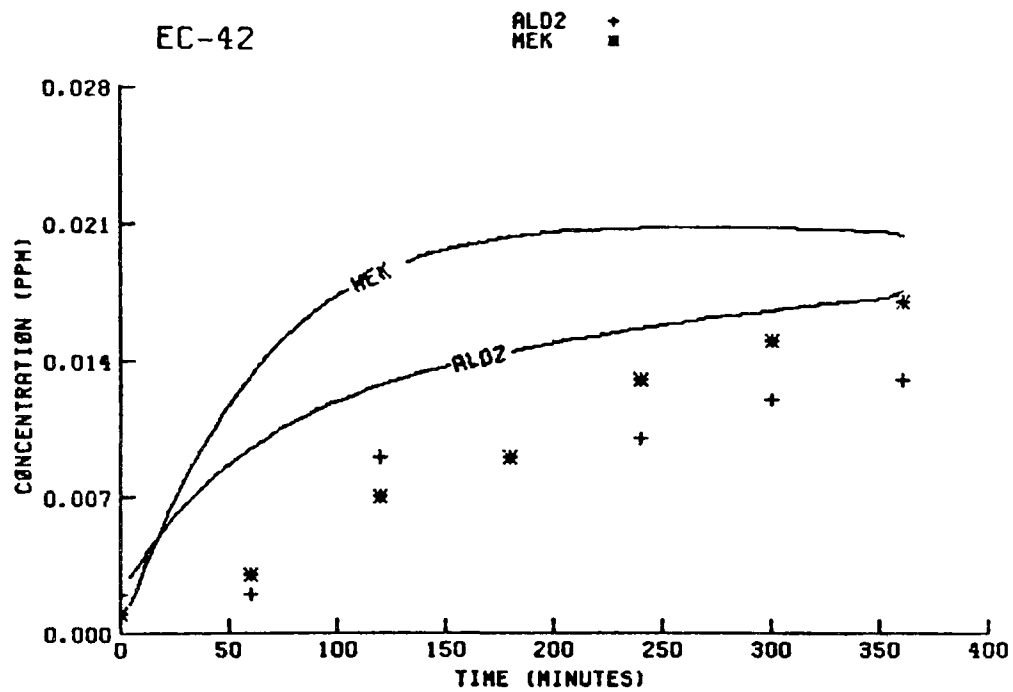


EC-41

BUT ■

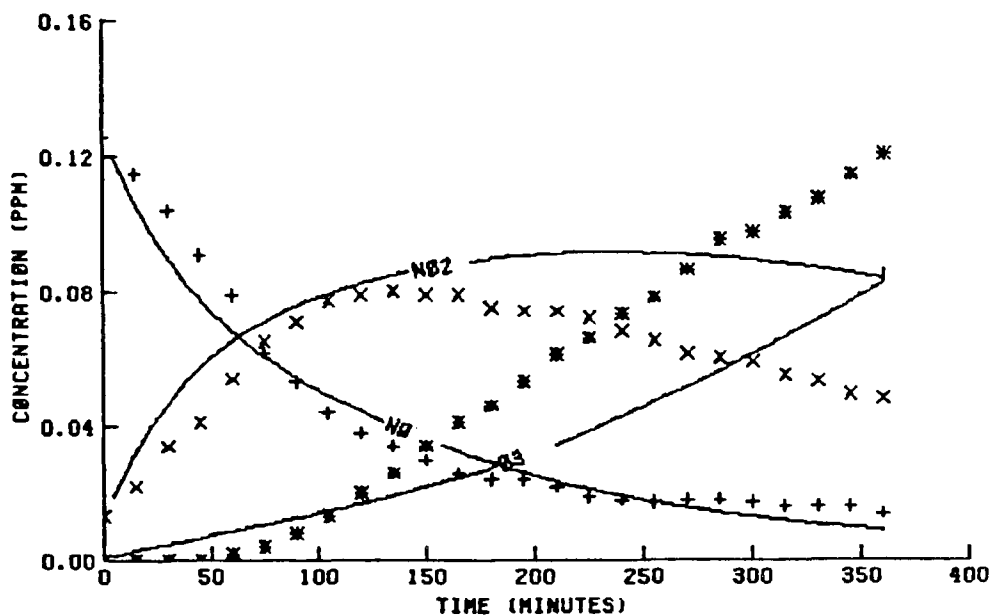






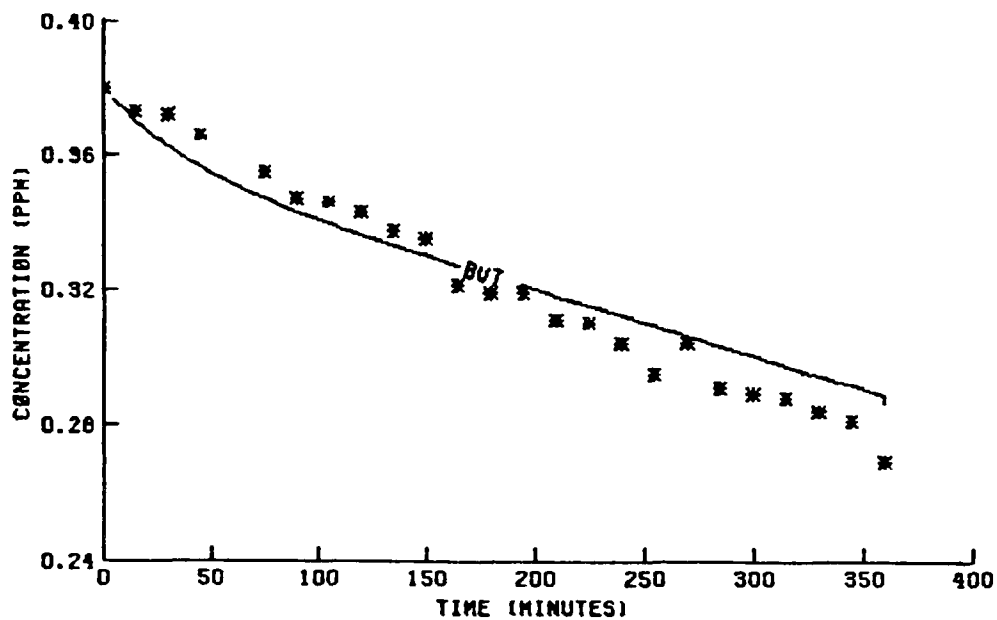
EC-43

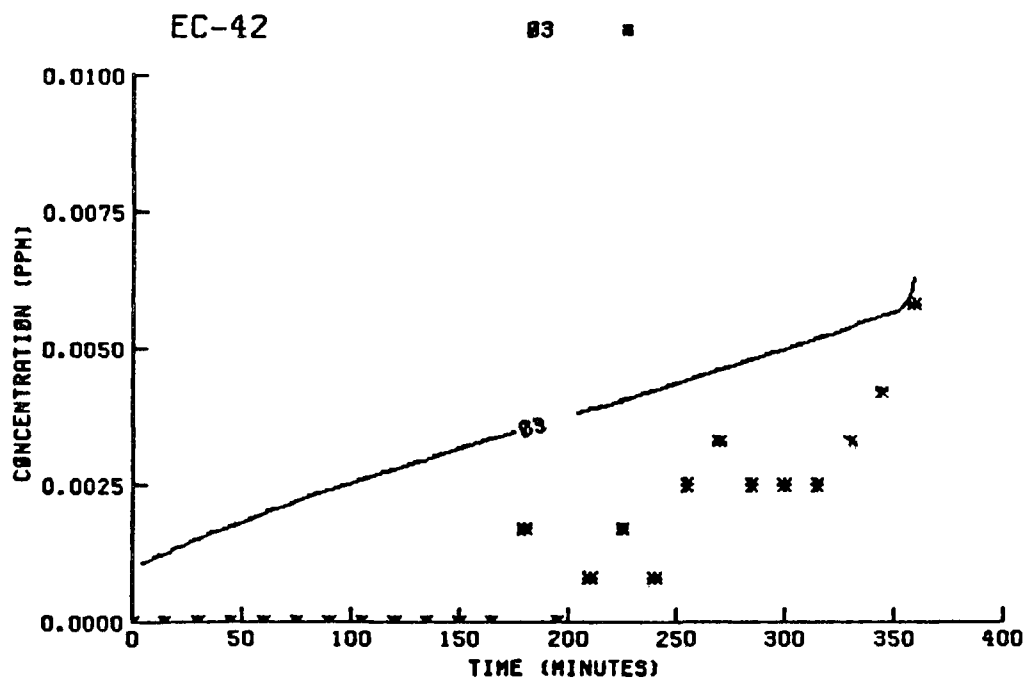
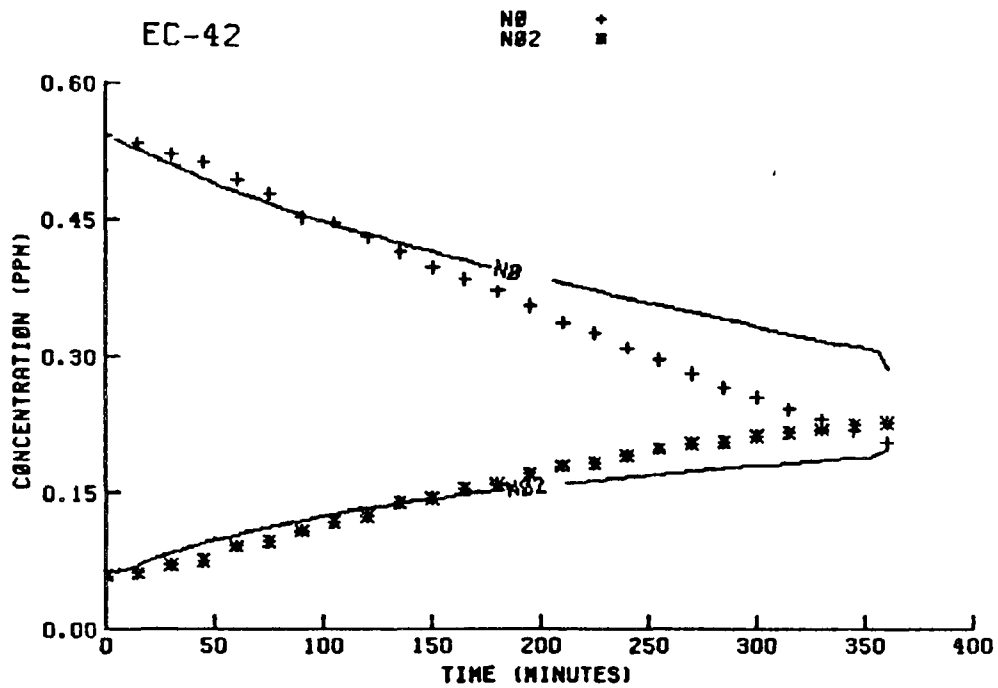
NO2 x
NO +
O3 ■

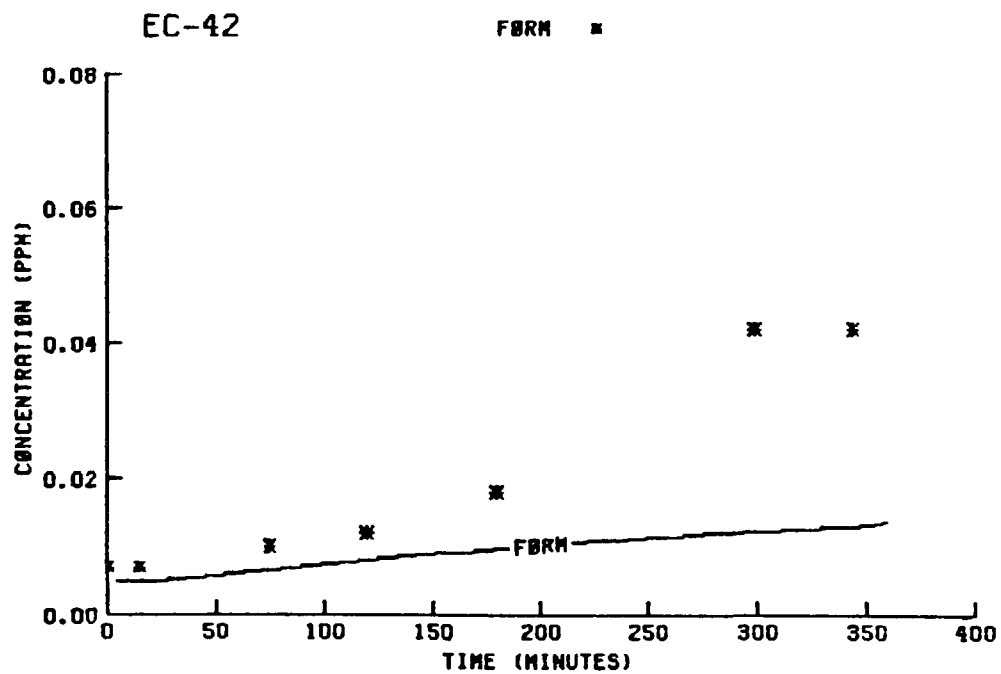
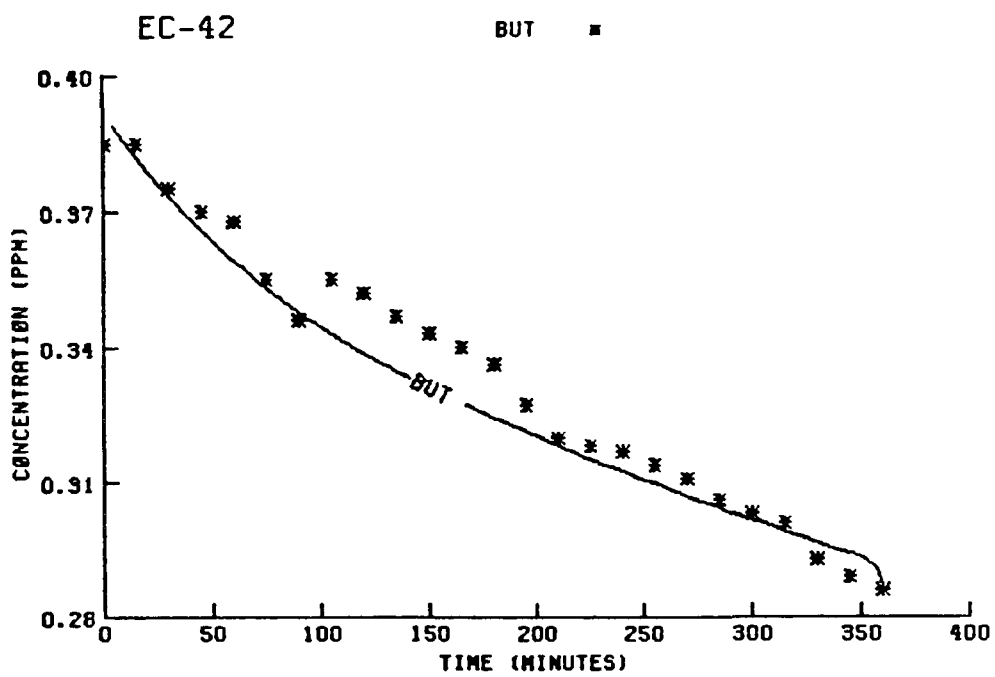


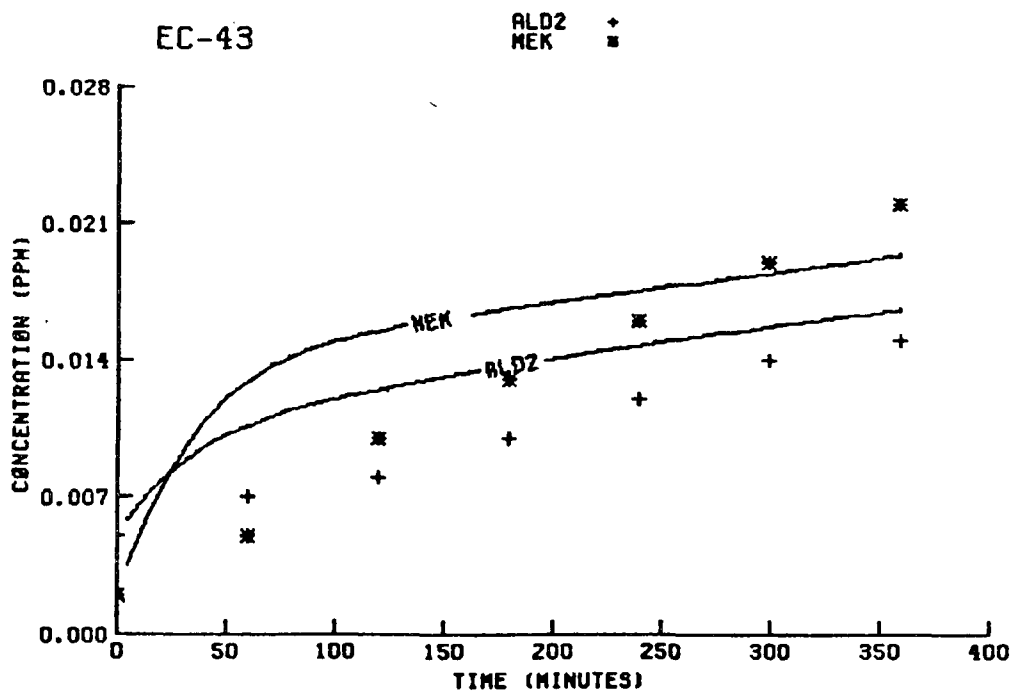
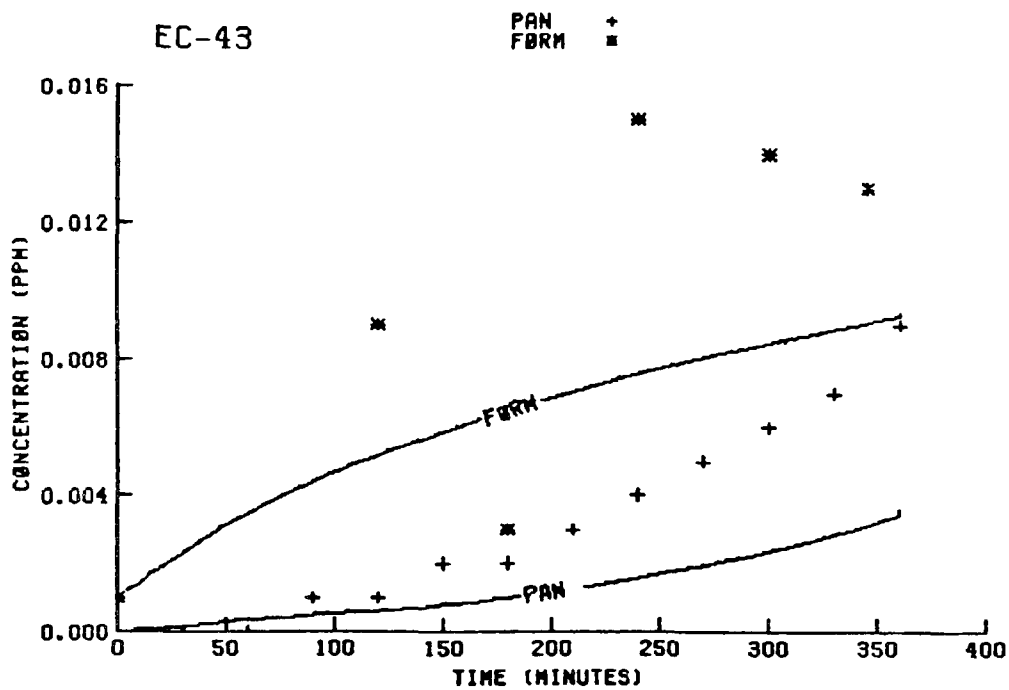
EC-43

BUT ■



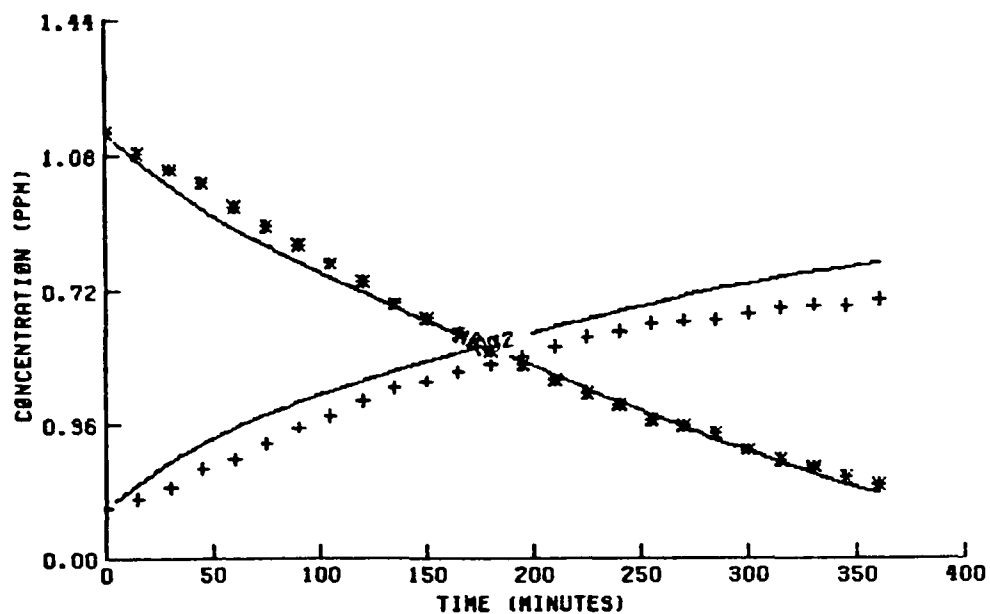






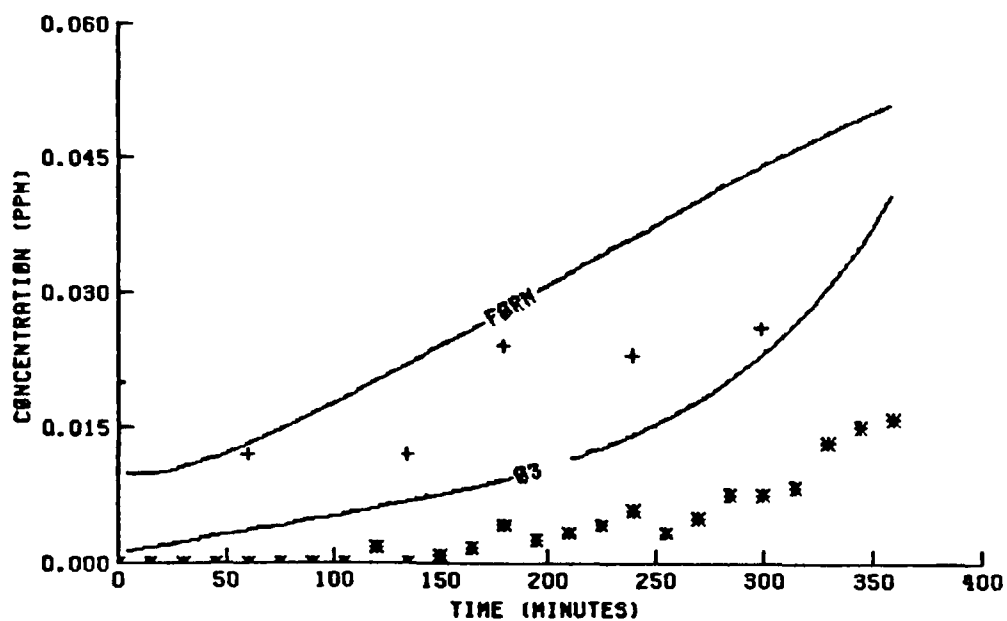
EC-44

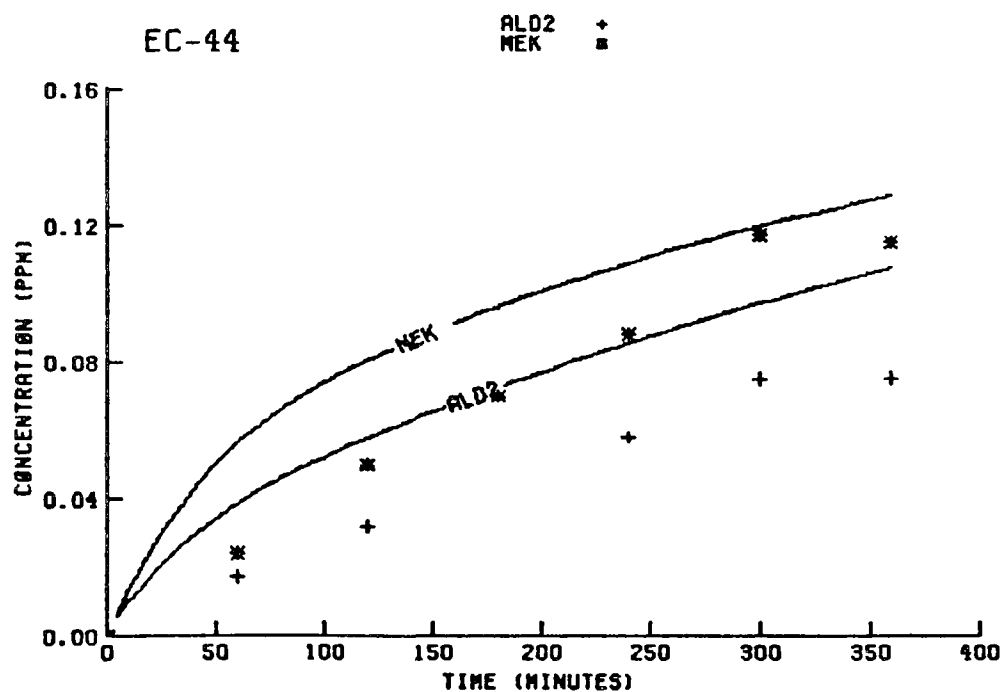
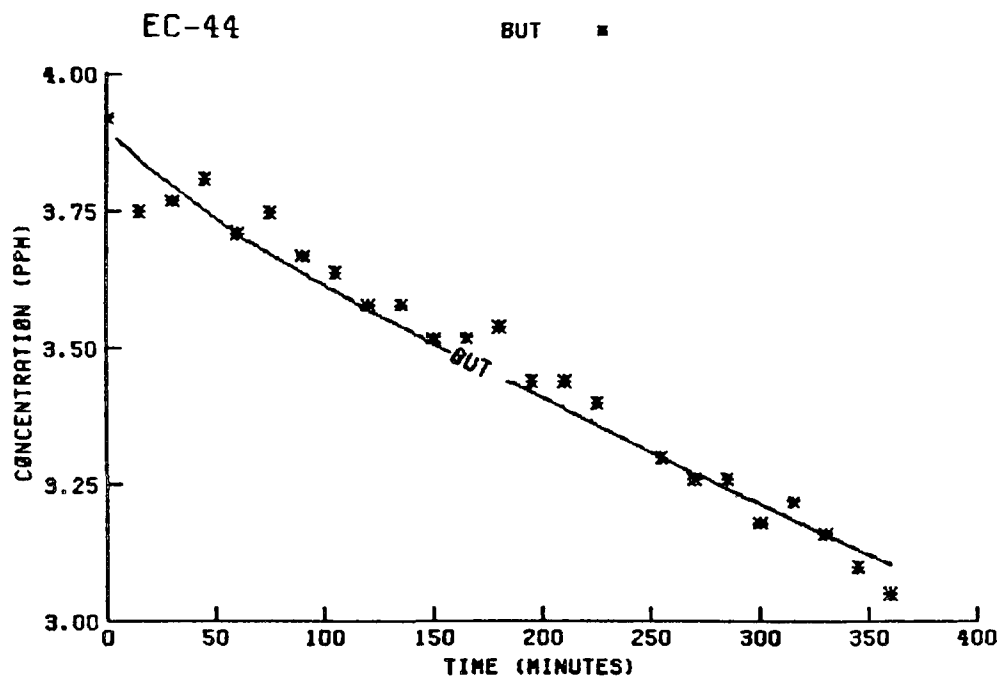
N02 +
N0 *

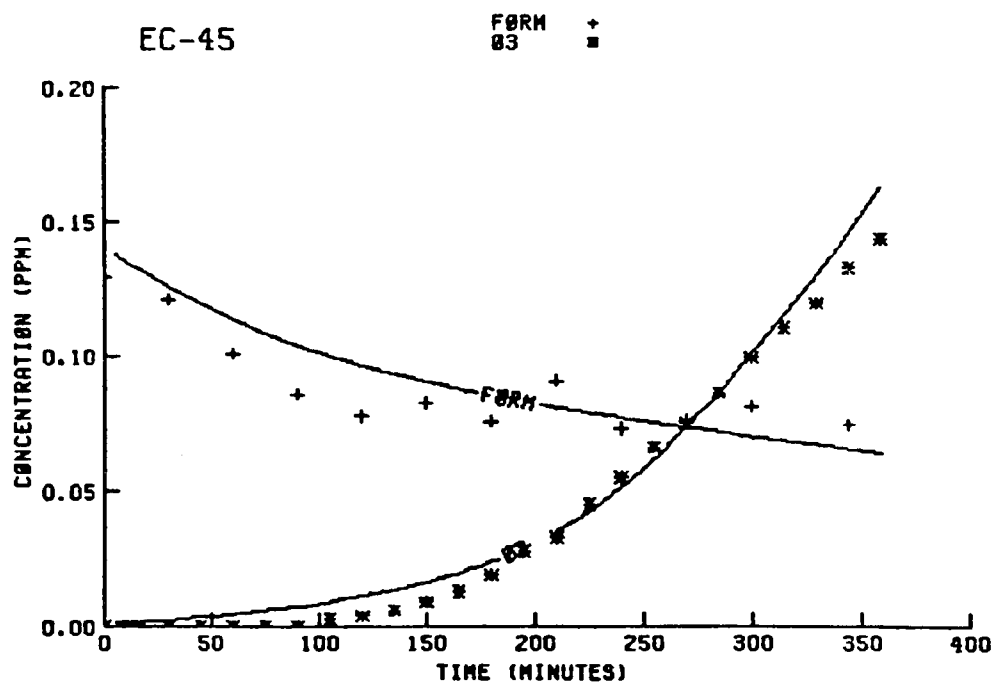
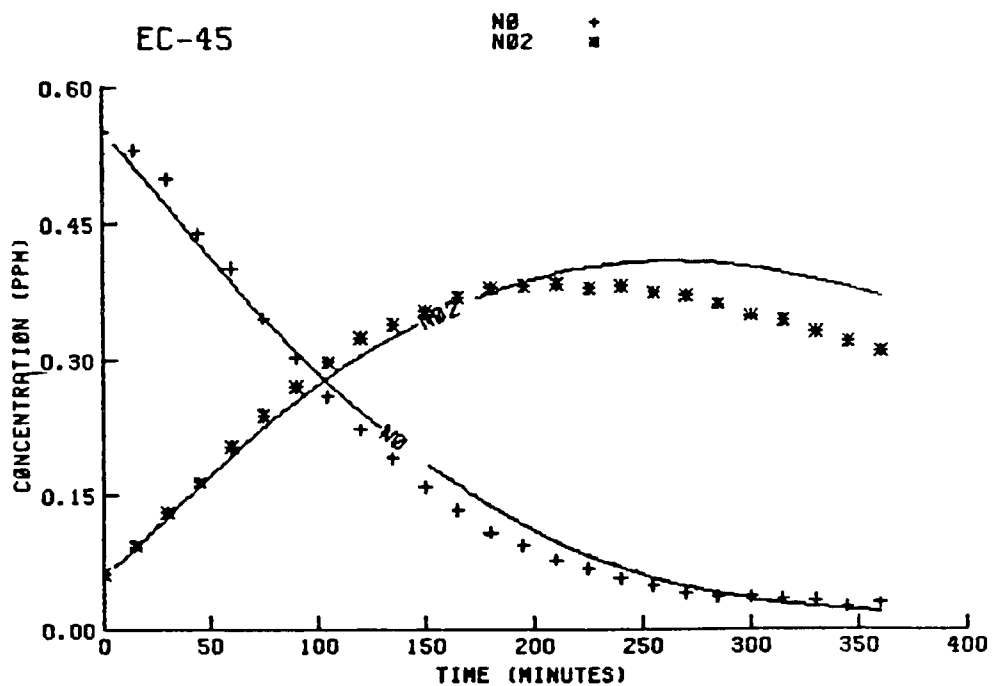


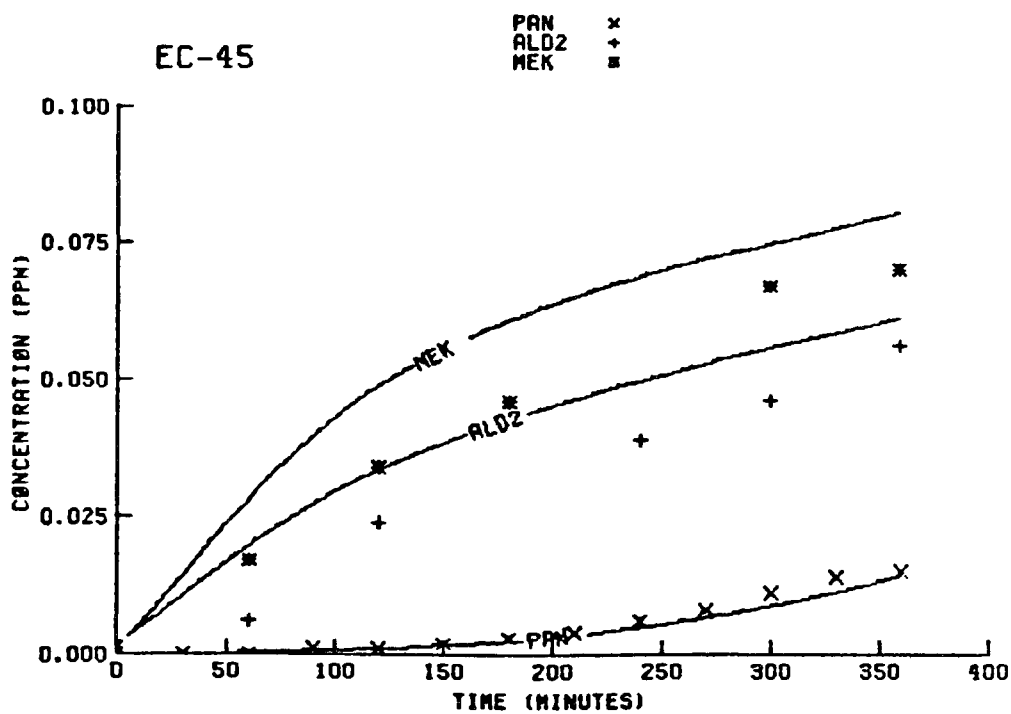
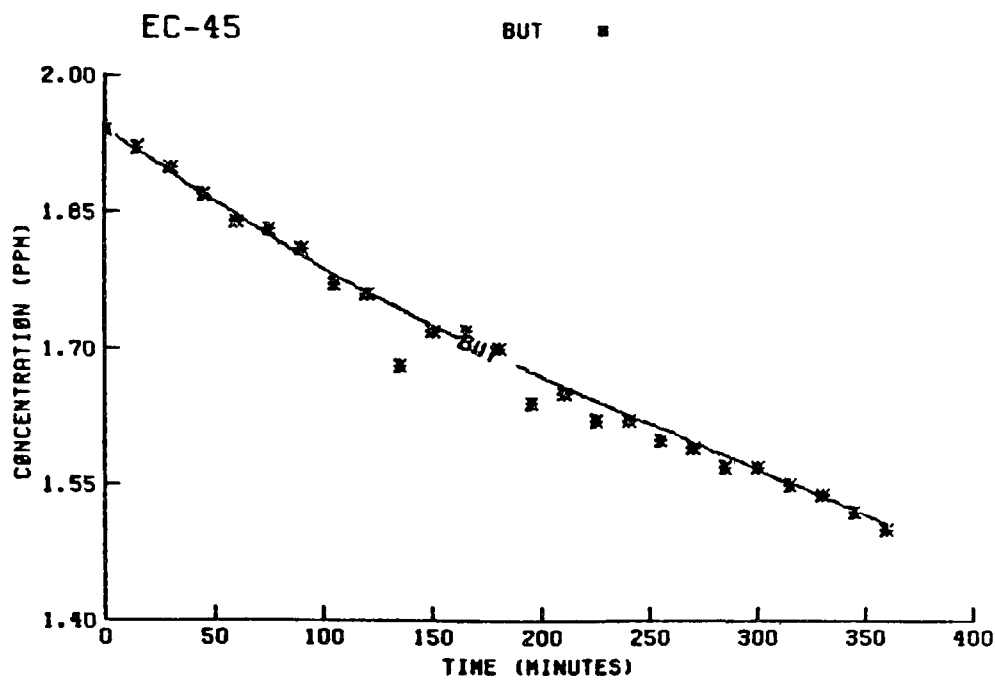
EC-44

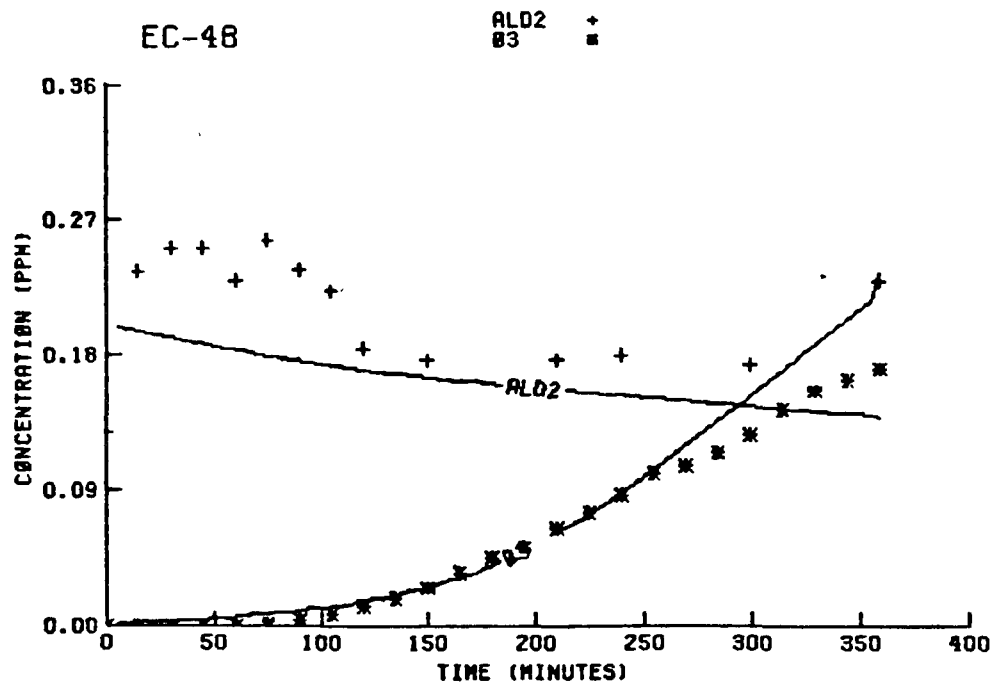
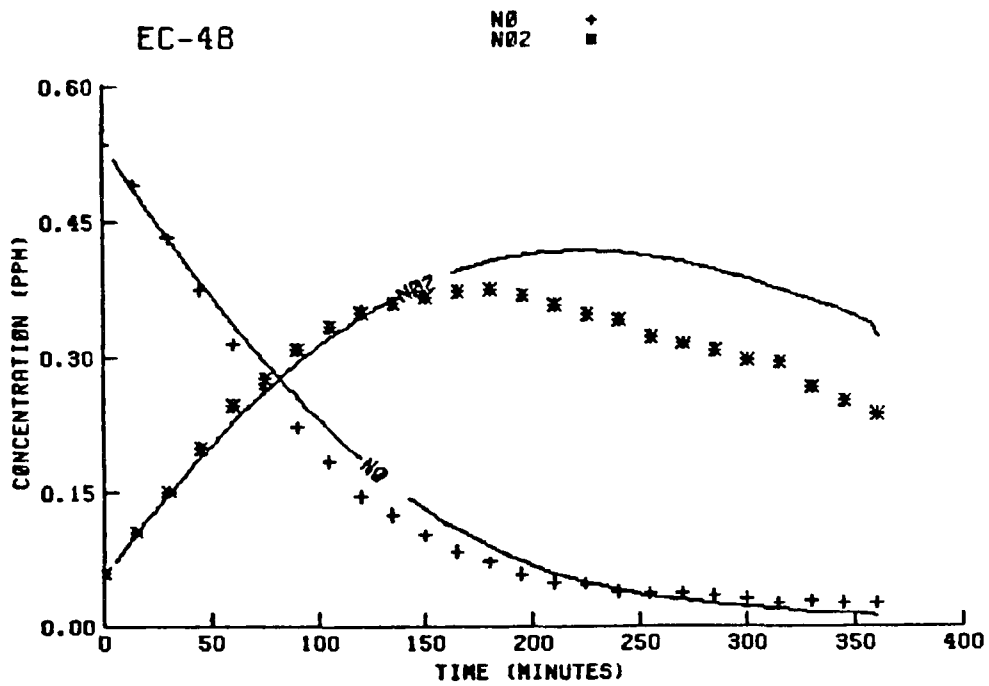
FORM +
03 *

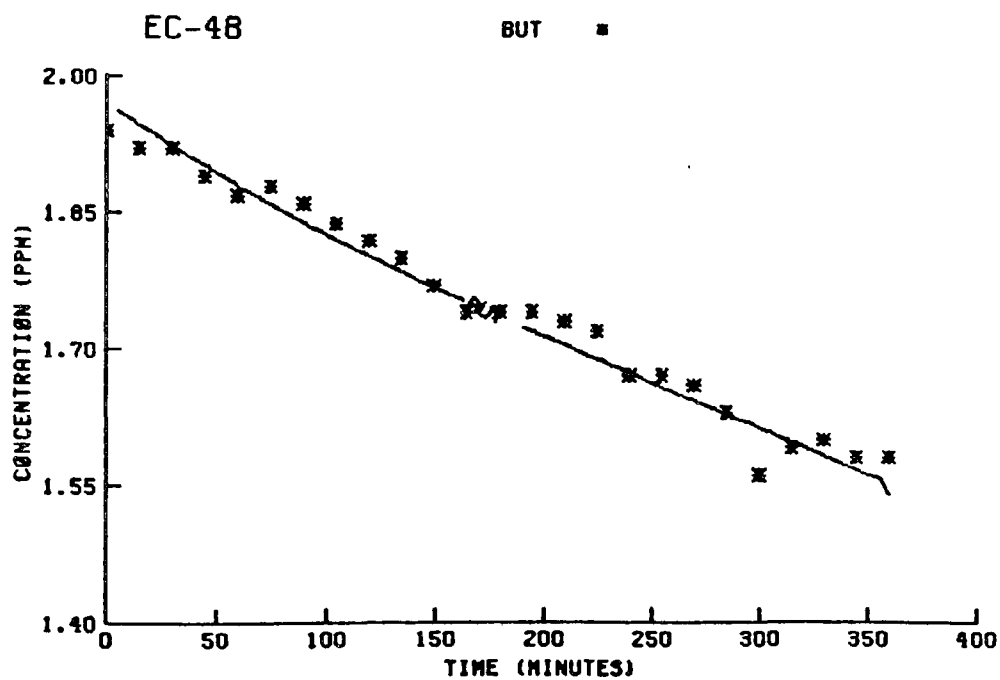
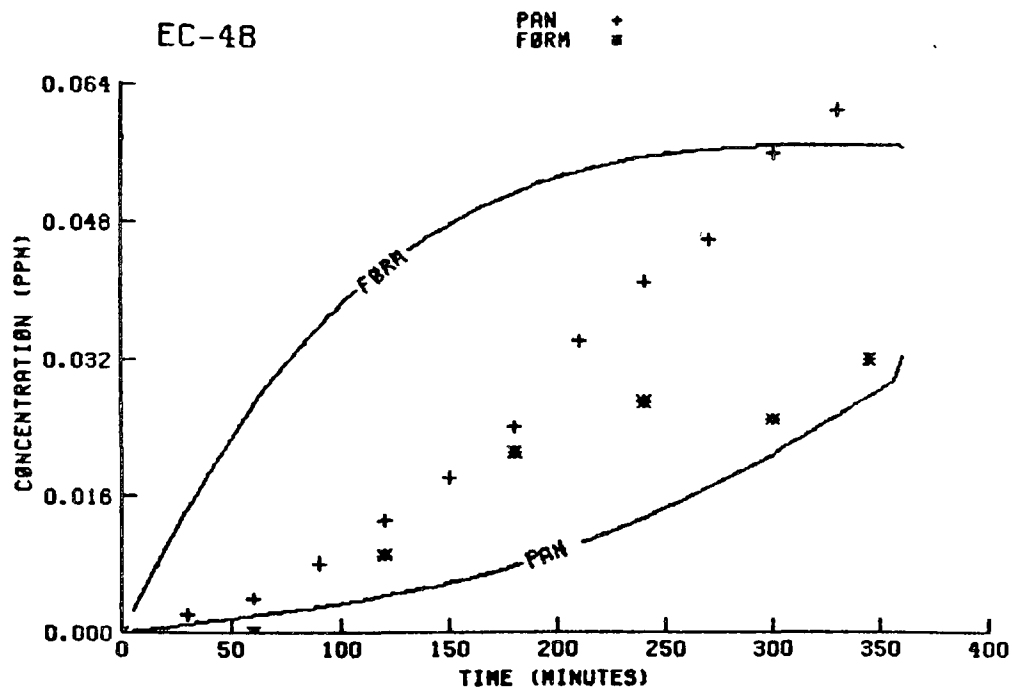






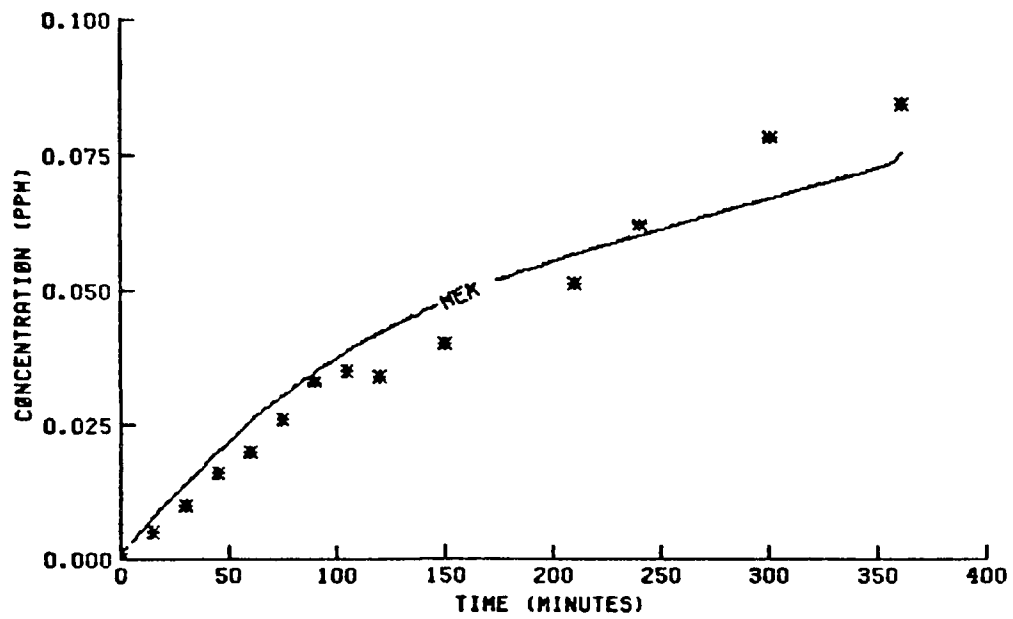






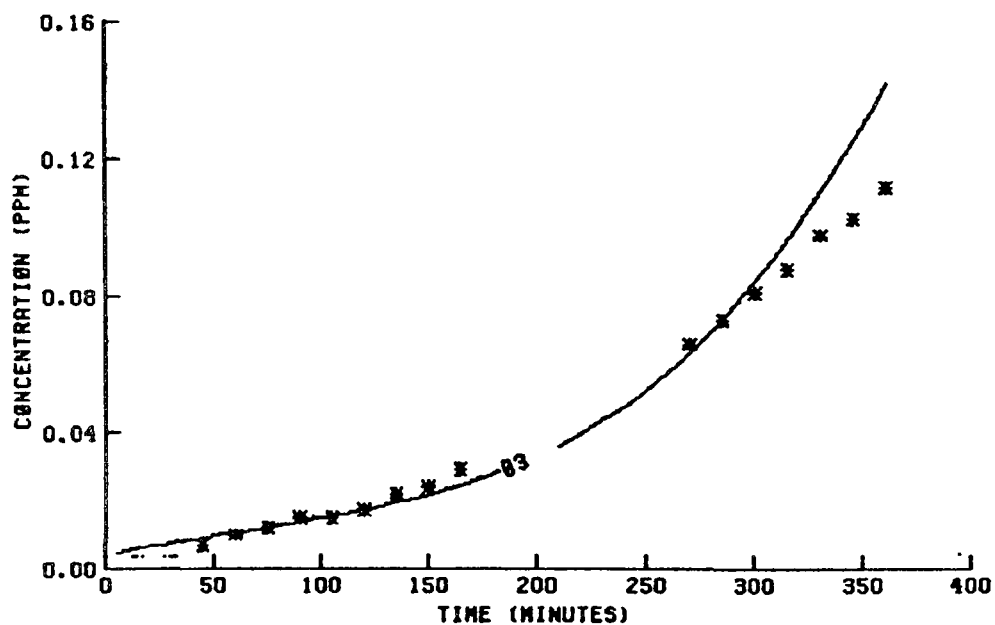
EC-48

MEK ■



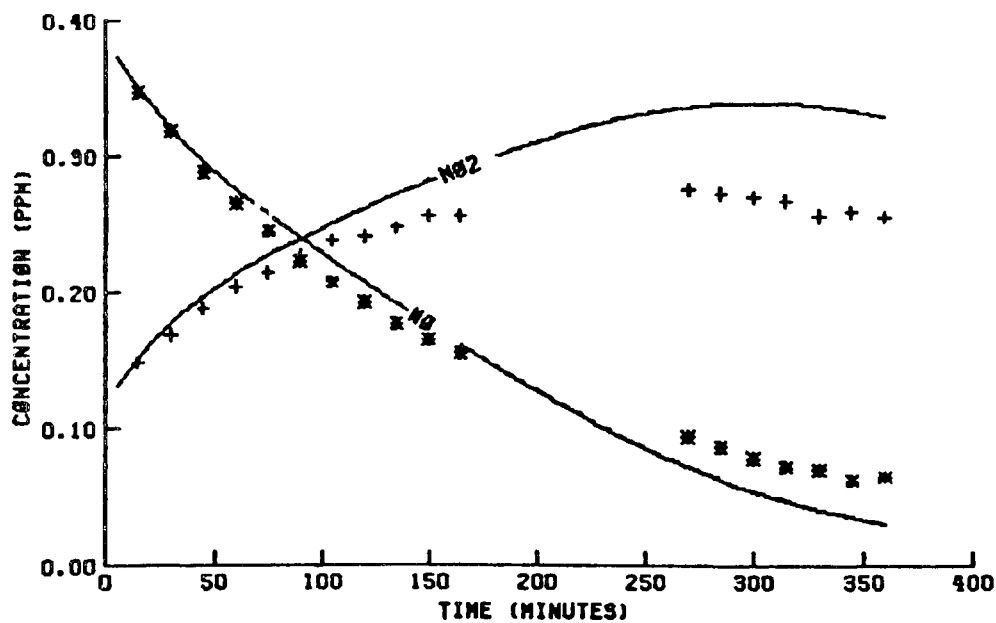
EC-162

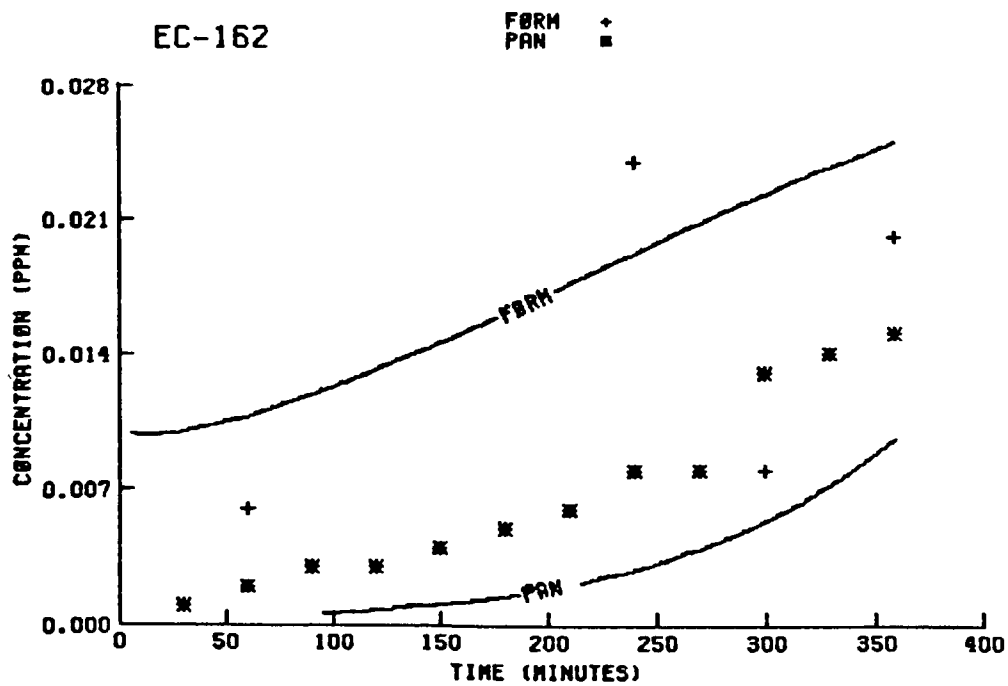
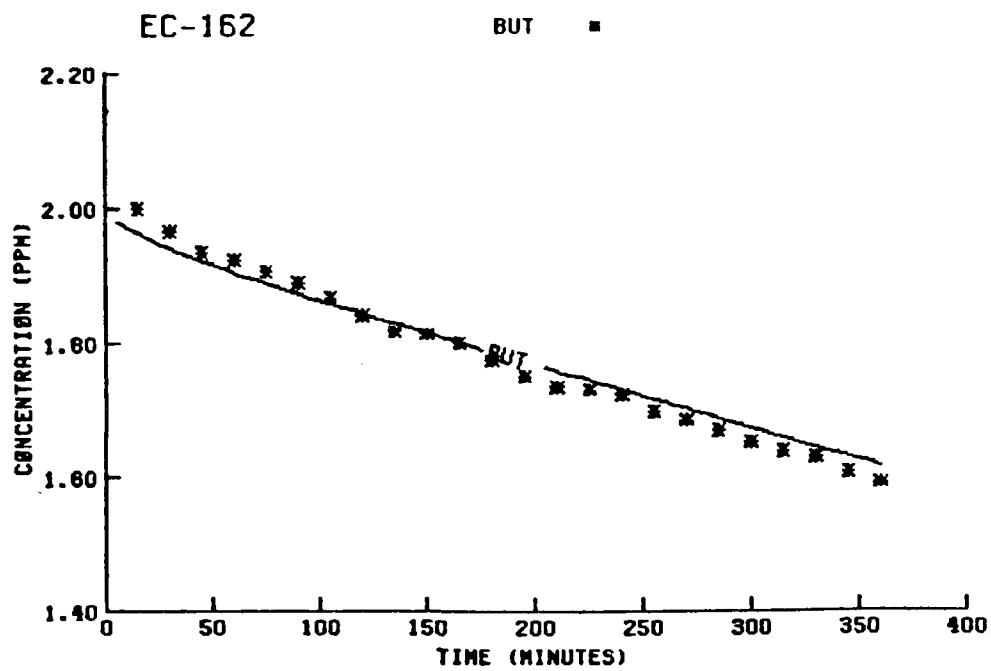
83 *

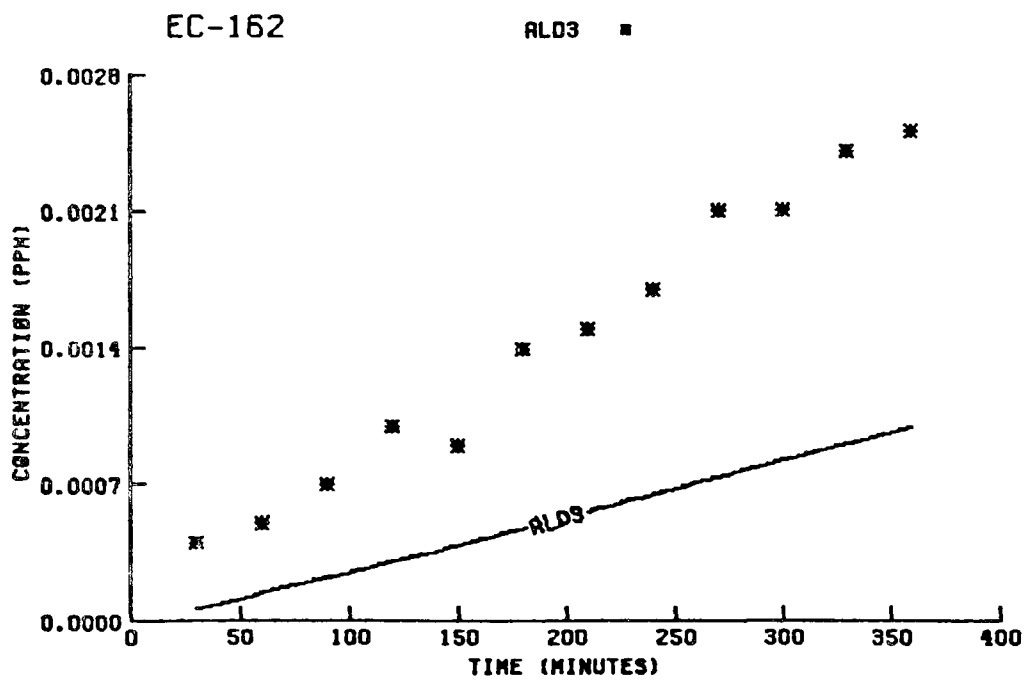
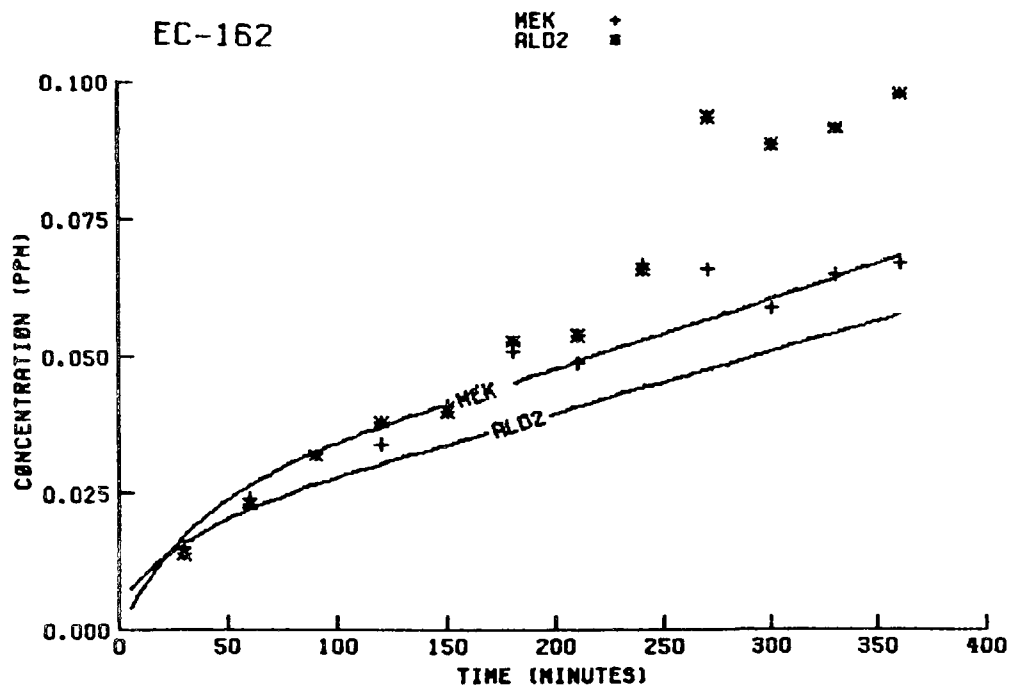


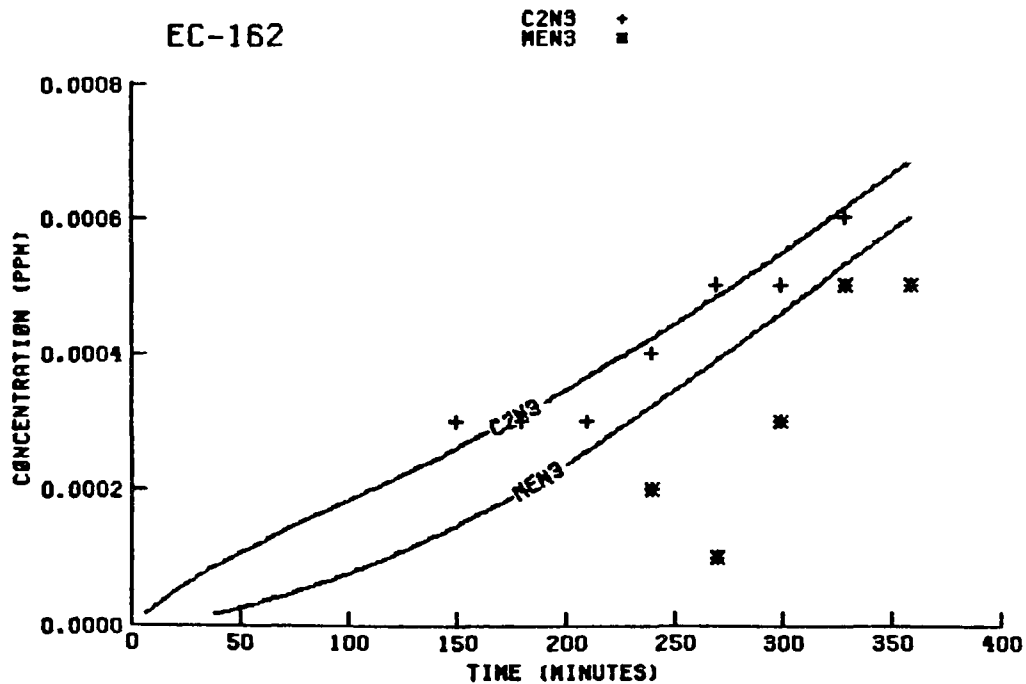
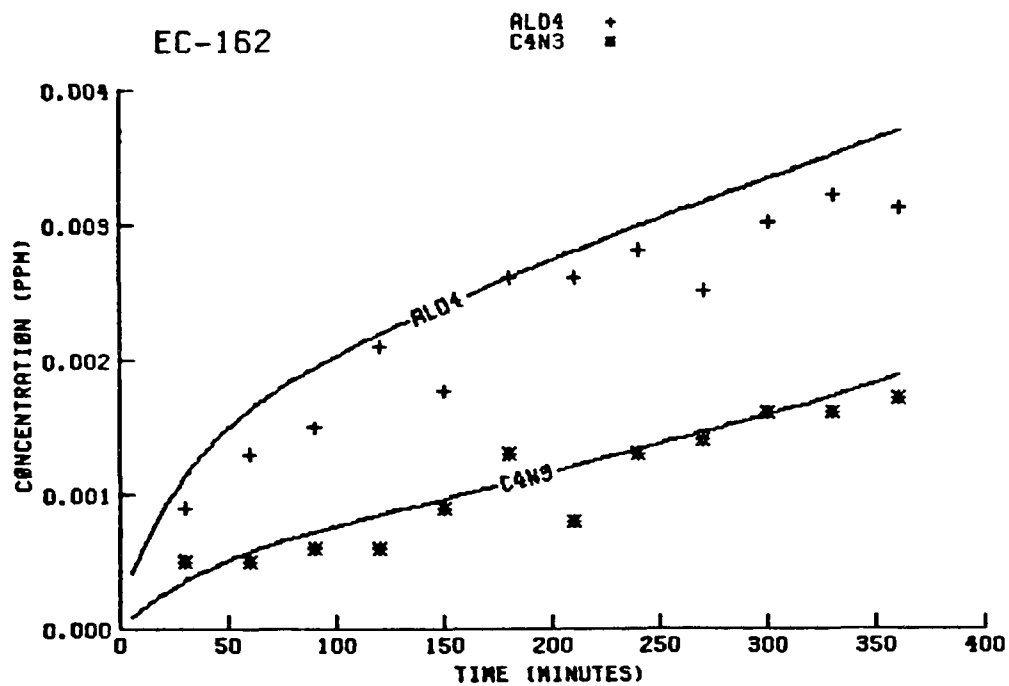
EC-162

N82 +
N8 *



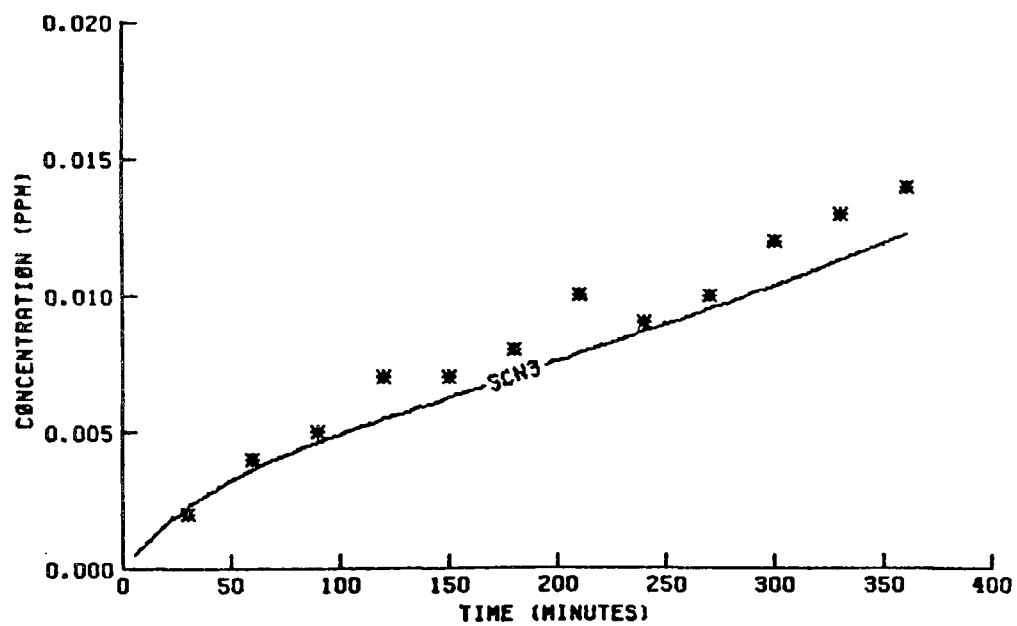






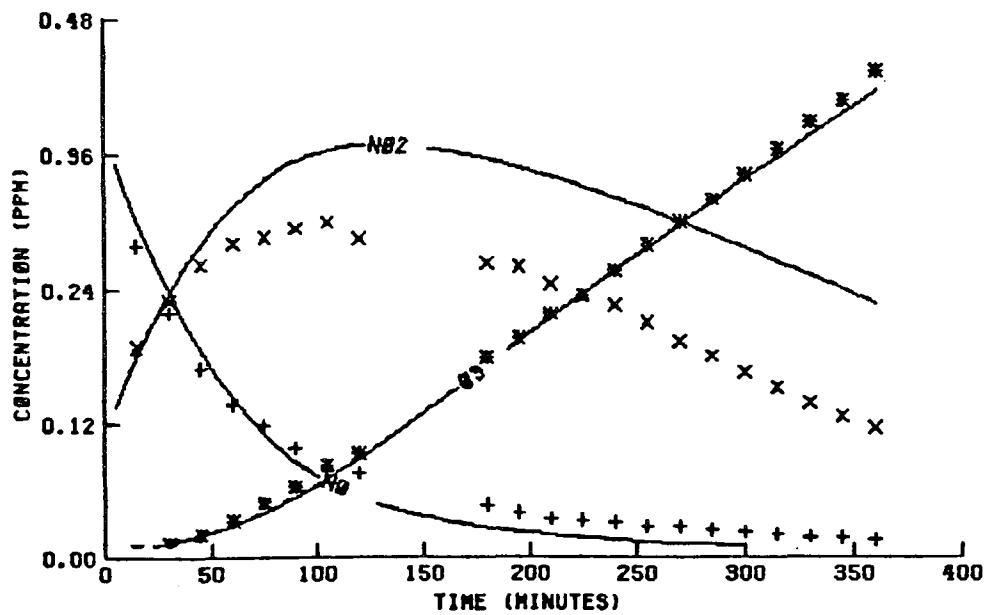
EC-162

SCN3 ■



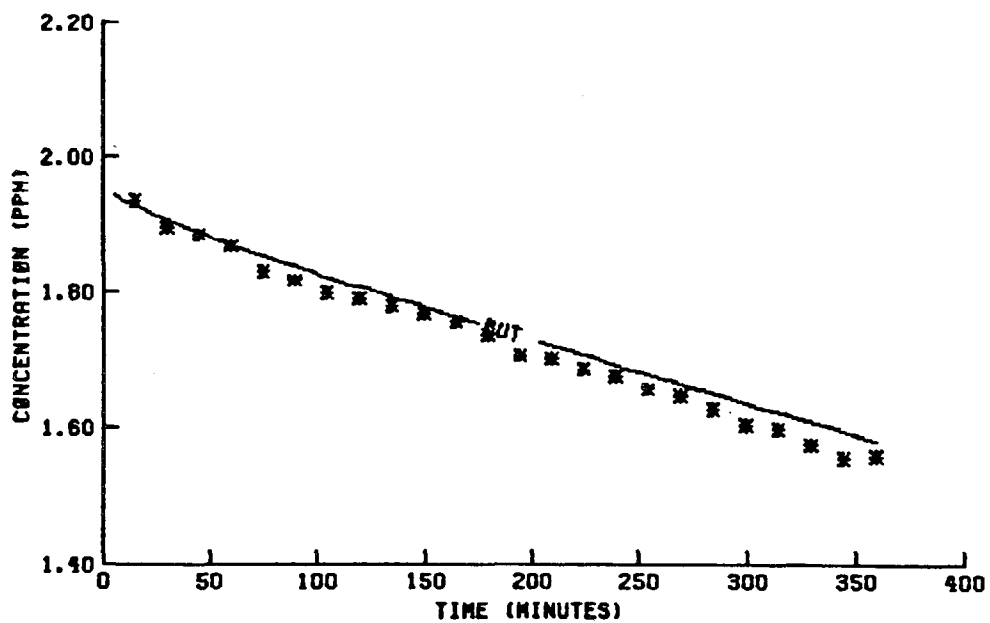
EC-163

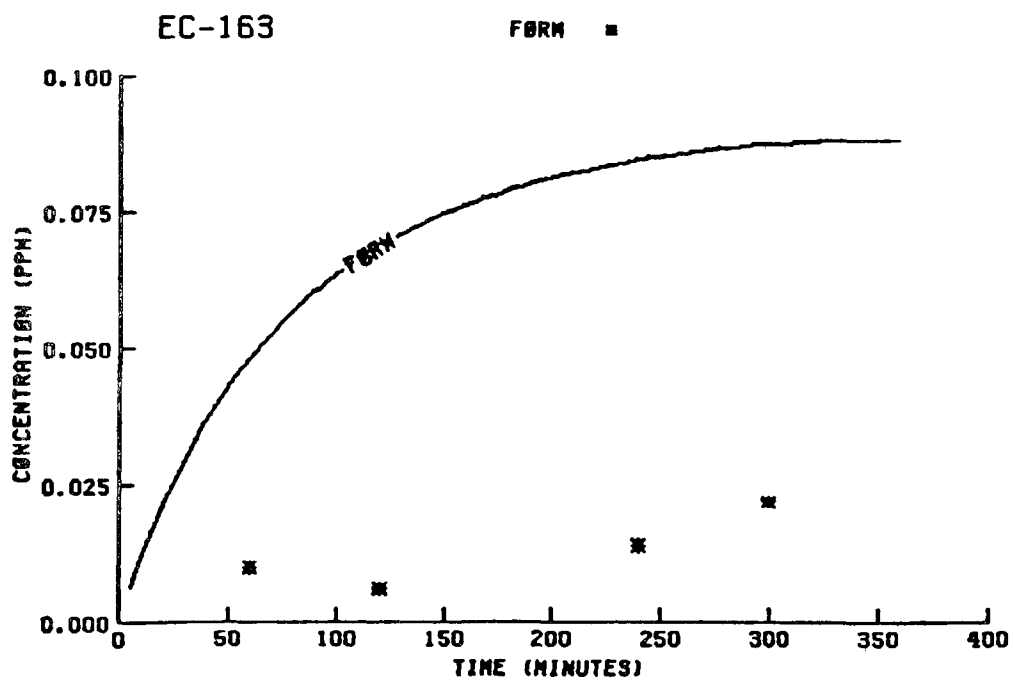
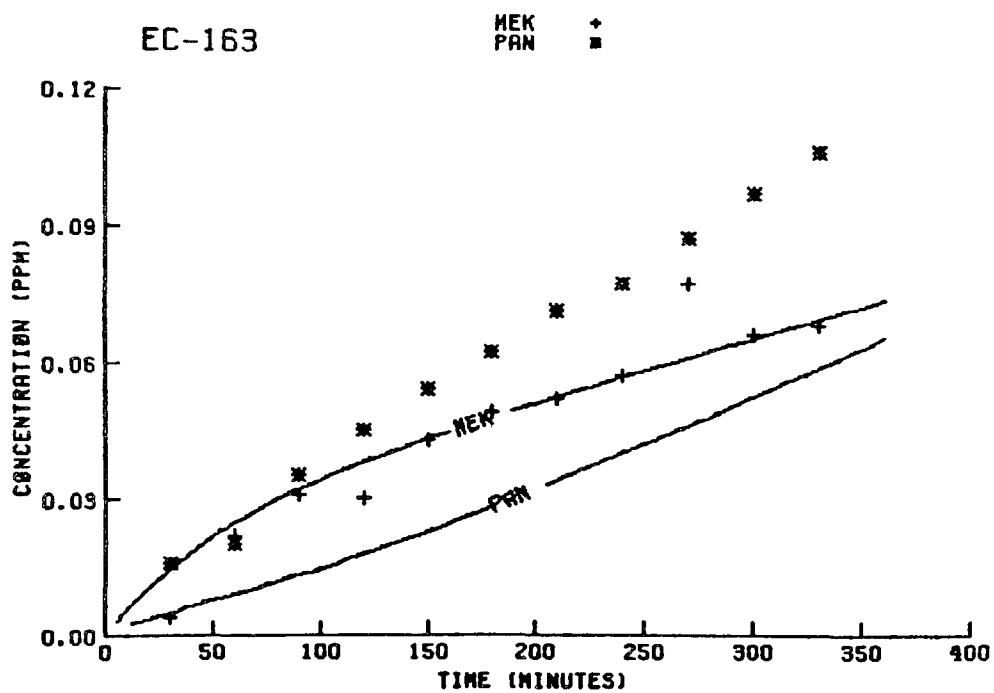
NO₂ x
NO +
O₃ ■

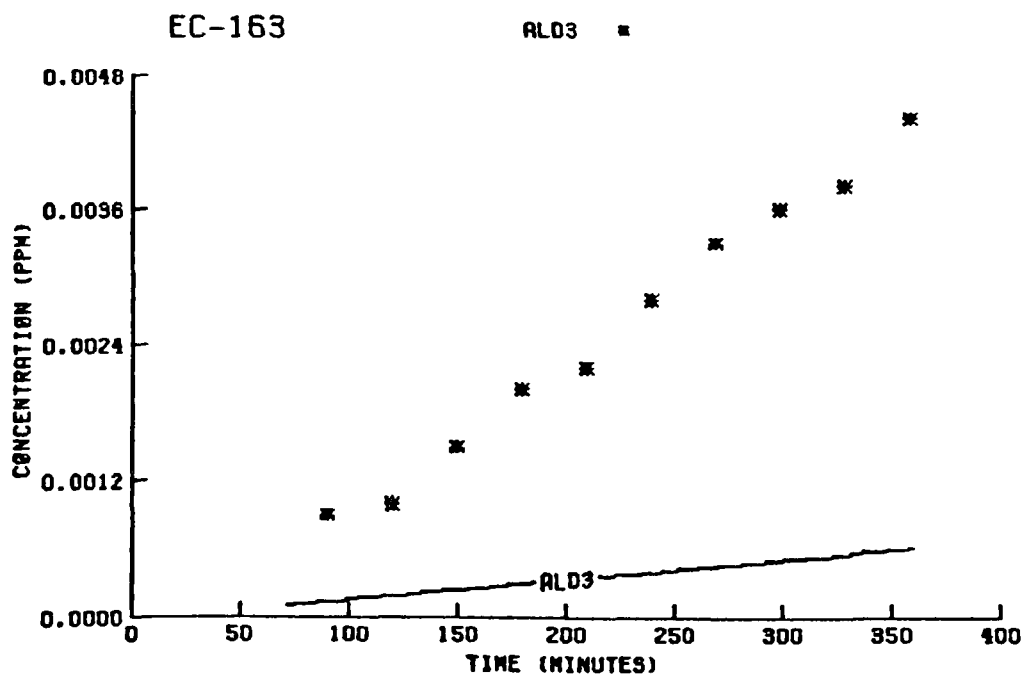
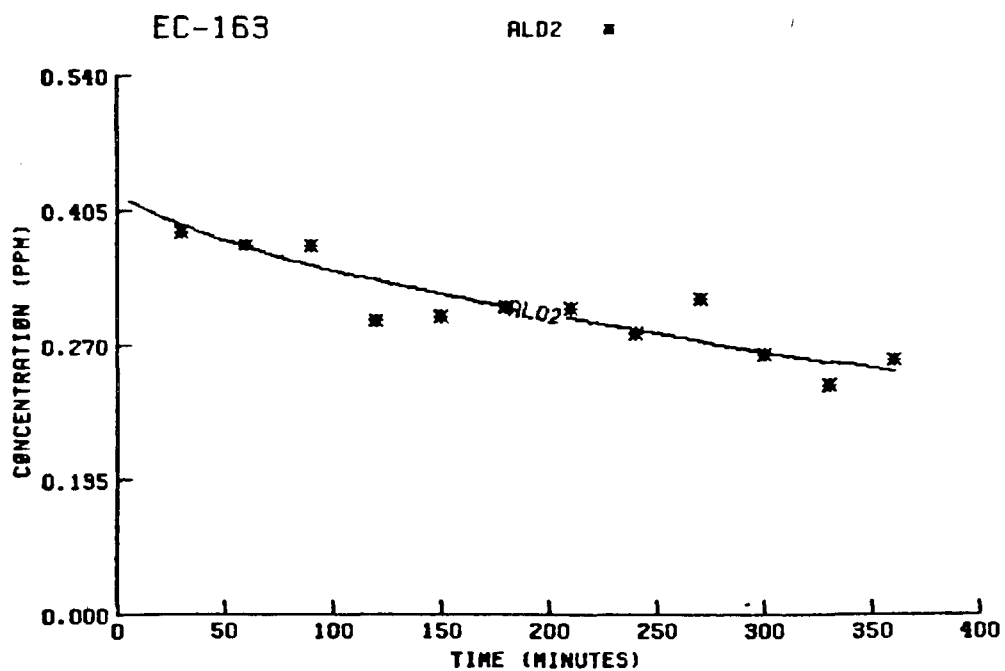


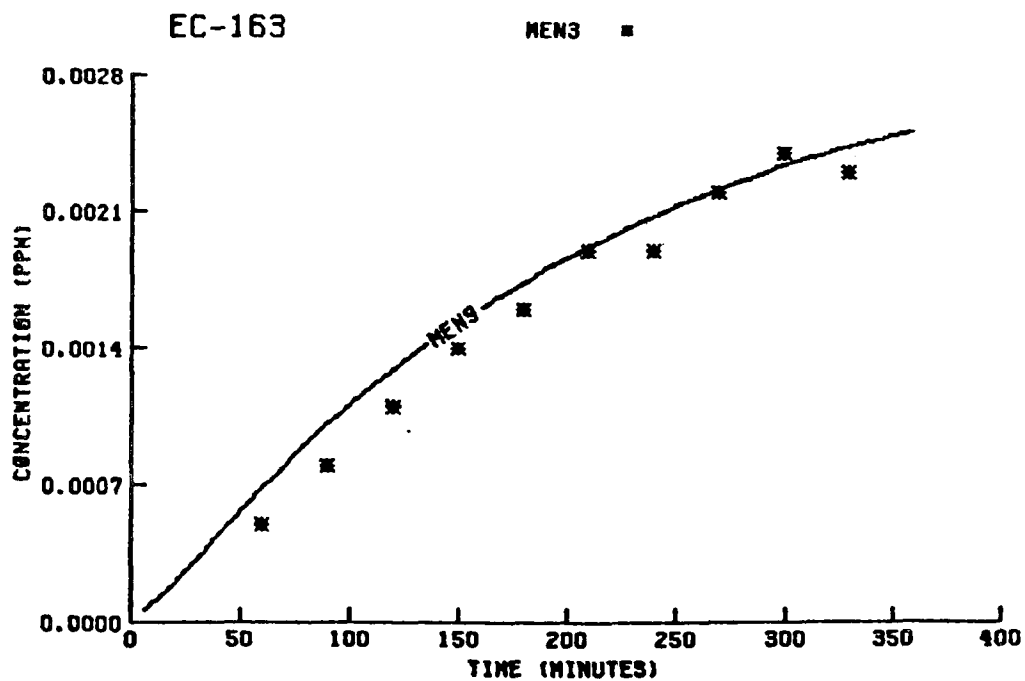
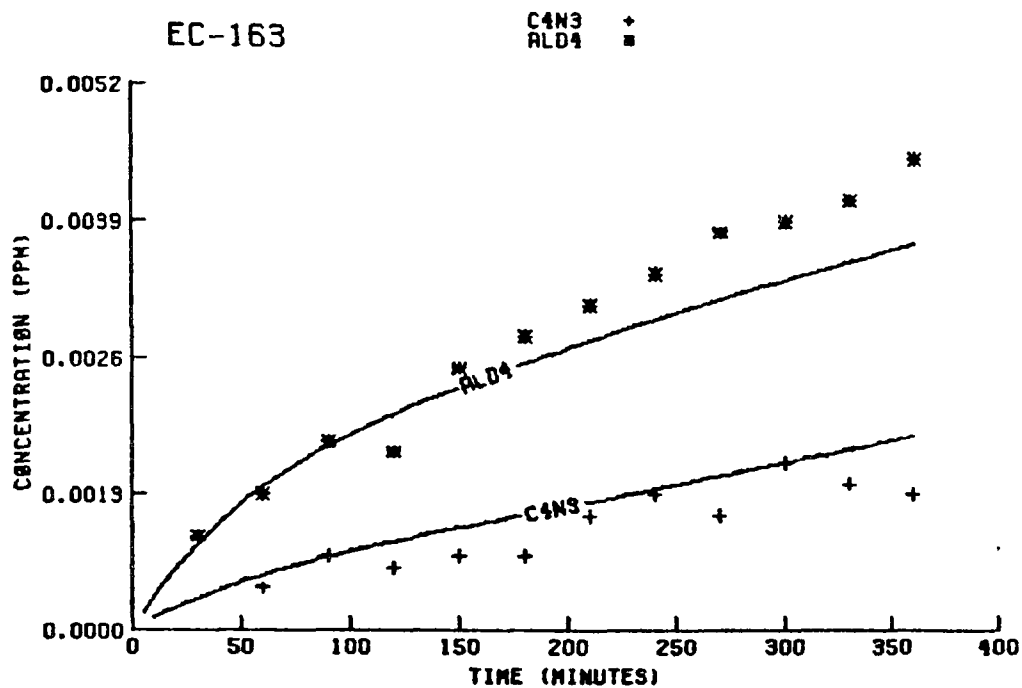
EC-163

BUT ■



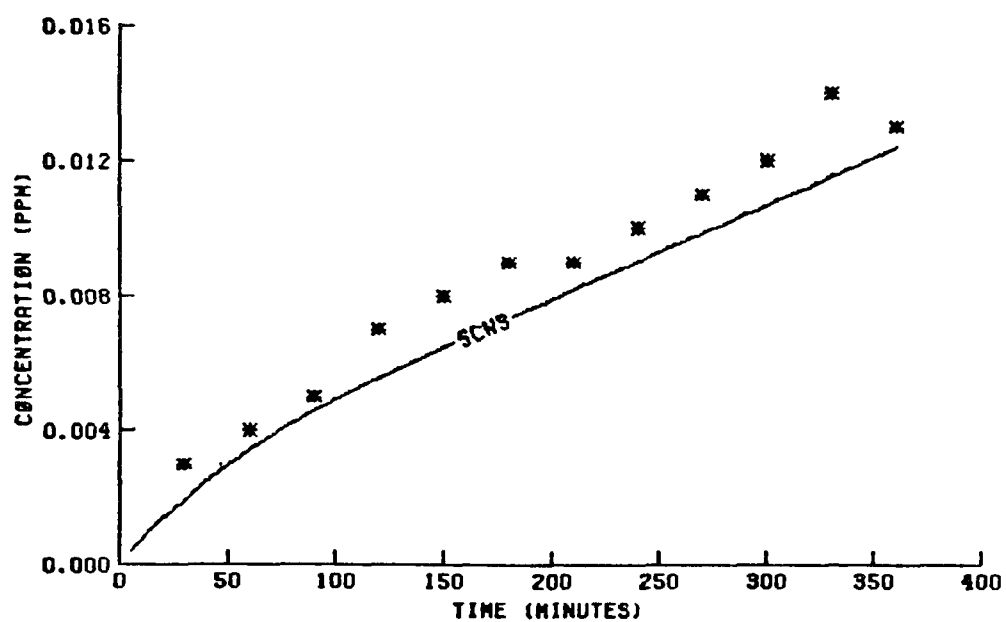






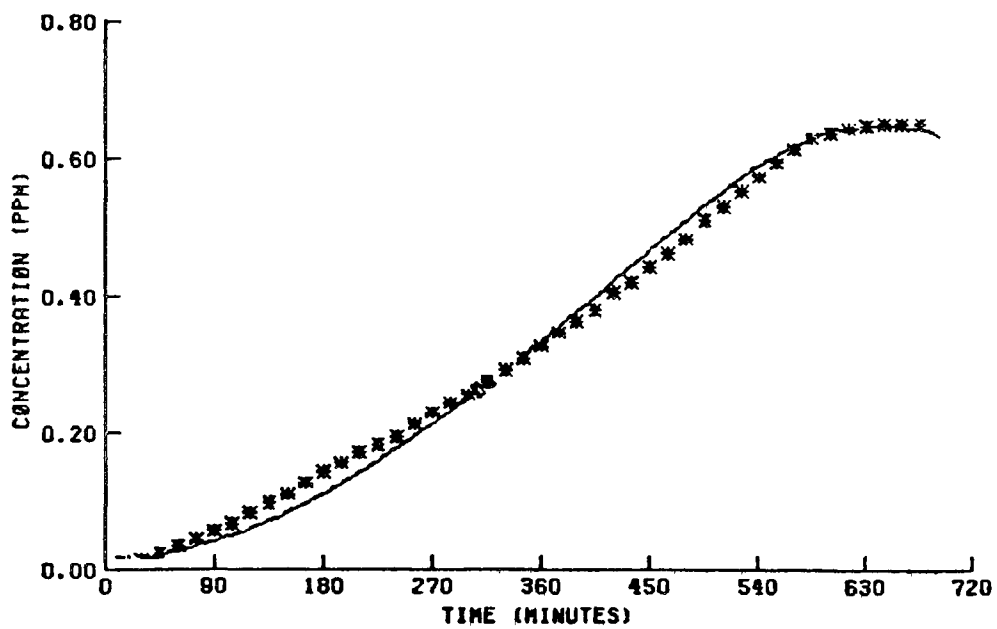
EC-163

SCN3 ■



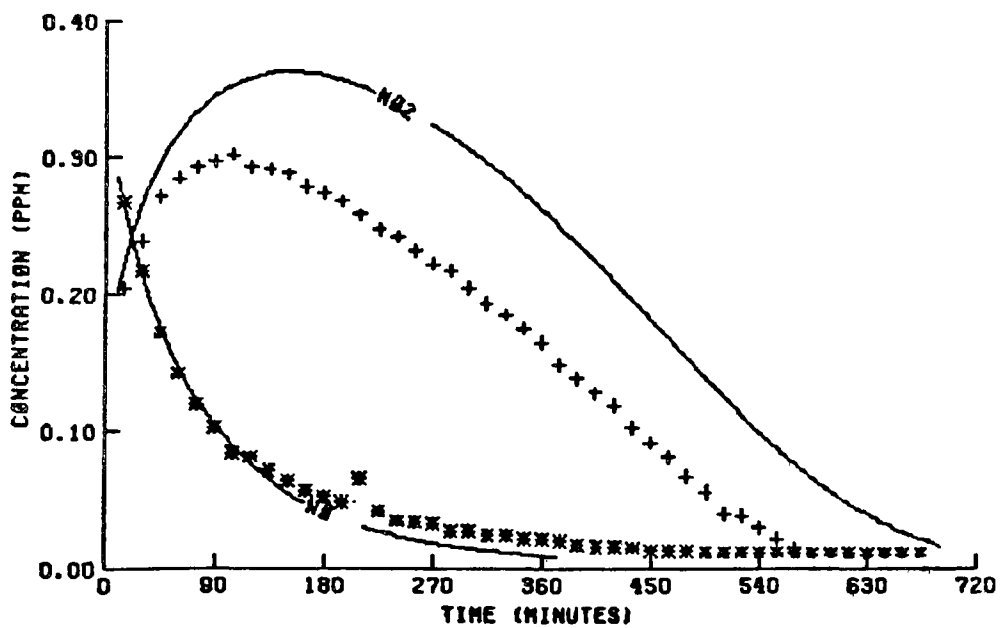
EC-168

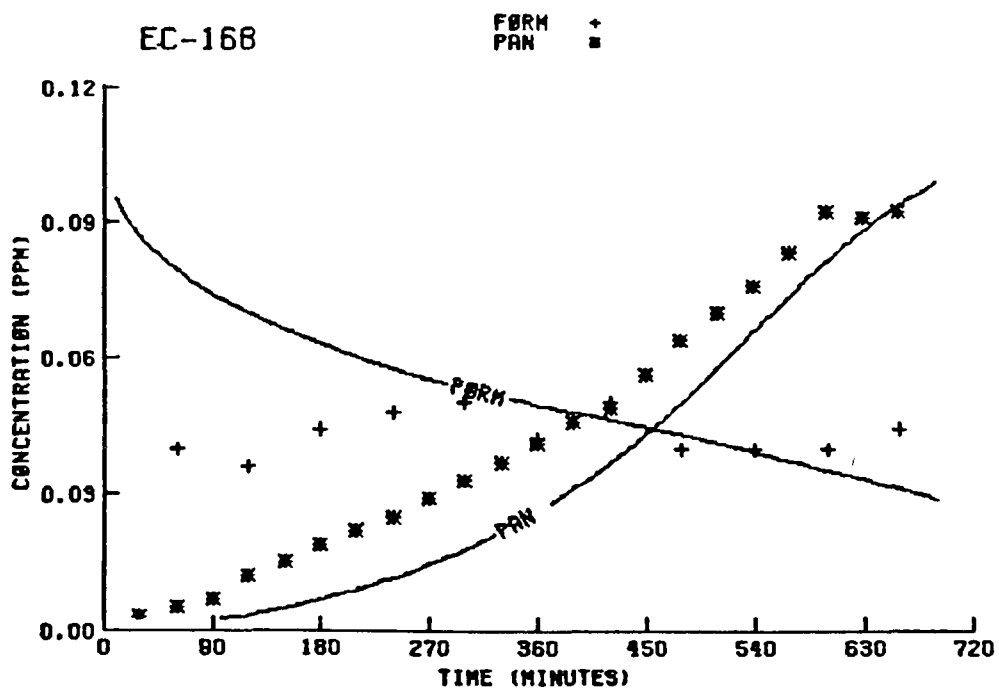
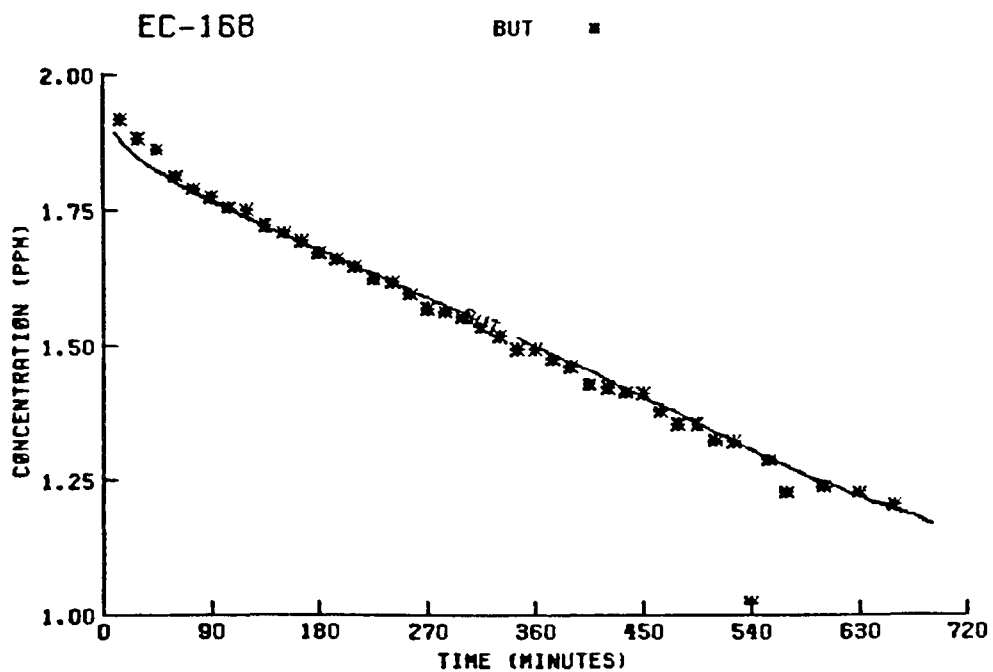
83 *

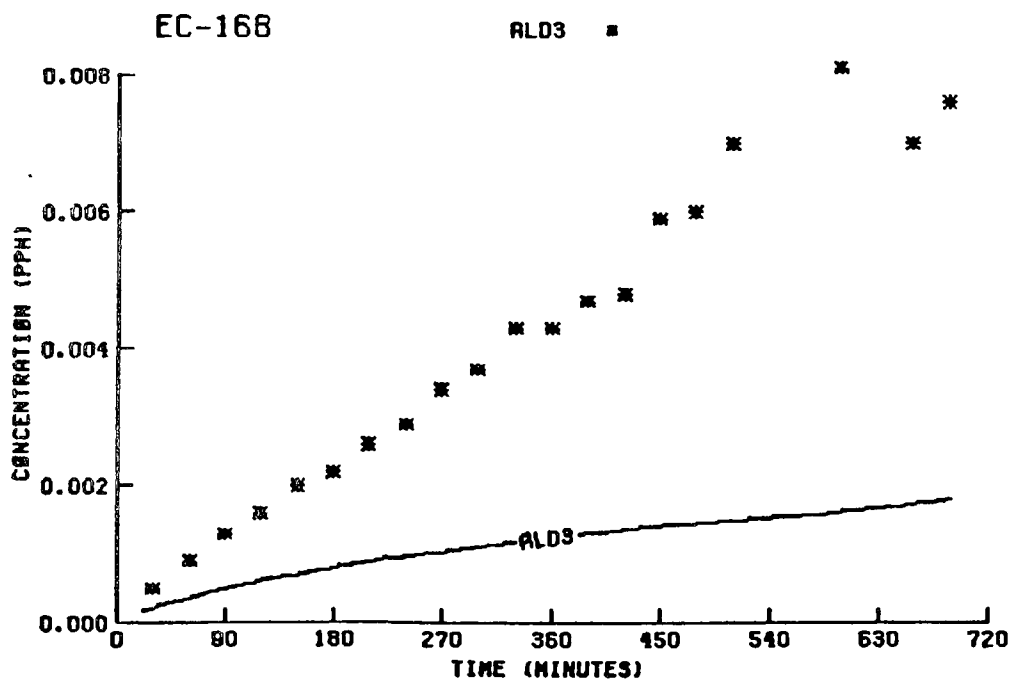
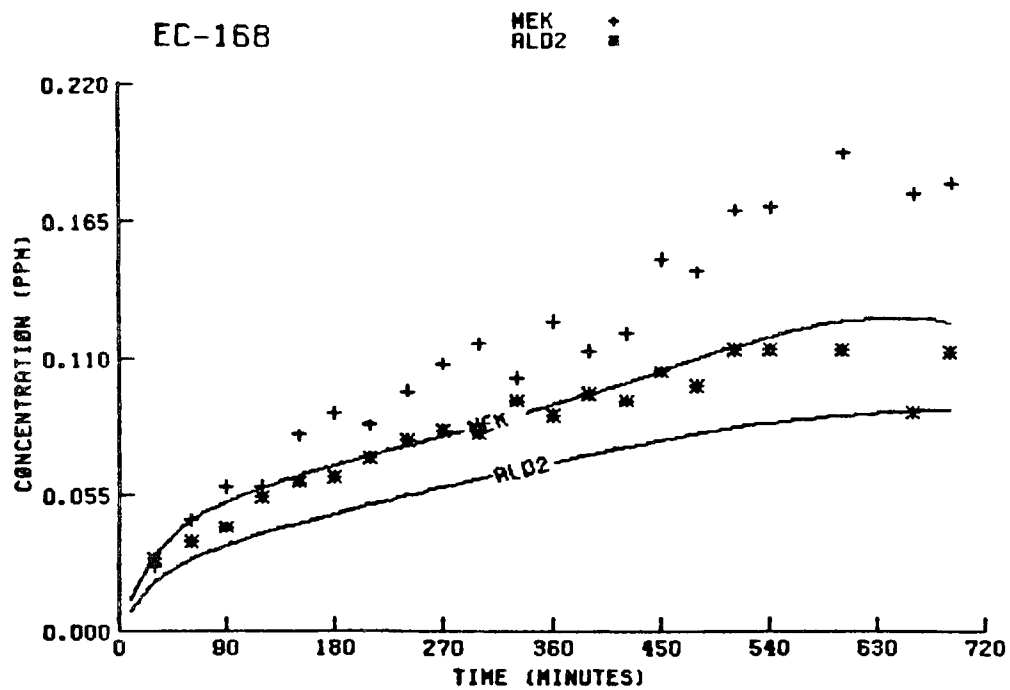


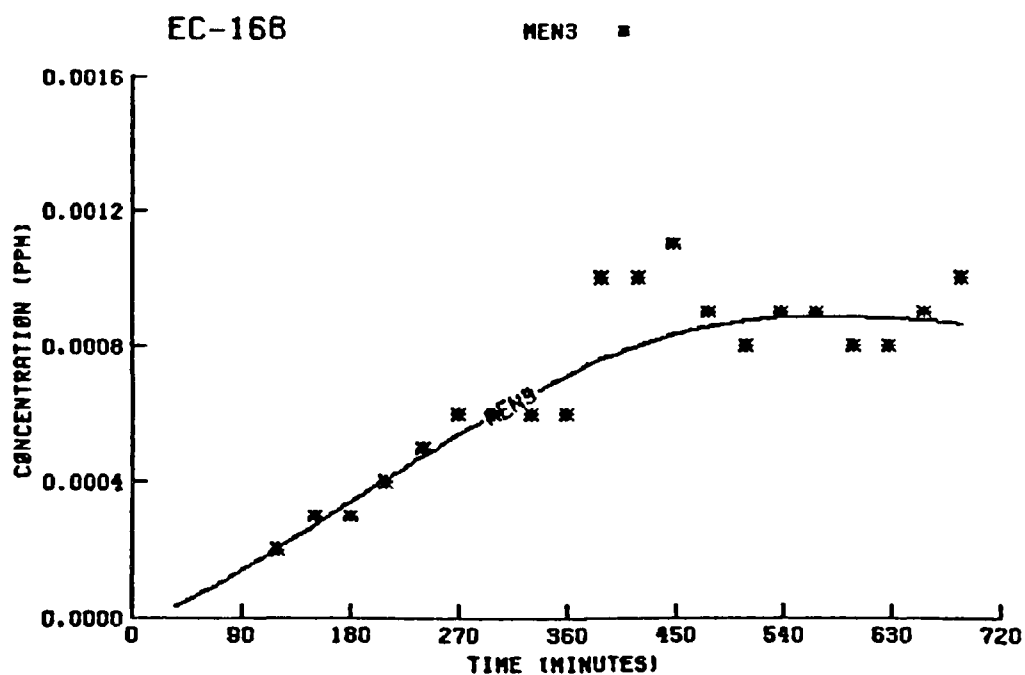
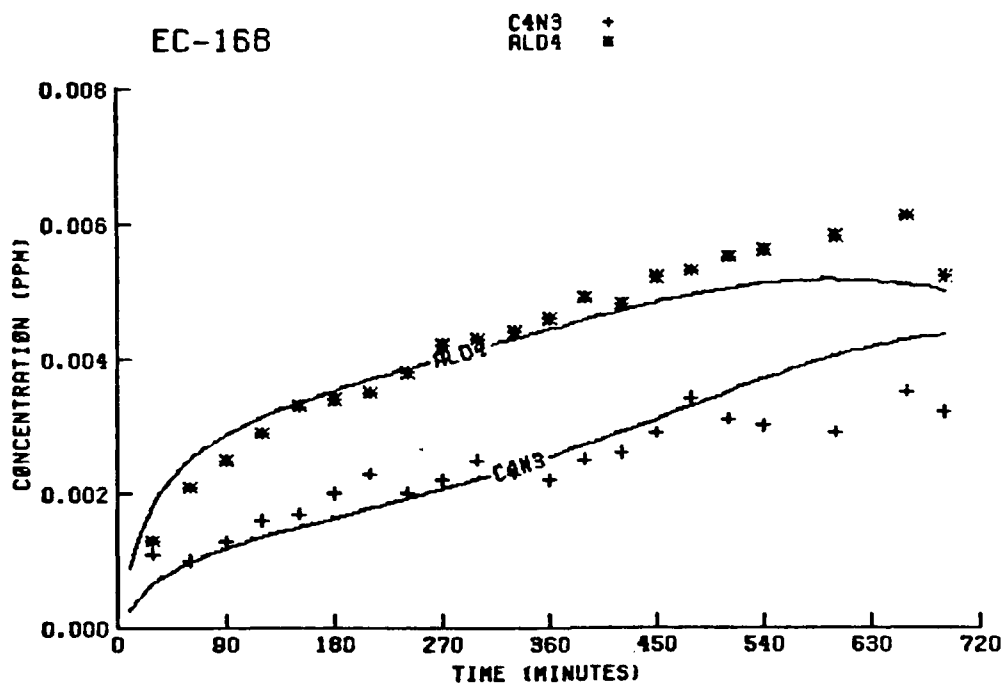
EC-168

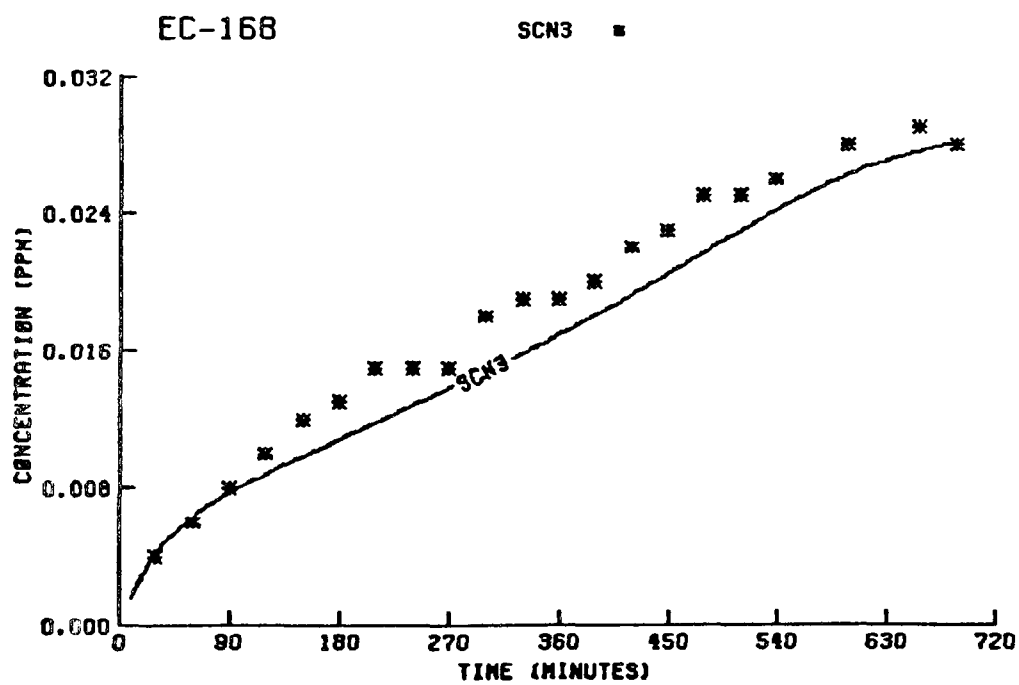
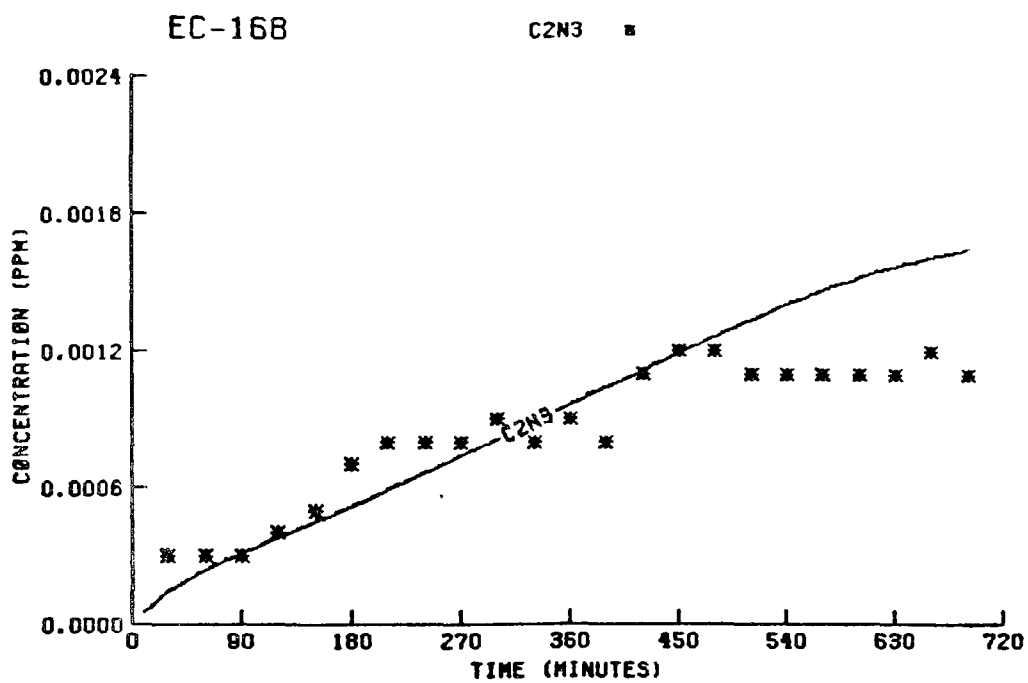
N82 +
N8 *







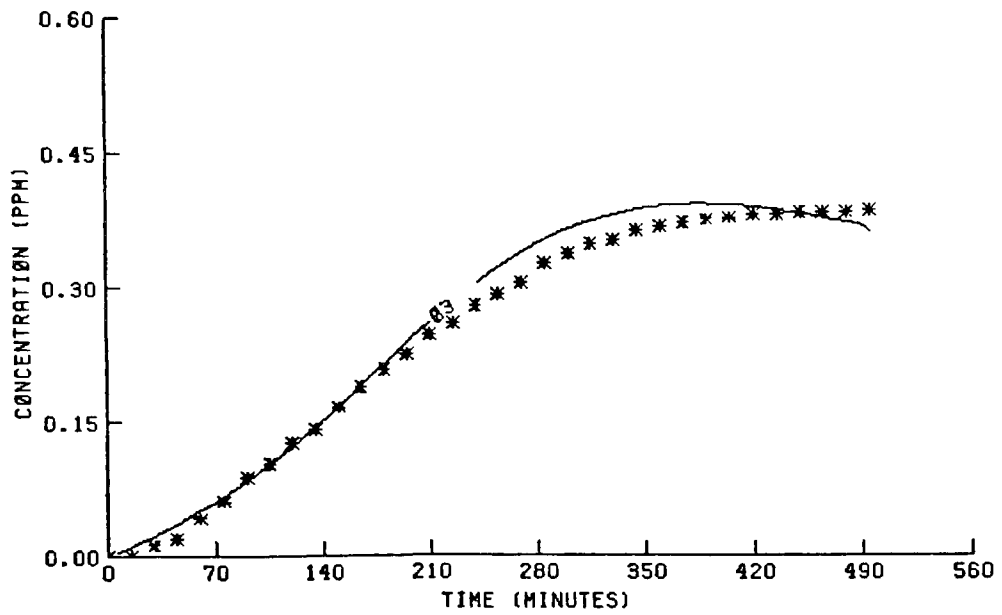




EC-178

O₃

■



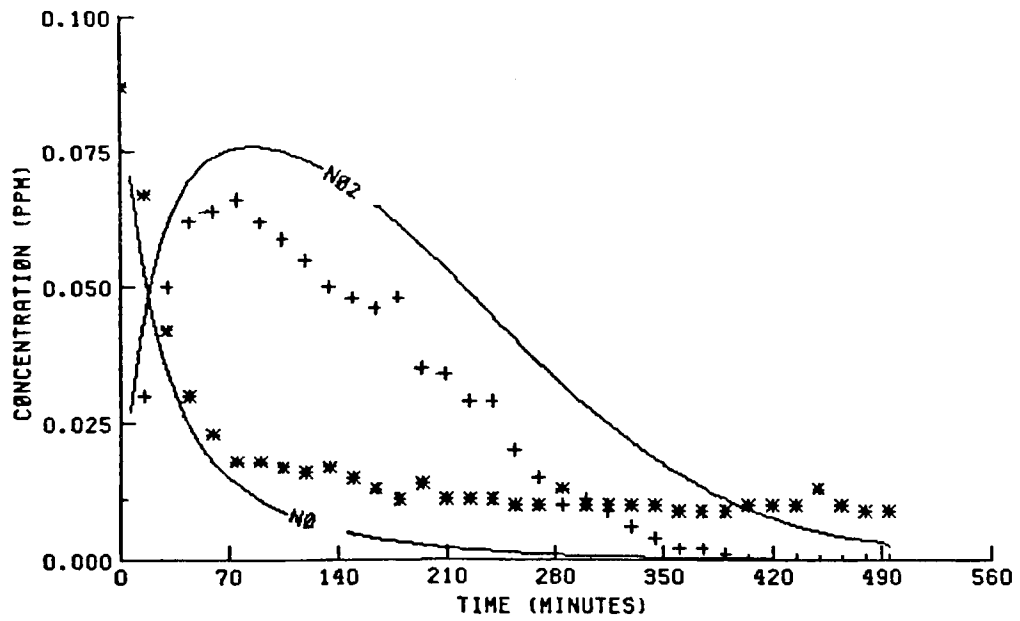
EC-178

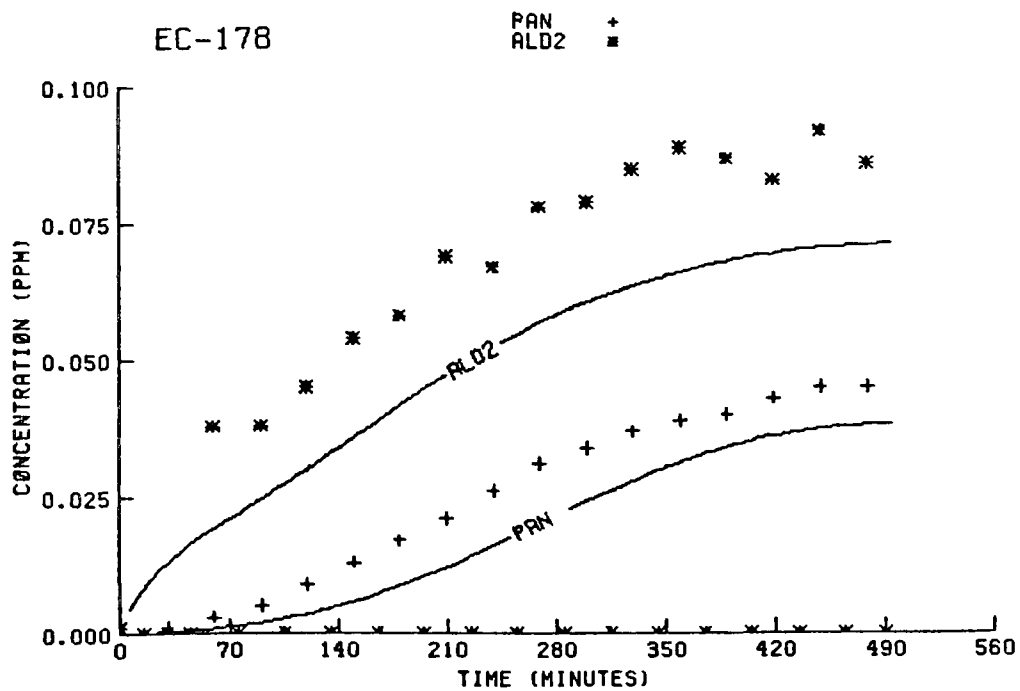
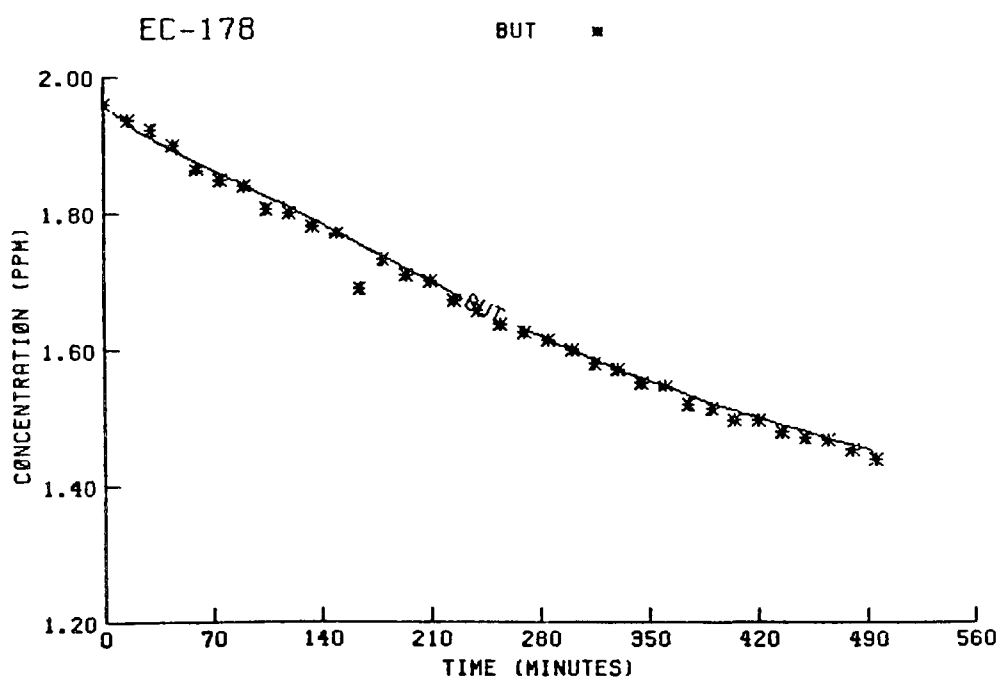
N₂O

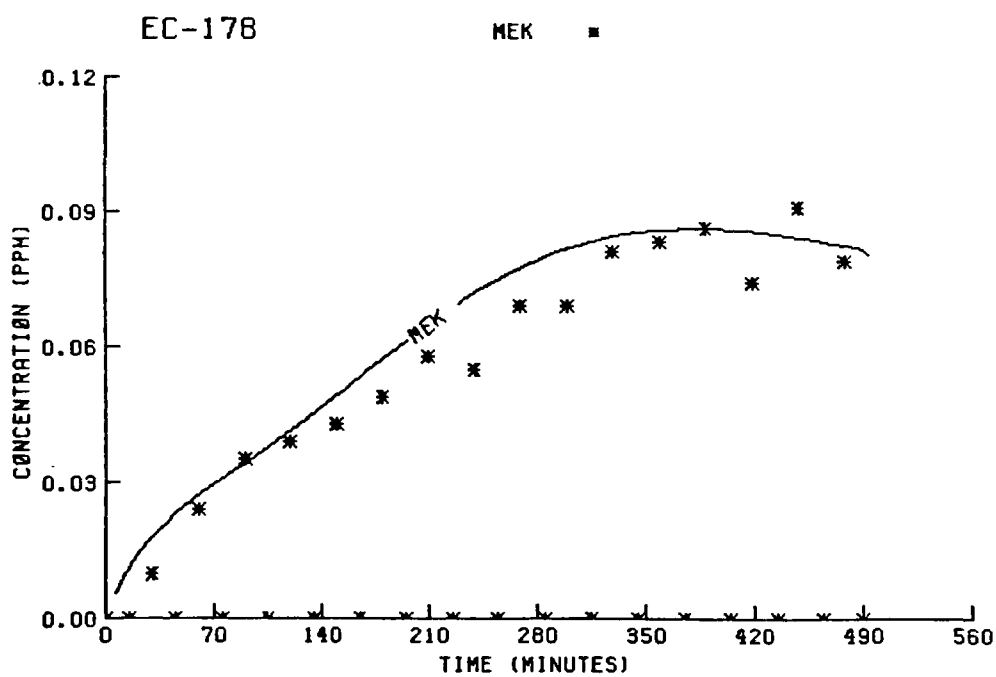
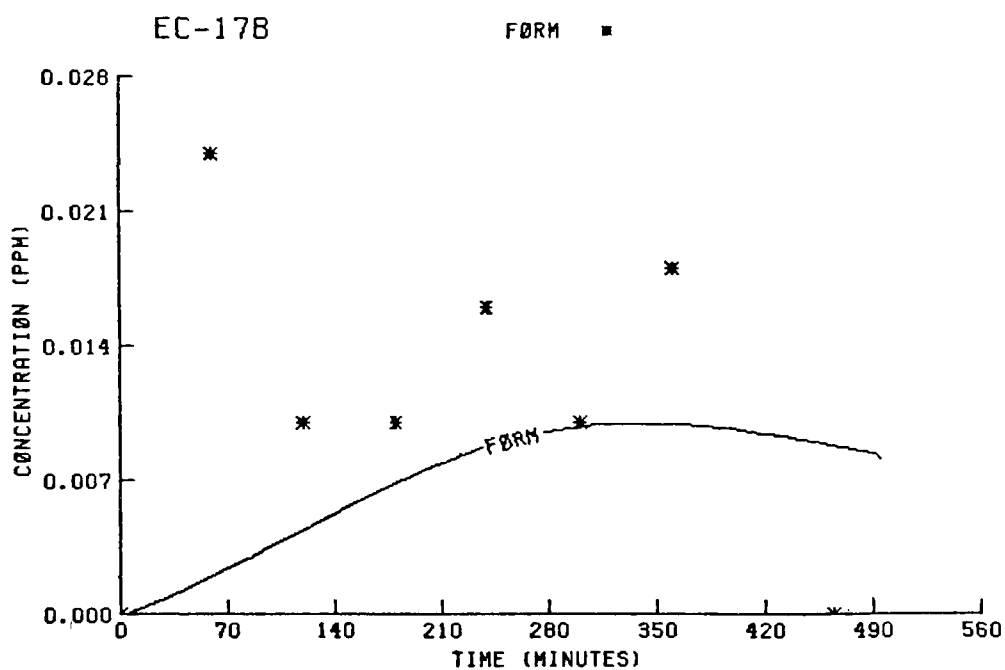
+

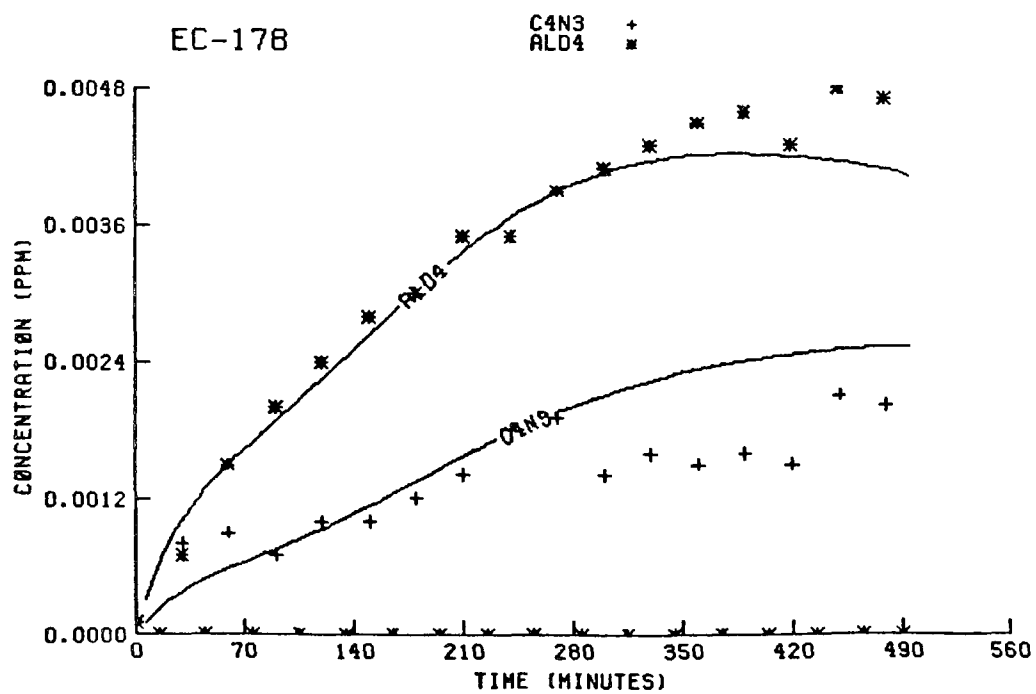
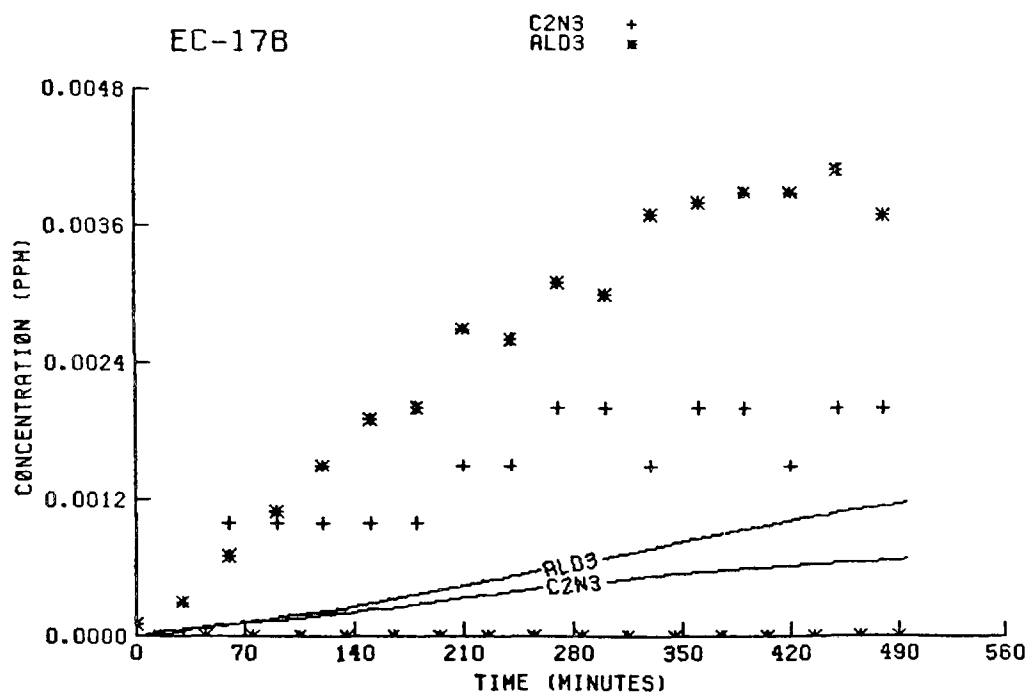
N₂

■



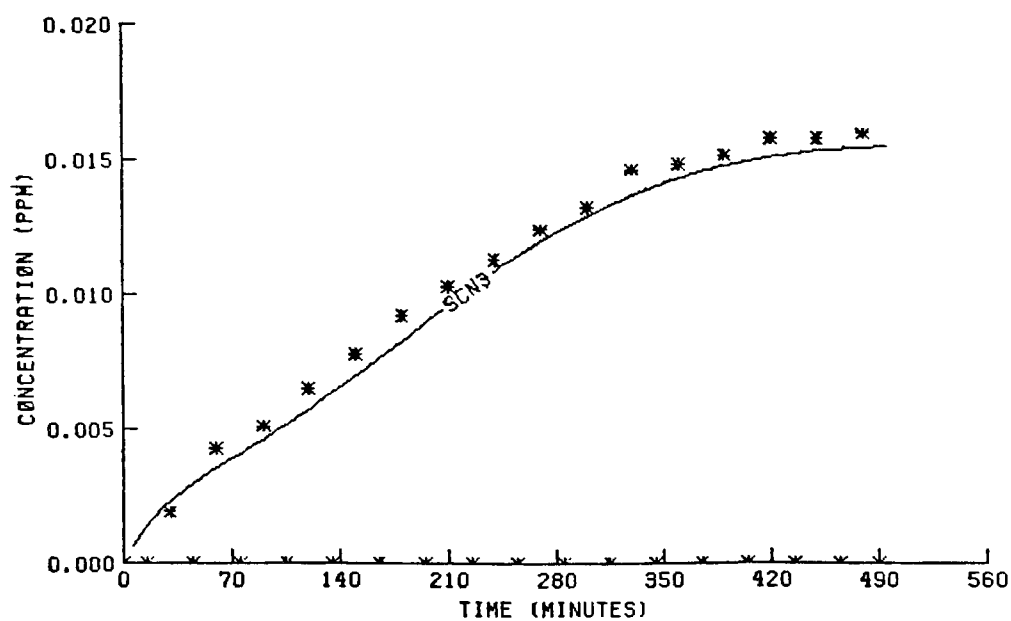




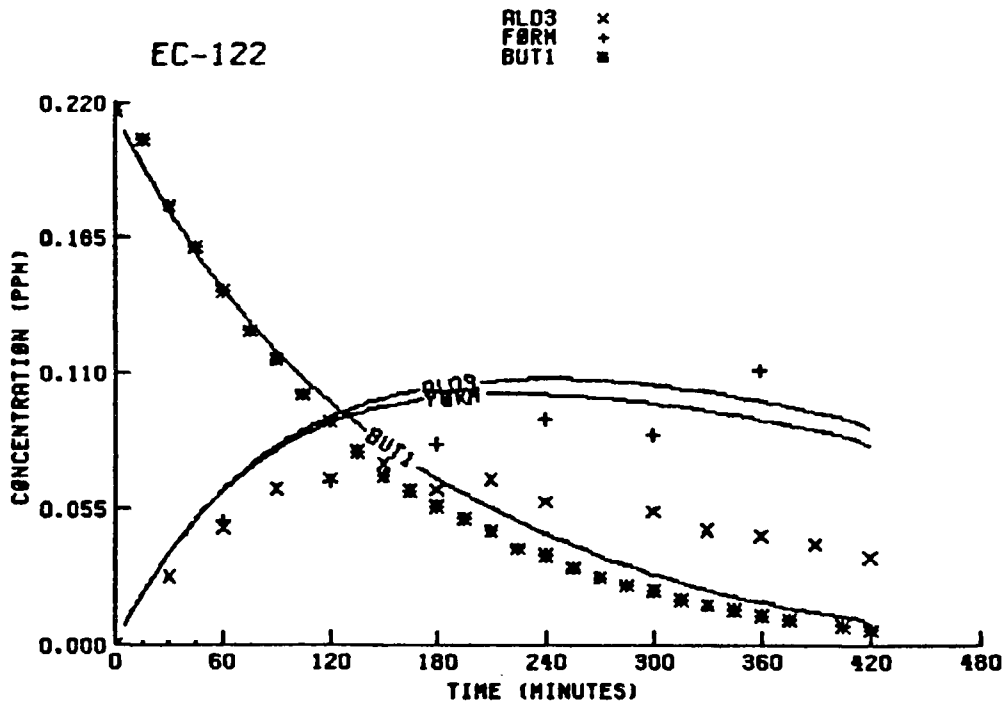
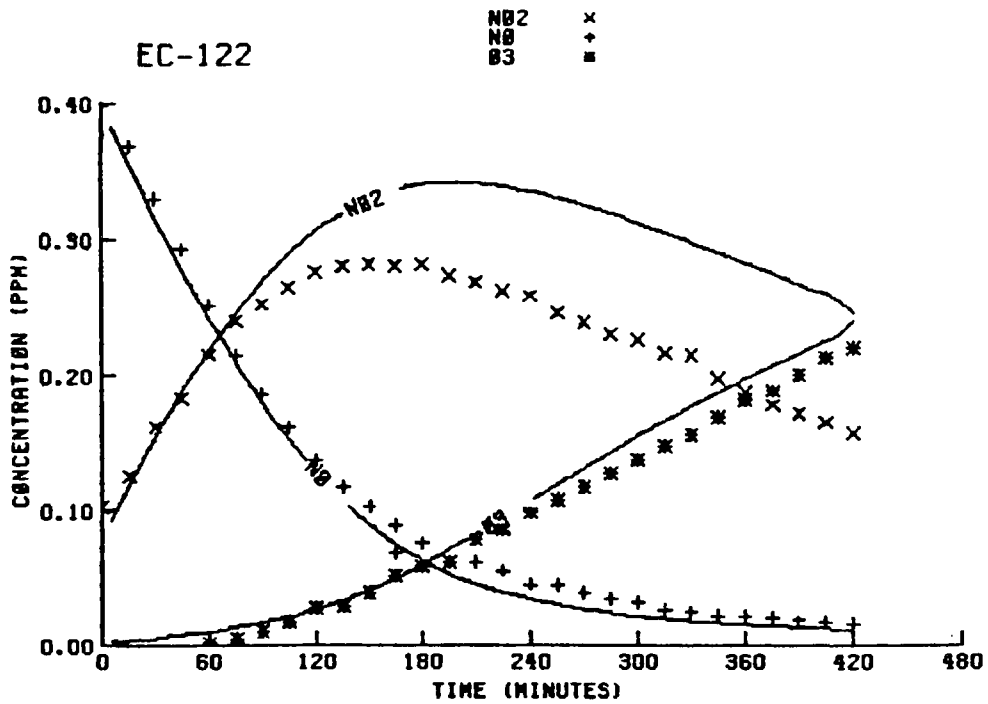


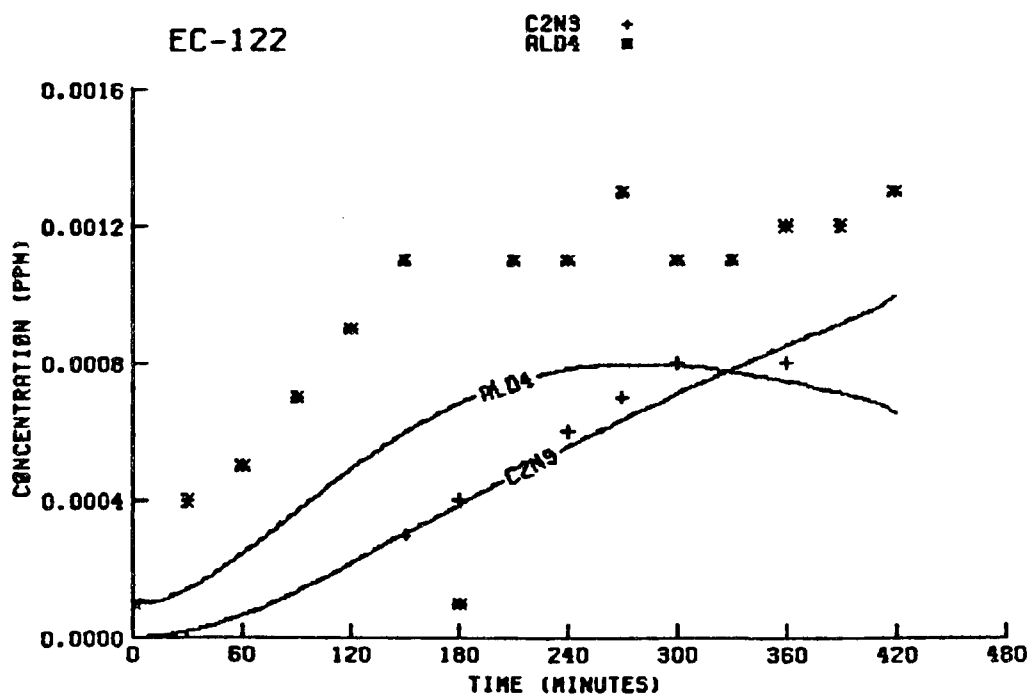
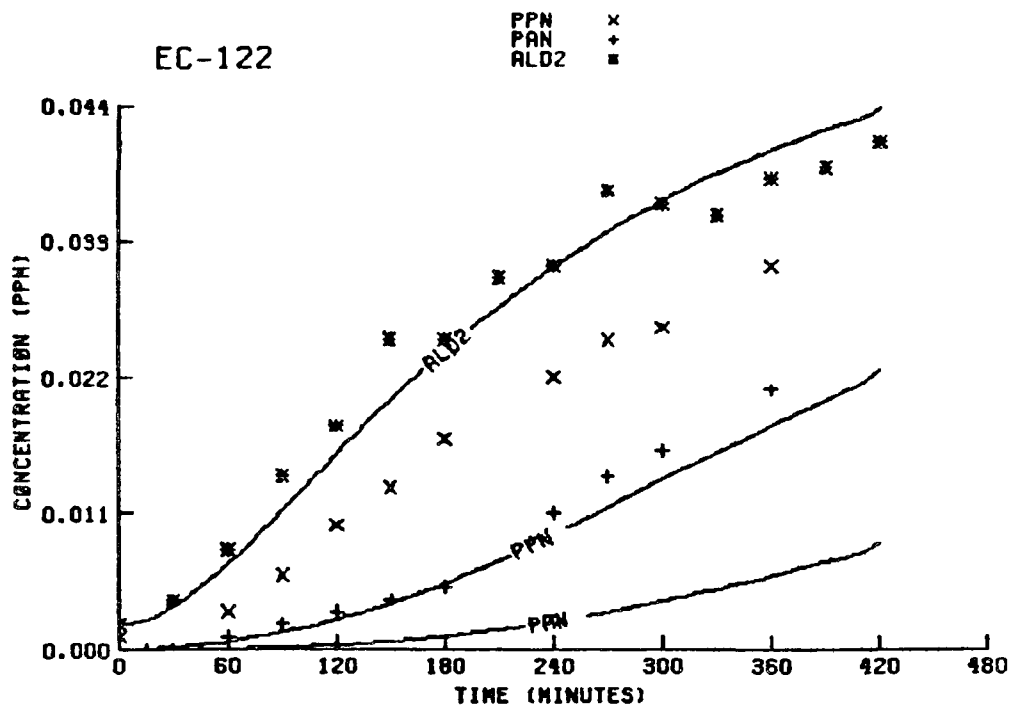
EC-178

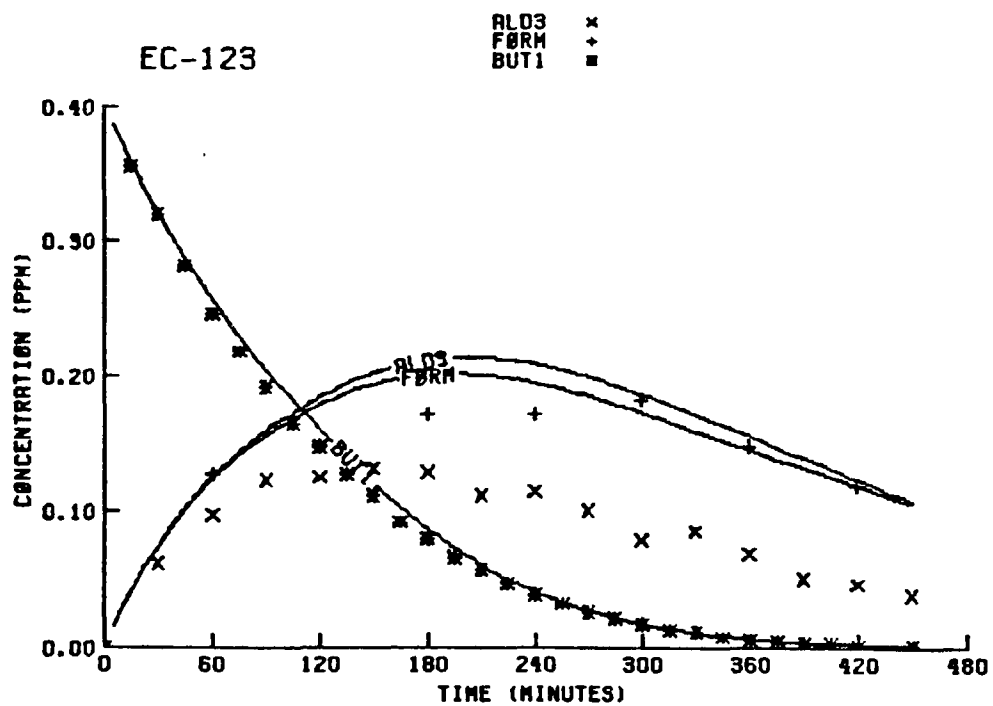
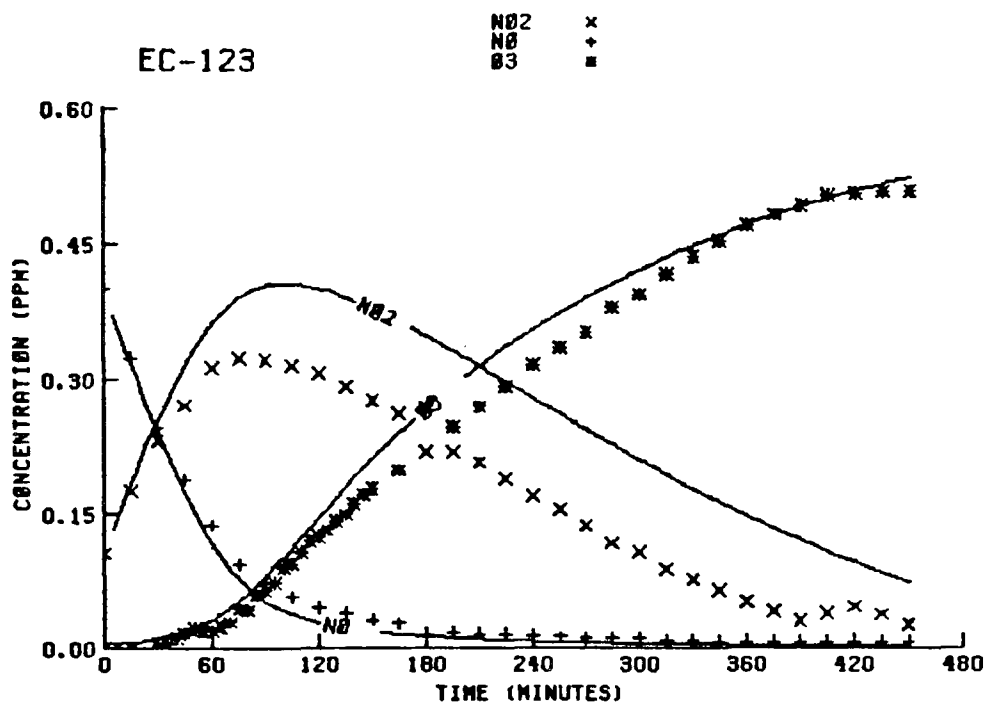
SCN3 ■

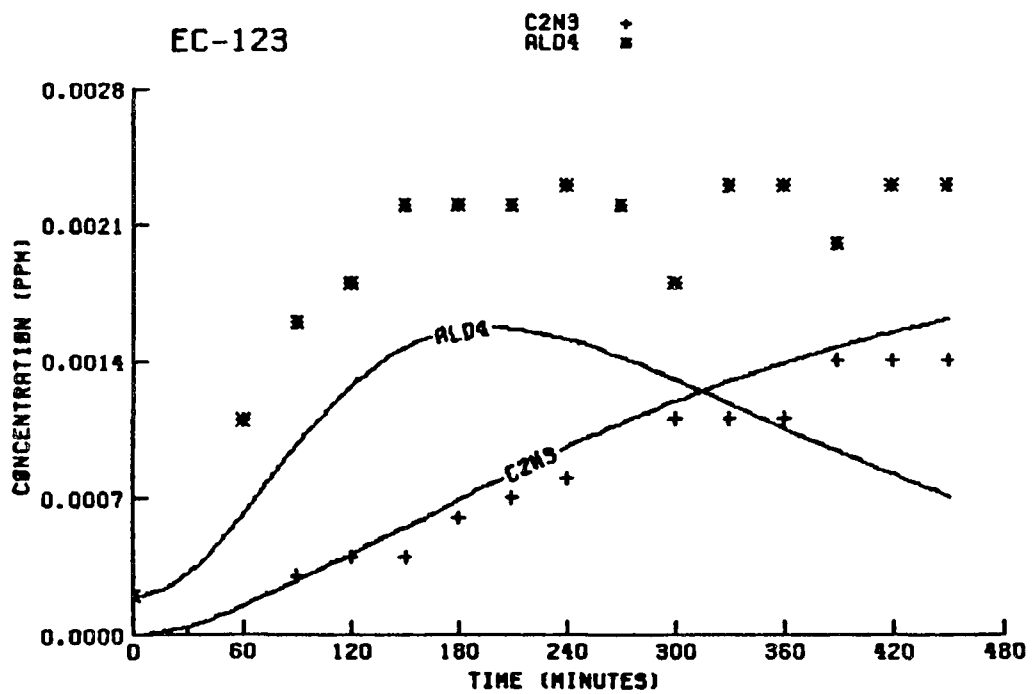
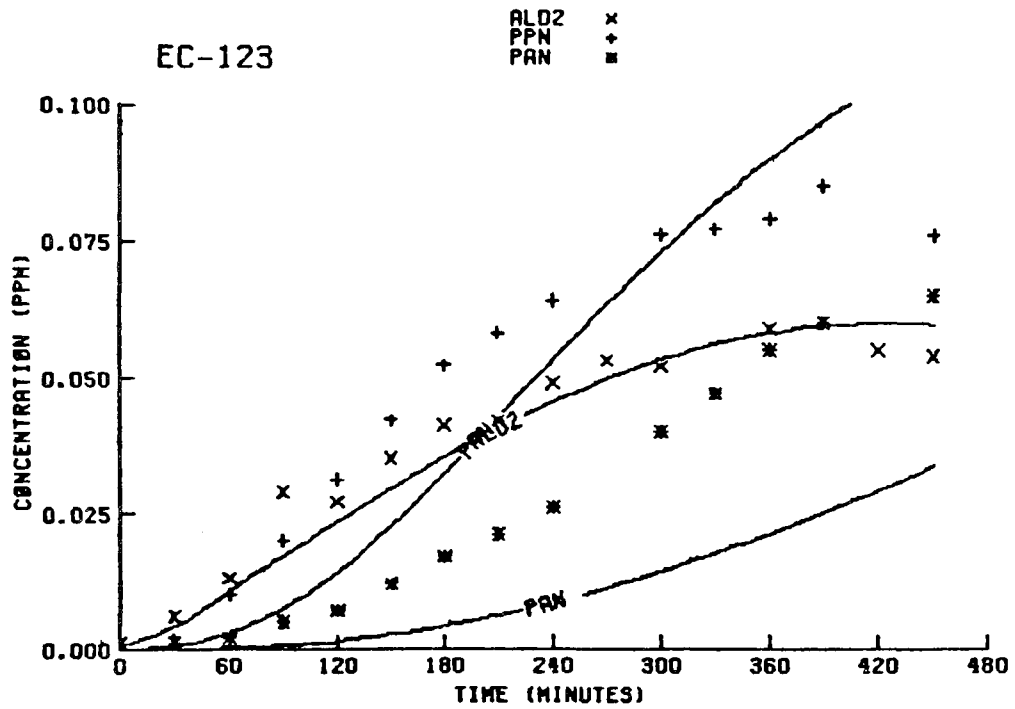


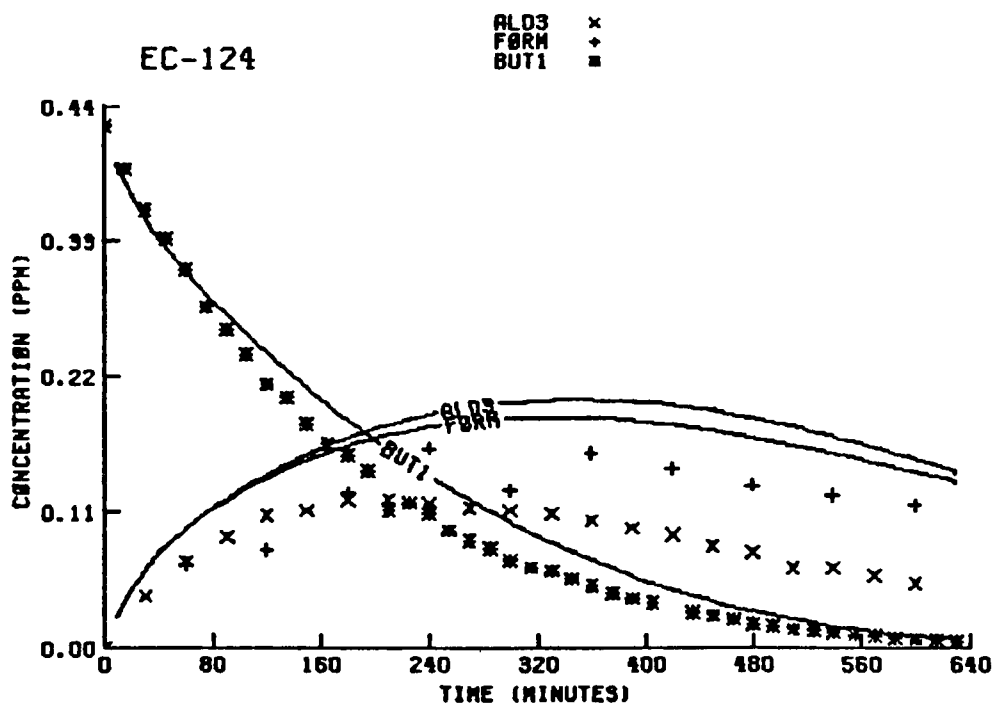
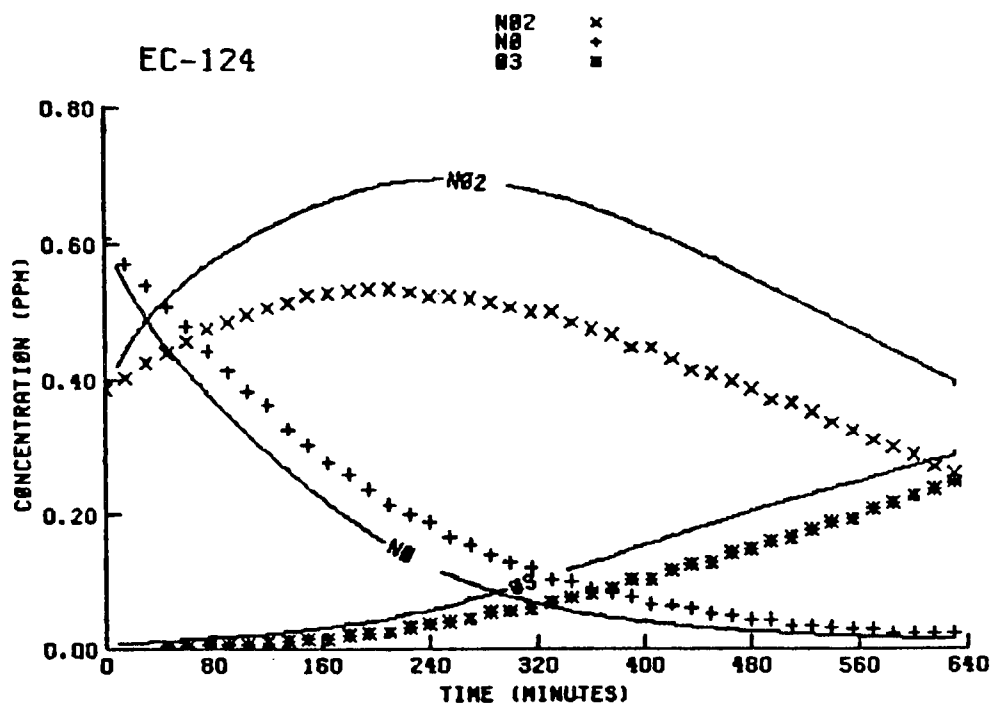
UCR 1-BUTENE EXPERIMENTS

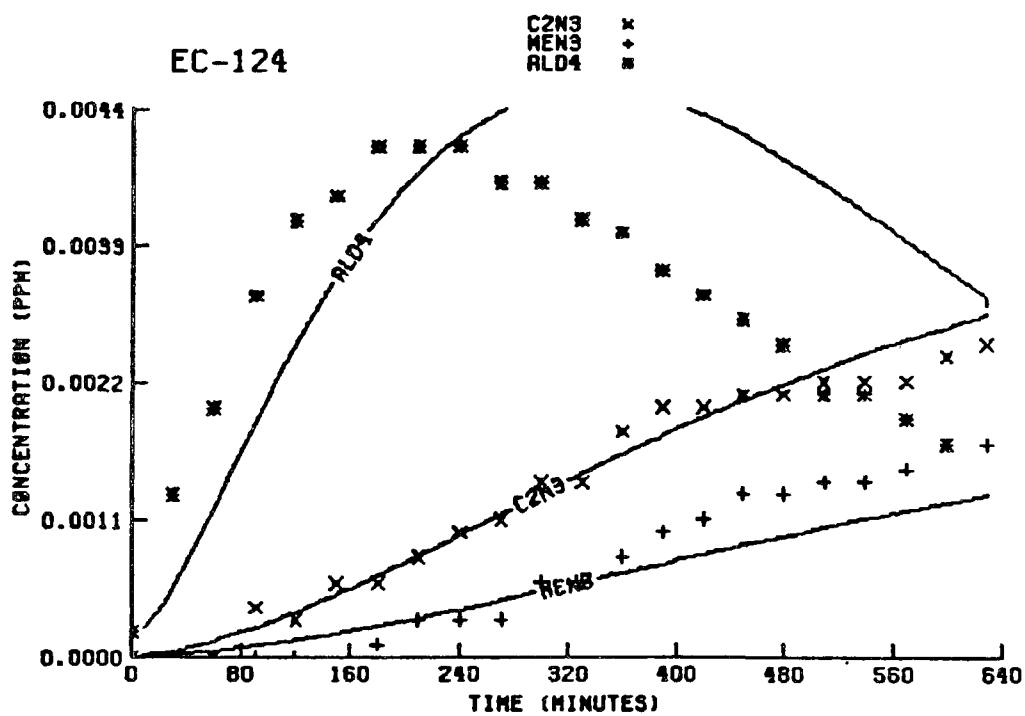
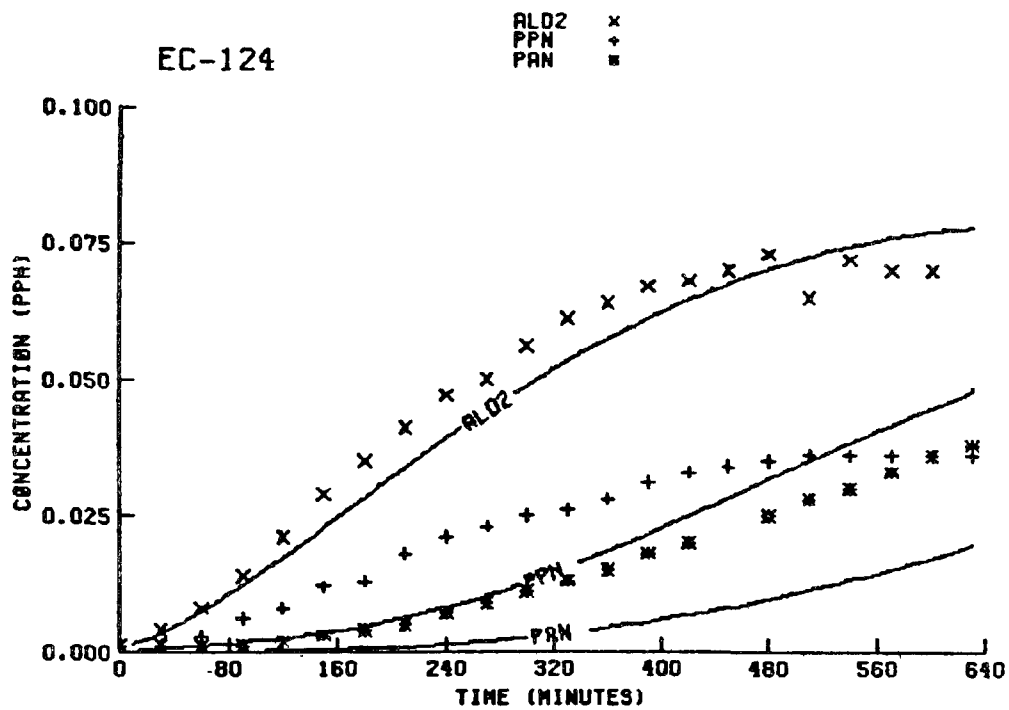




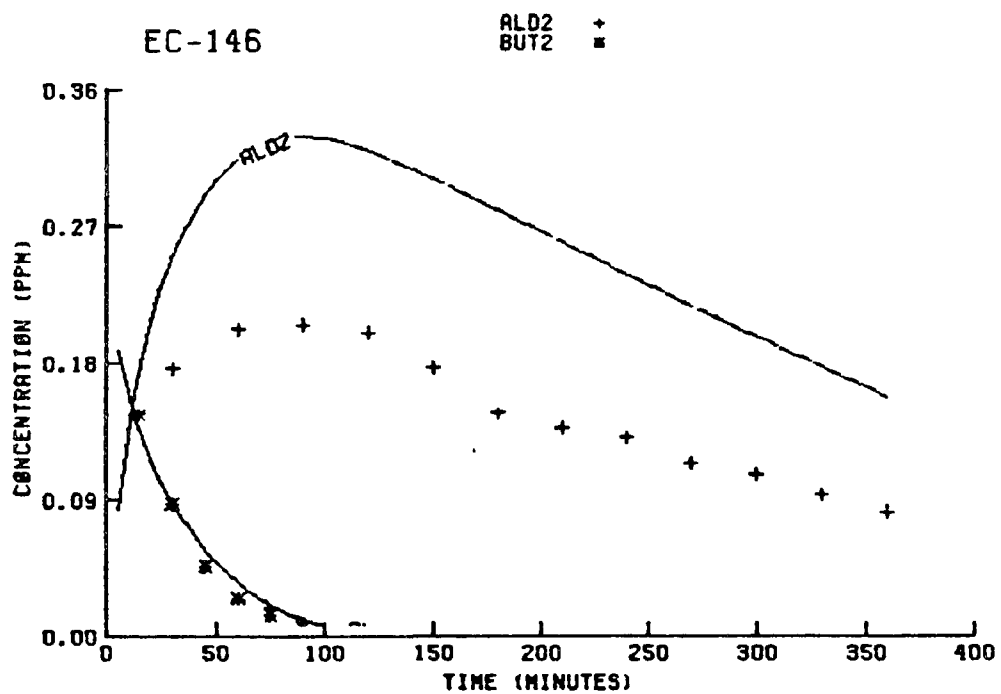
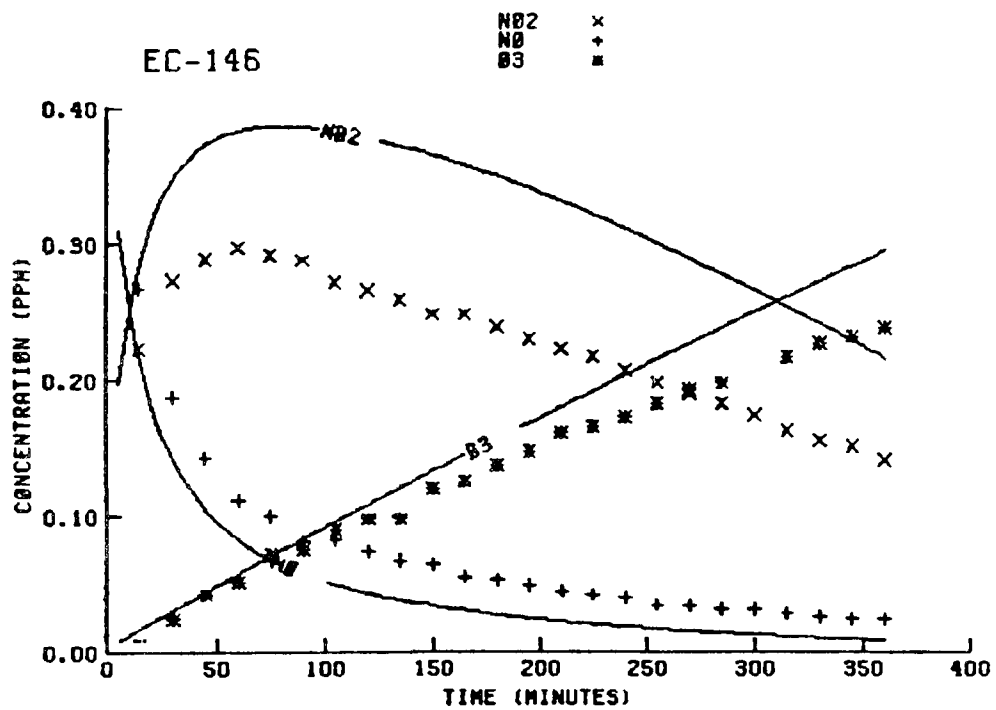


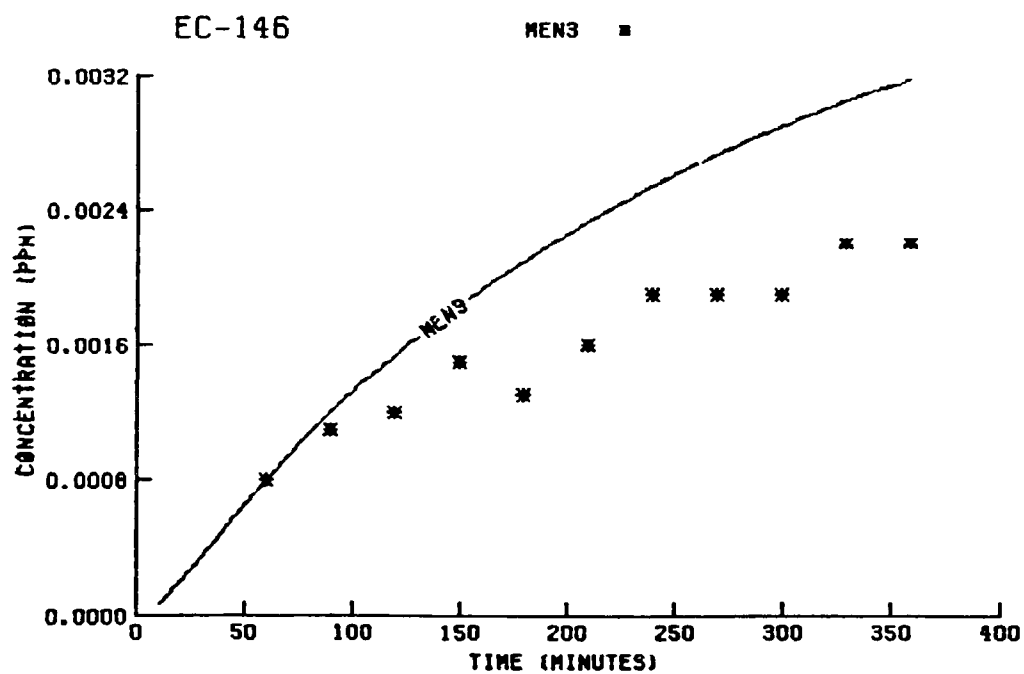
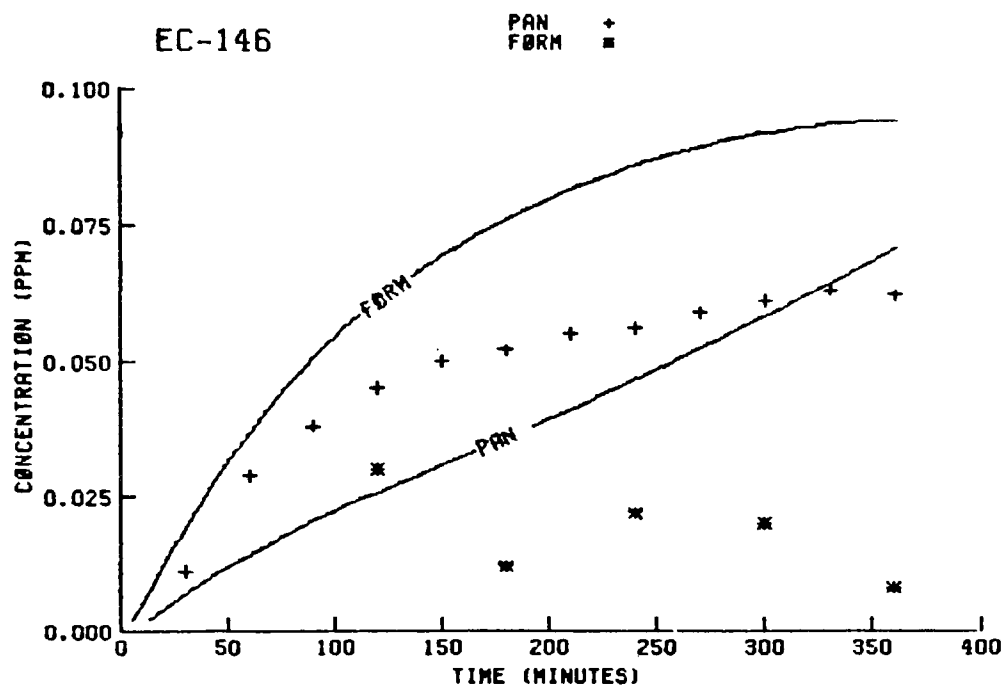


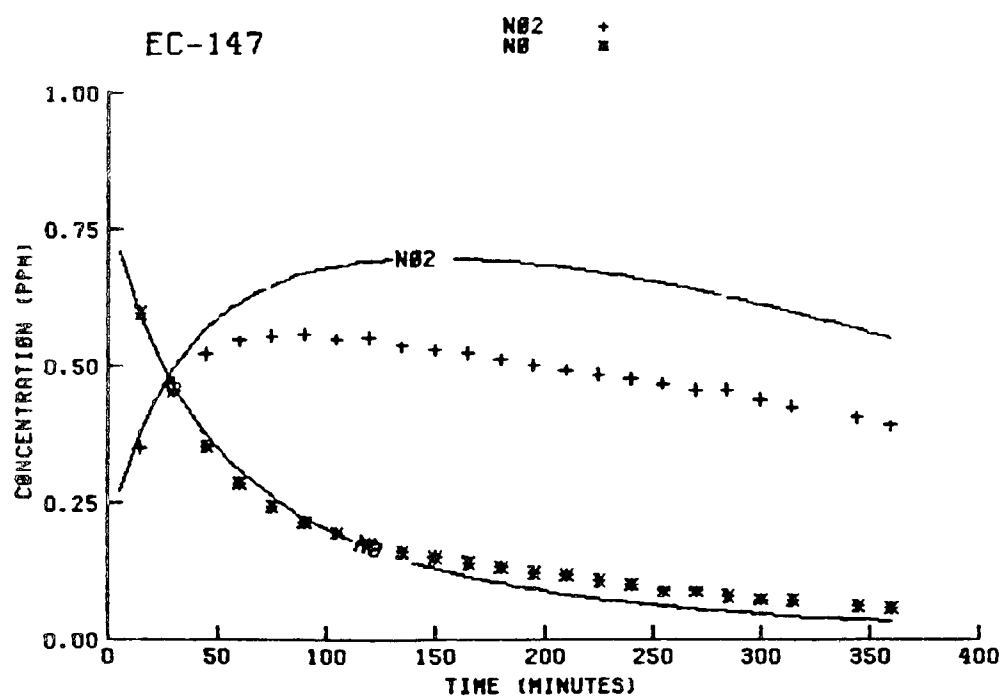
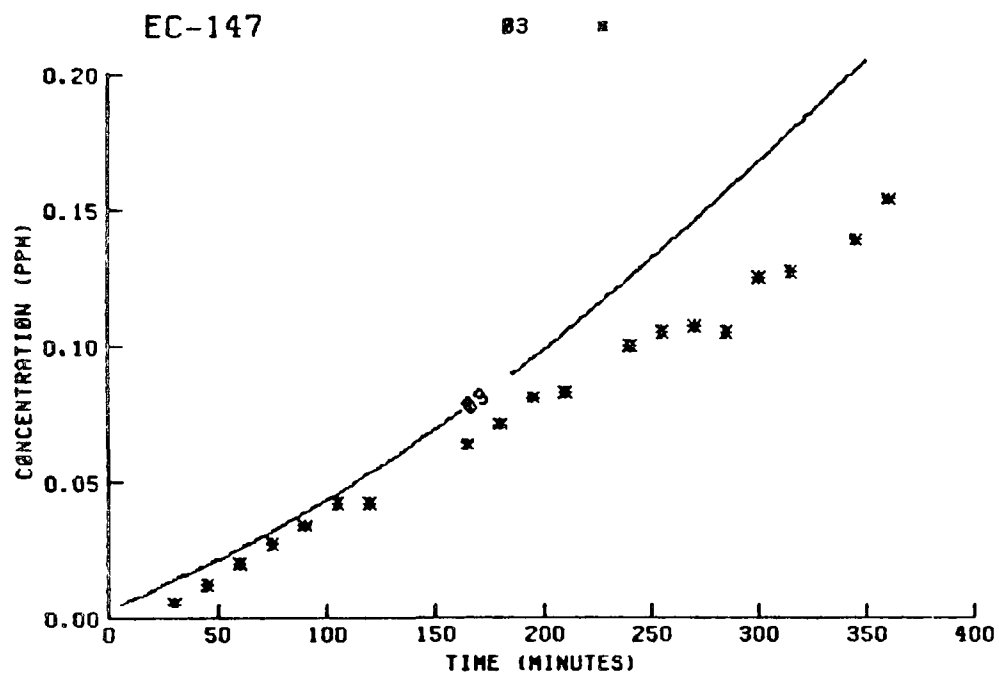


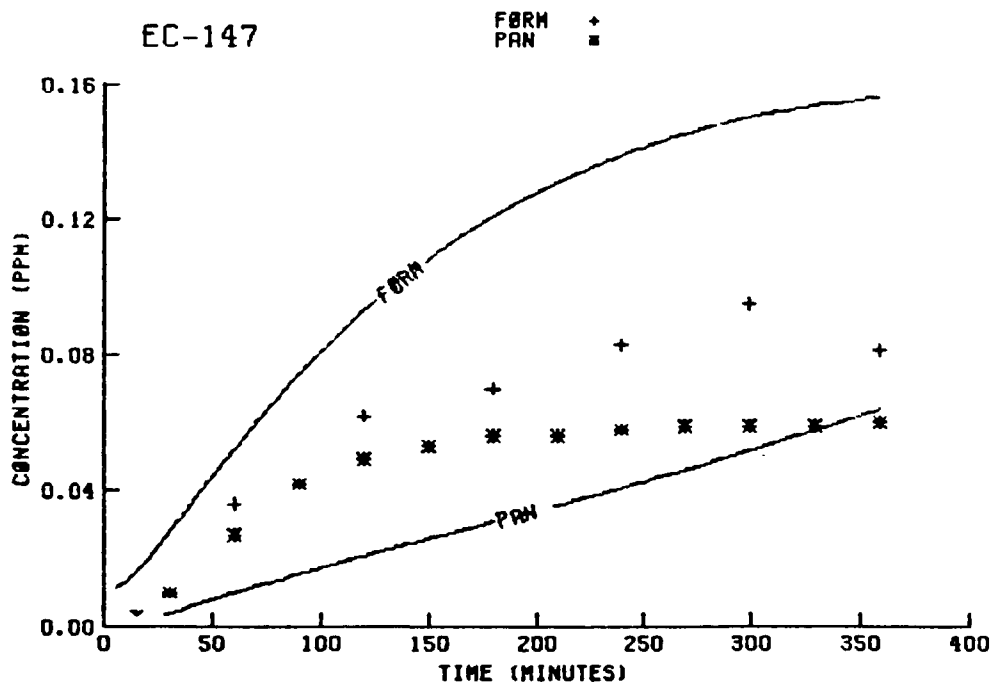
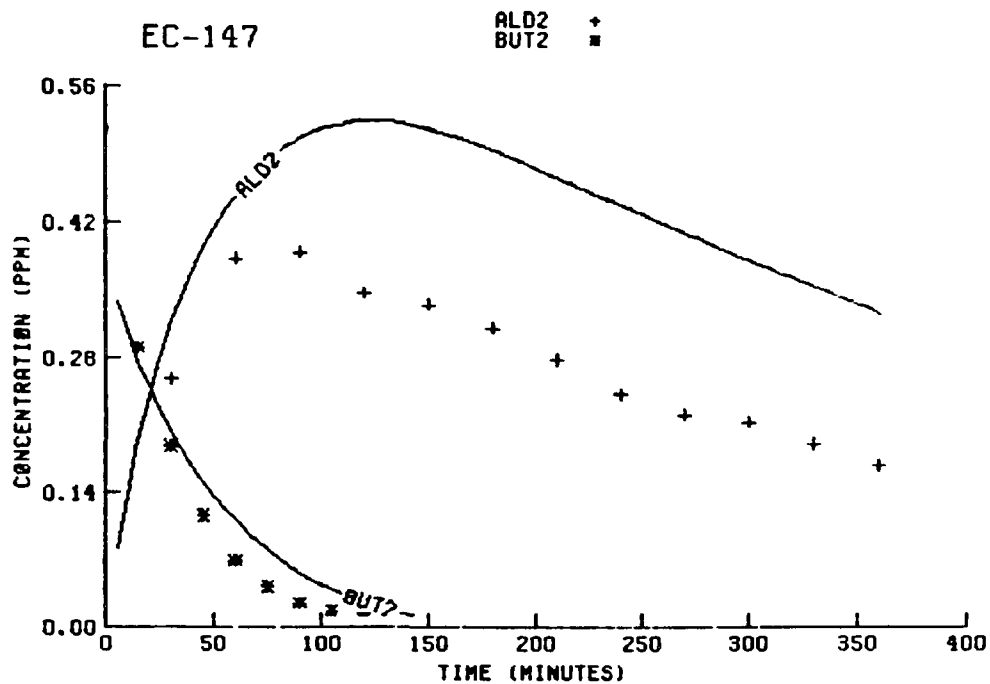


UCR TRANS-2-BUTENE EXPERIMENTS



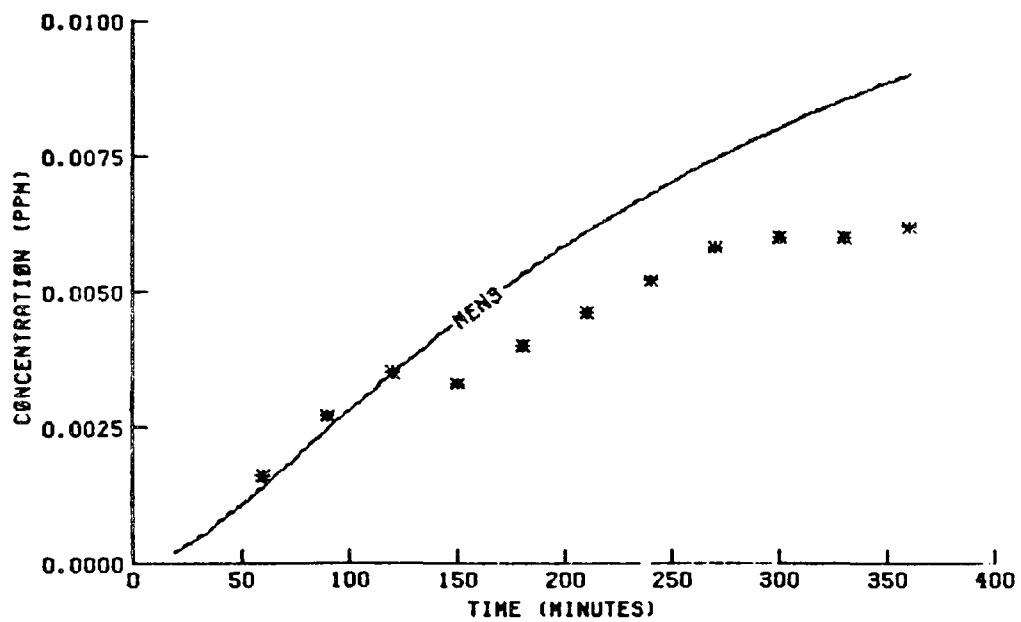






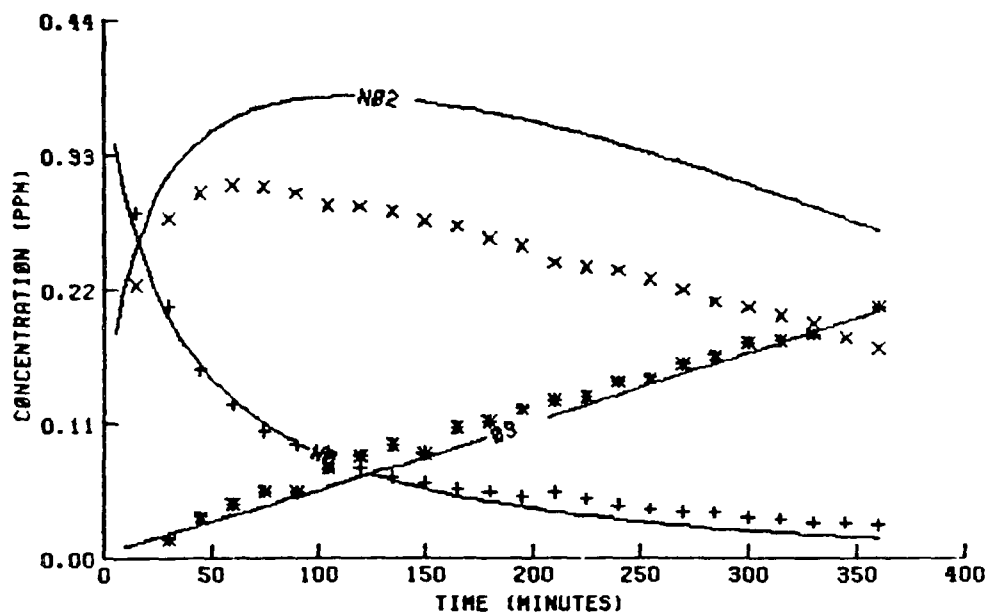
EC-147

MEN3



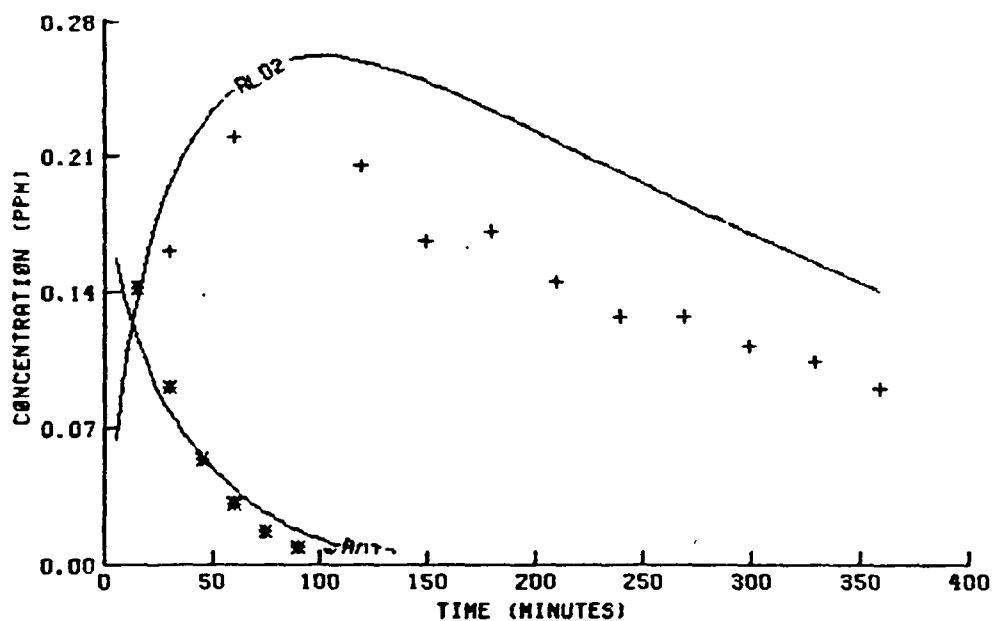
EC-157

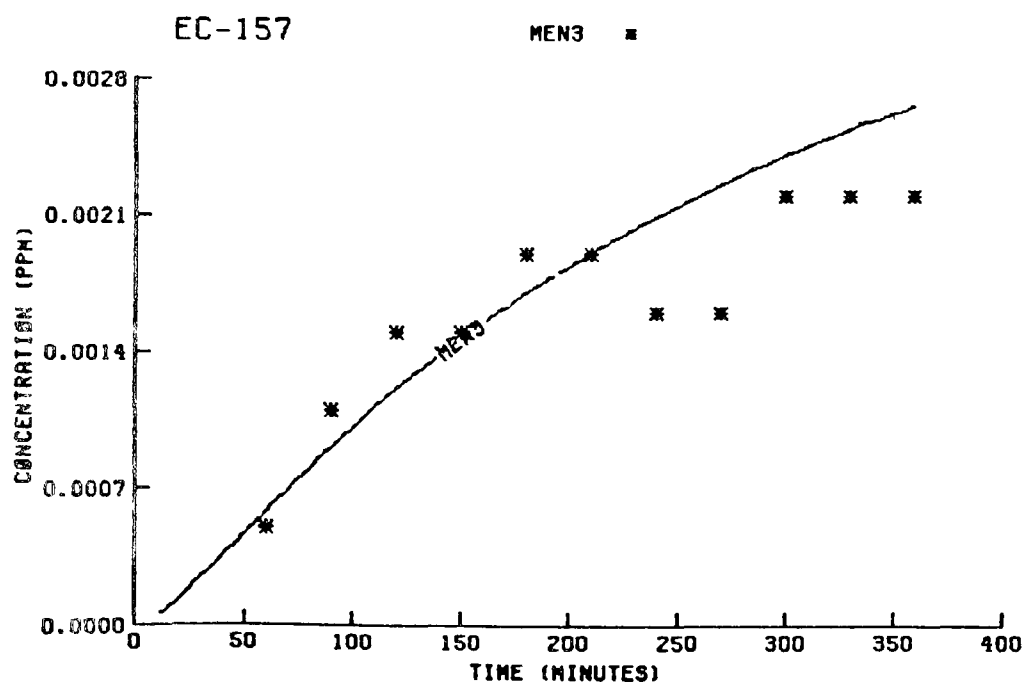
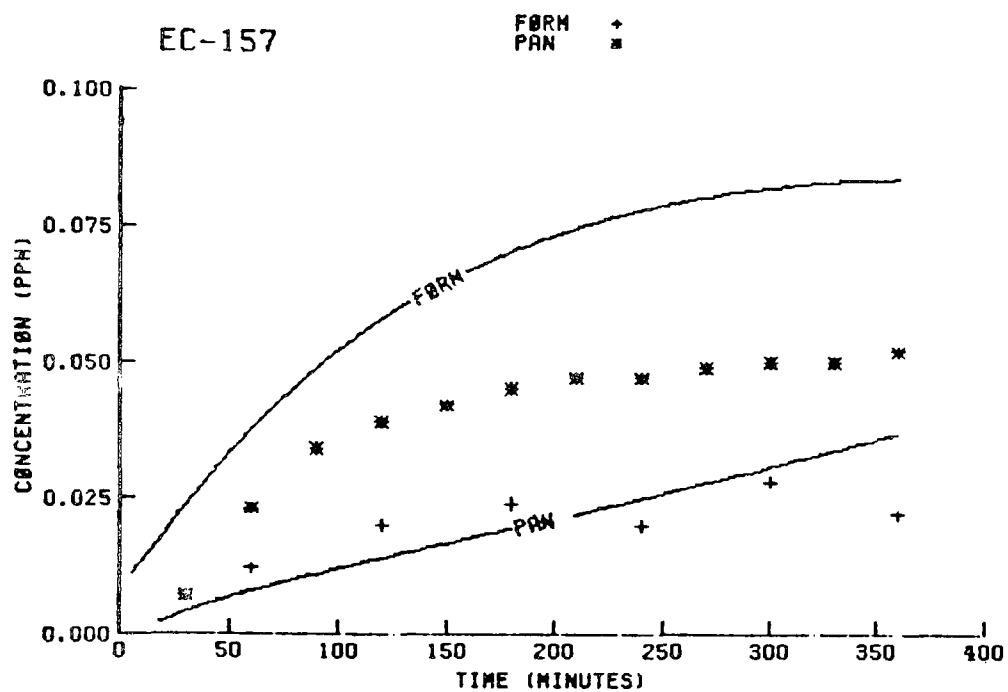
NO2 x
NB +
B3 ■



EC-157

ALD2 +
BUT2 ■

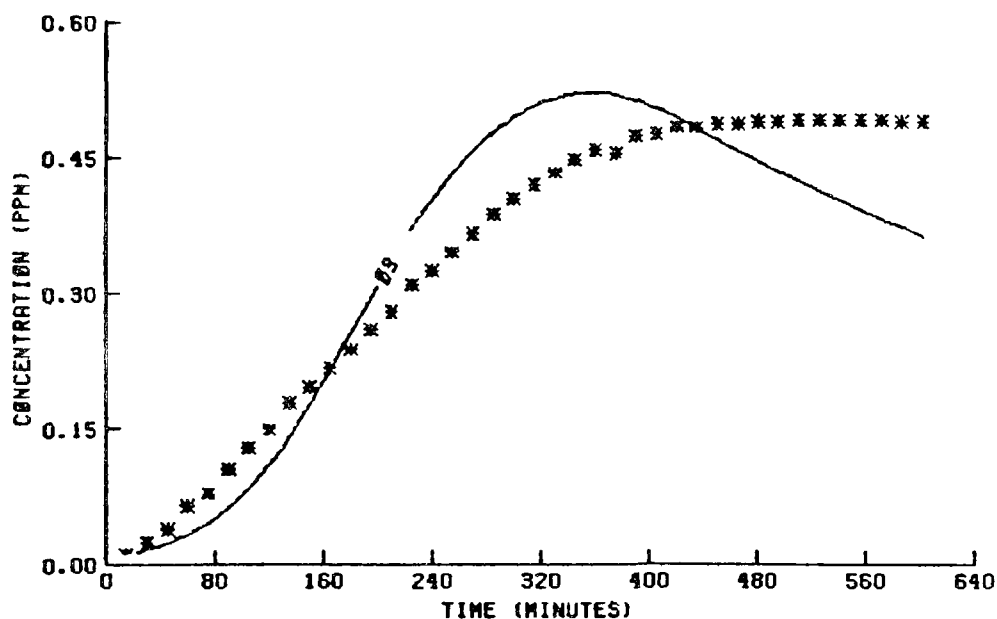




UCR 2,3-DIMETHYLBUTANE EXPERIMENTS

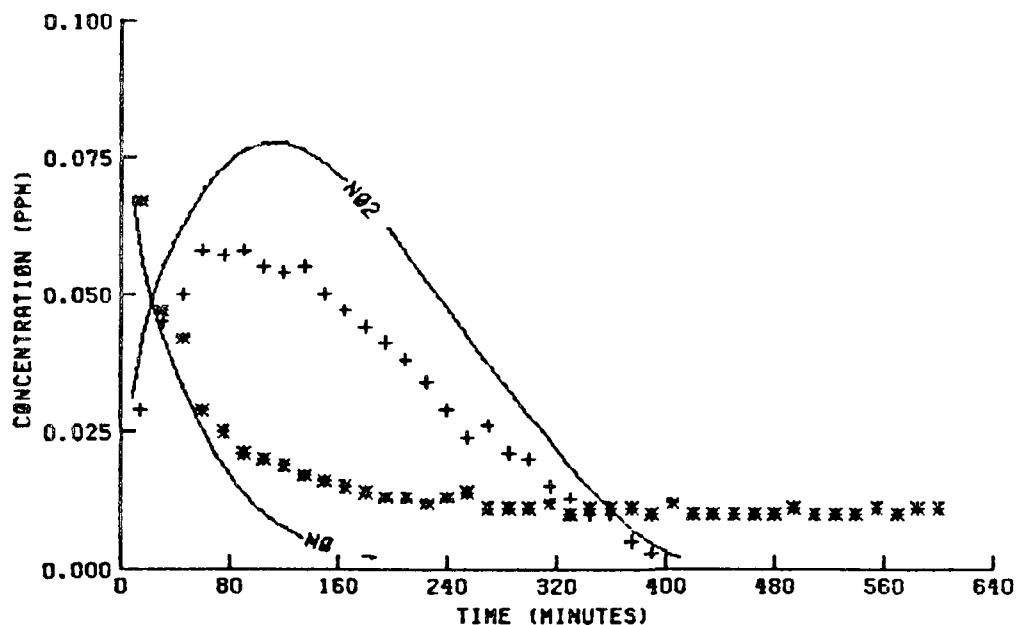
EC-165

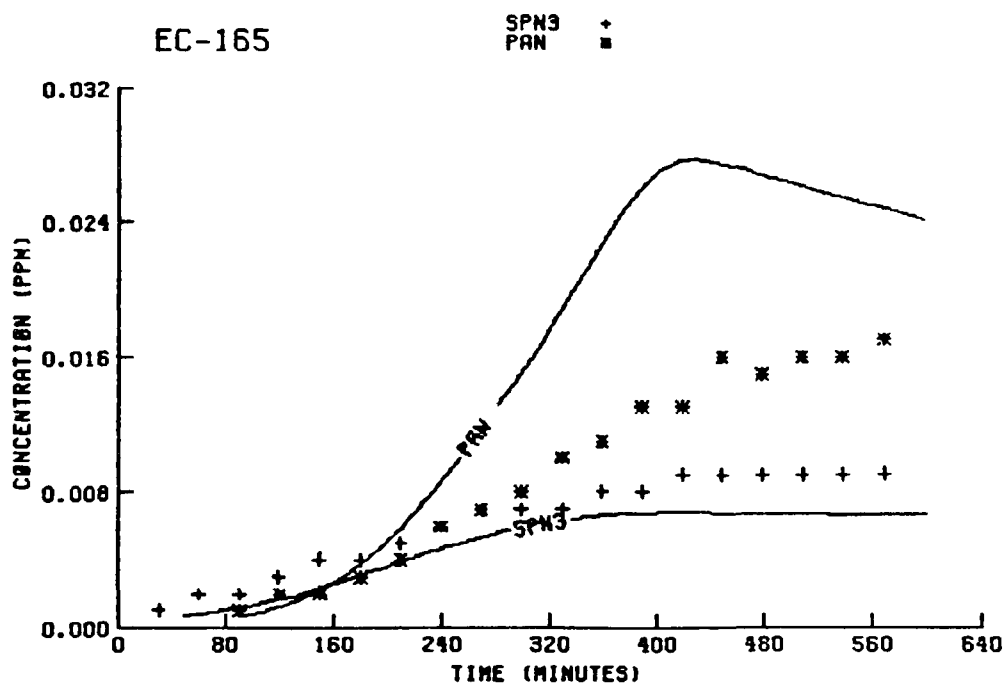
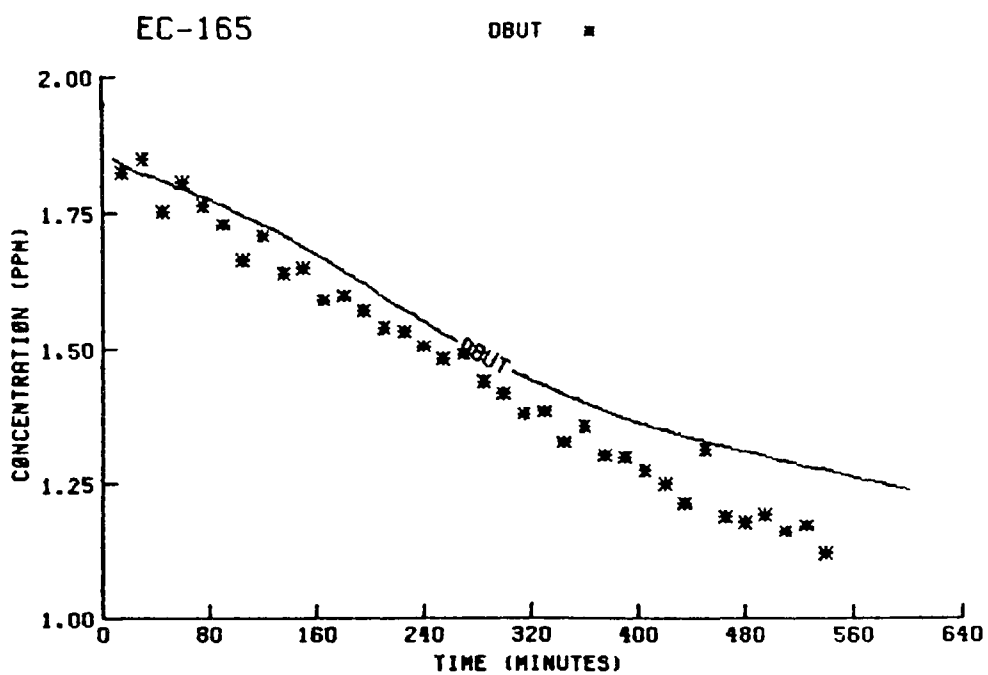
03 *



EC-165

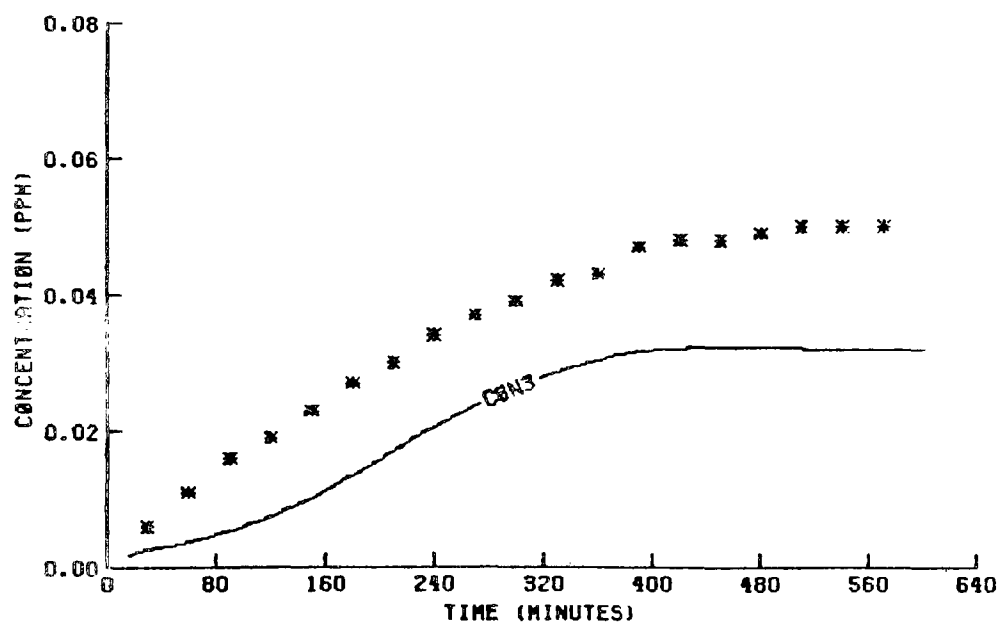
N02 +
N0 *





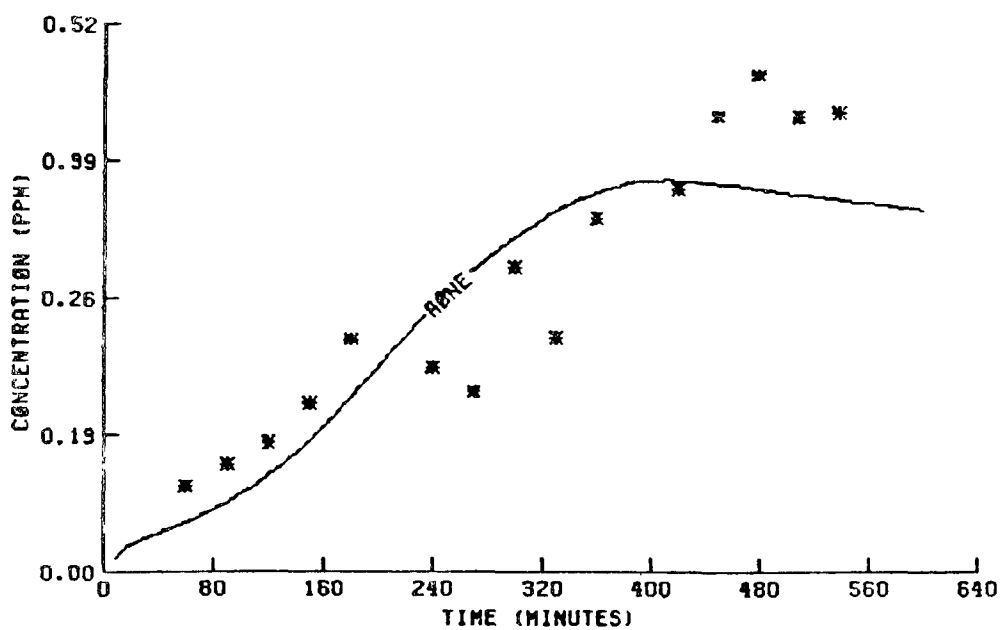
EC-165

C6N3



EC-165

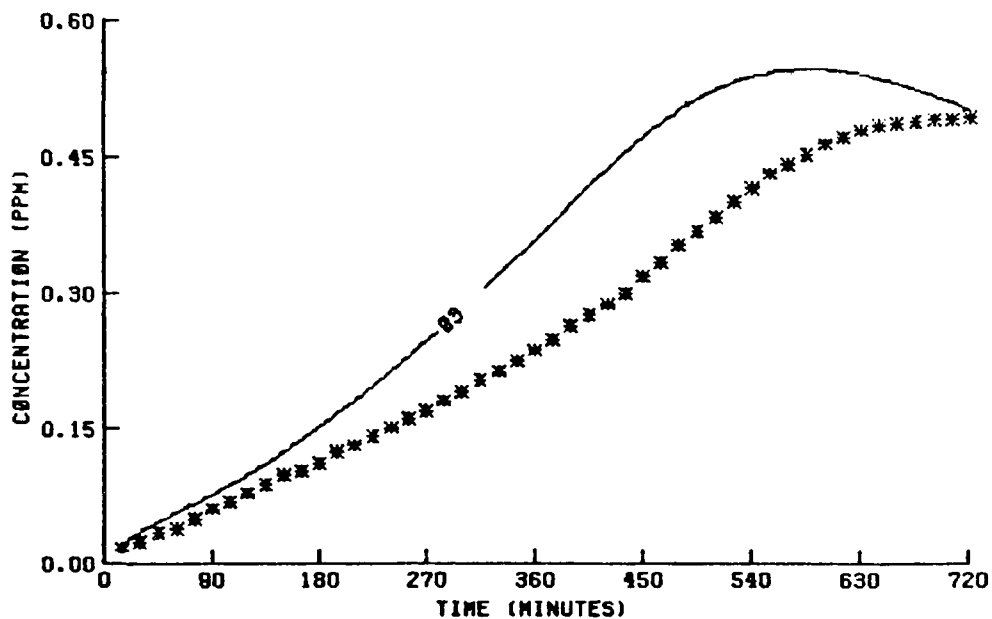
R8NE



EC-169

83

■



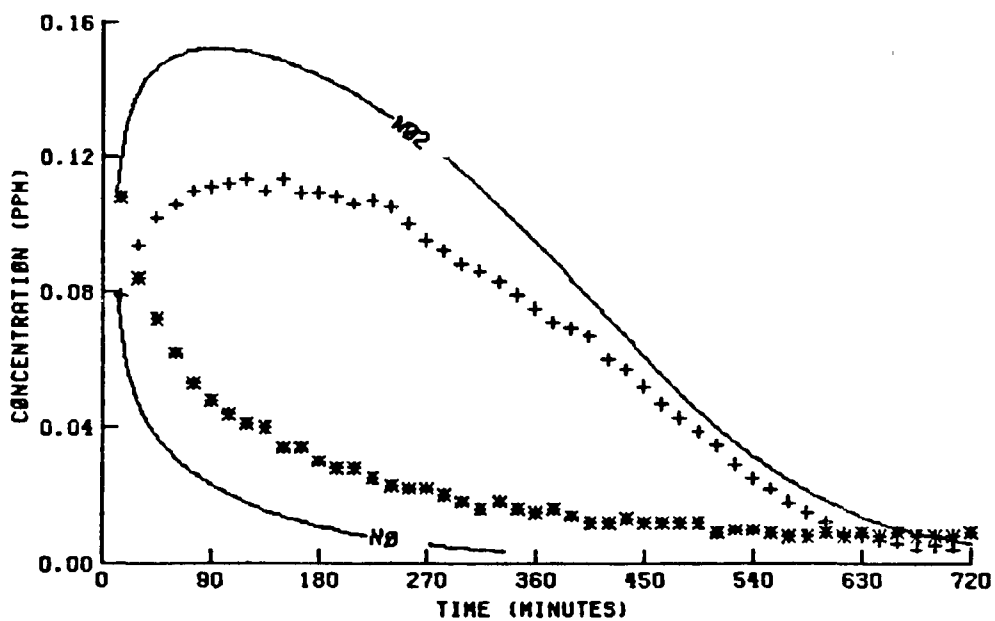
EC-169

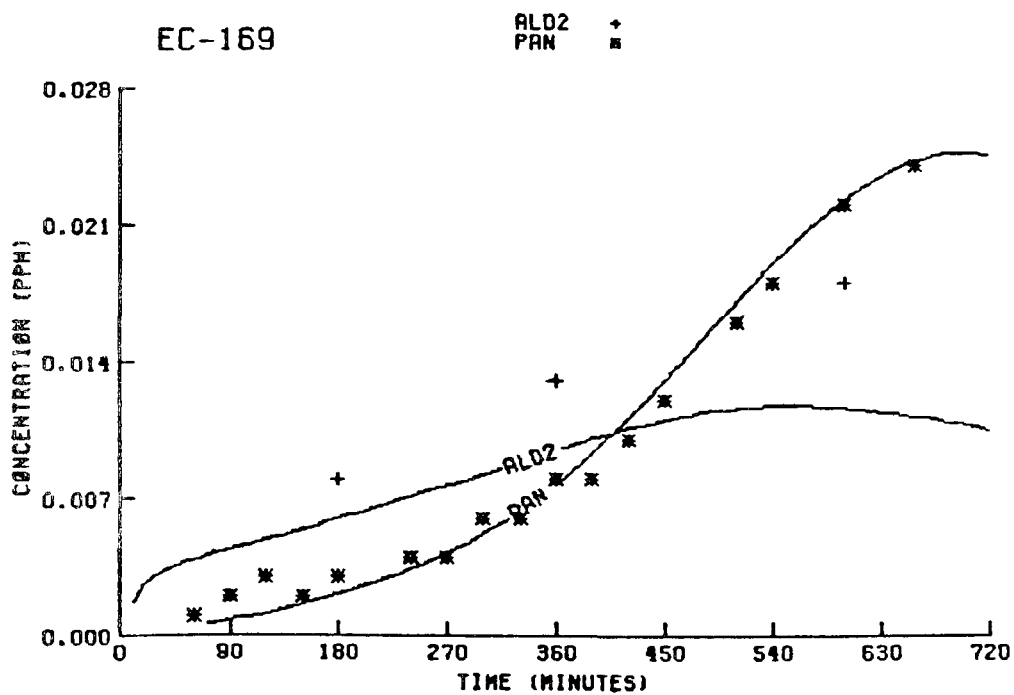
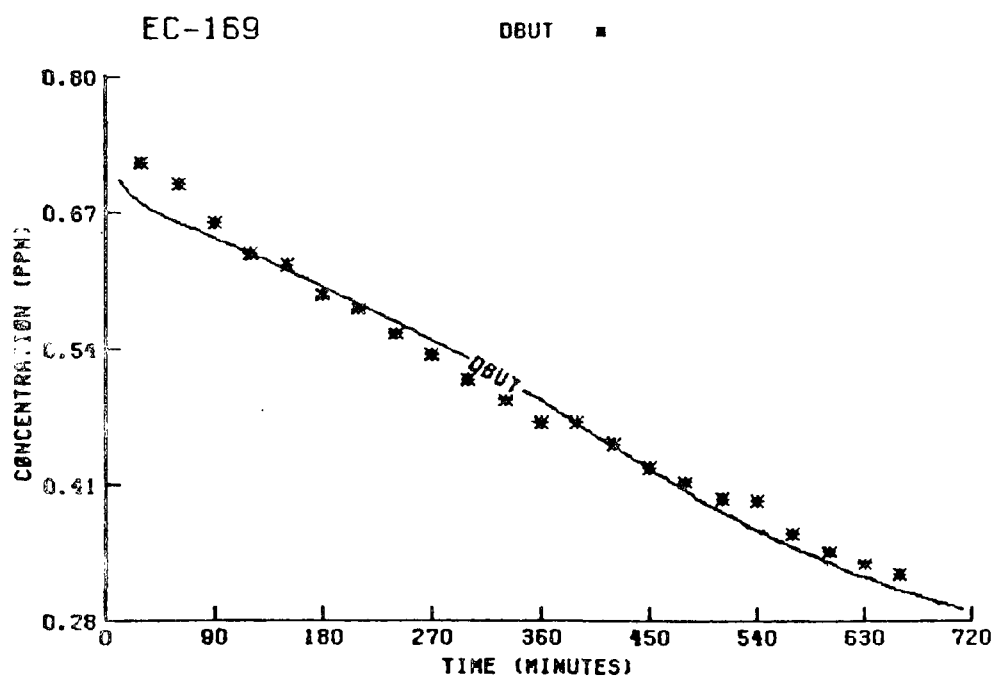
N02

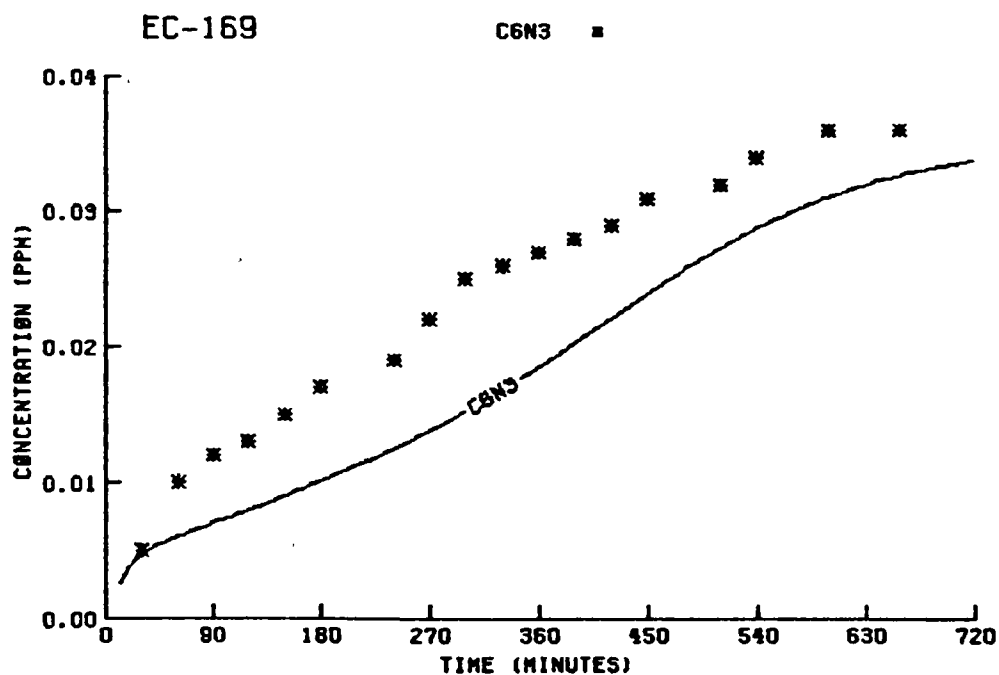
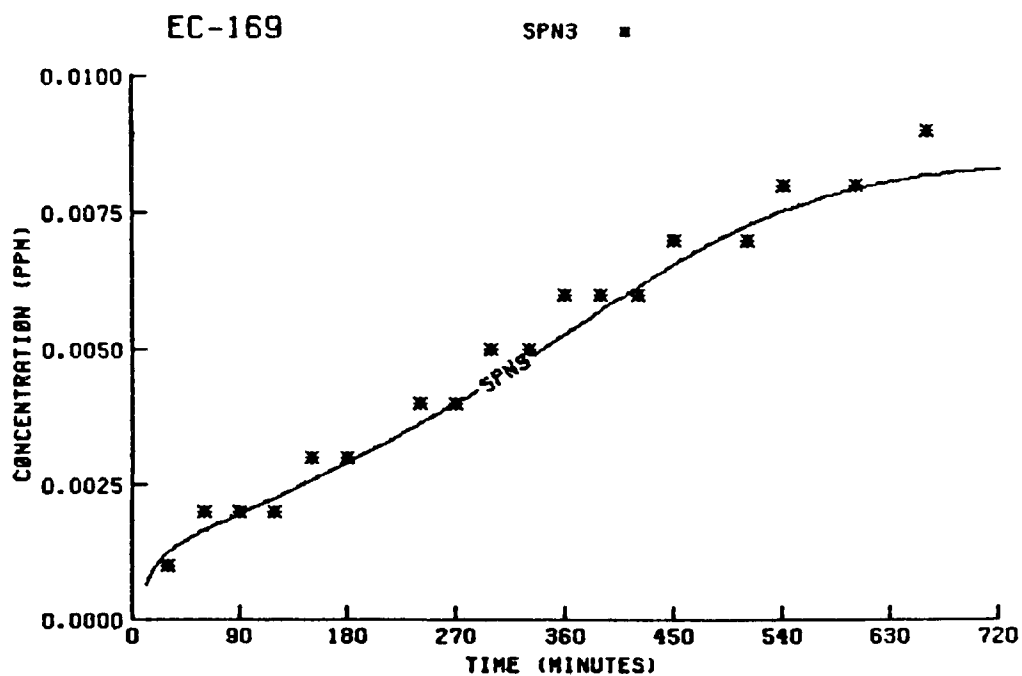
+

N0

■



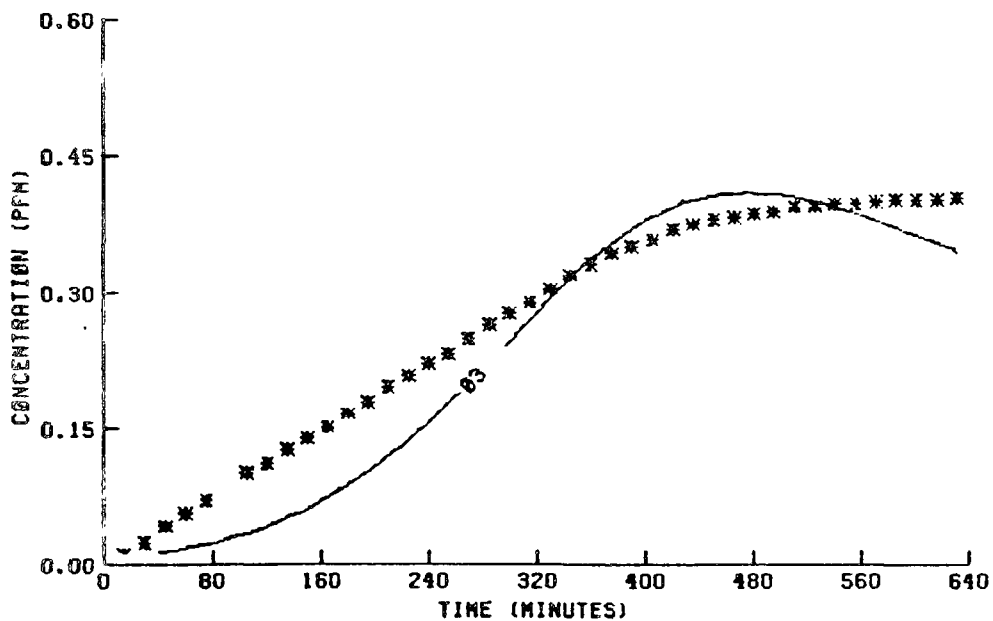




EC-171

03

■



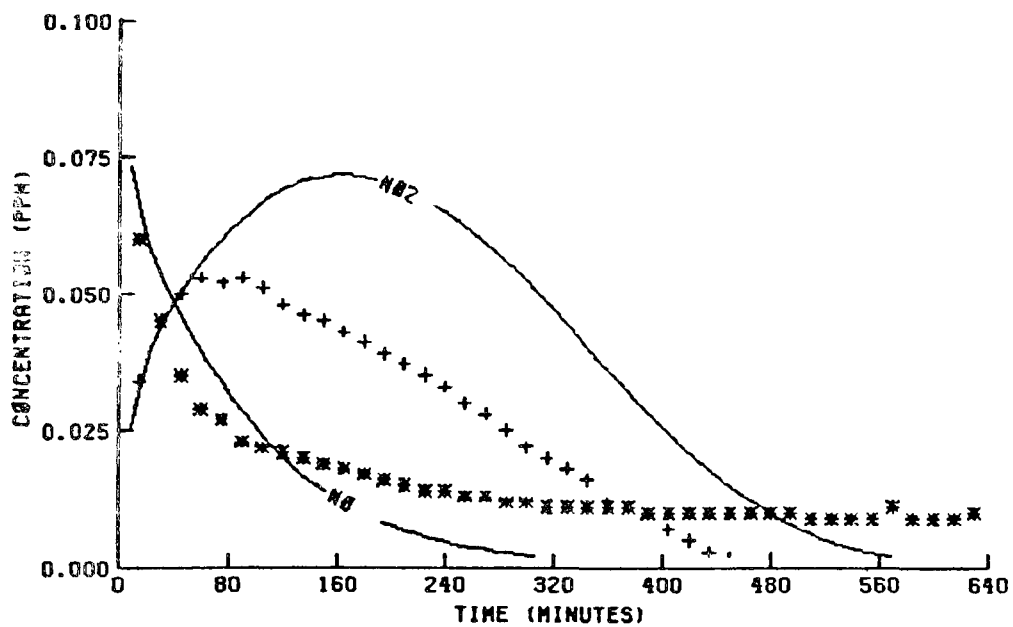
EC-171

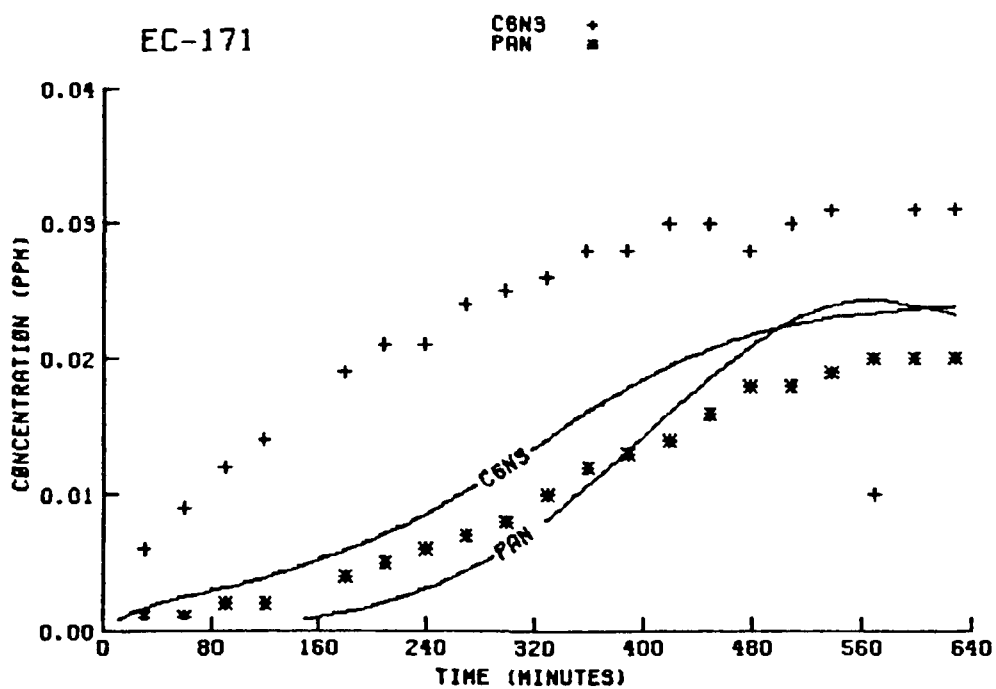
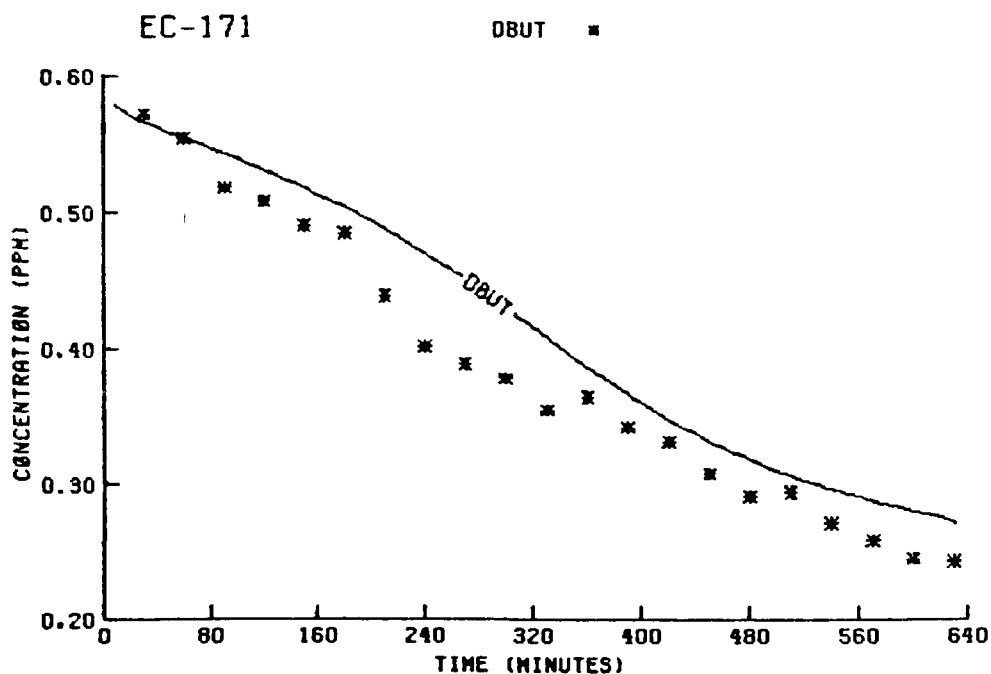
NB2

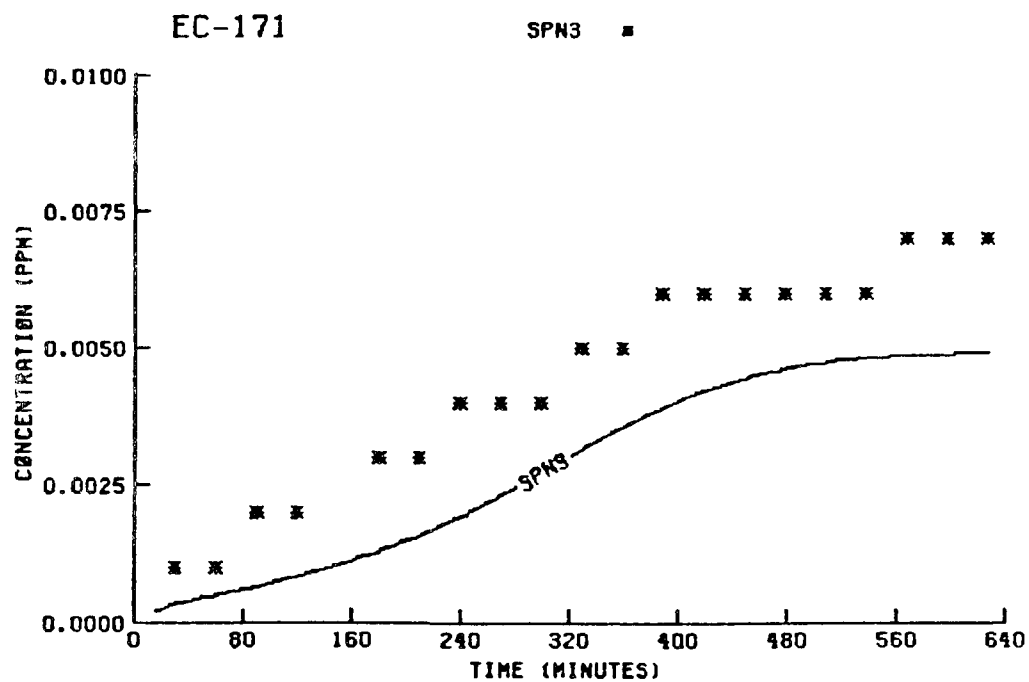
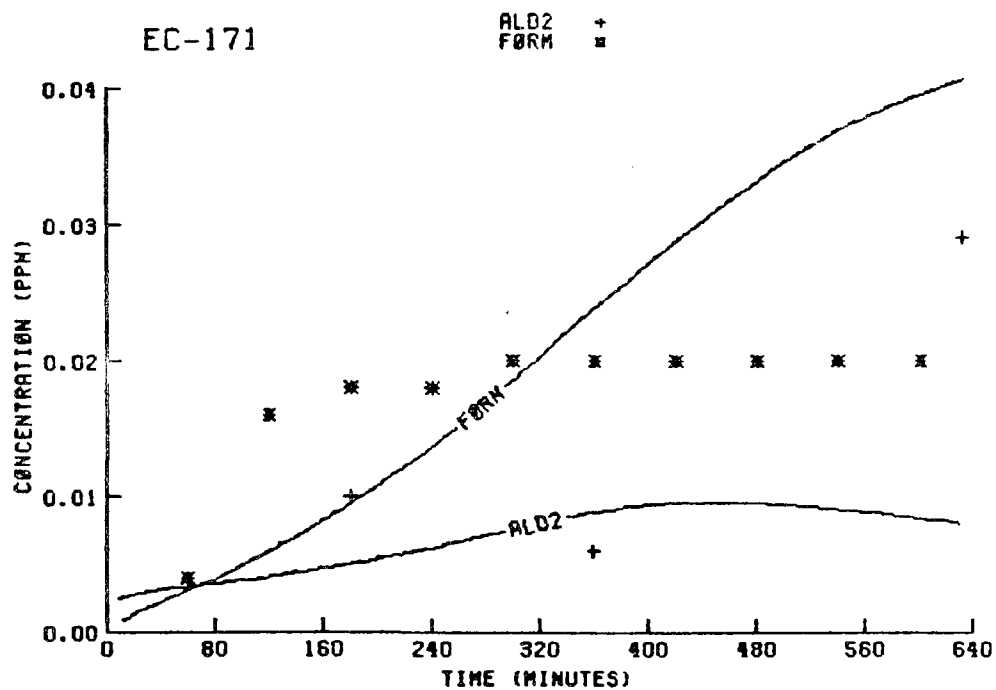
+

NB

■

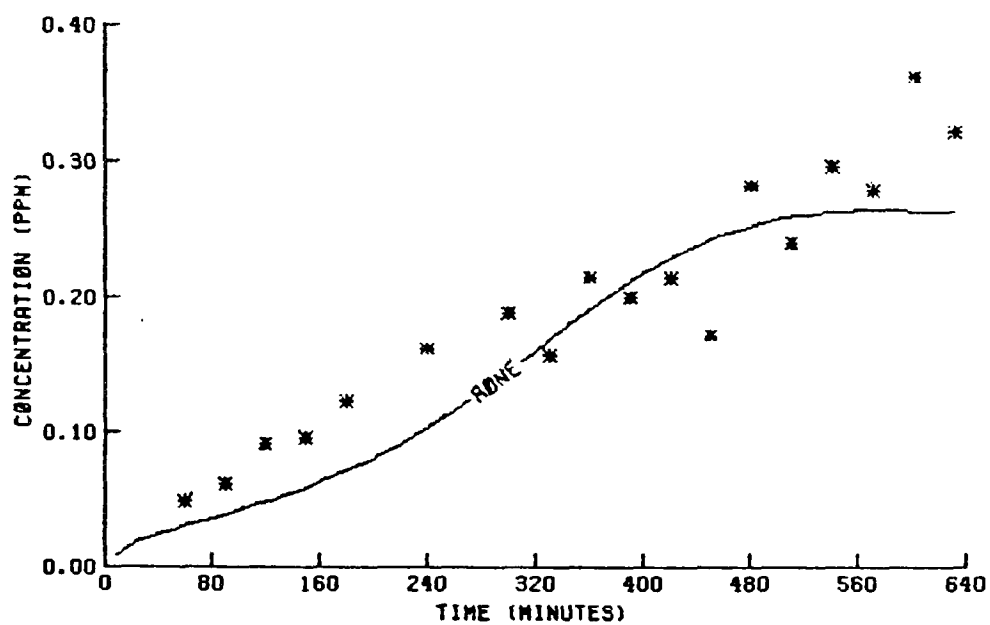






EC-171

ADNE *

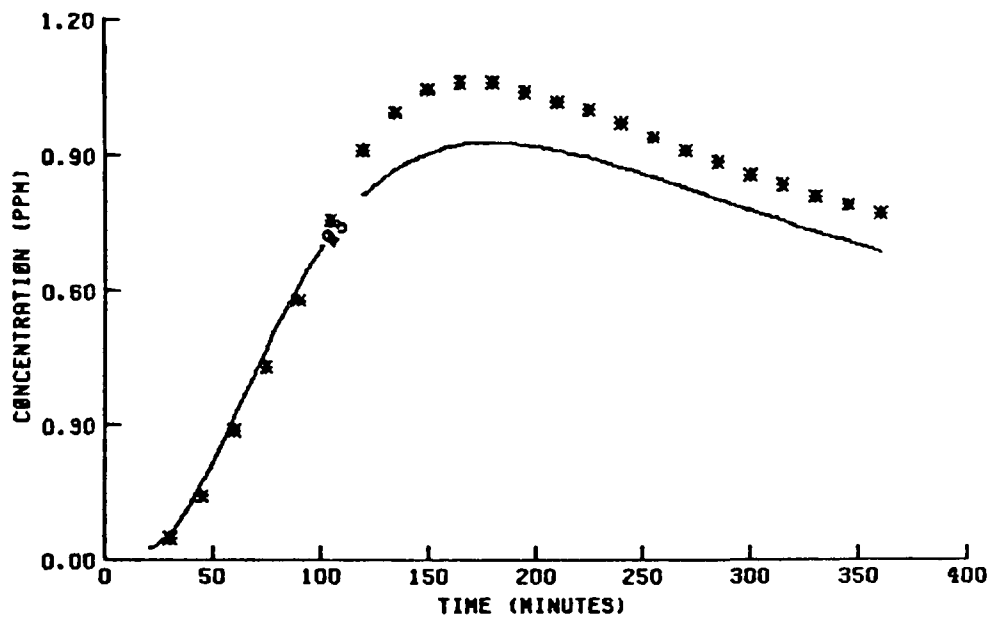


UCR ETHYLENE/PROPYLENE EXPERIMENTS

EC-144

83

■



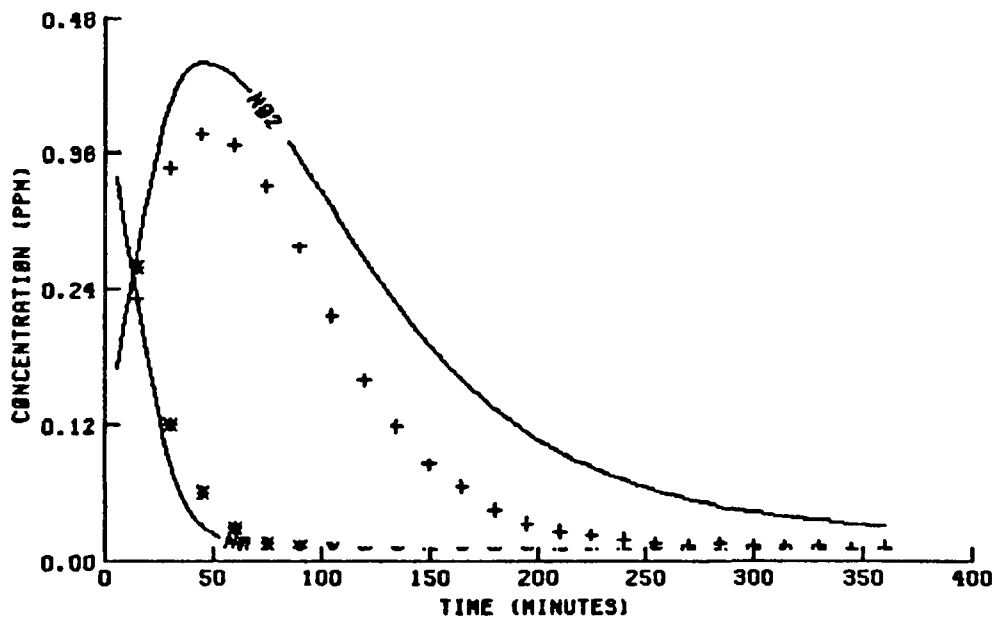
EC-144

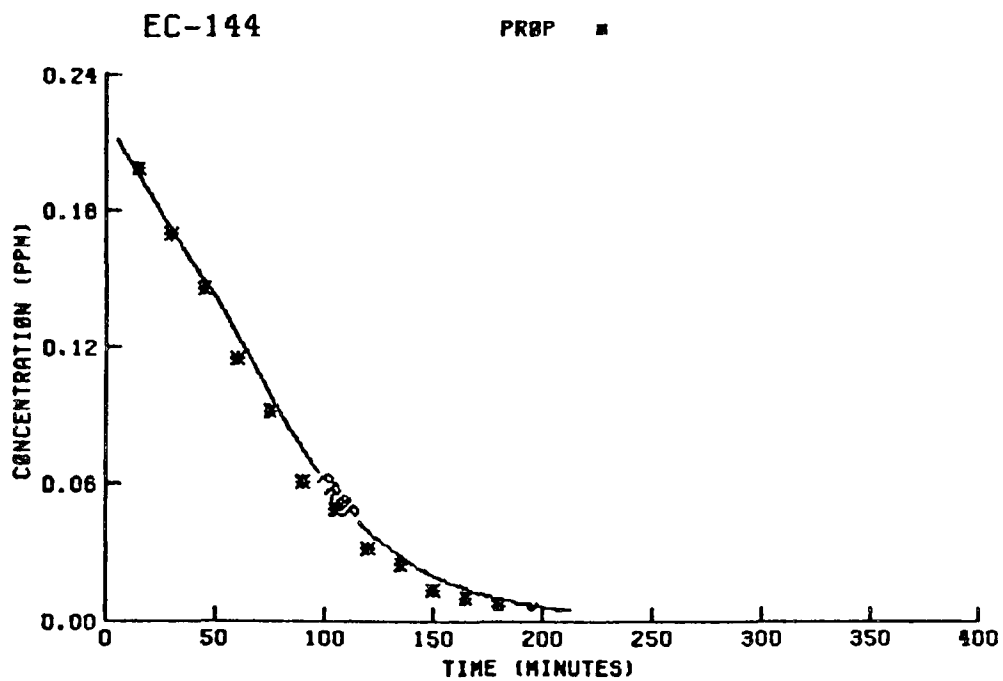
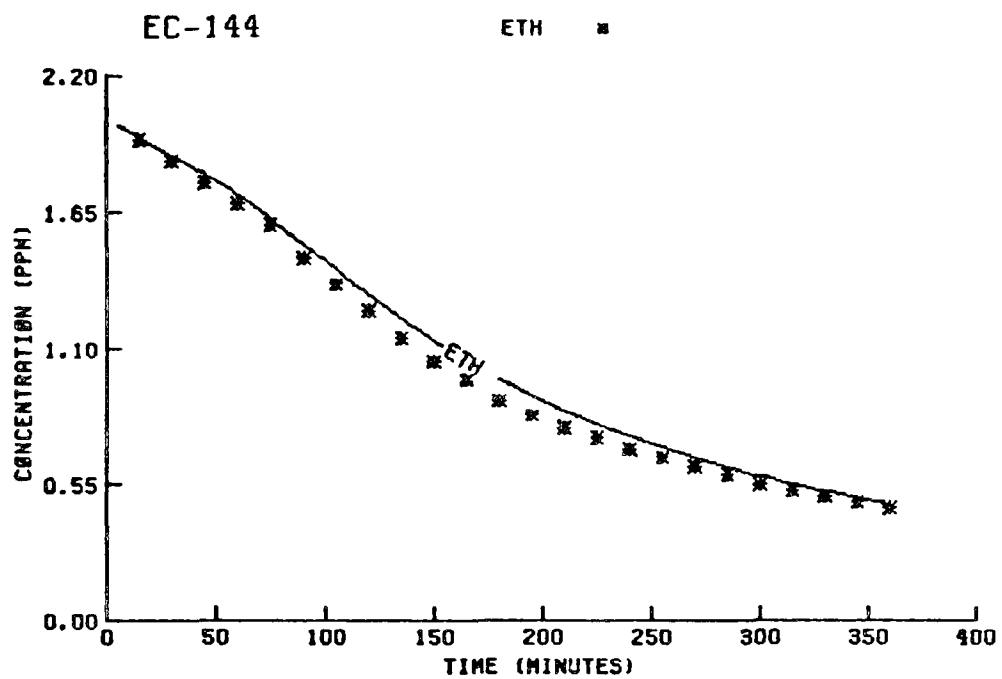
N82

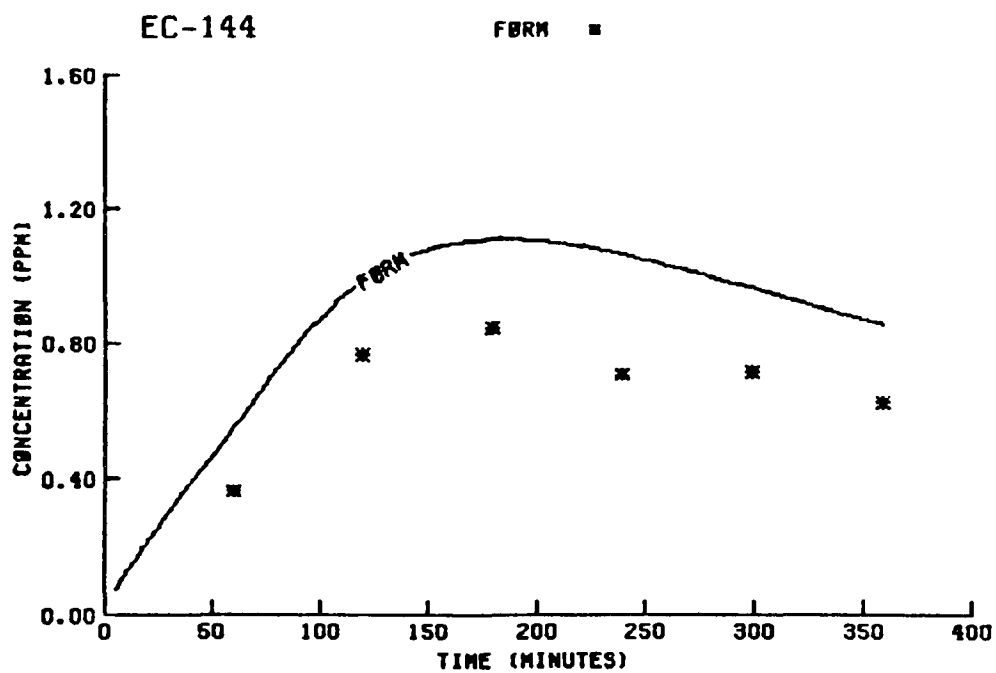
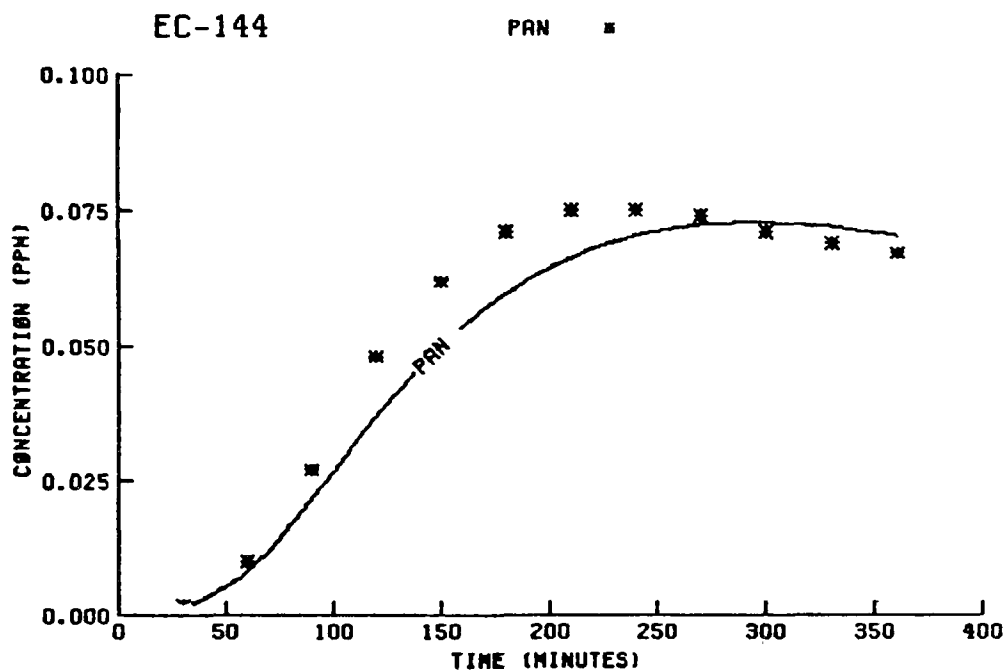
+

N8

■

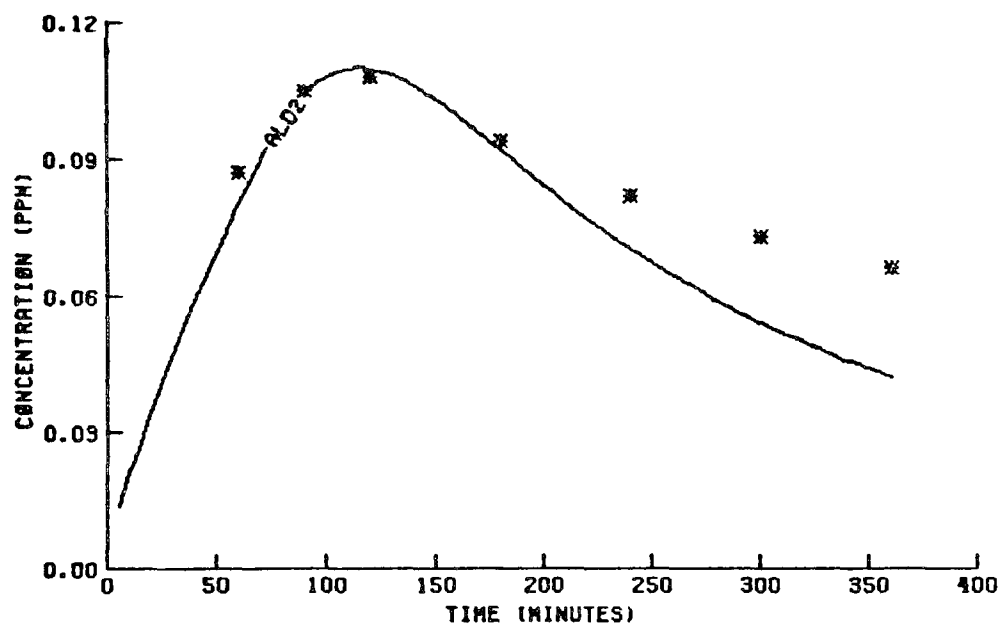


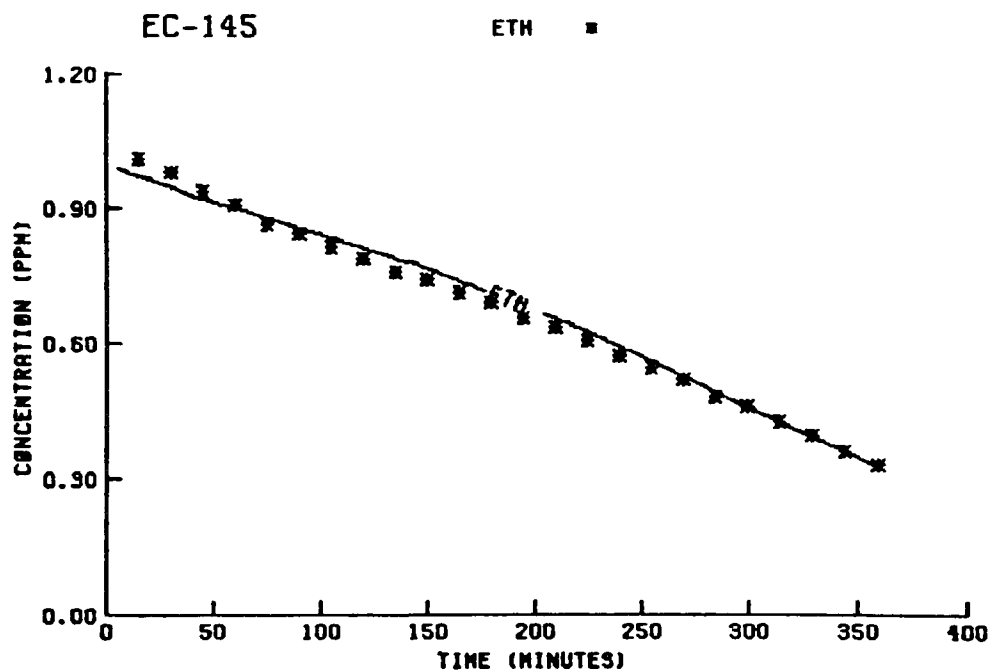
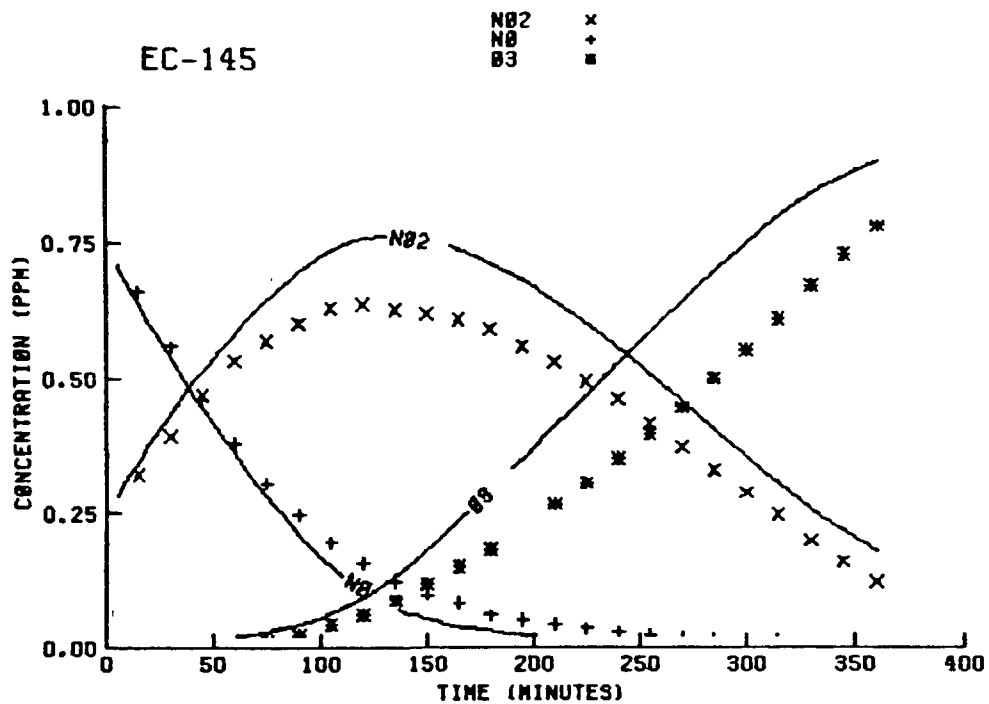




EC-144

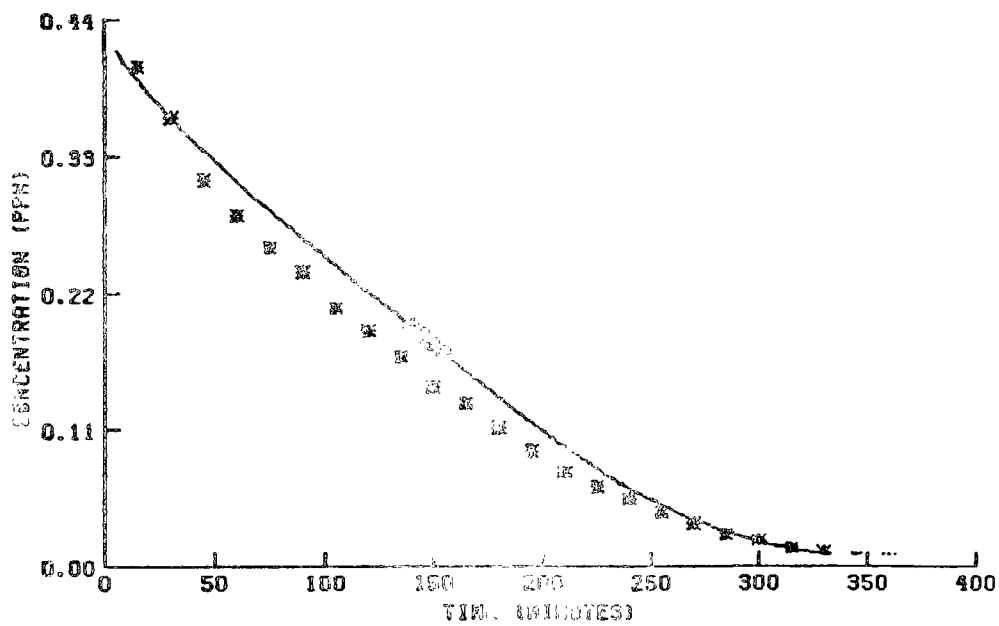
ALD2 ■





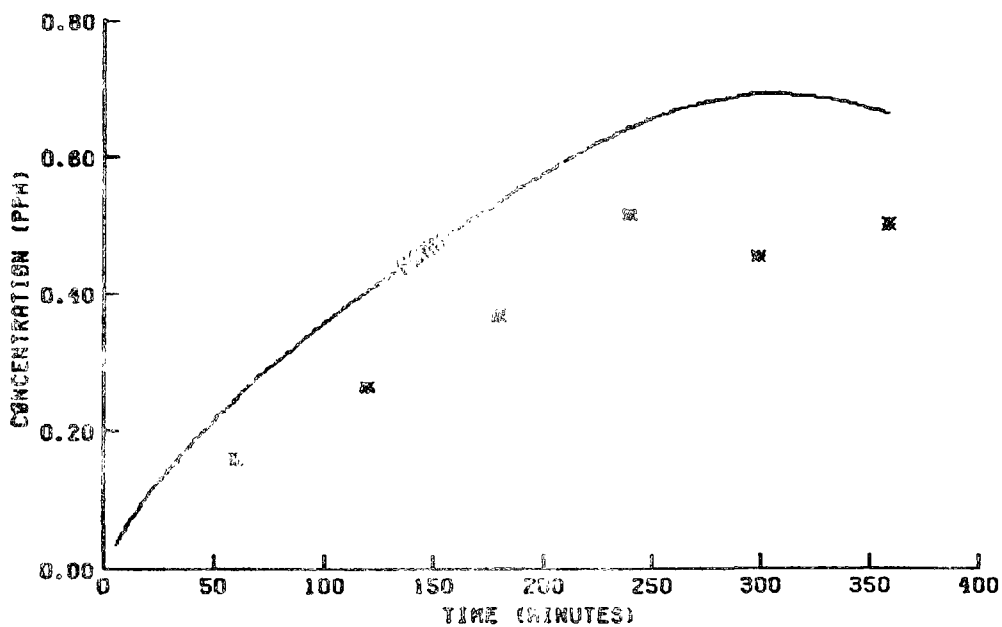
EC-145

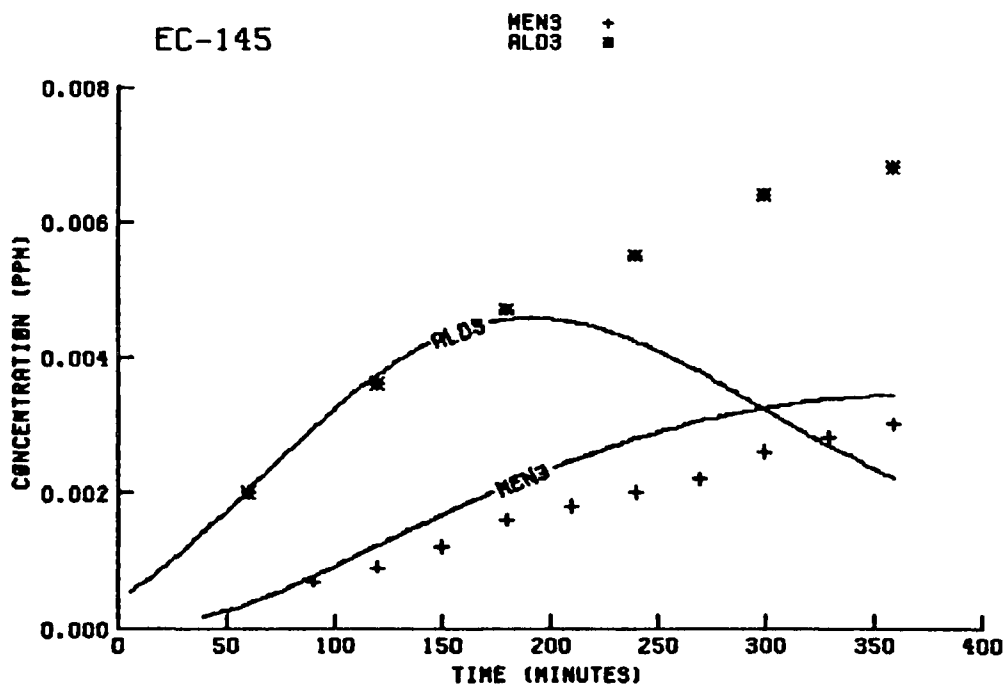
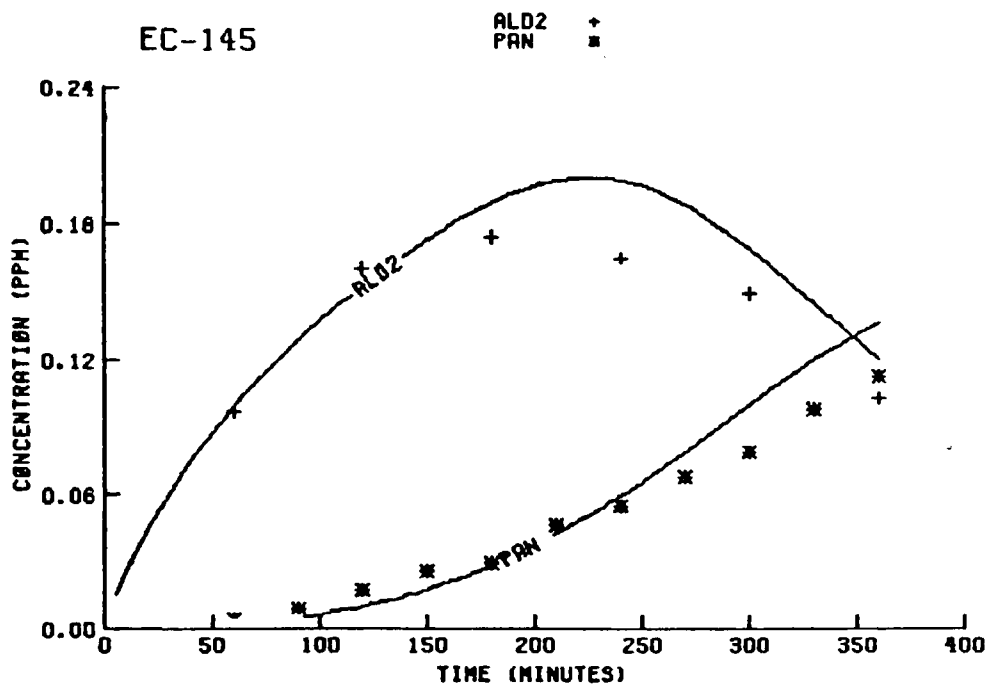
PWBP

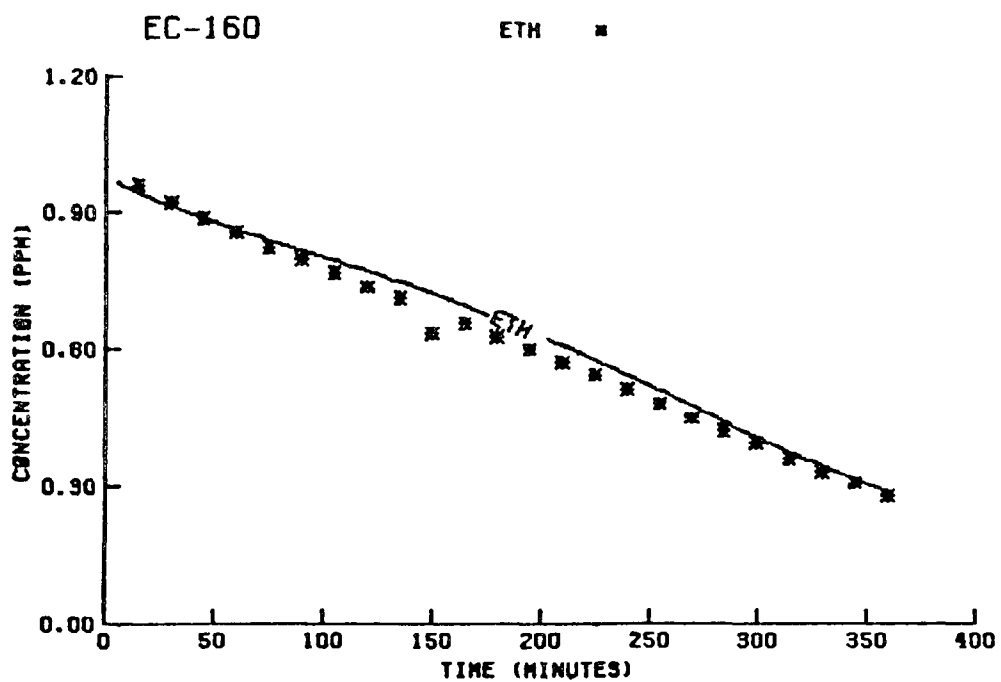
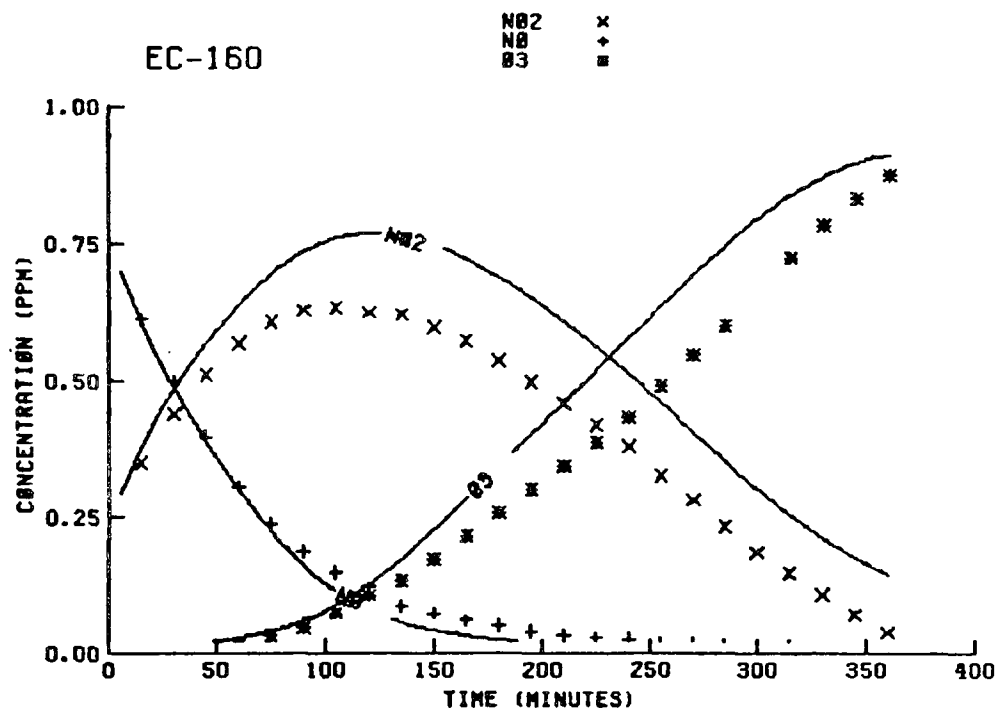


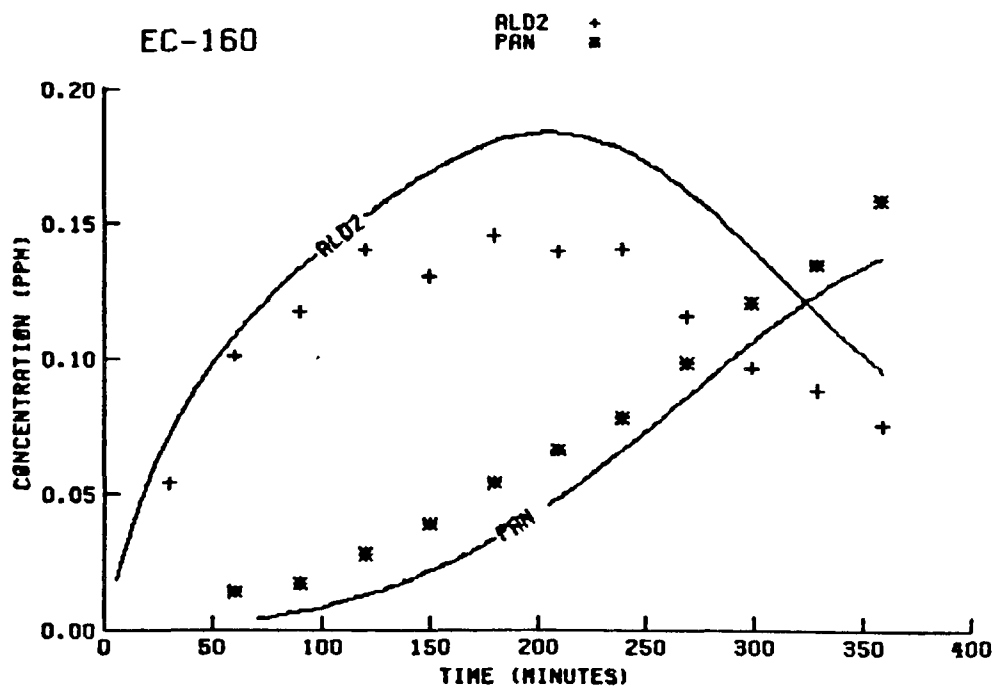
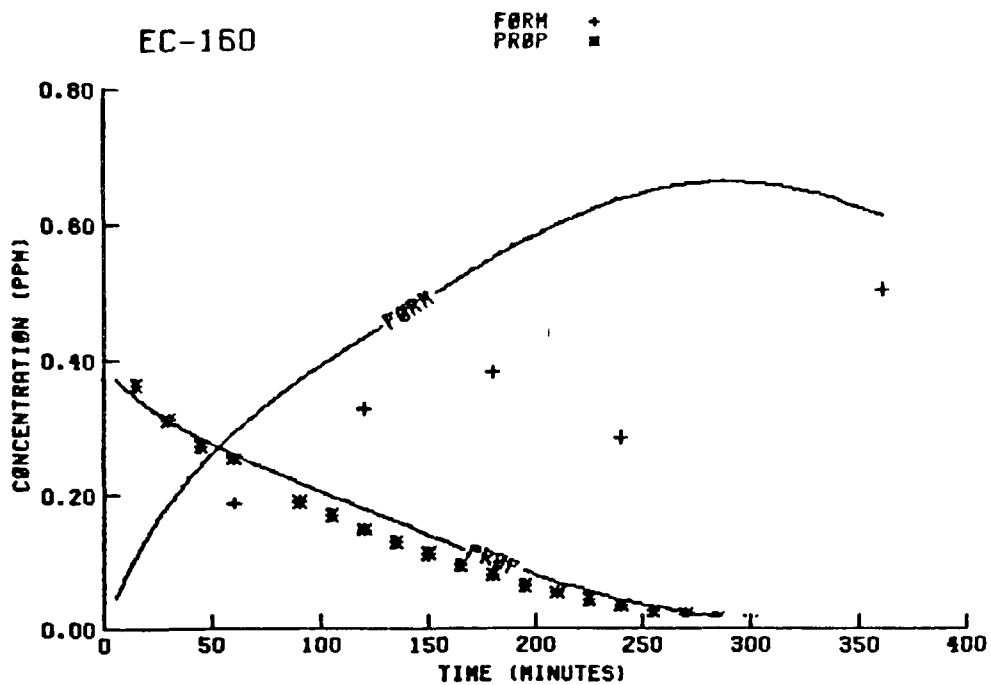
EC-145

FORM



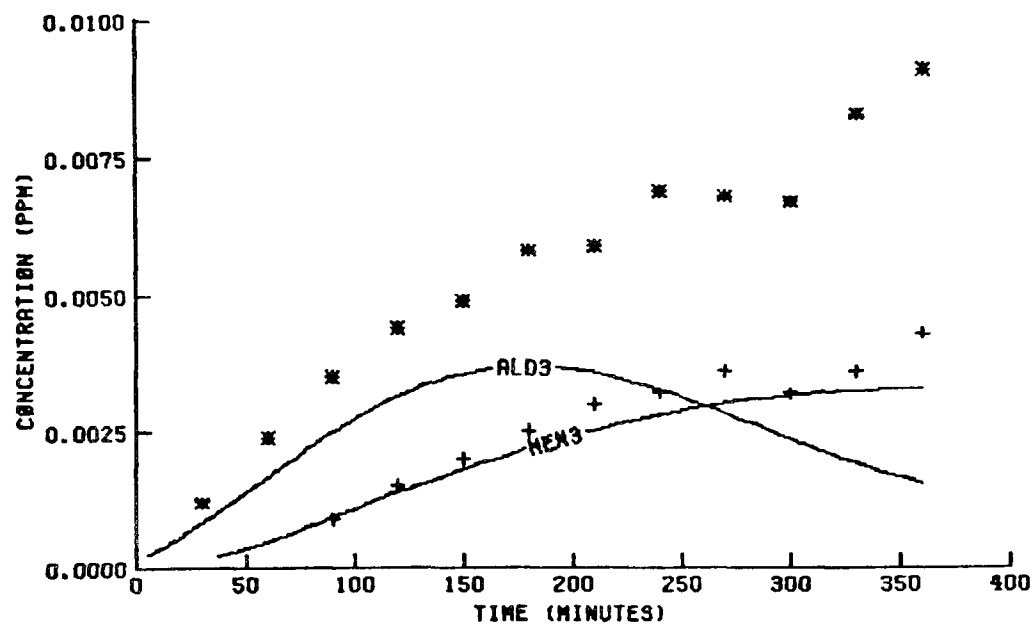




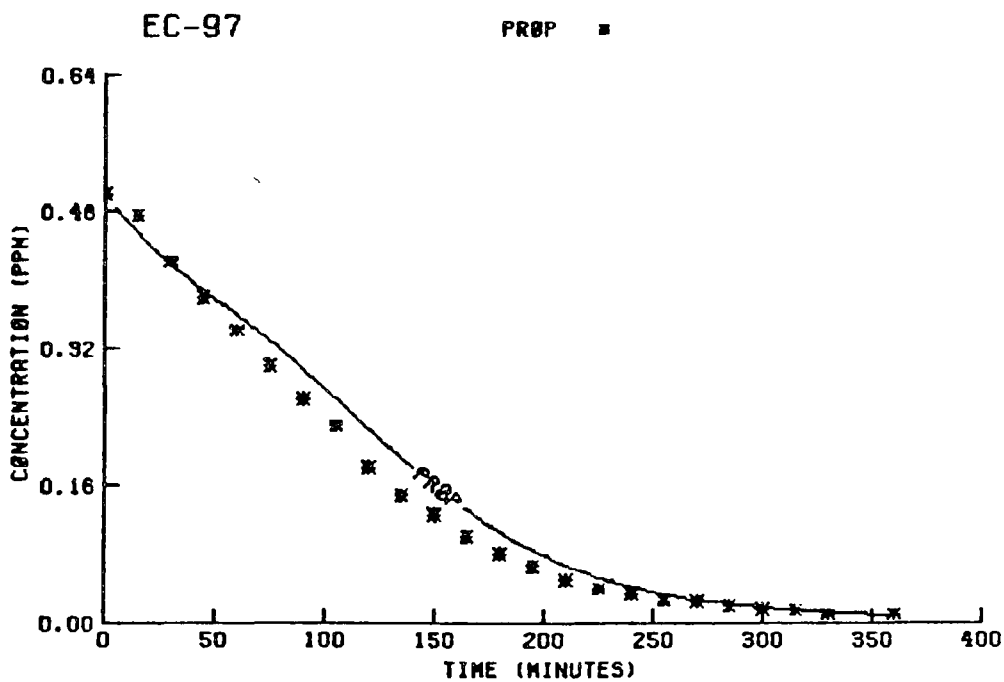
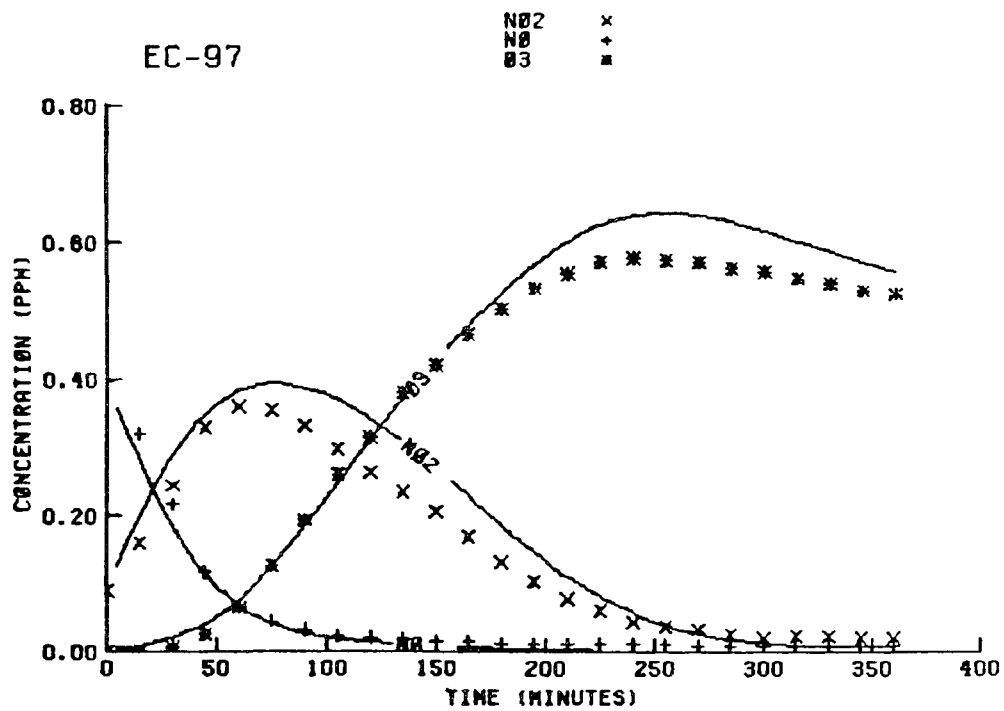


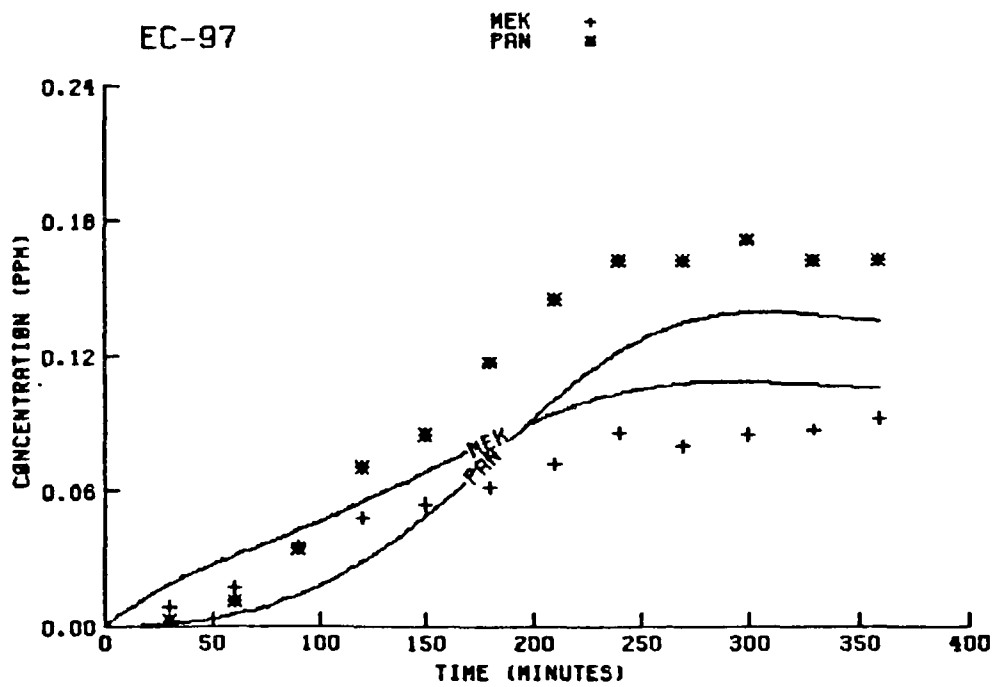
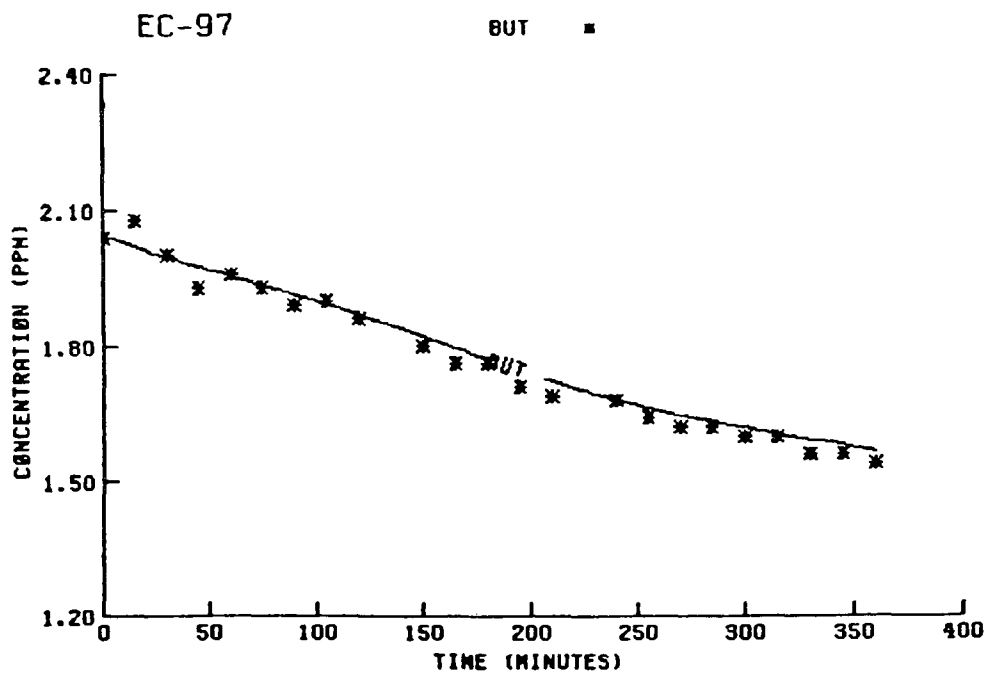
EC-160

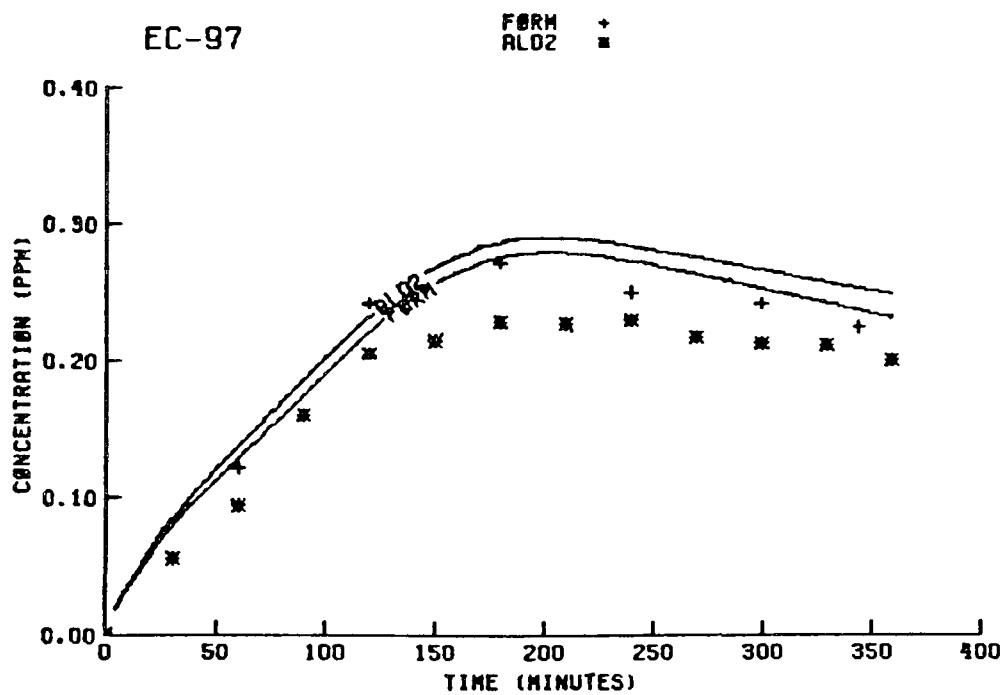
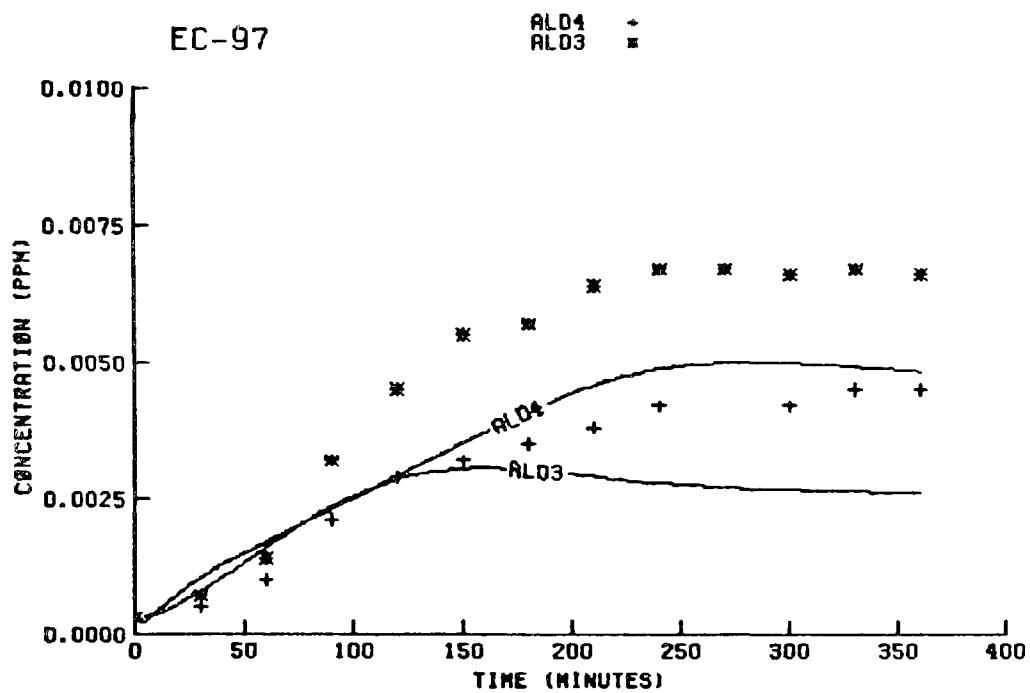
MEN3 +
ALD3 *

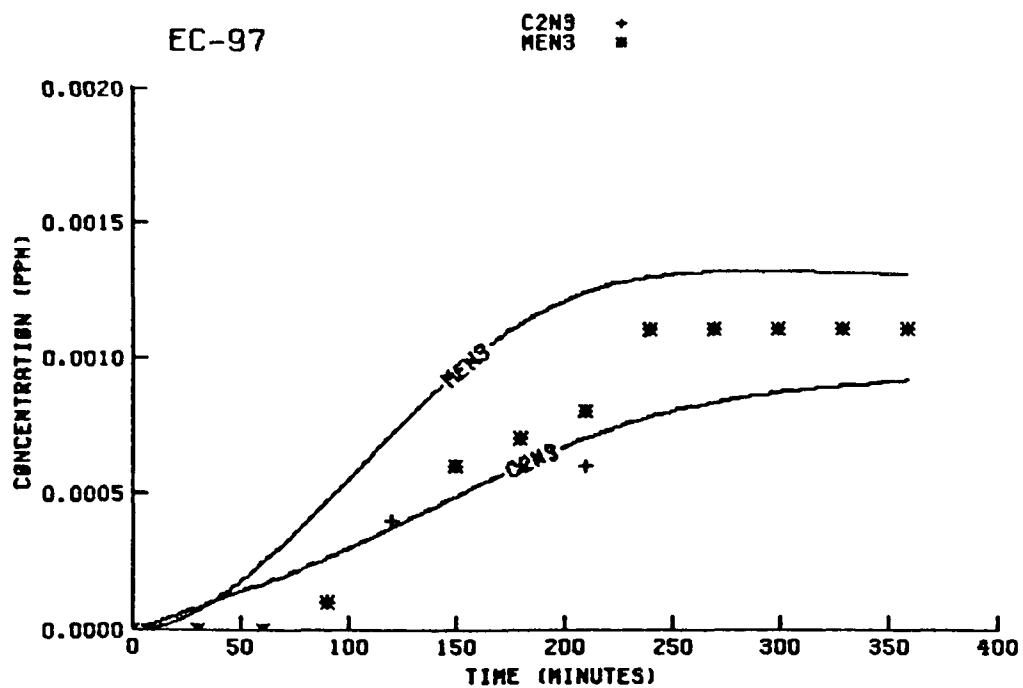
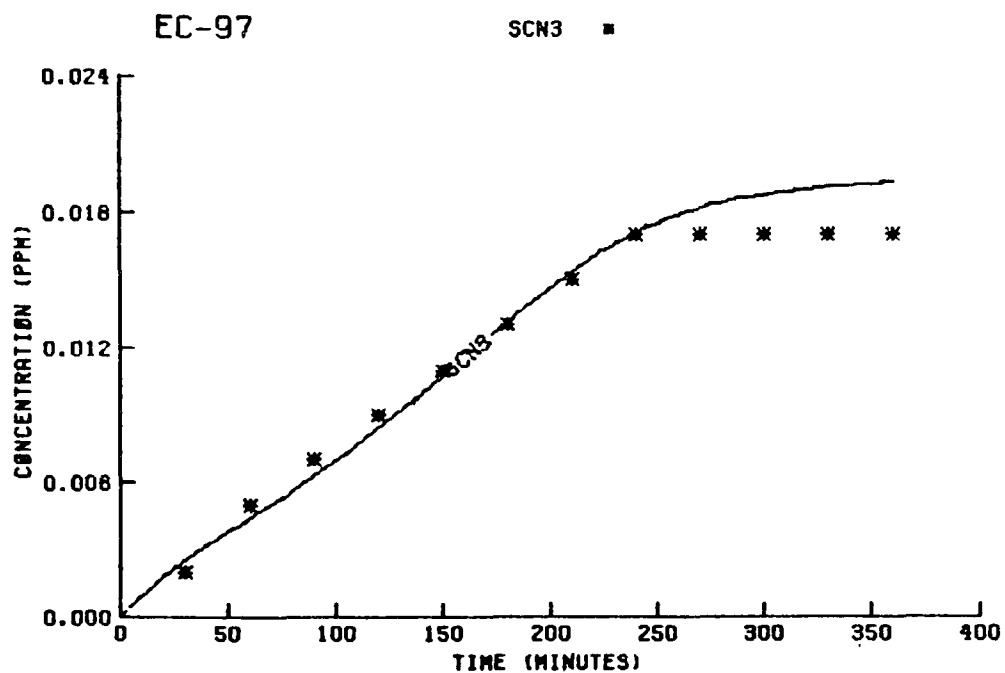


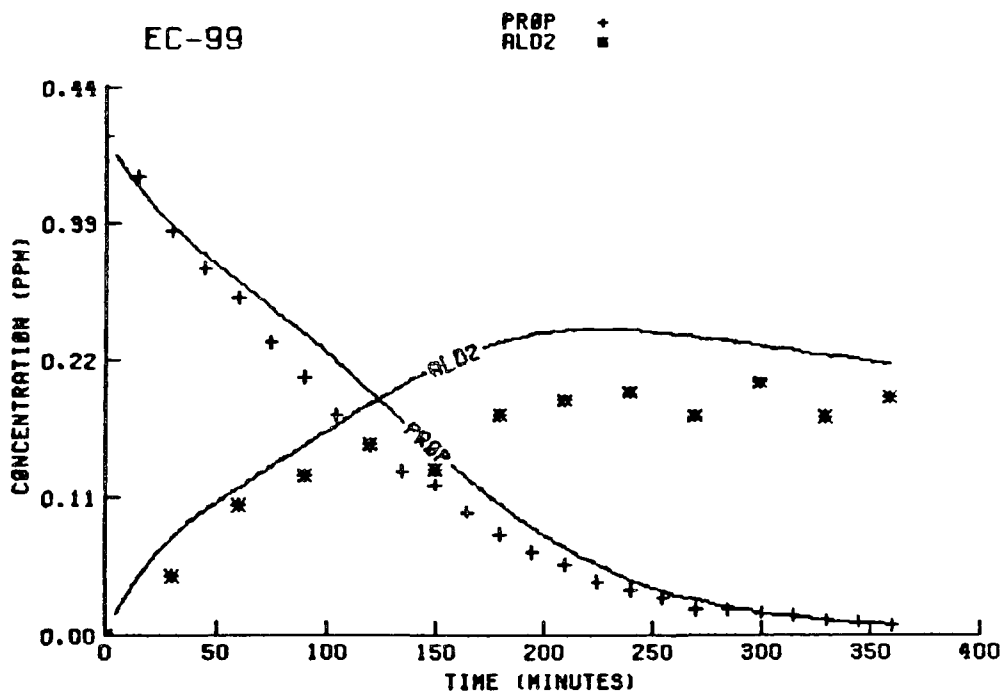
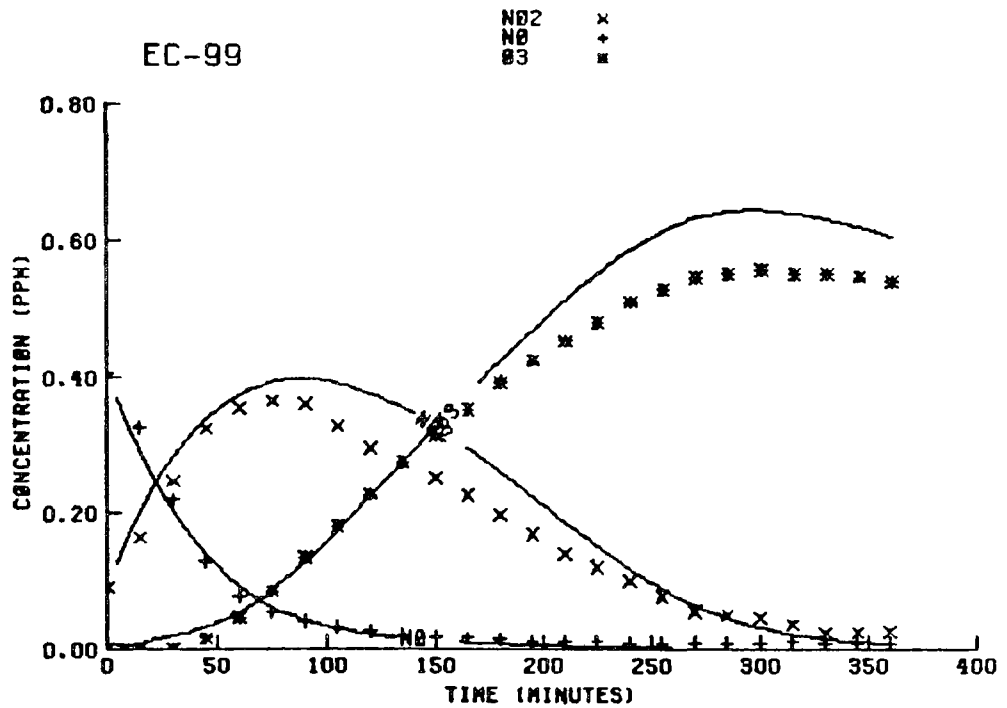
UCR PROPYLENE/BUTANE EXPERIMENTS

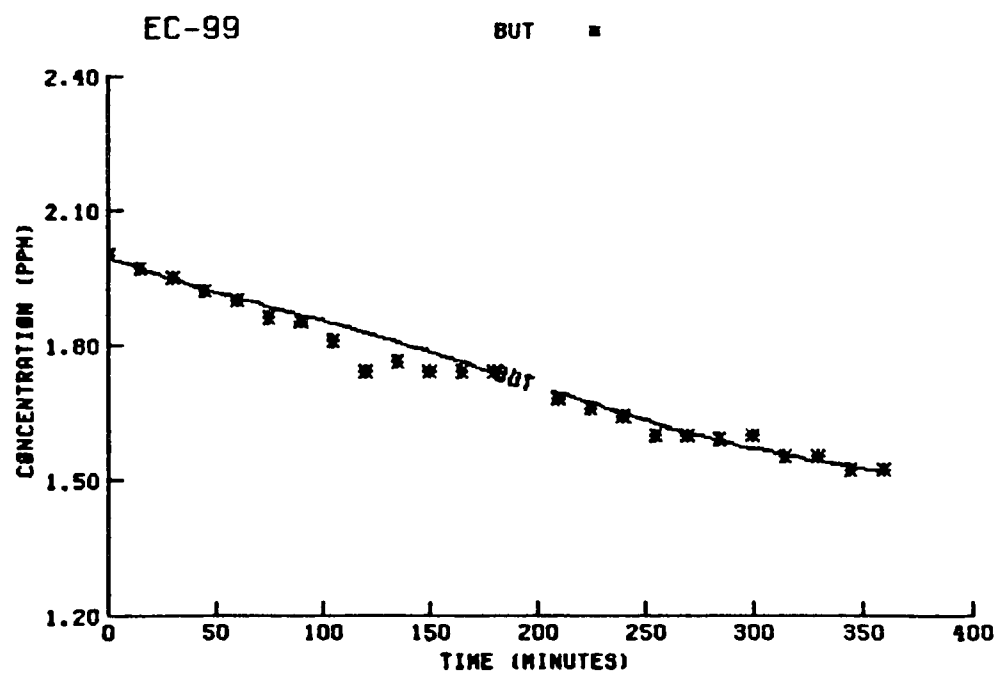
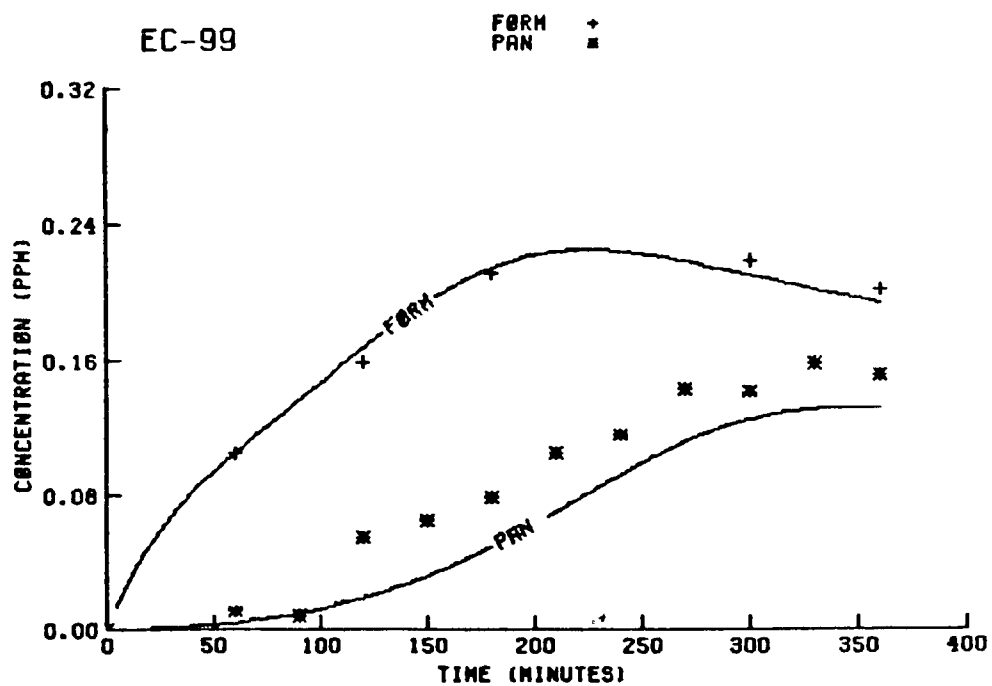


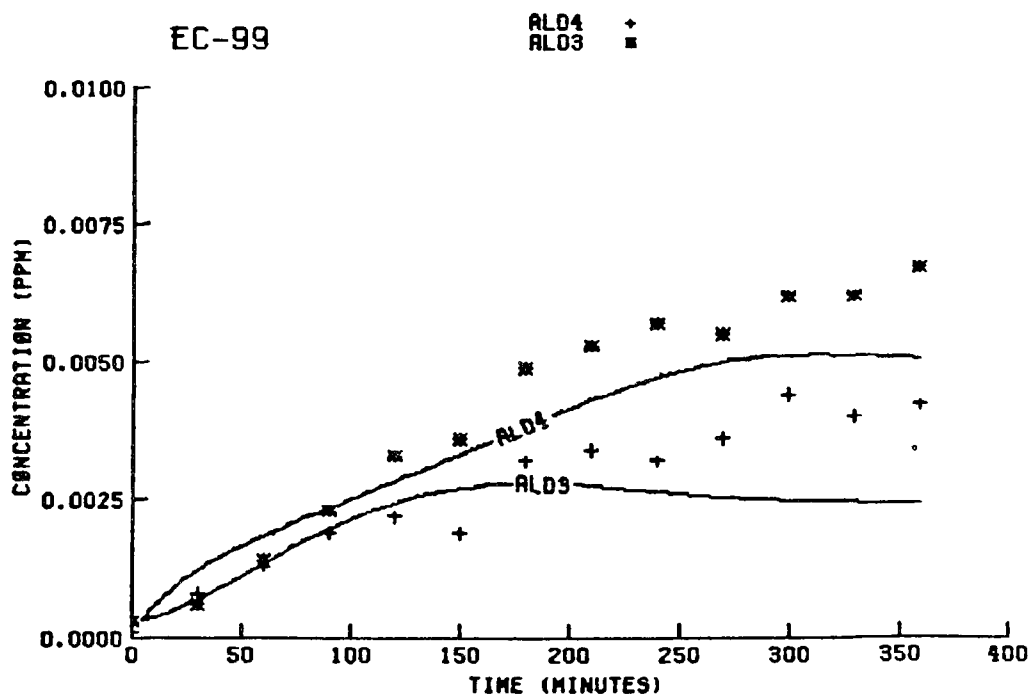
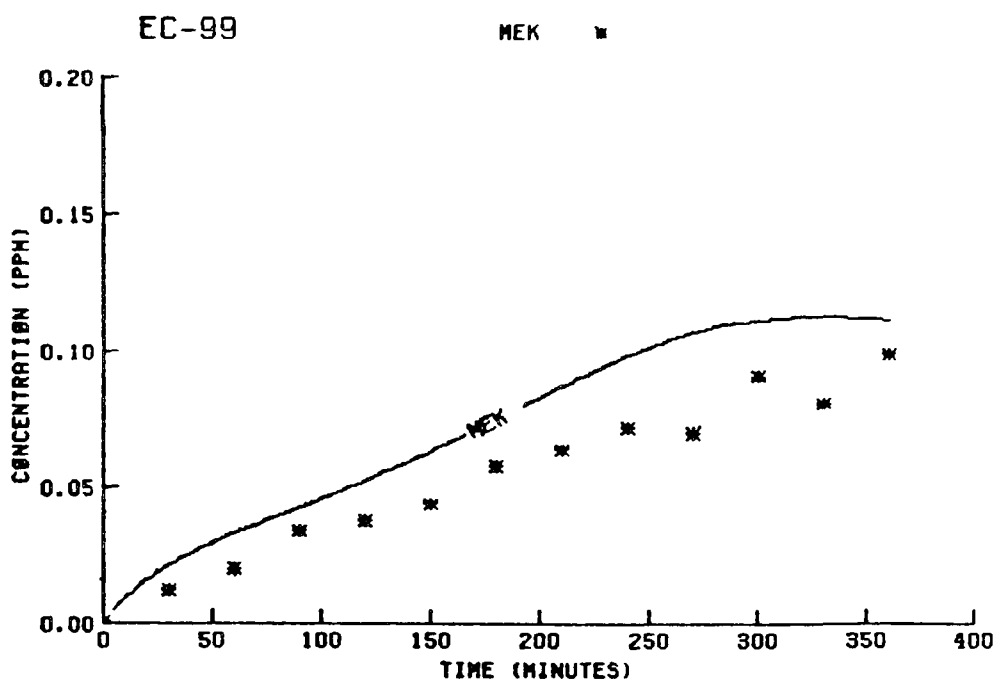


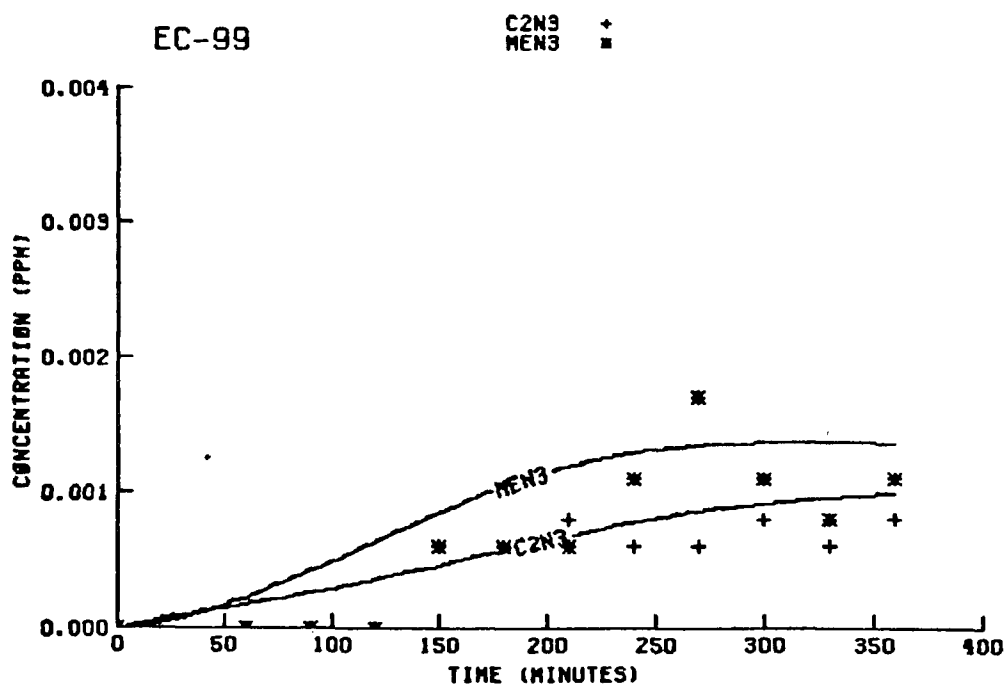
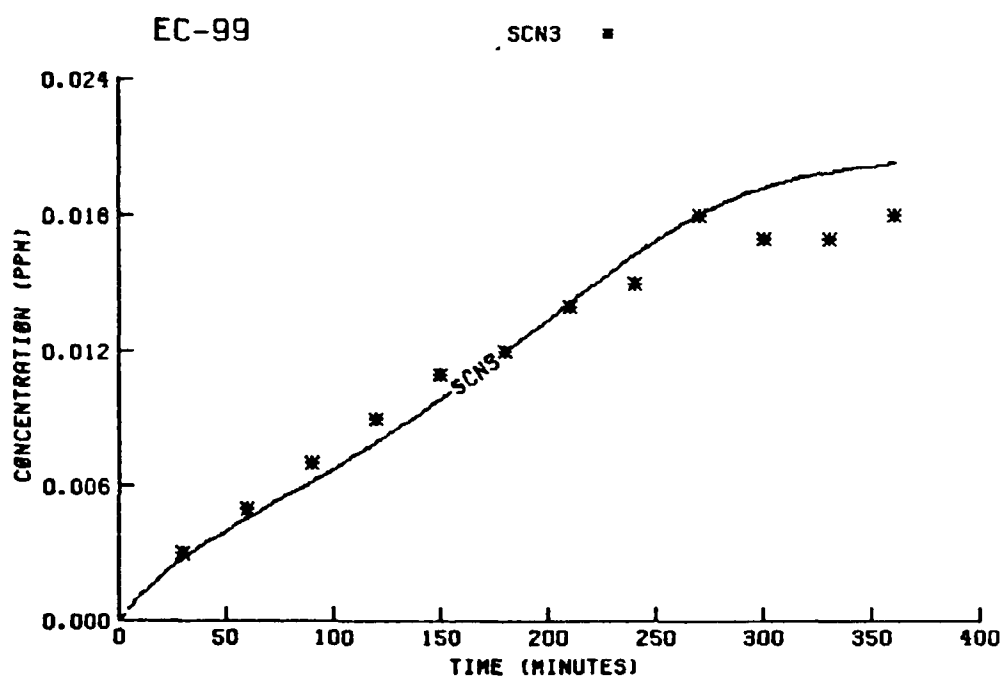






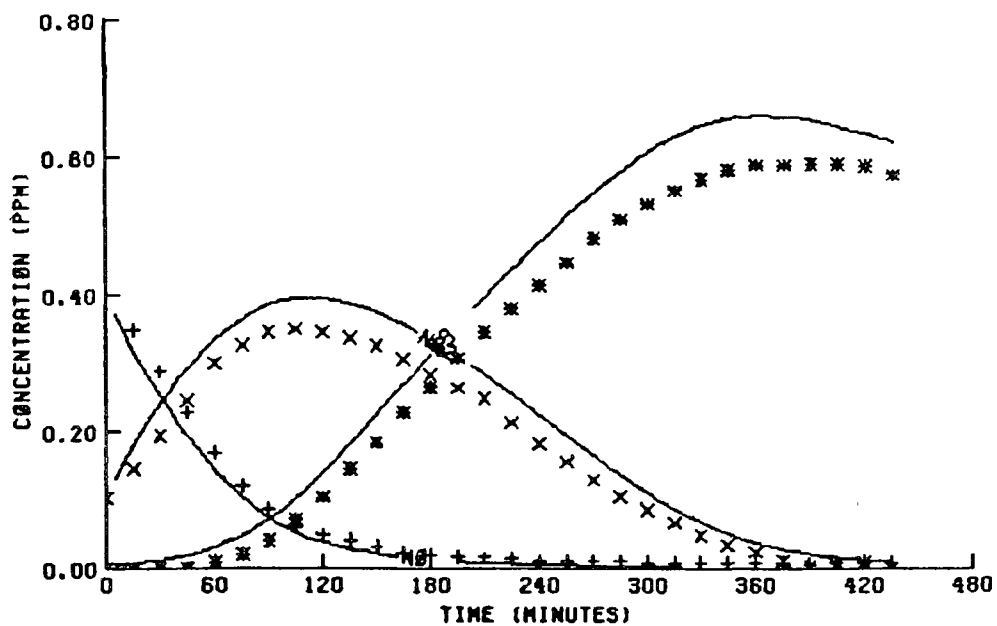






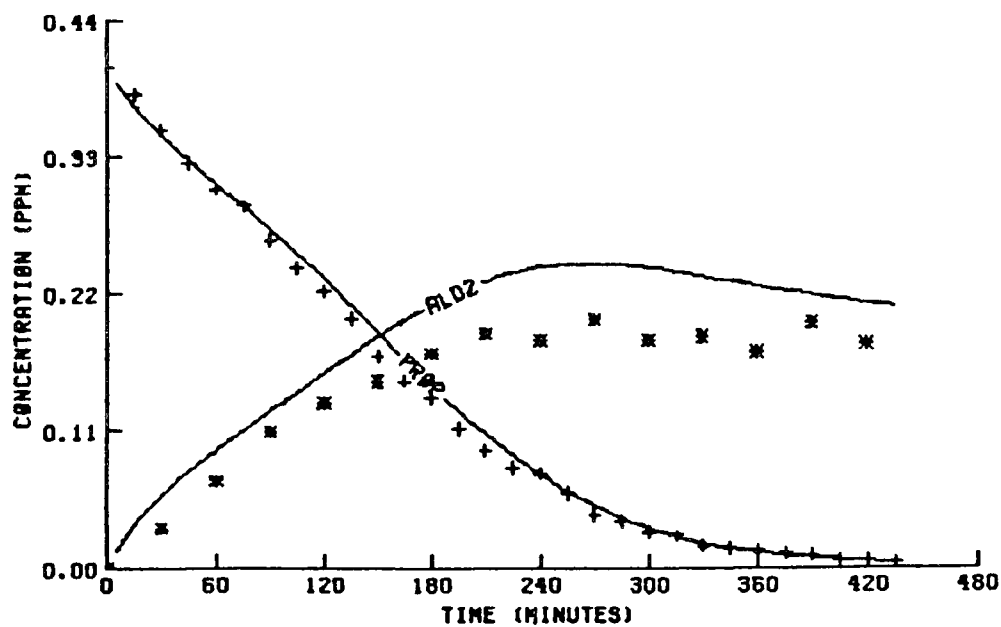
EC-106

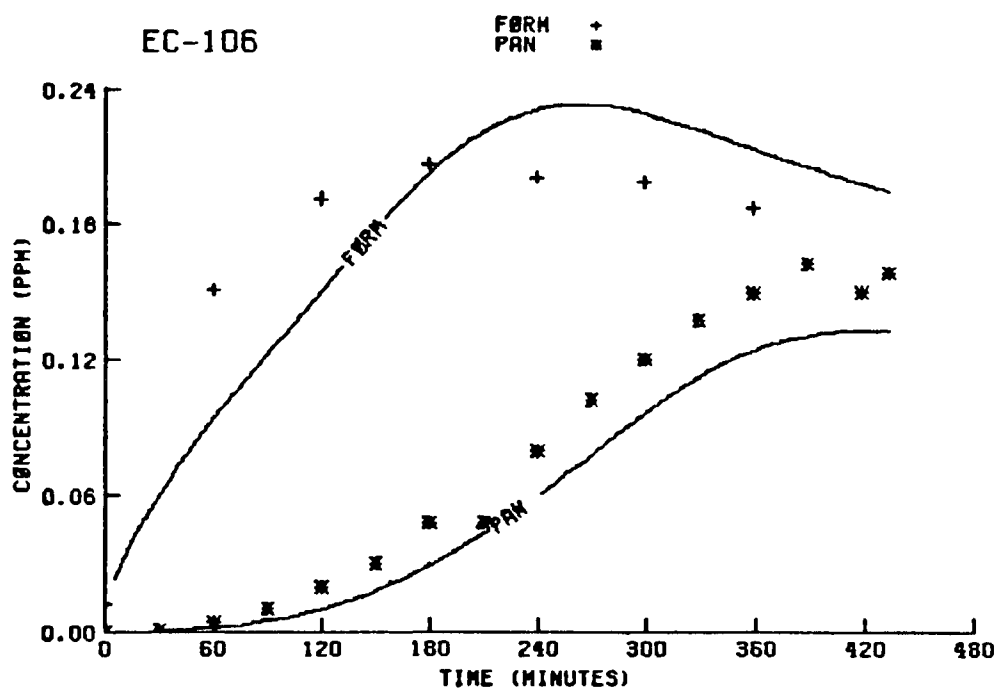
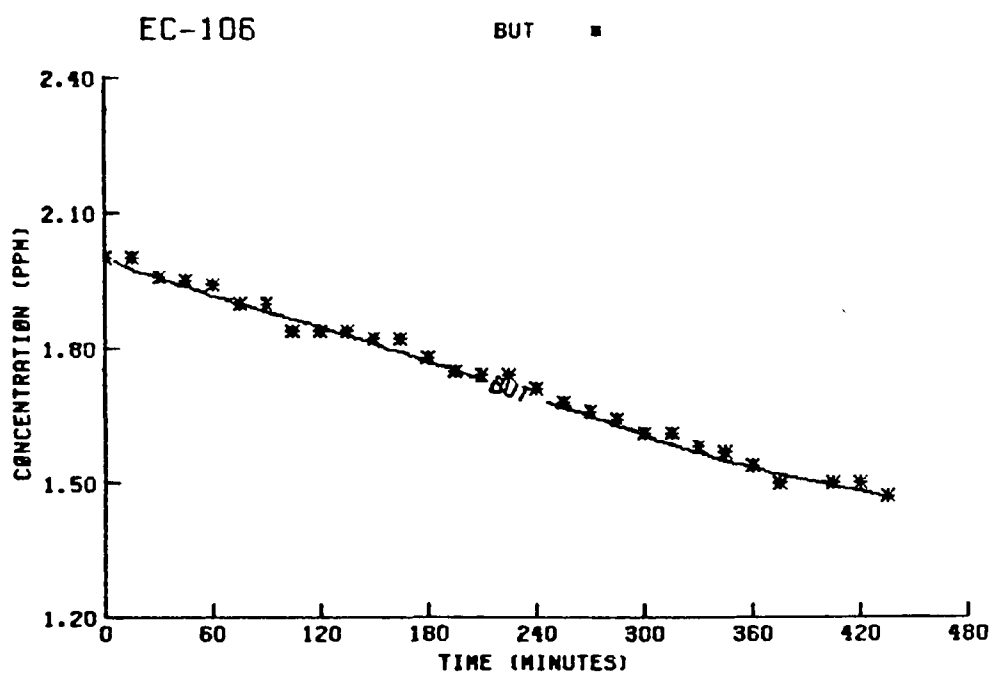
N02 x
N0 +
03 ■

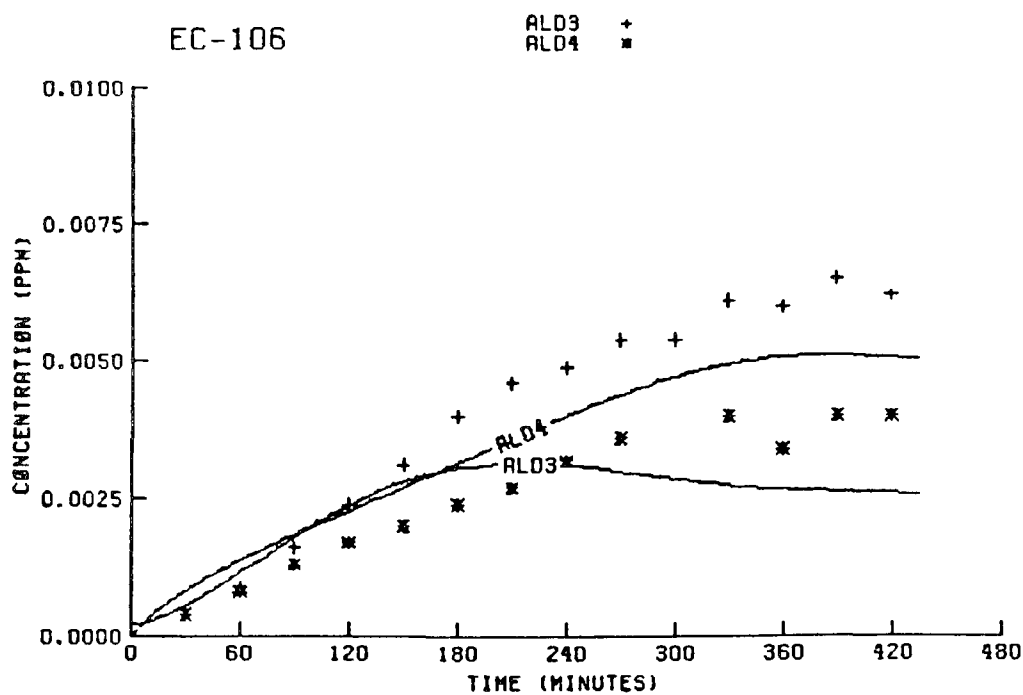
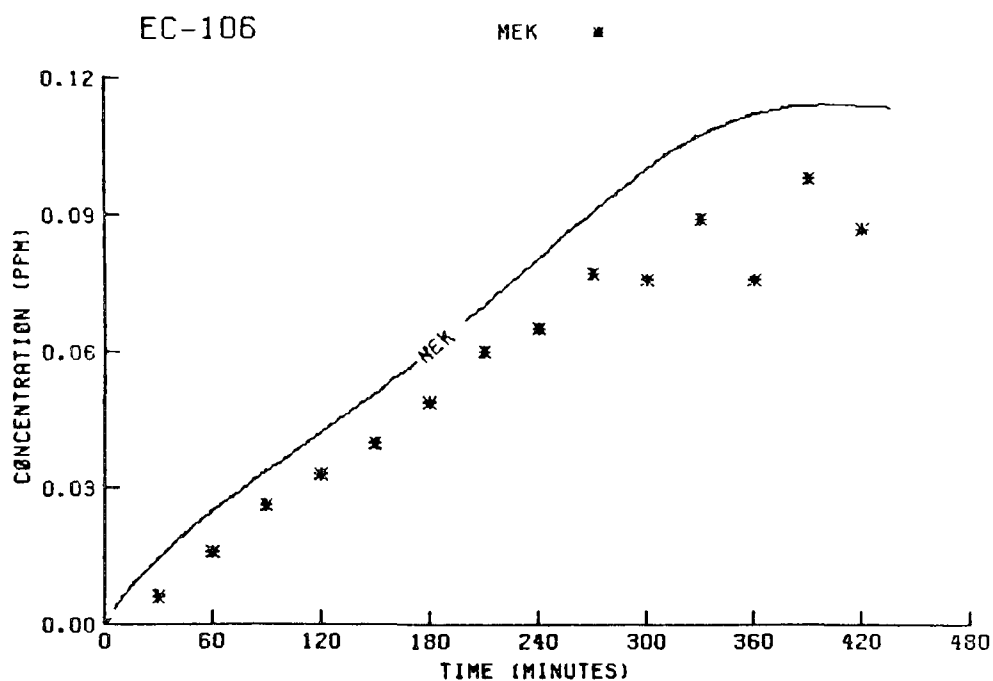


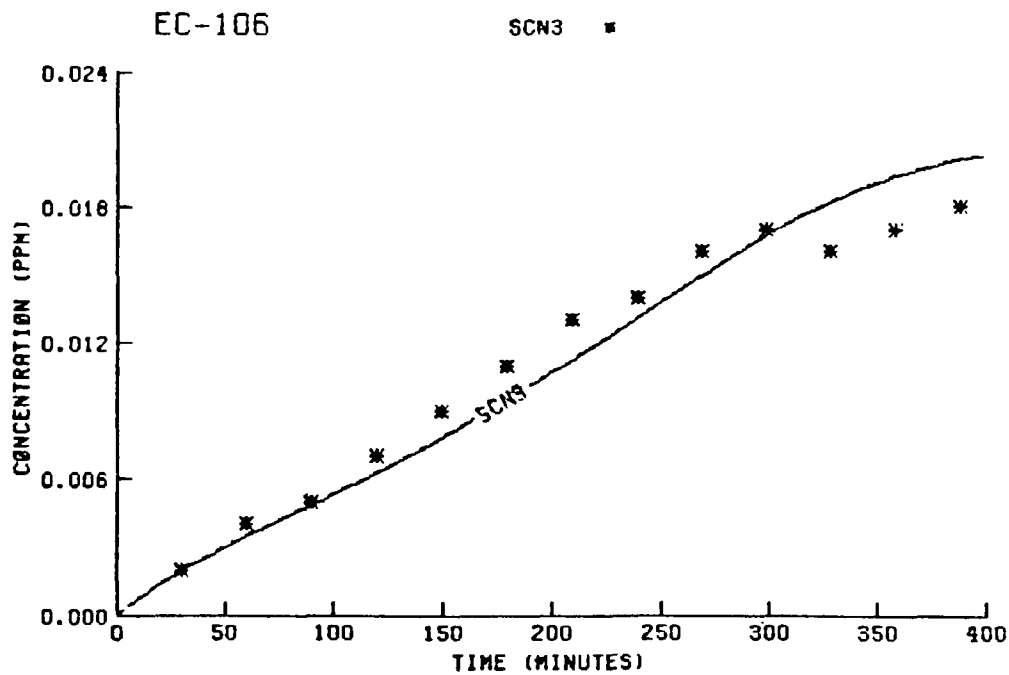
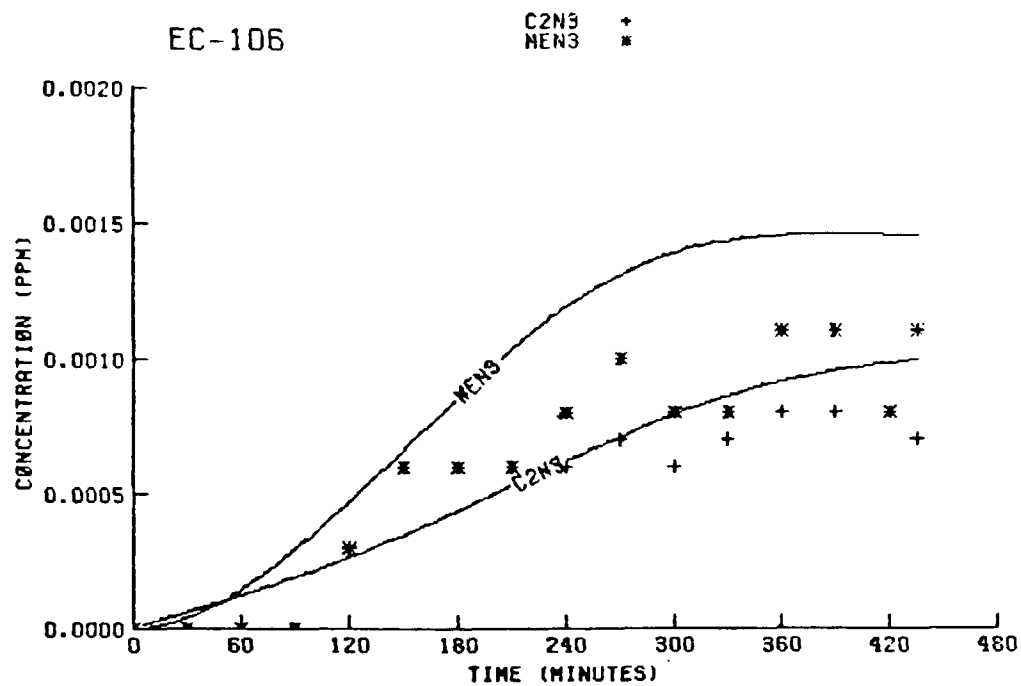
EC-106

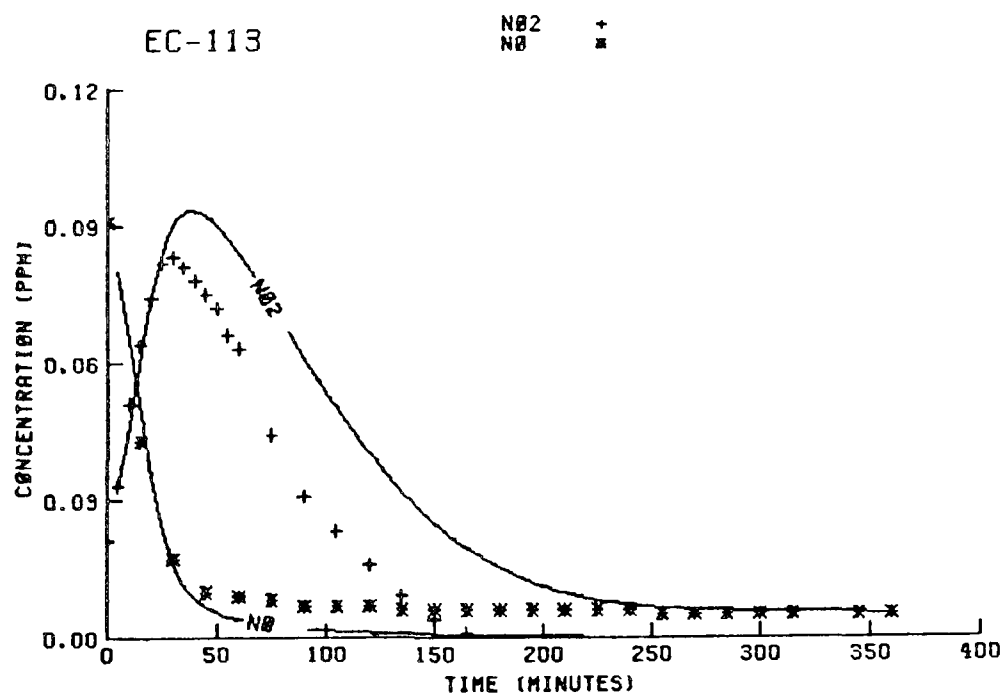
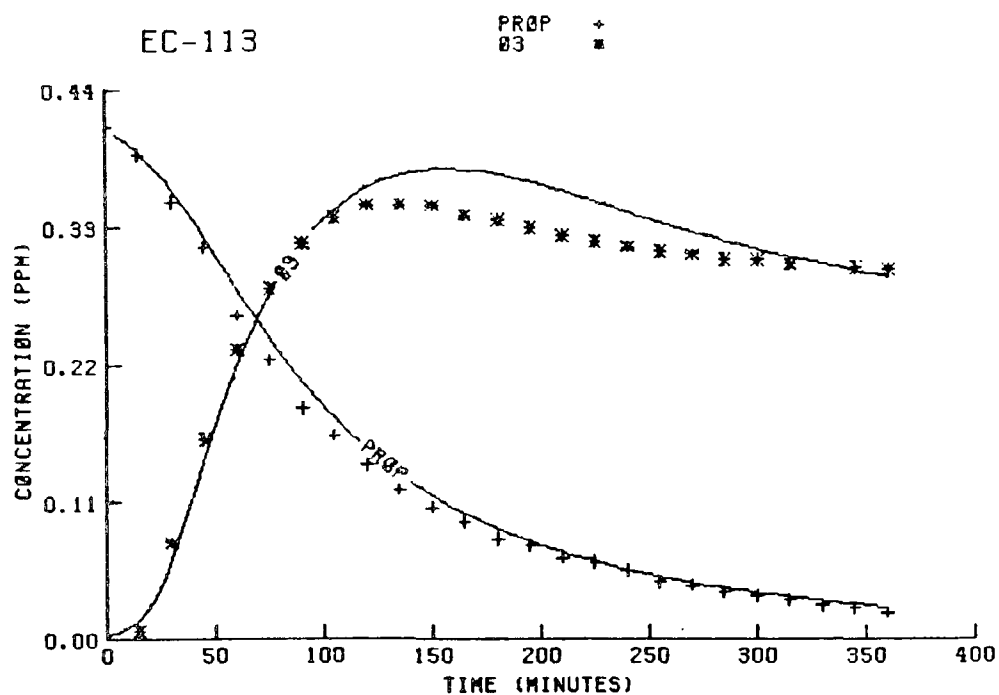
PR0P +
ALD2 ■

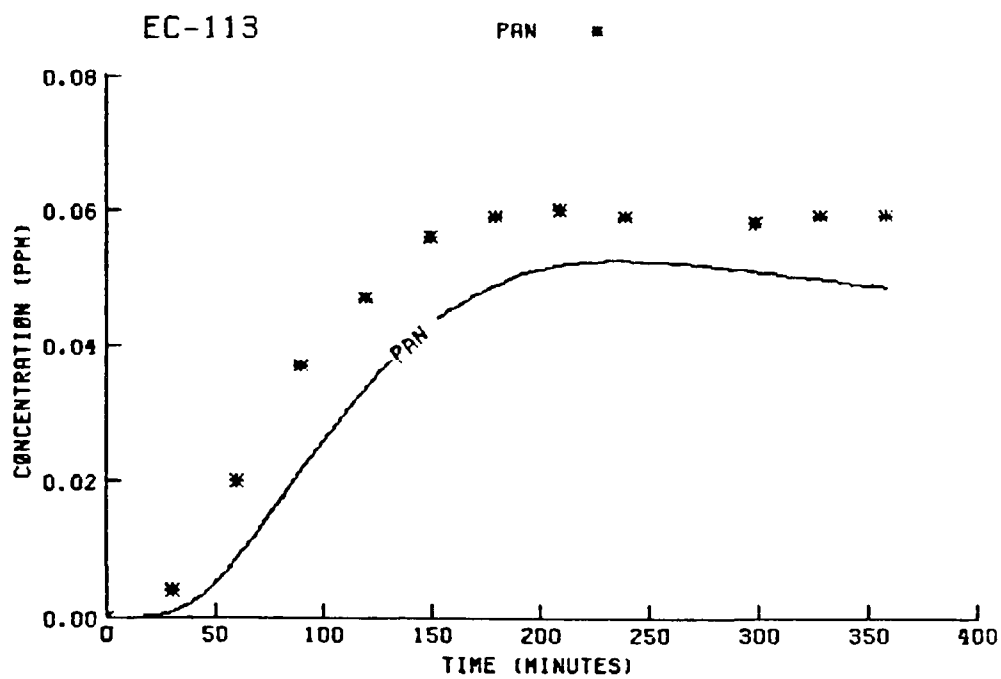
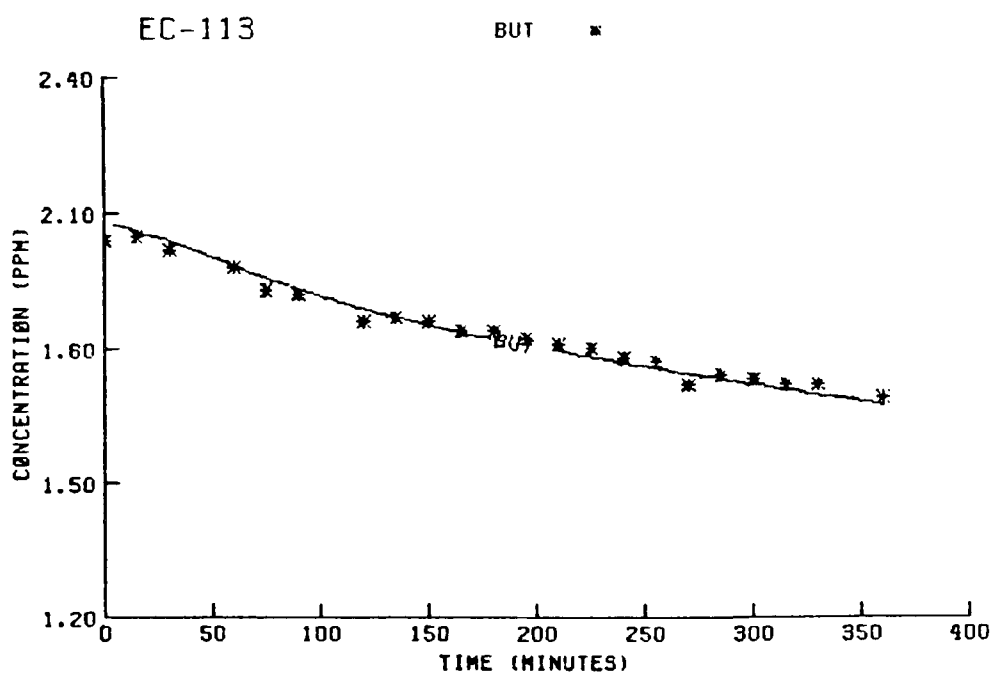


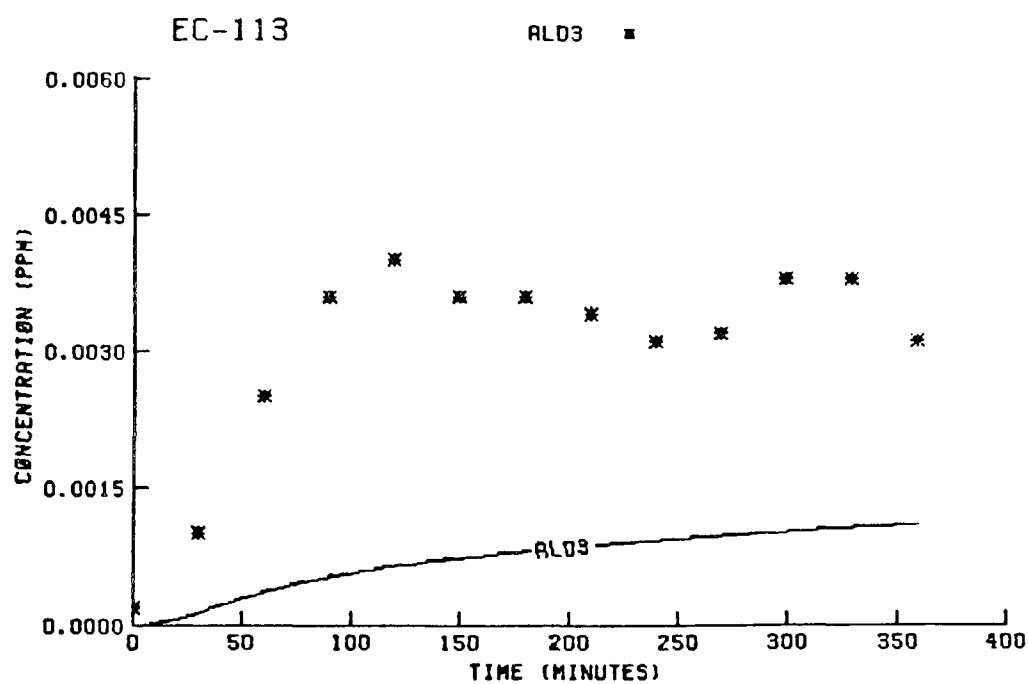
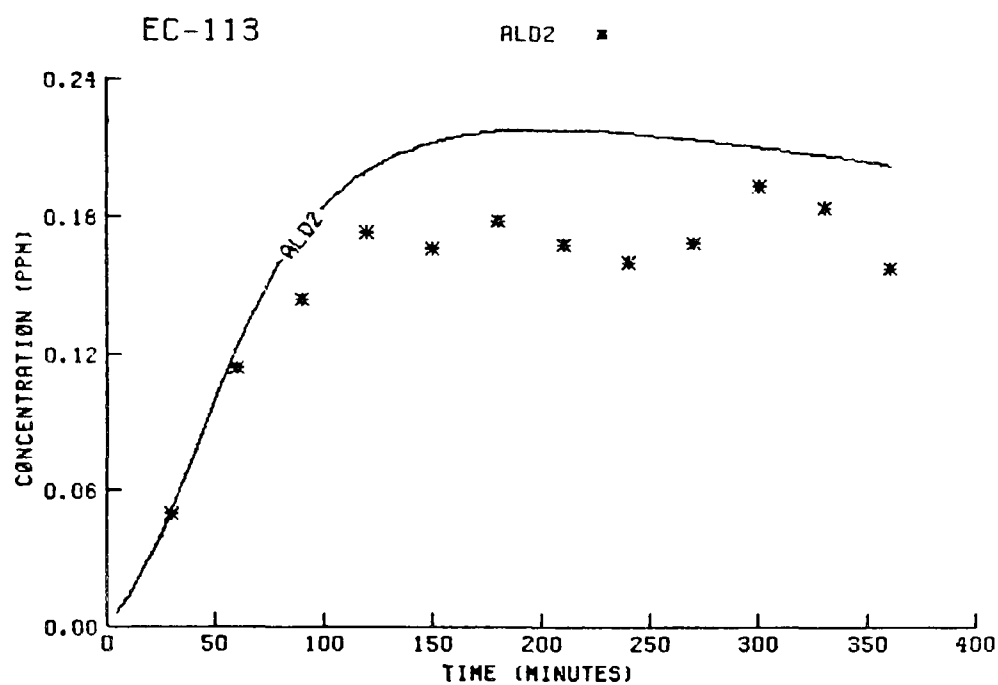


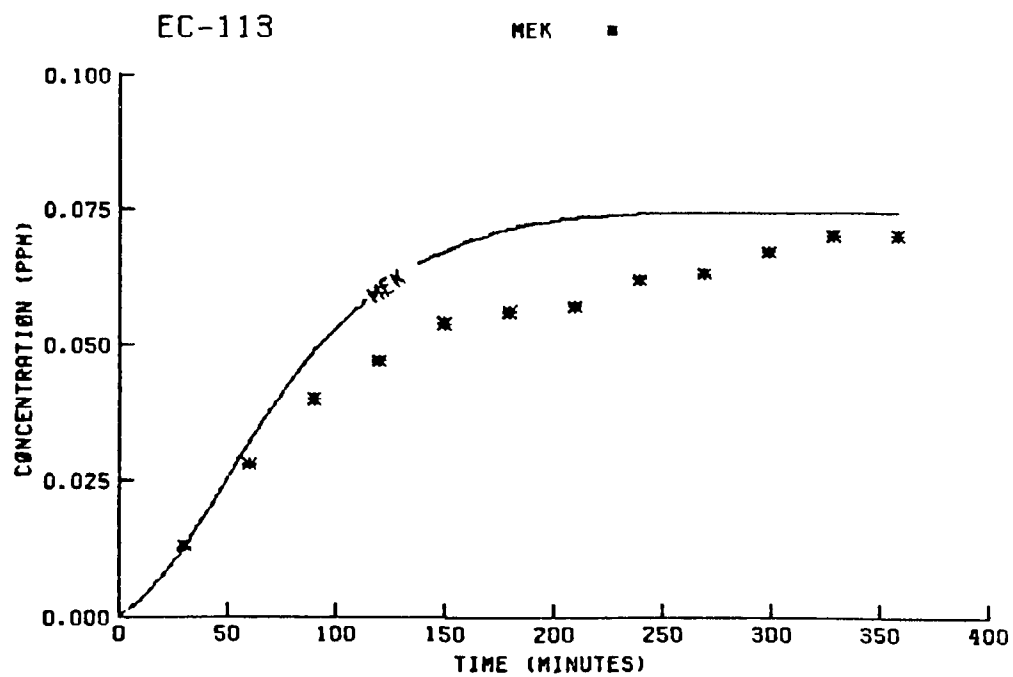
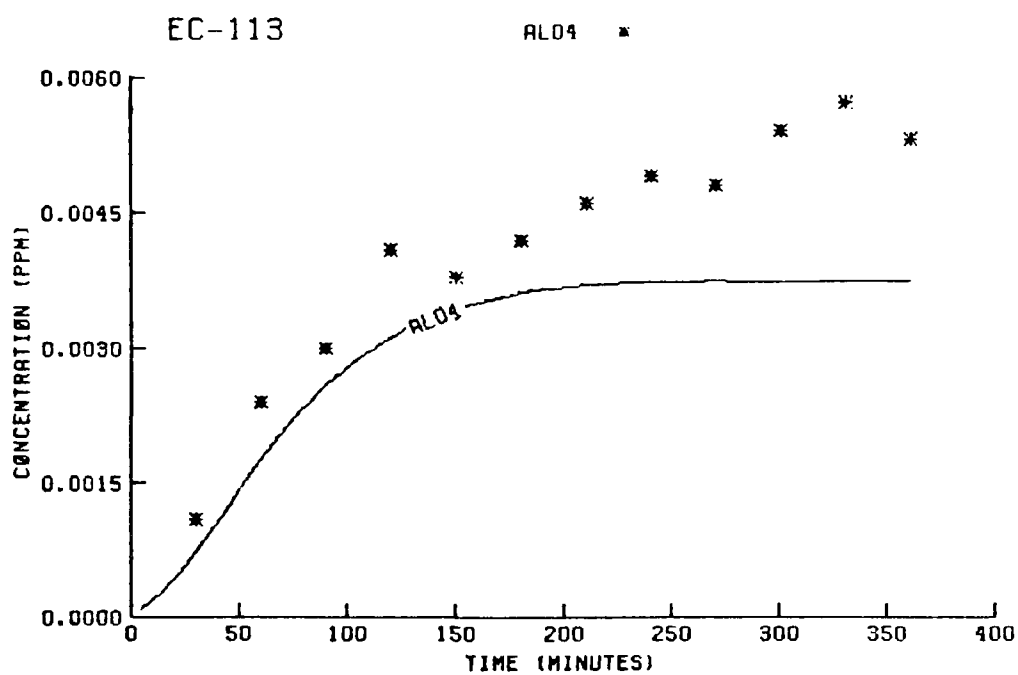


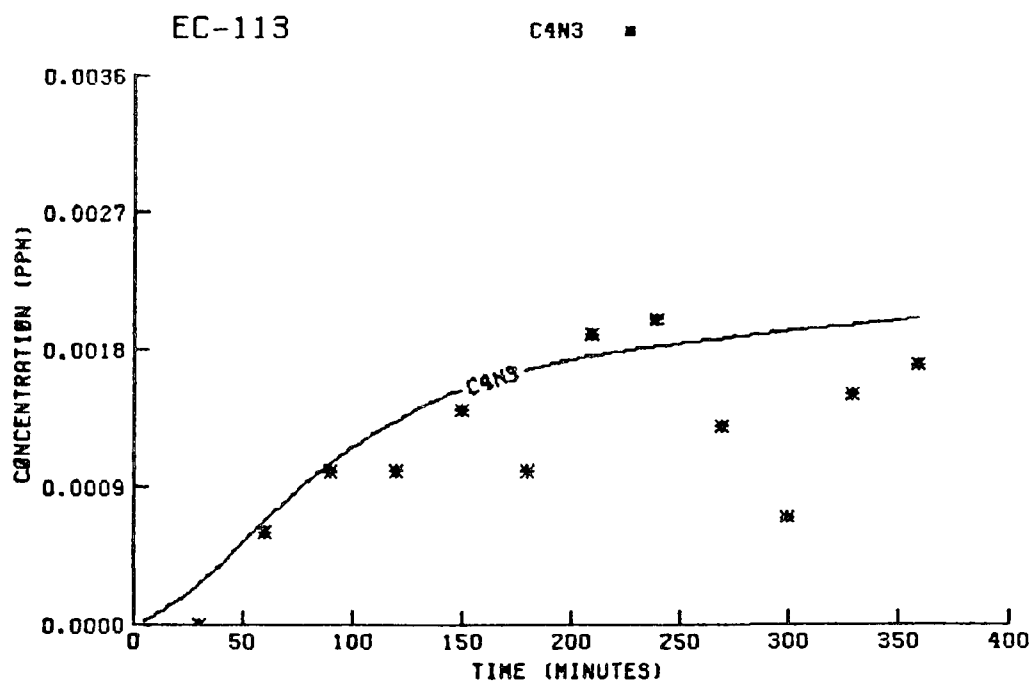
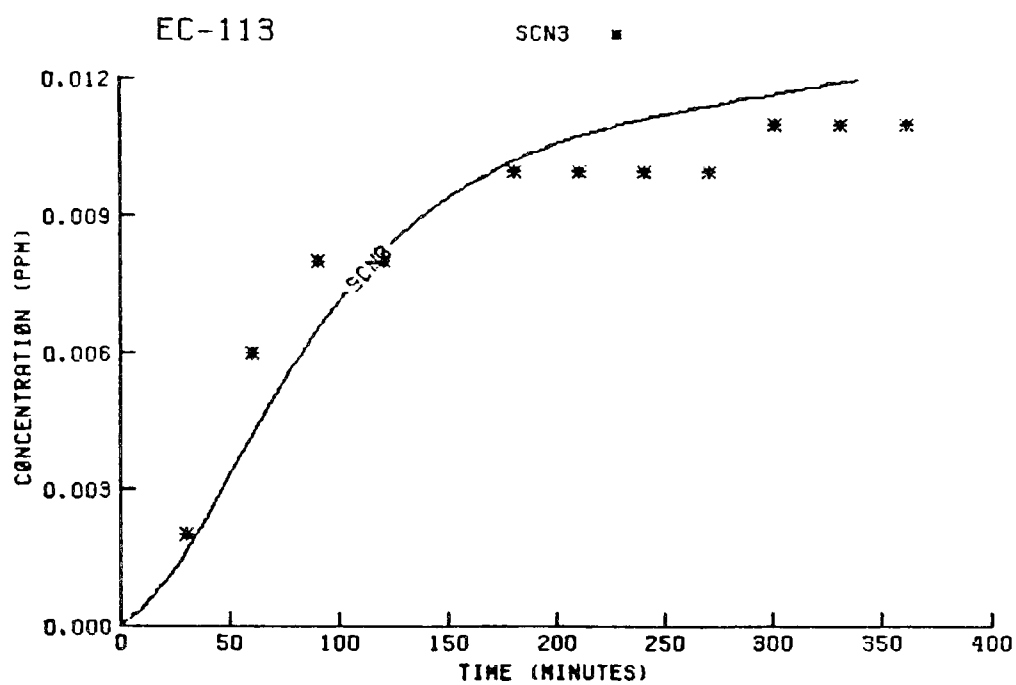


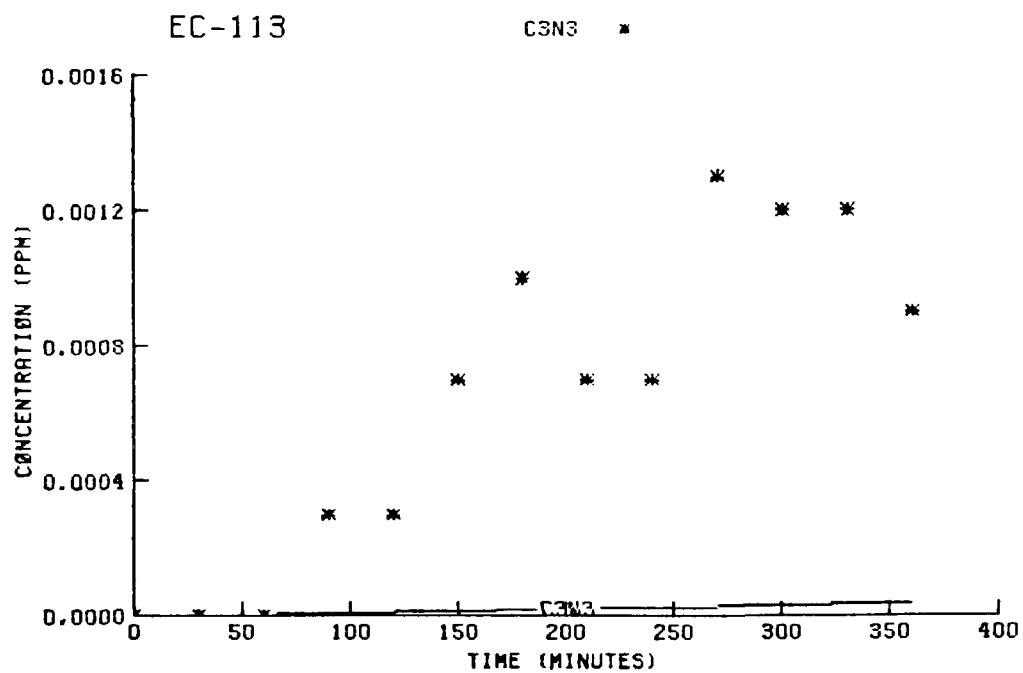


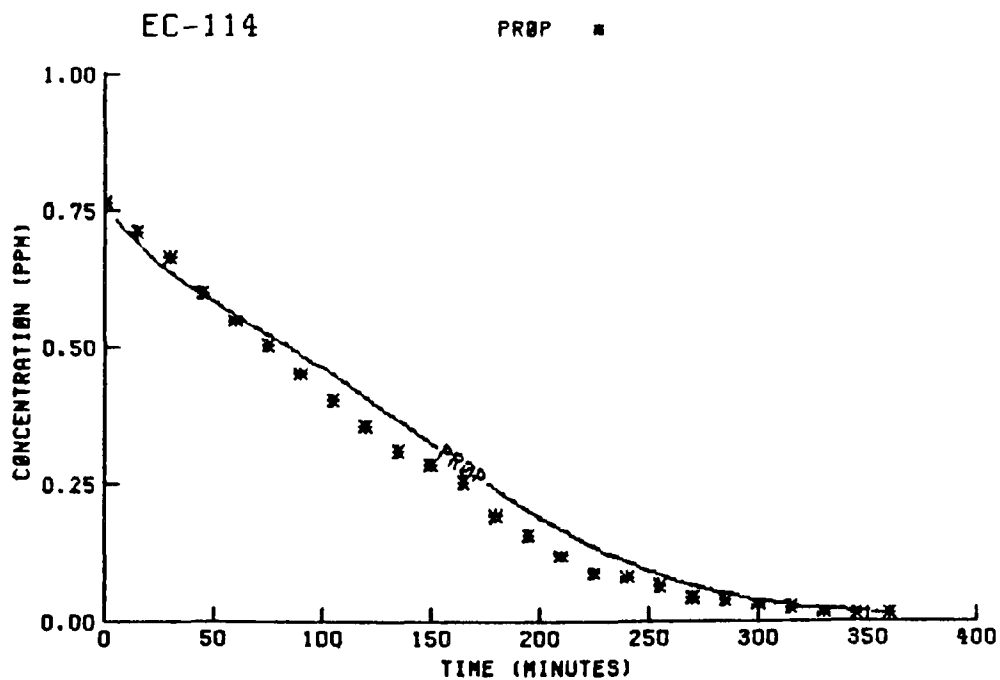
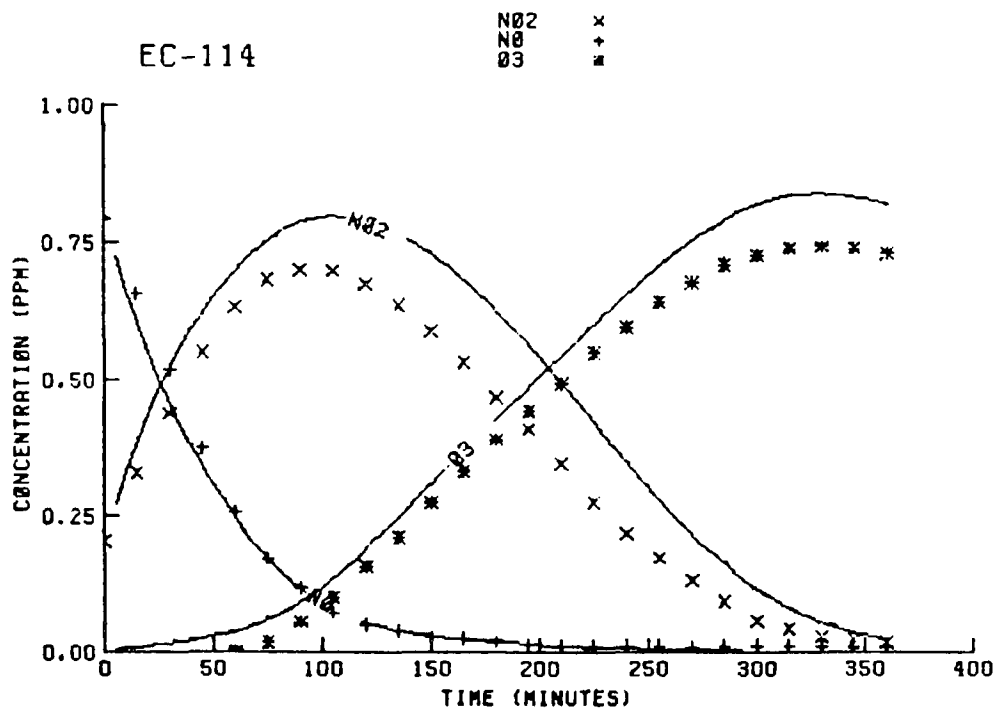


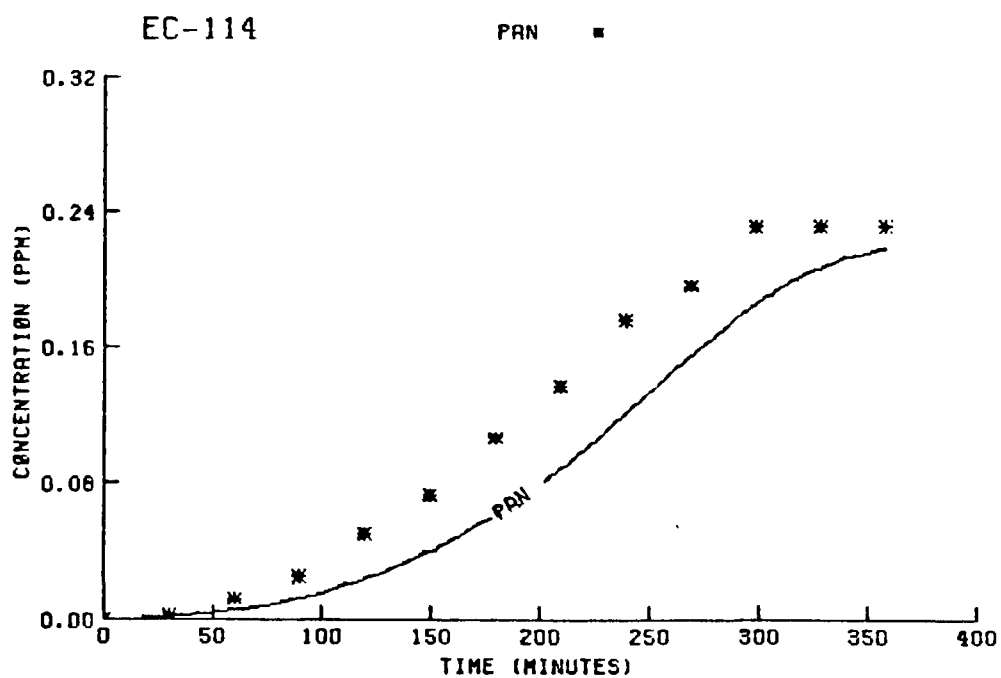
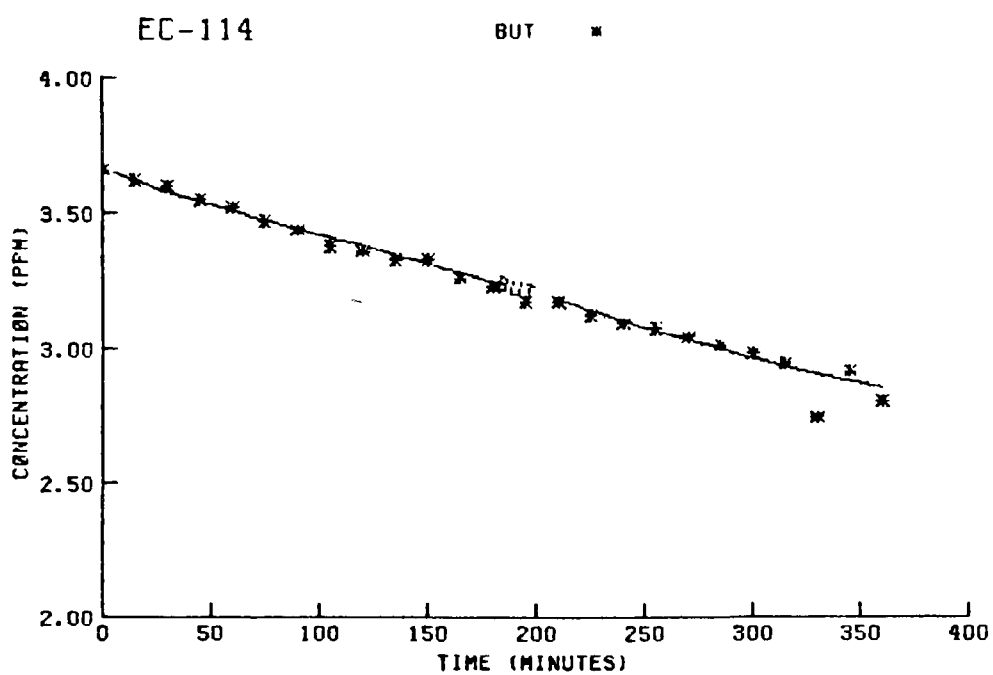






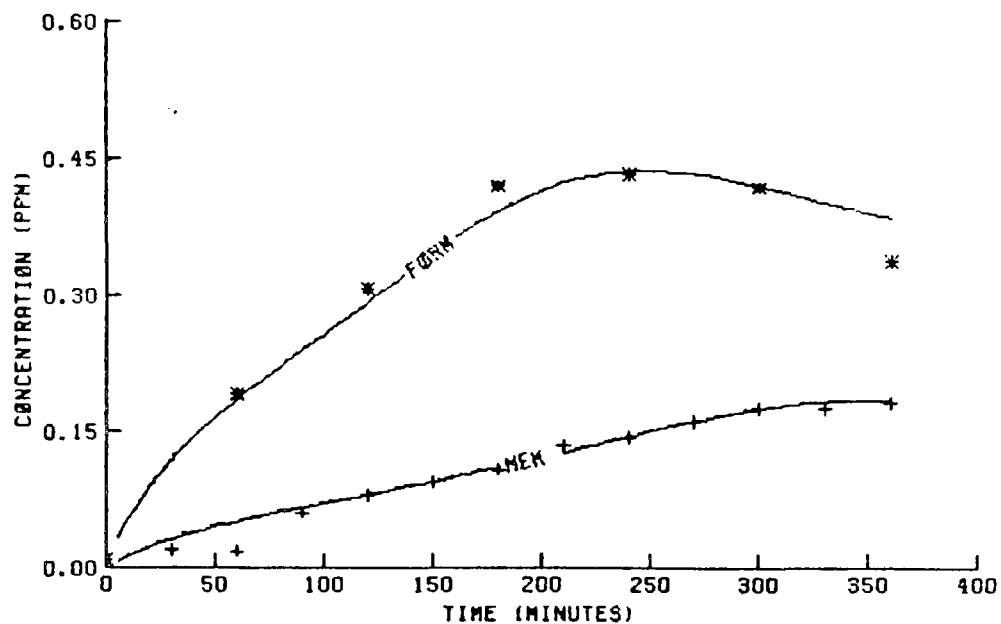






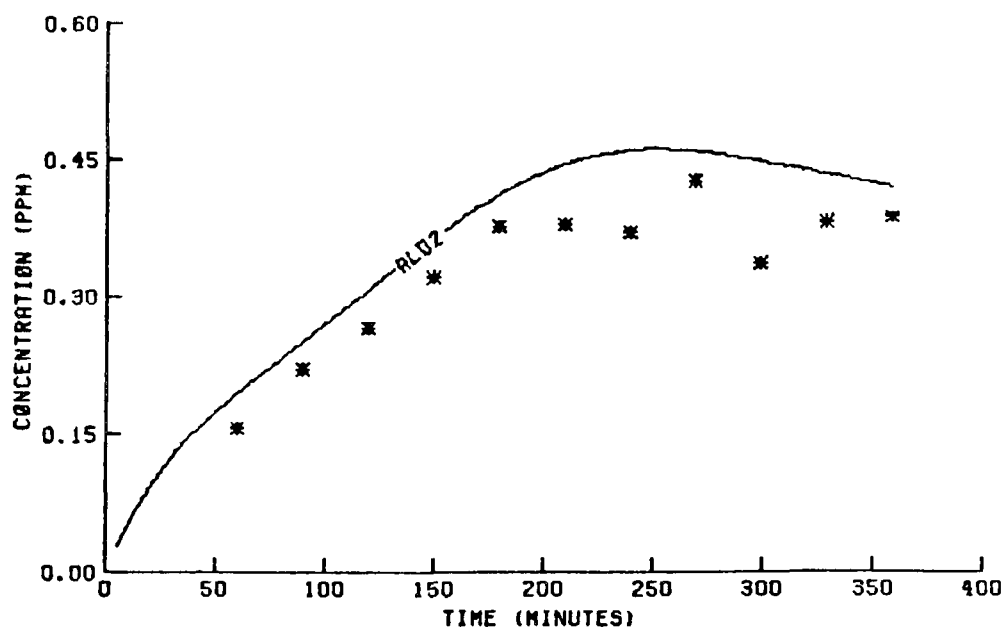
EC-114

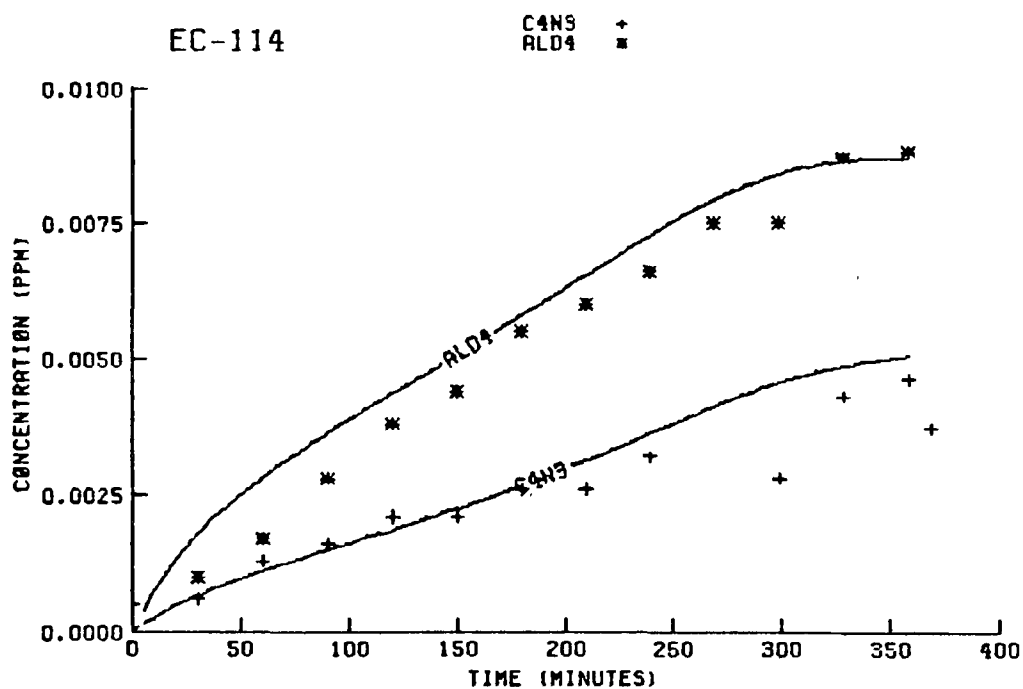
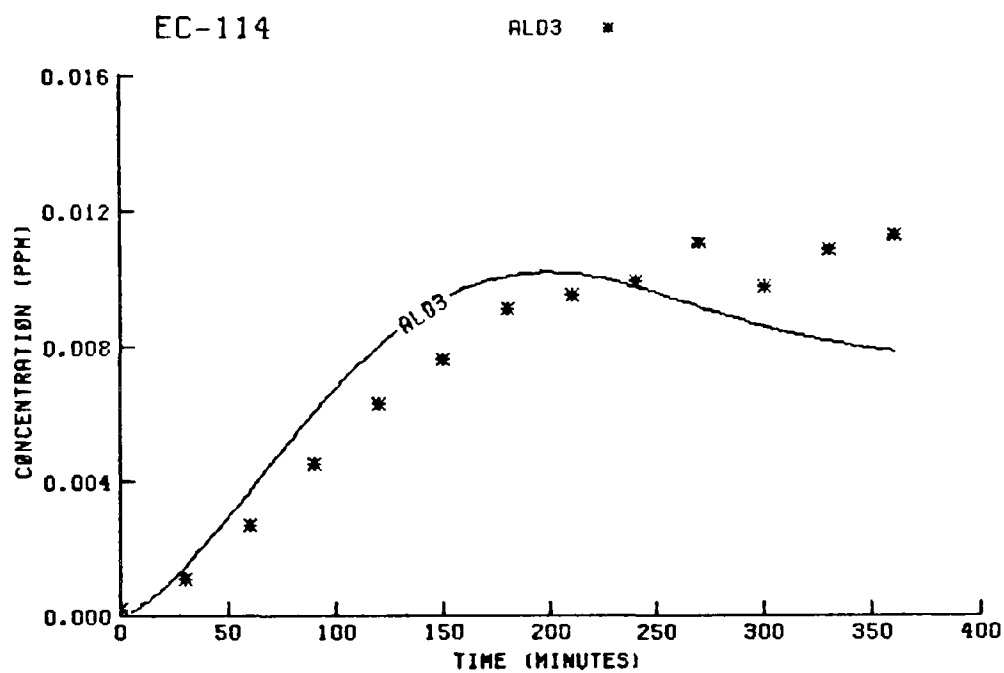
MEK +
FORM *



EC-114

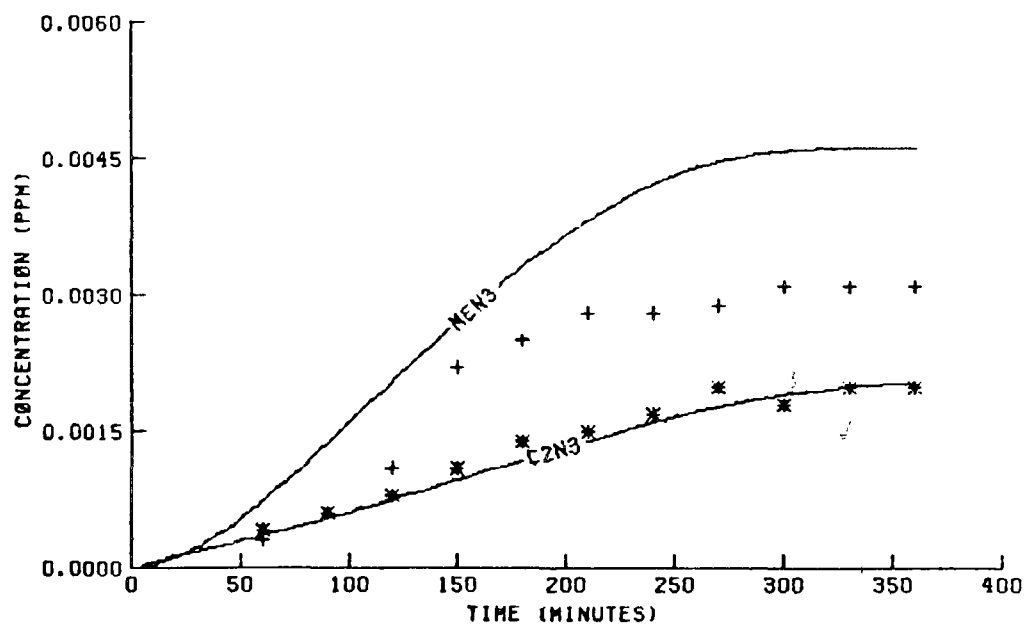
ALD2 *





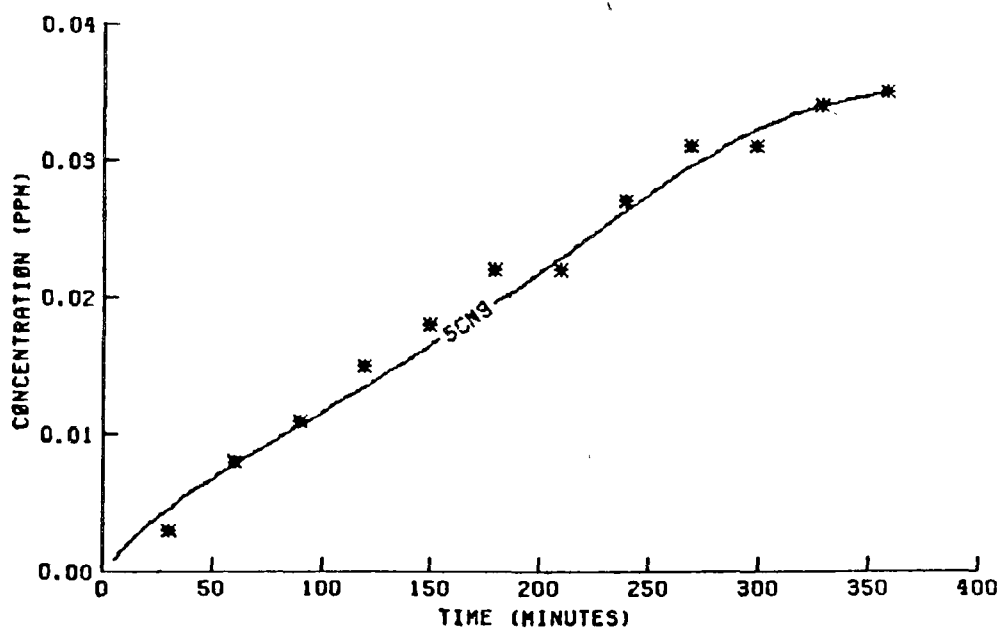
EC-114

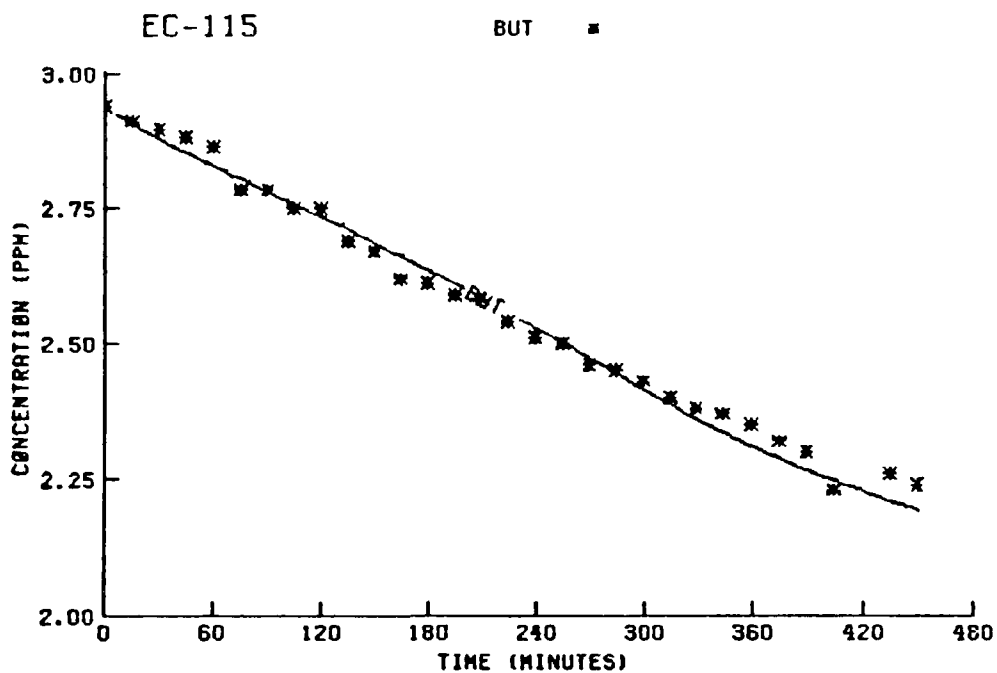
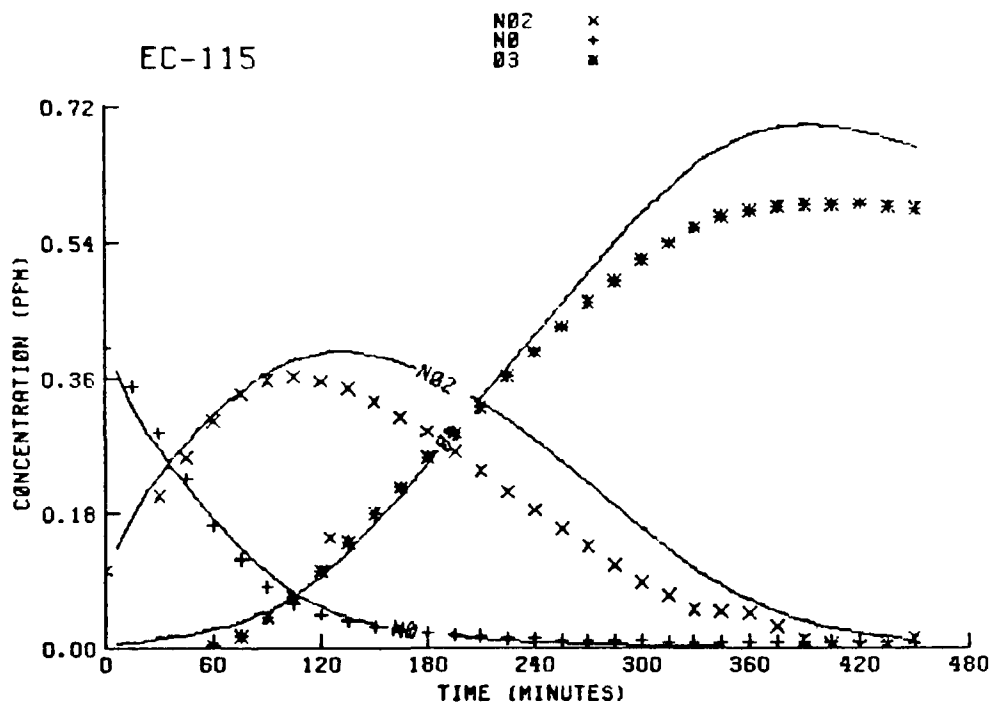
MEN3 +
C2N3 *

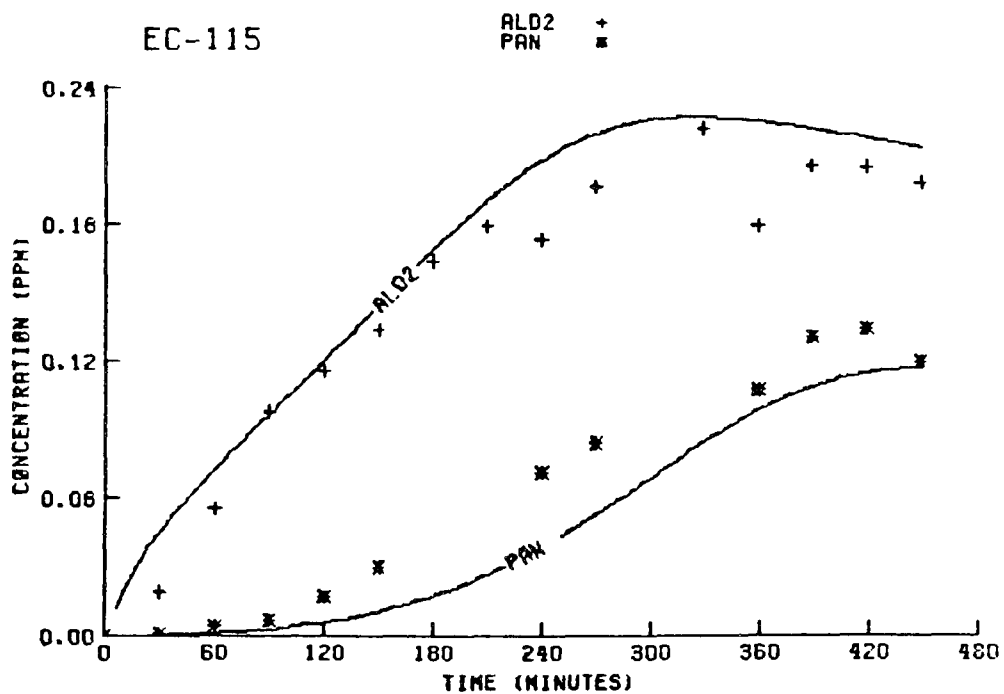
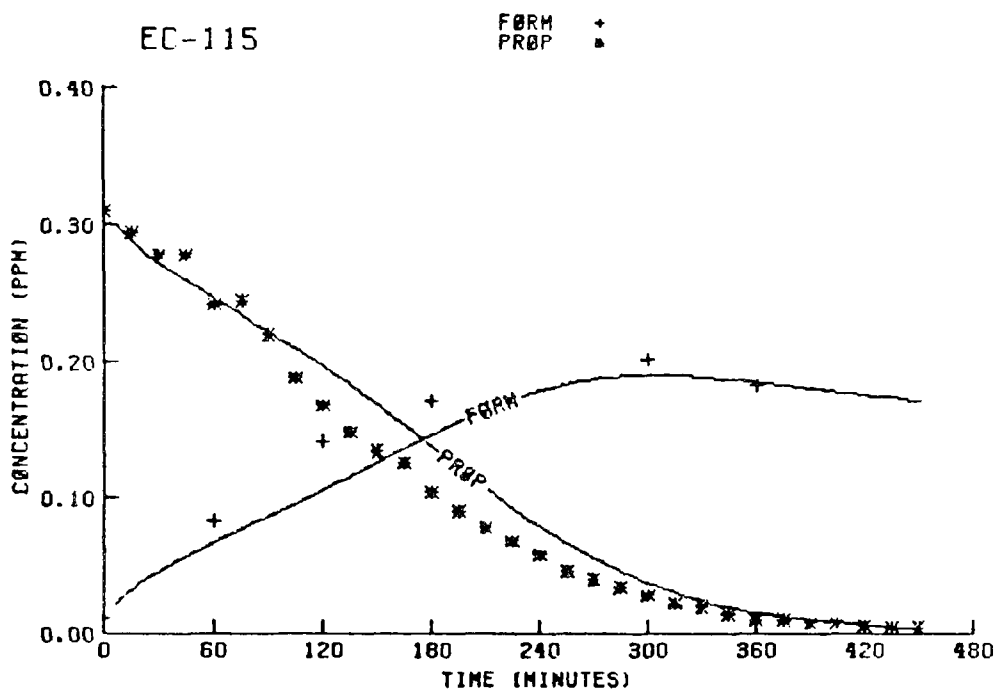


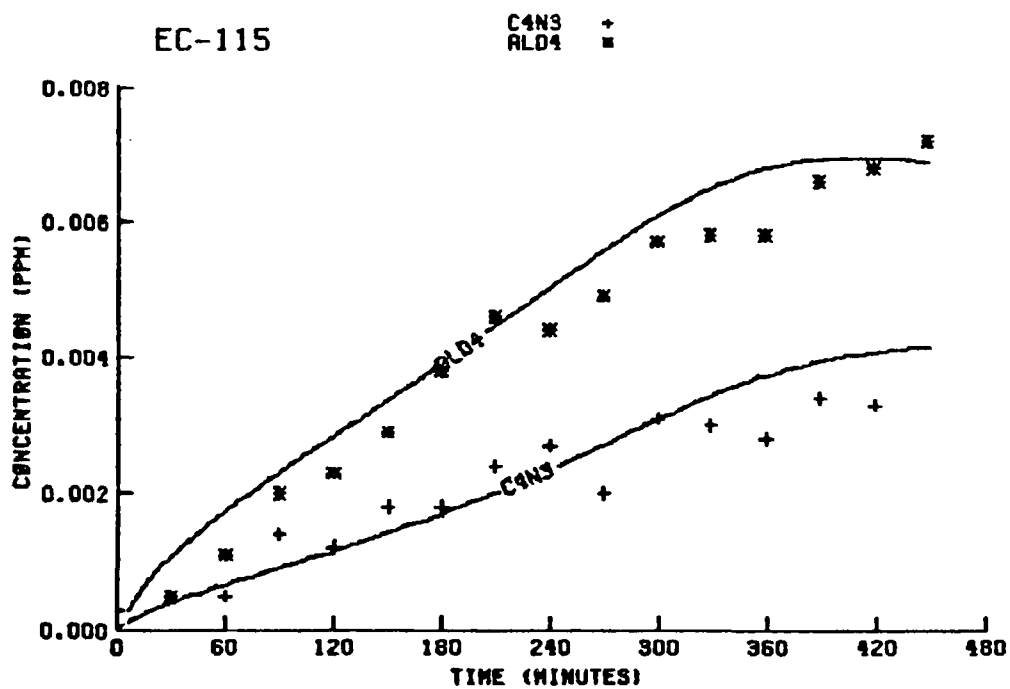
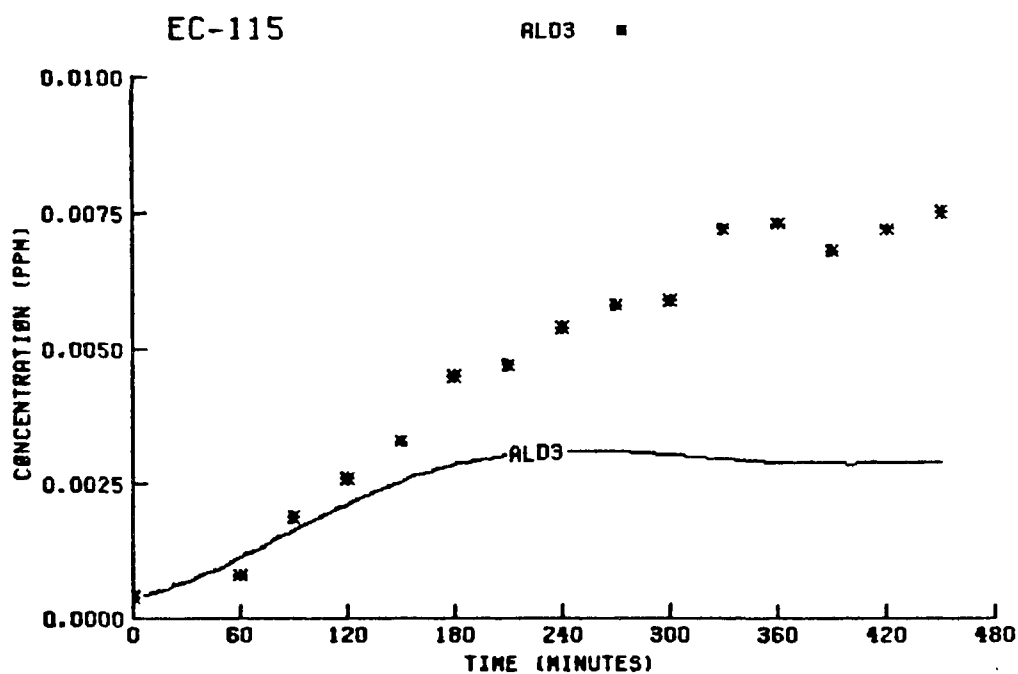
EC-114

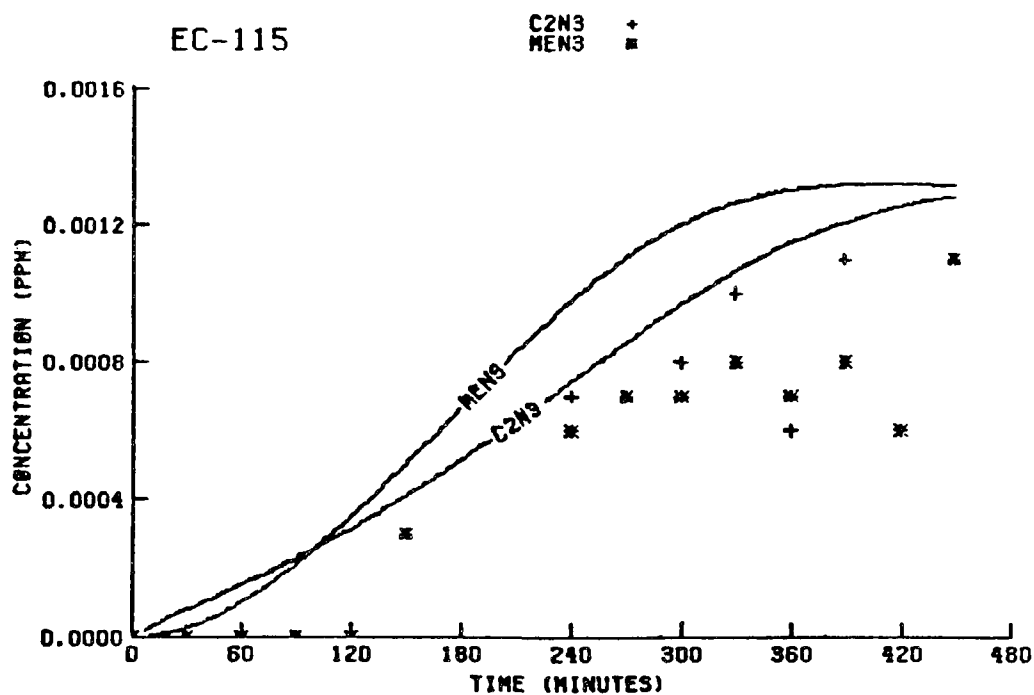
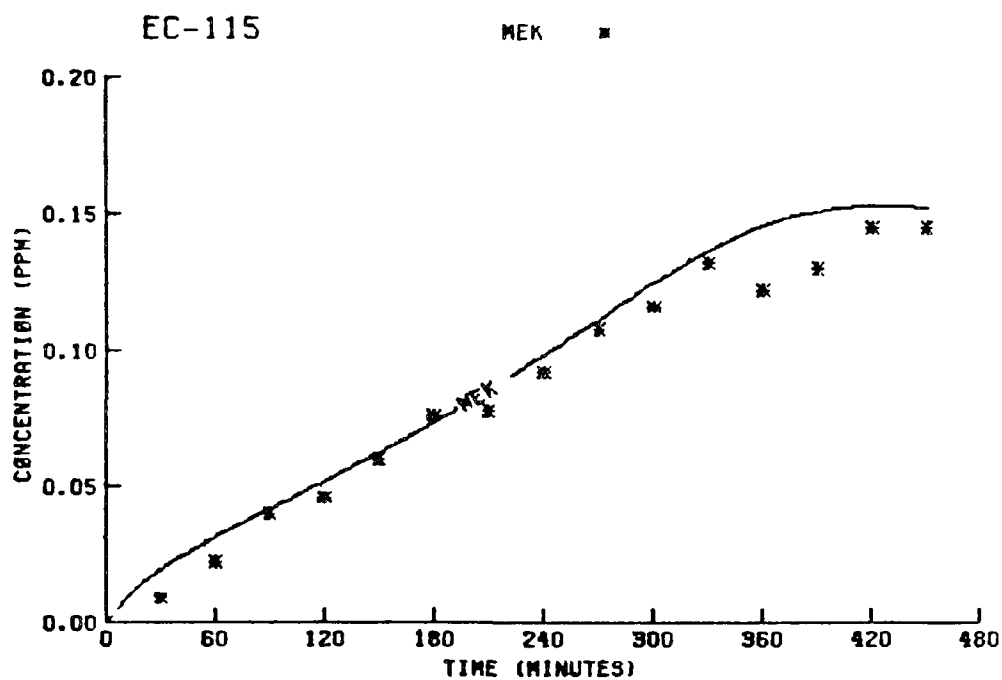
SCN3 *





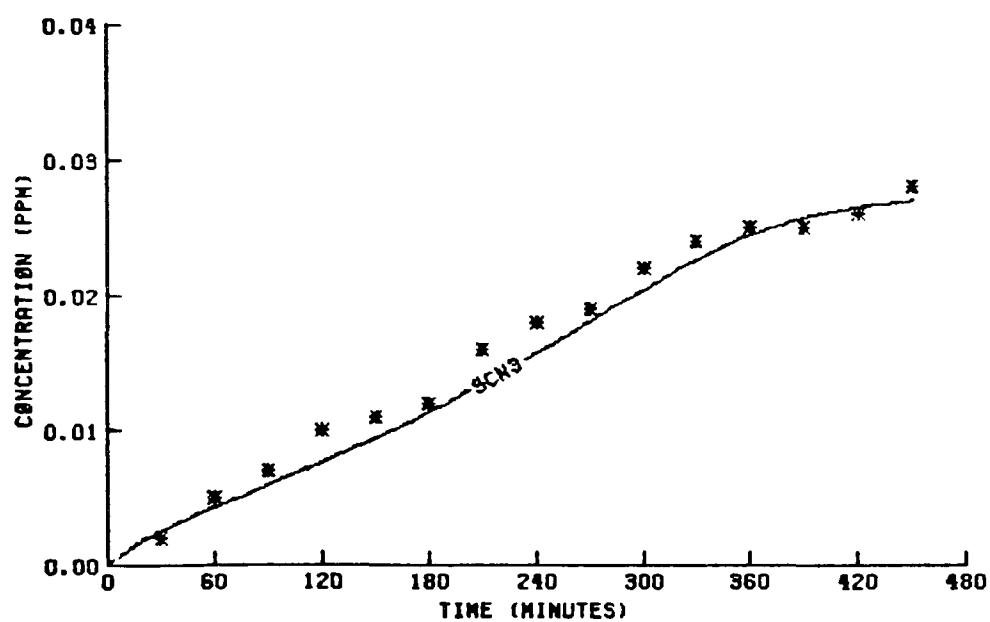


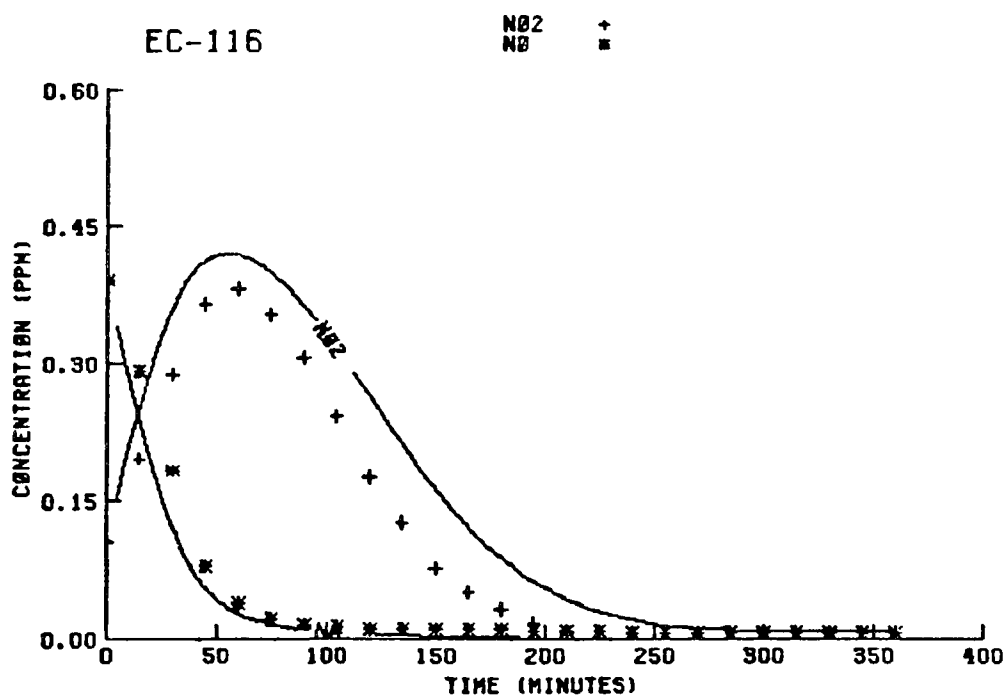
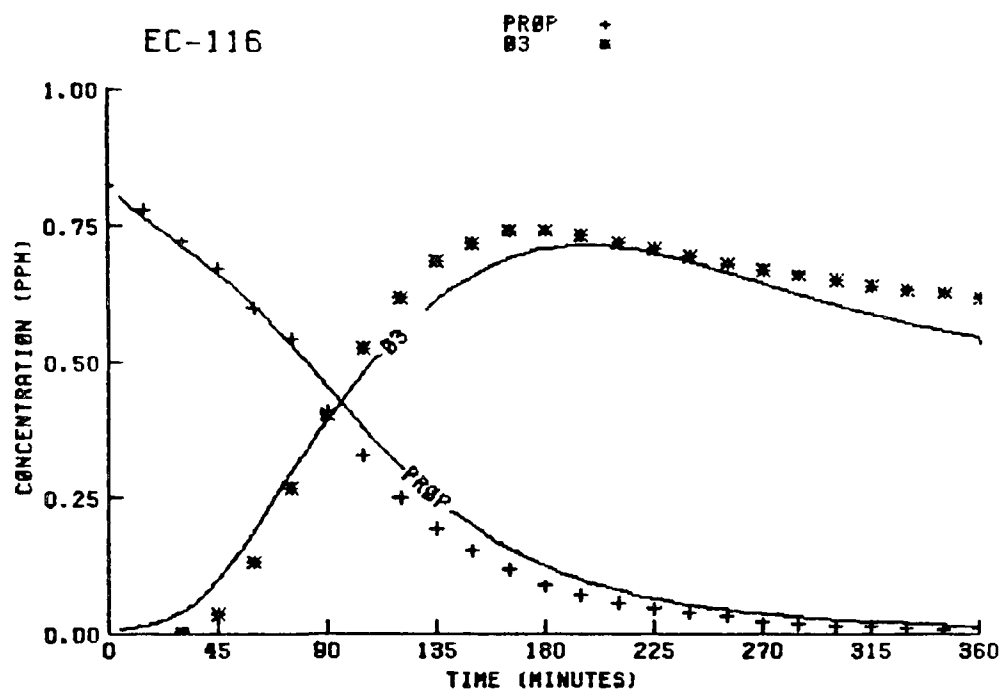


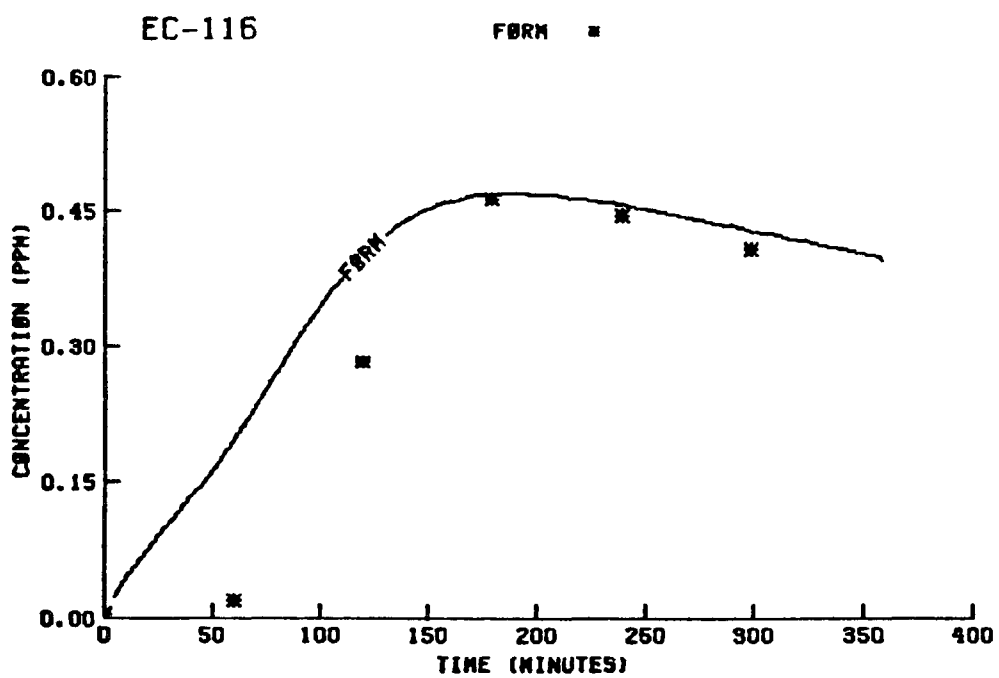
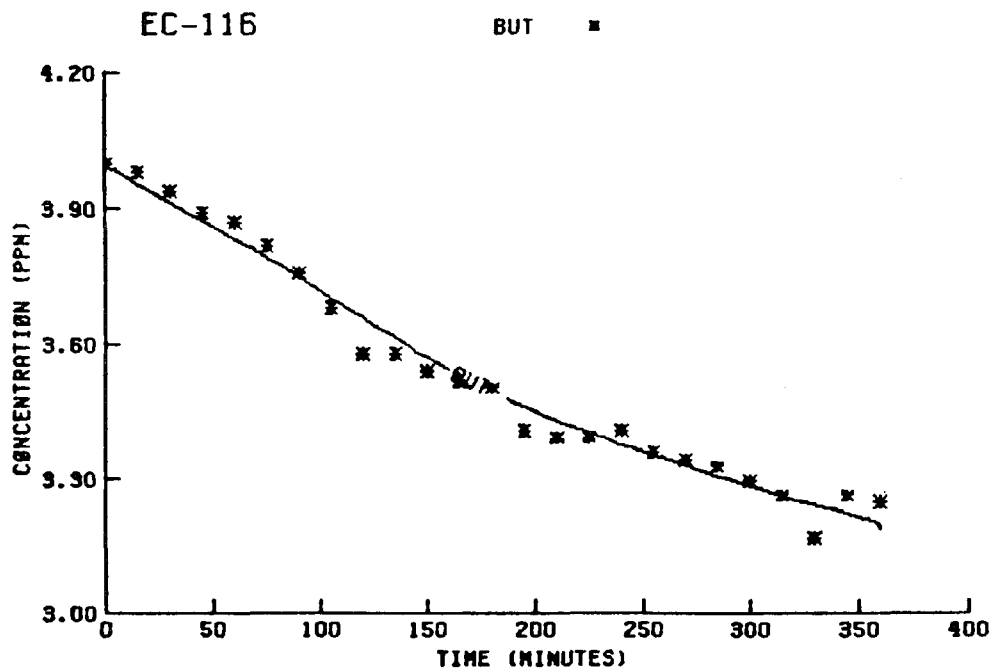


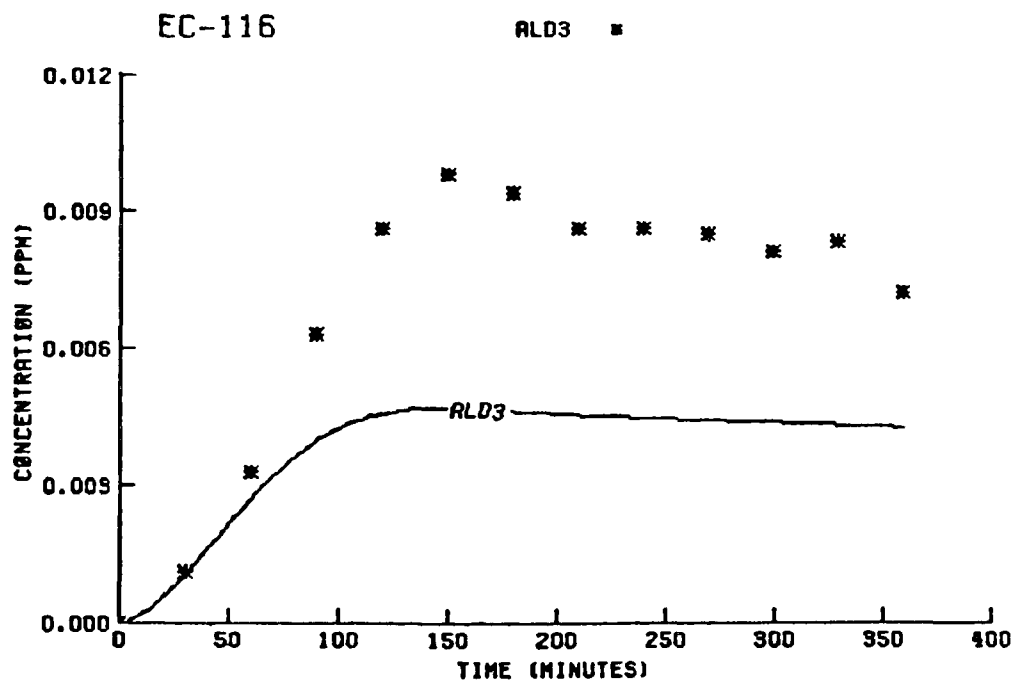
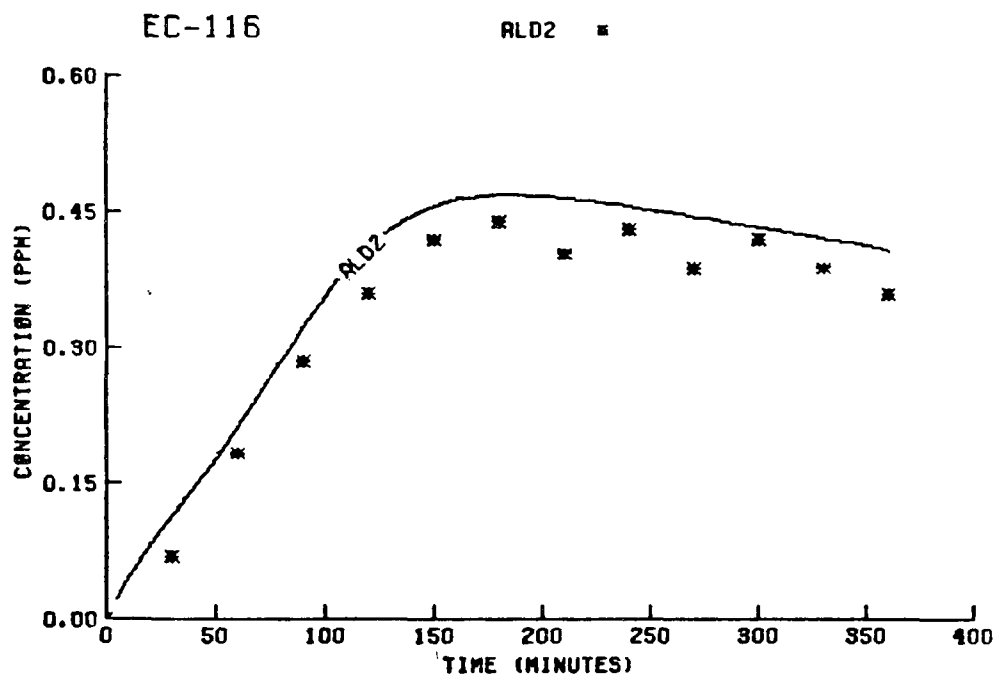
EC-115

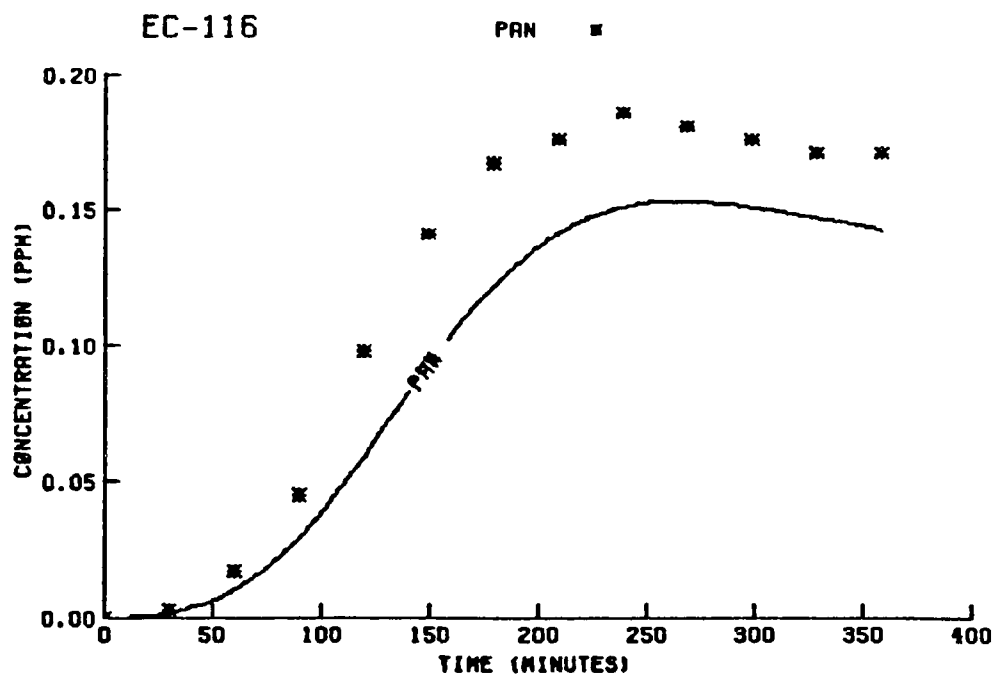
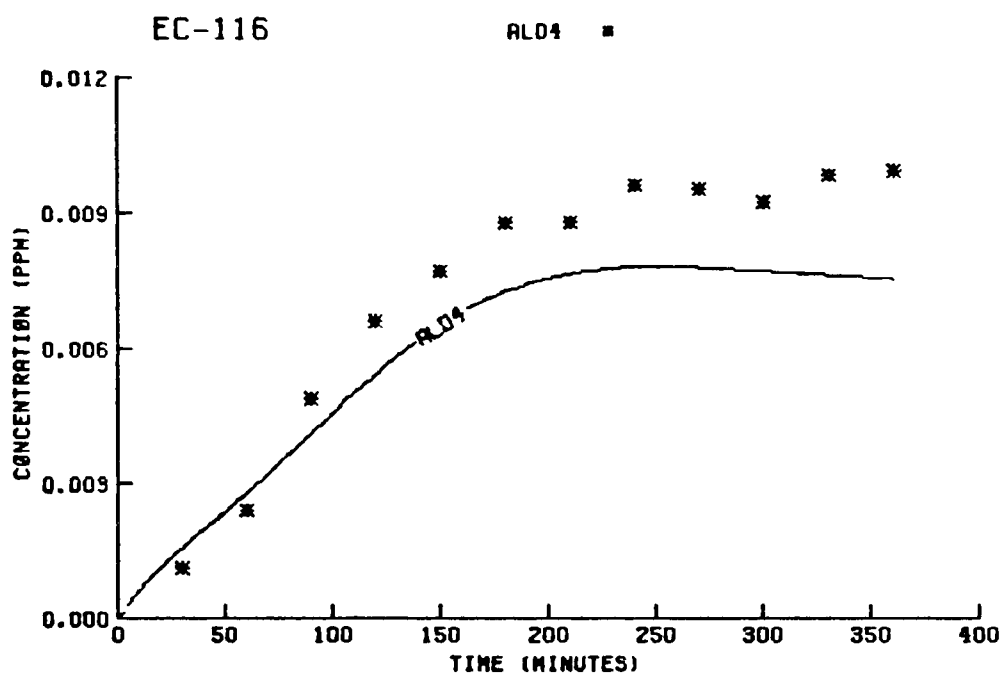
SCN3 ■

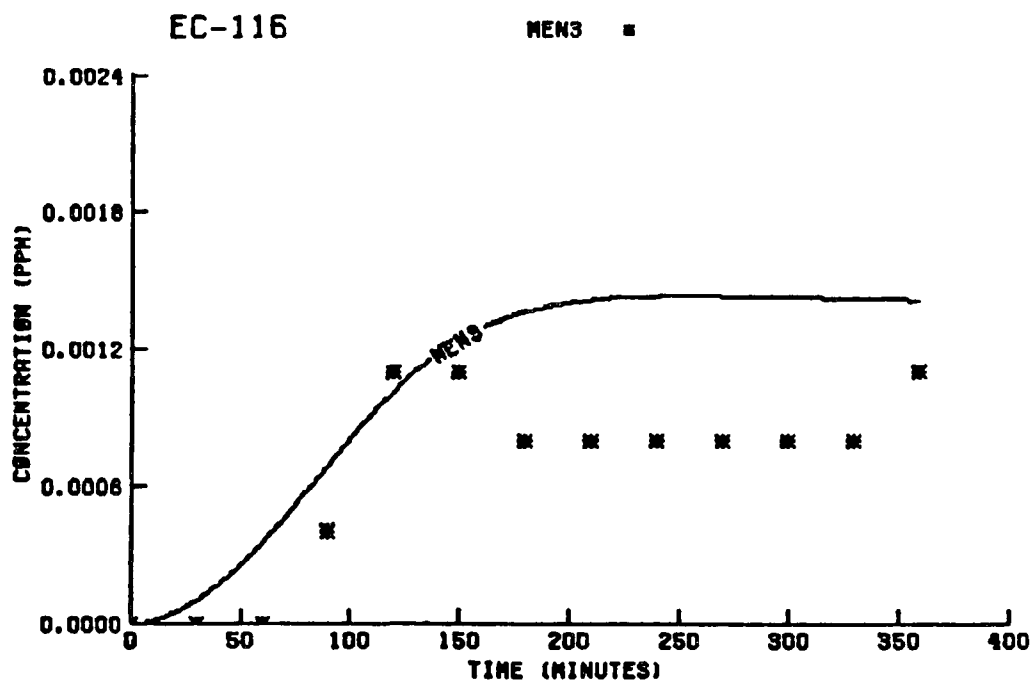
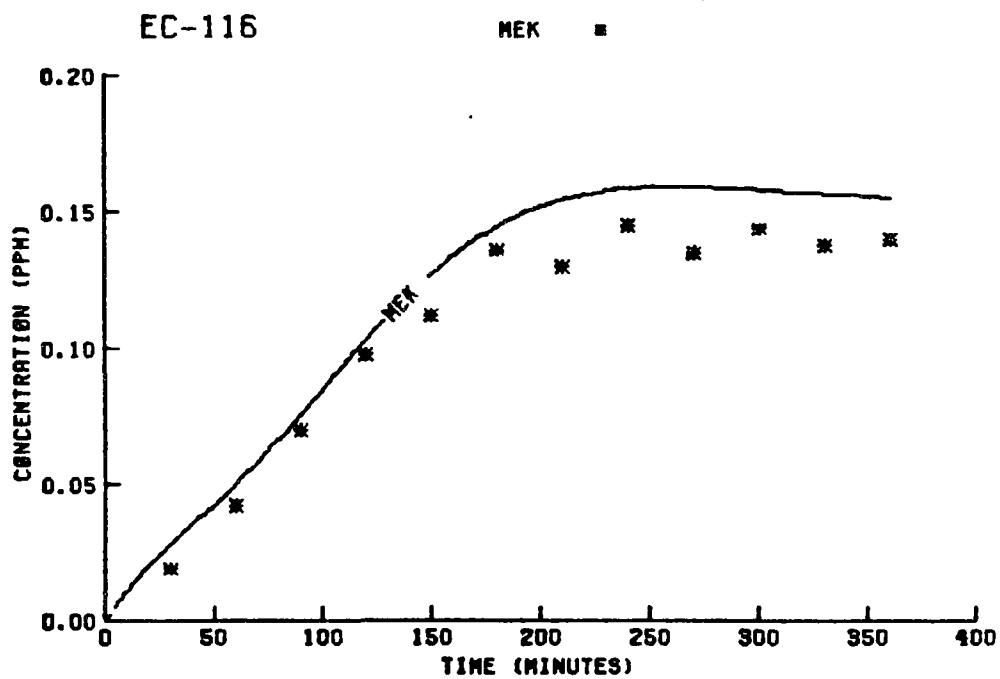


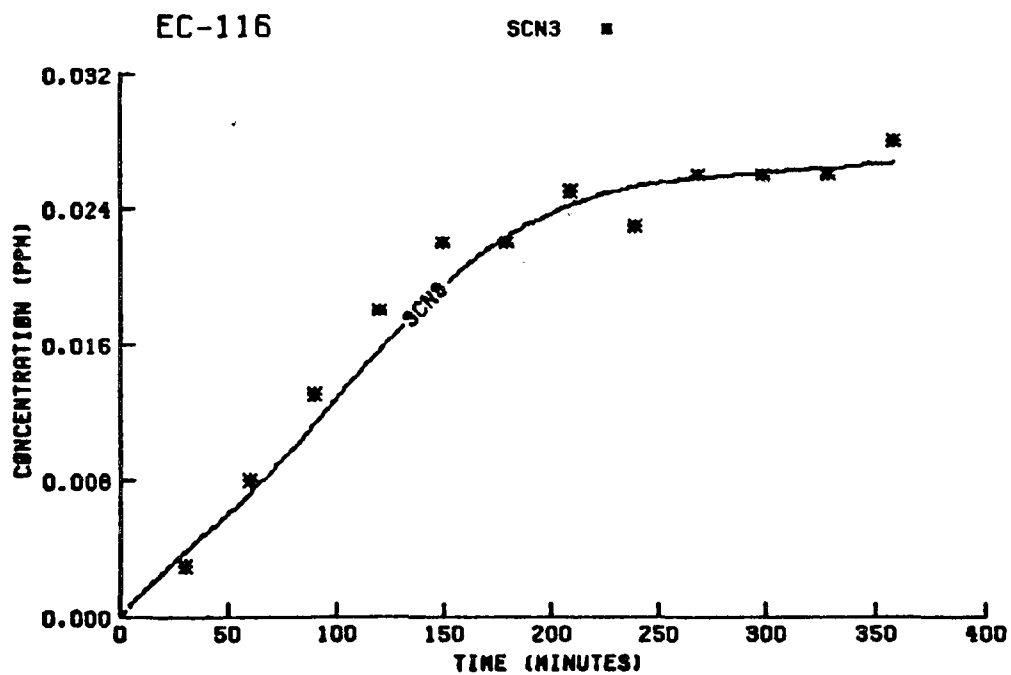
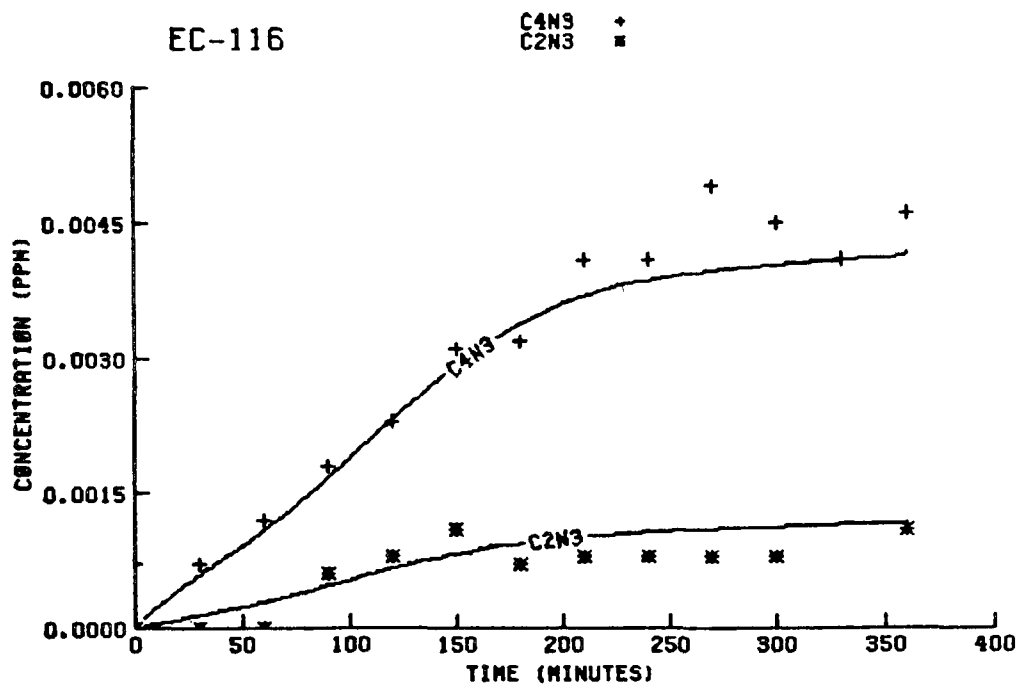








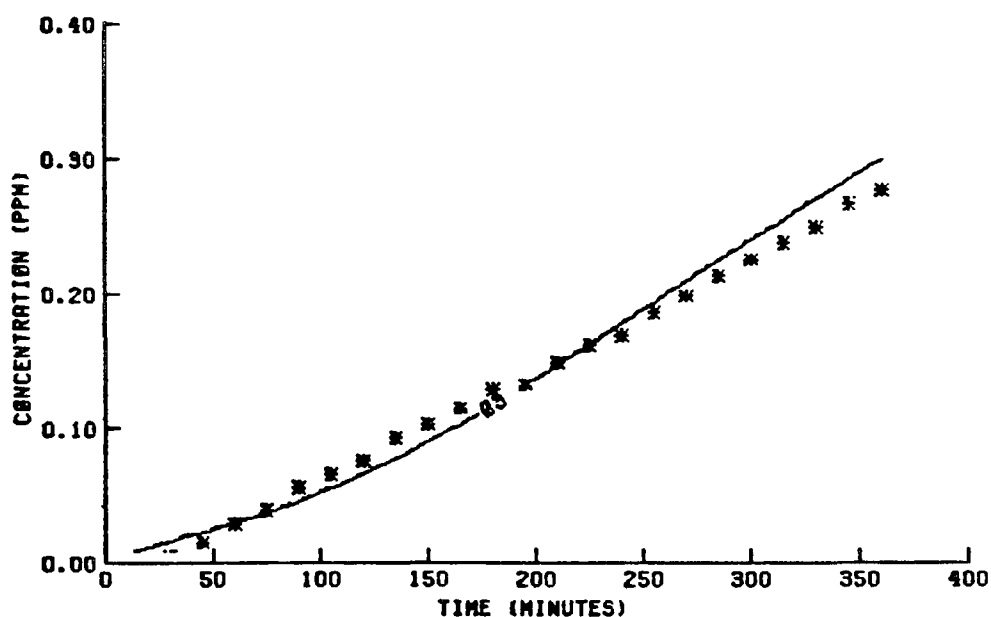




UCR PROPYLENE/TRANS-2-BUTENE EXPERIMENT

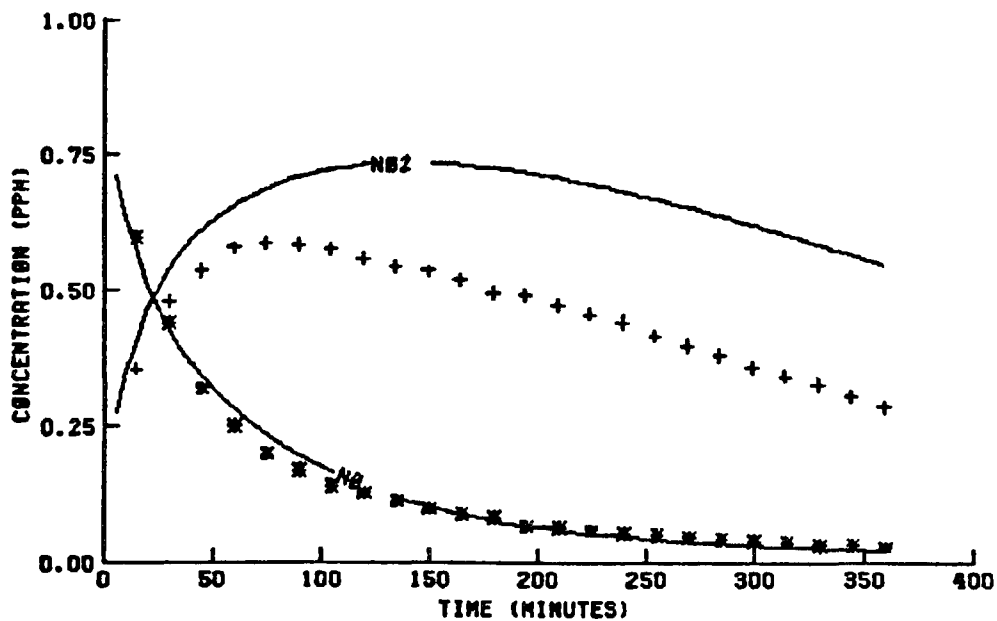
EC-149

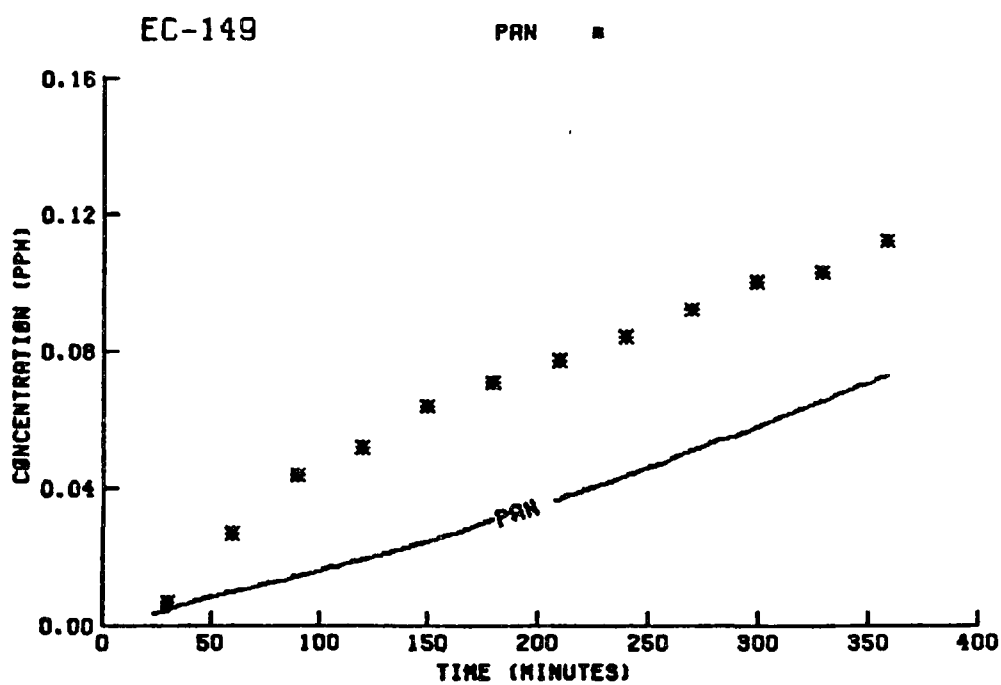
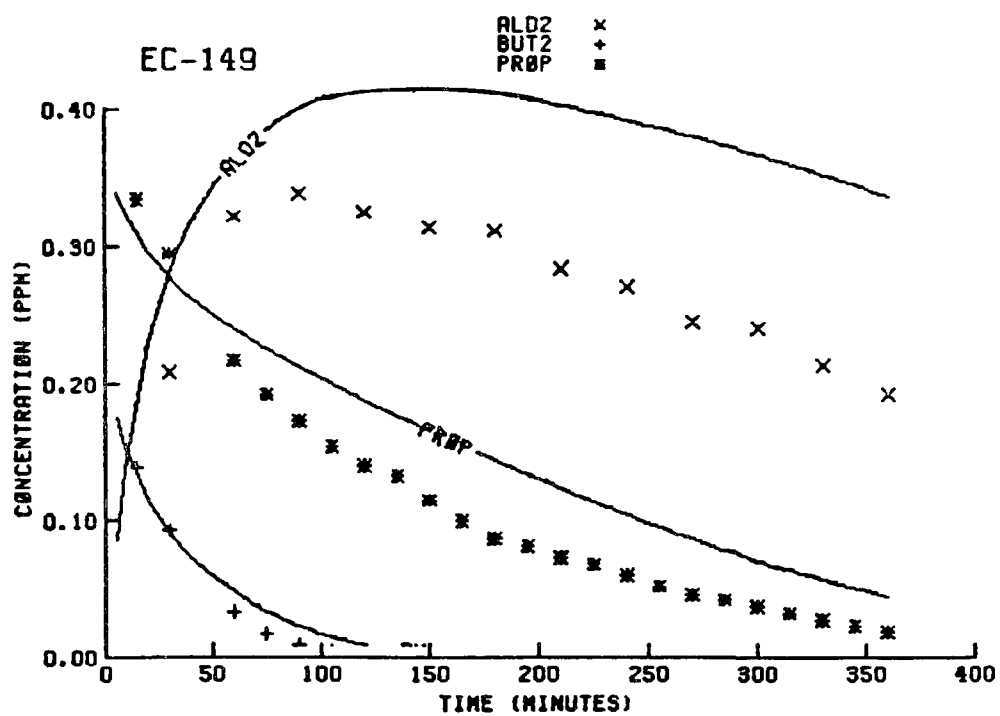
83 ■

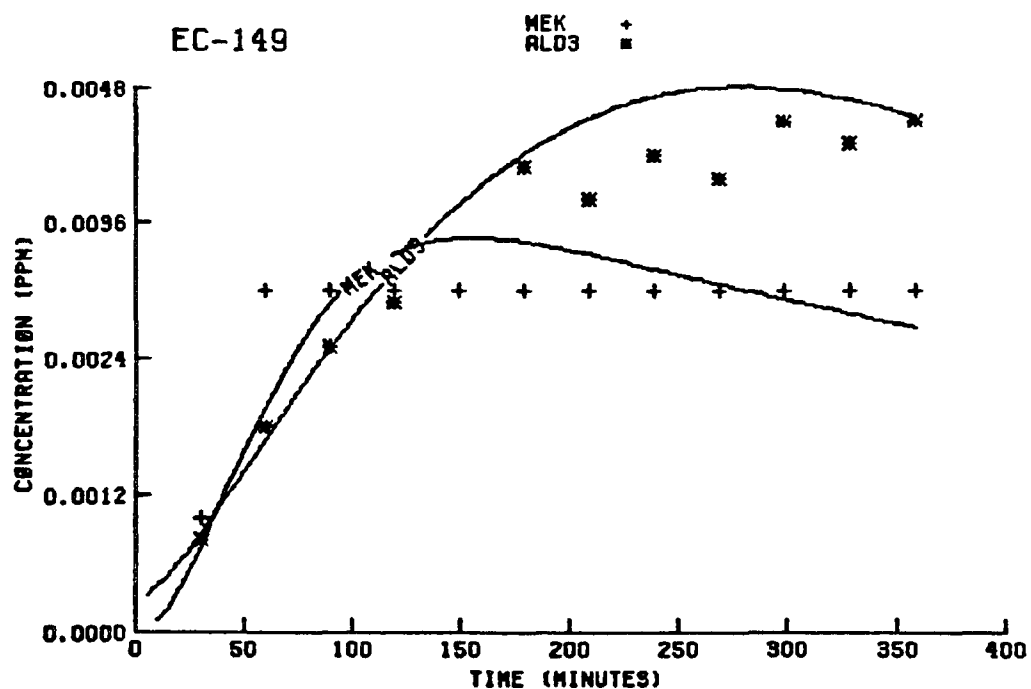
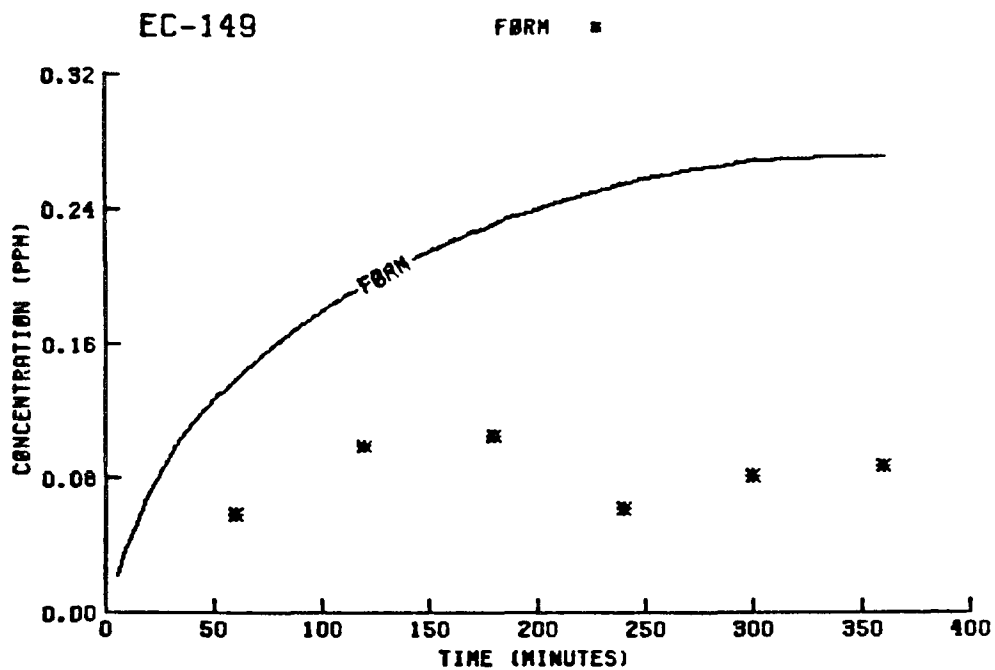


EC-149

NB2 +
NB ■

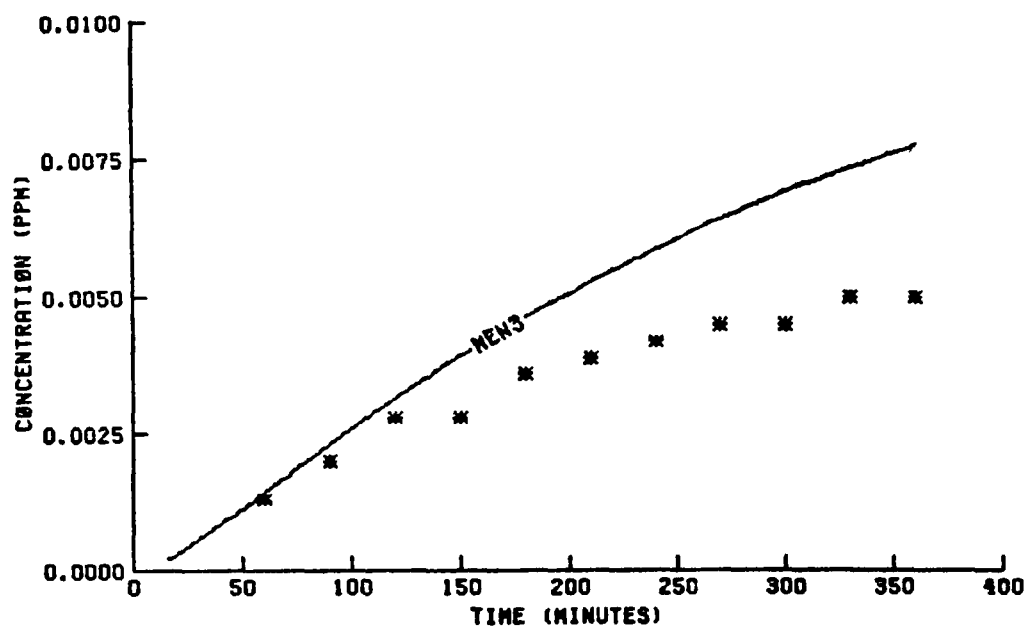




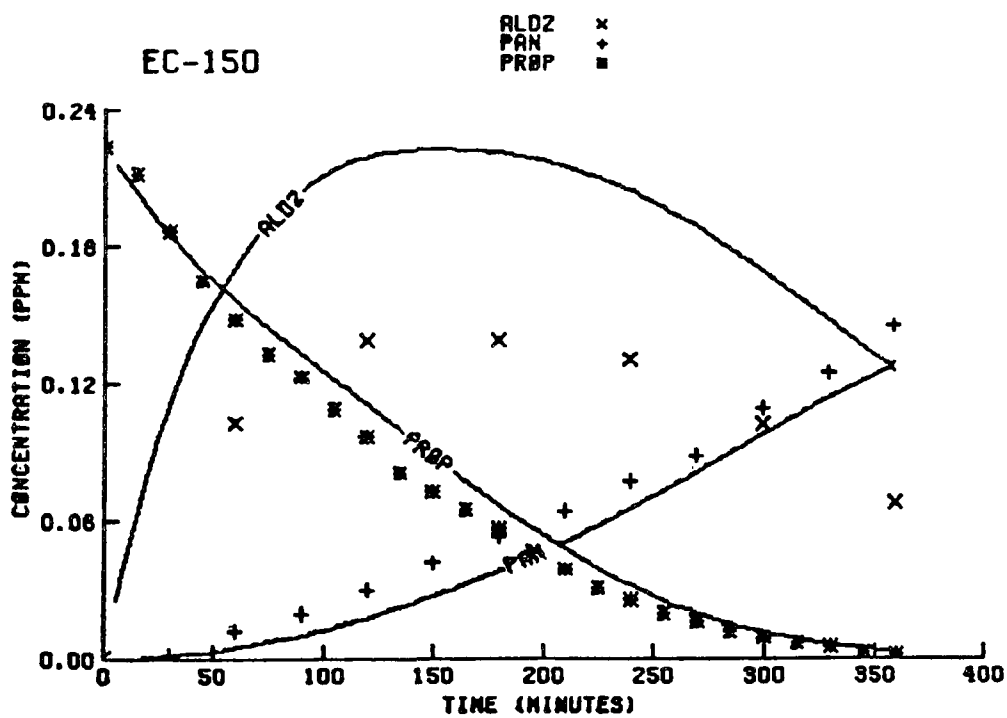
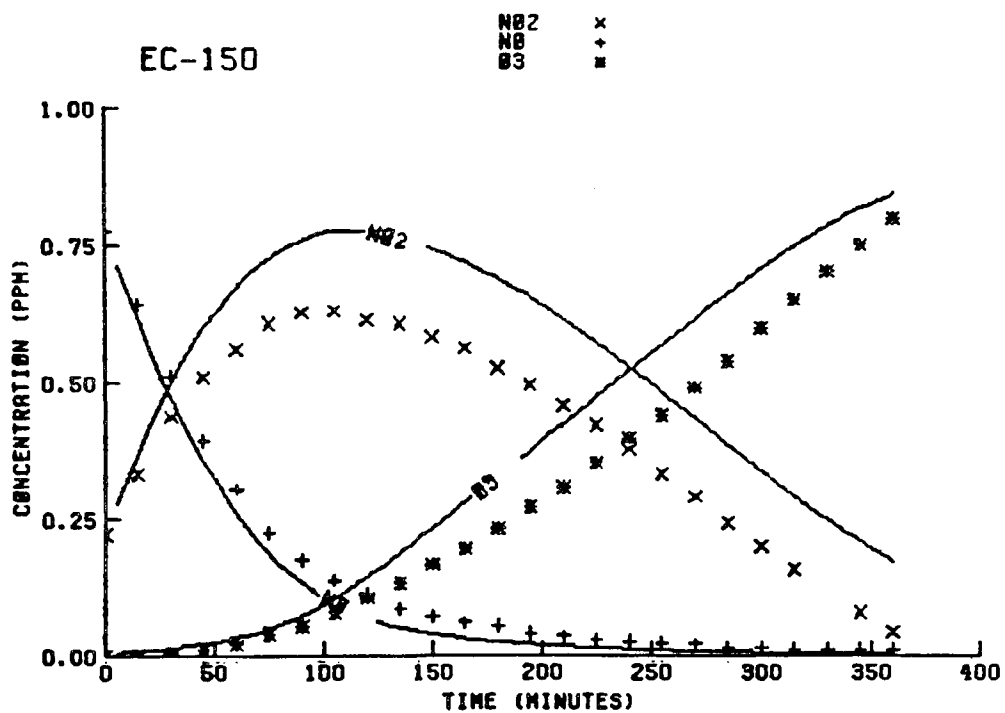


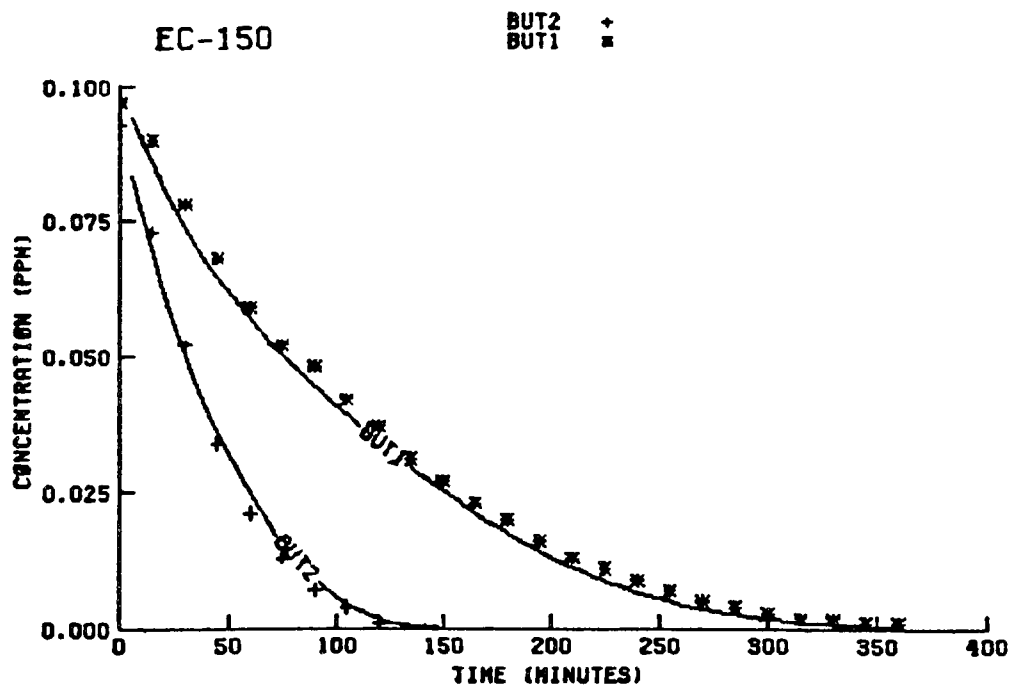
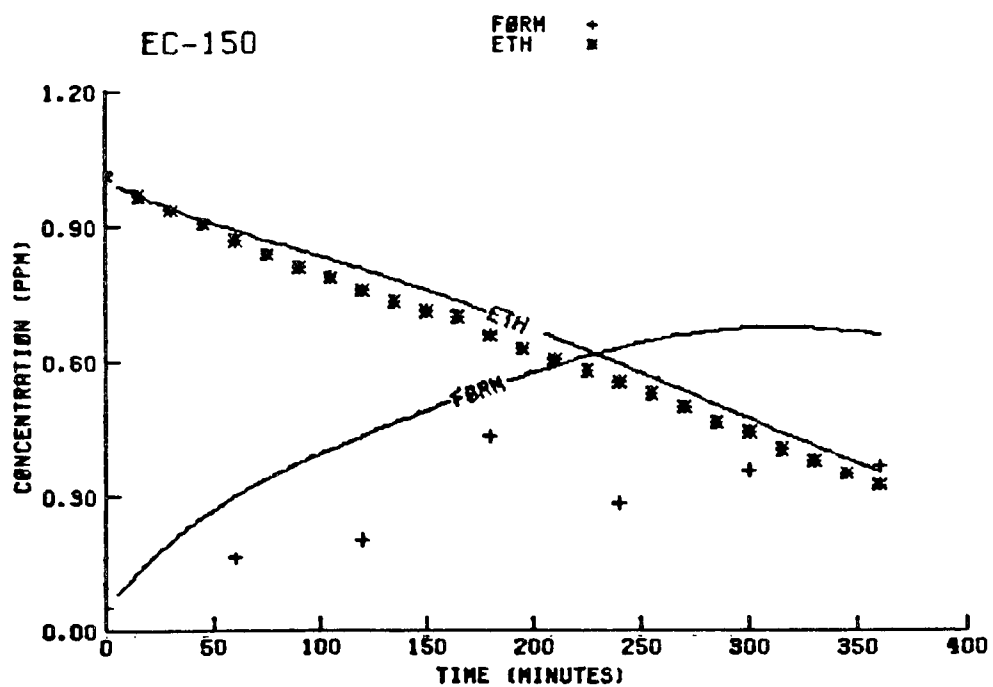
EC-149

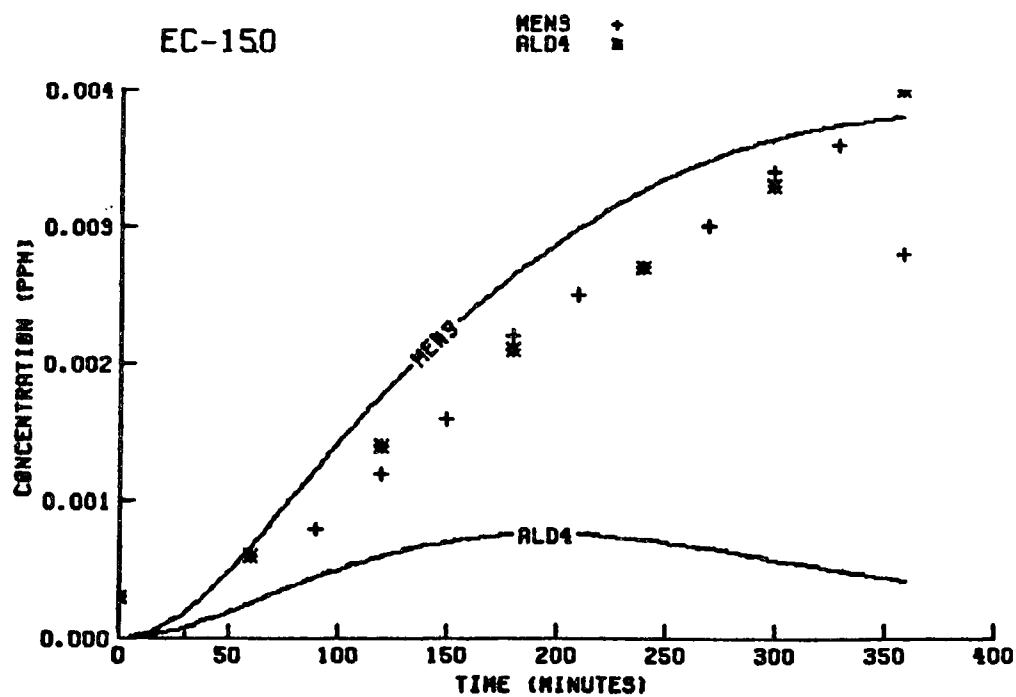
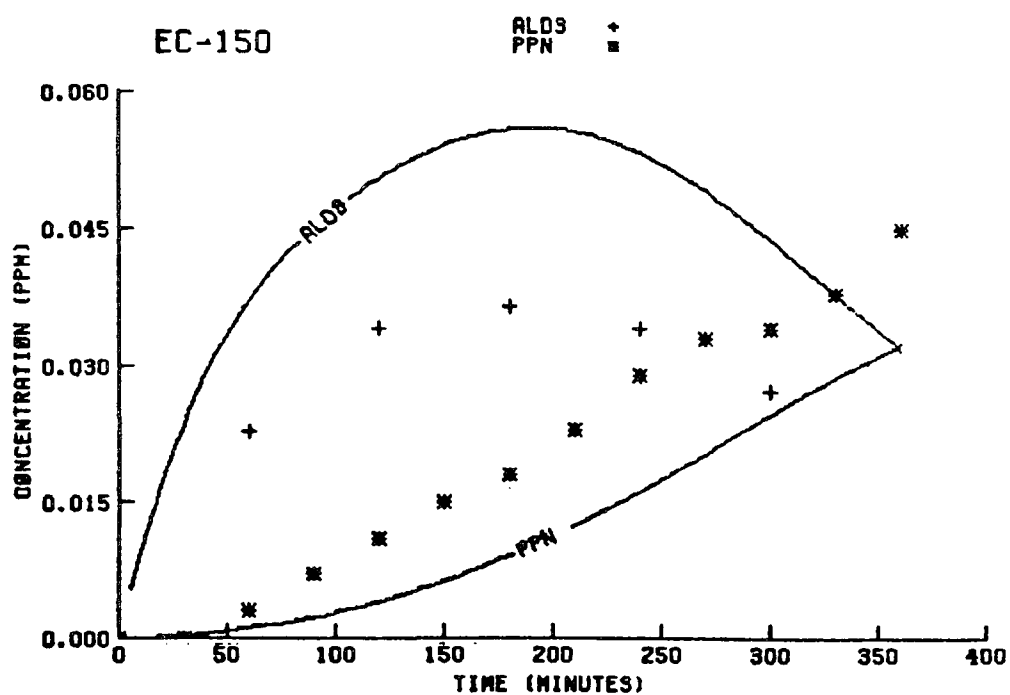
MEN3 ■



UCR MULTIOLEFIN EXPERIMENTS



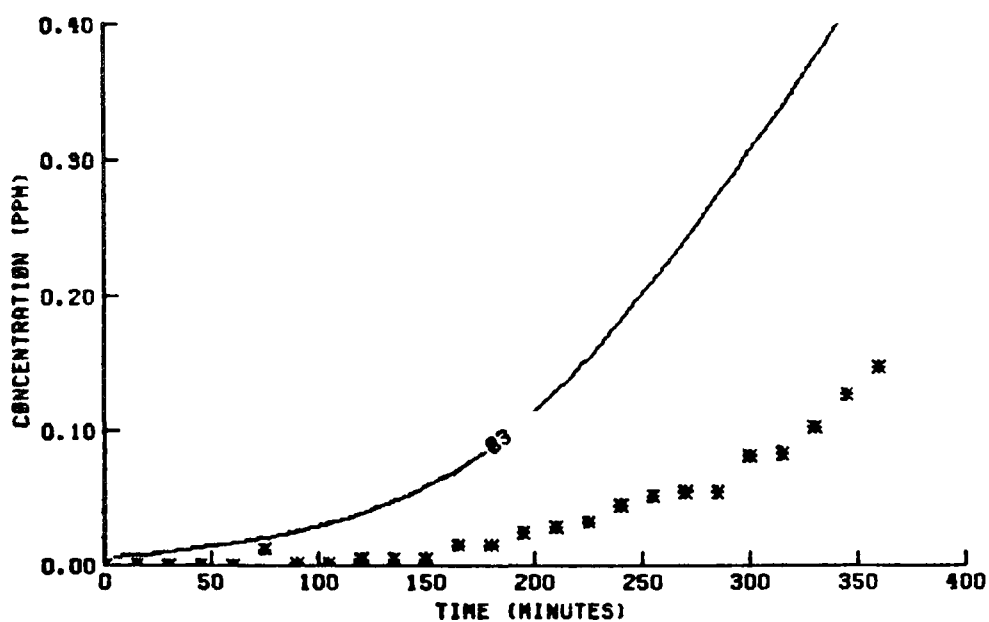




EC-151

83

■



EC-151

ETH

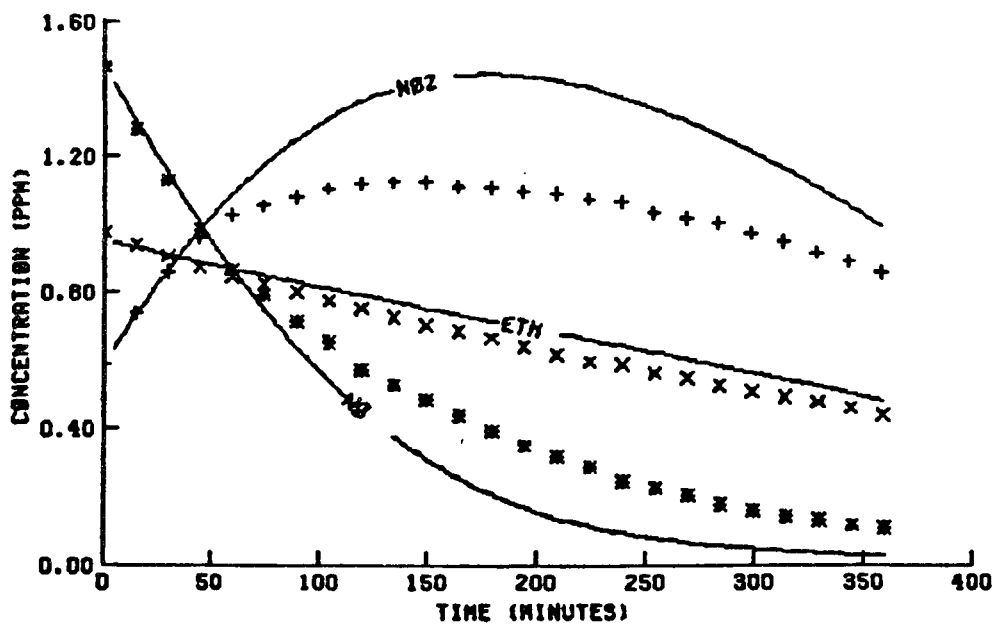
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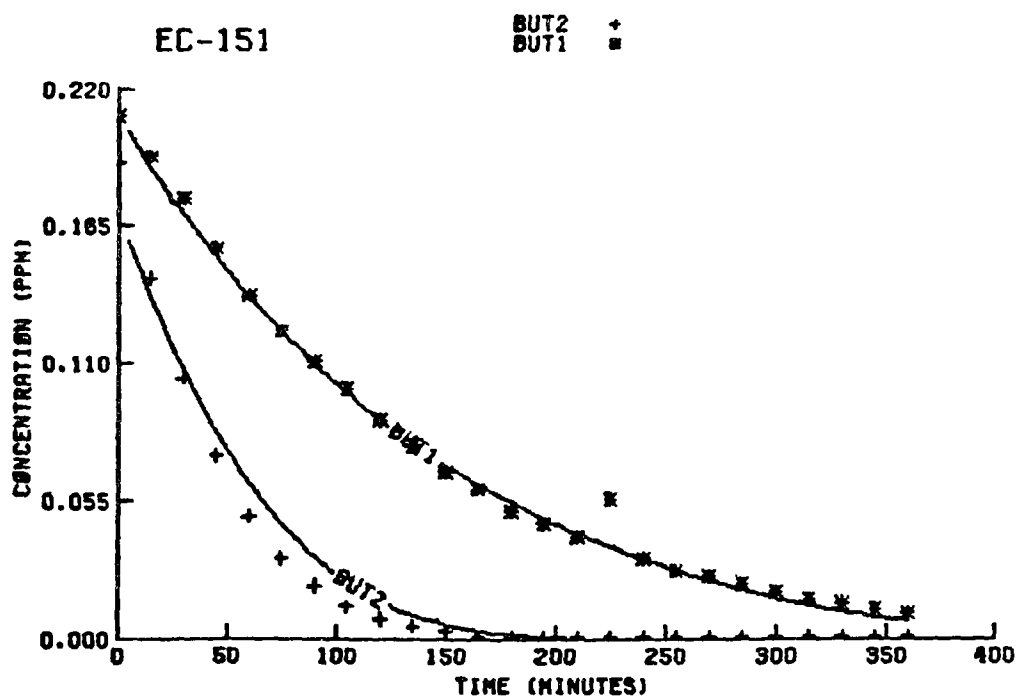
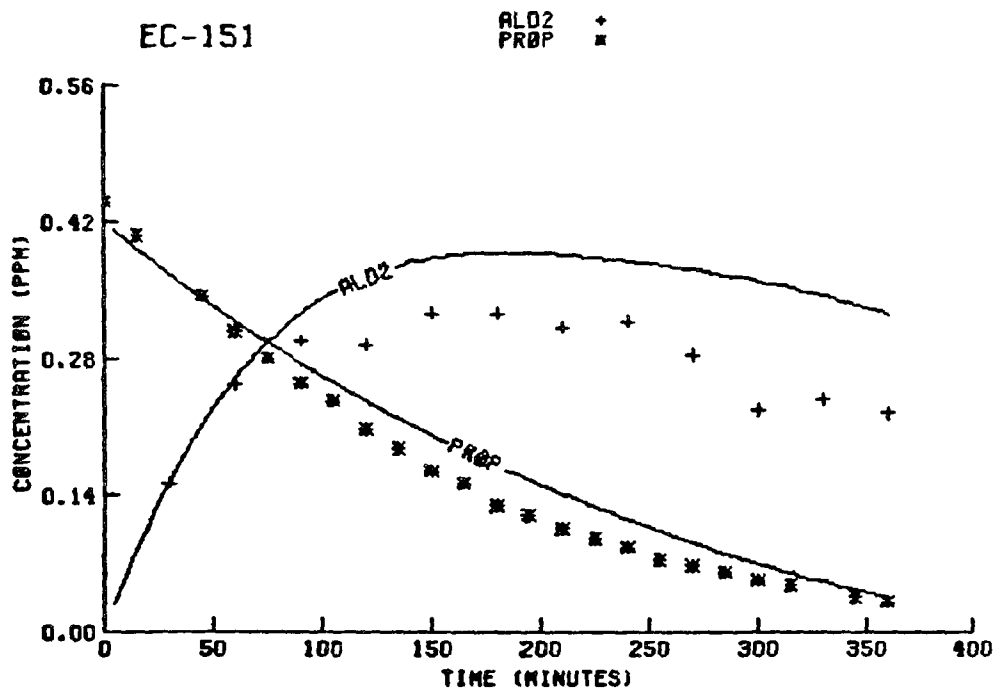
NB2

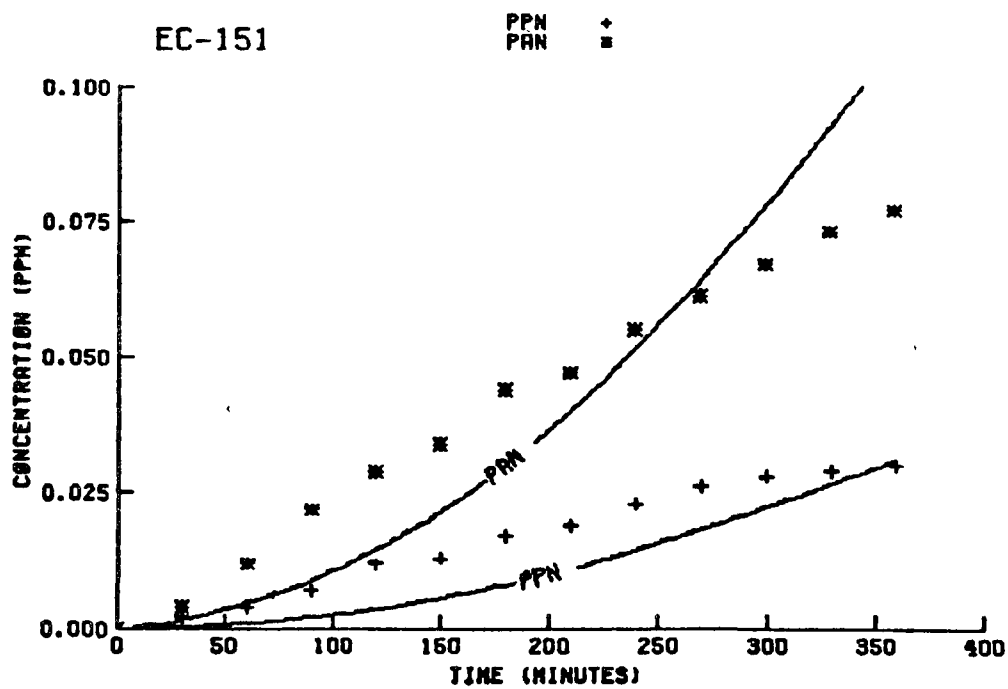
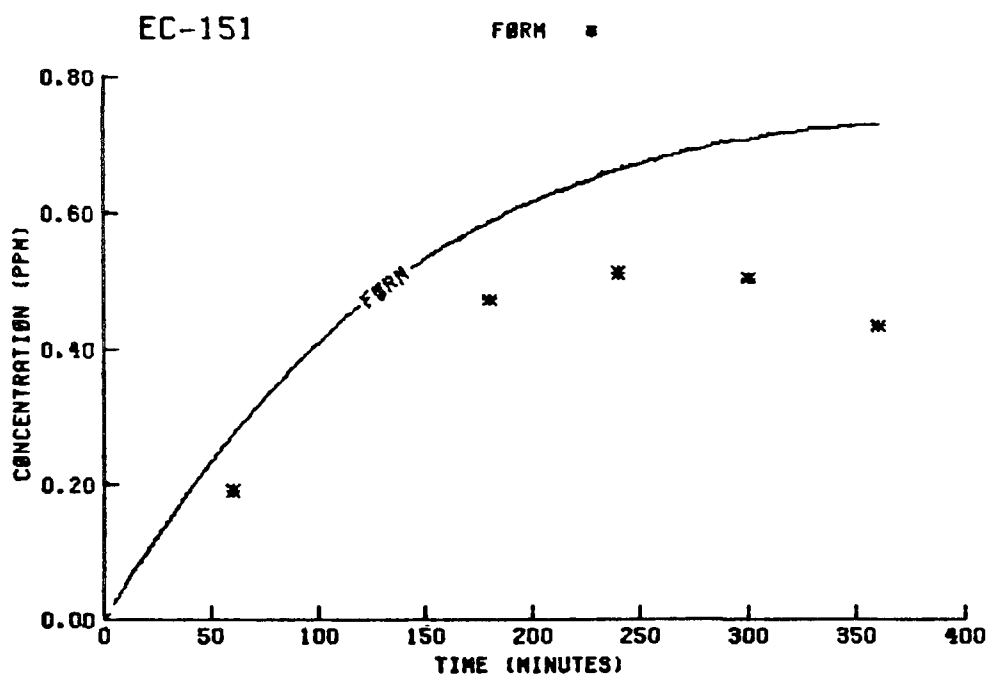
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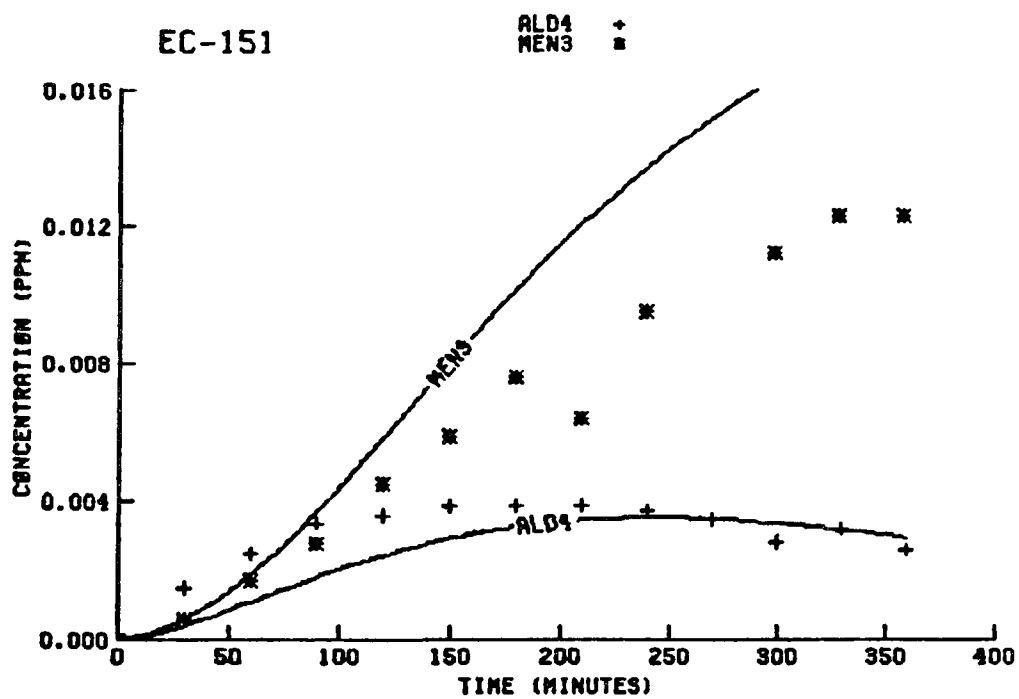
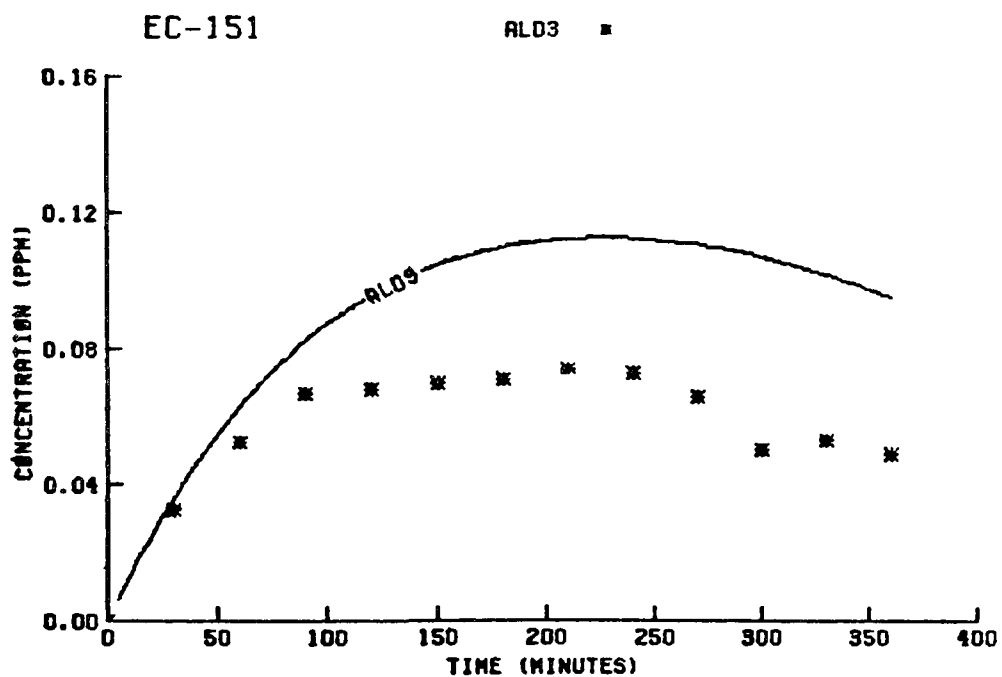
NB

■



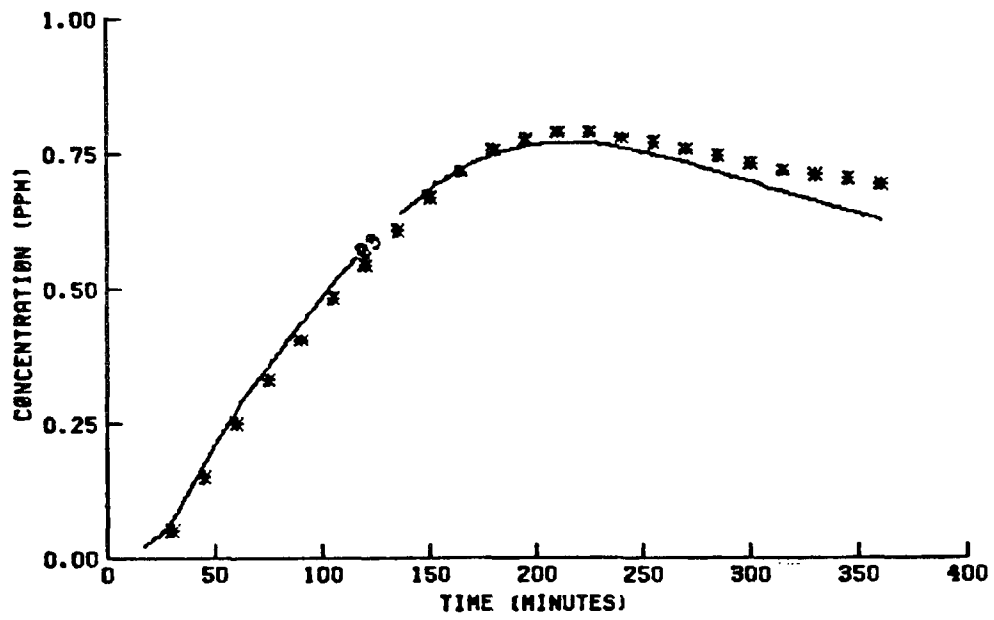






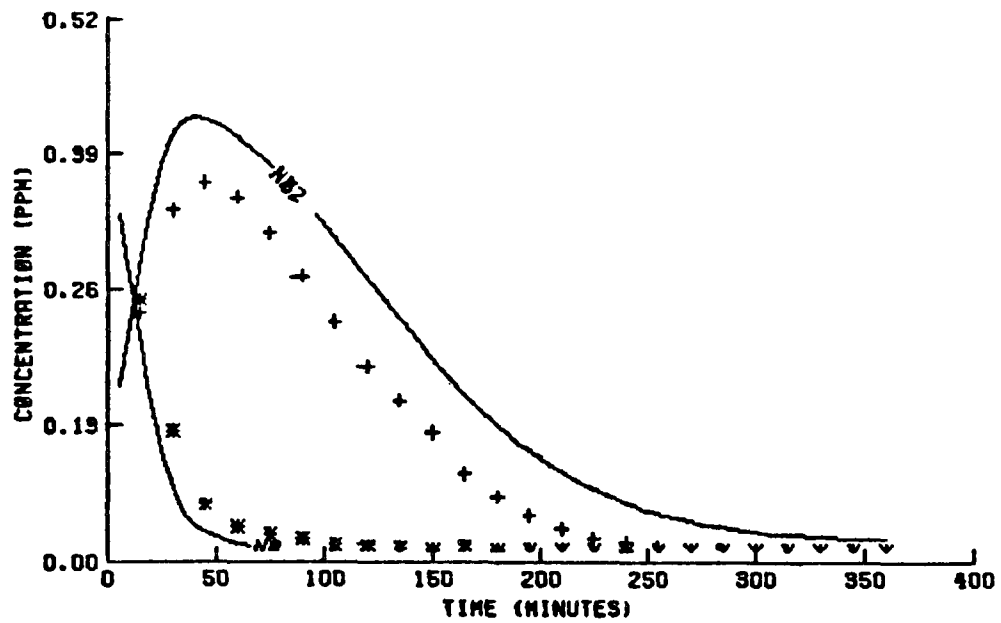
EC-152

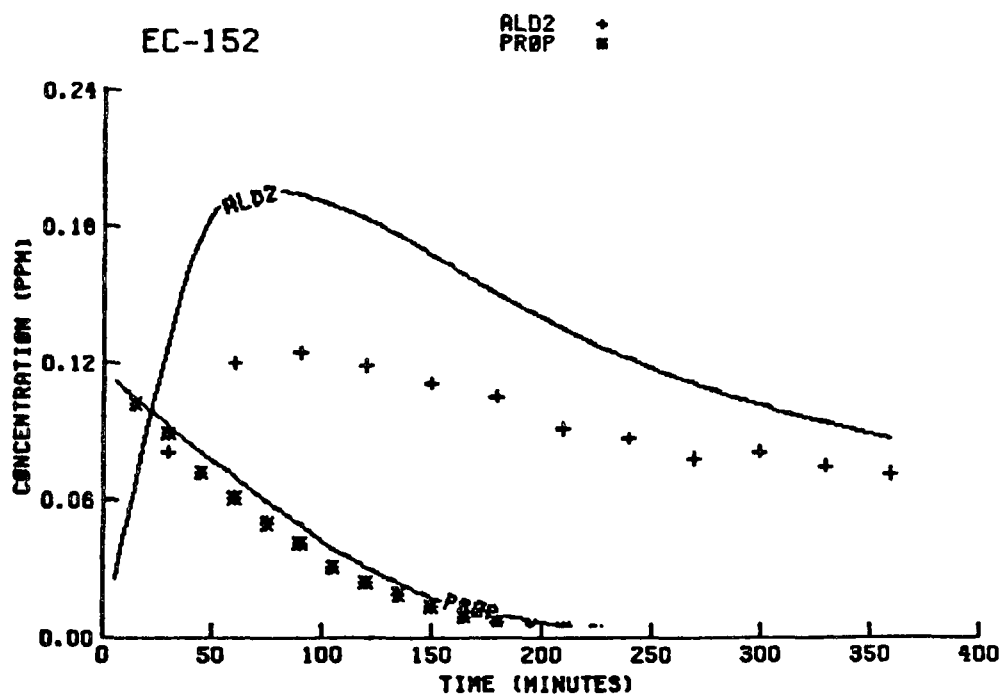
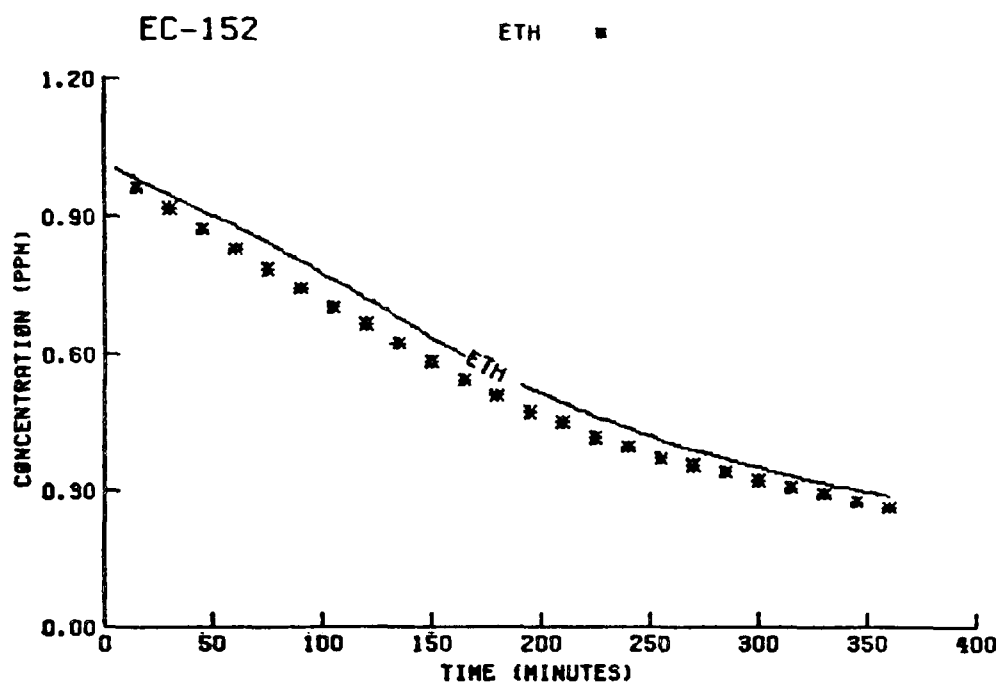
03 ■

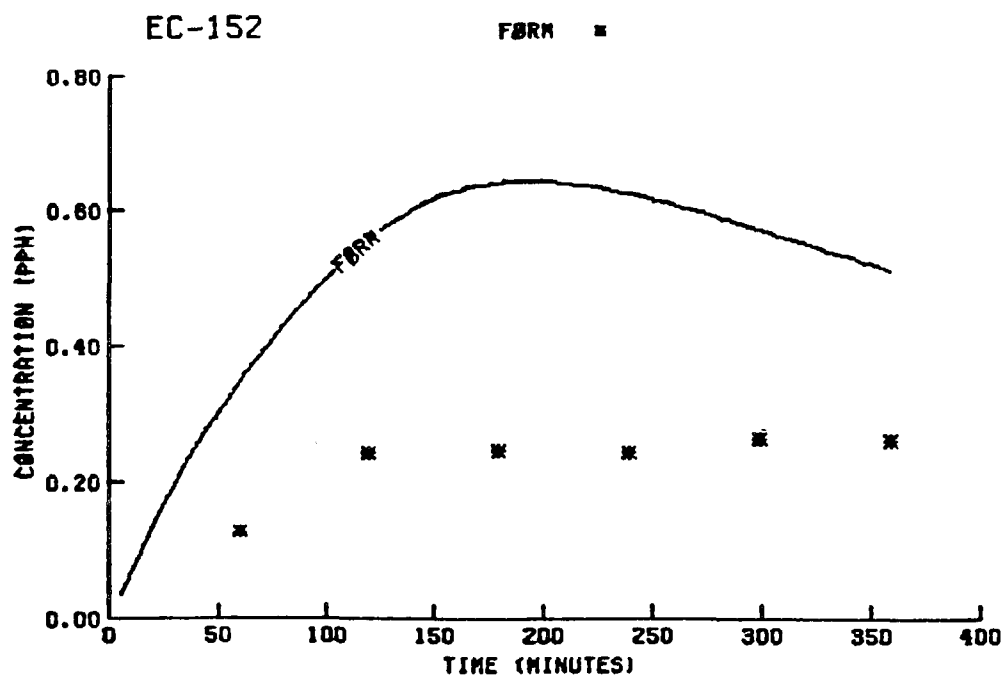
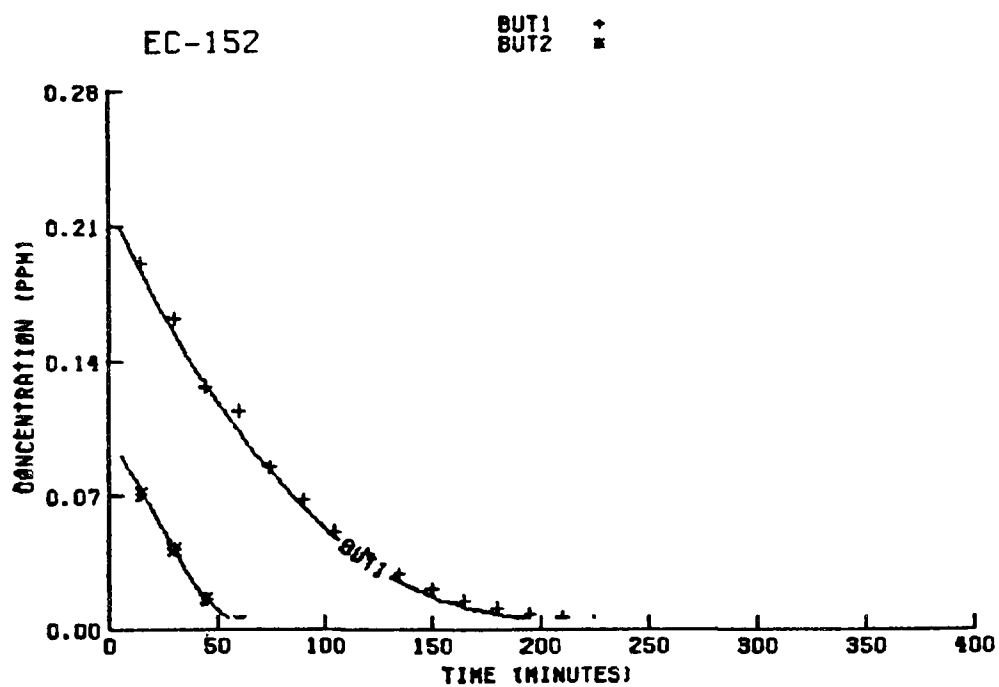


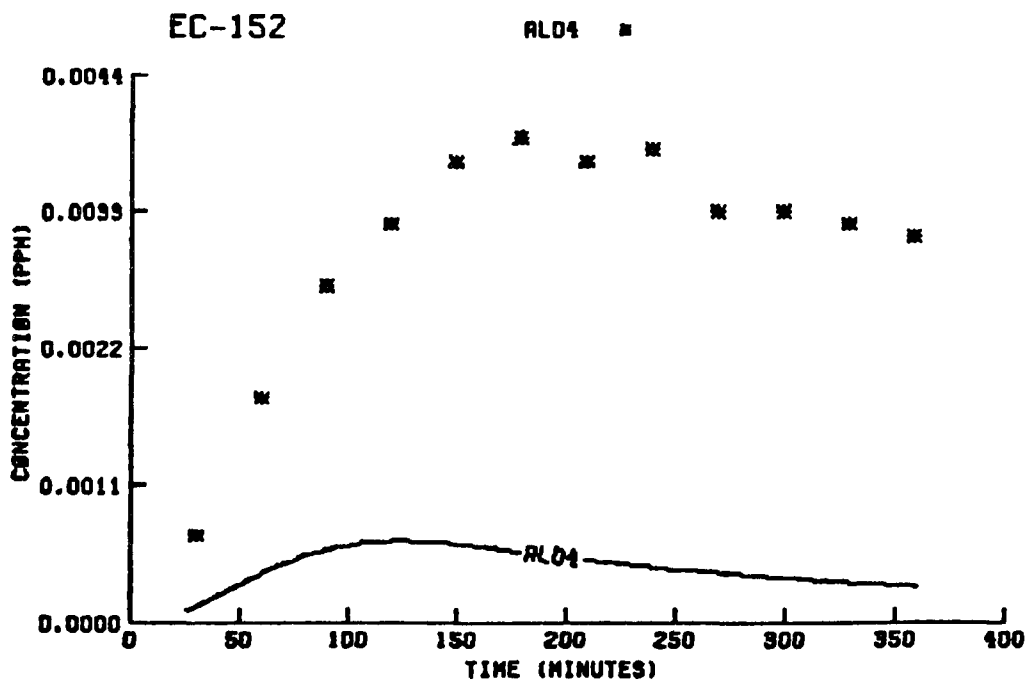
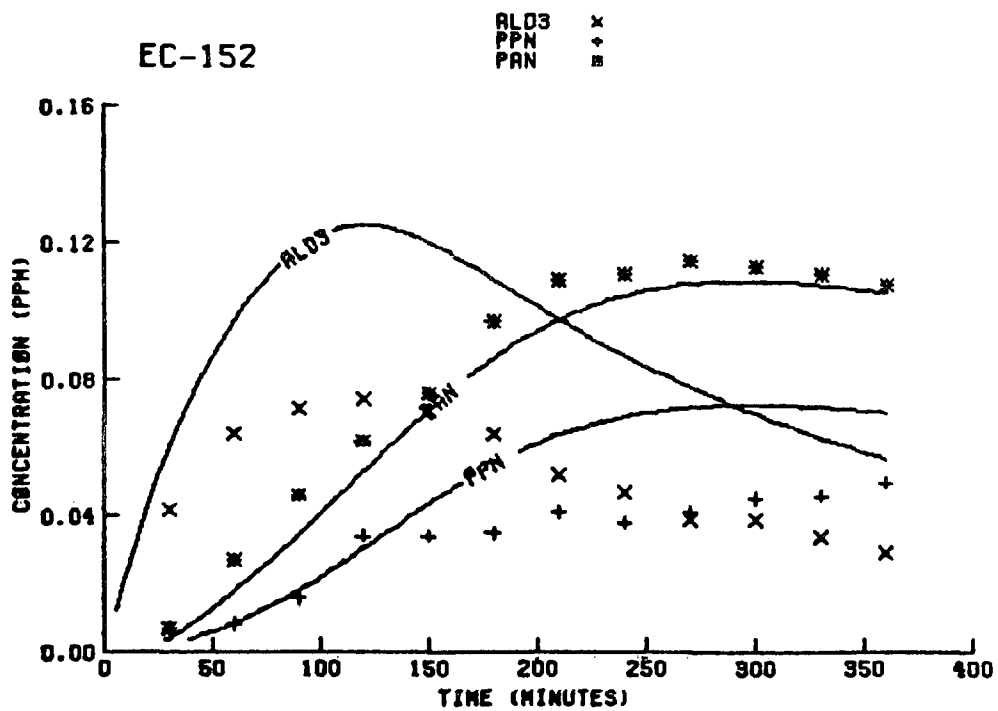
EC-152

N02 +
NB ■



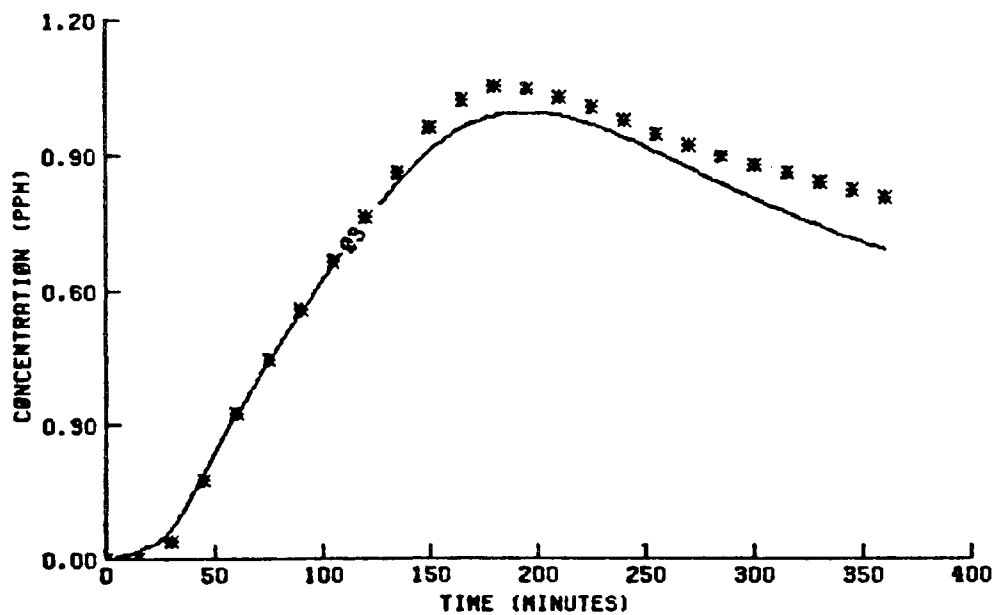






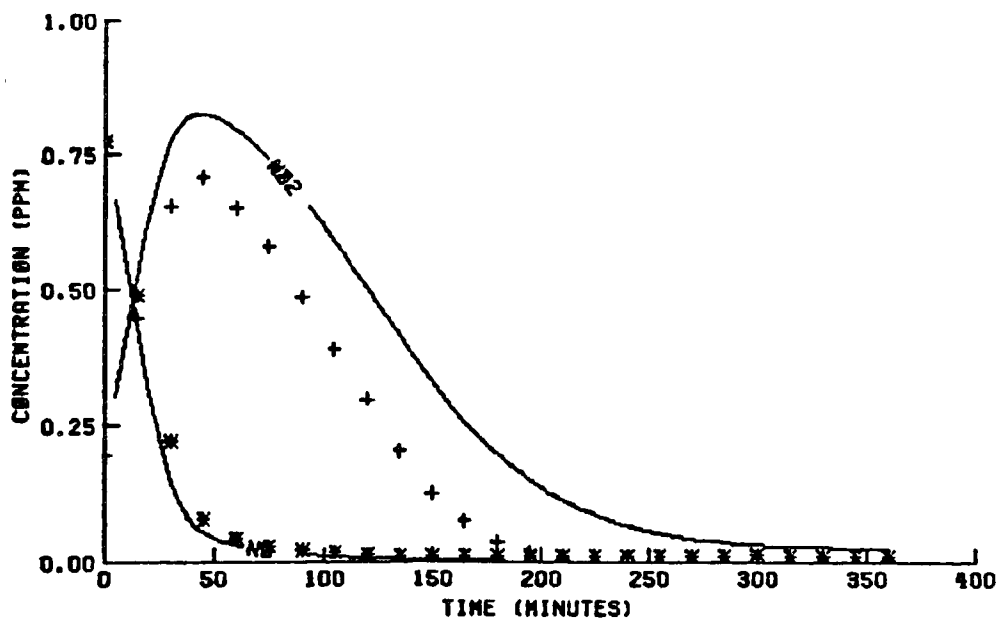
EC-153

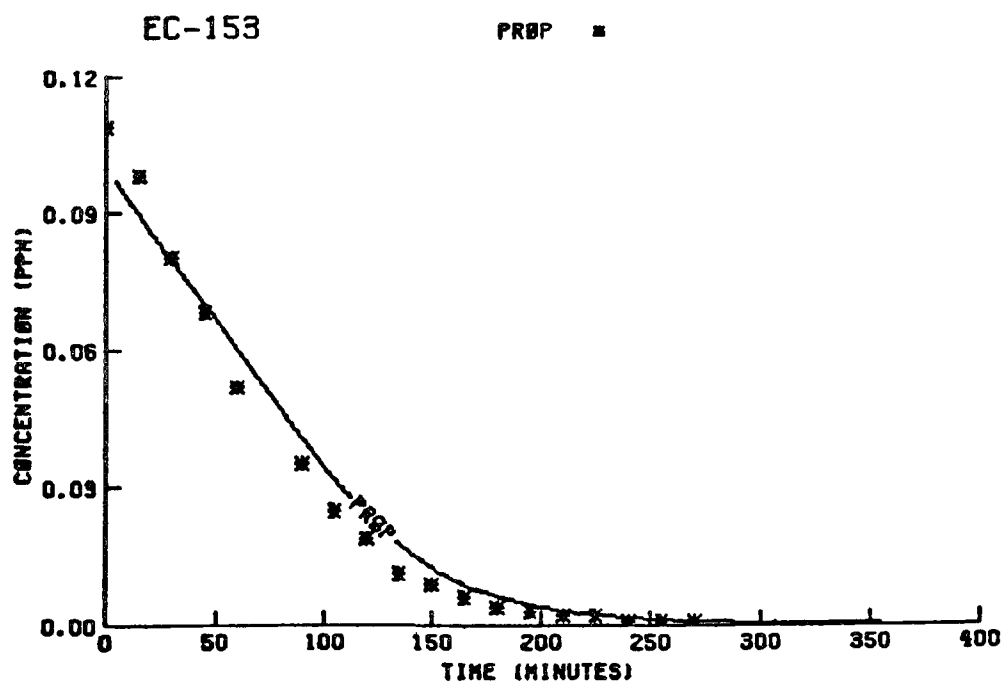
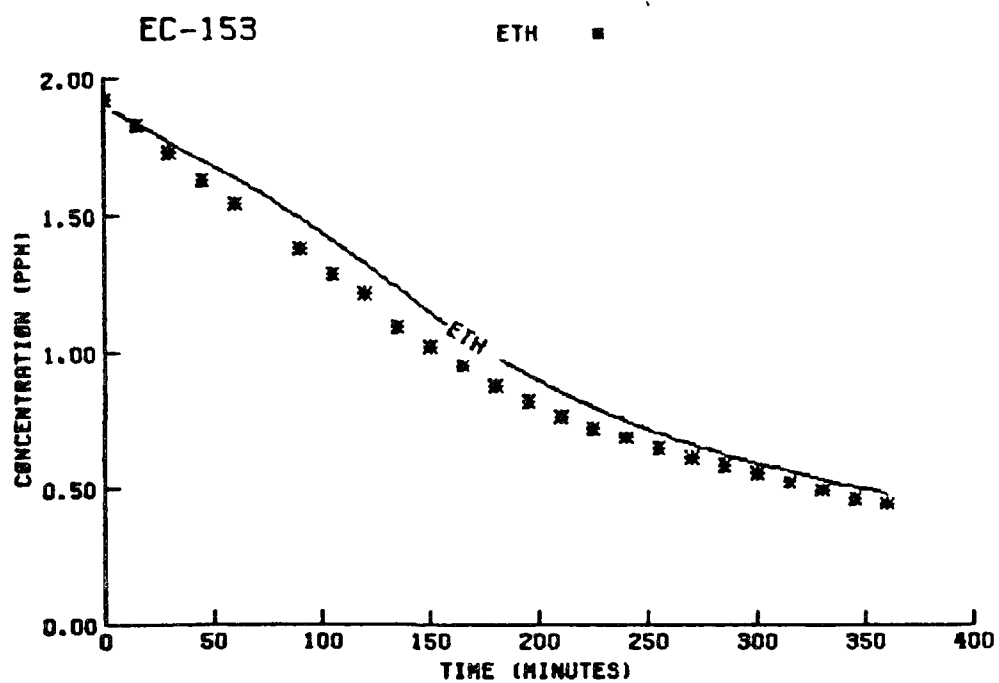
83 ■

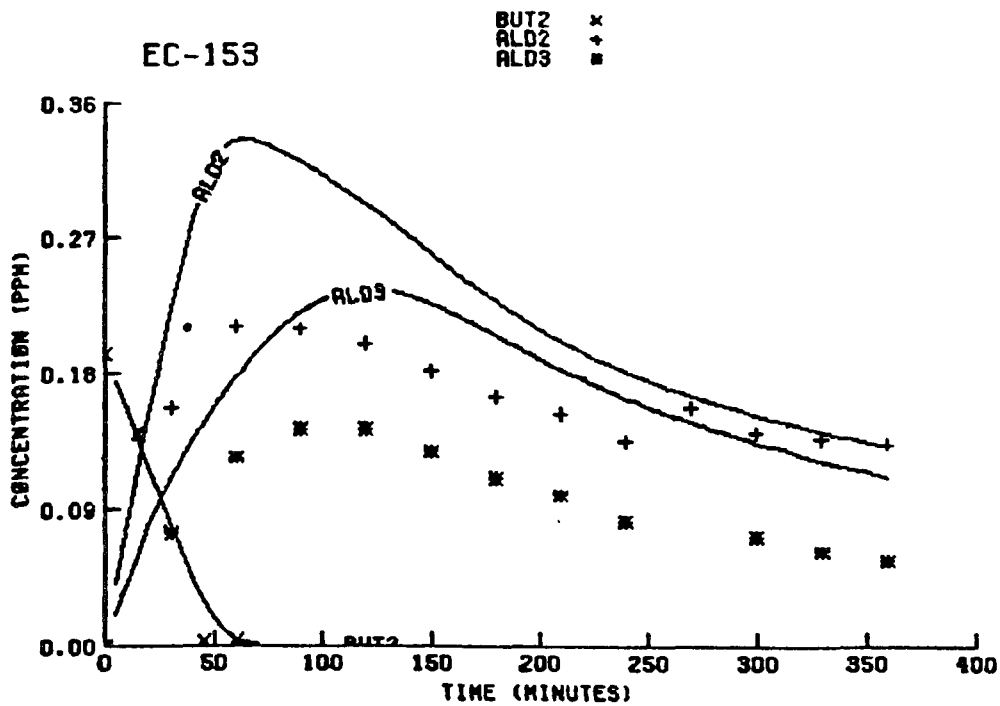
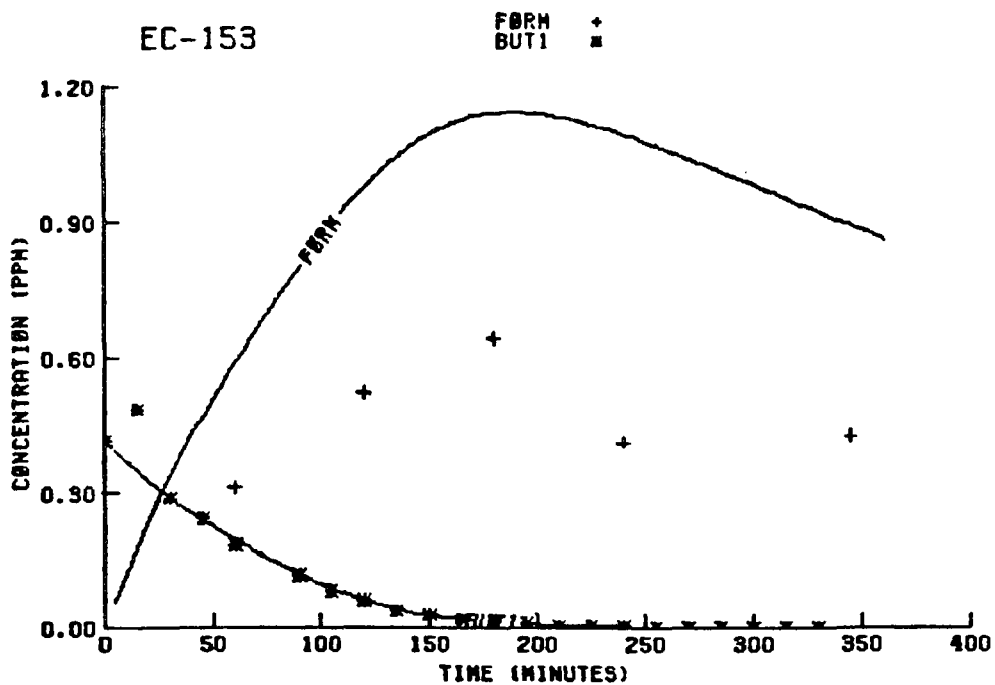


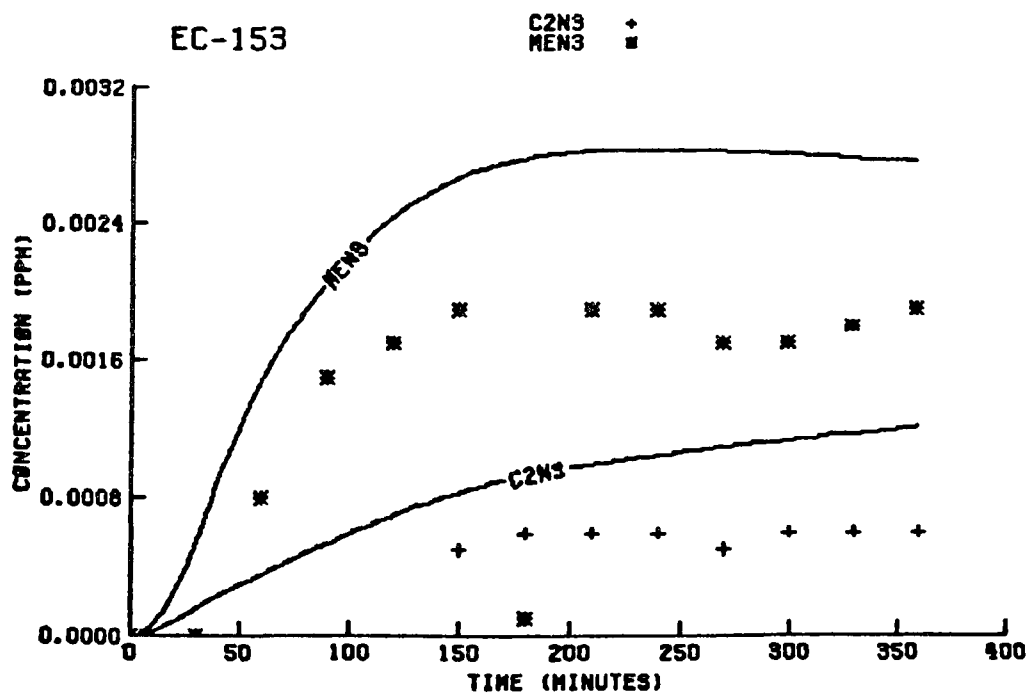
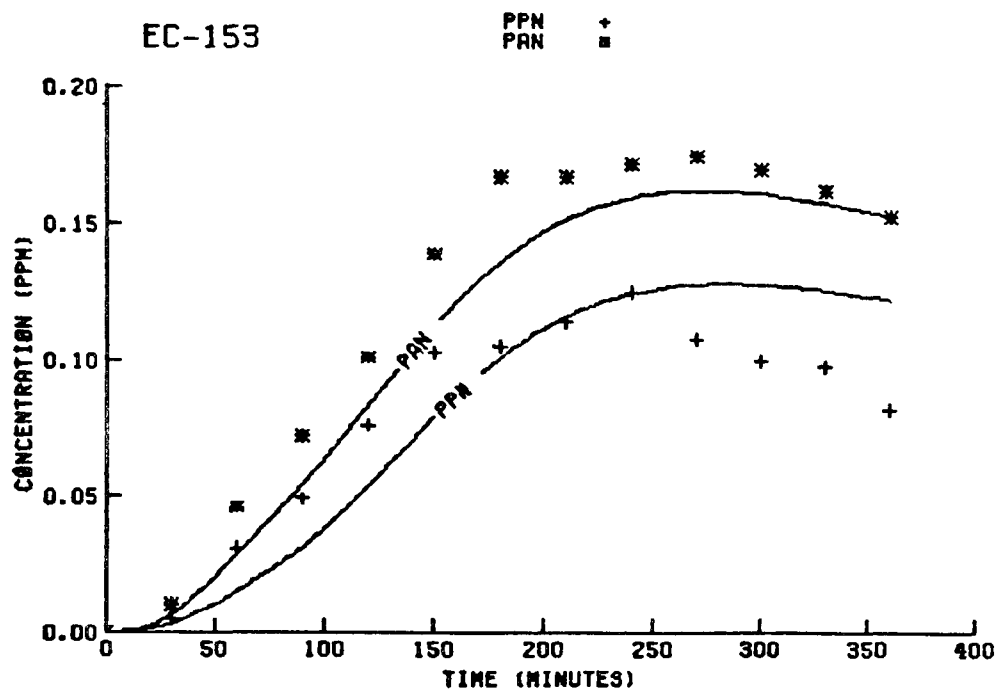
EC-153

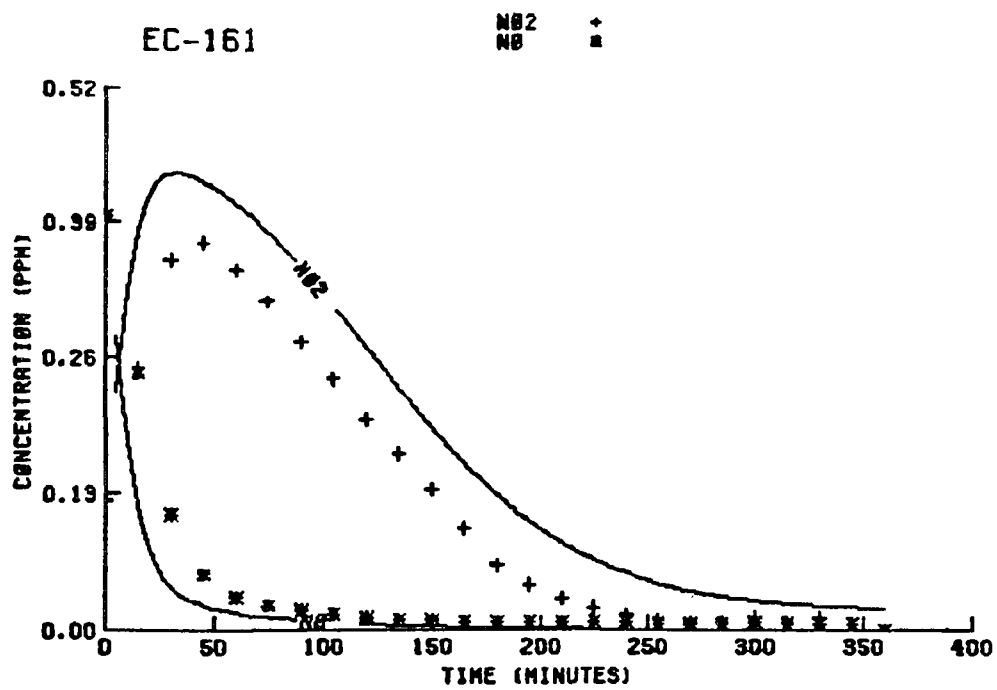
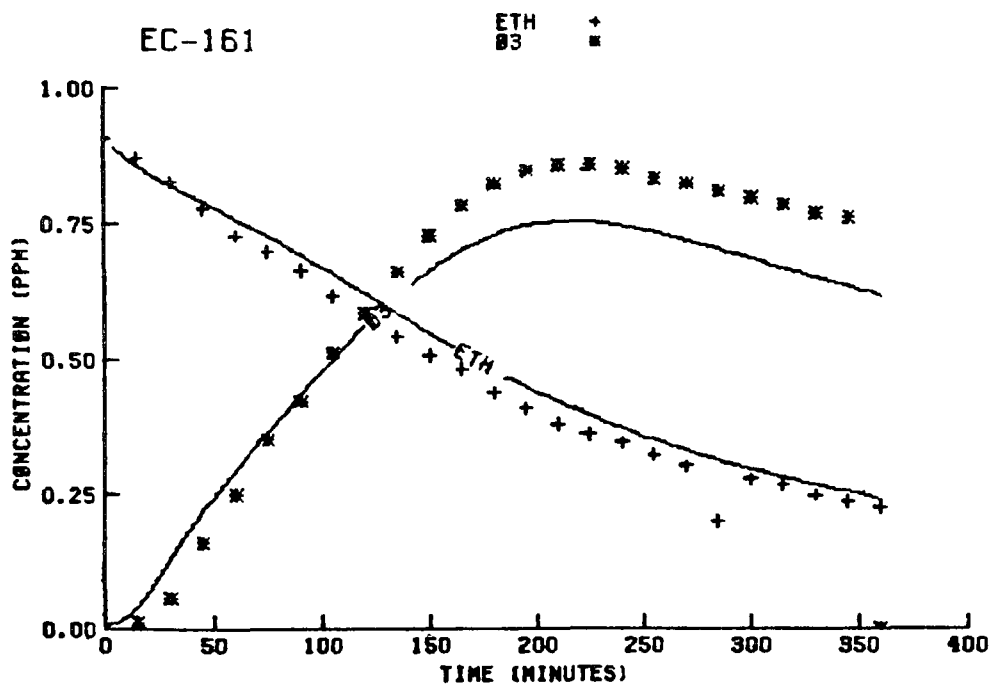
N82 +
N8 ■

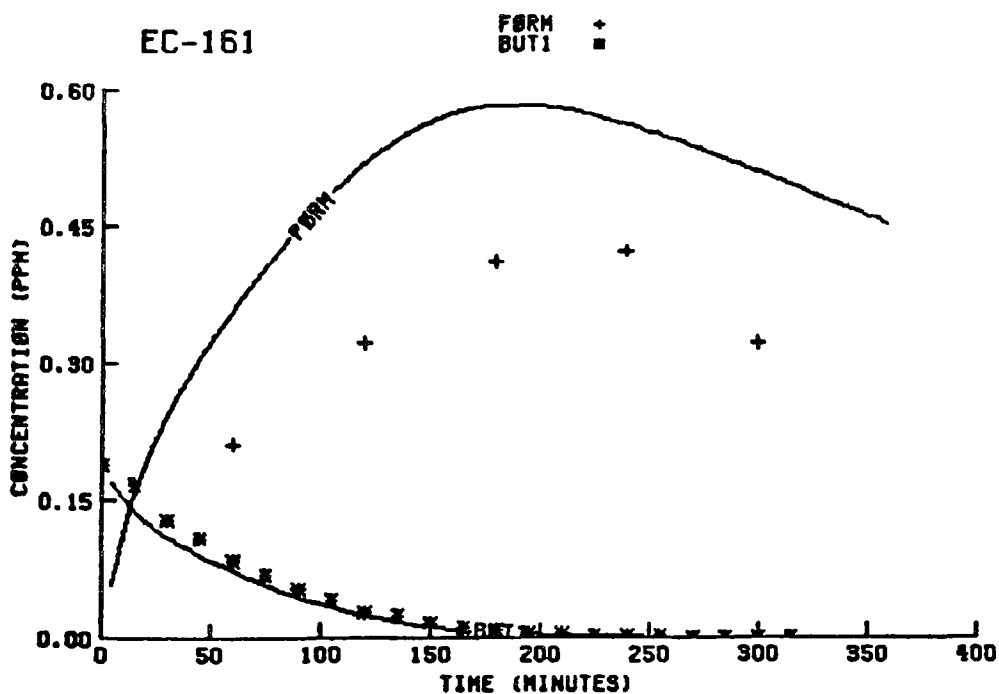
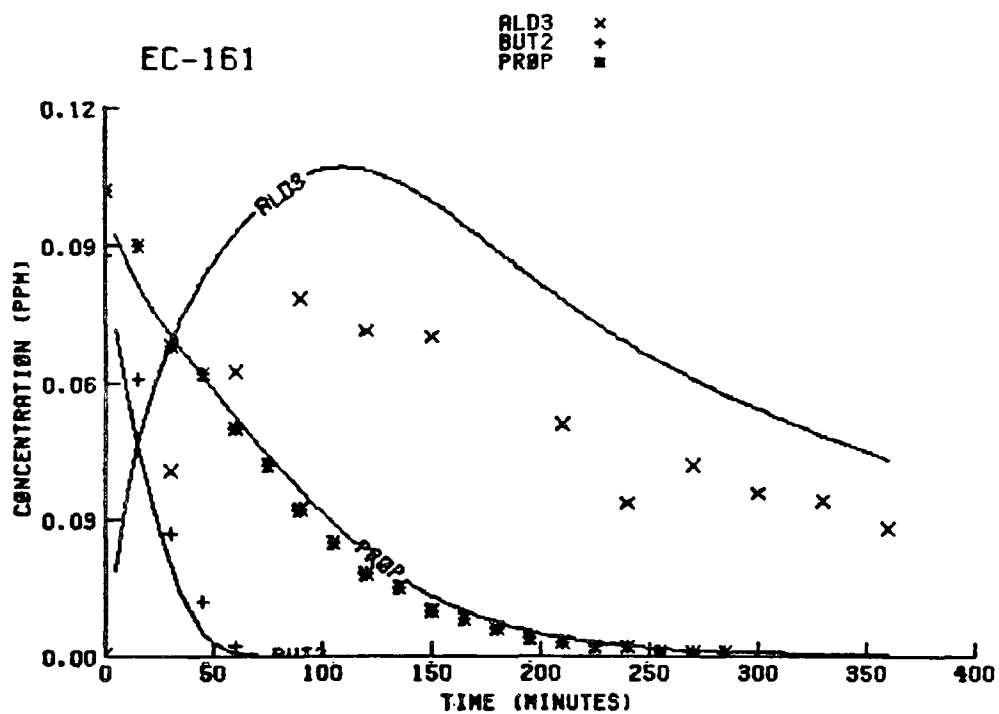


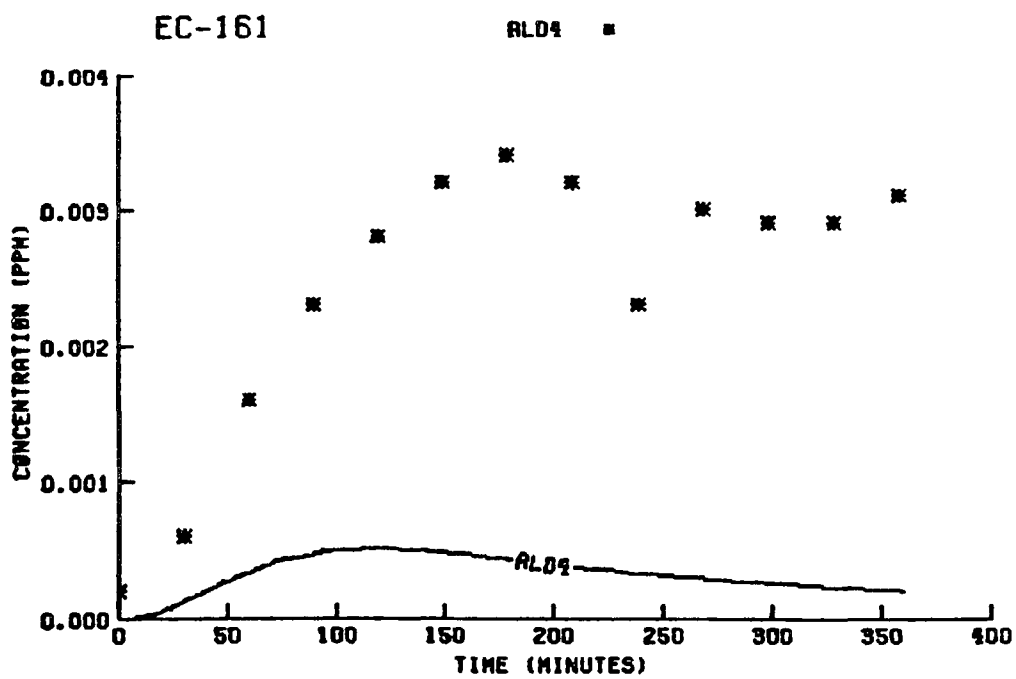
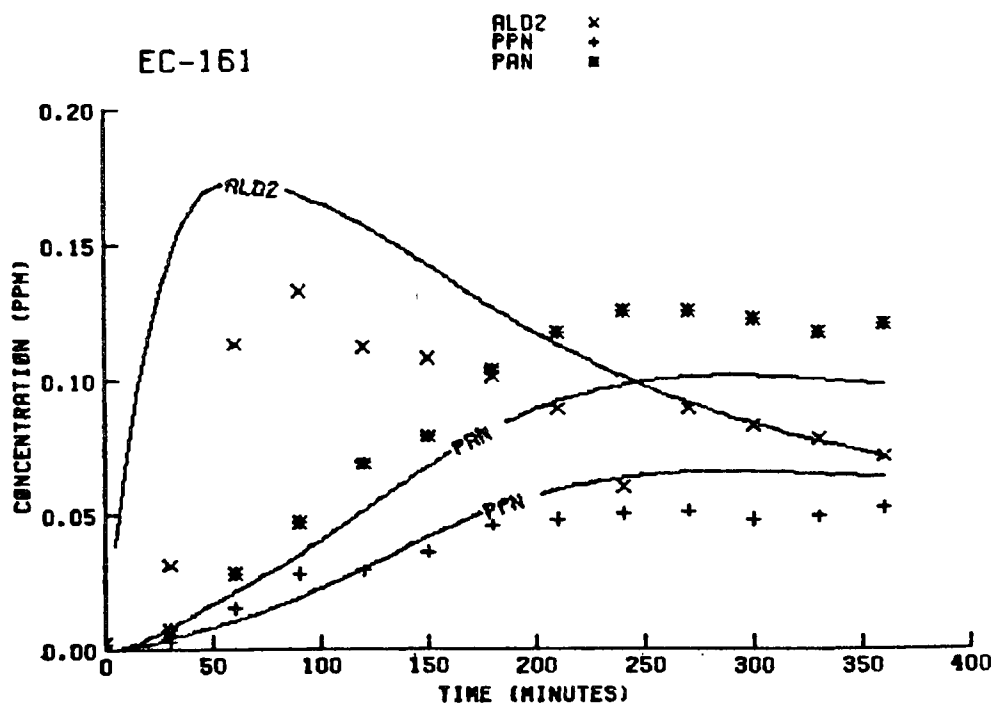


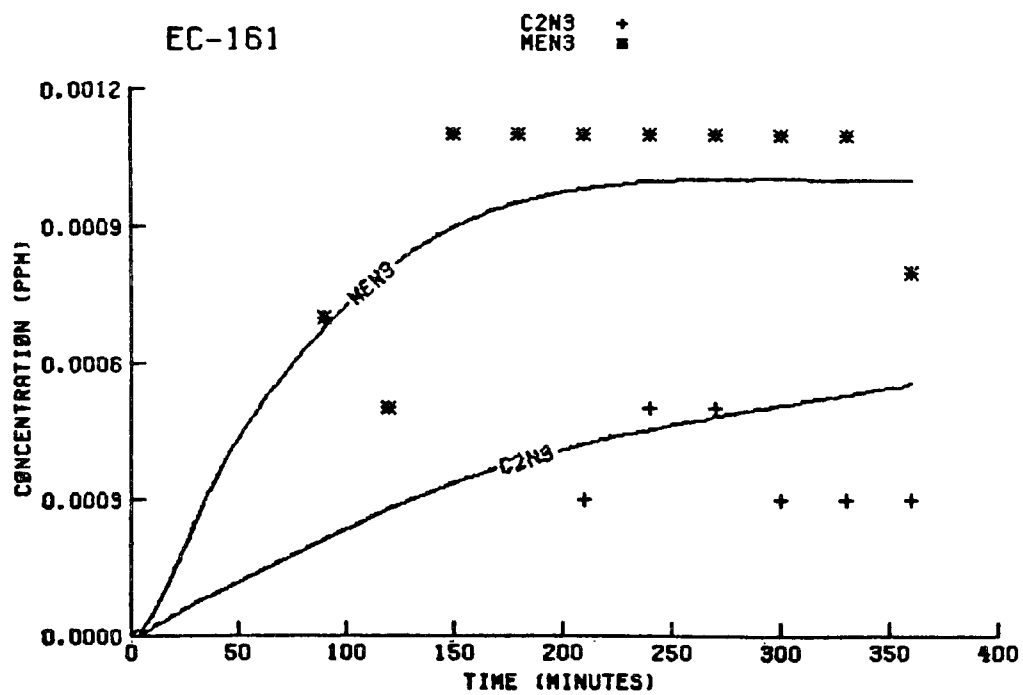










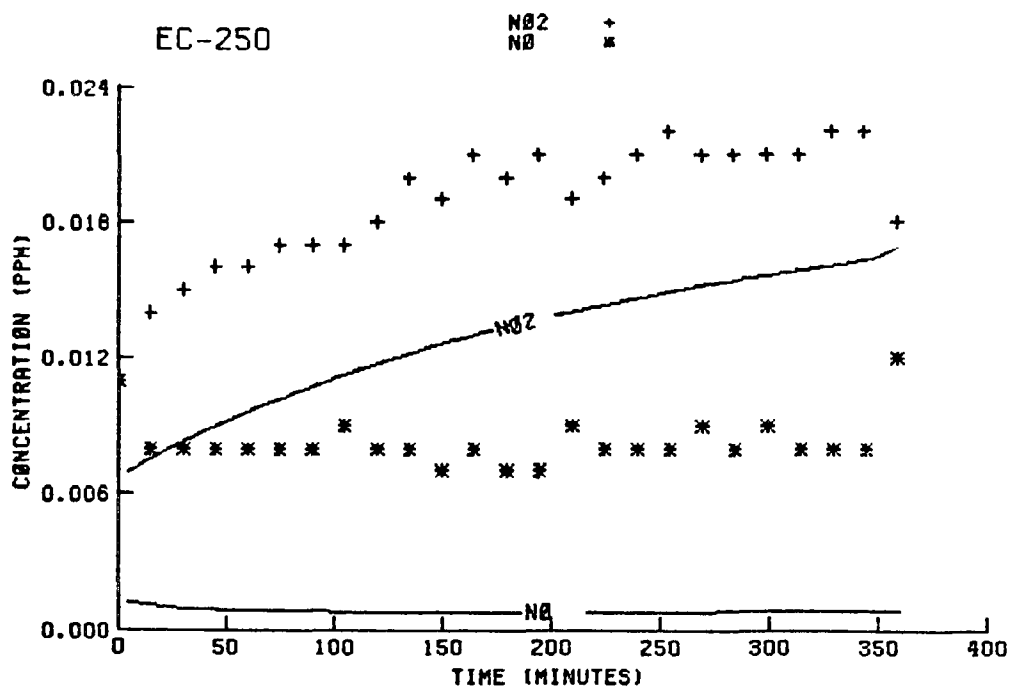
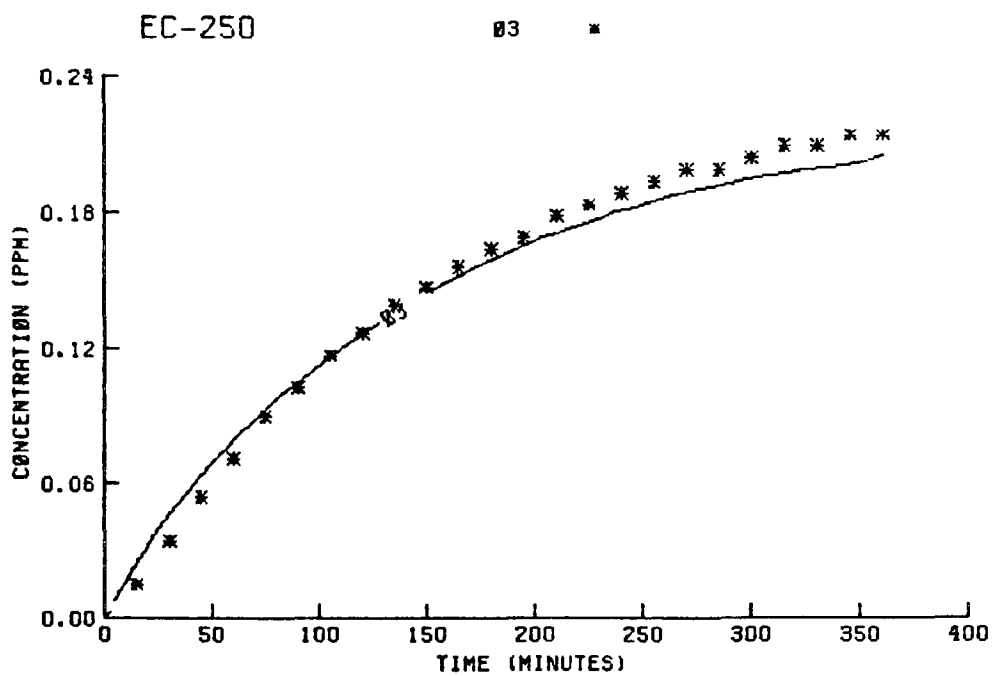


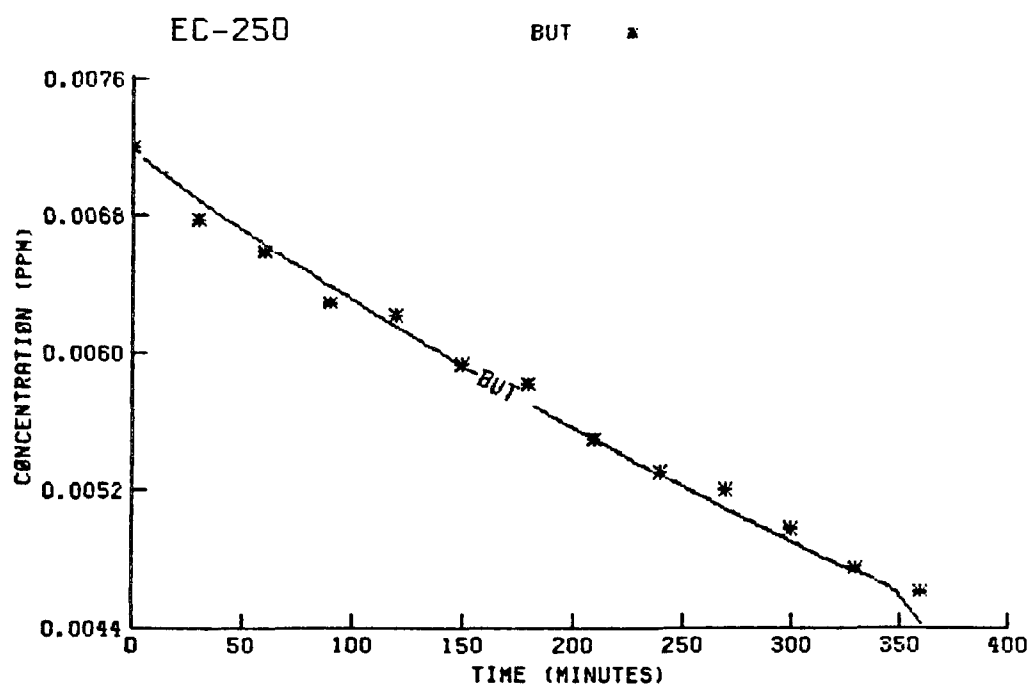
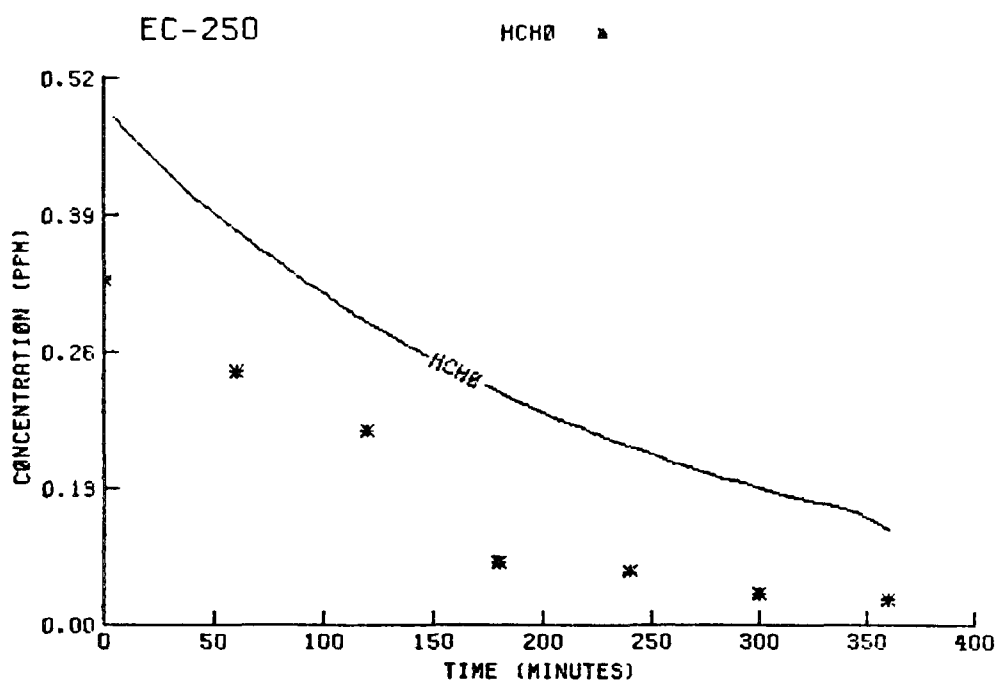
Part B

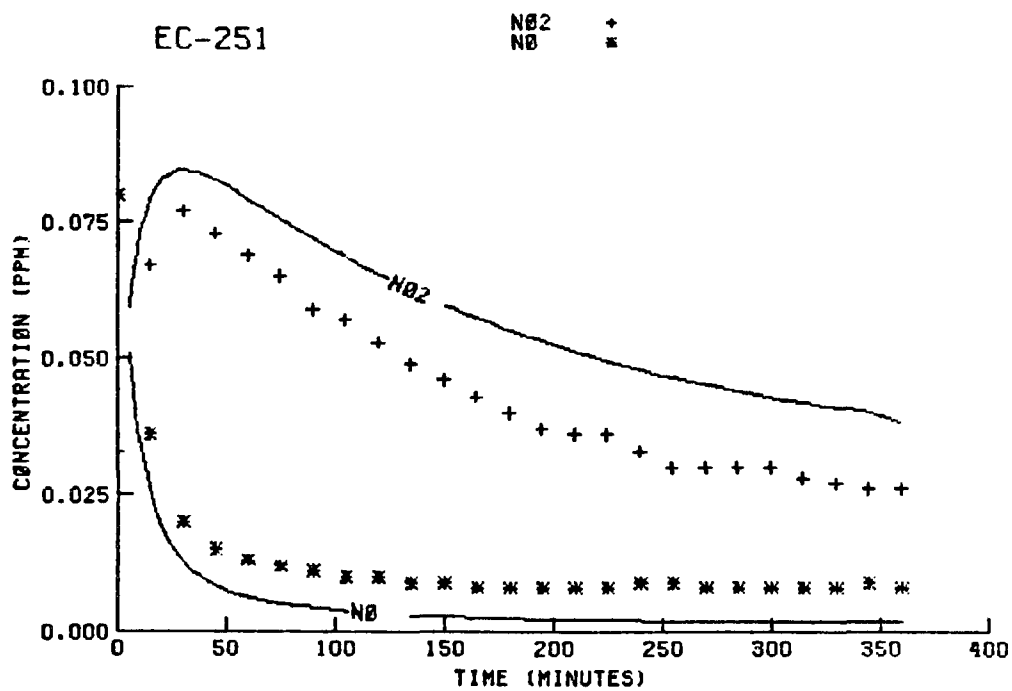
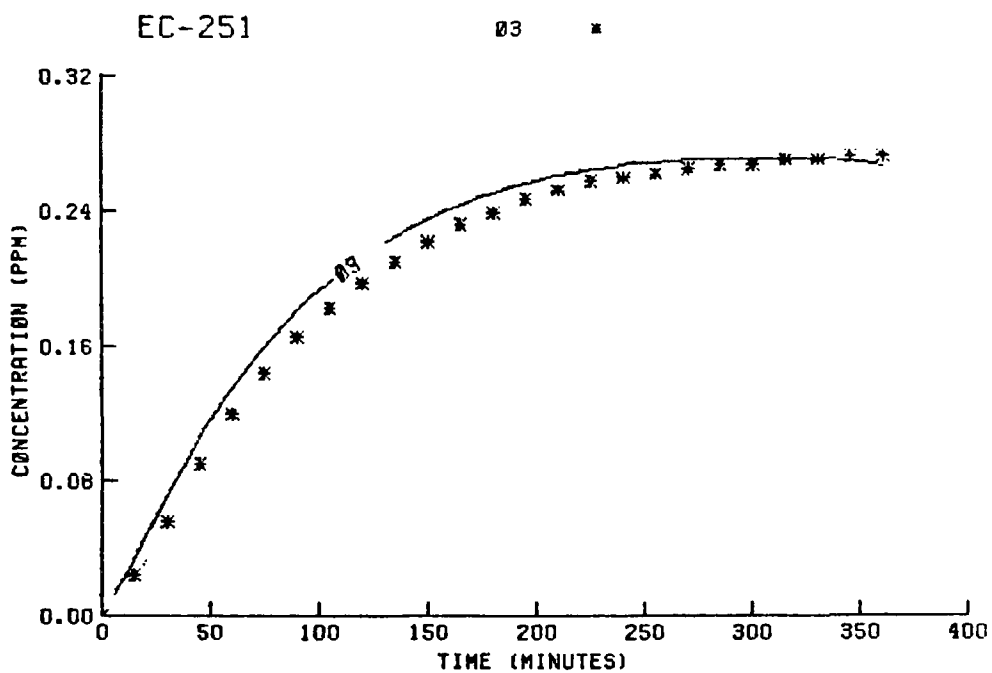
Simulation Results with the Carbon-Bond Mechanism

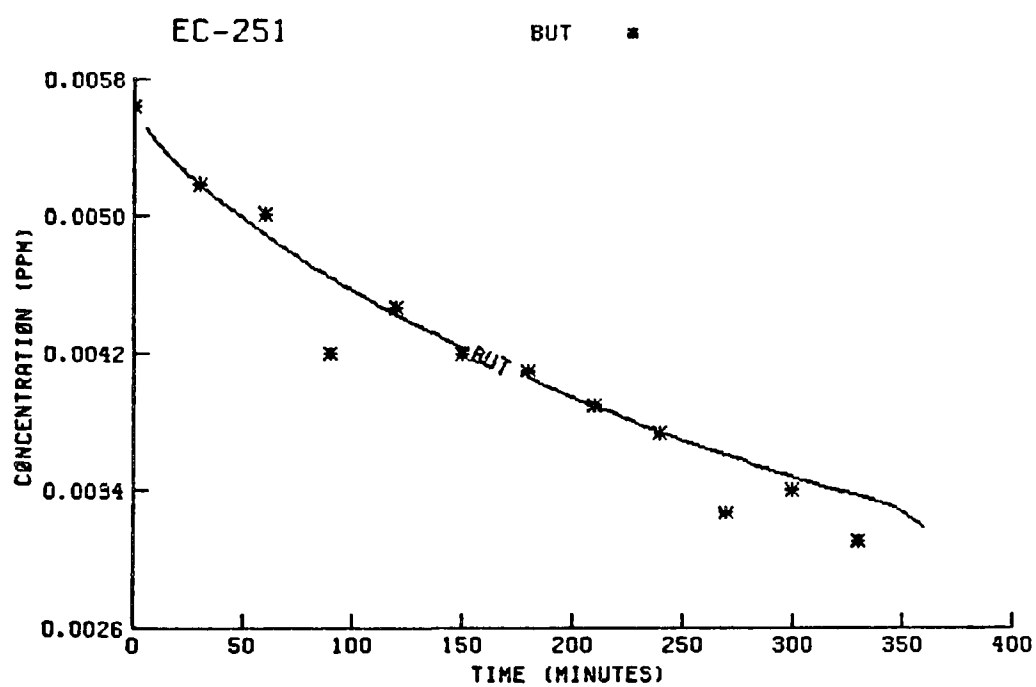
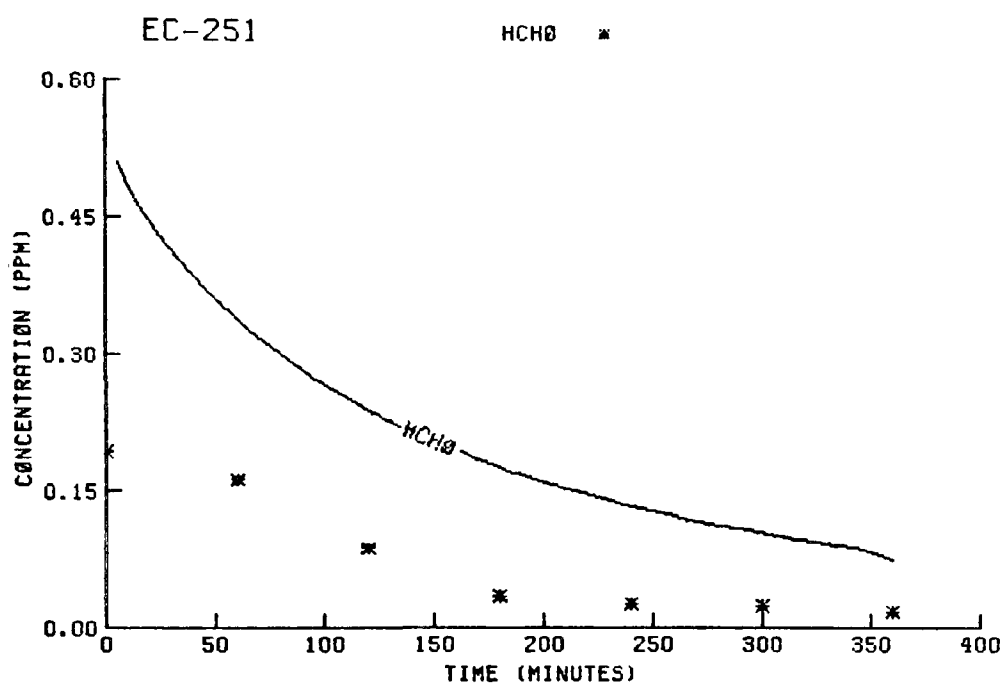
UCR FORMALDEHYDE EXPERIMENTS

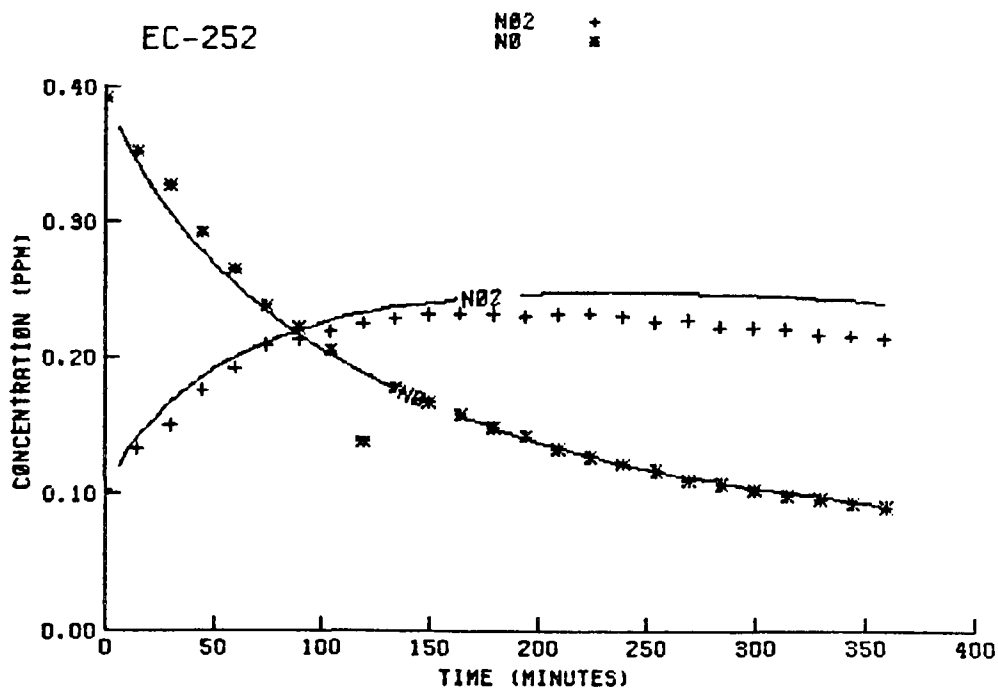
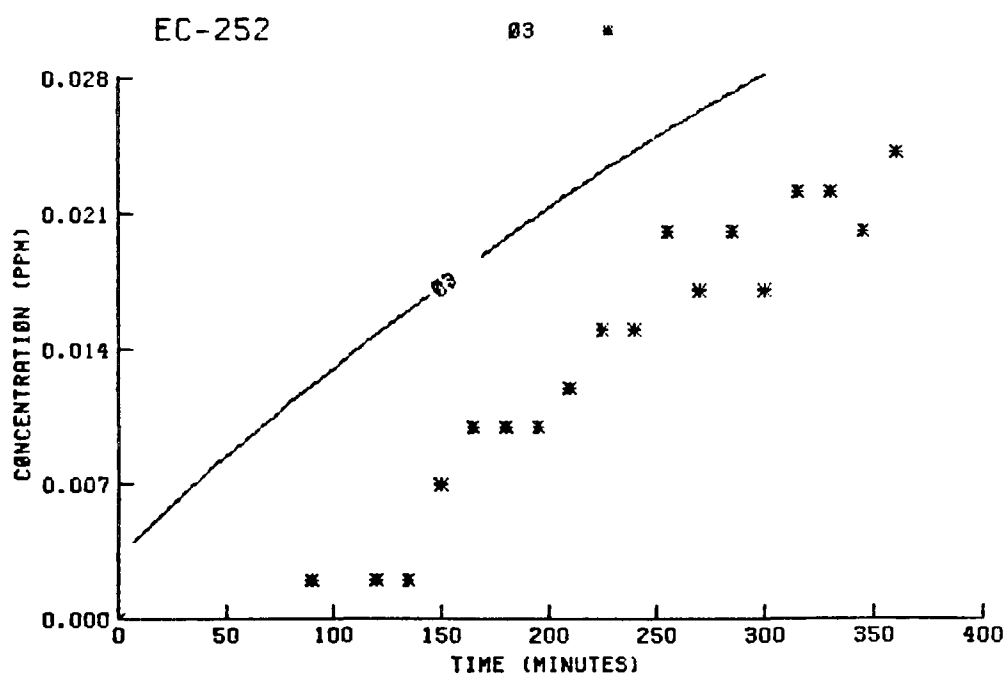
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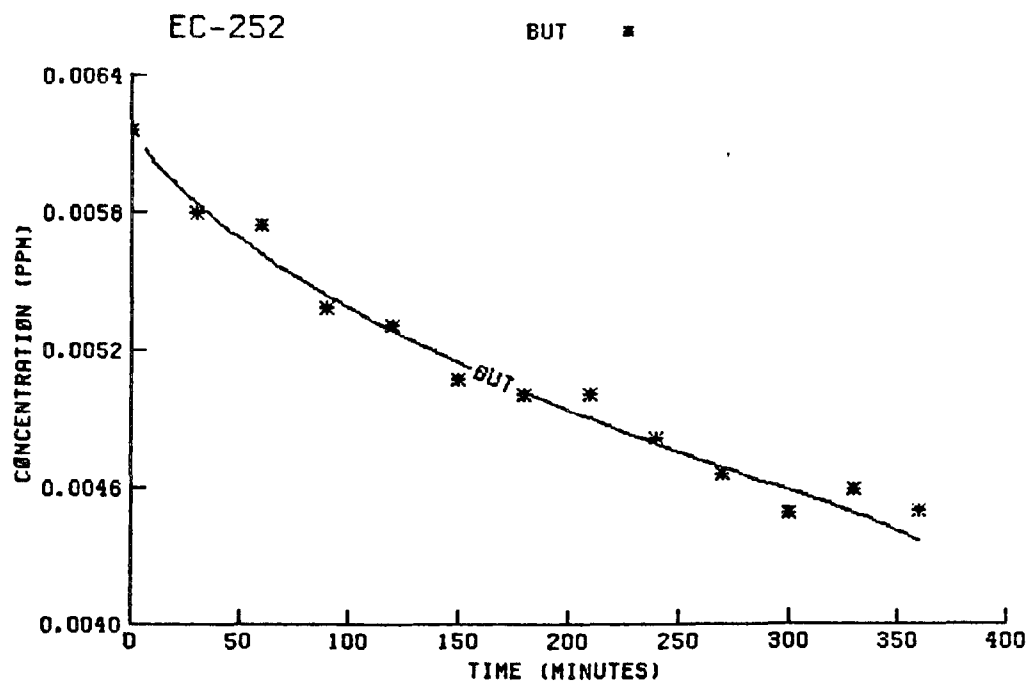
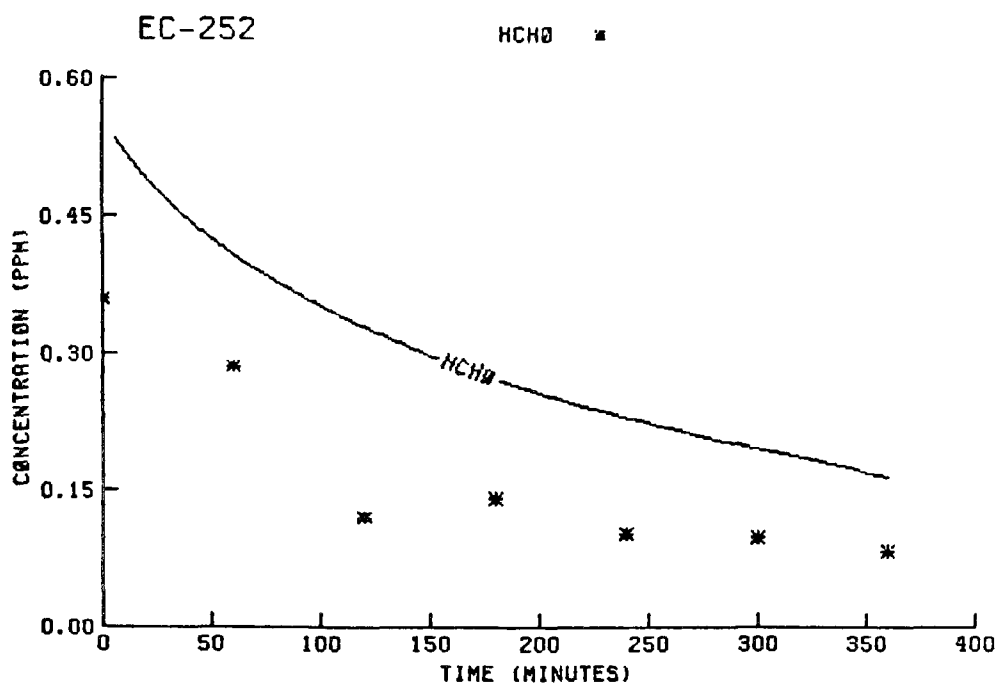






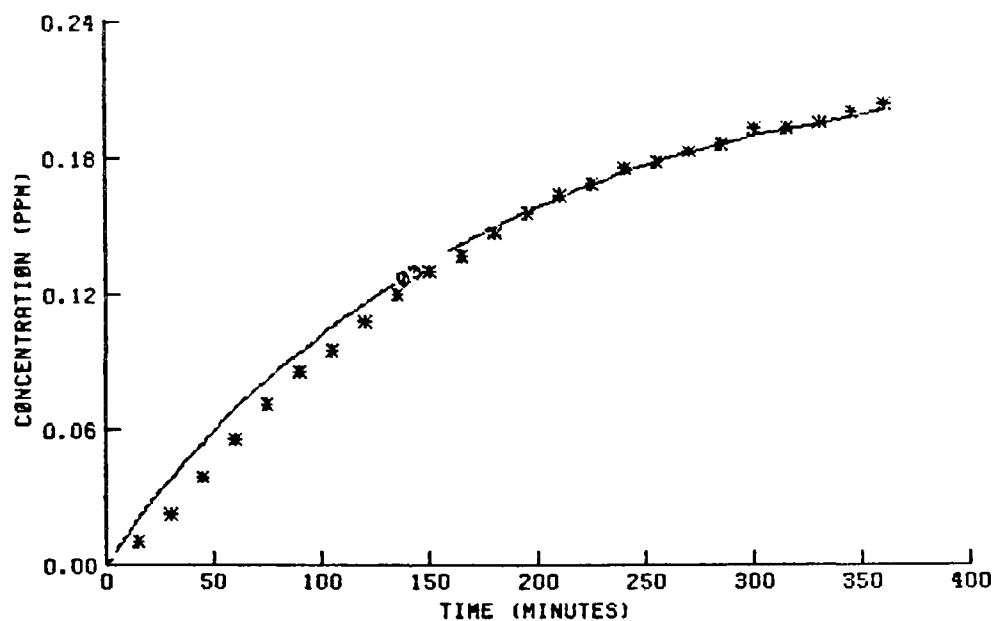






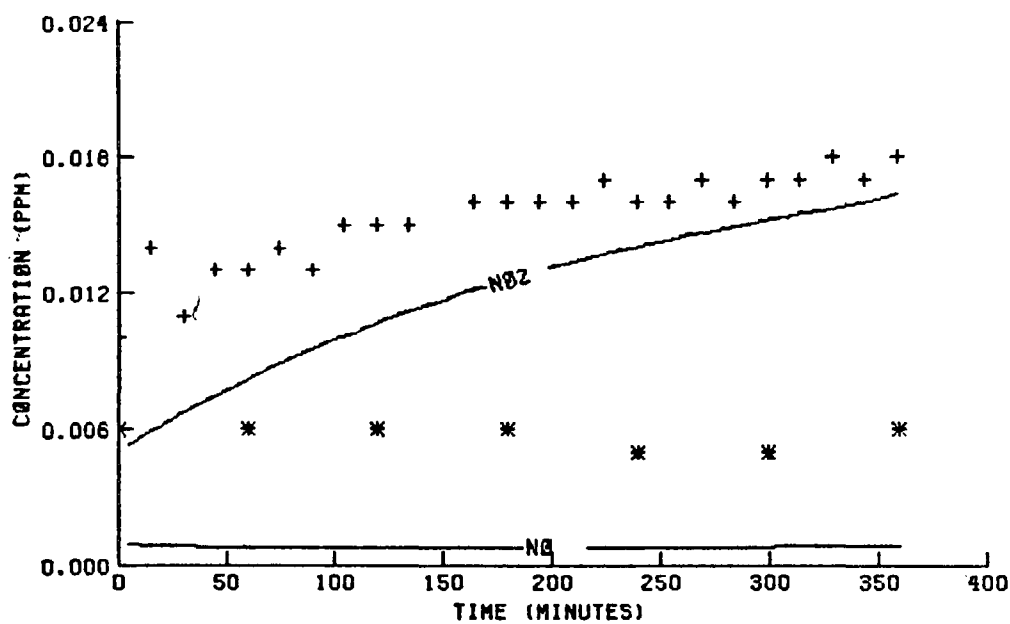
EC-255

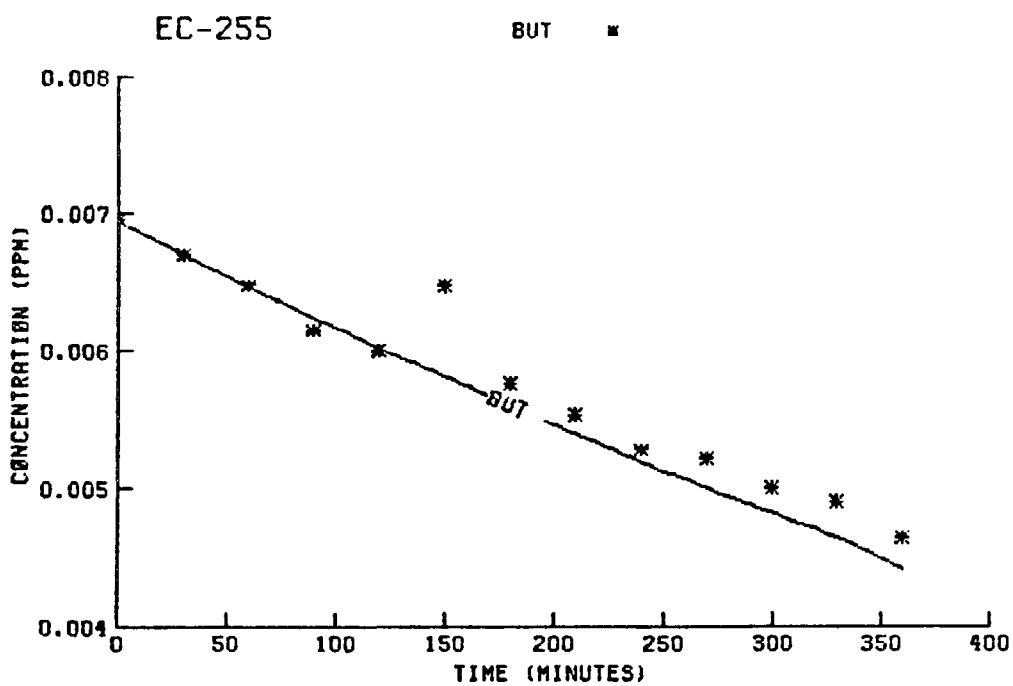
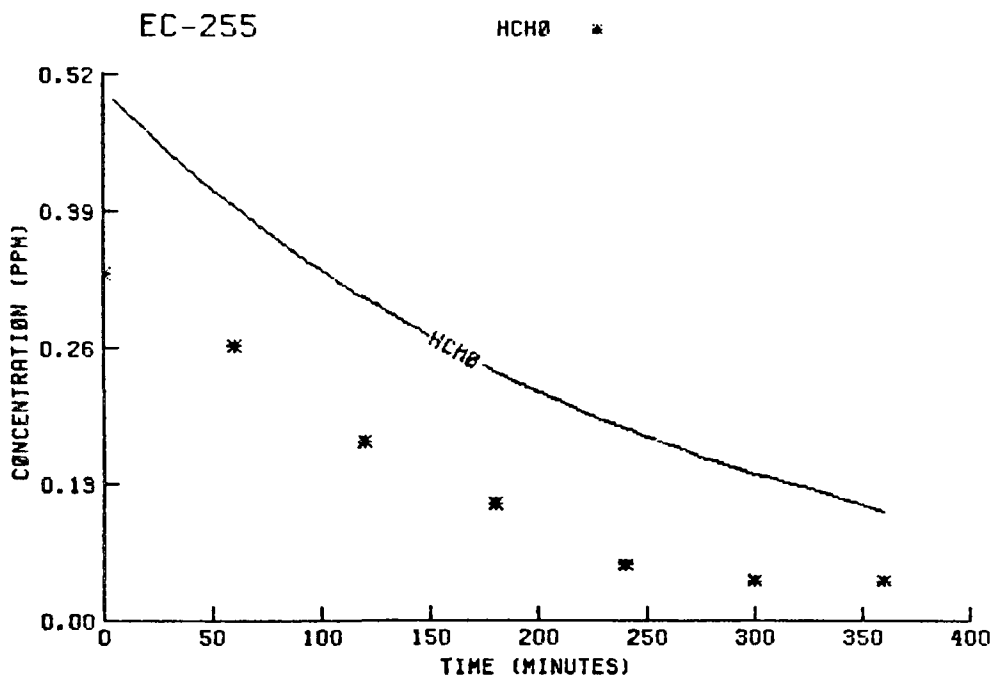
83 *



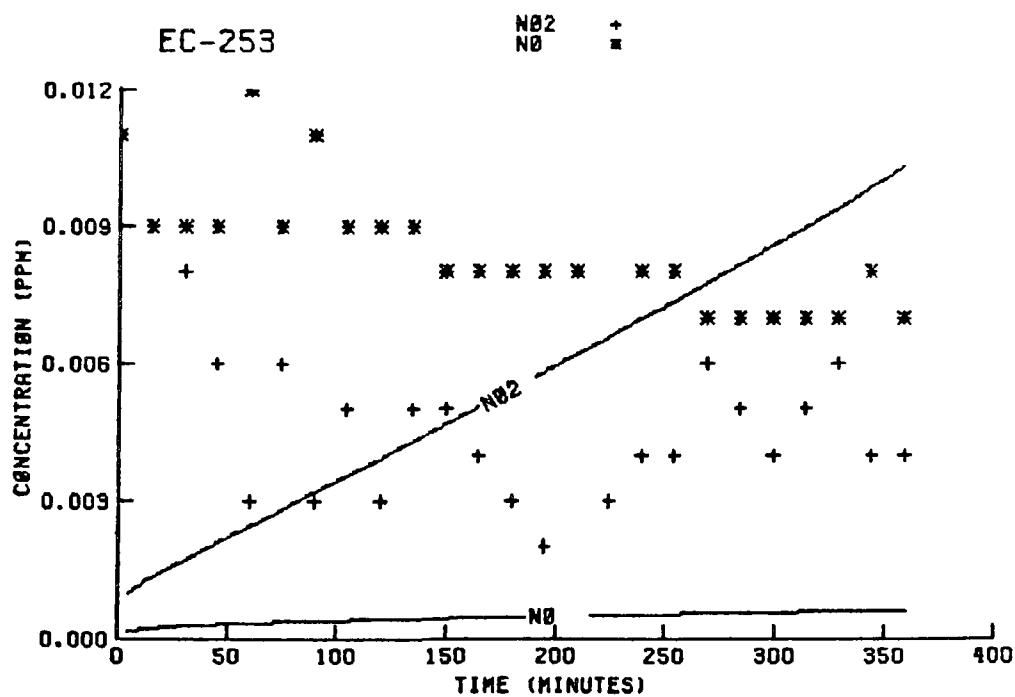
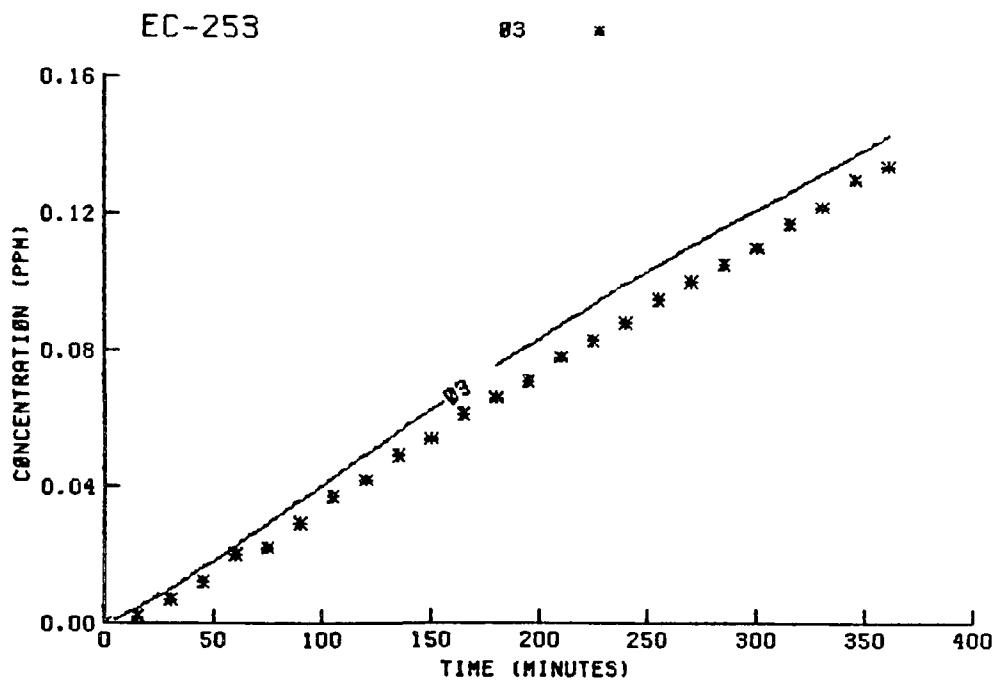
EC-255

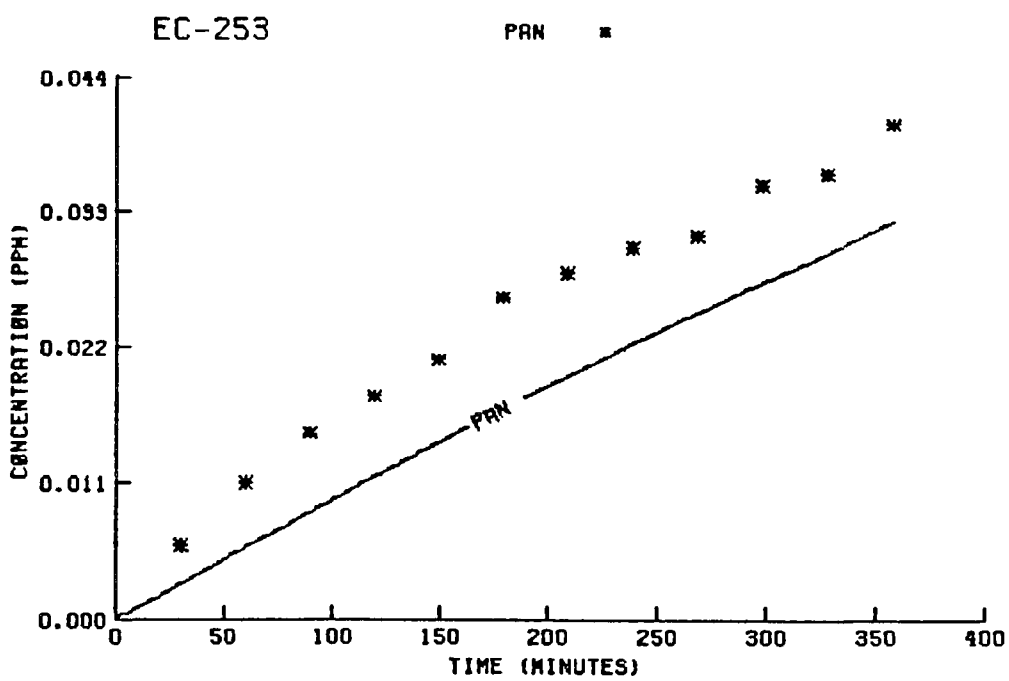
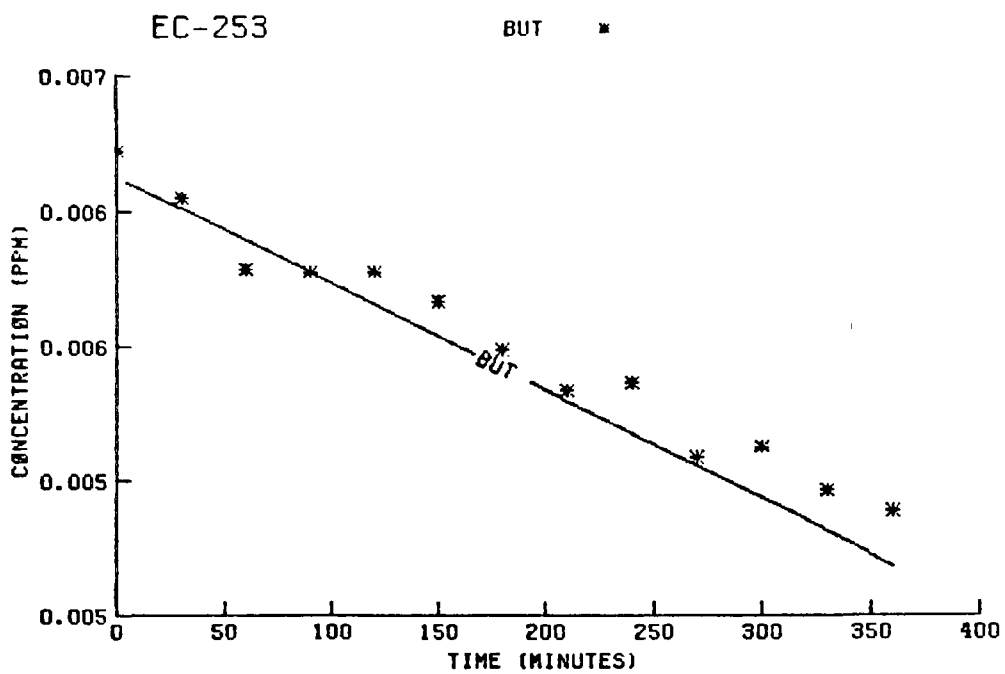
N82 +
N8 * □





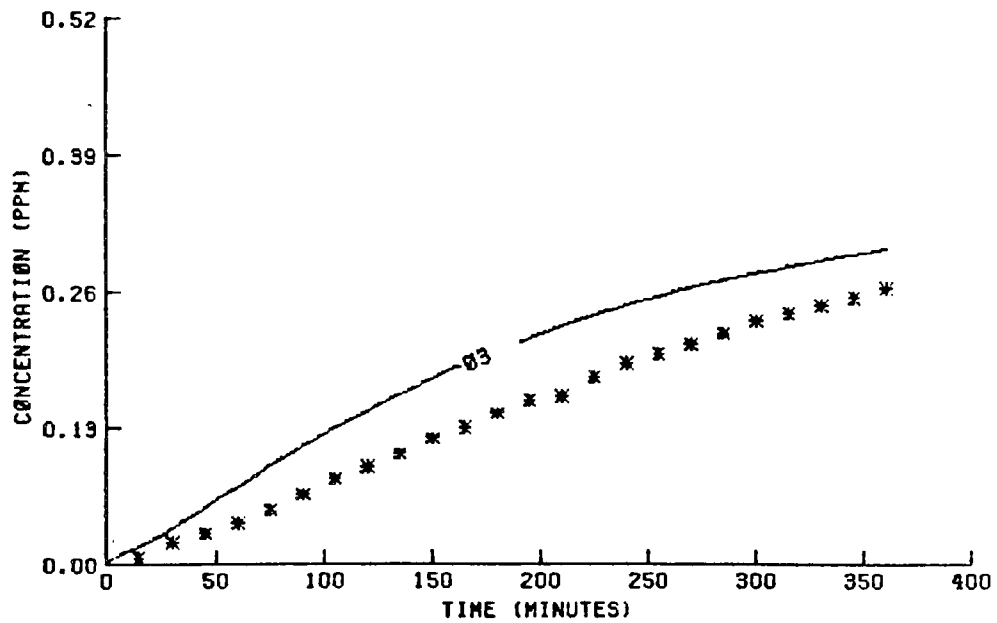
UCR ACETALDEHYDE EXPERIMENTS





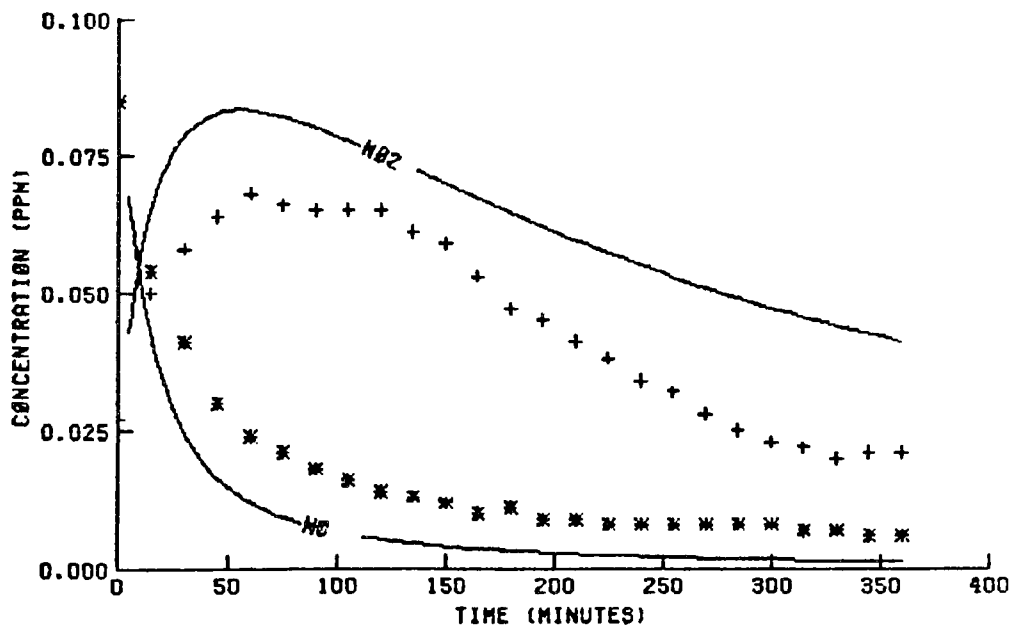
EC-254

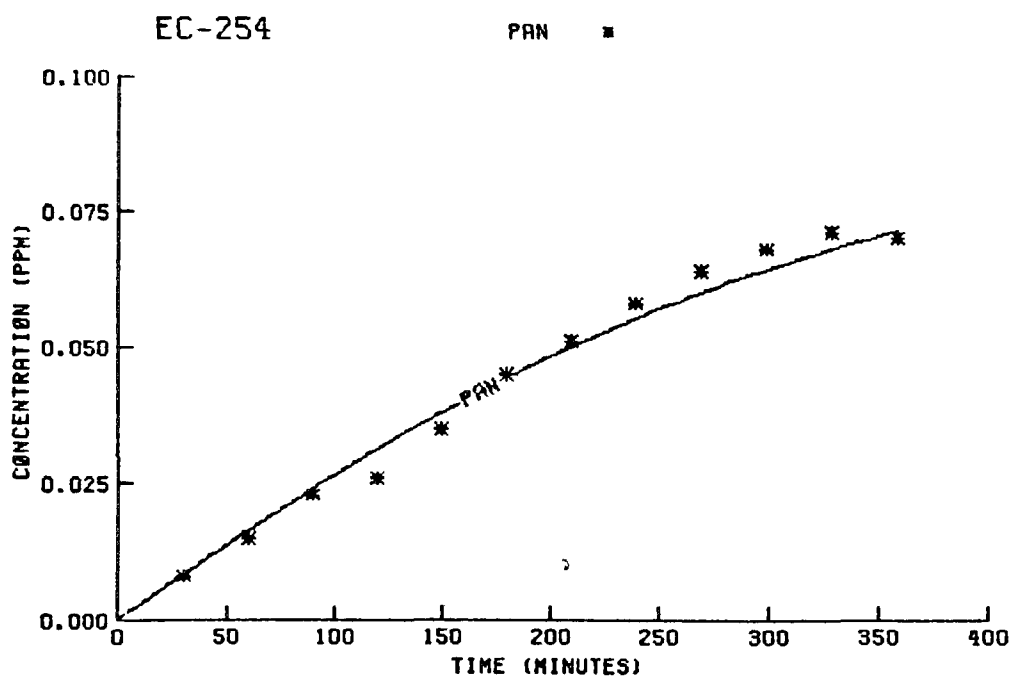
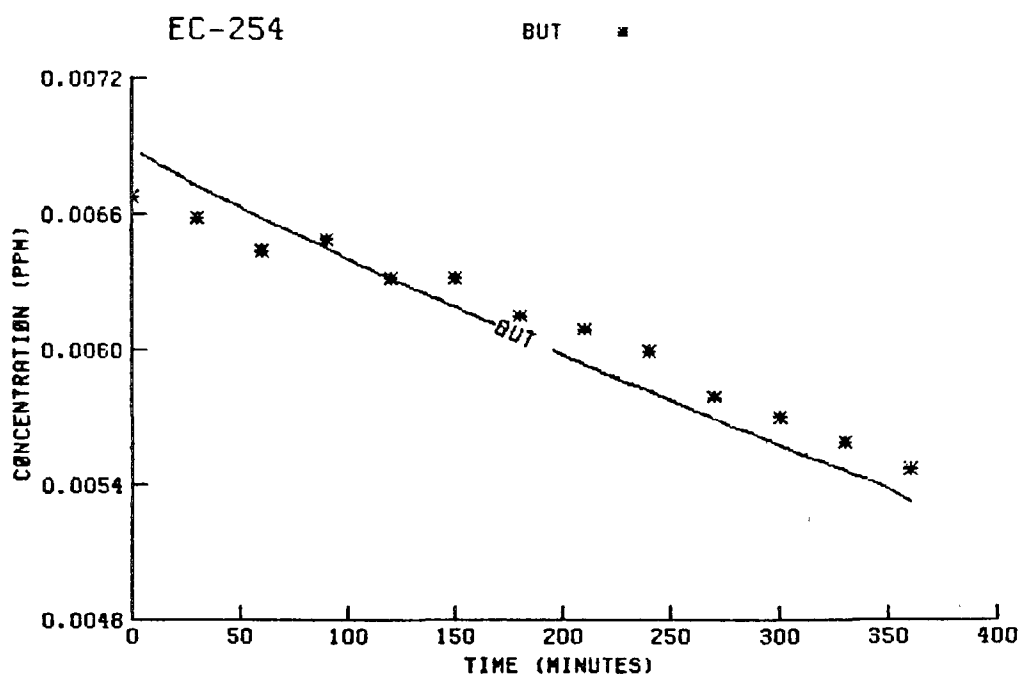
03 *



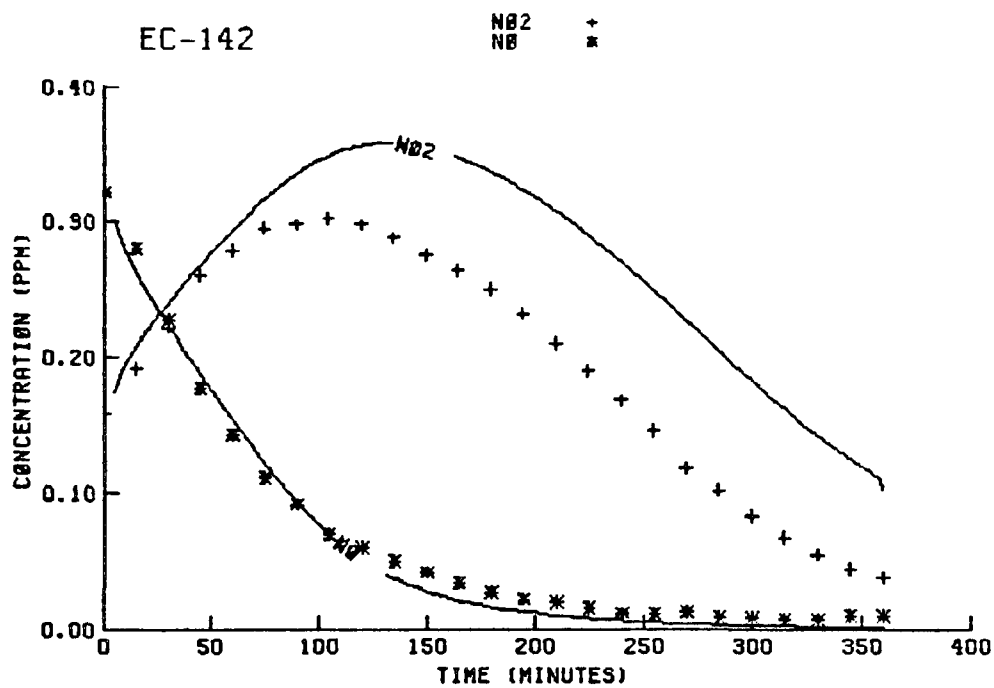
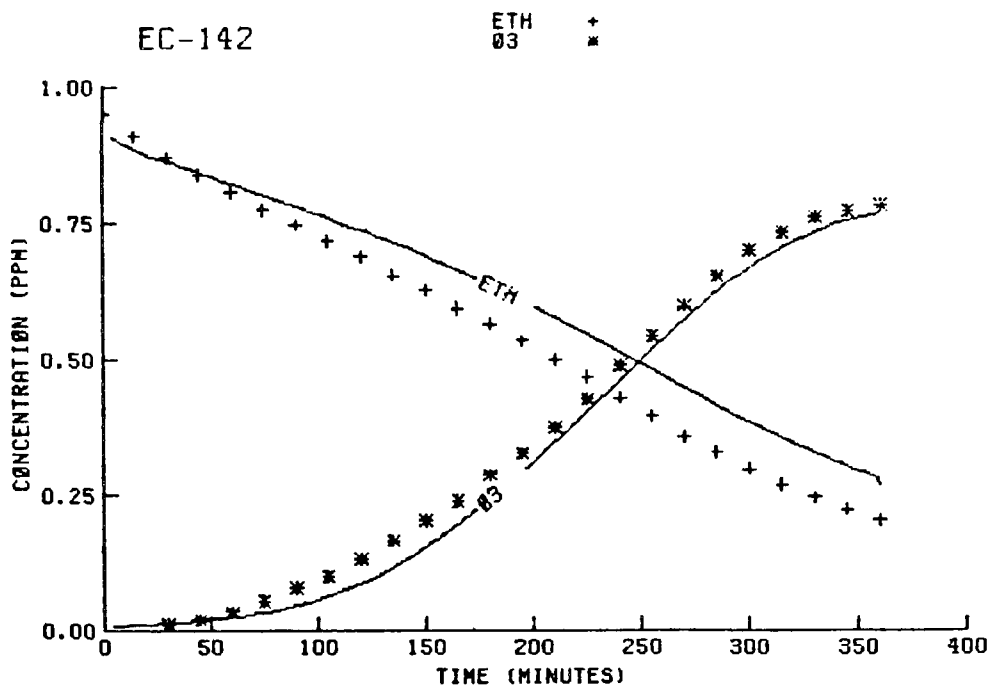
EC-254

NB2 +
NB *



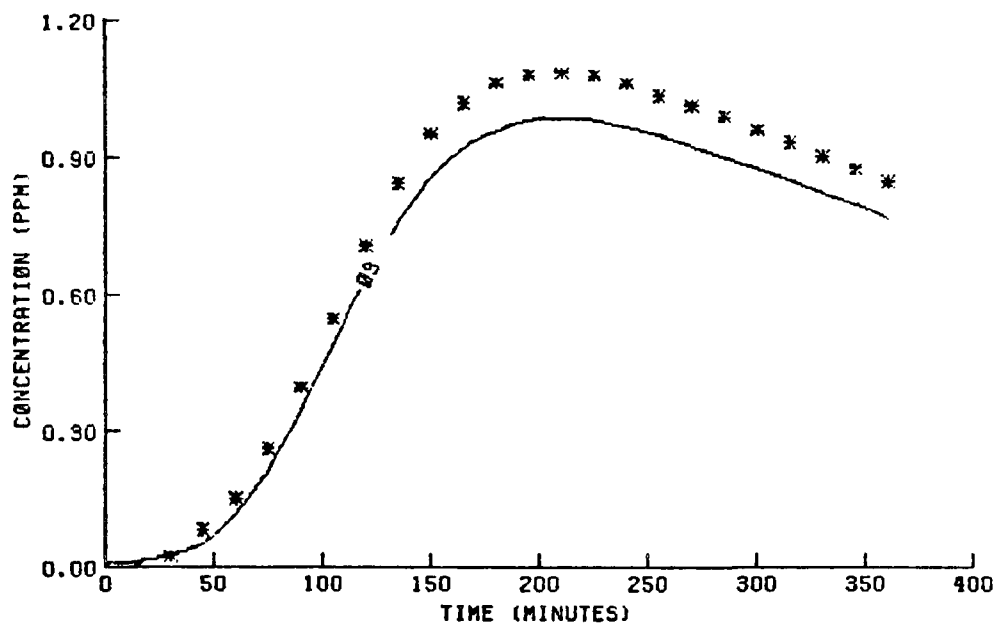


UCR ETHYLENE EXPERIMENTS



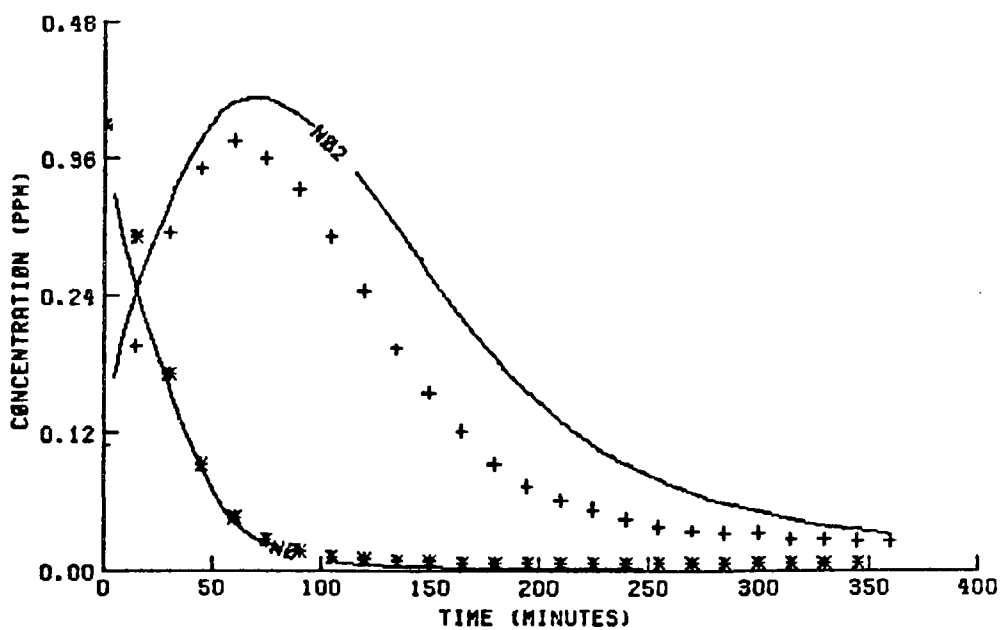
EC-143

03



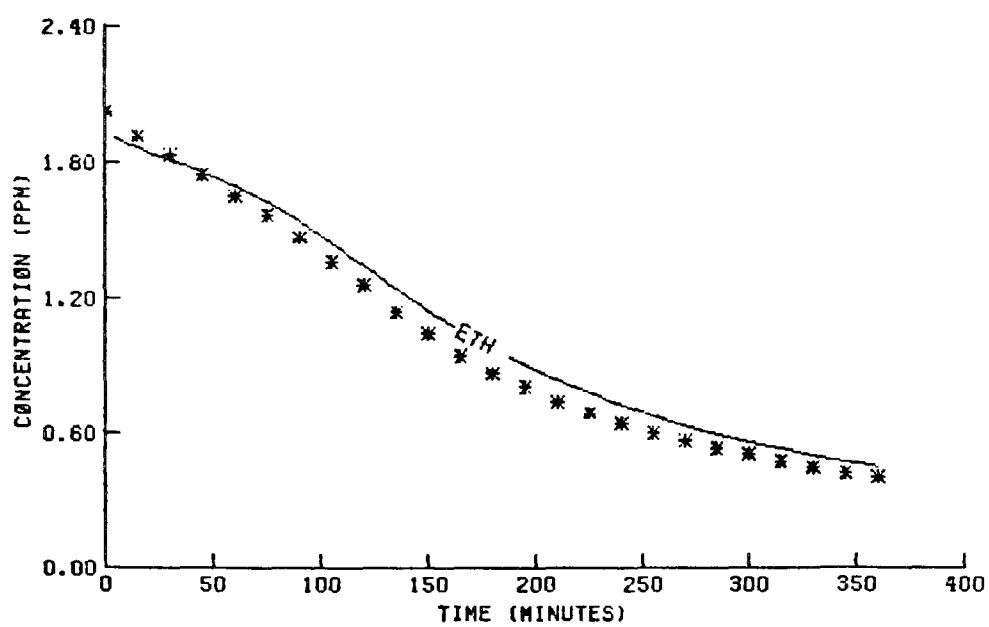
EC-143

N02 +
N0 *



EC-143

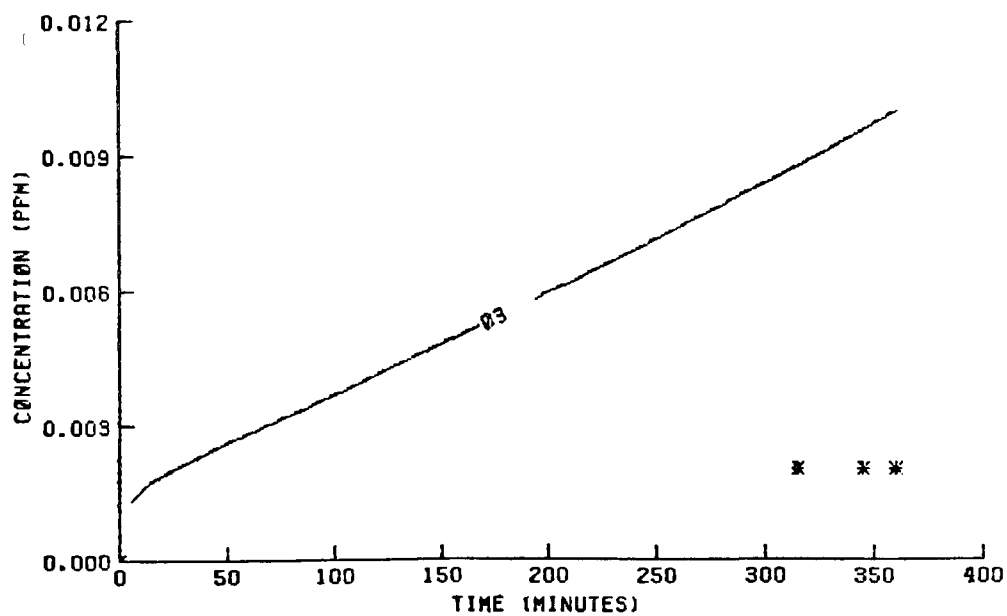
ETH *



UCR PROPYLENE EXPERIMENTS

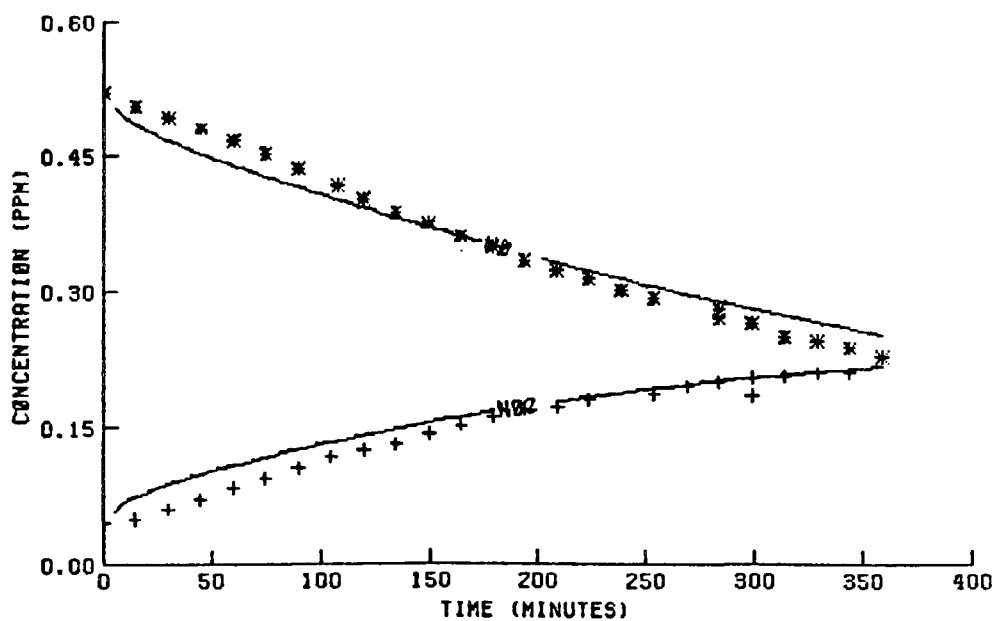
EC-256

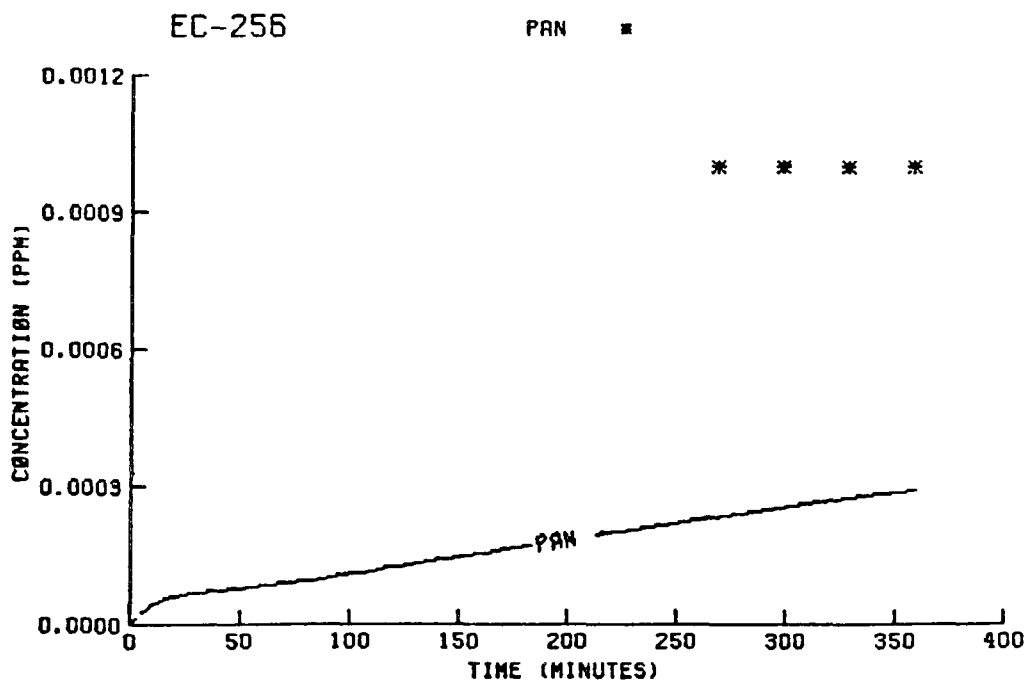
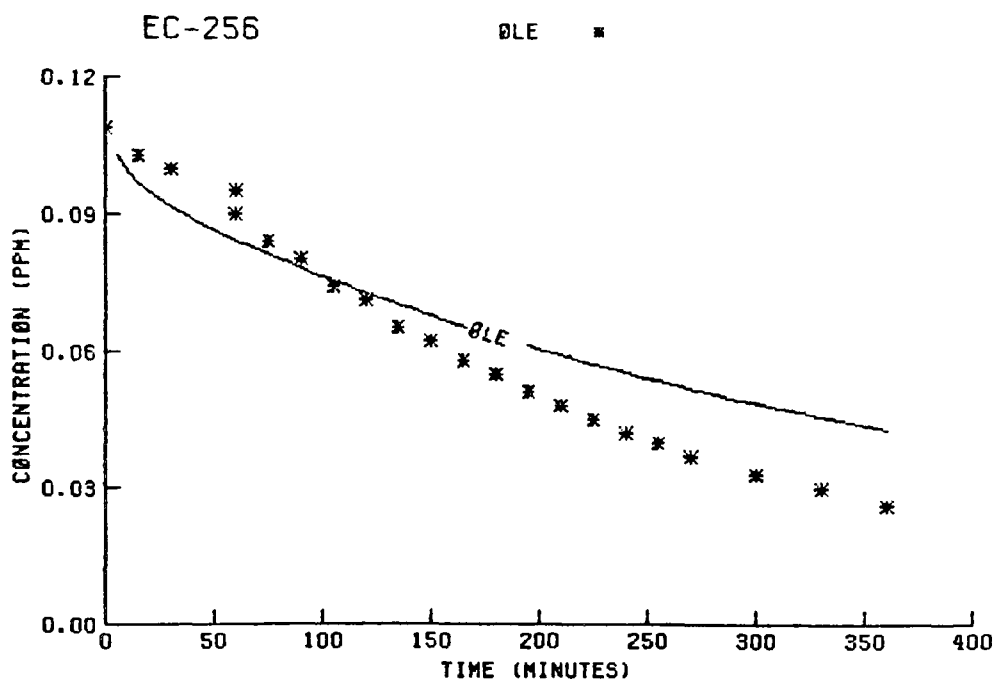
03 *

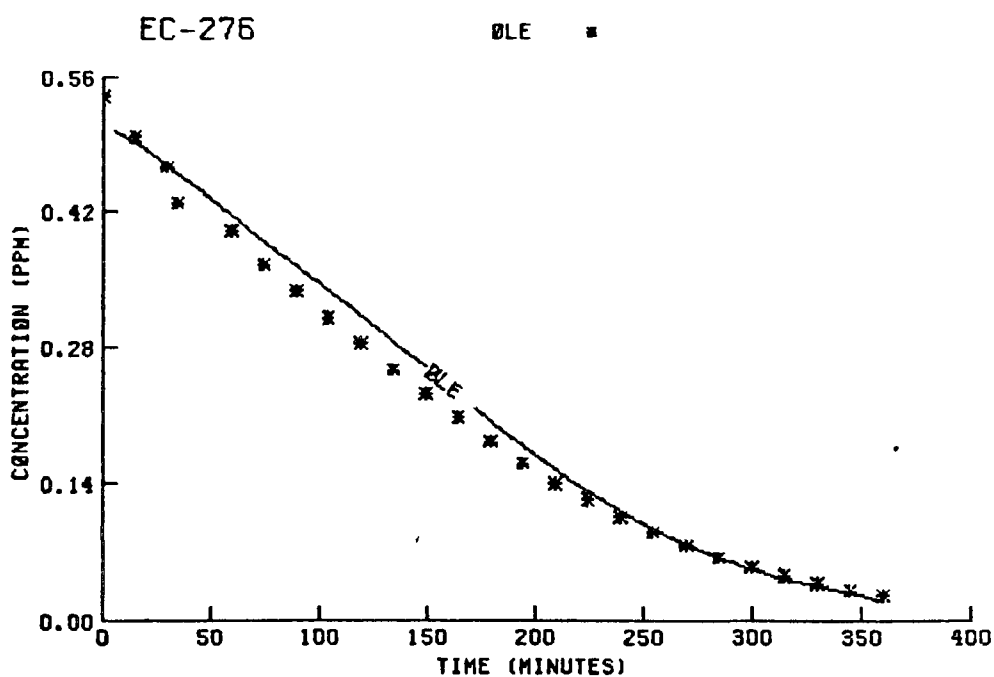
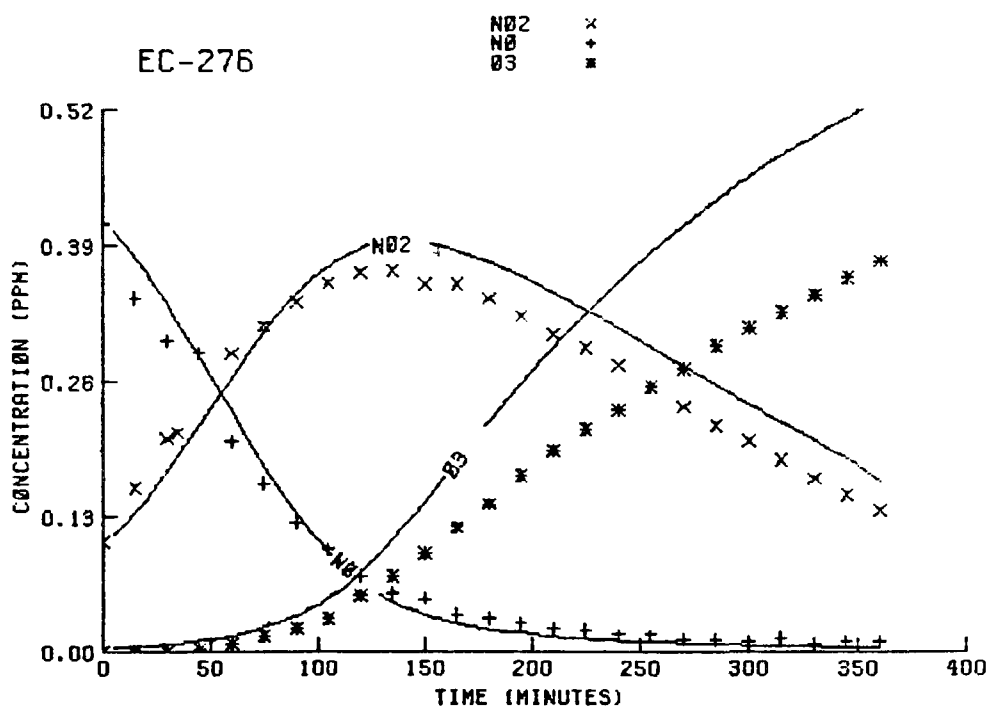


EC-256

NB2 +
N0 *

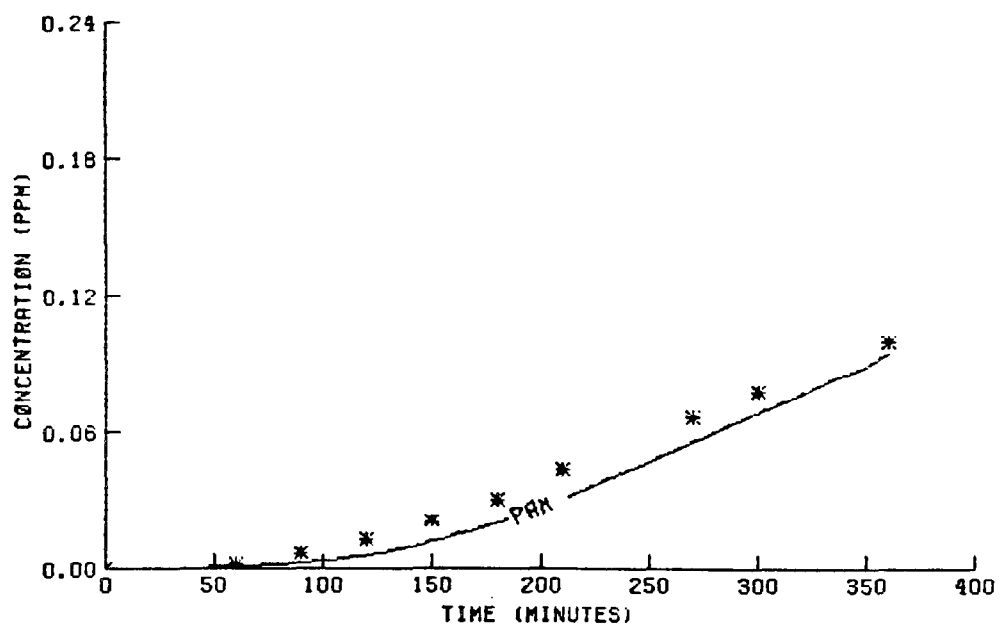






EC-276

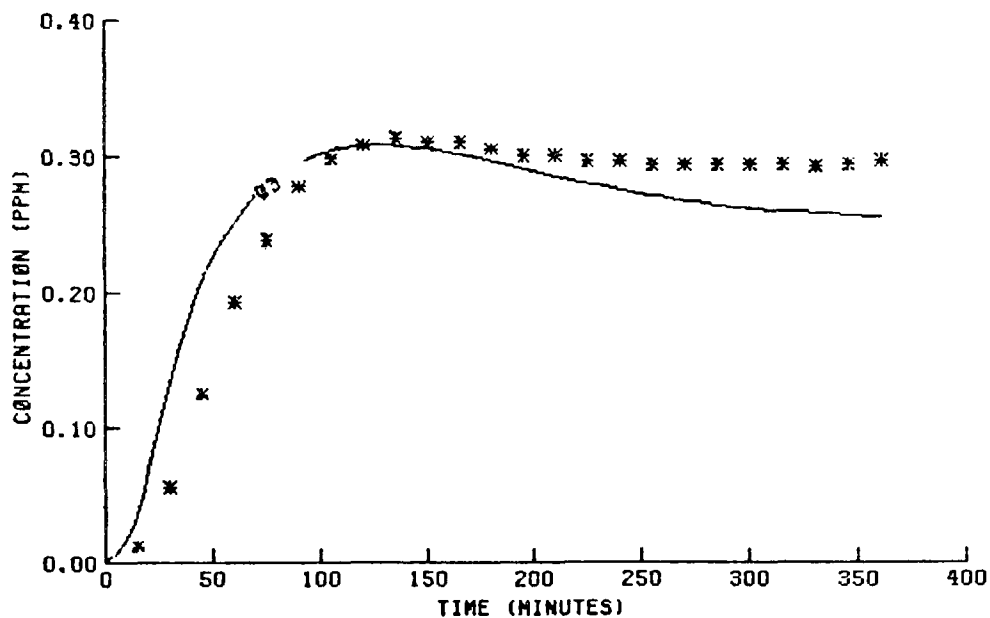
PAN *



EC-277

03

*

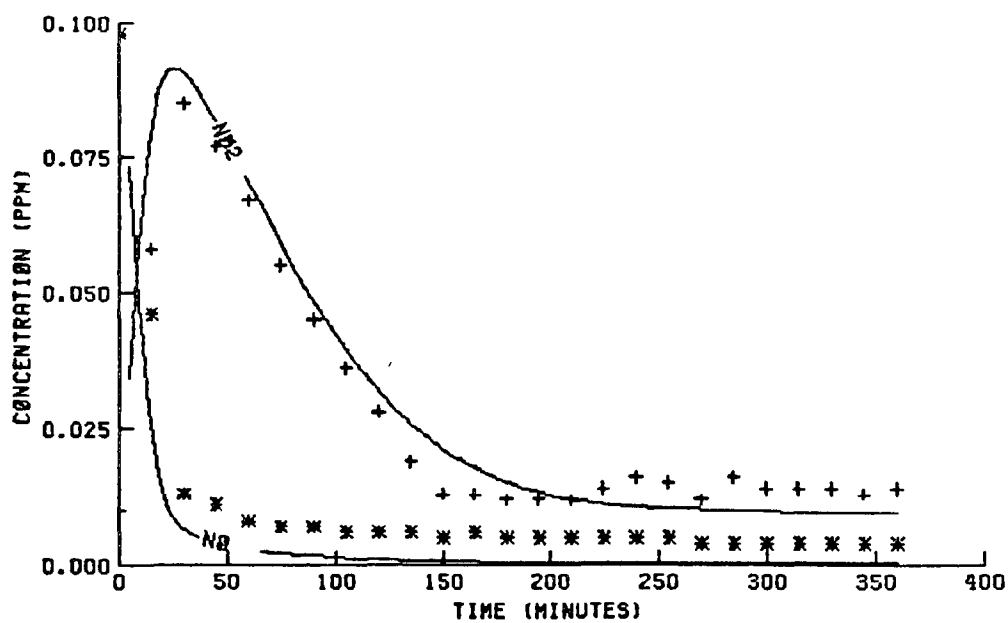


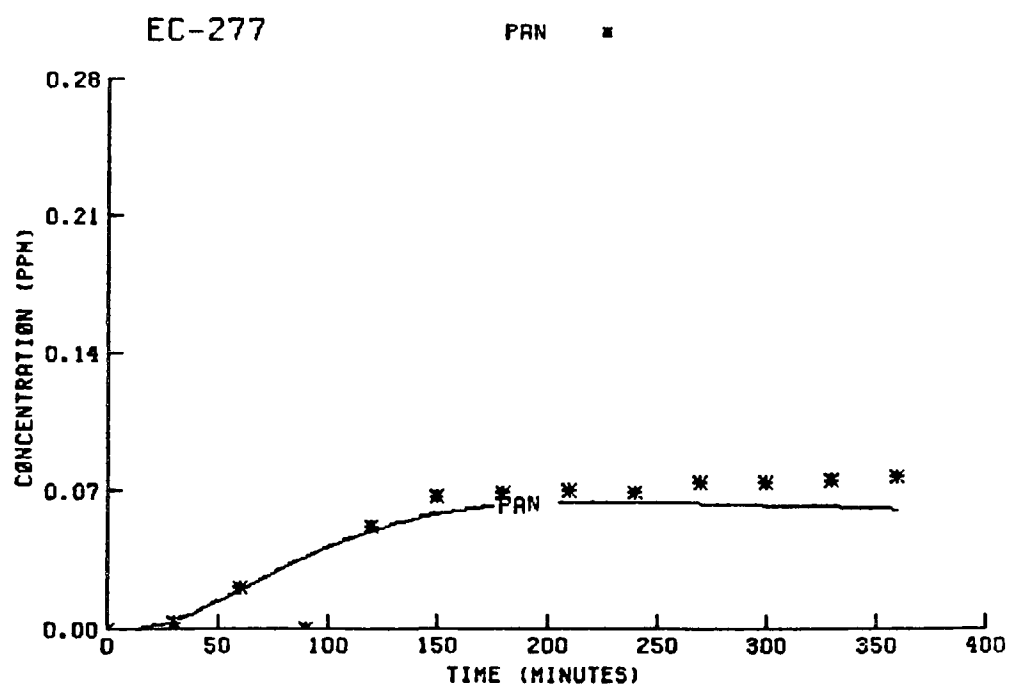
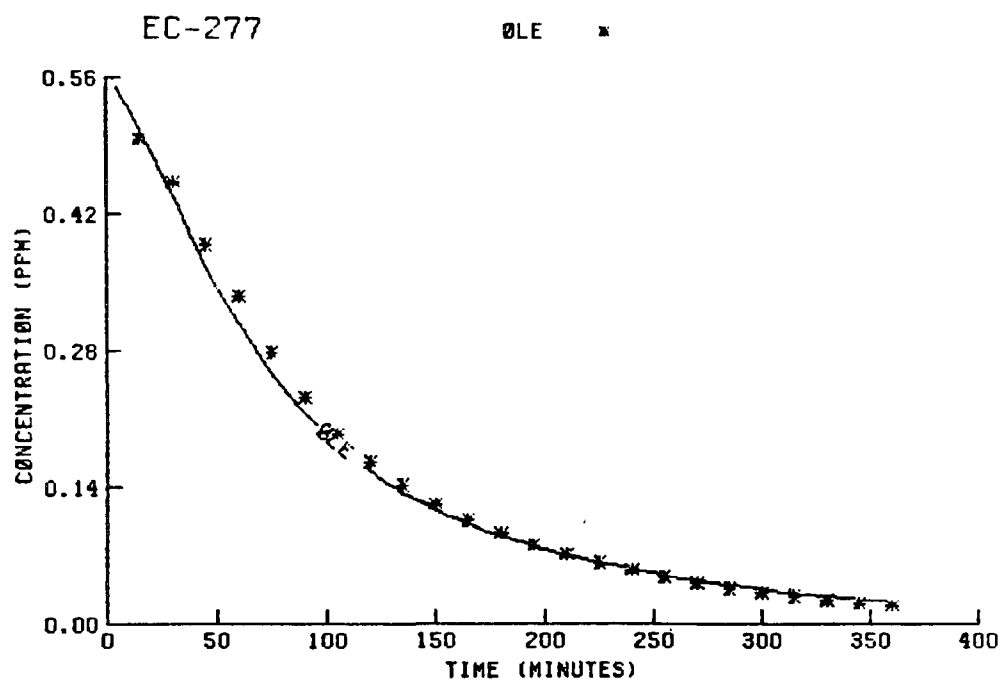
EC-277

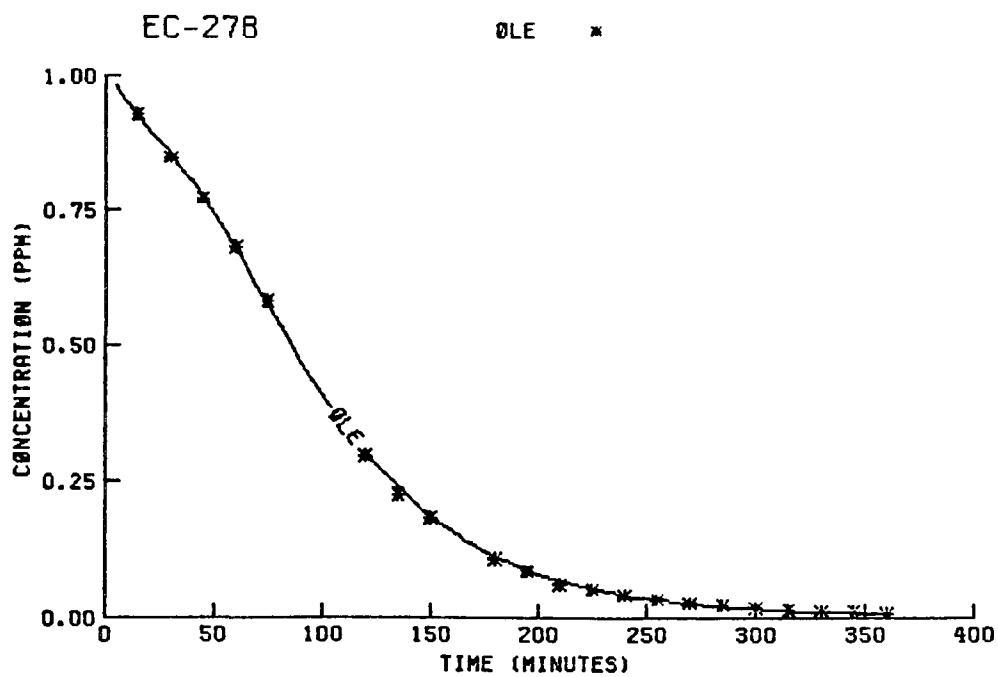
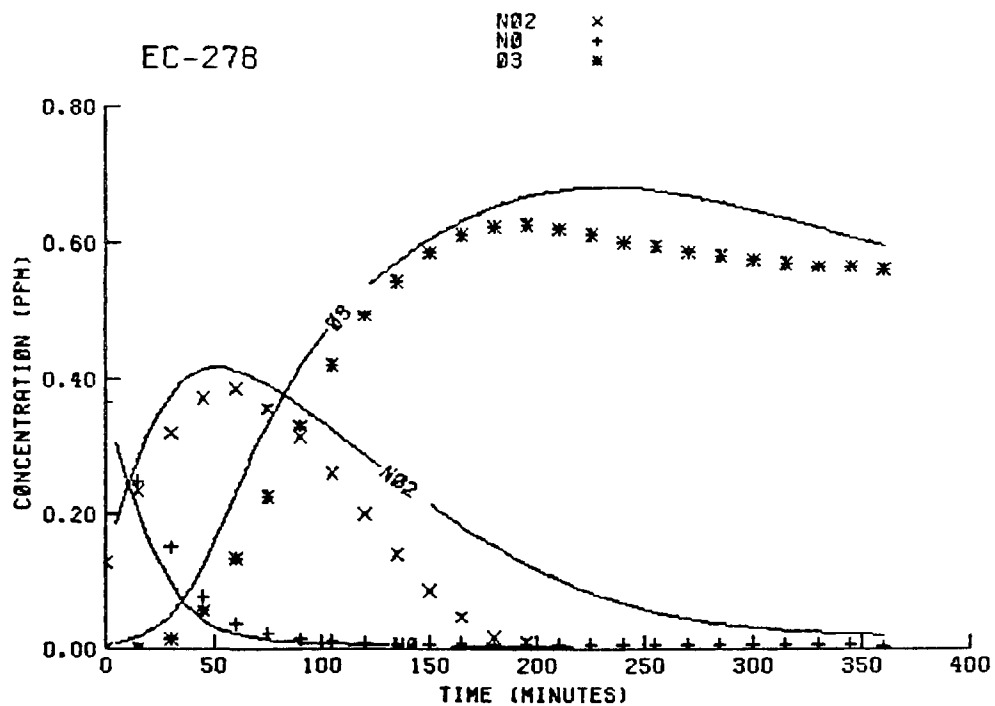
N02
N0

+

*

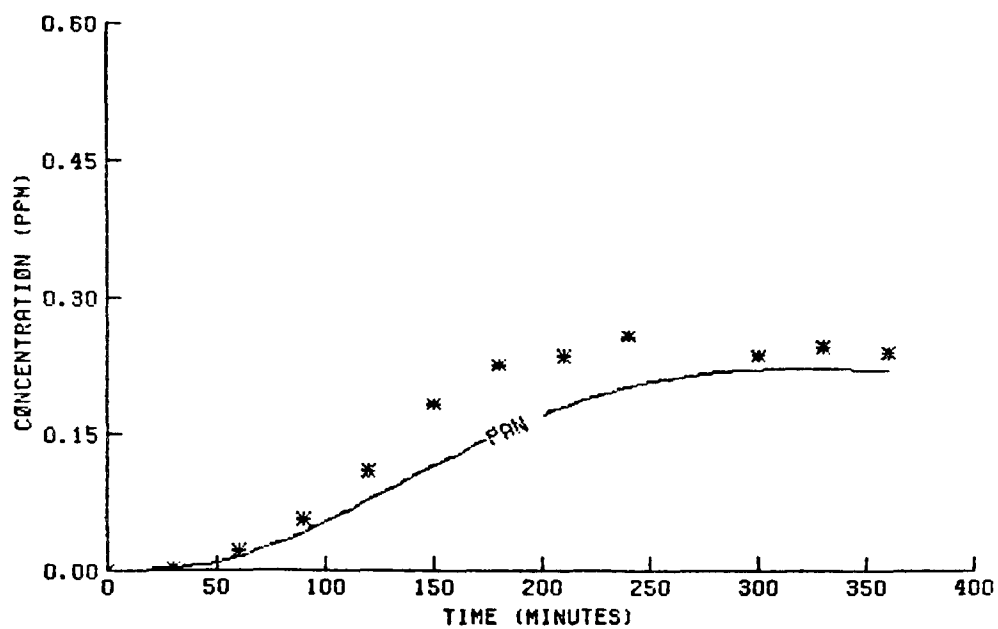


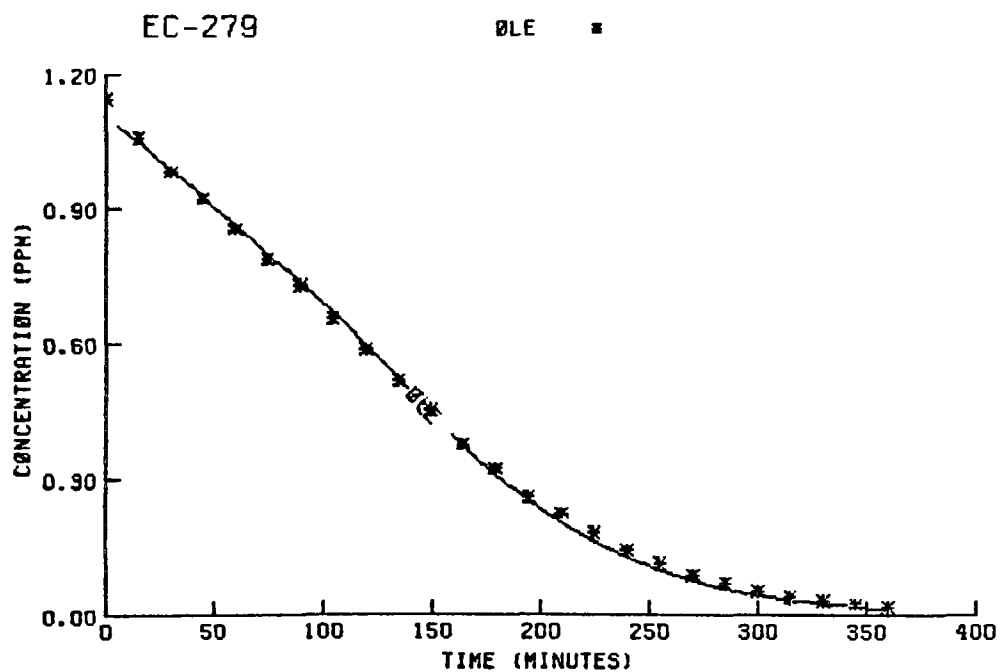
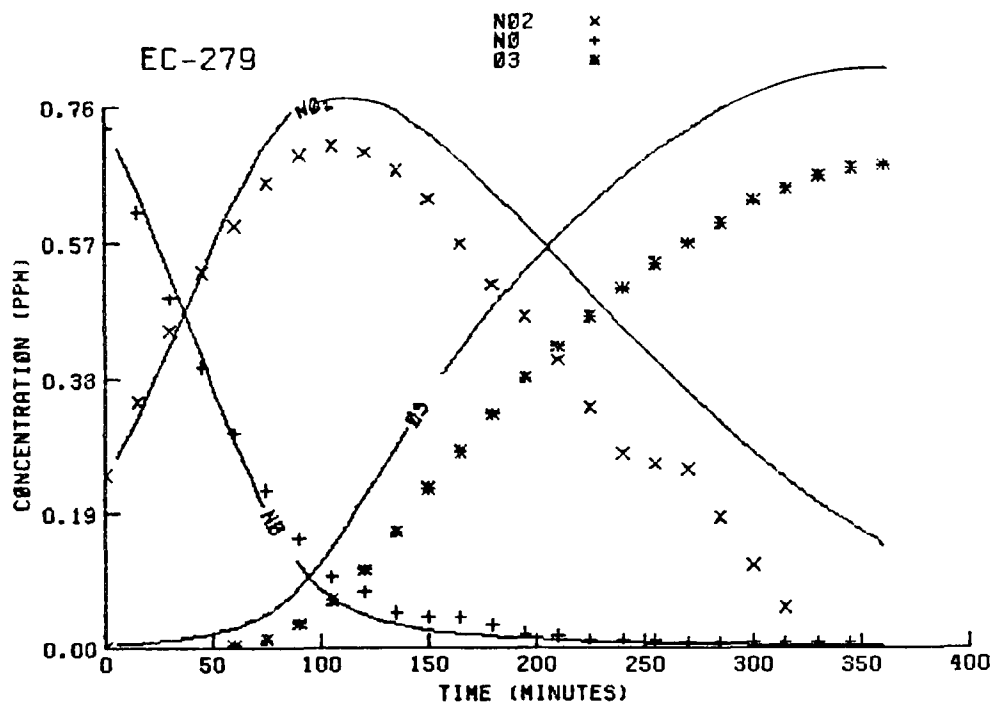




EC-278

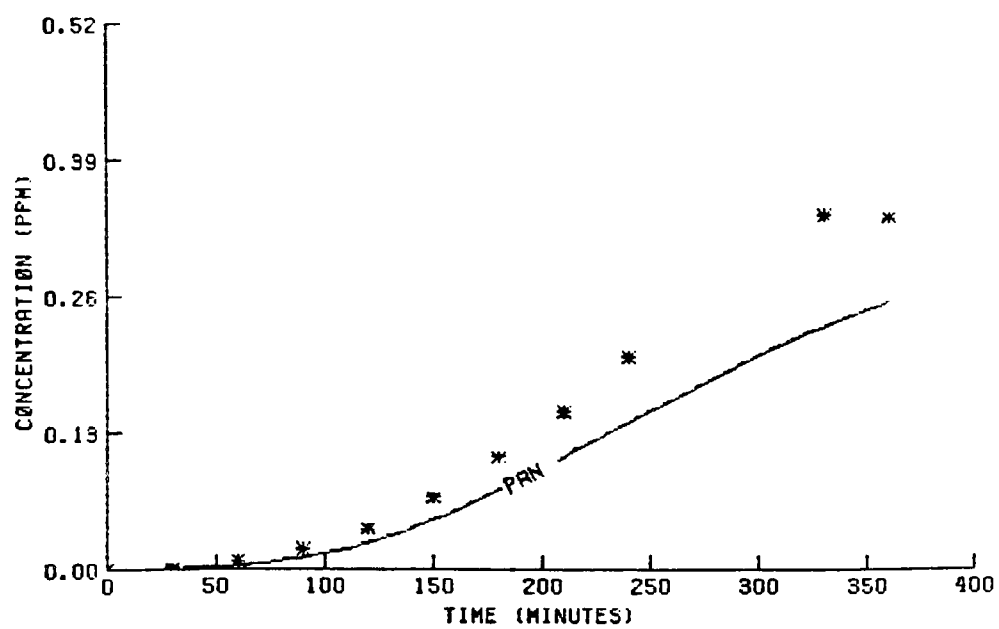
PAN *



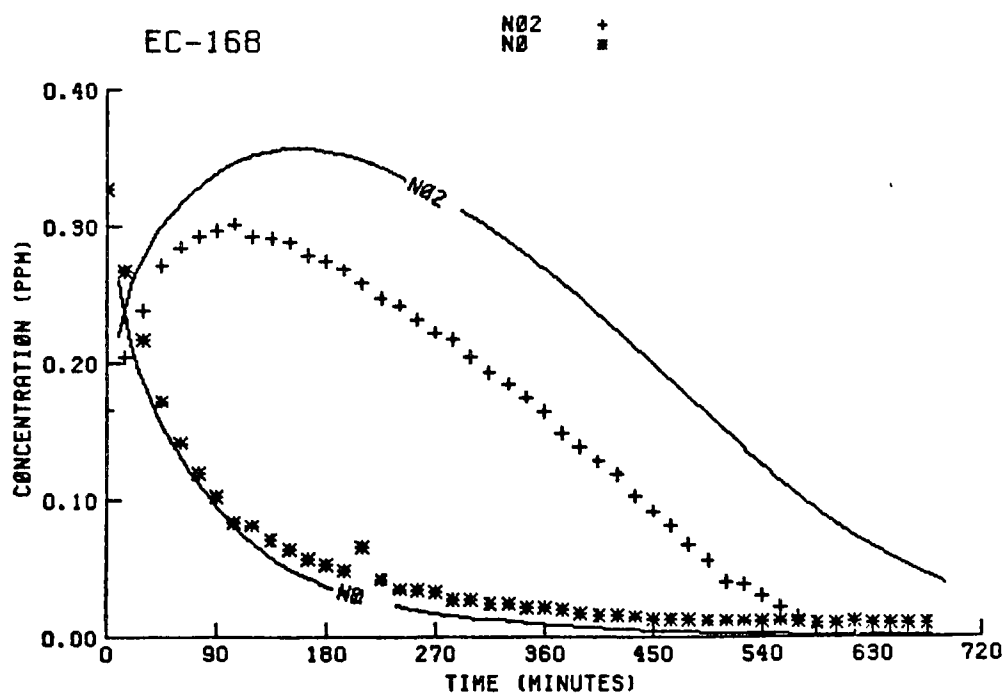
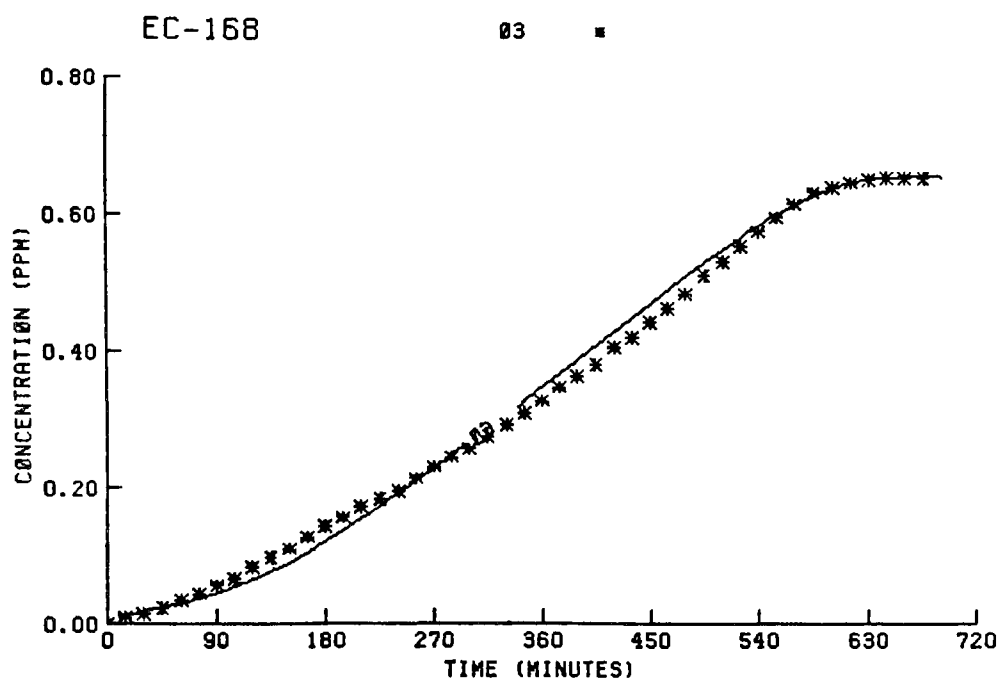


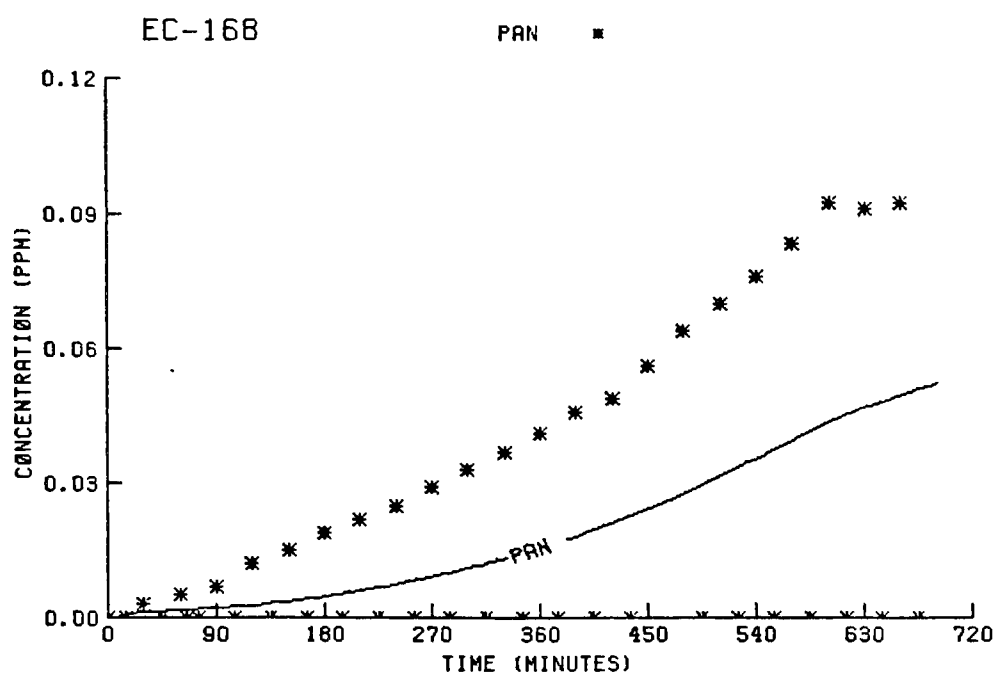
EC-279

PAN *



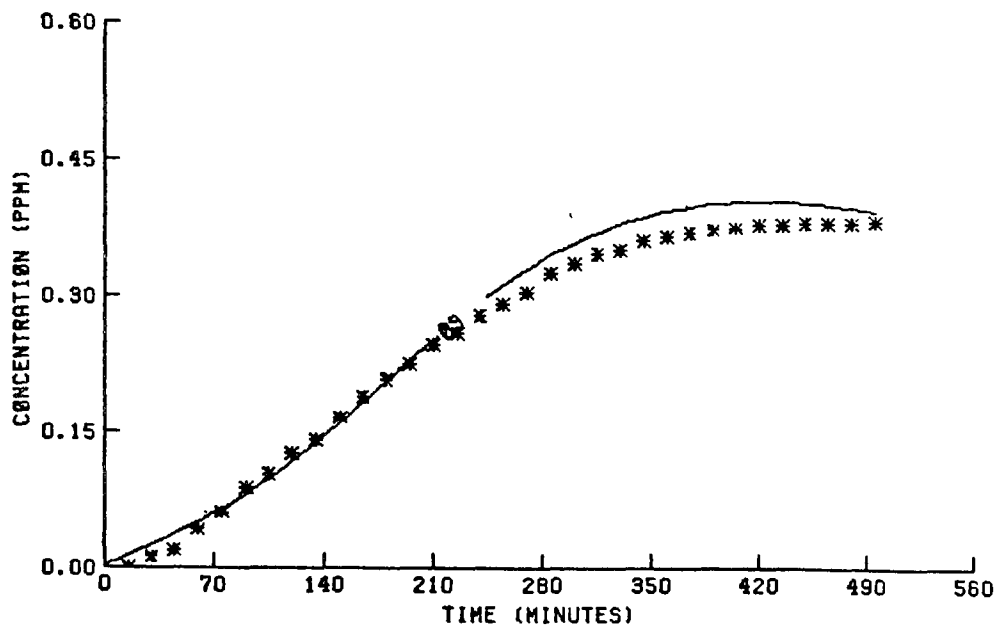
UCR BUTANE EXPERIMENTS





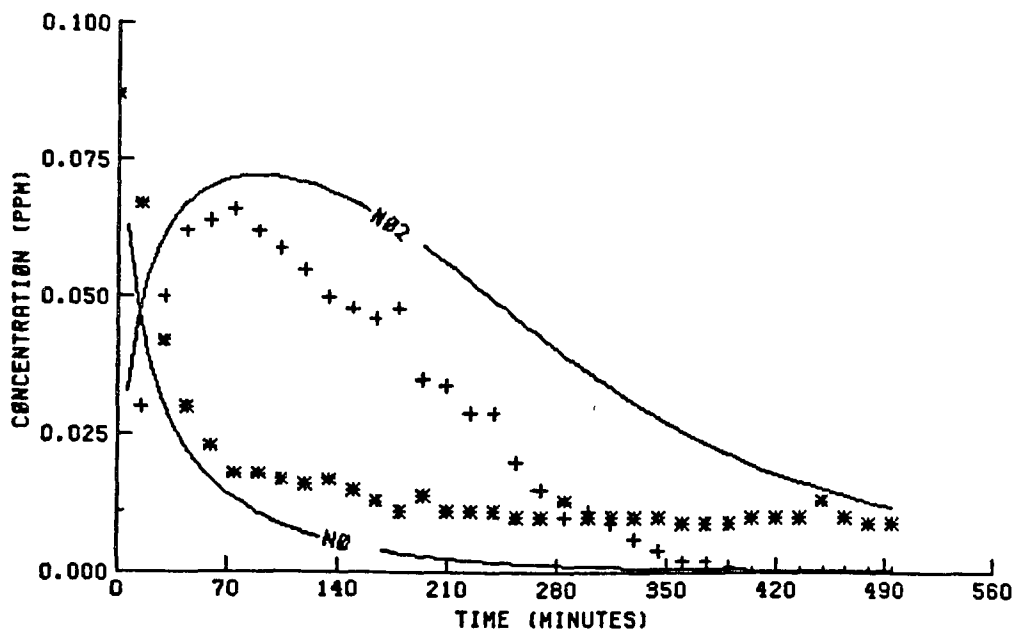
EC-178

03



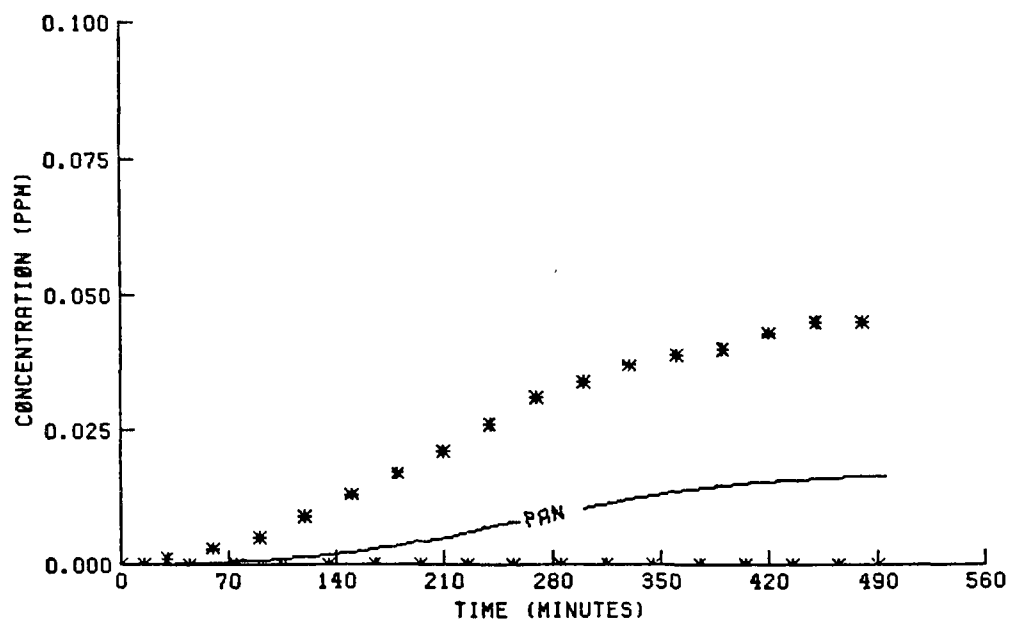
EC-178

N02 +
N0 *

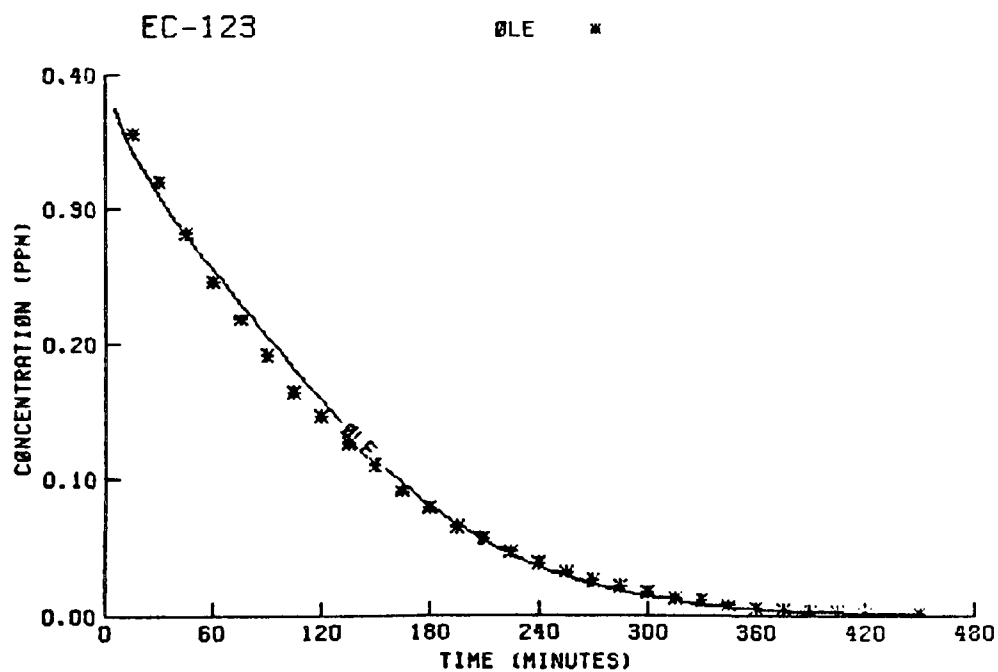
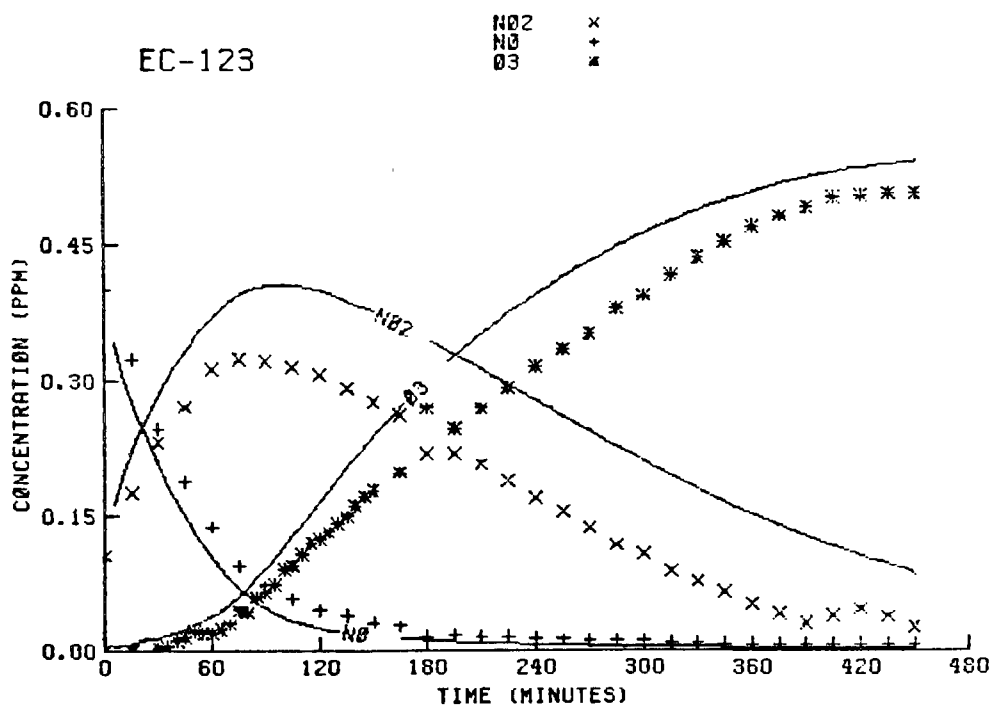


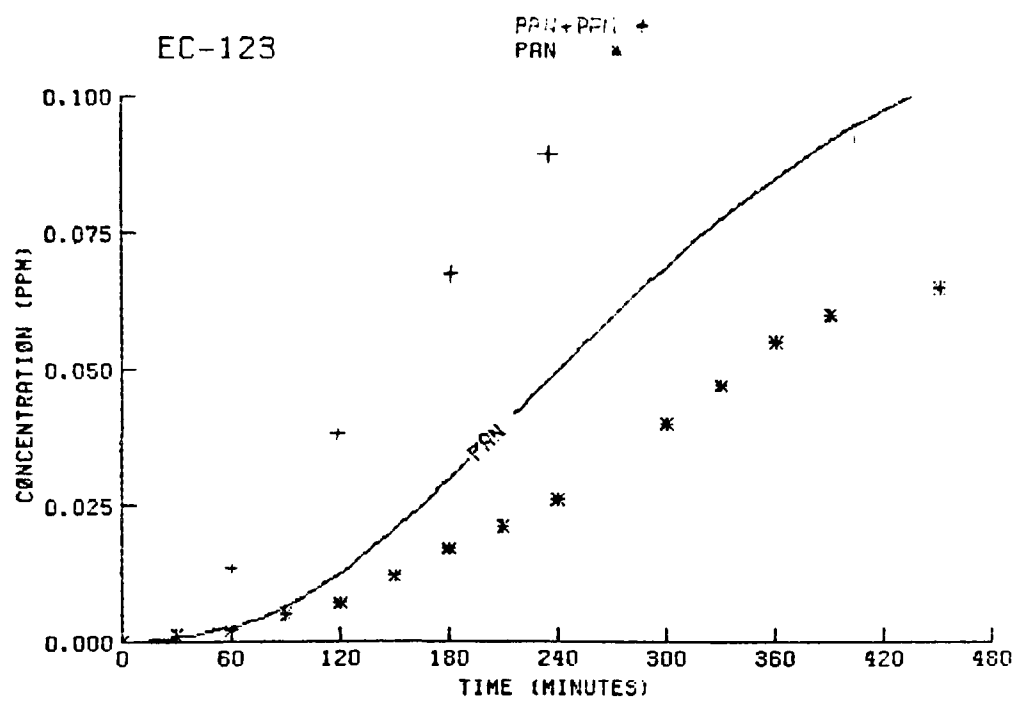
EC-178

PAN *



UCR 1-BUTENE EXPERIMENTS

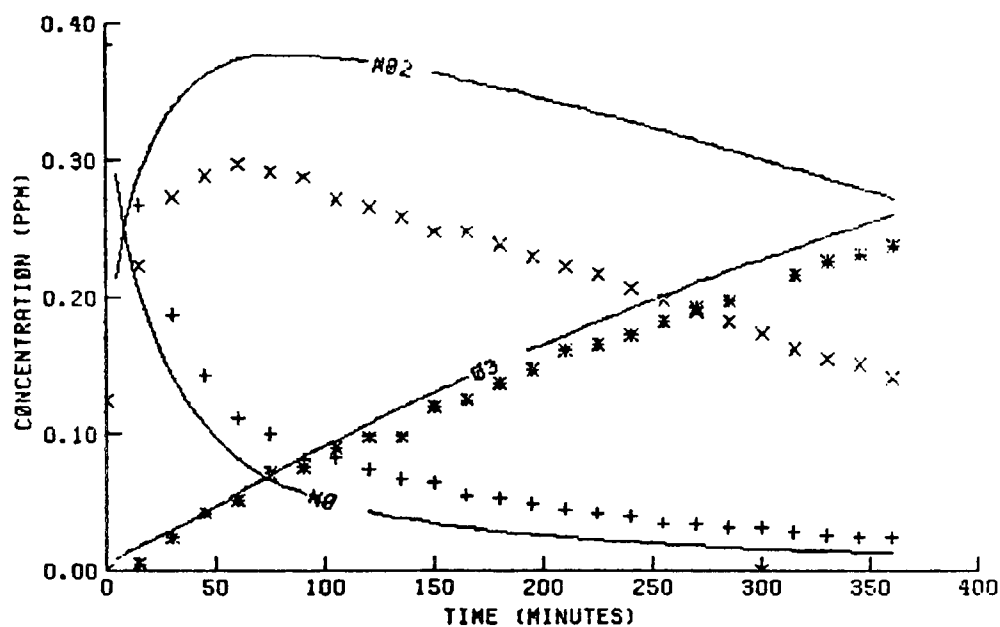




UCR TRANS-2-BUTENE EXPERIMENTS
(With trans-2-butene treated as an olefin)

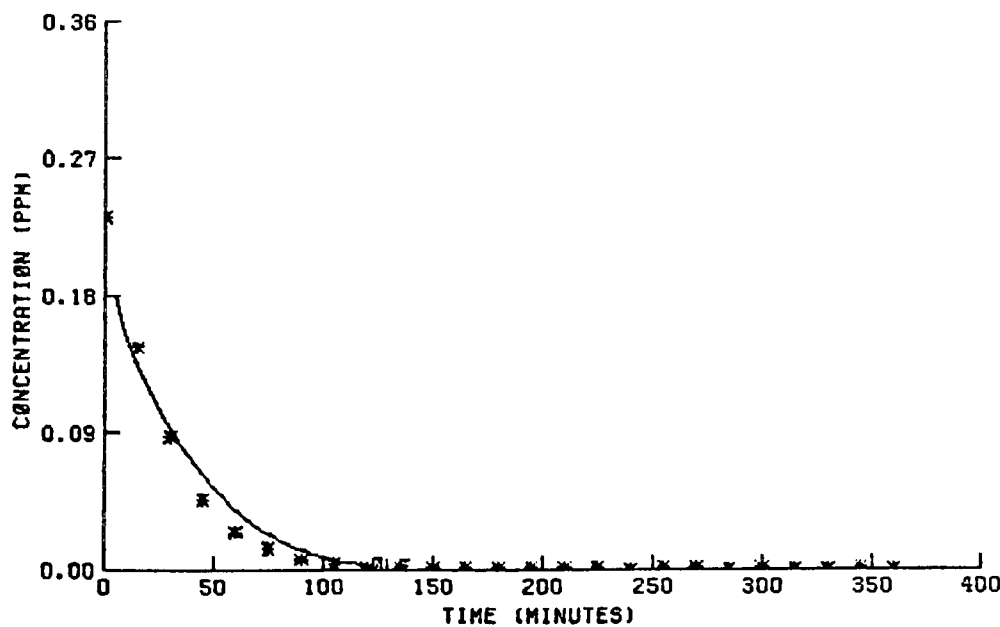
EC-146

N02 x
N0 +
03 *



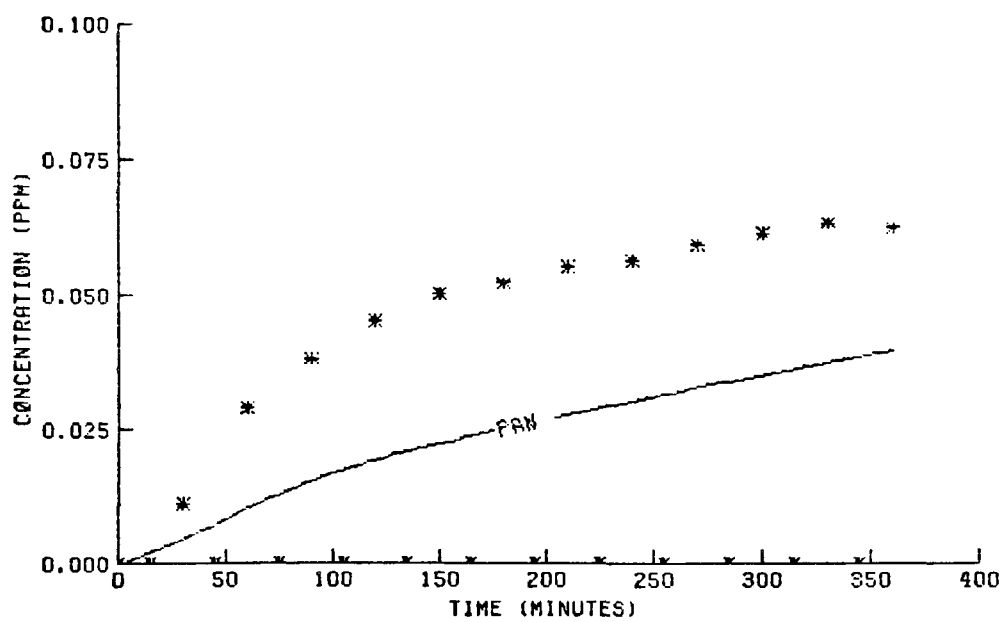
EC-146

0LE *

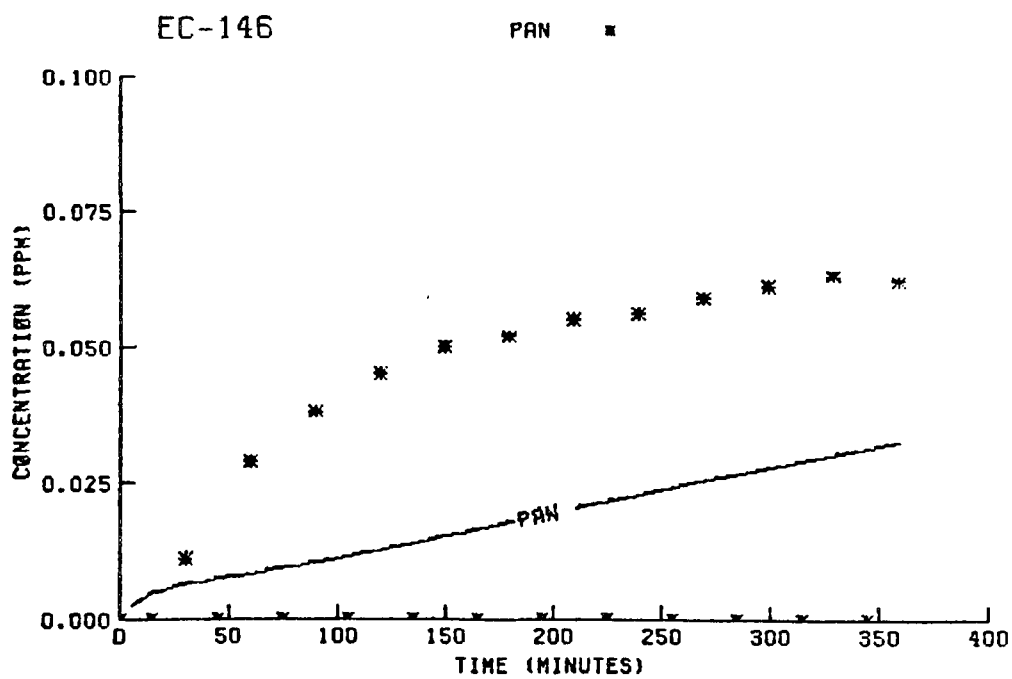
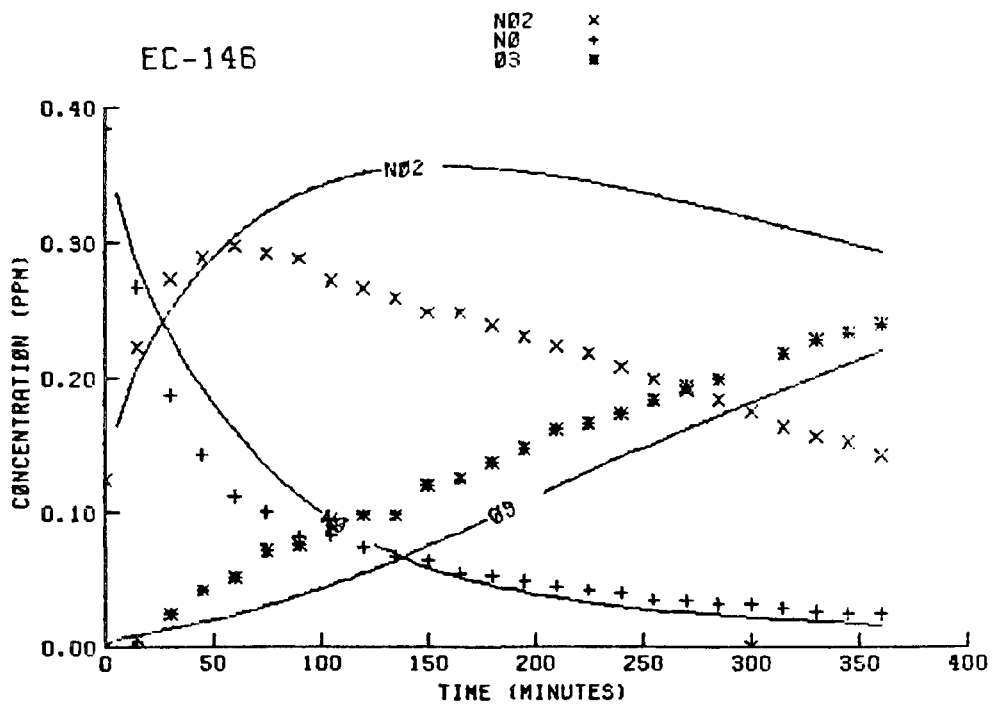


EC-146

PAN *



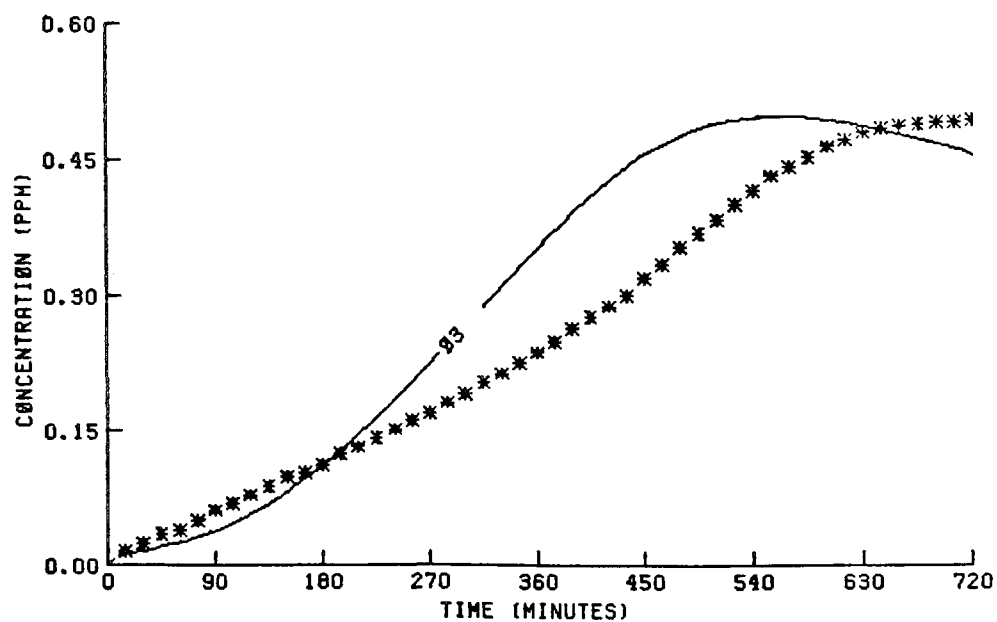
UCR TRANS-2-BUTENE EXPERIMENTS
(with trans-2-butene treated as a carbonyl)



UCR 2,3-DIMETHYLBUTANE EXPERIMENTS

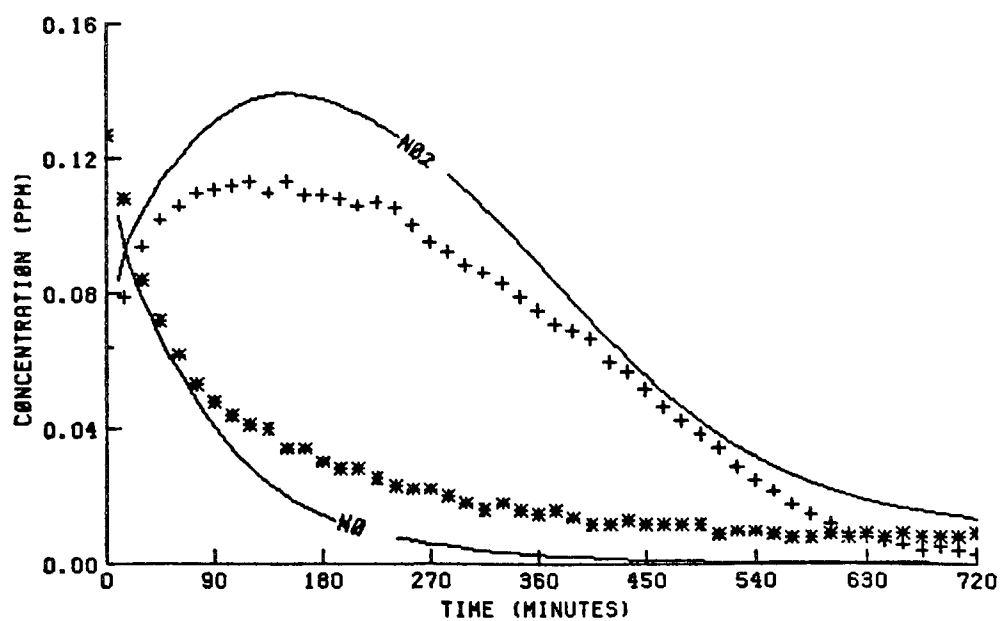
EC-169

03 *



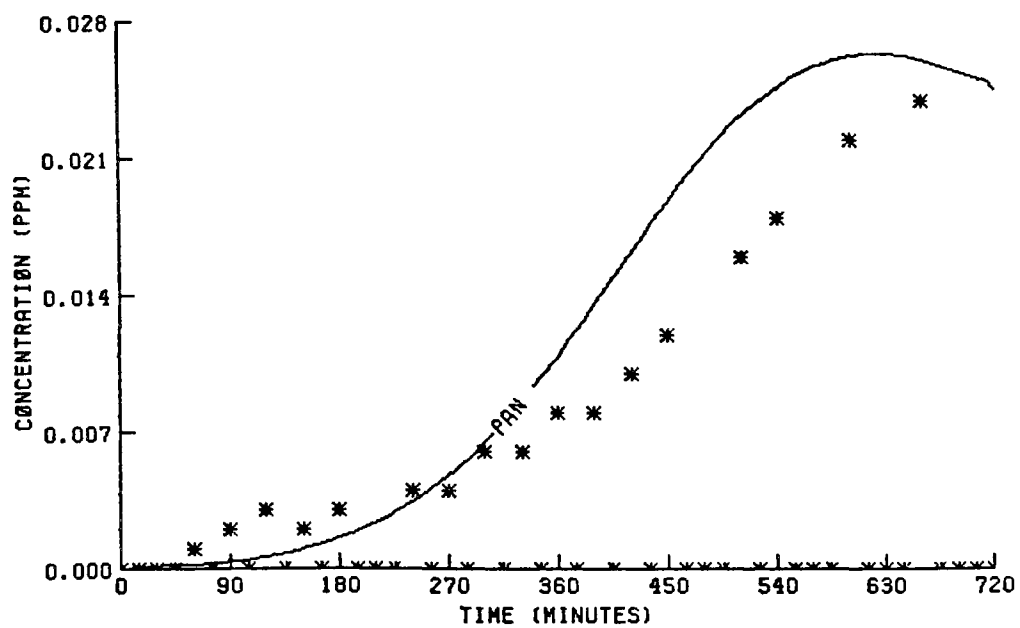
EC-169

N02 +
N0 *

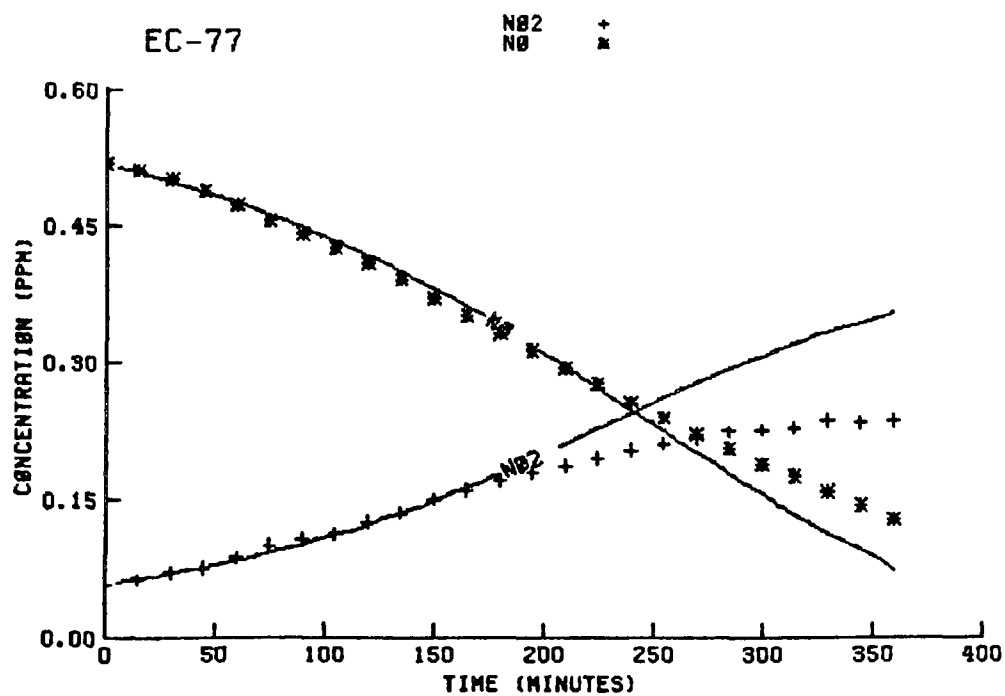
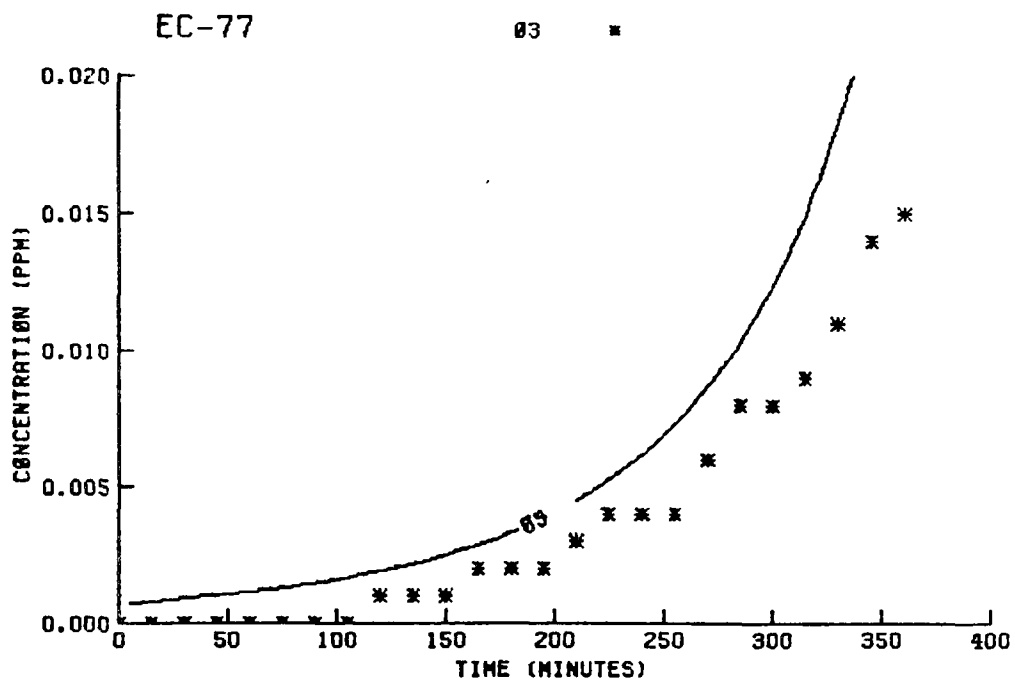


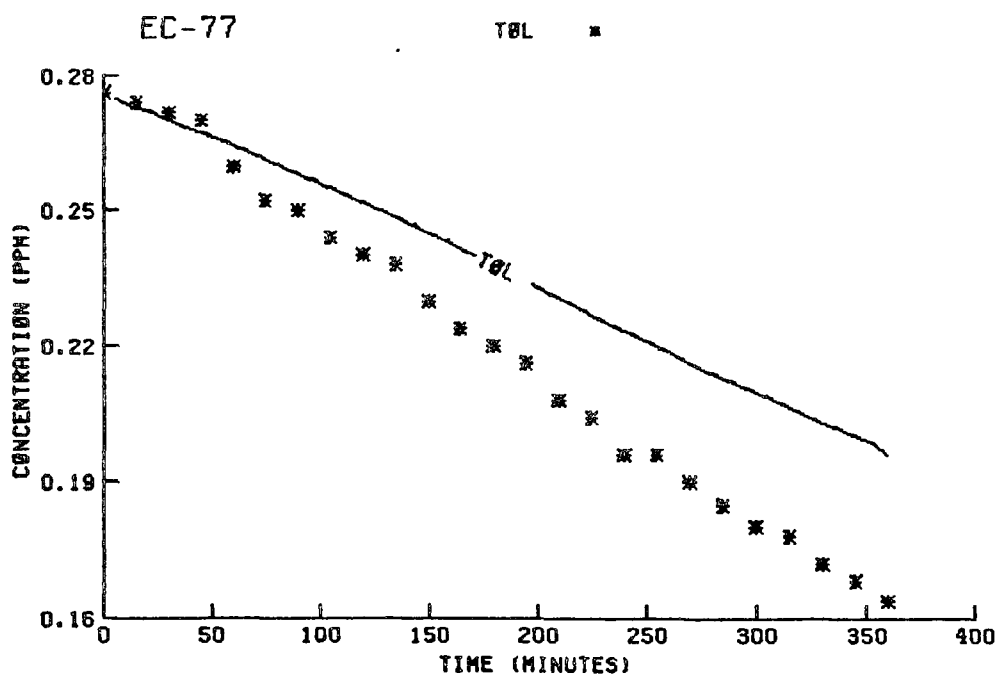
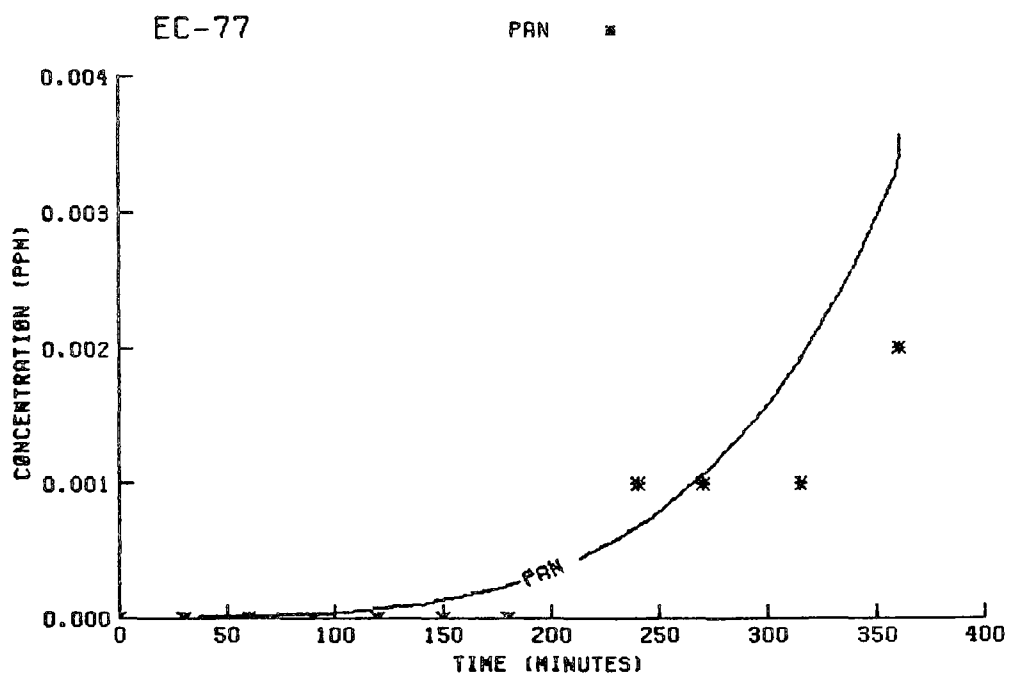
EC-169

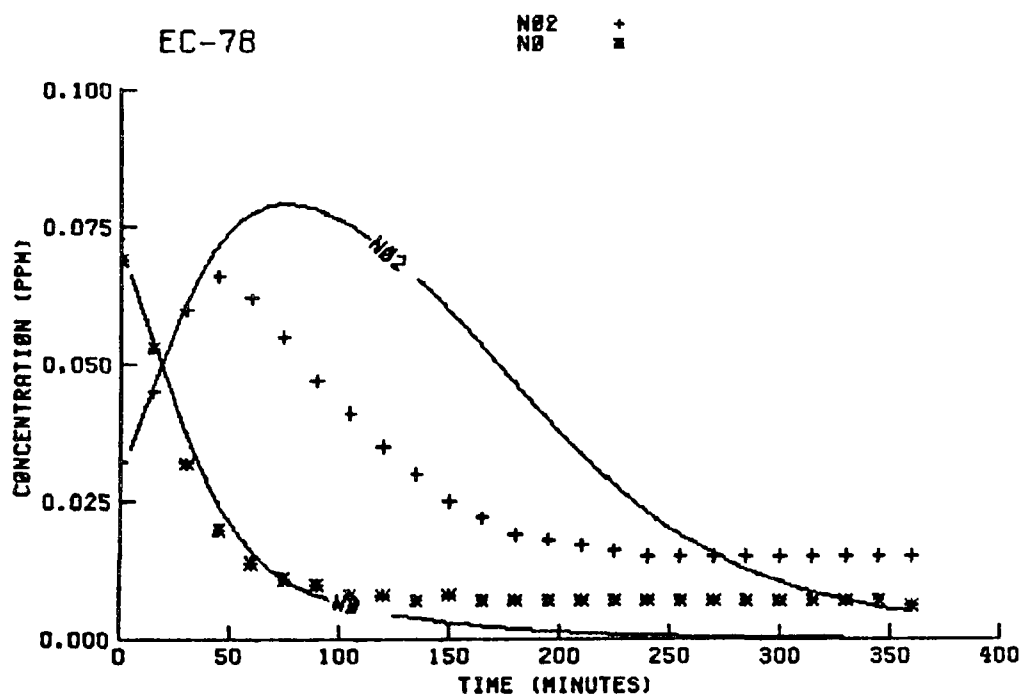
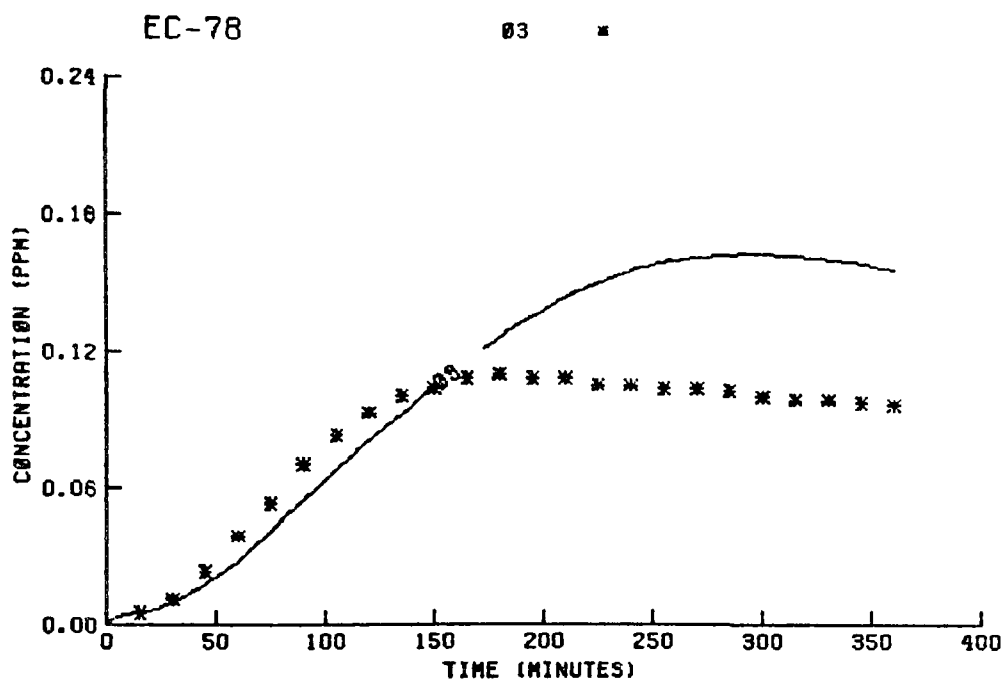
PAN

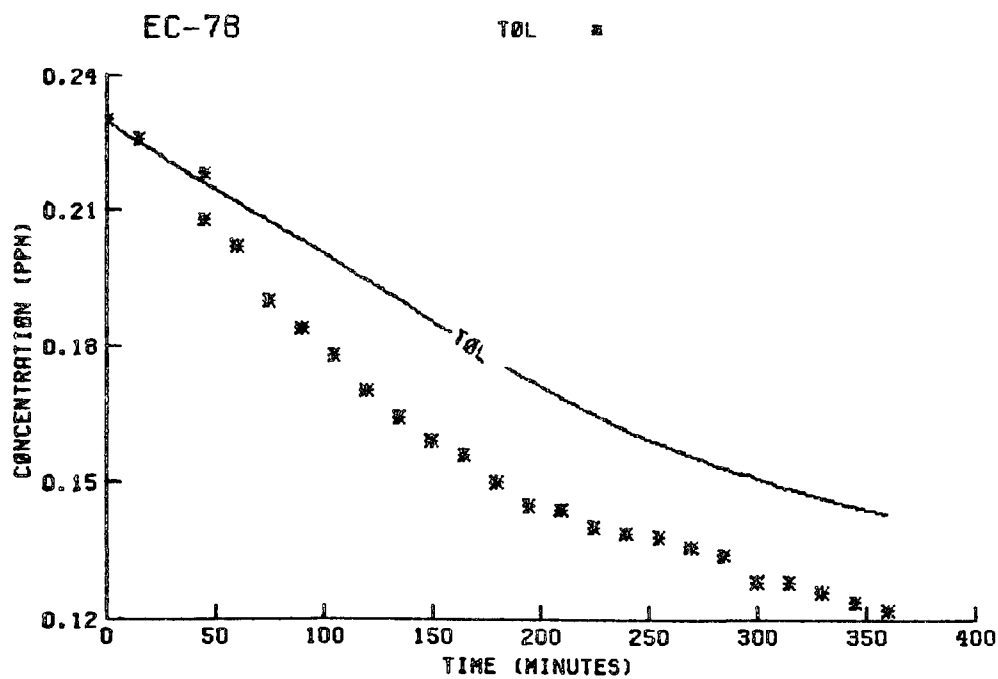
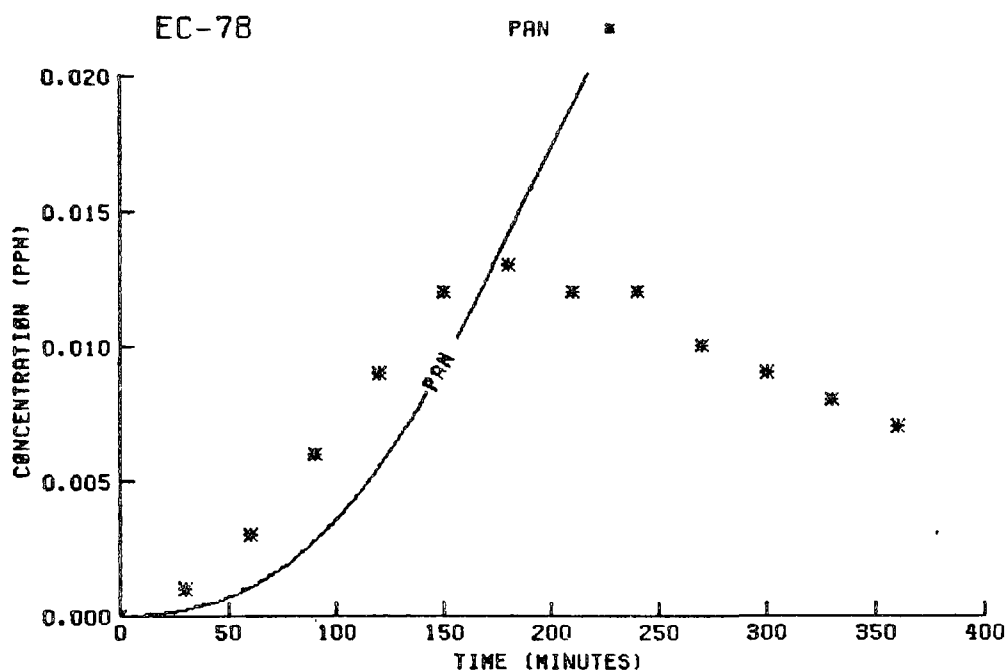


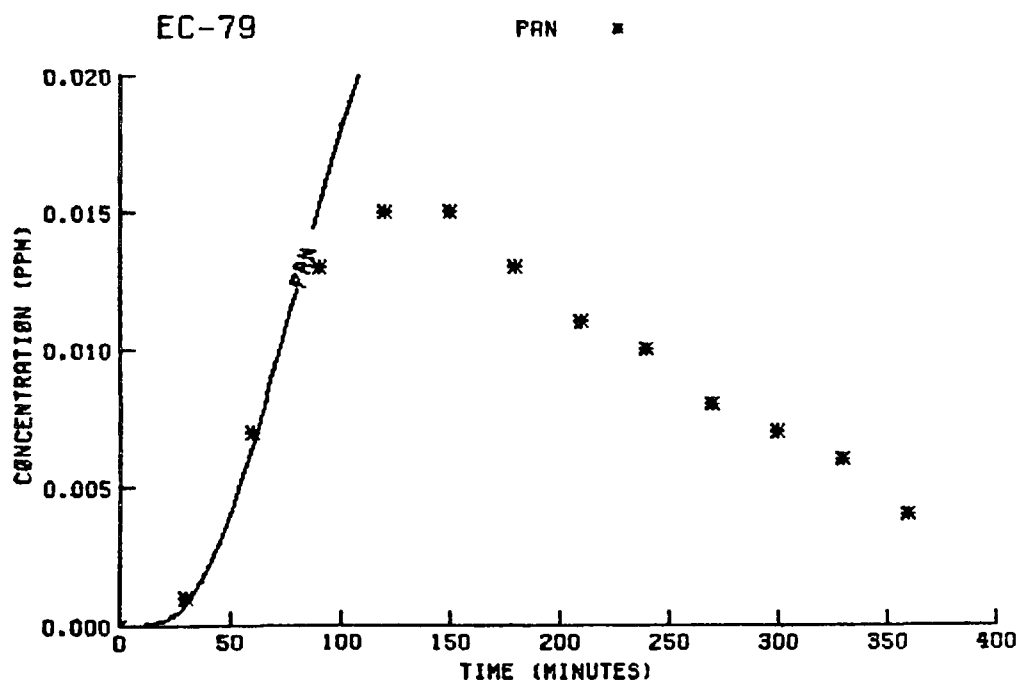
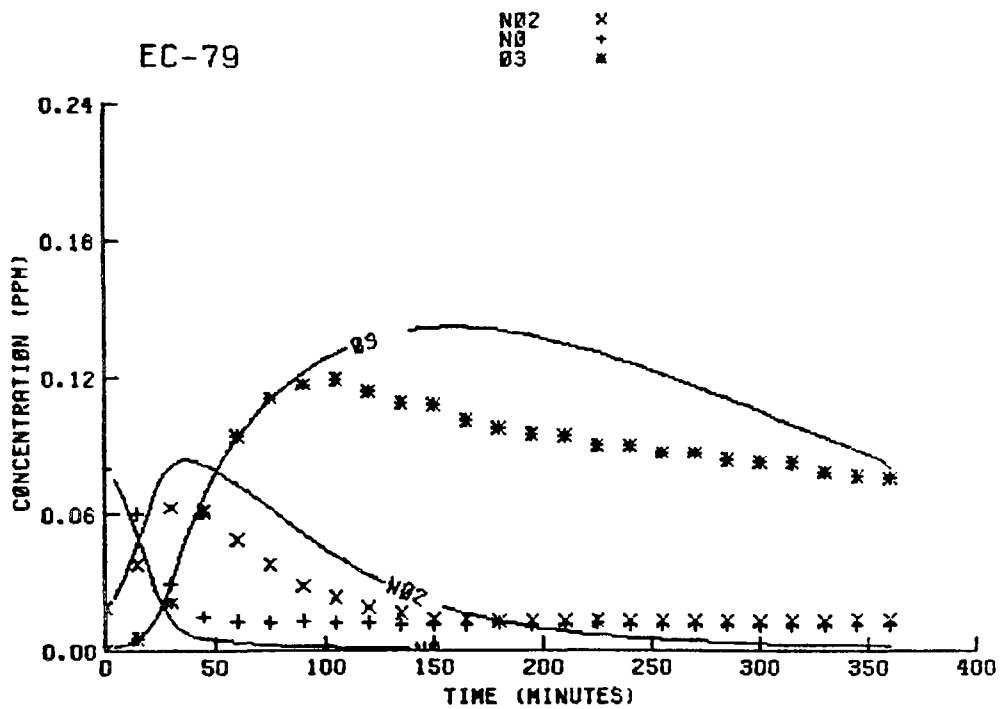
UCR TOLUENE EXPERIMENTS

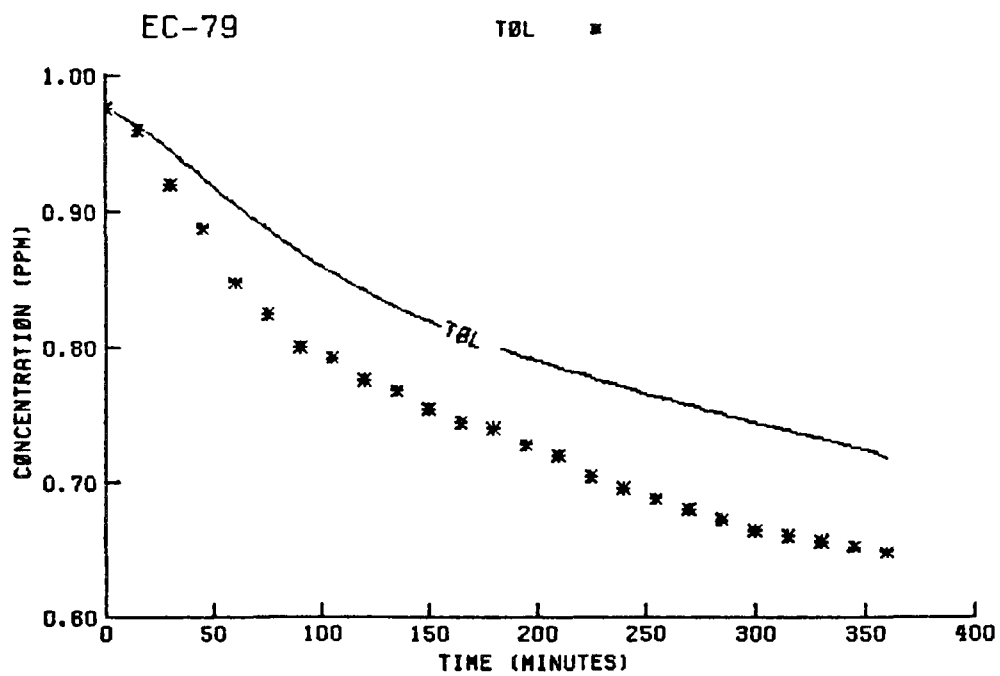






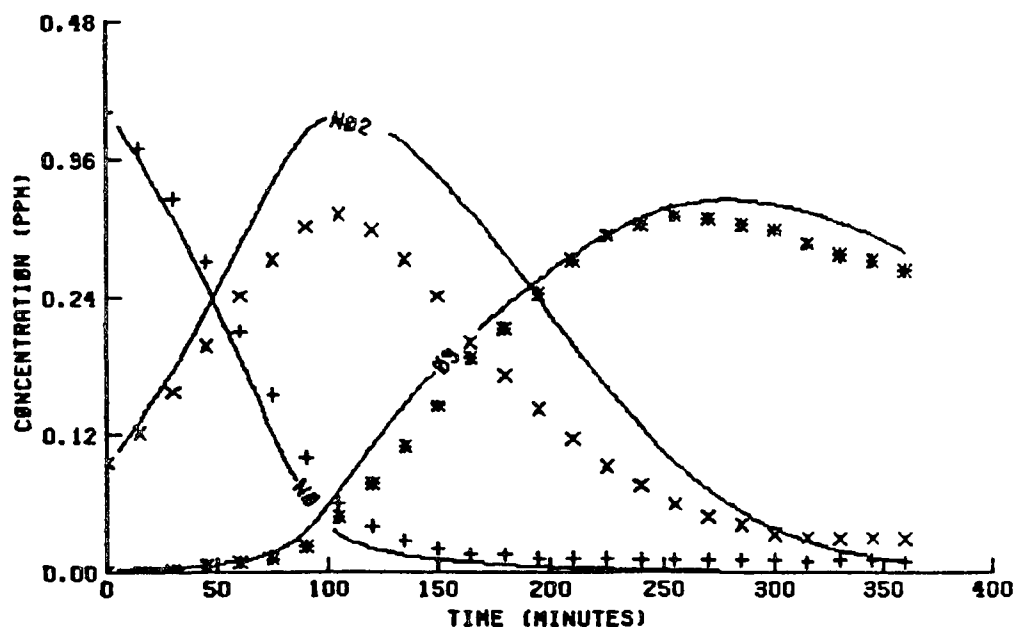






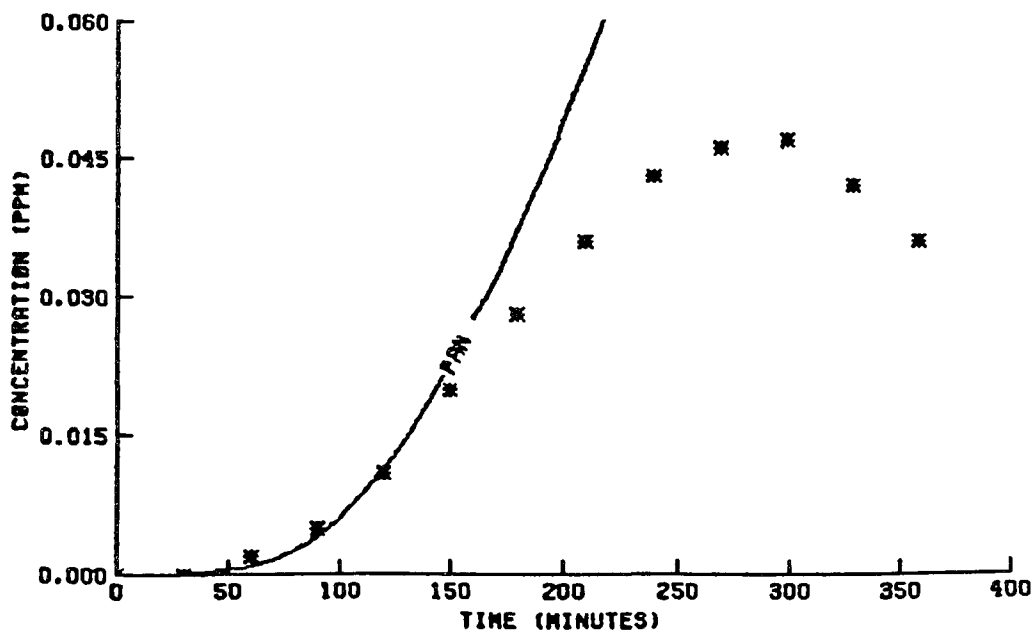
EC-80

NO₂ x
NO +
O₃ ■



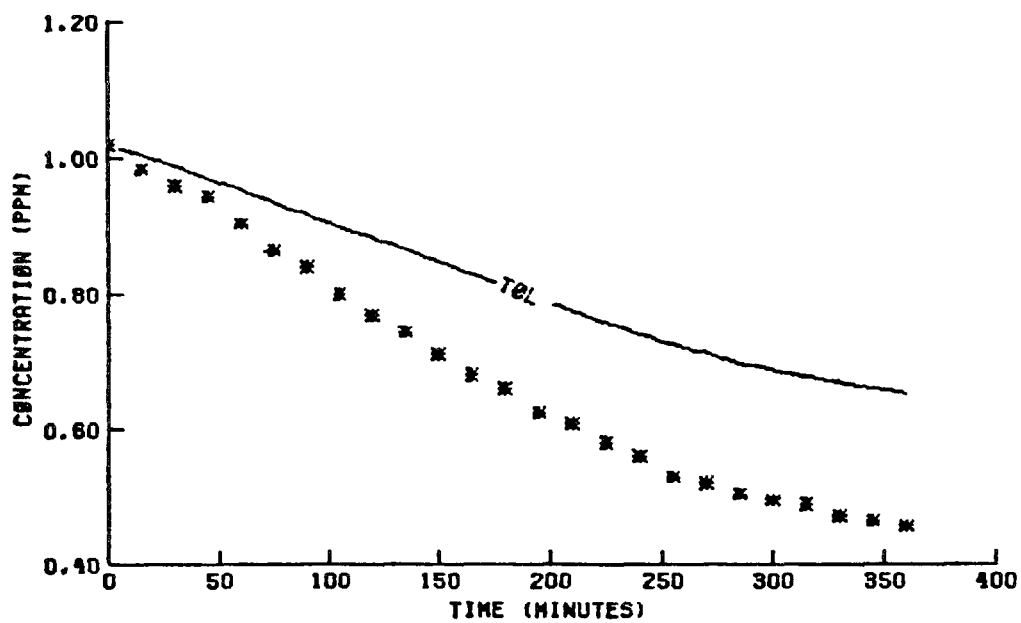
EC-80

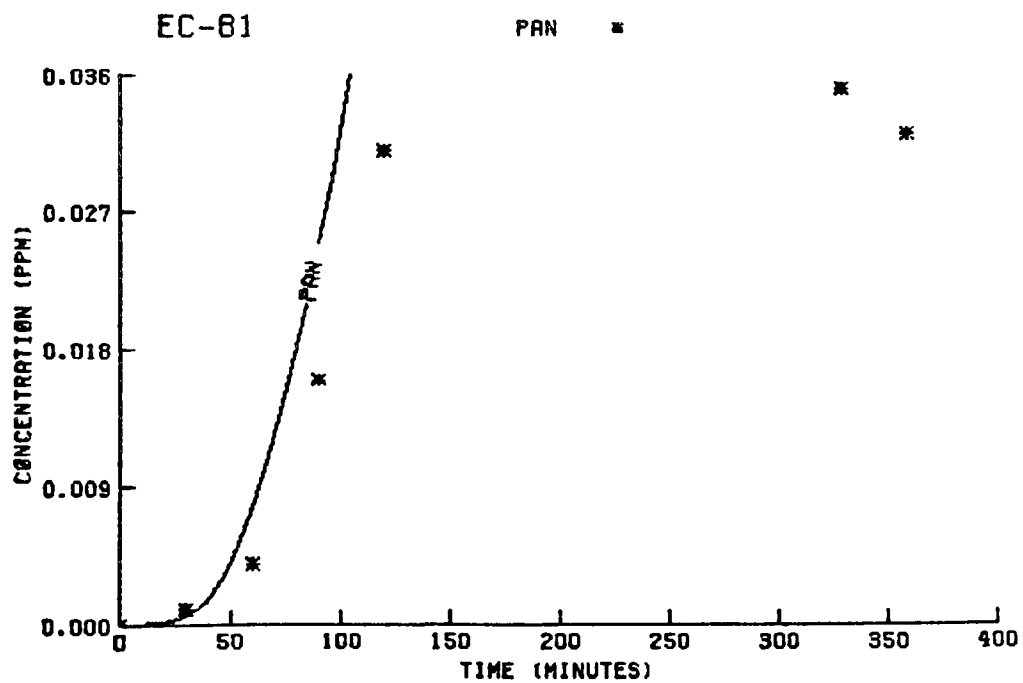
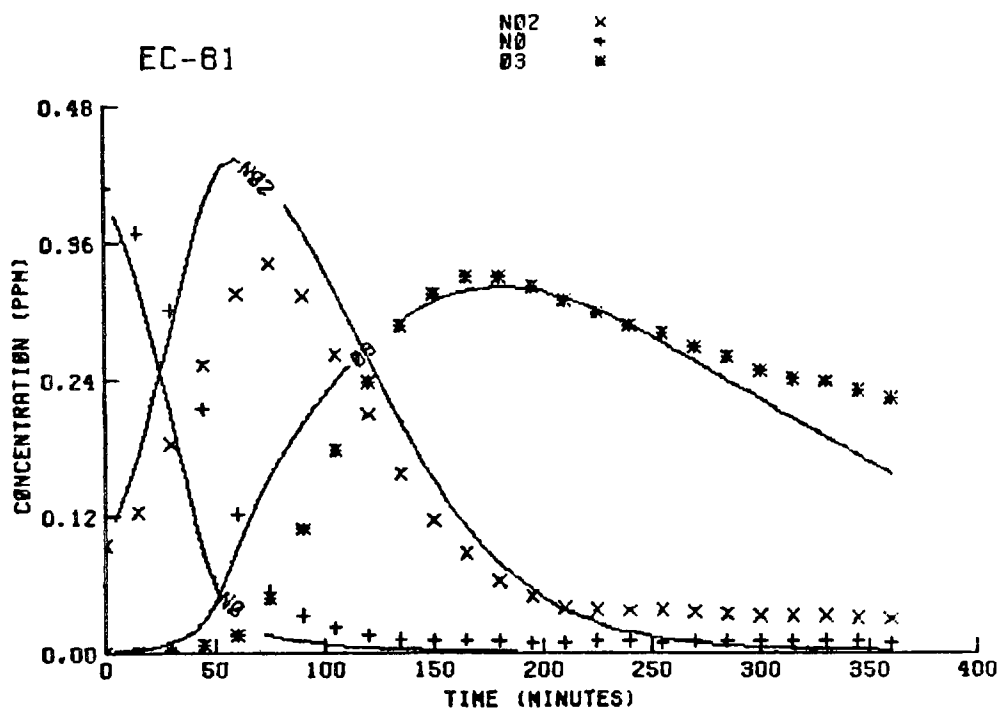
PAN ■



EC-80

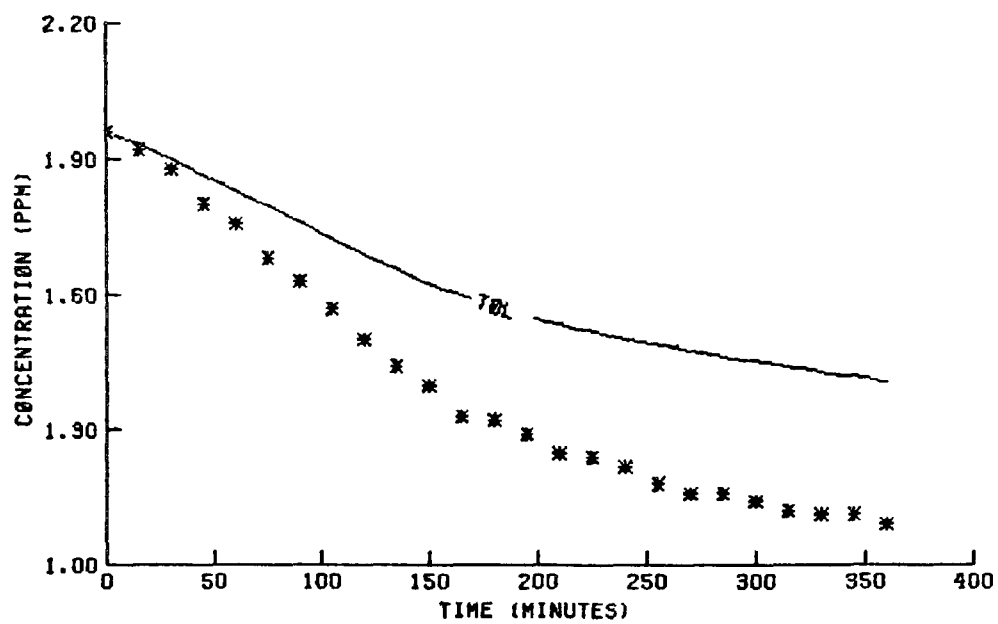
TOL ■

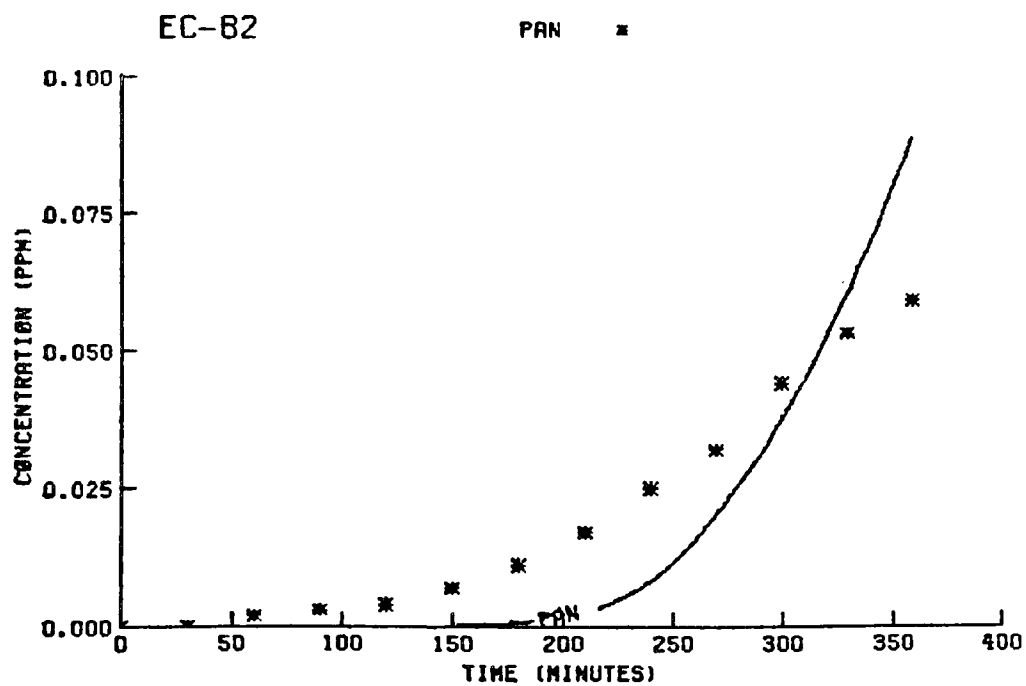
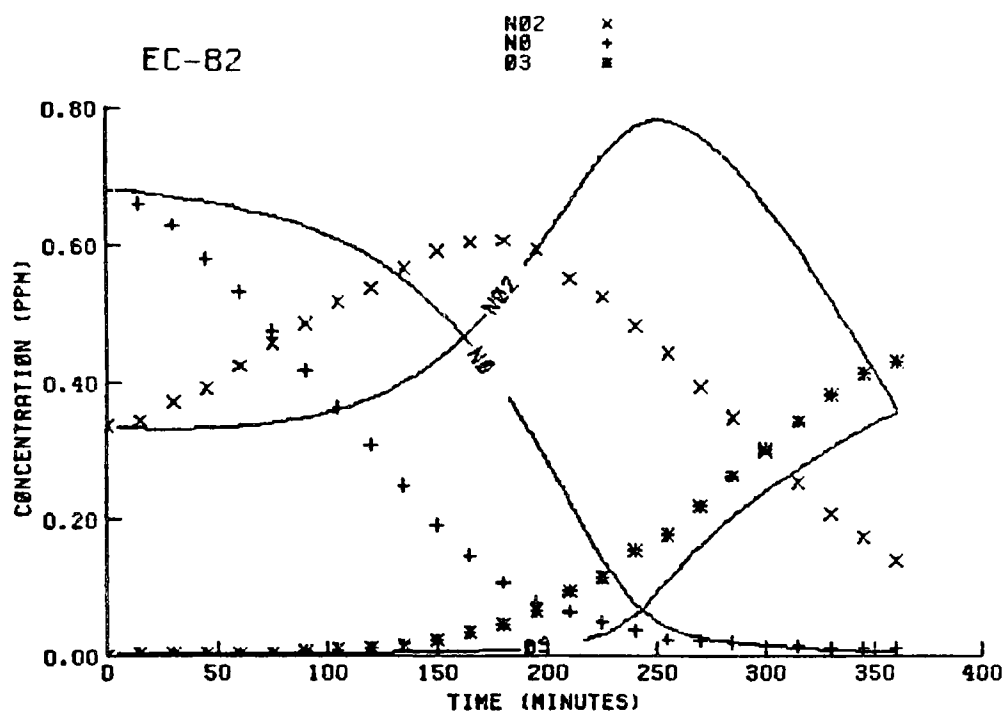




EC-81

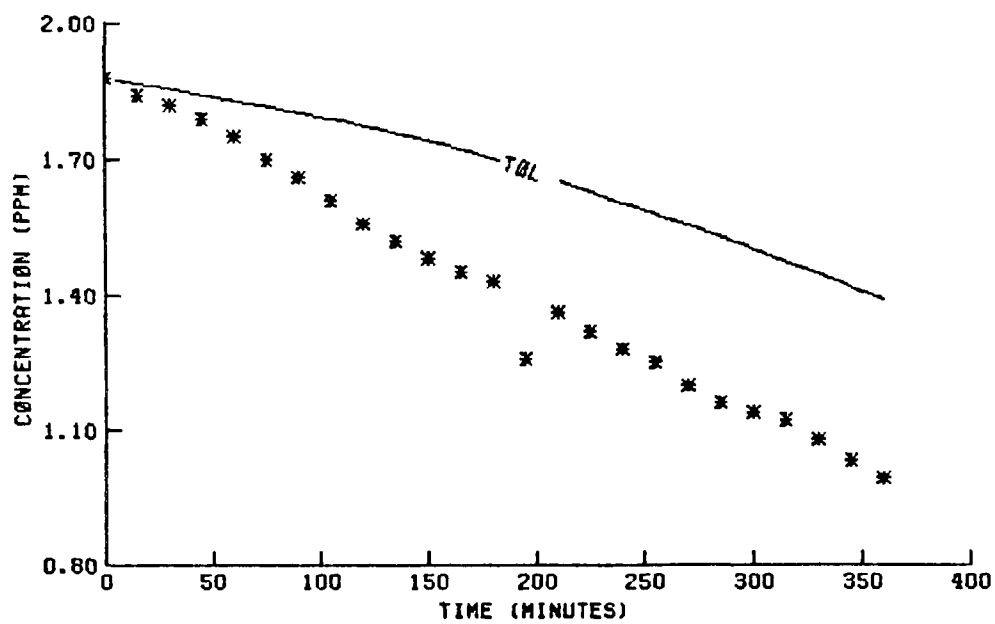
TOL ■

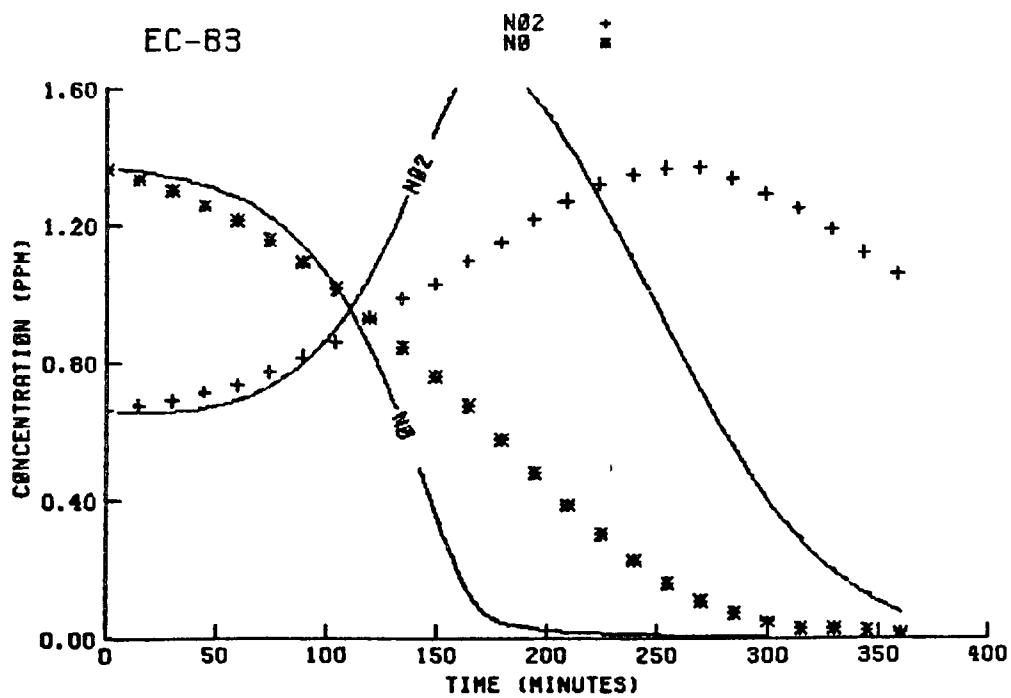
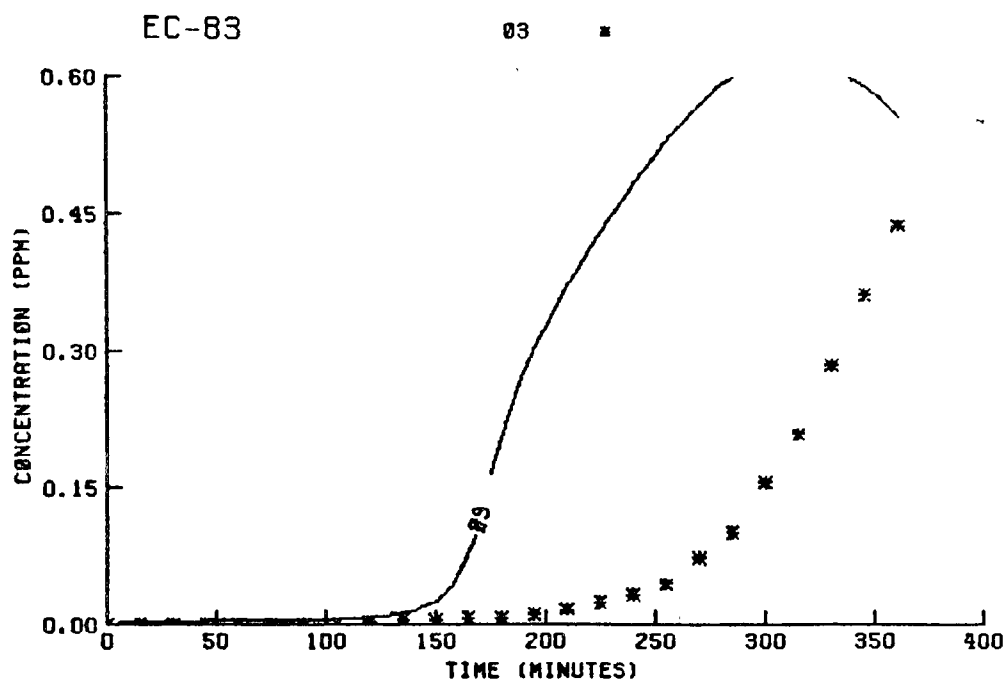


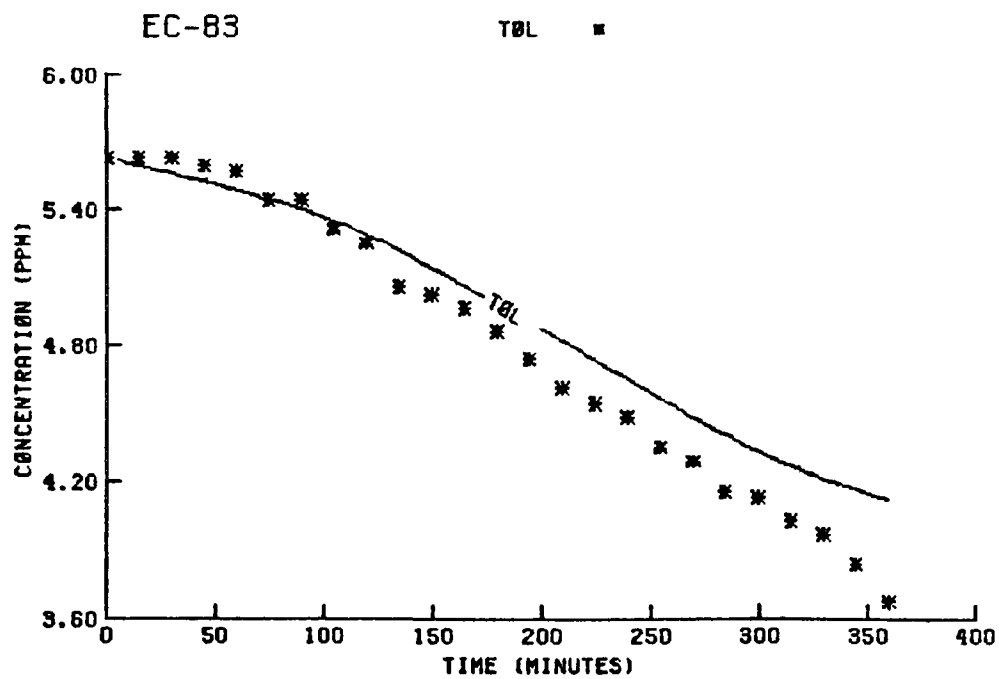
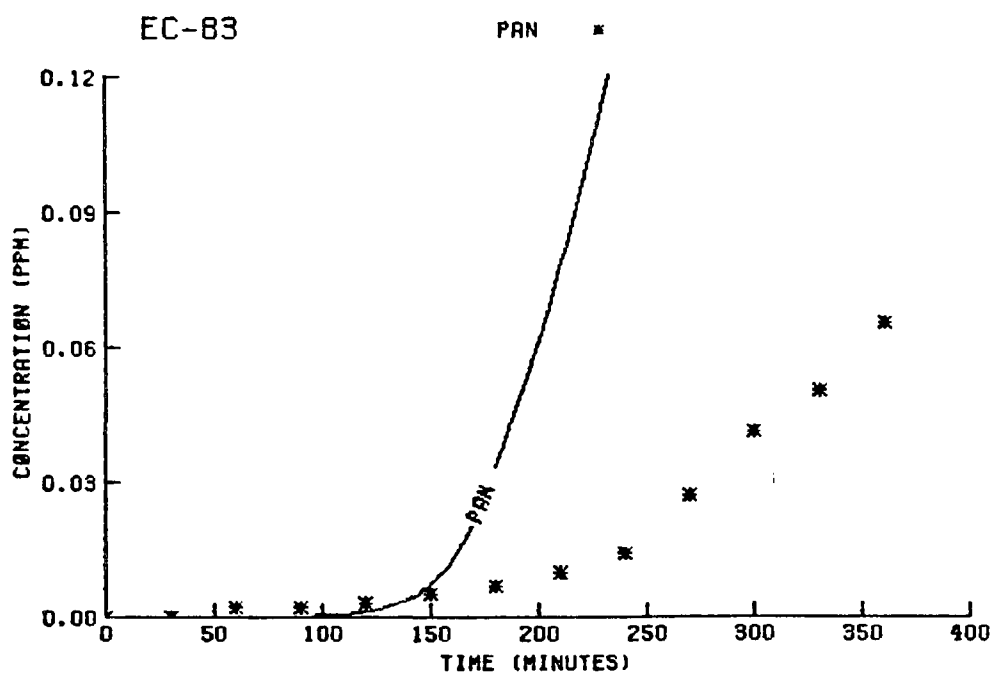


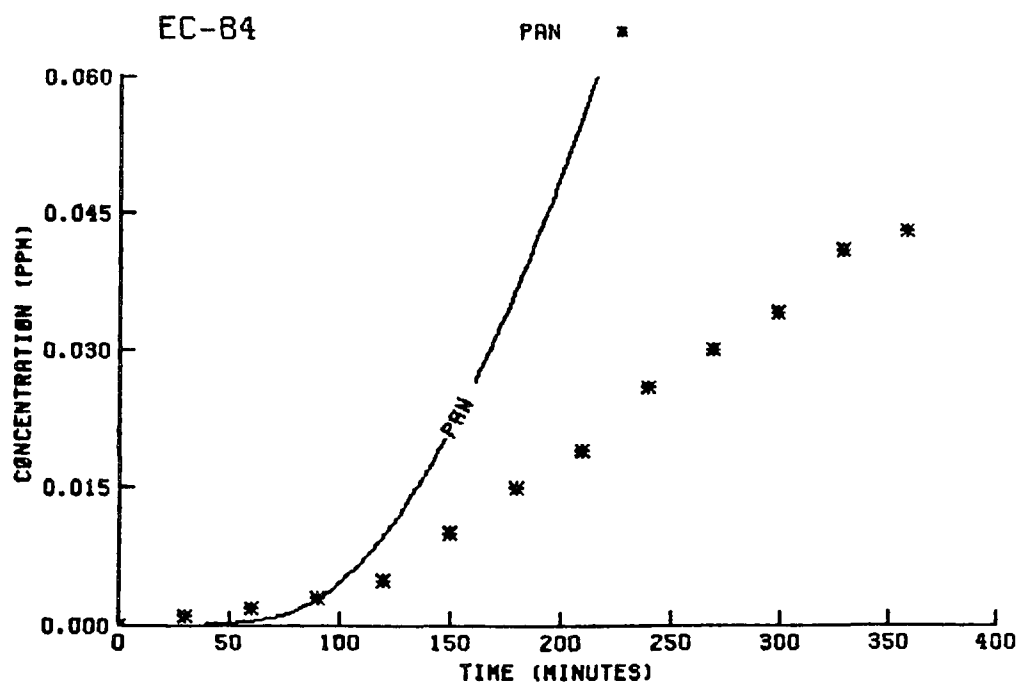
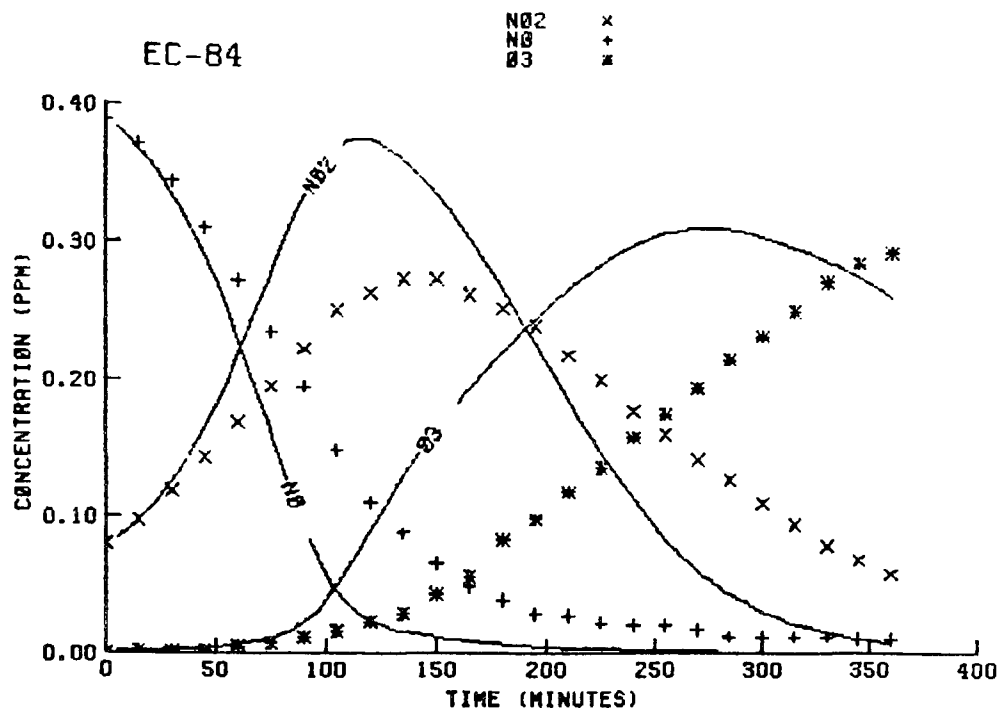
EC-82

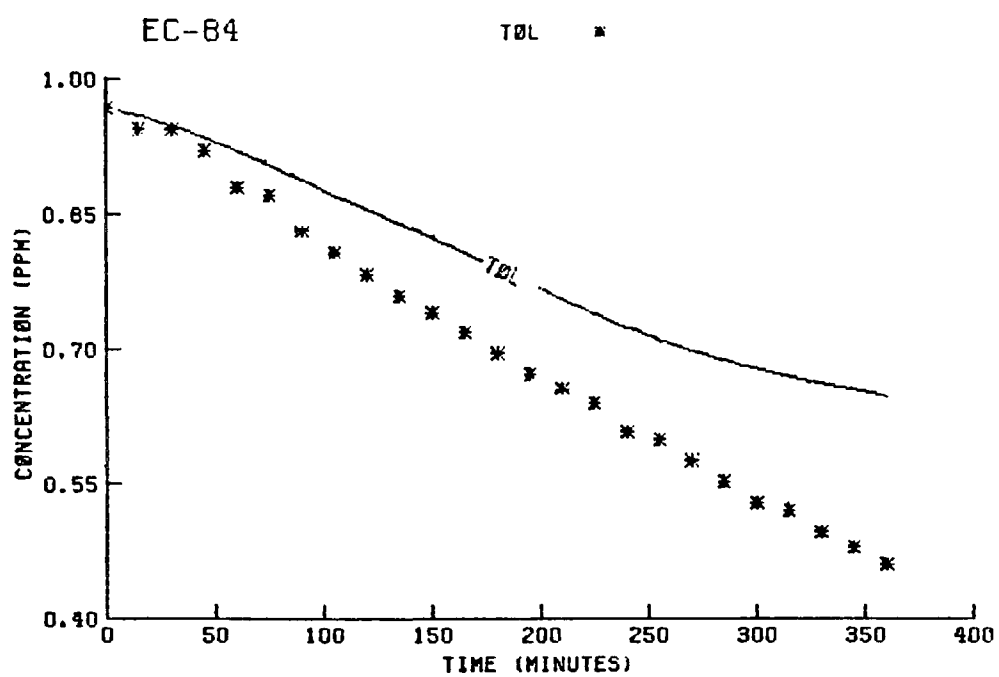
TOL ■

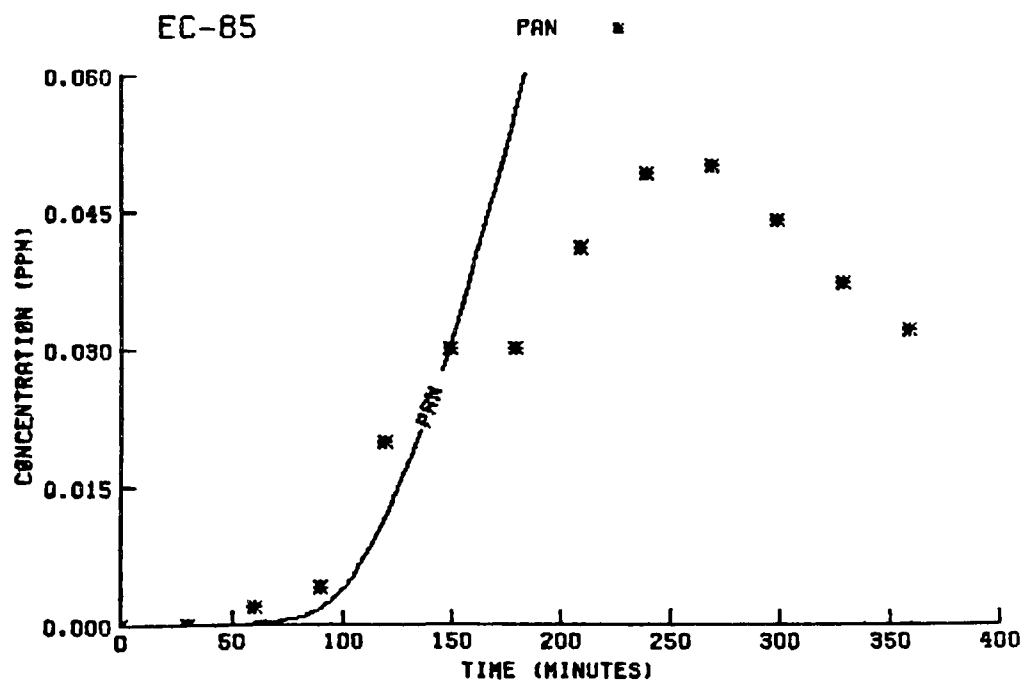
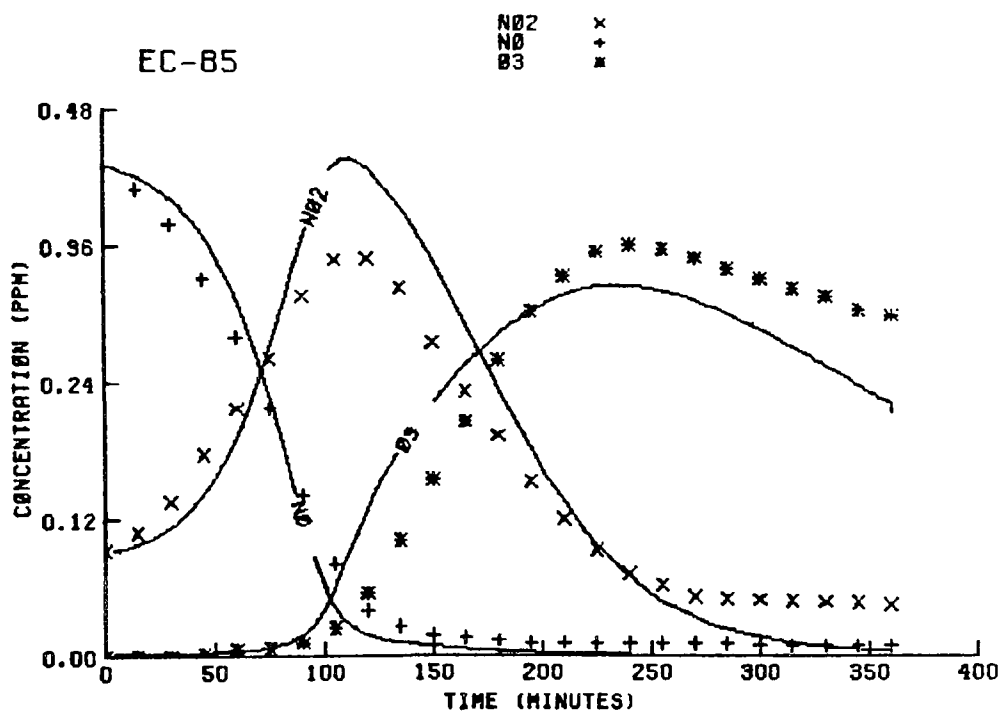






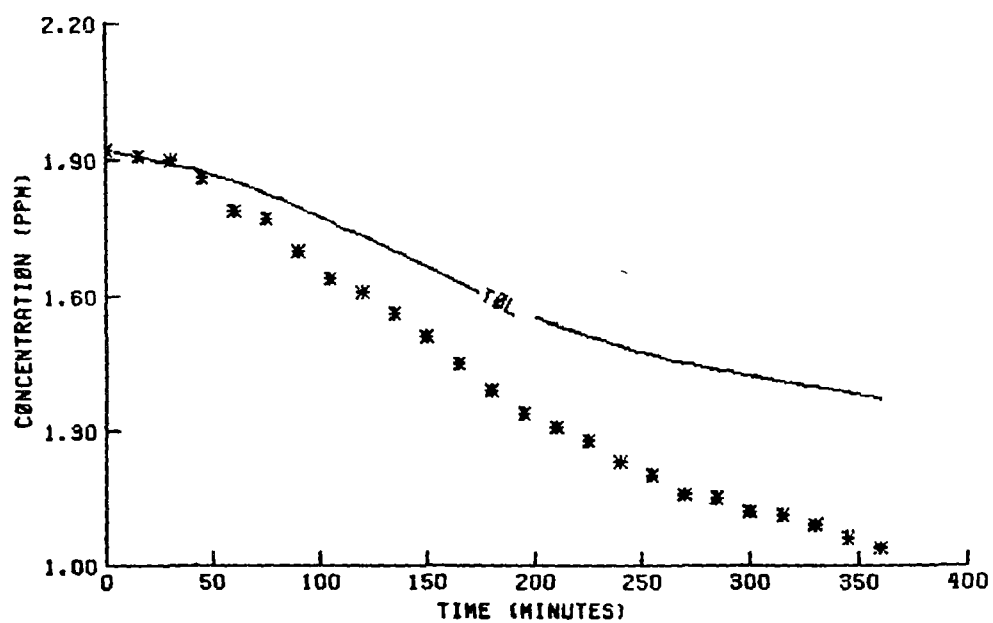


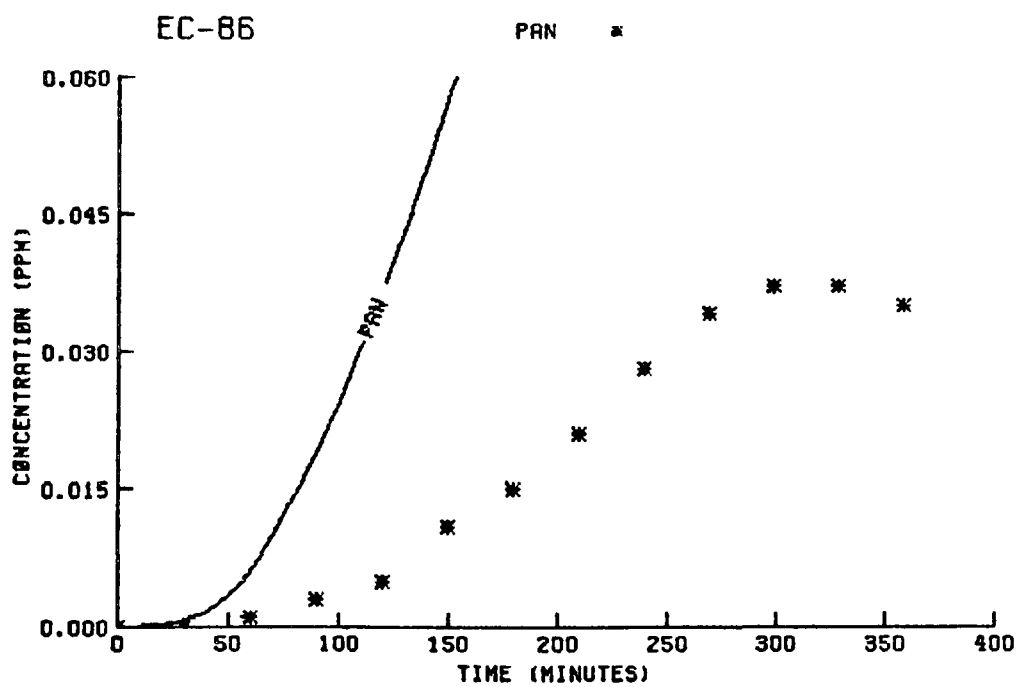
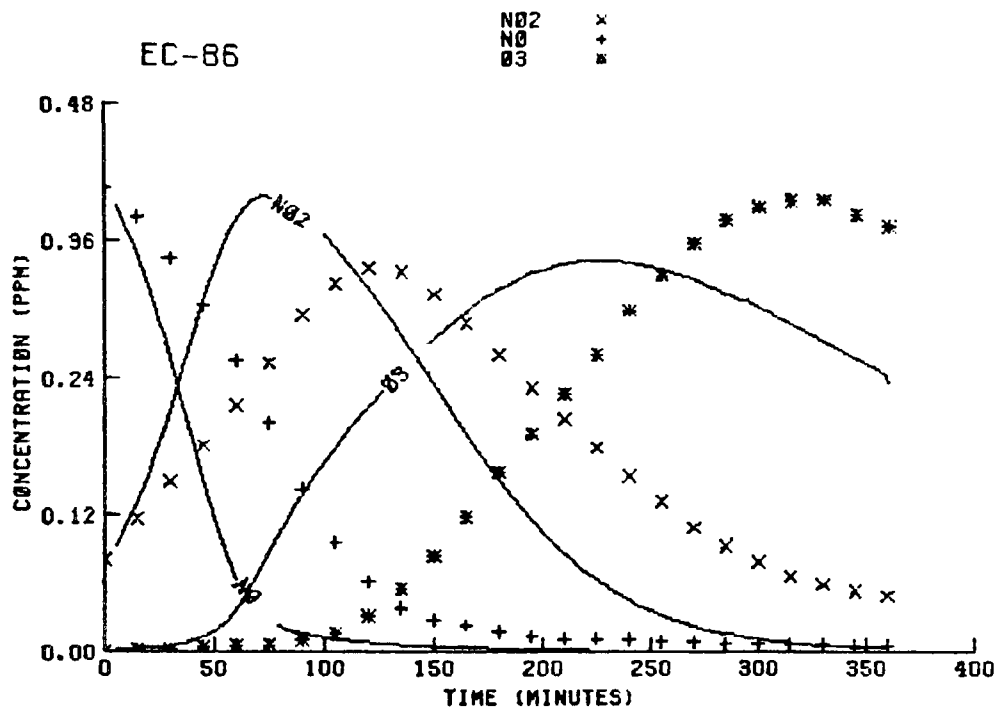




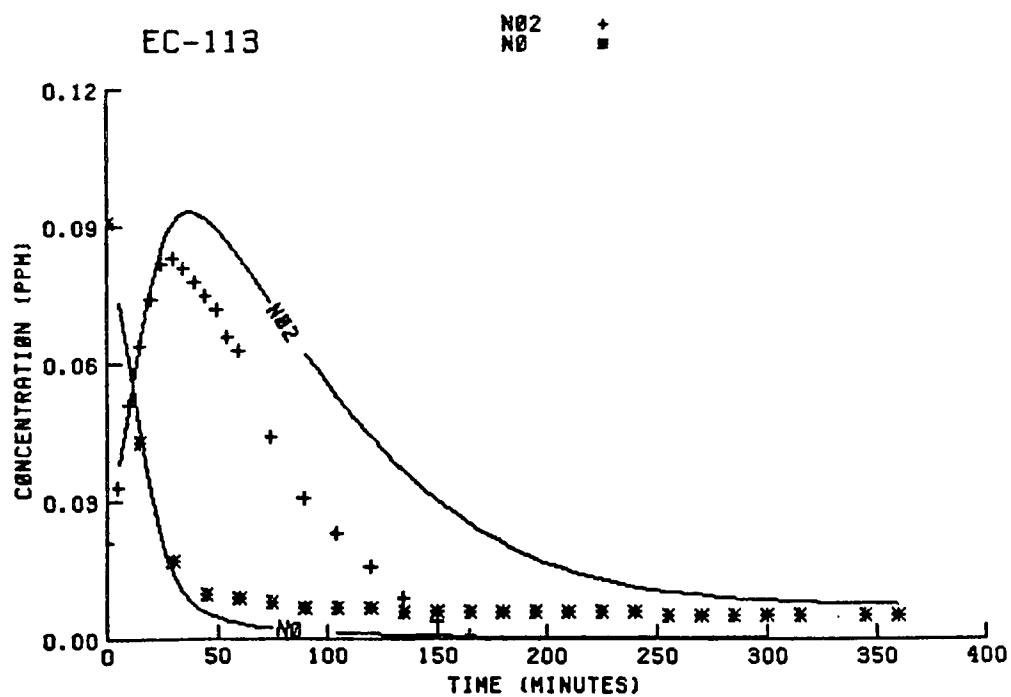
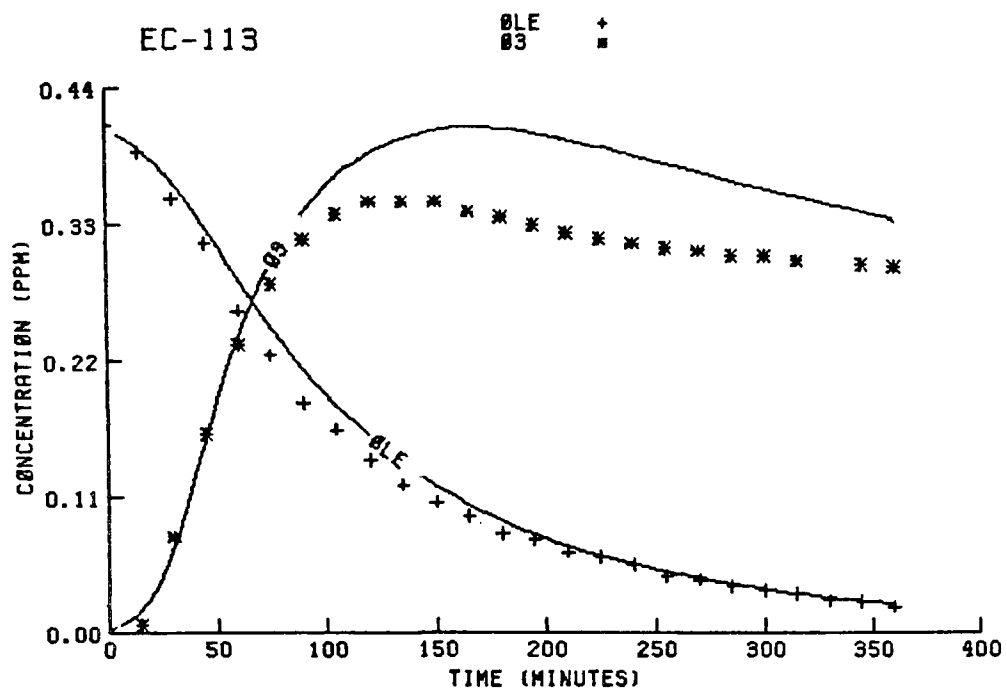
EC-85

TOL *



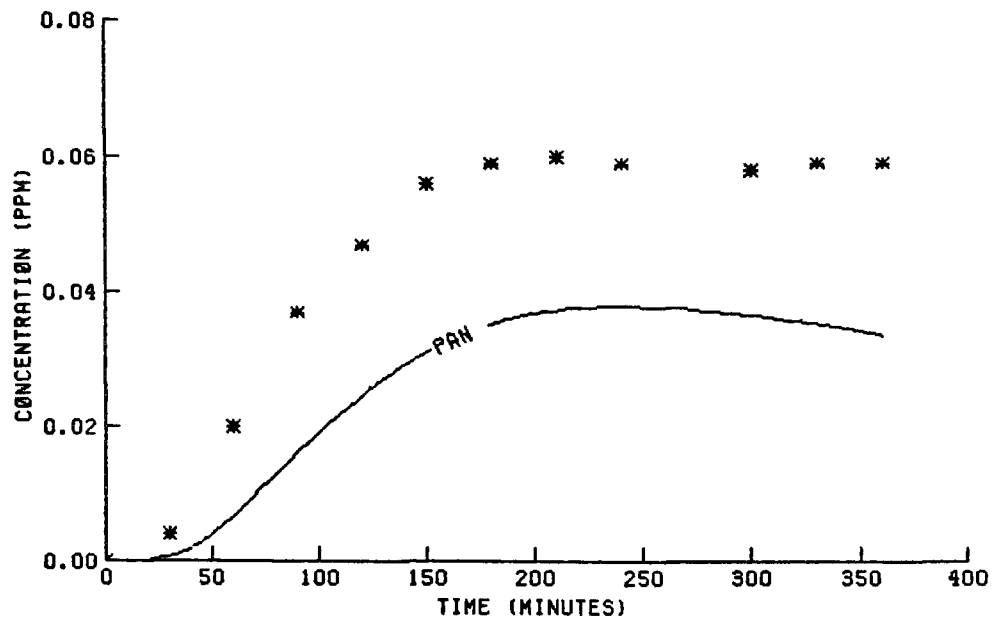


UCR PROPYLENE/BUTANE EXPERIMENTS



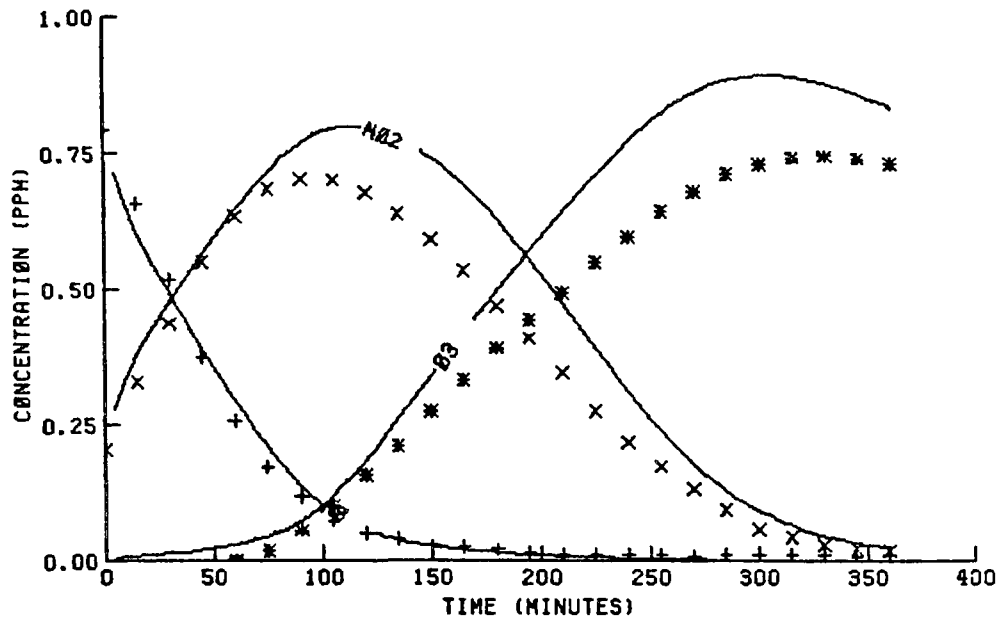
EC-113

PAN



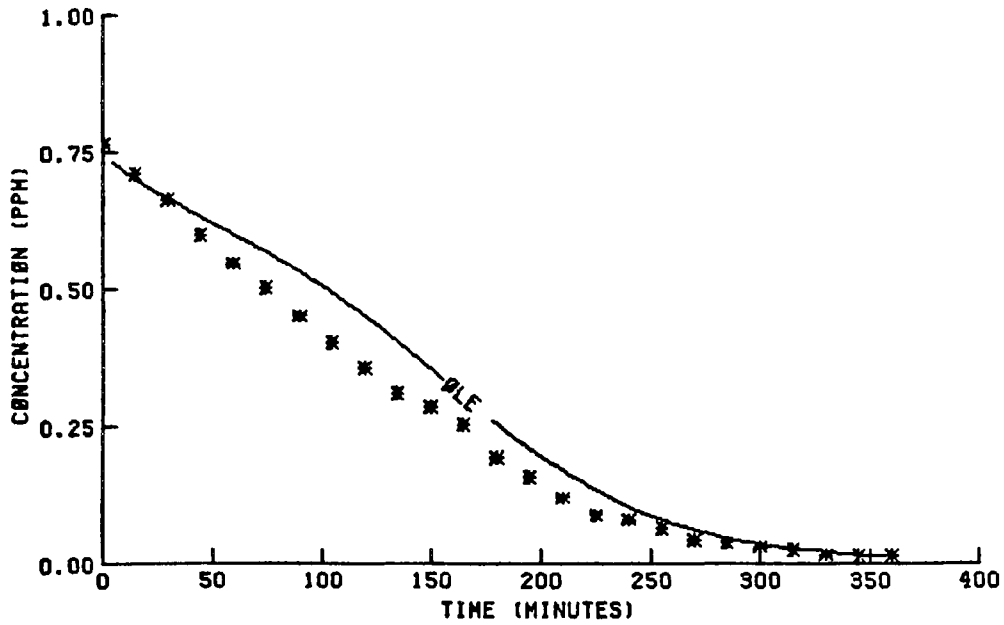
EC-114

NO₂ x
NO +
O₃ ■



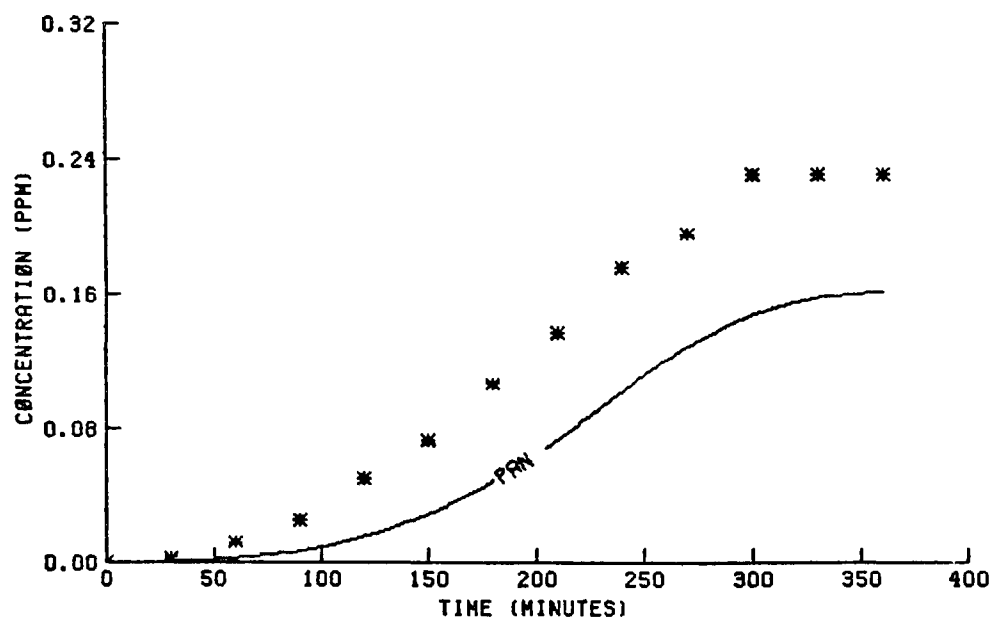
EC-114

O₃LE ■



EC-114

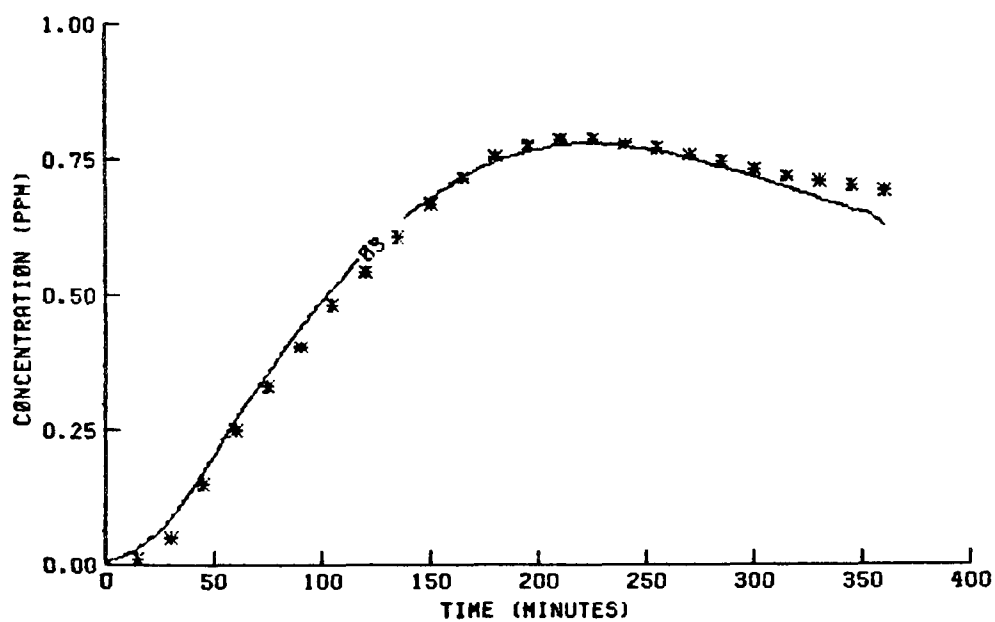
PAN ■



UCR MULTIOLEFIN EXPERIMENTS

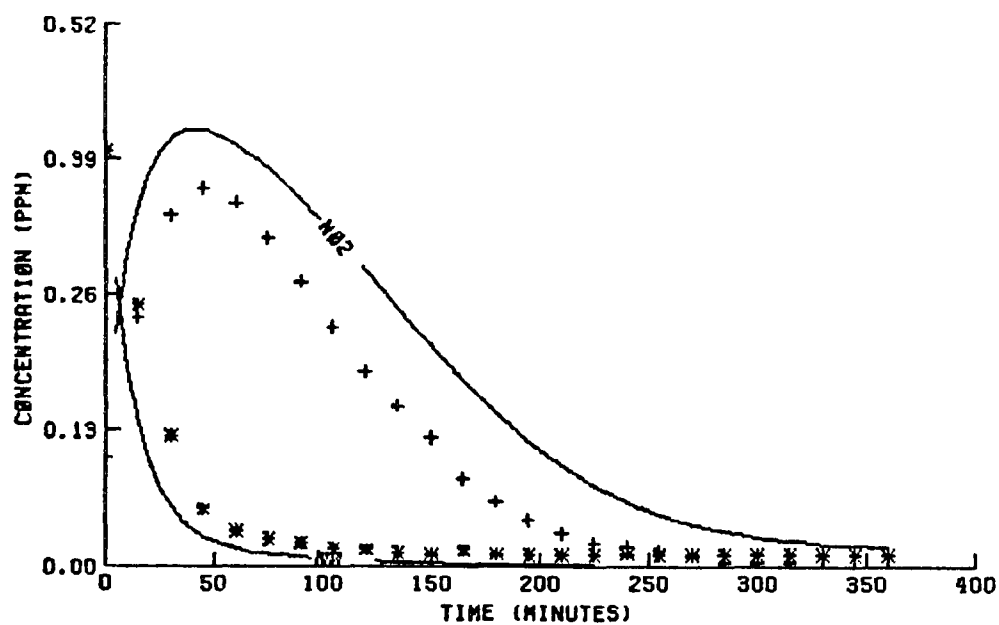
EC-152

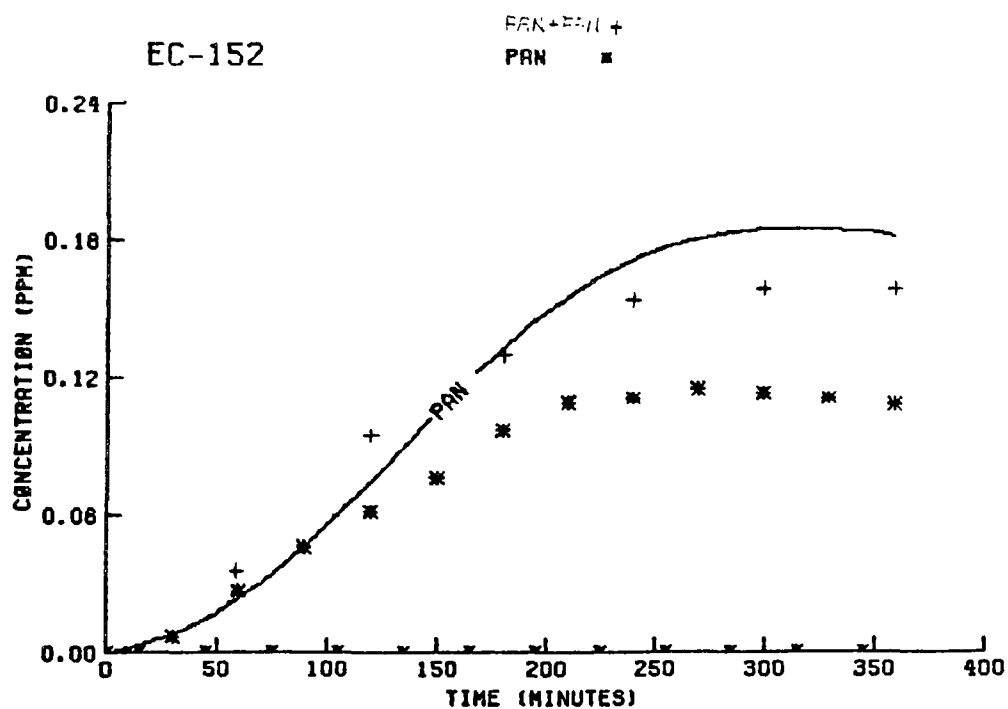
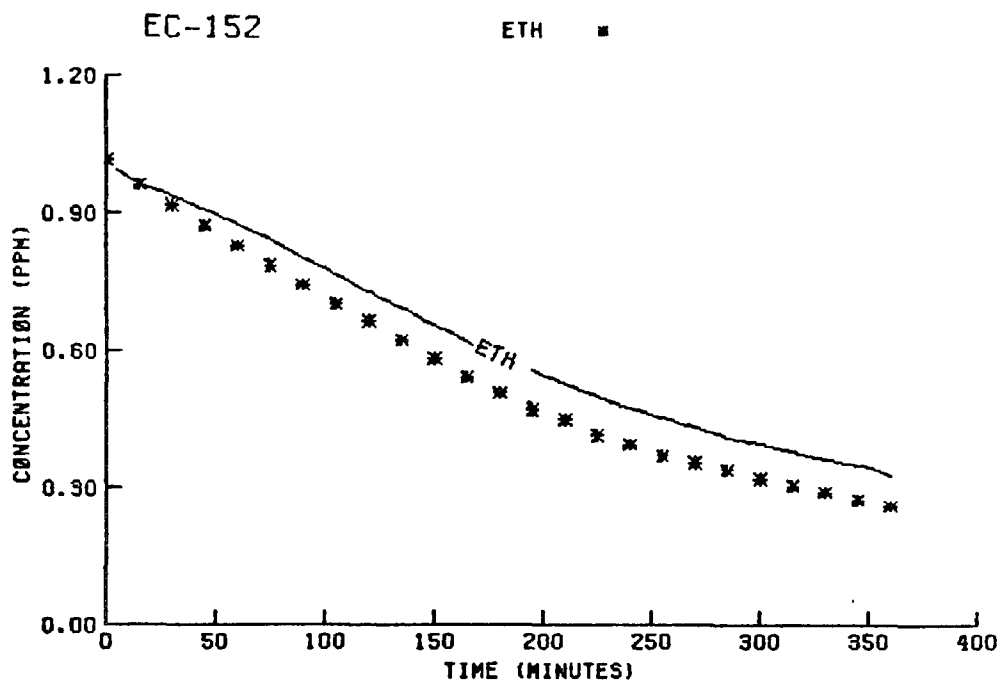
03 *



EC-152

N02 +
N0 *

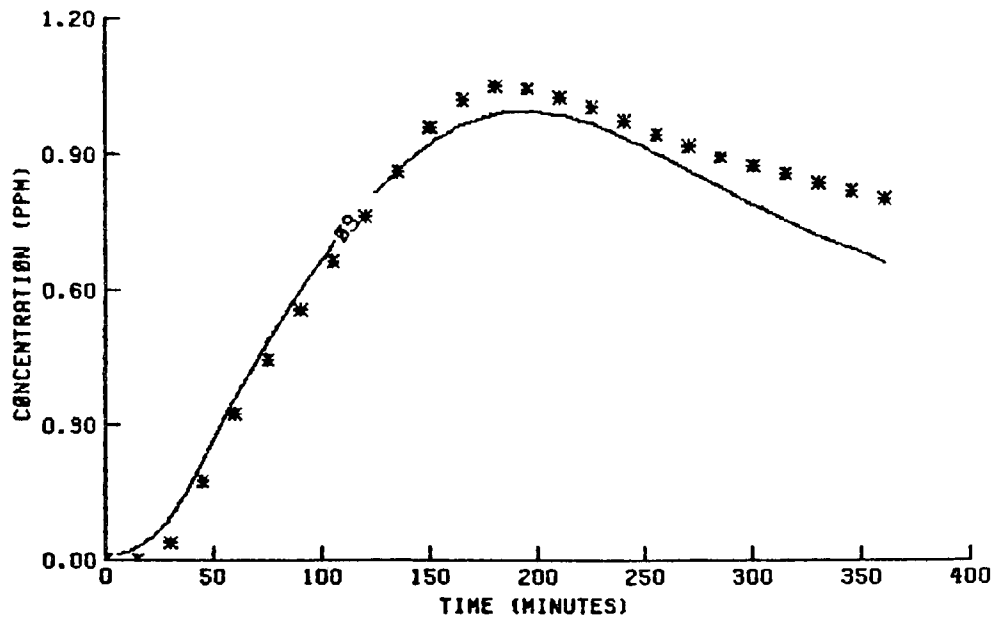




EC-153

03

*



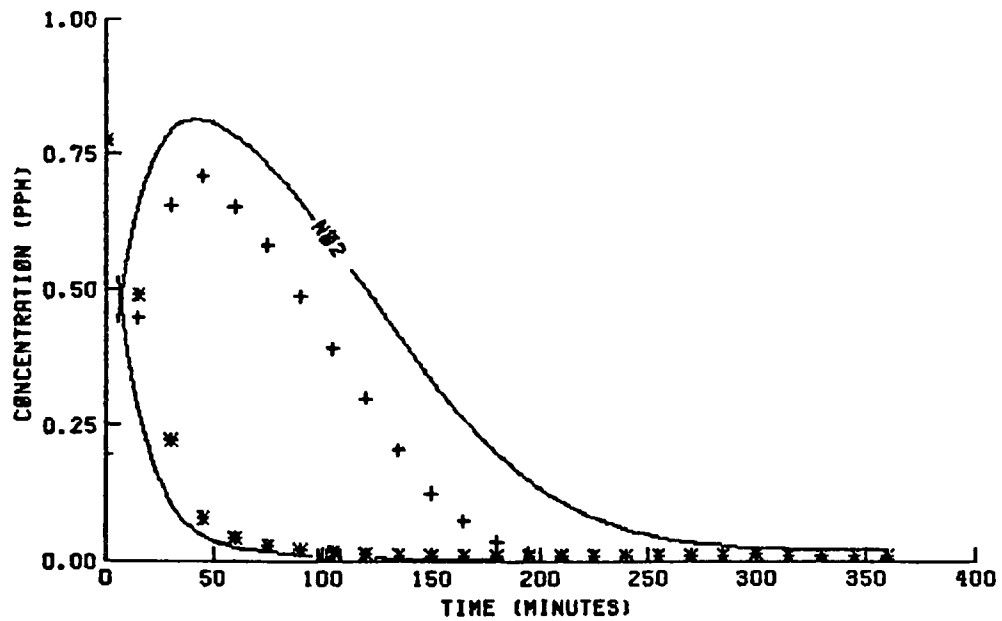
EC-153

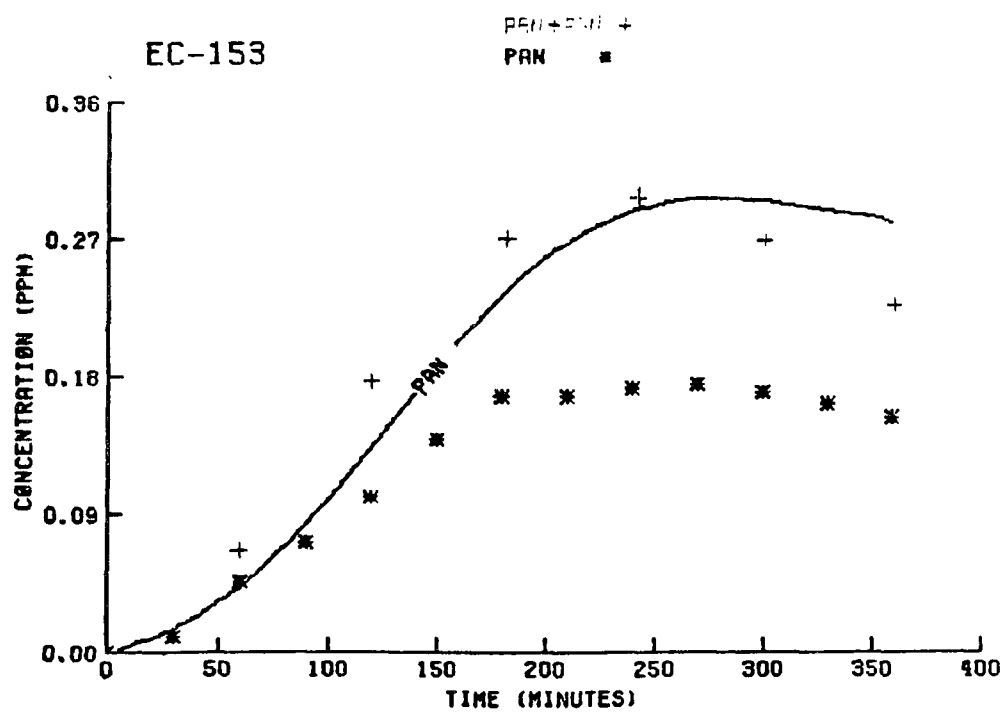
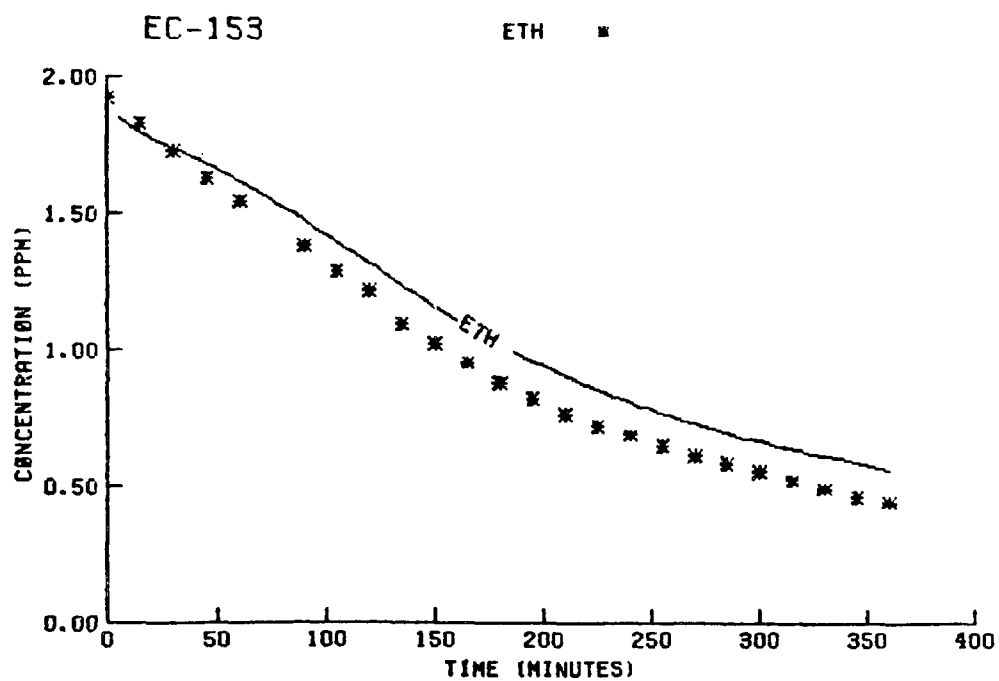
N02

+

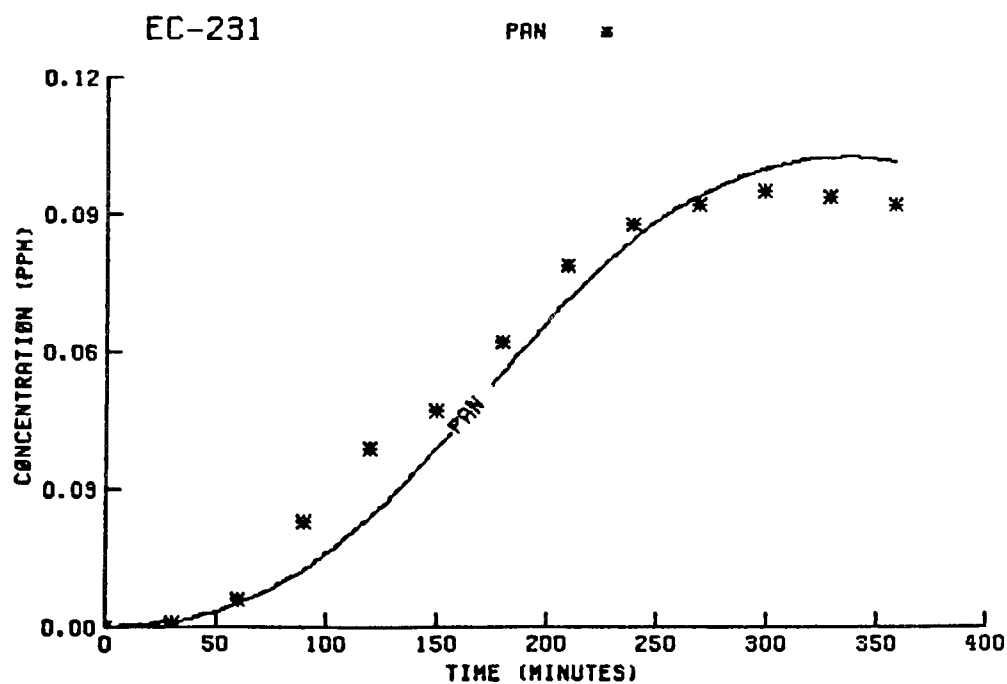
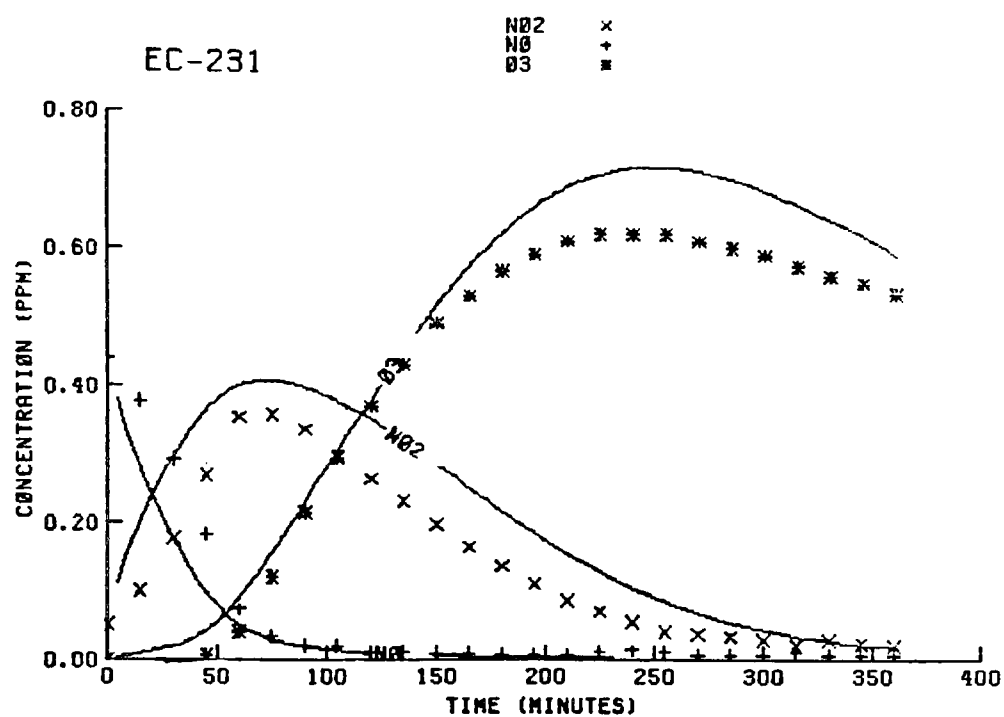
N0

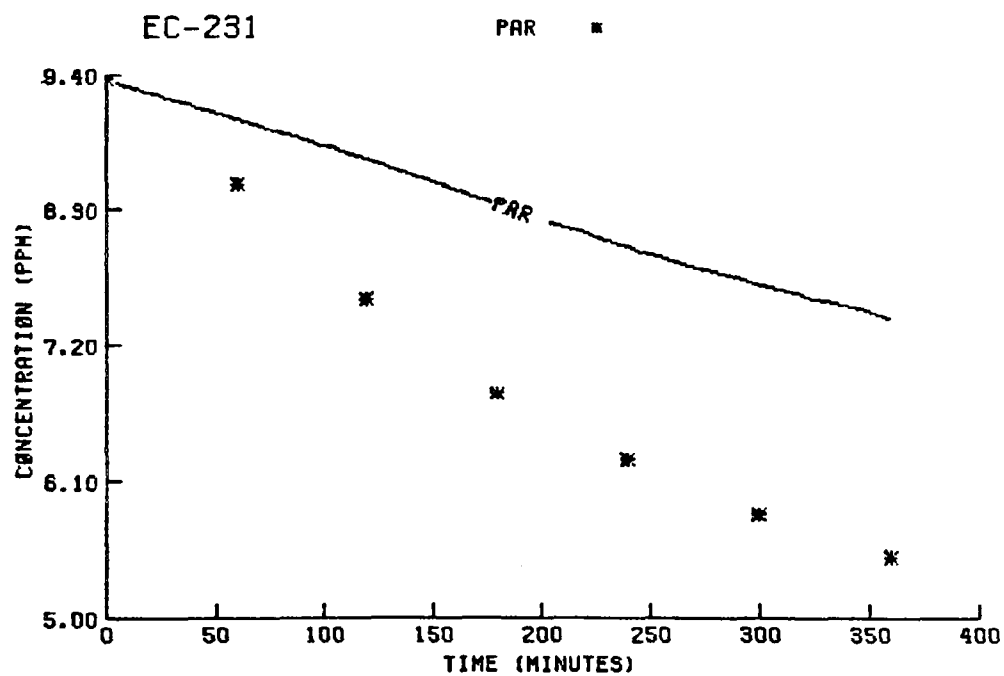
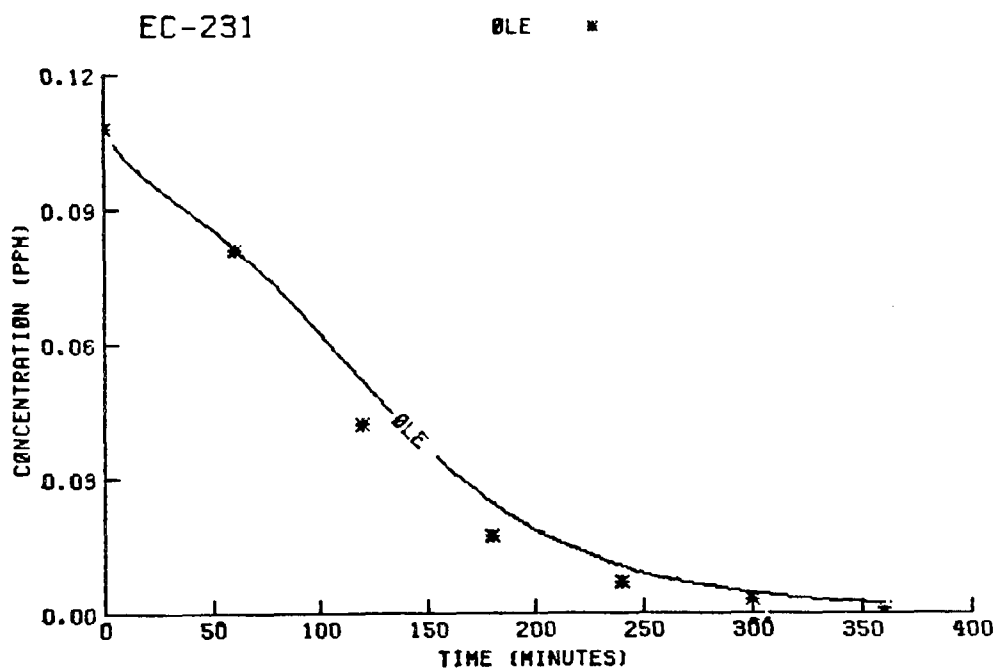
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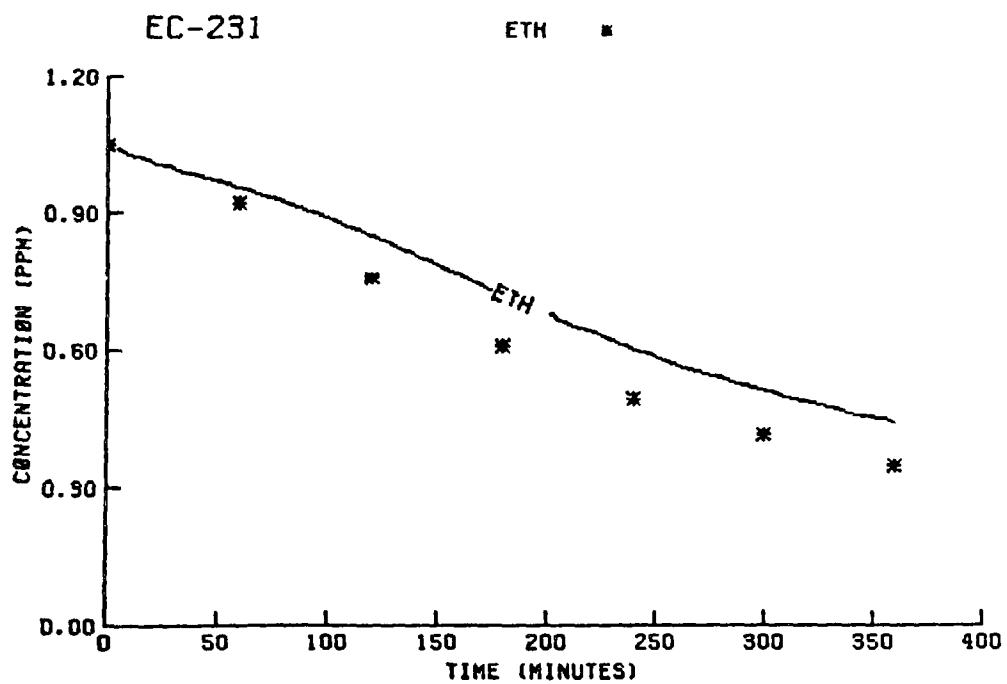
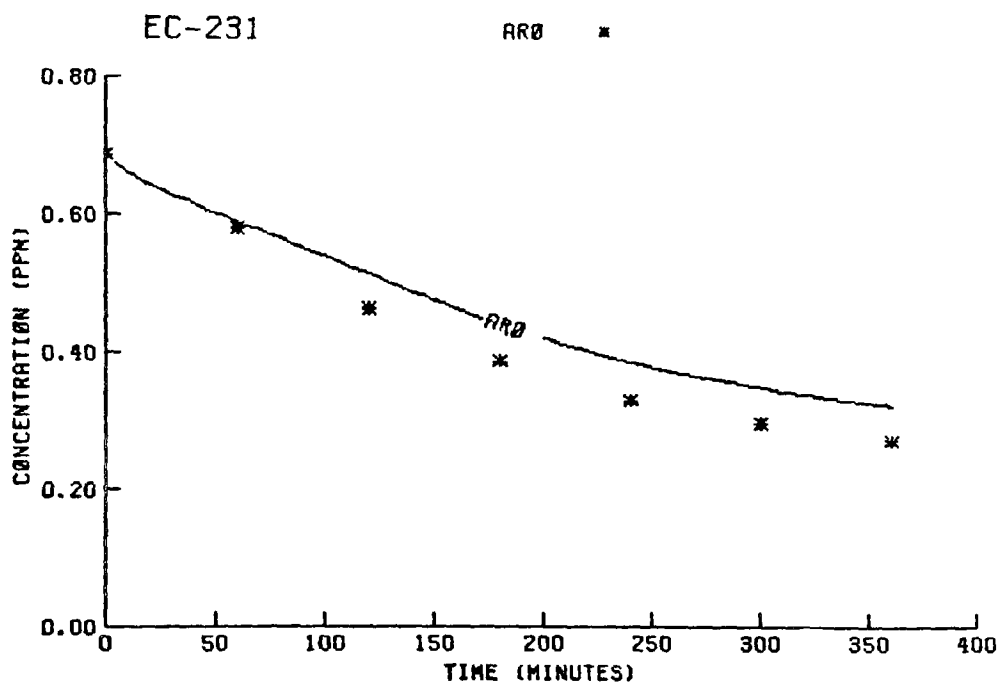


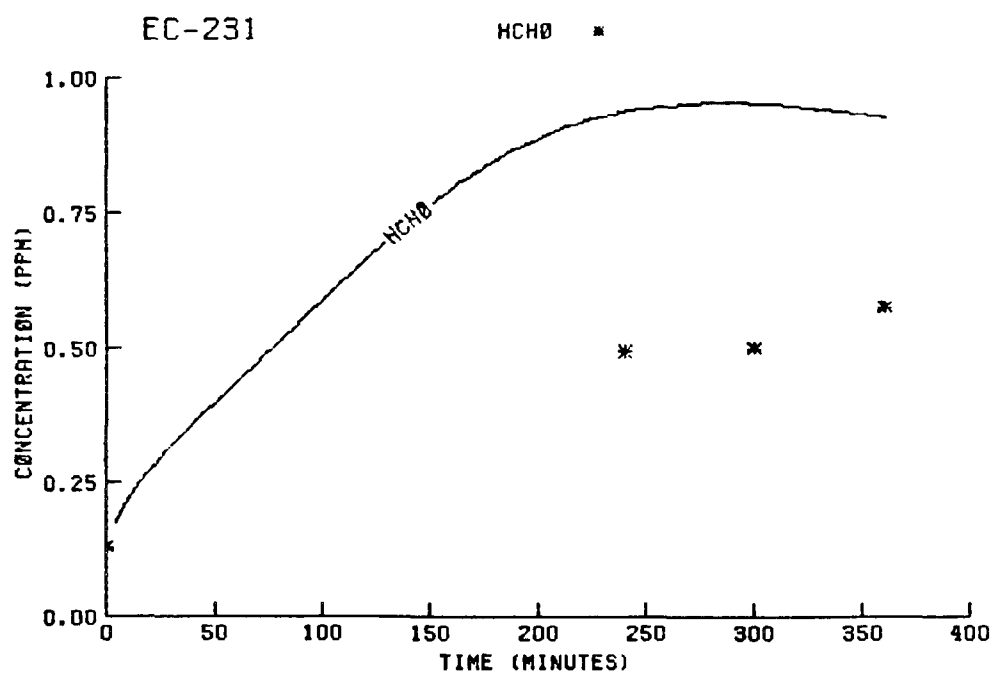


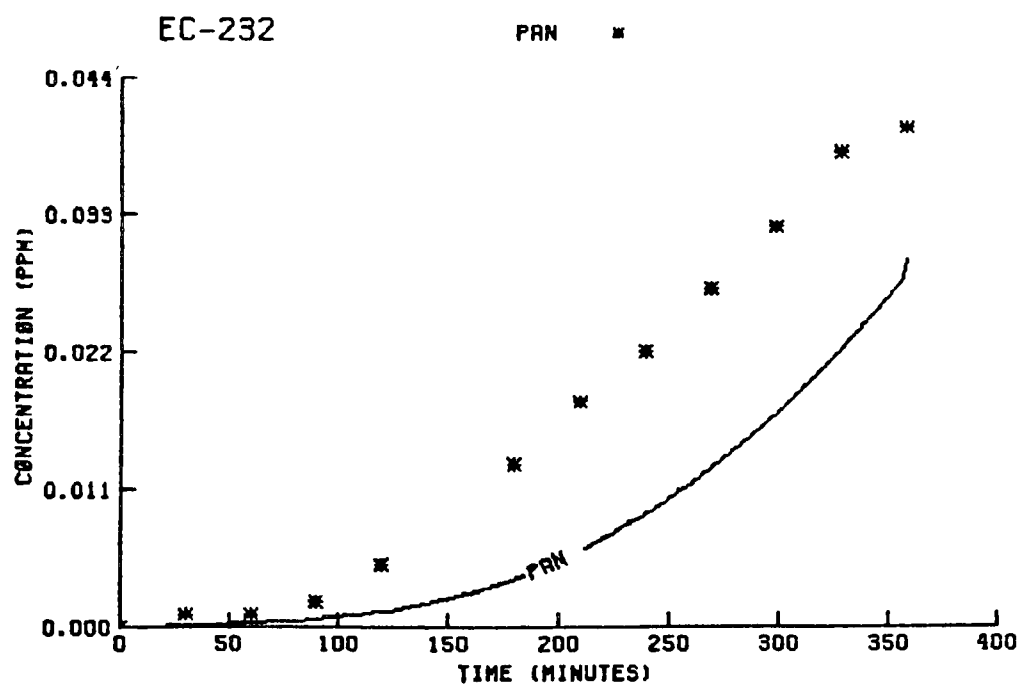
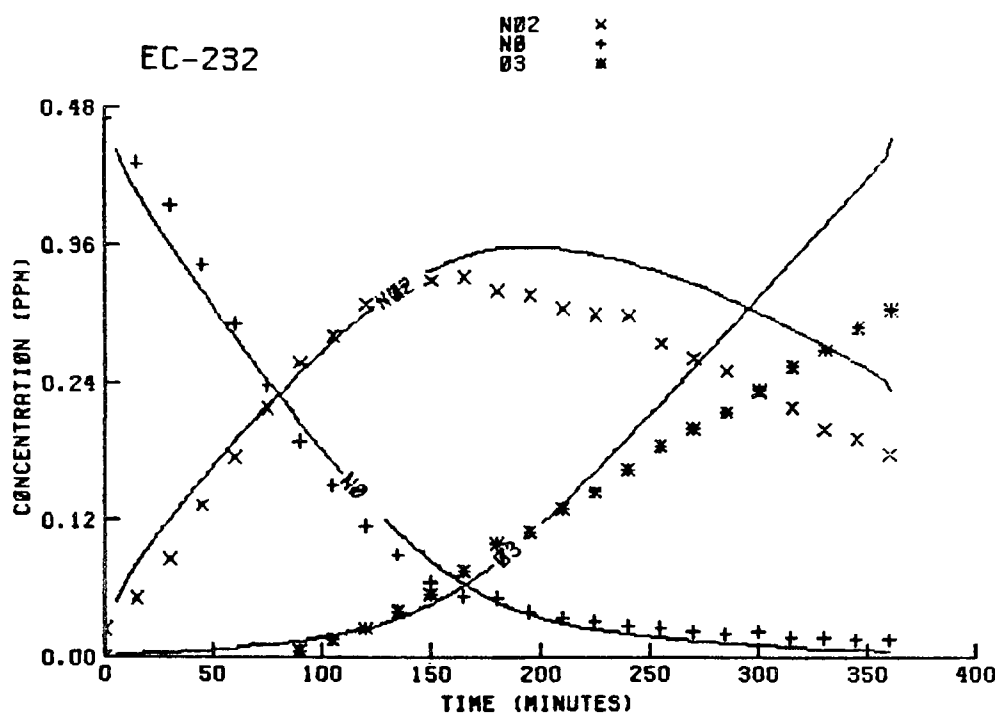
UCR SEVEN-HYDROCARBON EXPERIMENTS

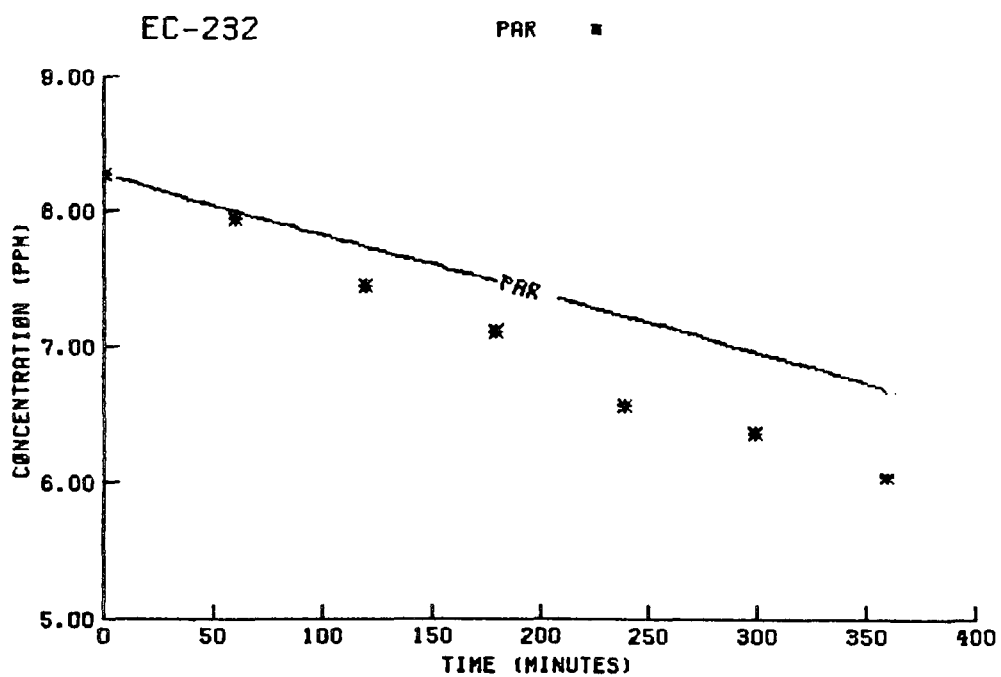
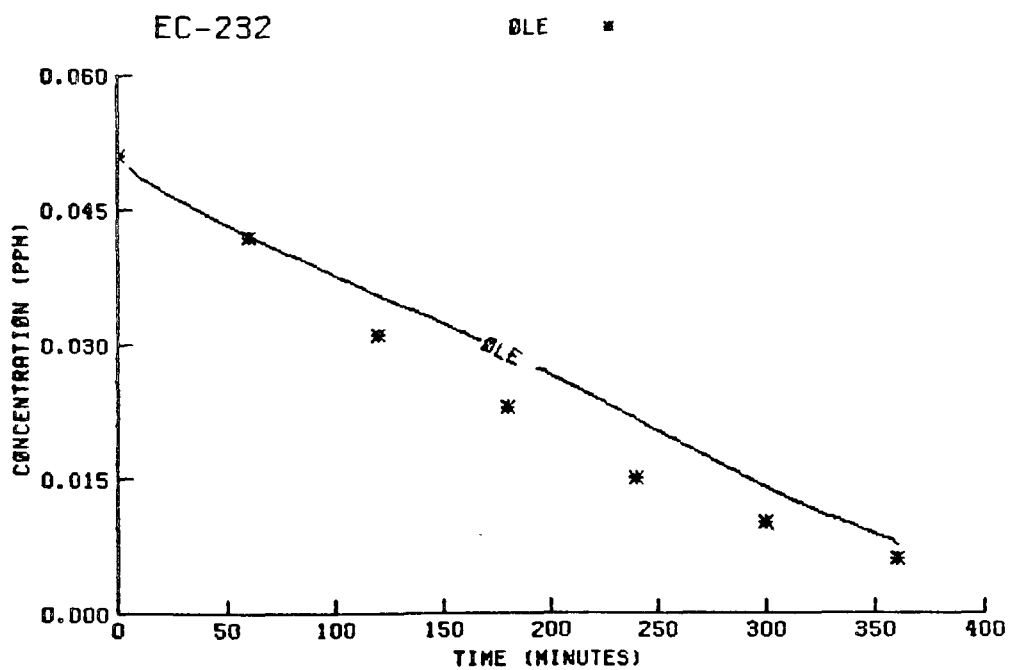


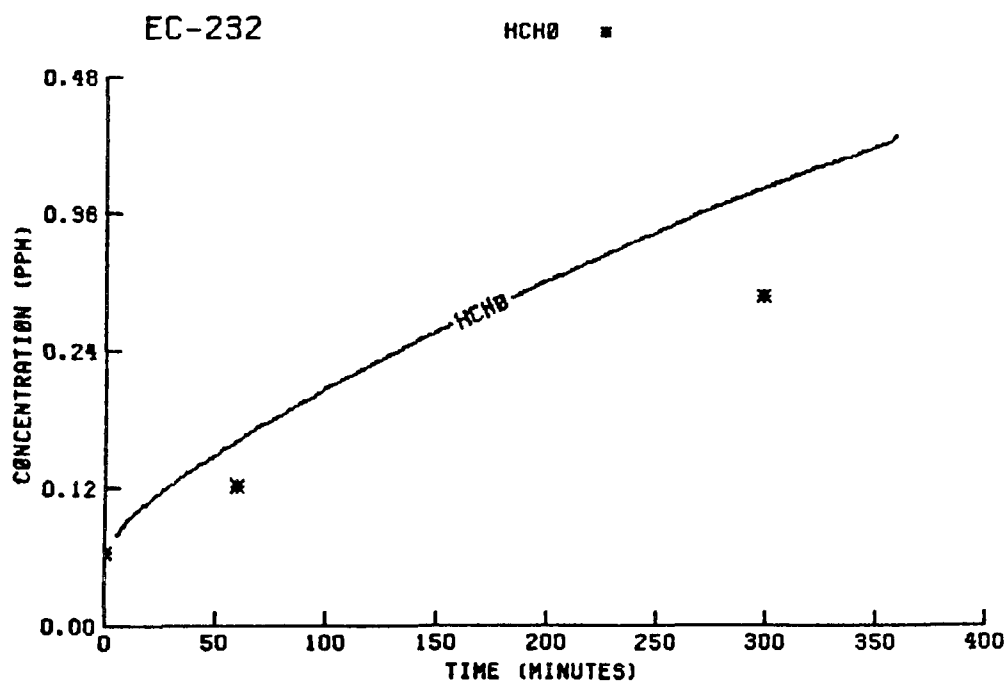
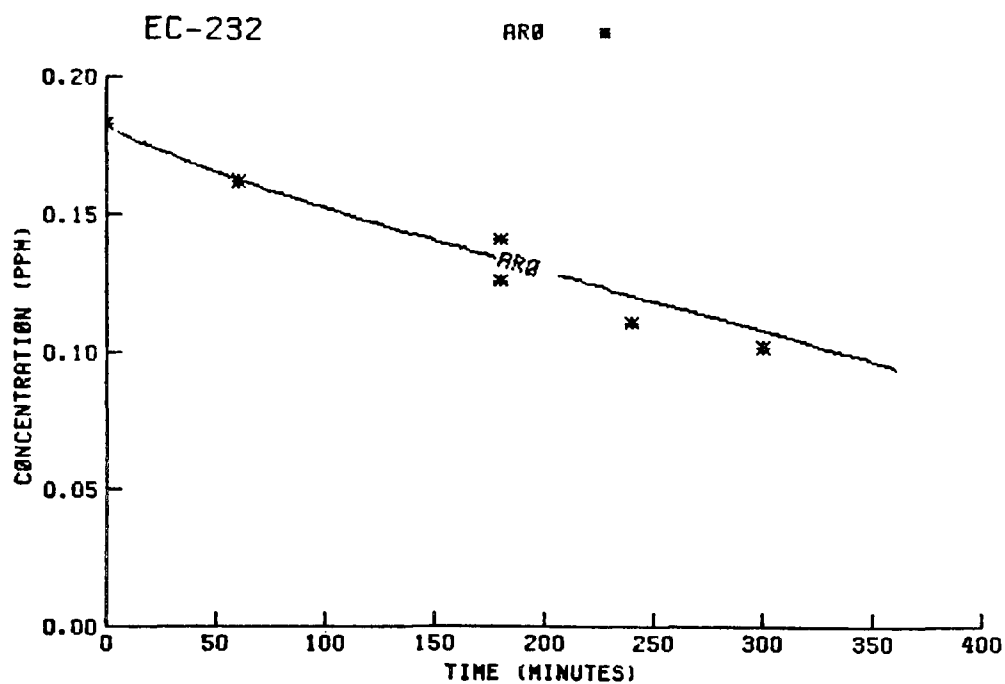






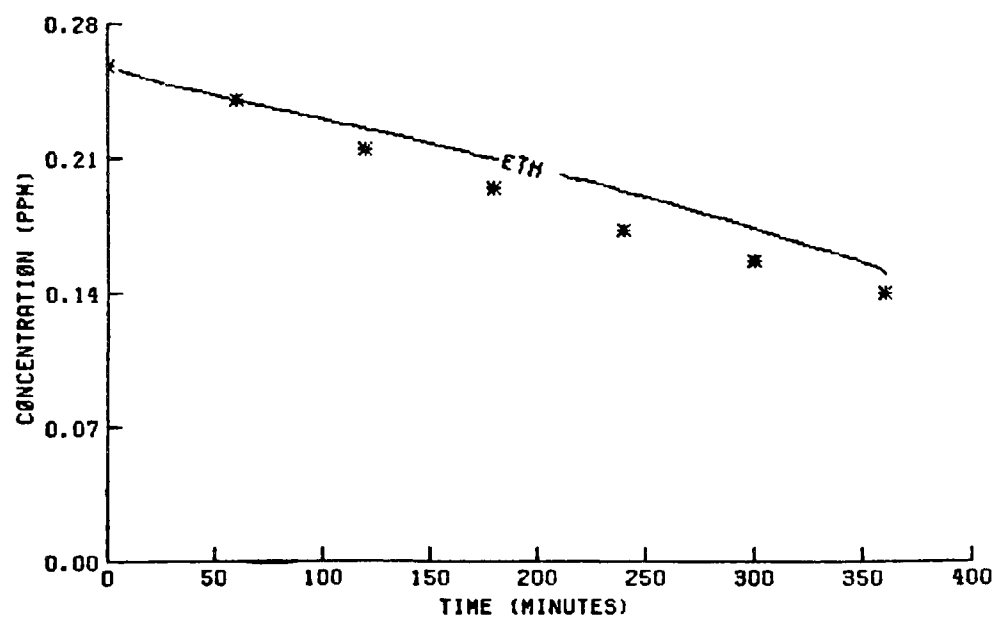






EC-232

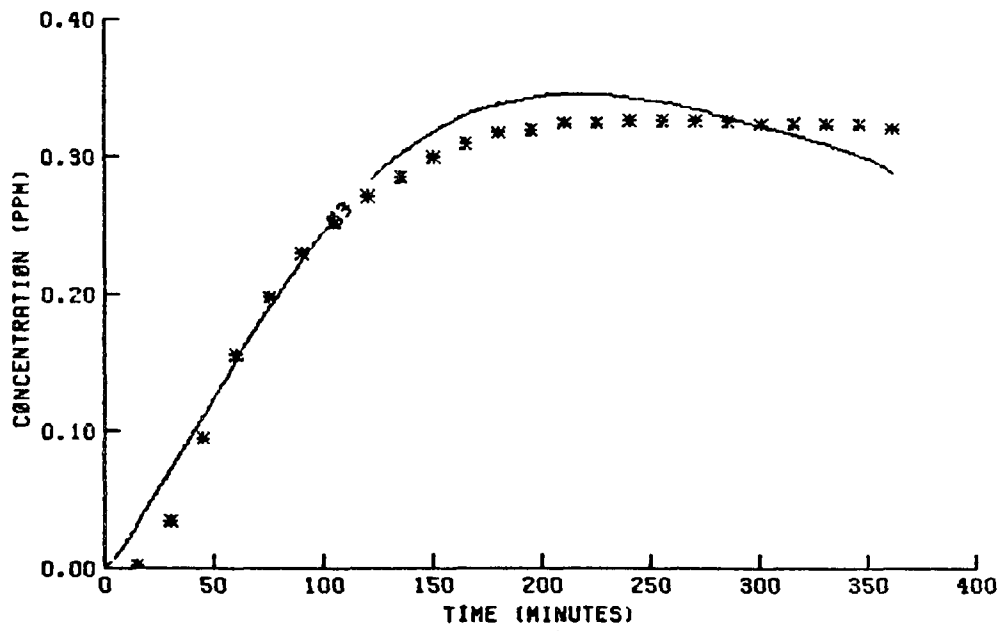
ETH *



EC-233

03

■



EC-233

PAN

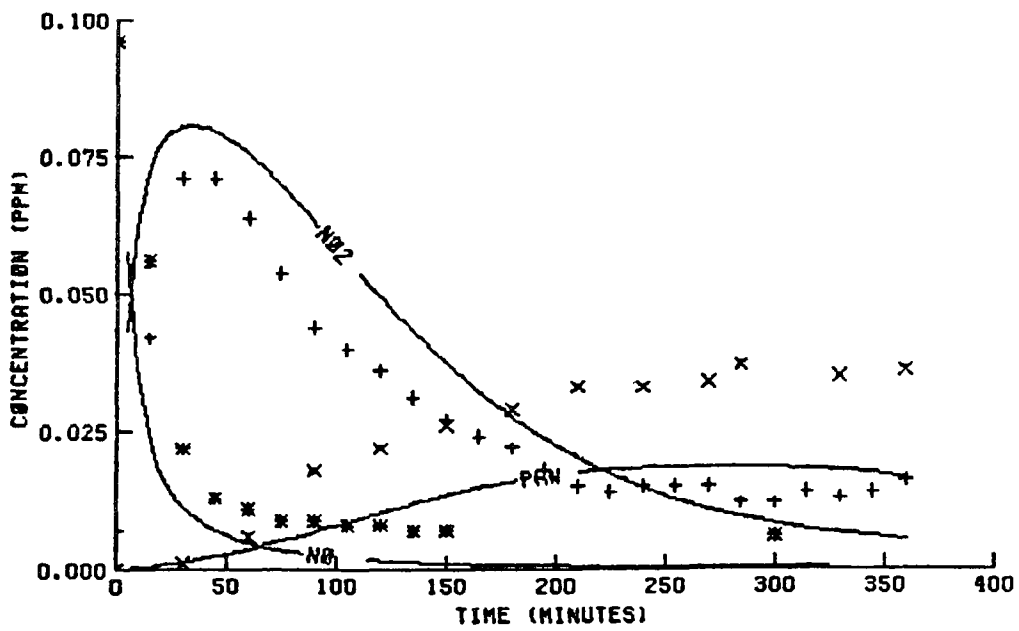
x

N02

+

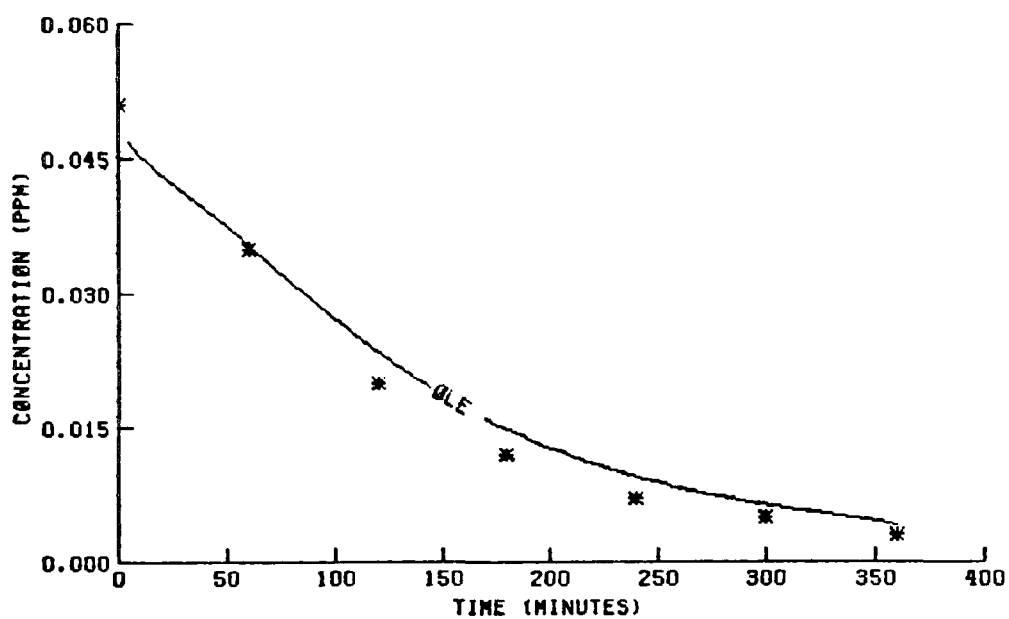
N0

■



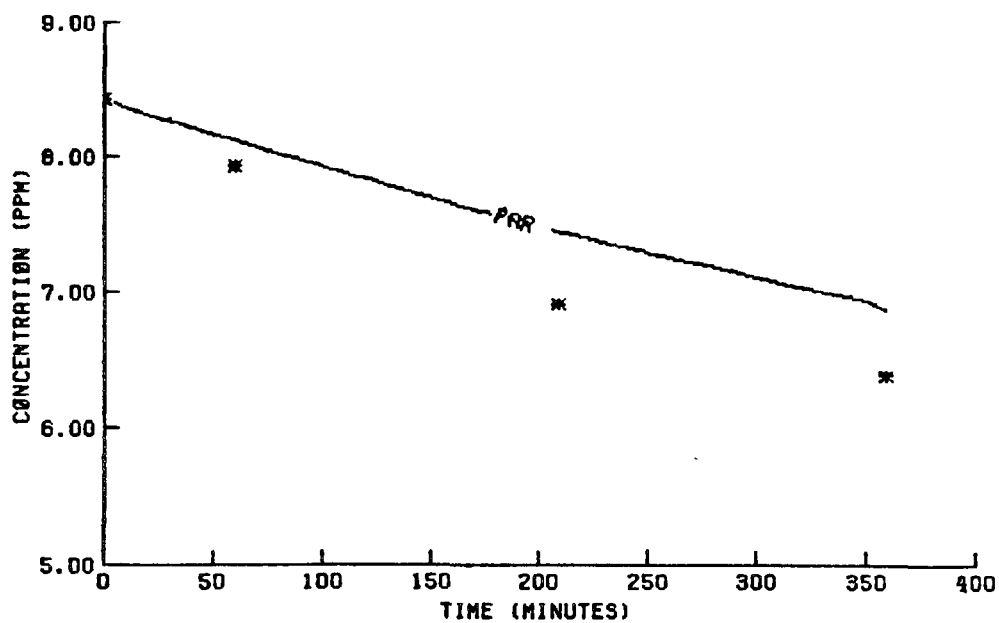
EC-233

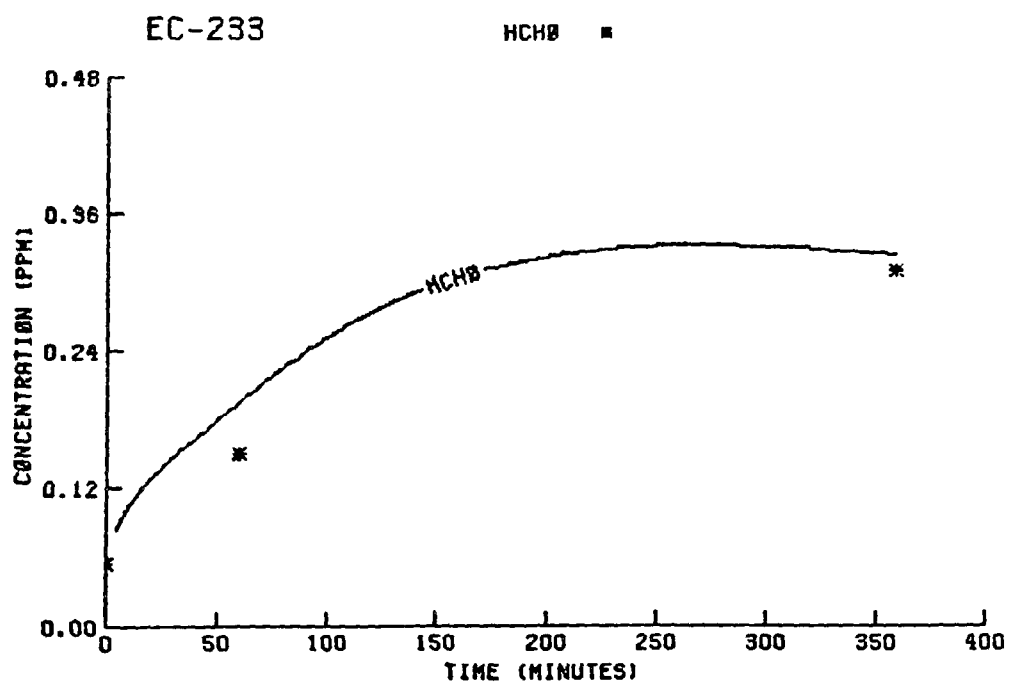
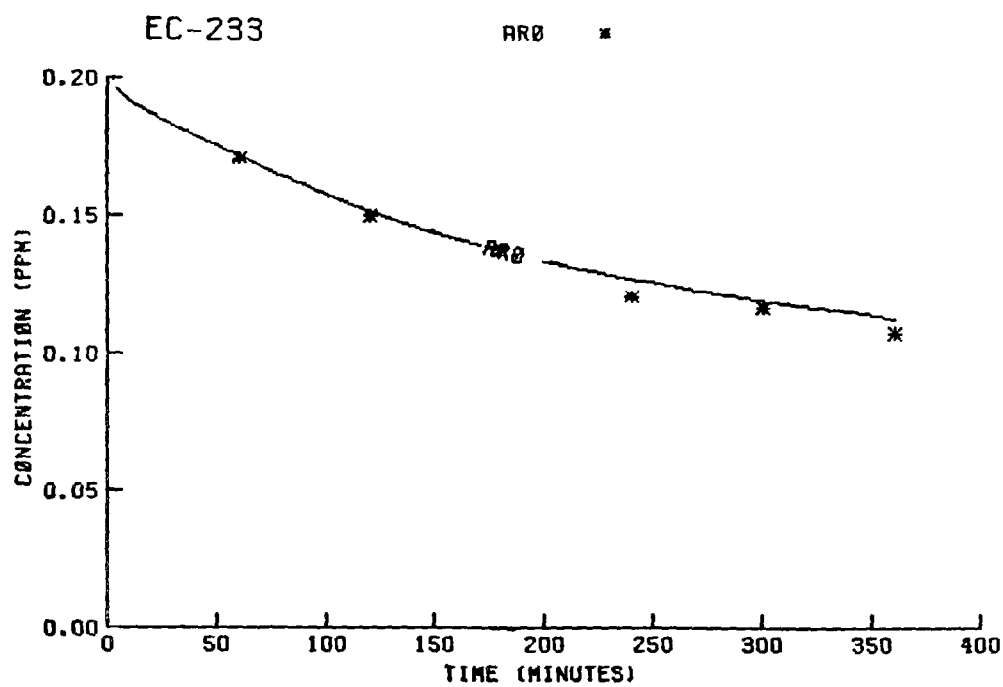
BLE *



EC-233

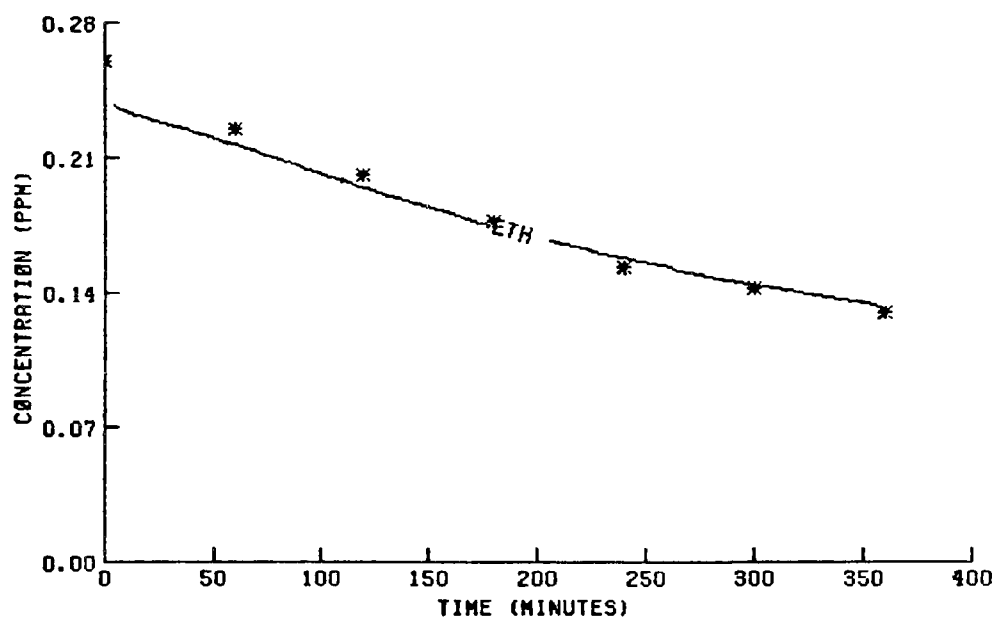
PAR *

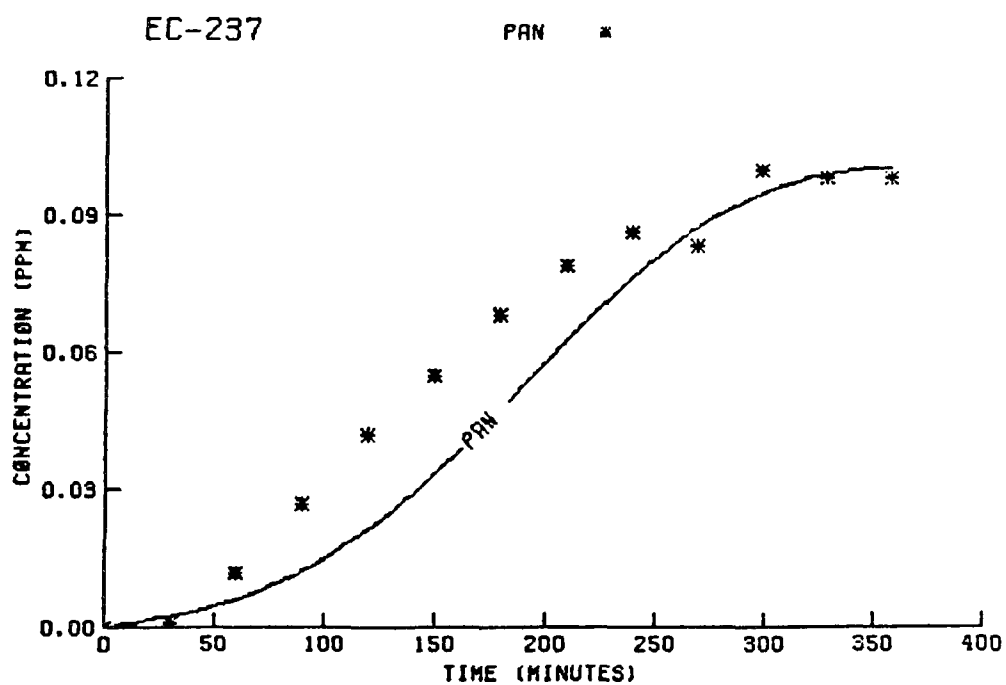
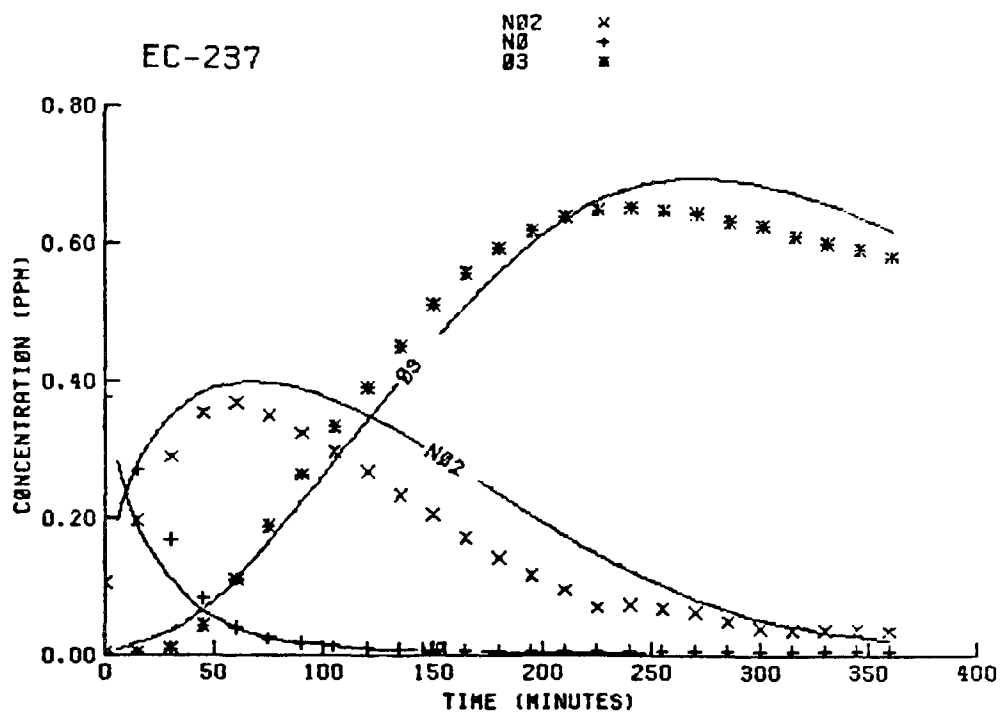


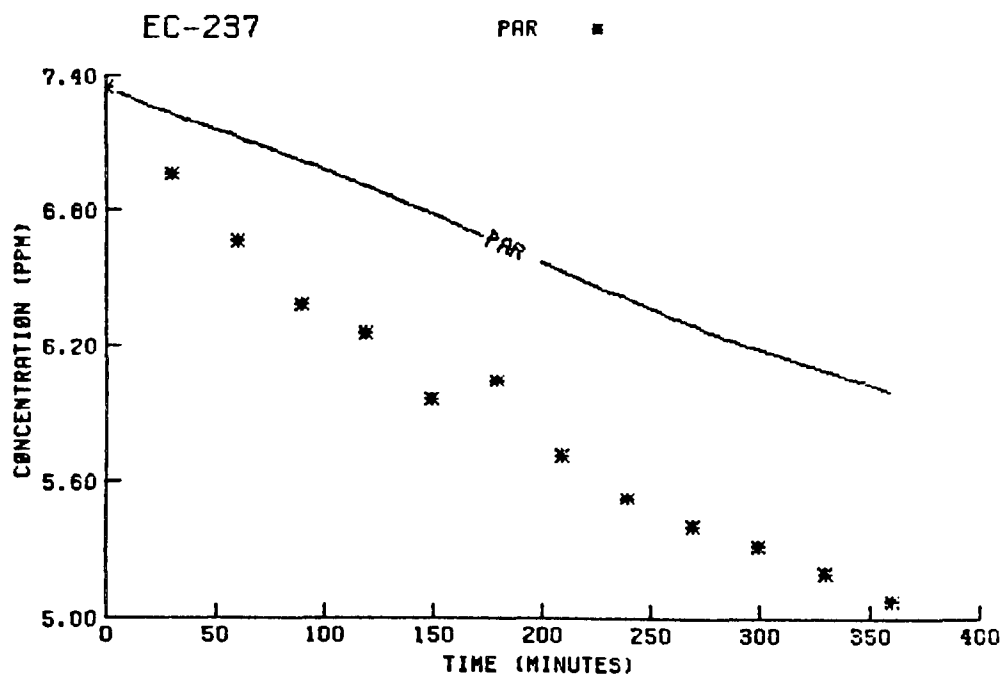
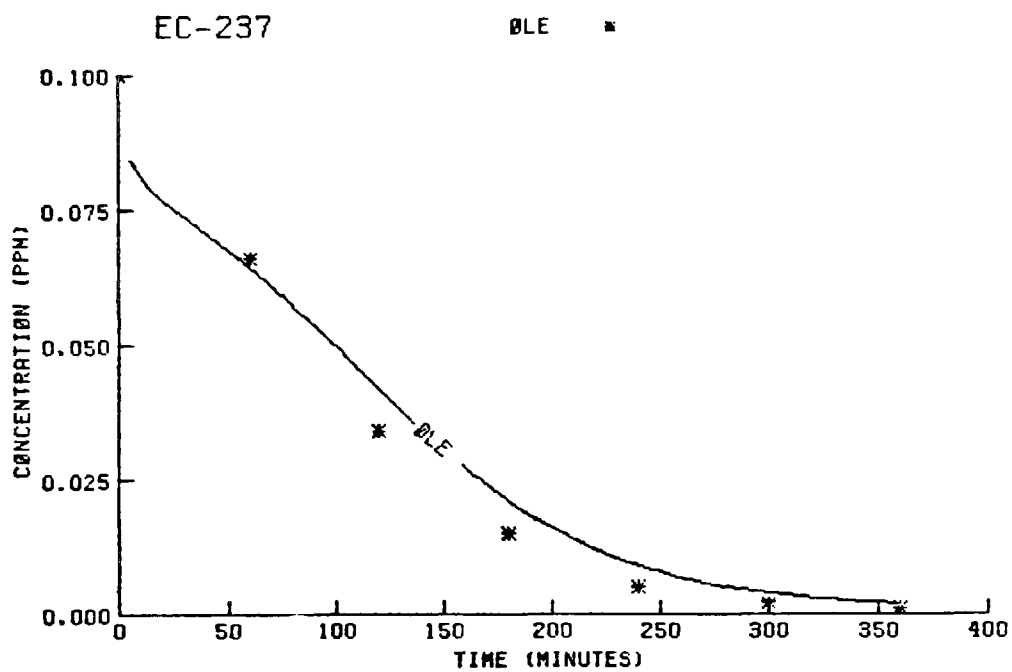


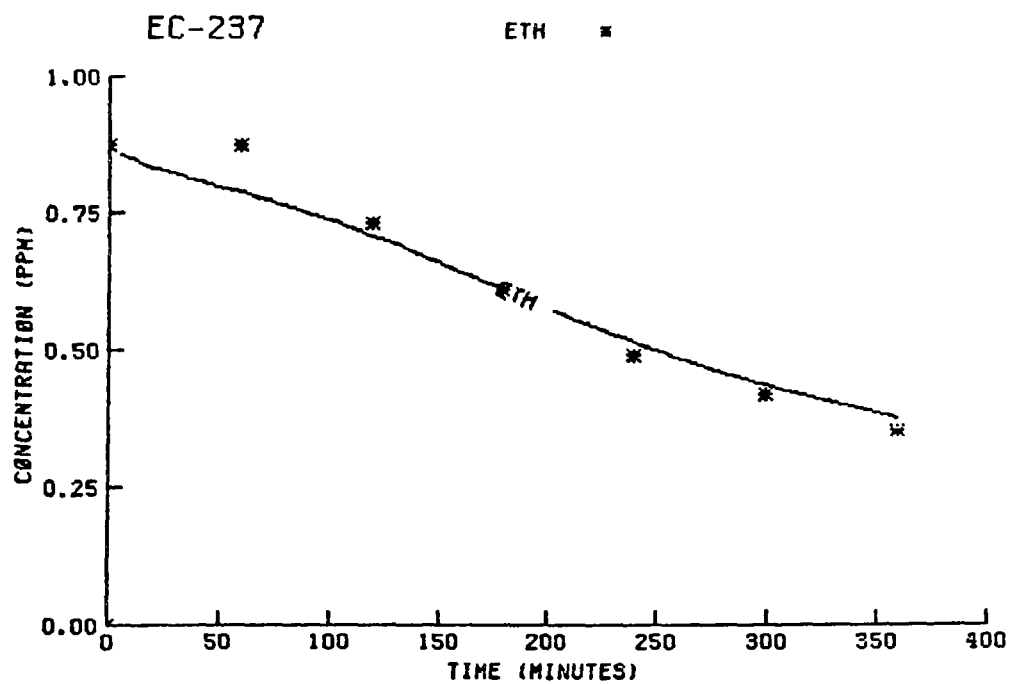
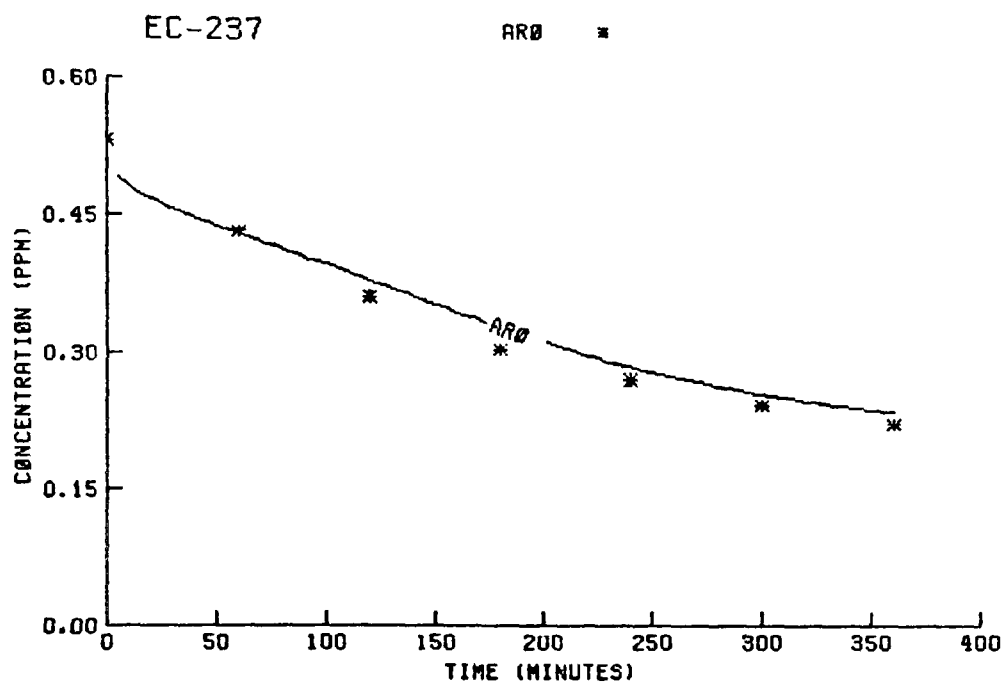
EC-233

ETH *



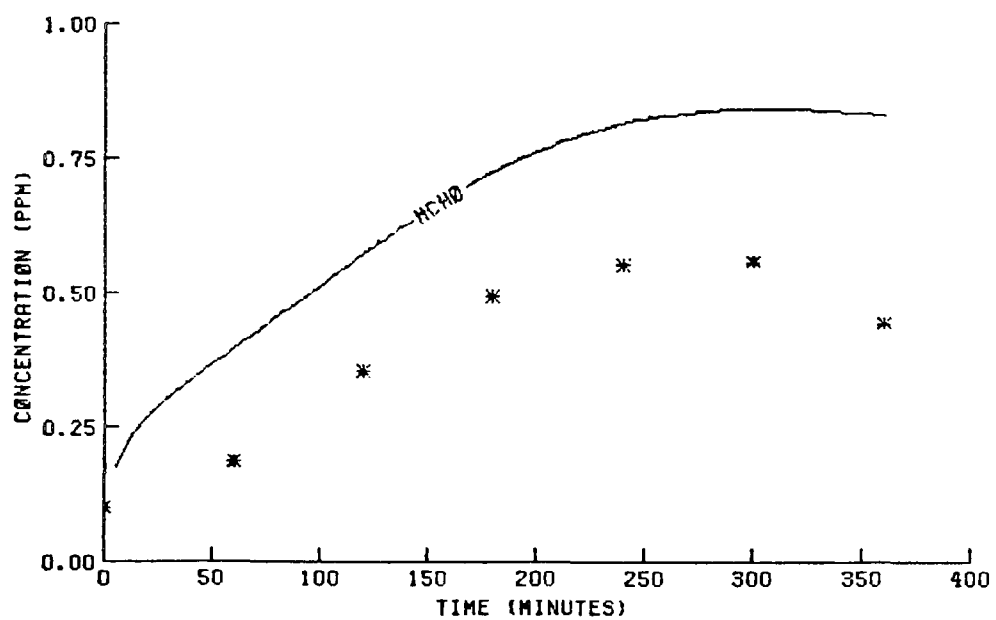


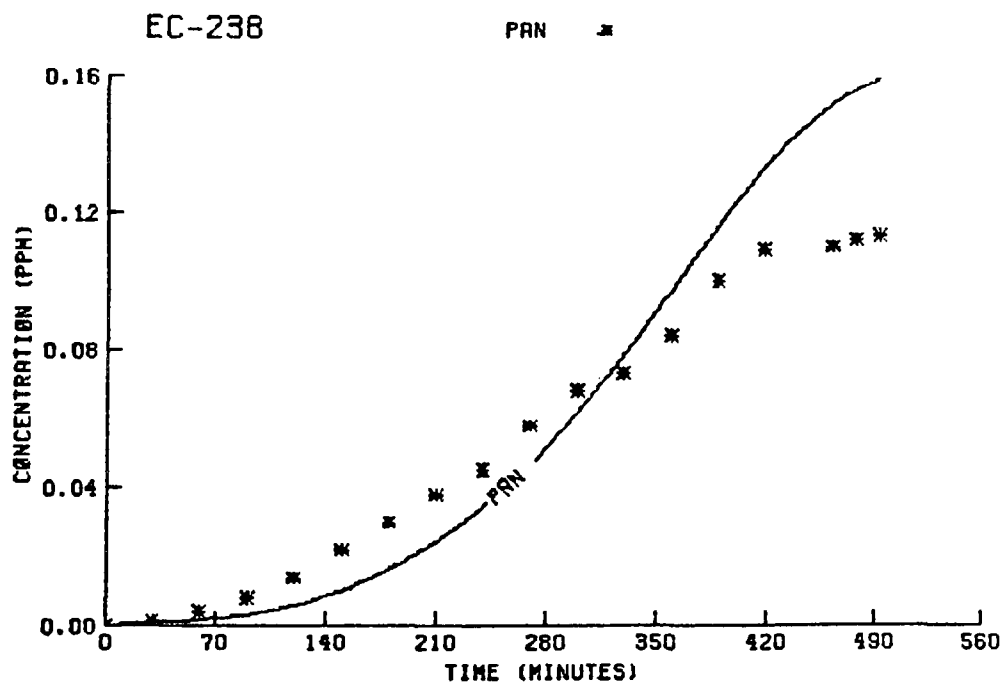
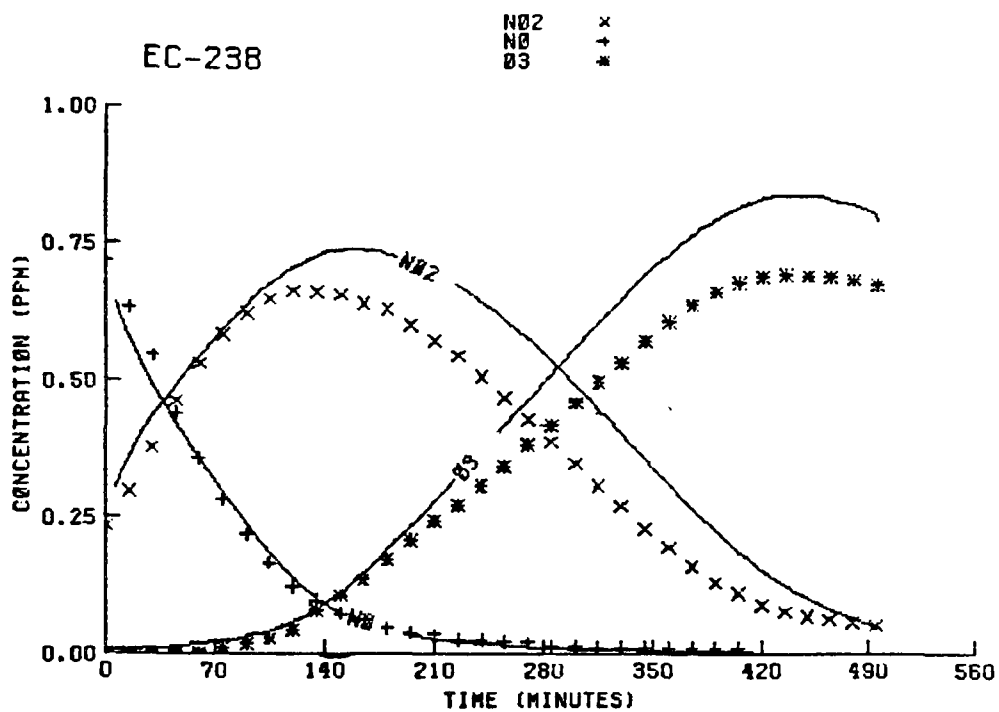


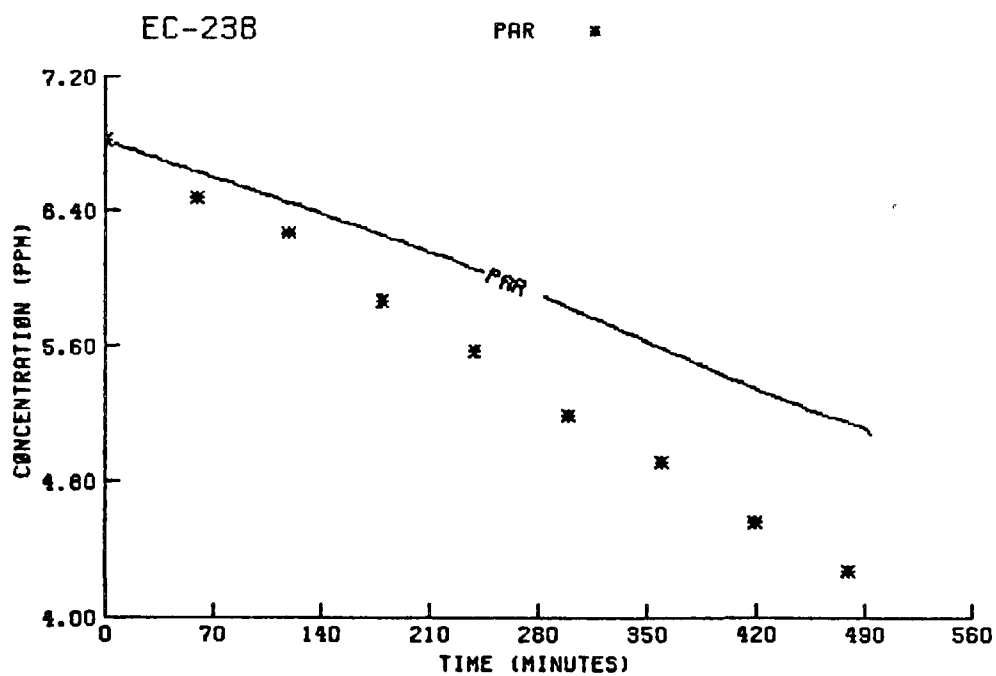
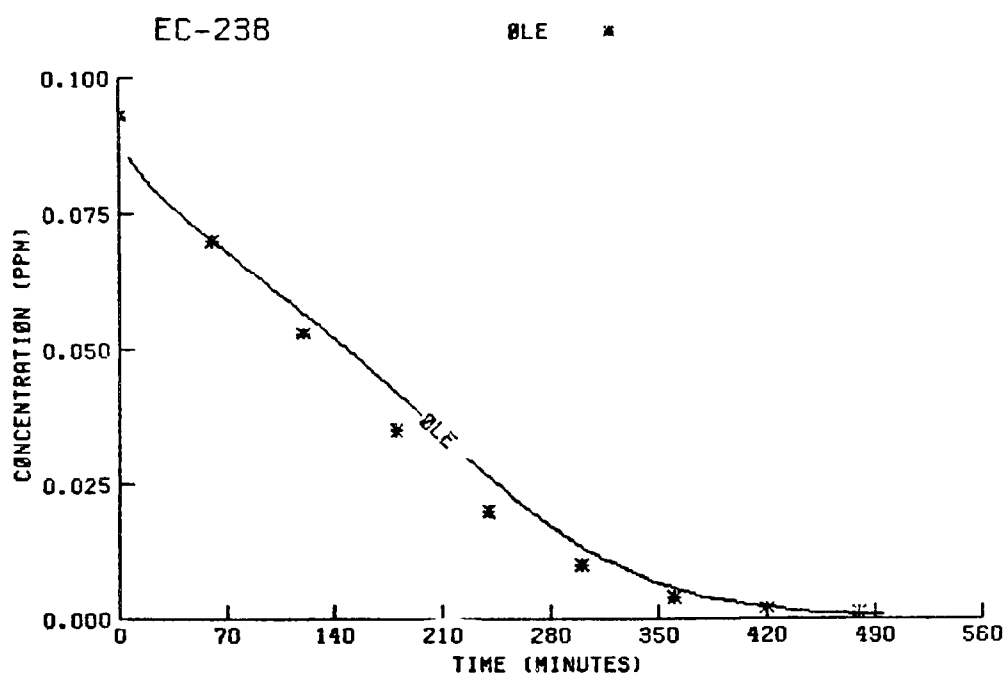


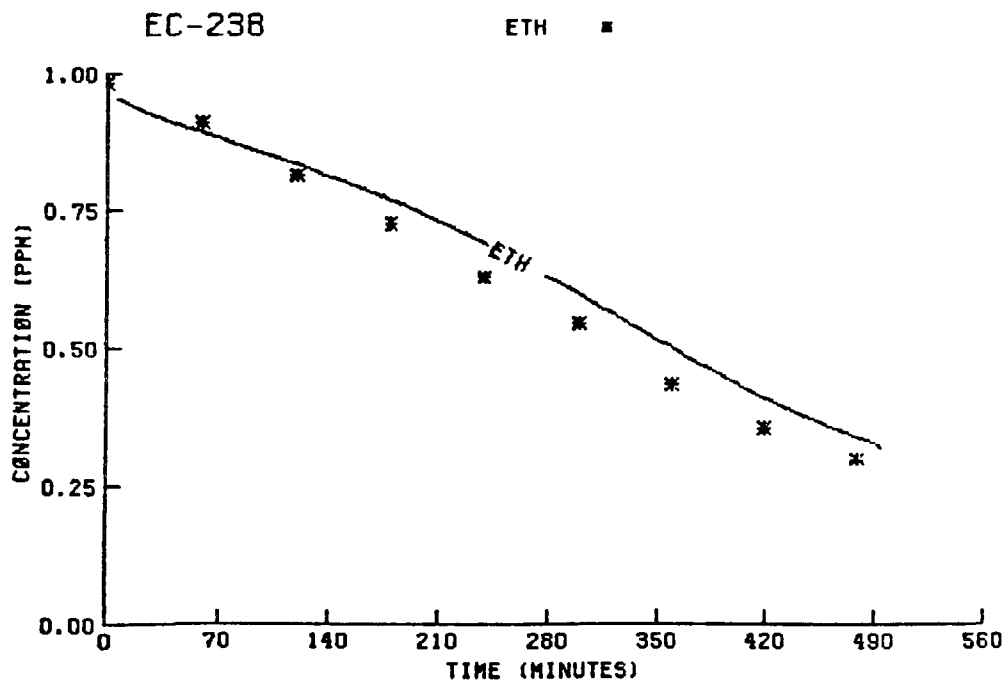
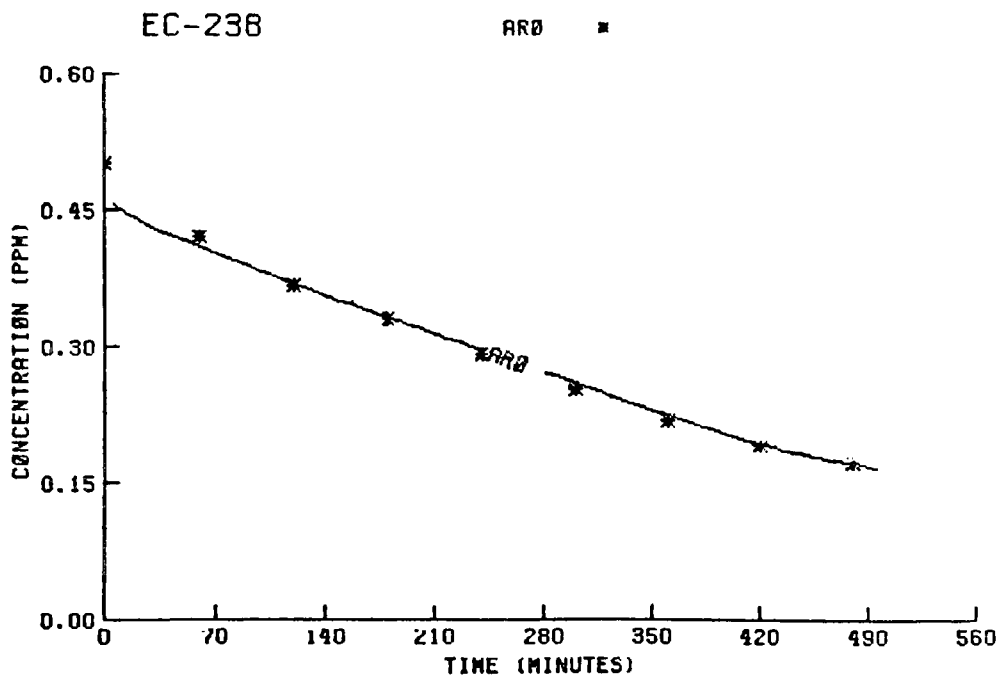
EC-237

HCHO *



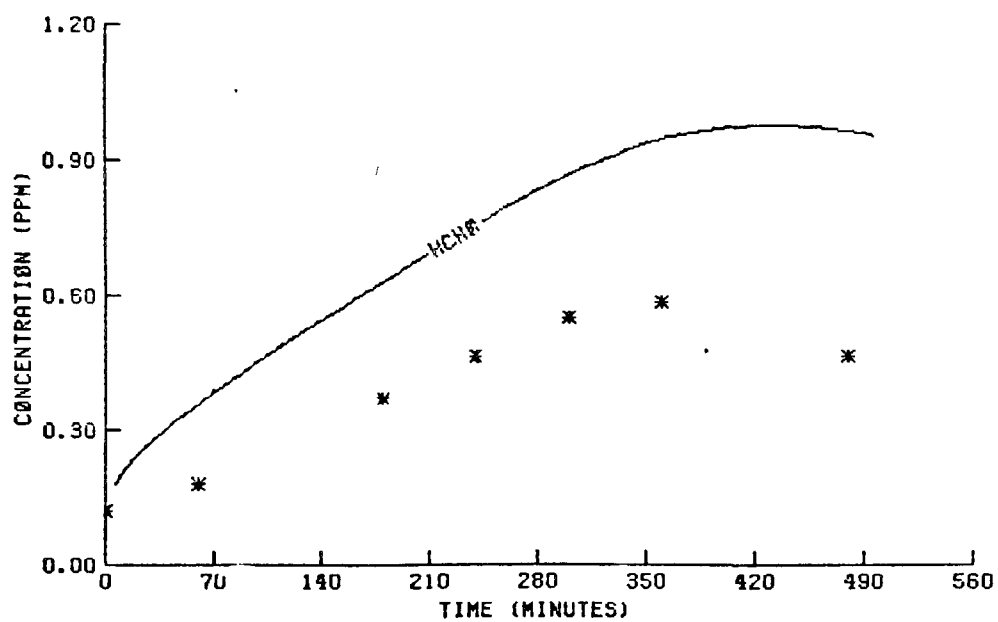






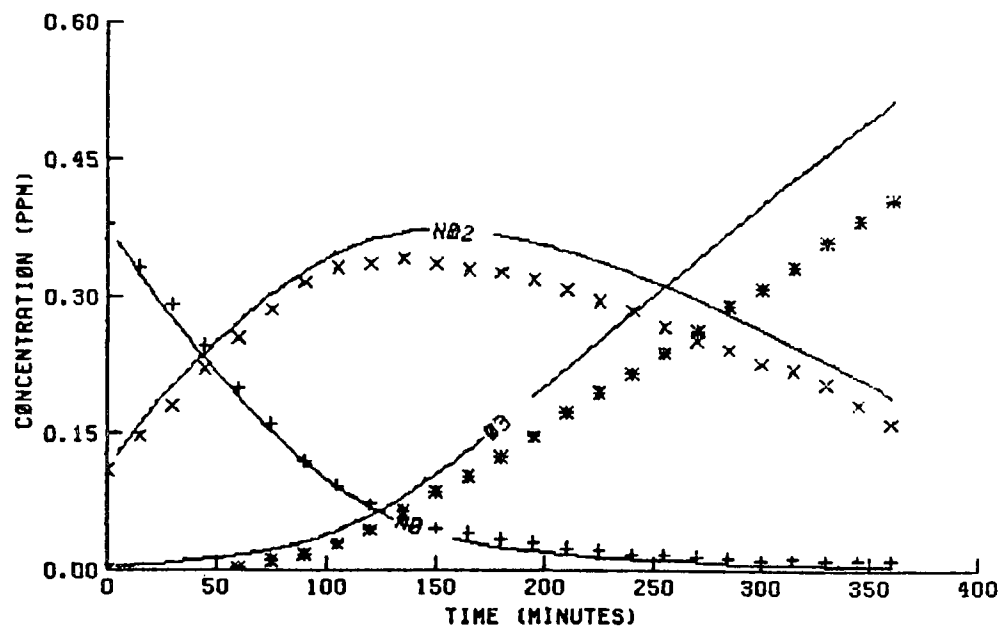
EC-238

HCHO *



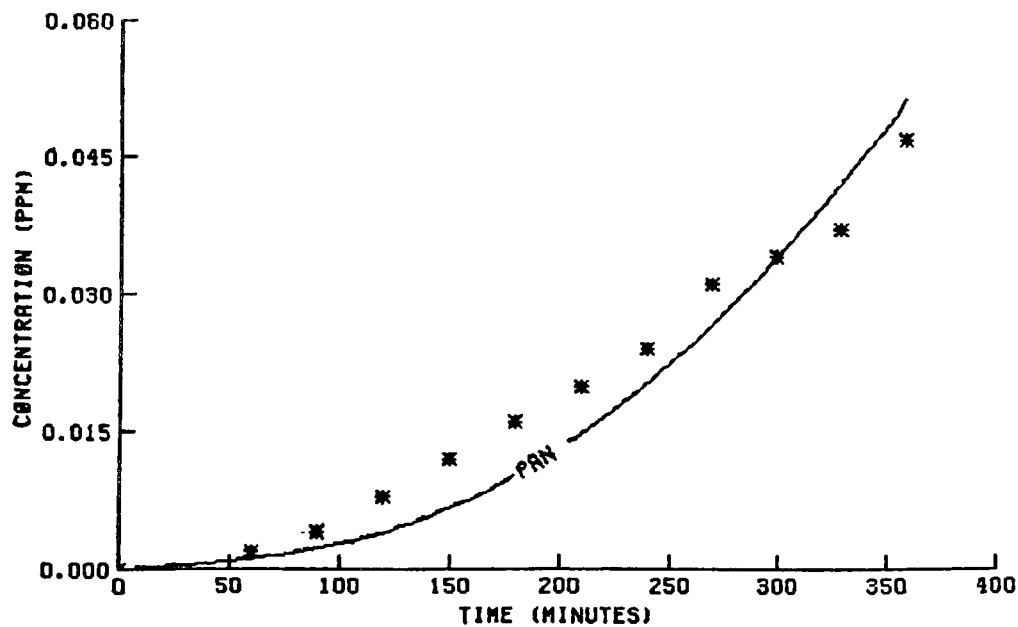
EC-241

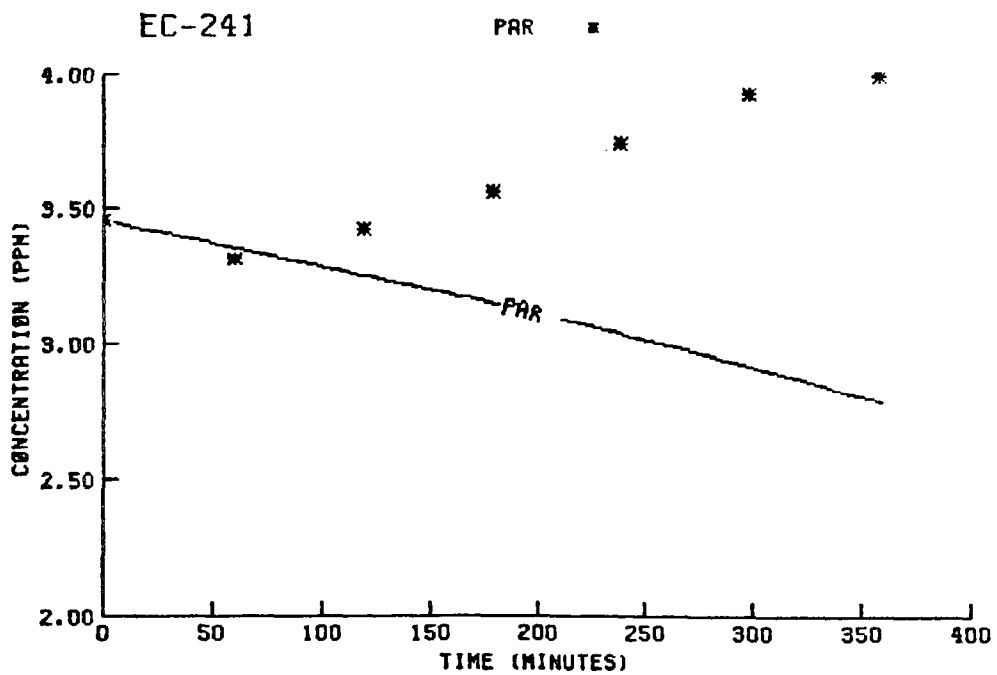
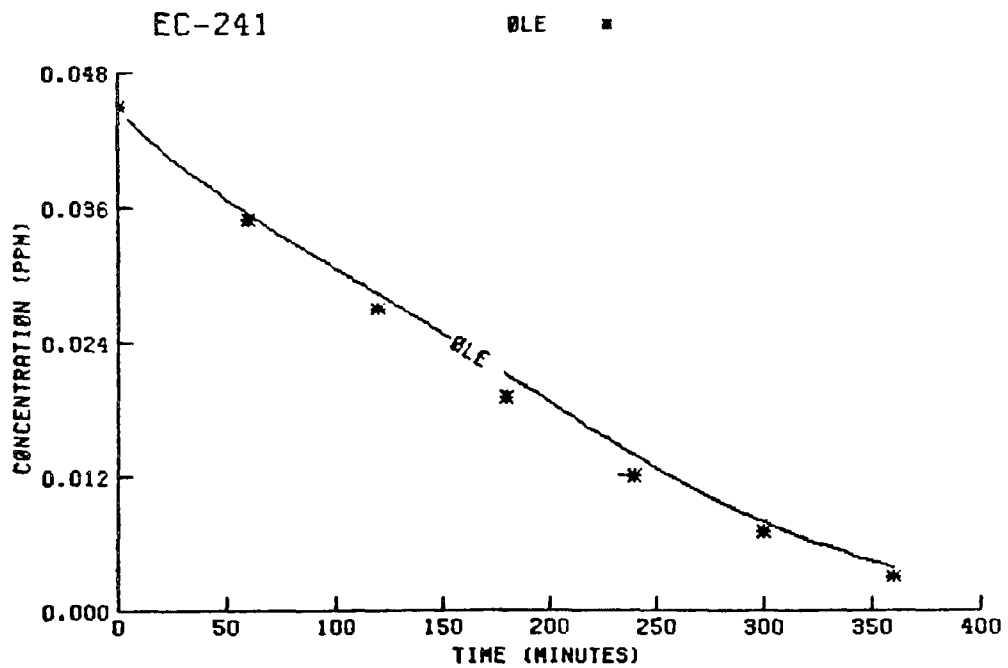
NO2 x
 NO +
 O3 *

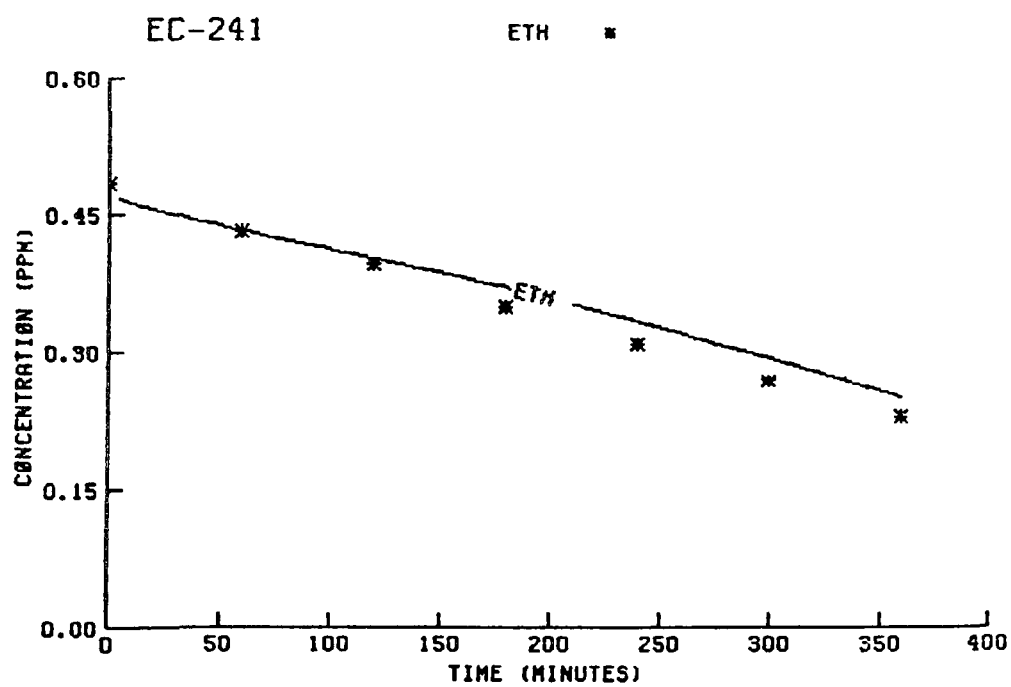
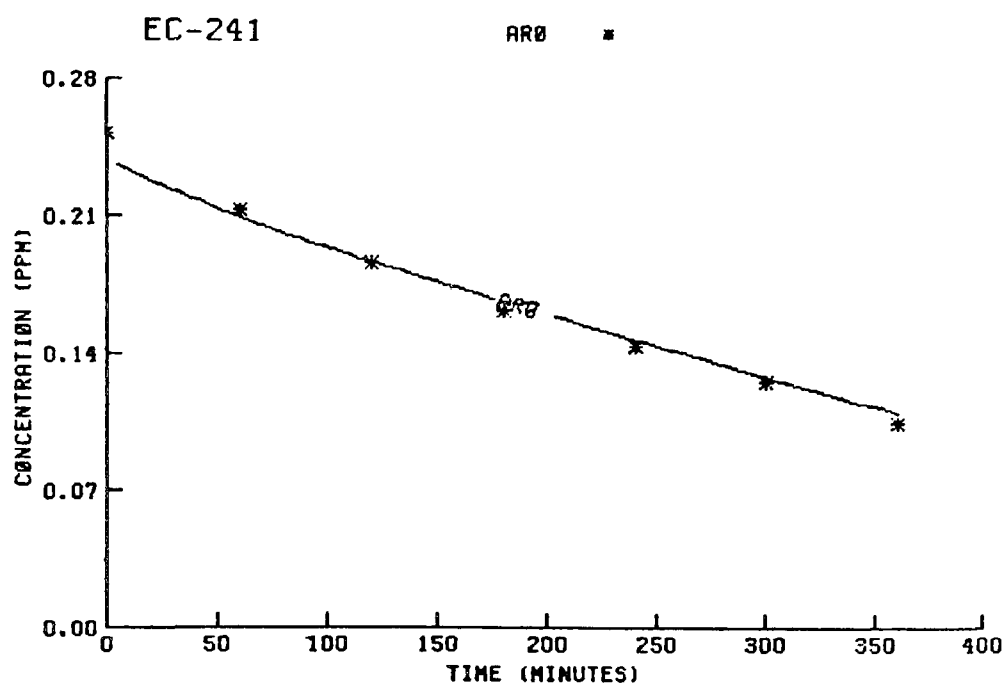


EC-241

PAN *

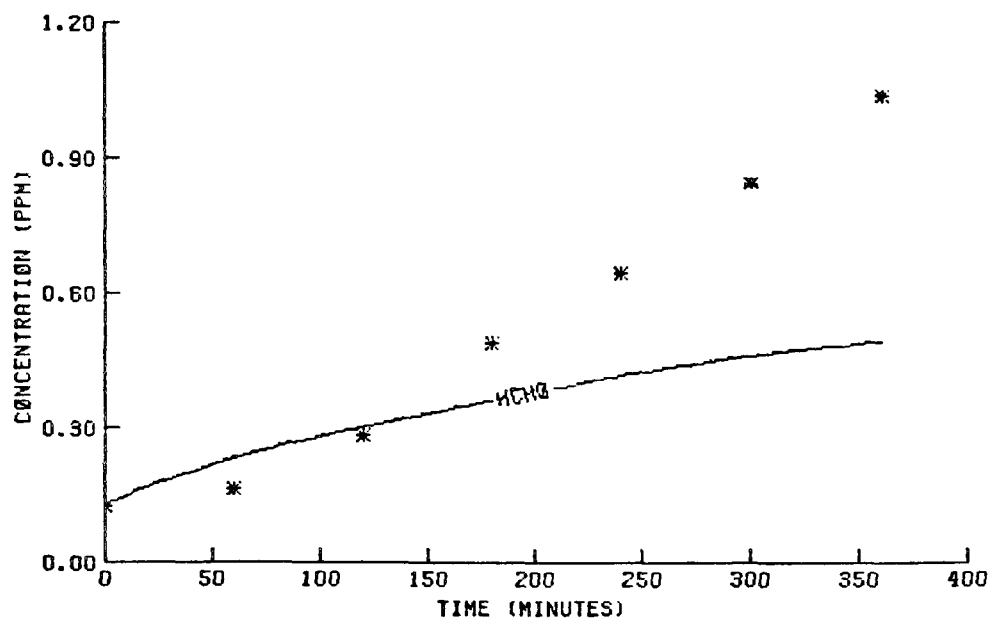


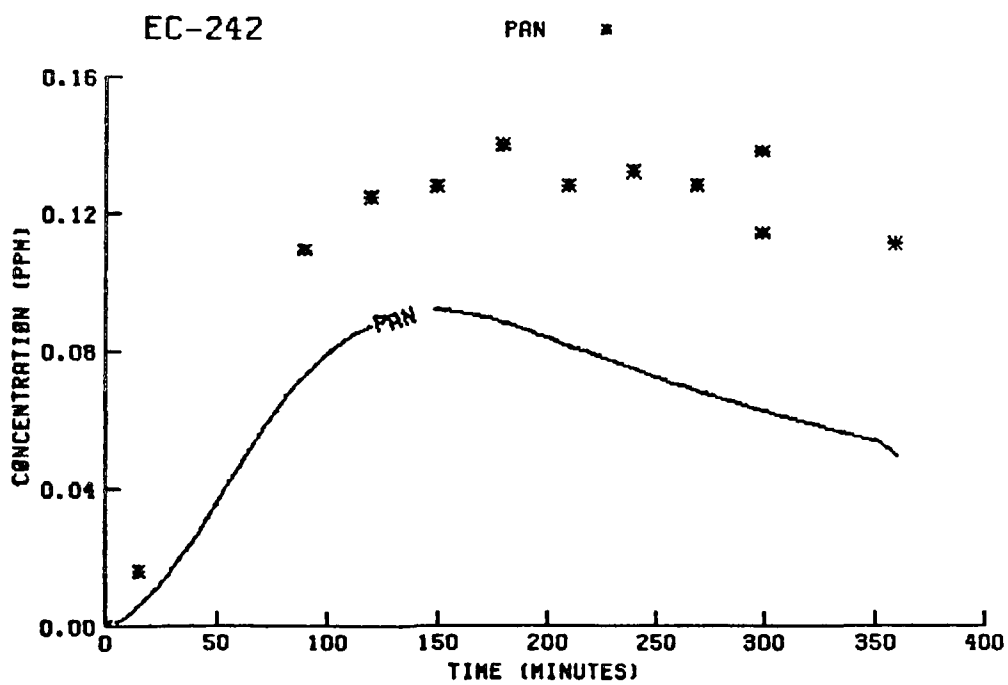
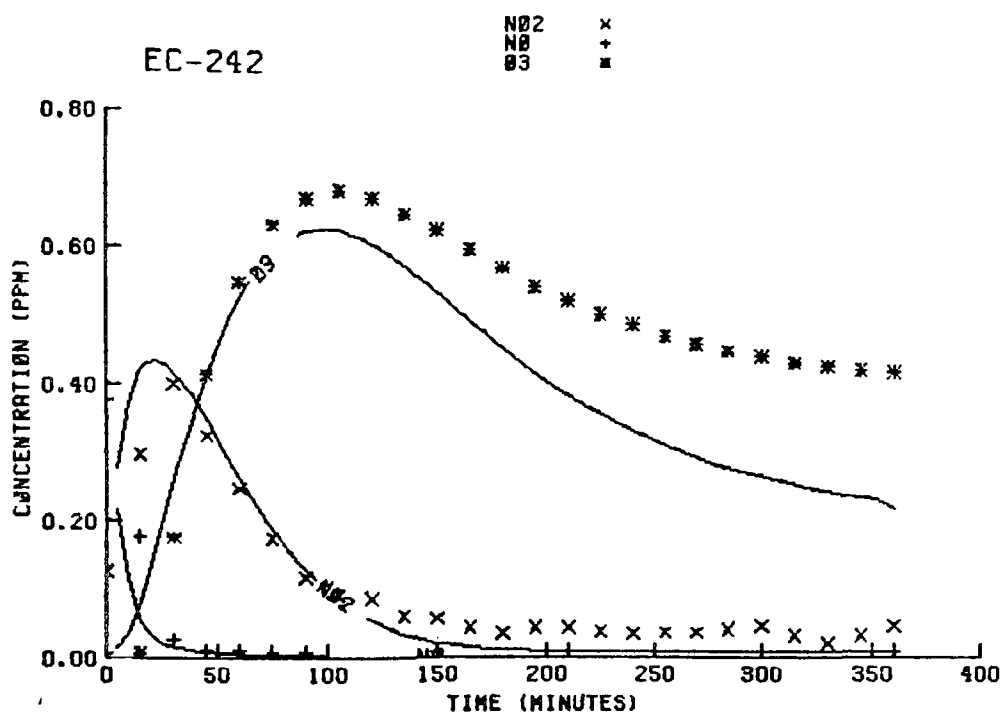


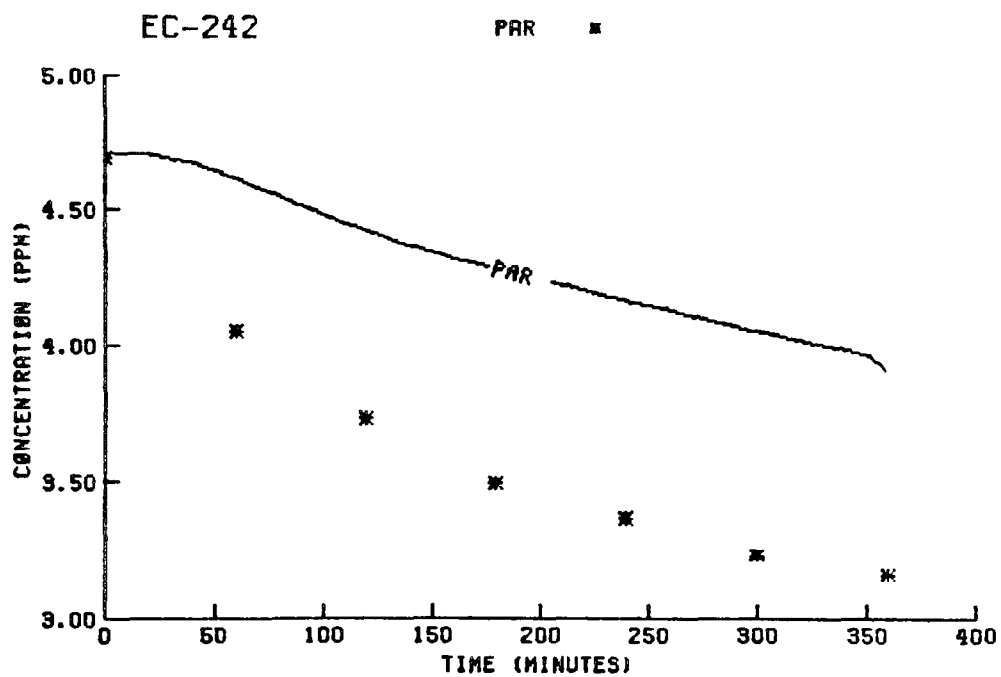
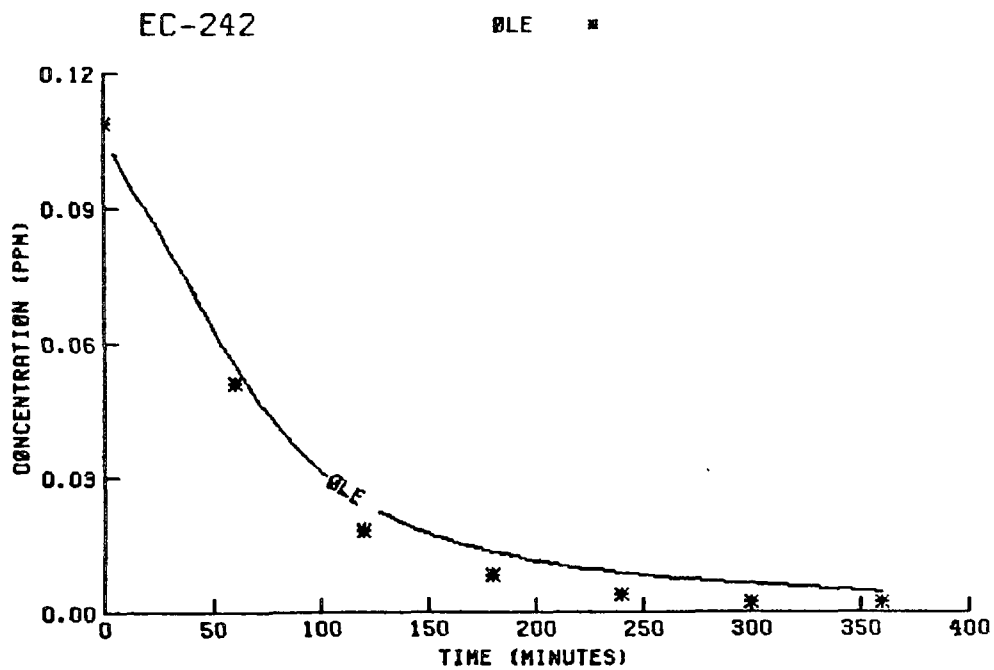


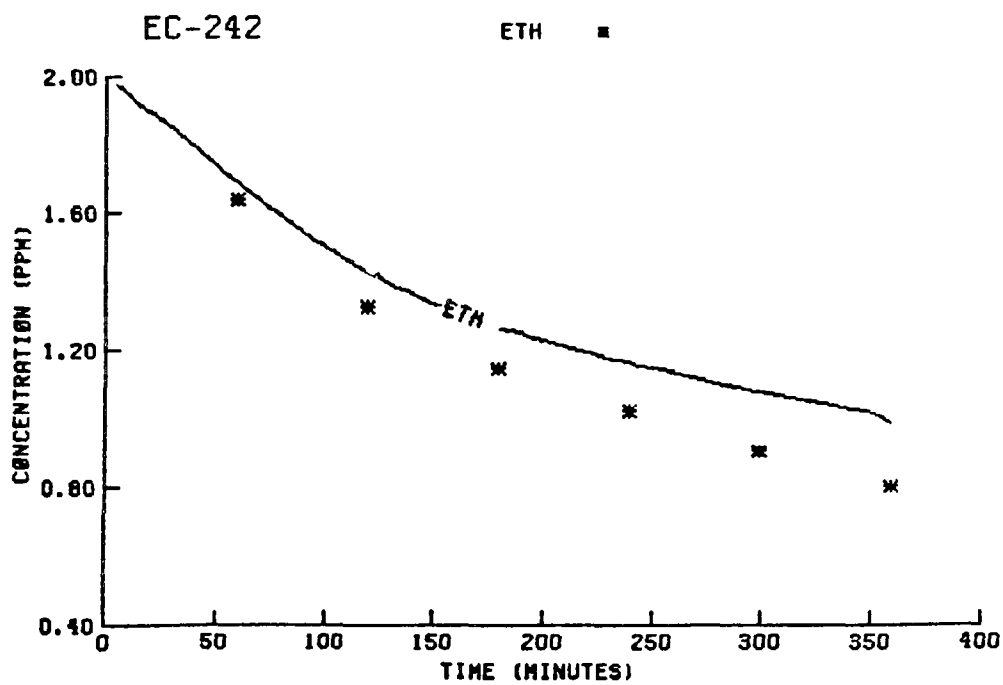
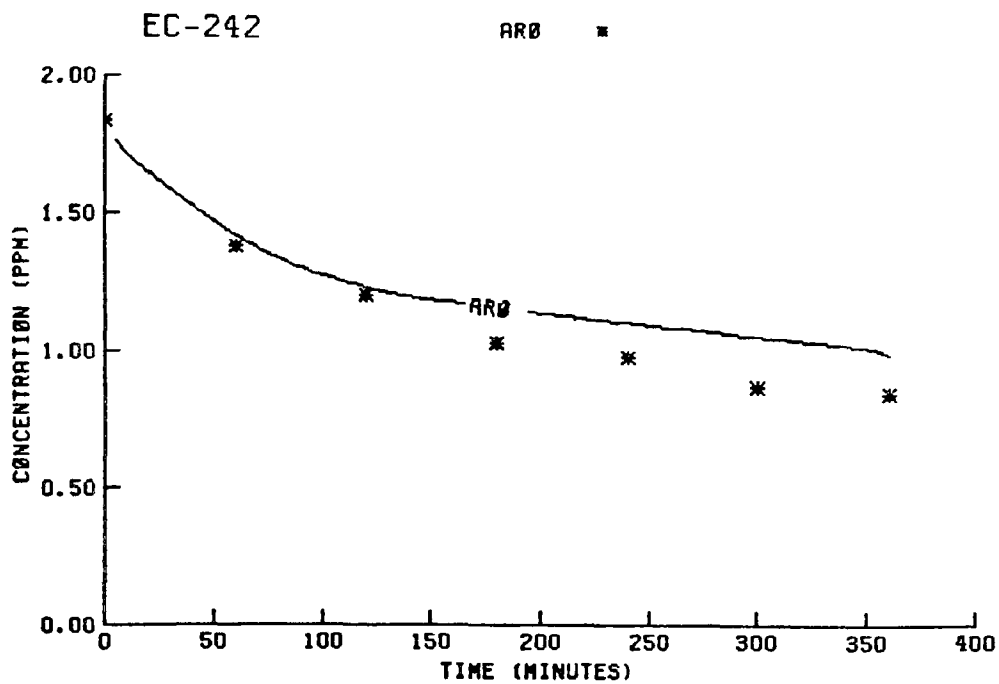
EC-241

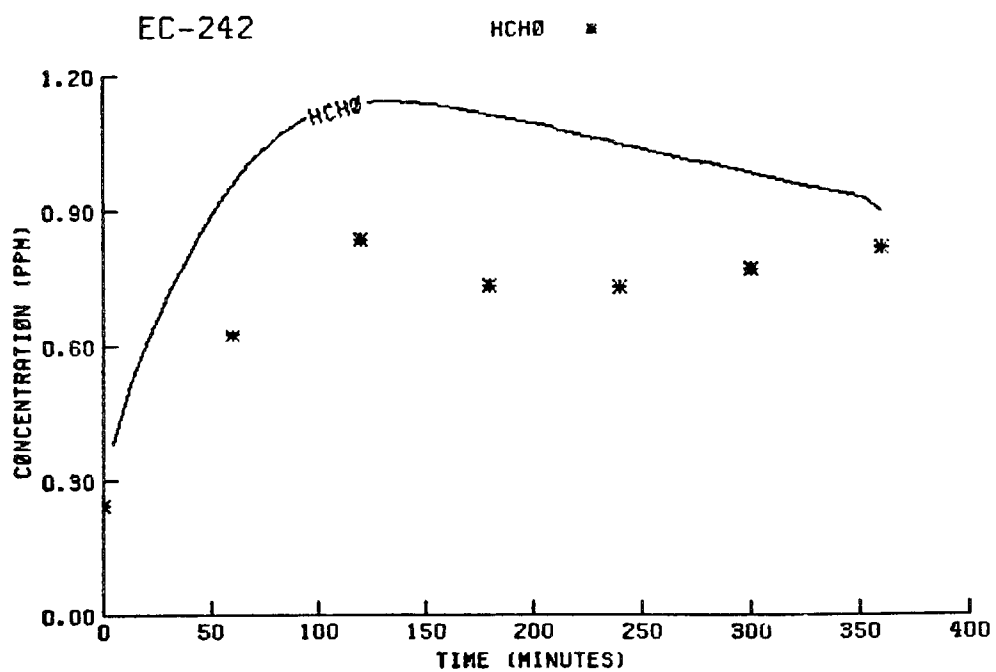
HCHO *

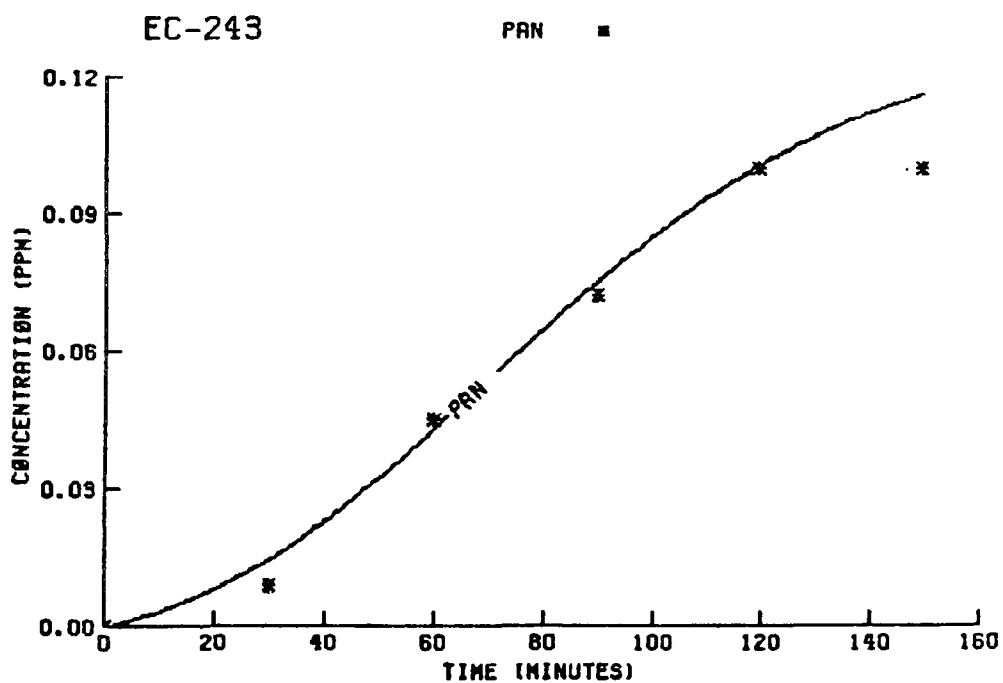
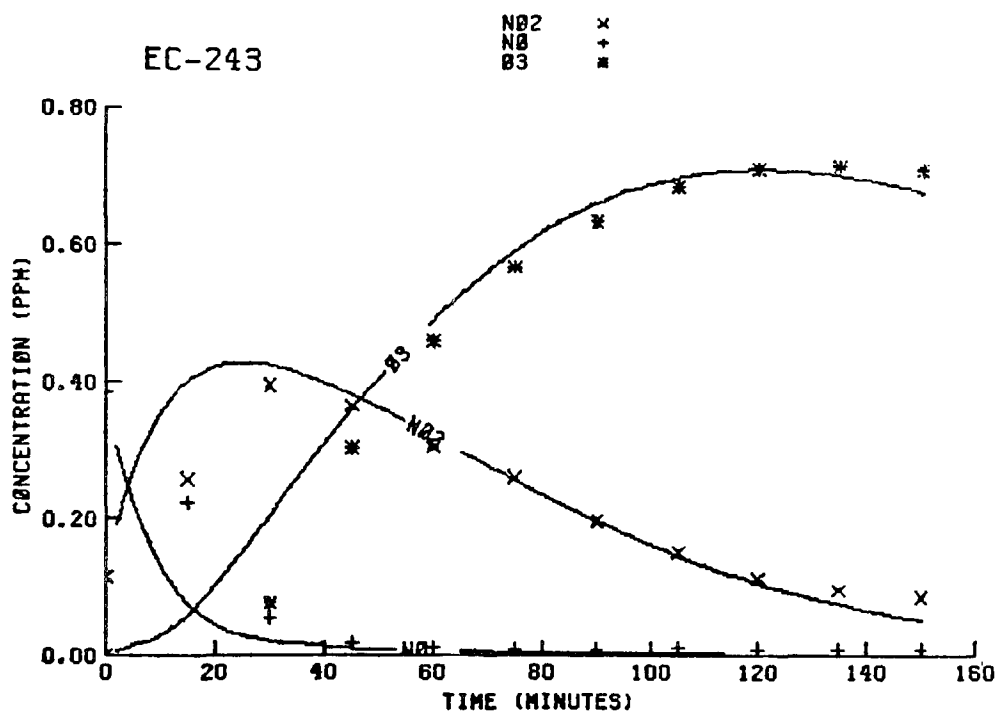


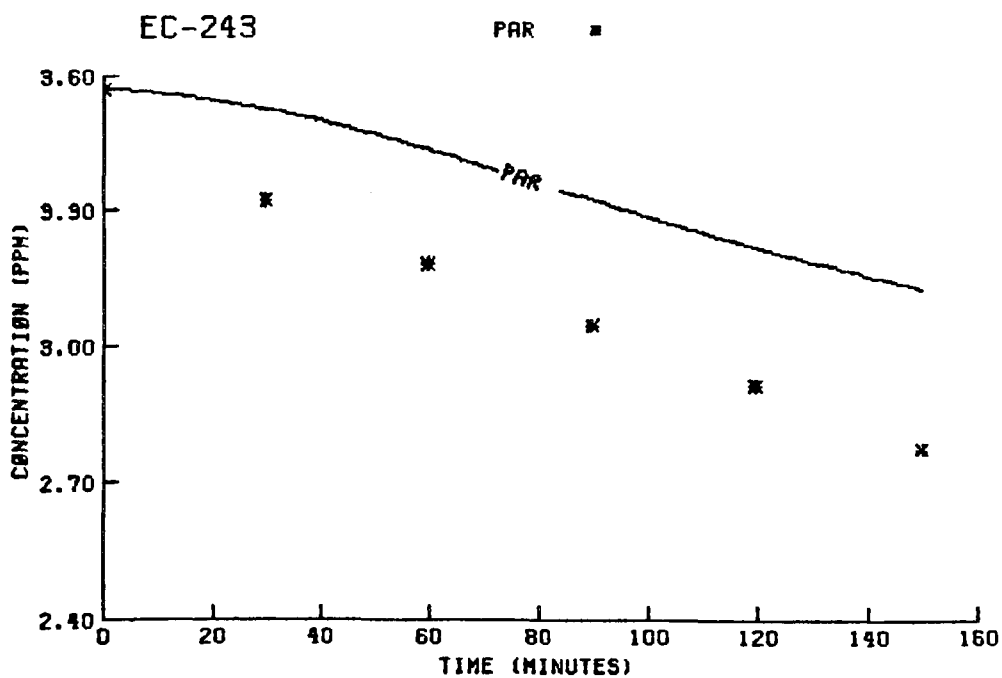
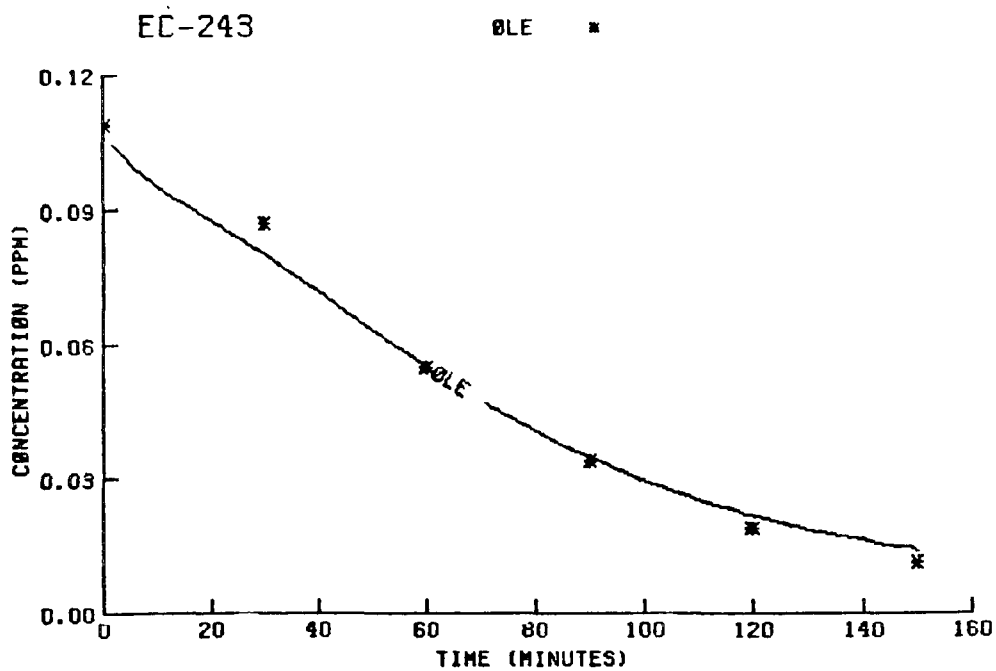


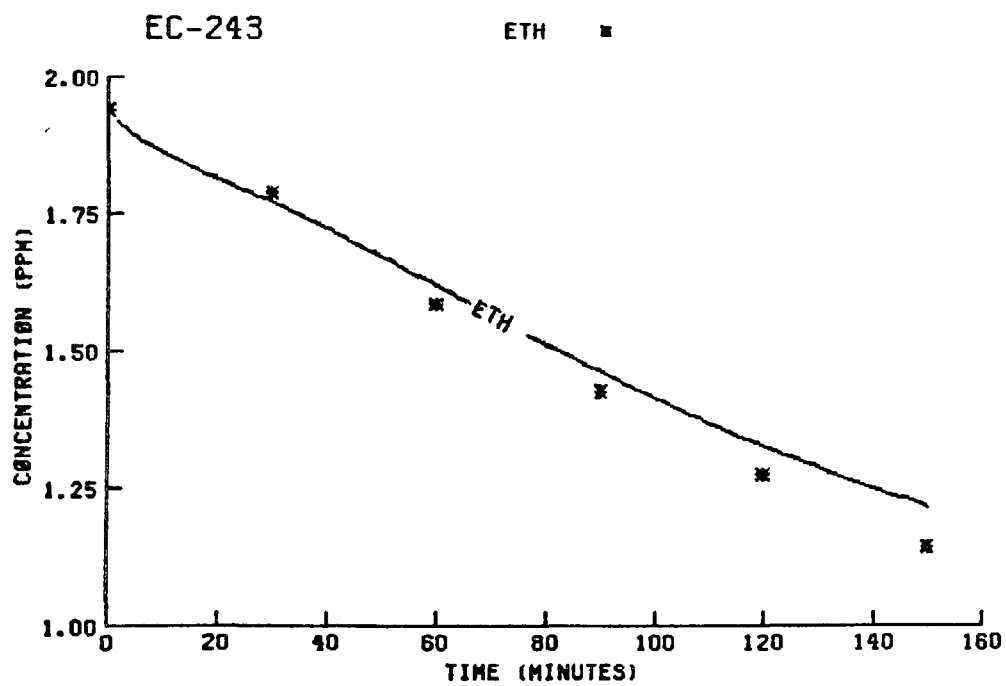
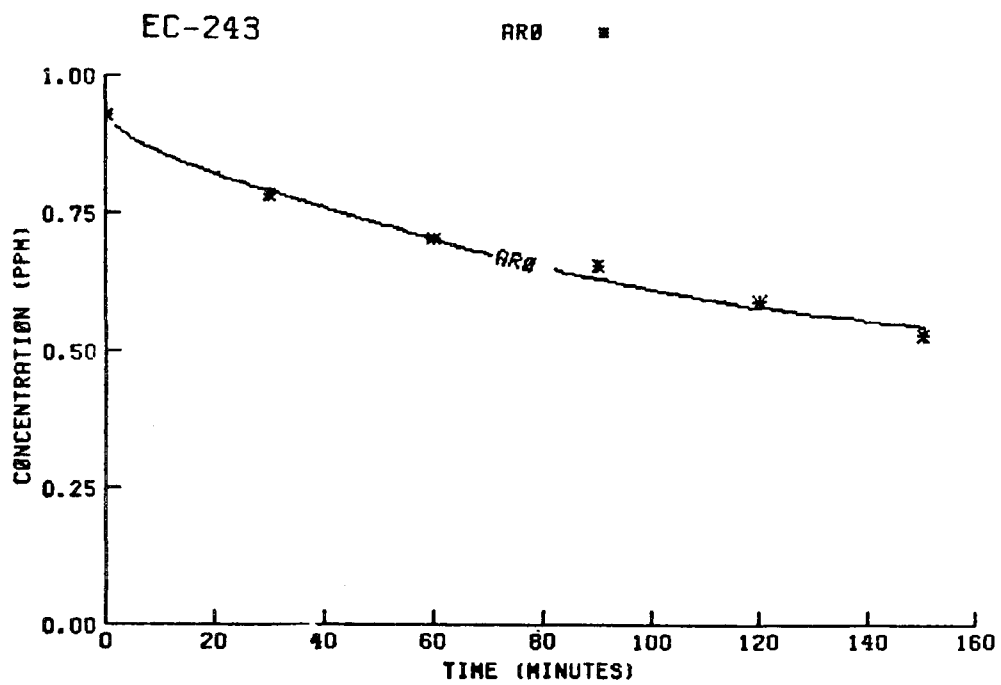


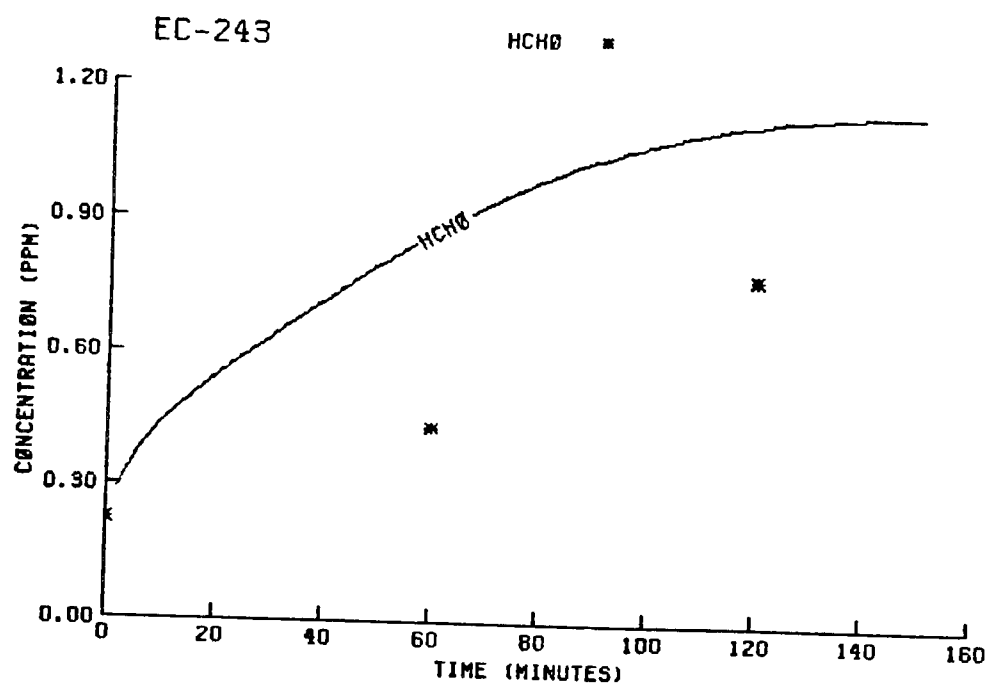


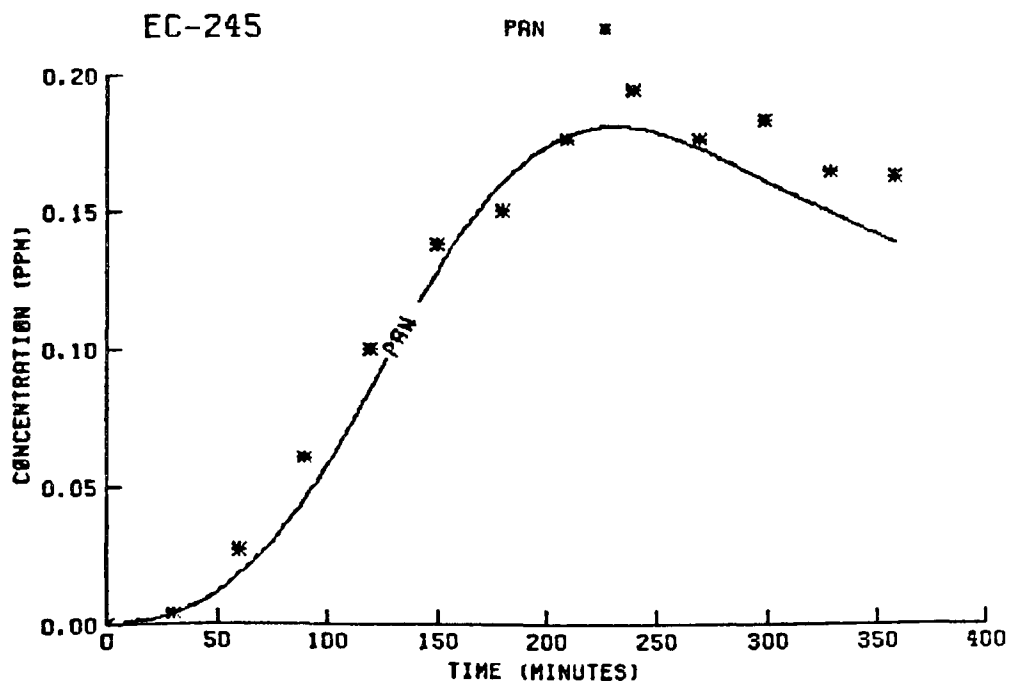
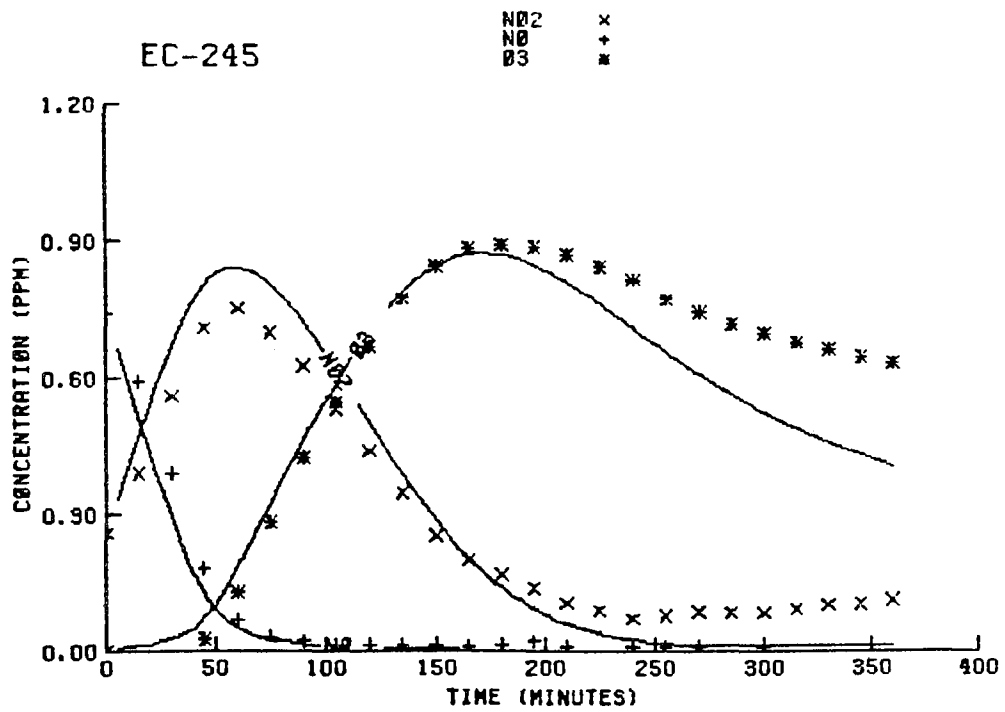






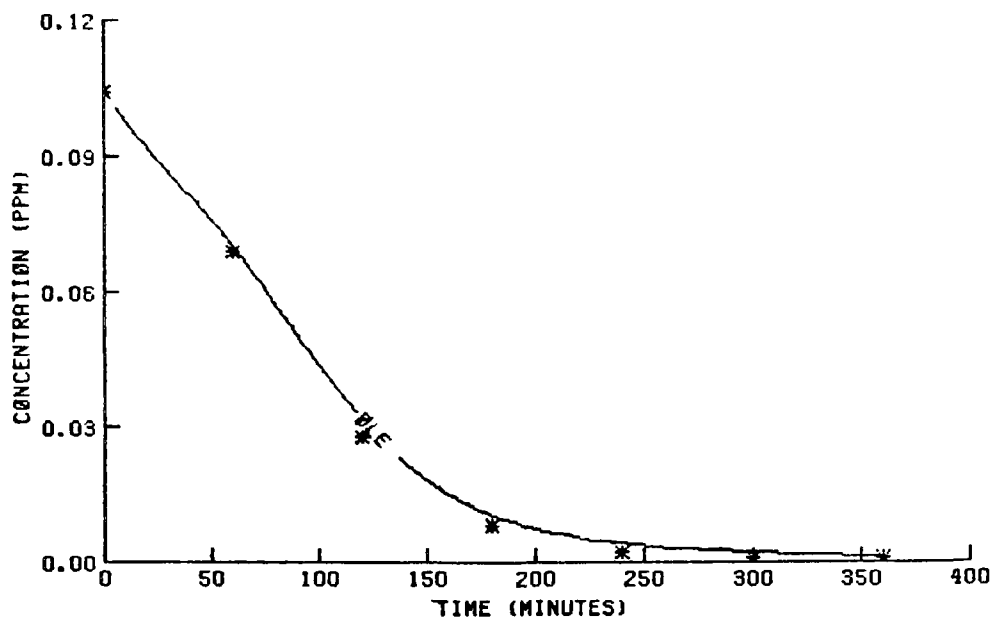






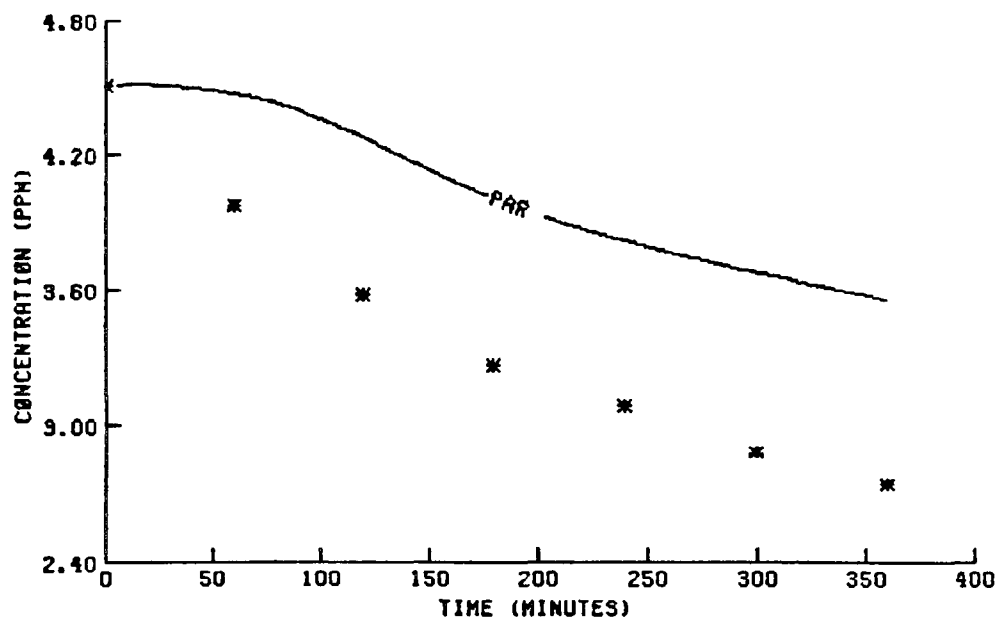
EC-245

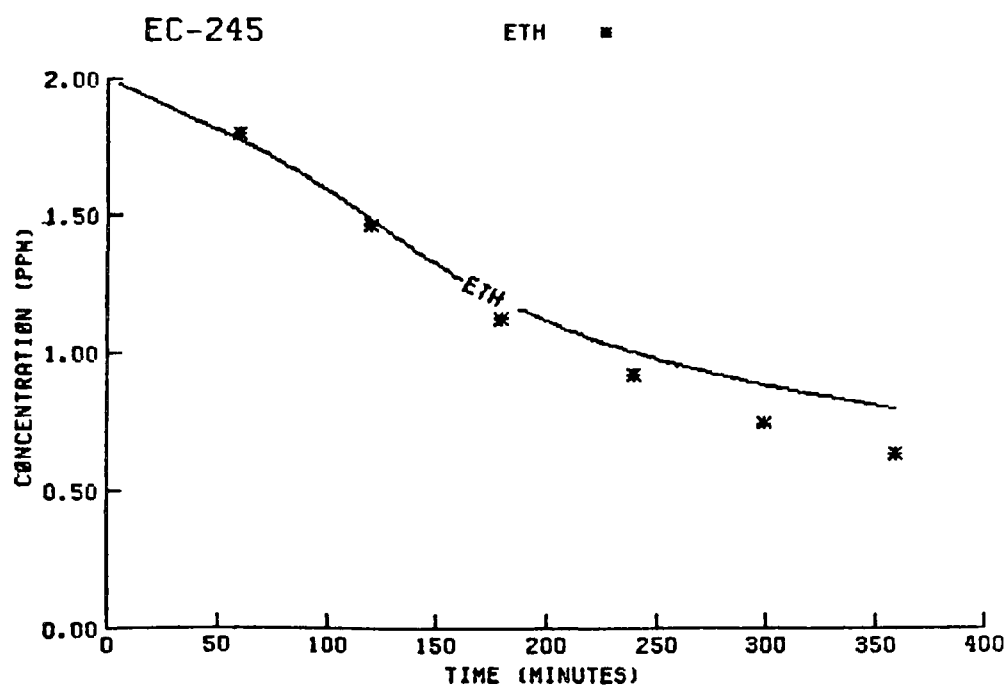
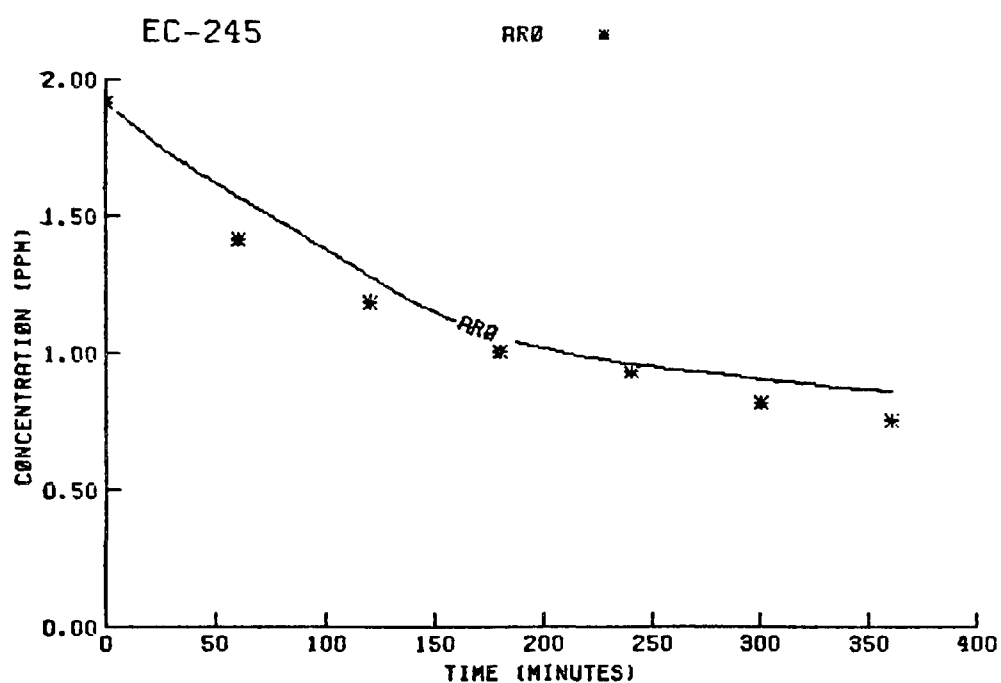
OLE *

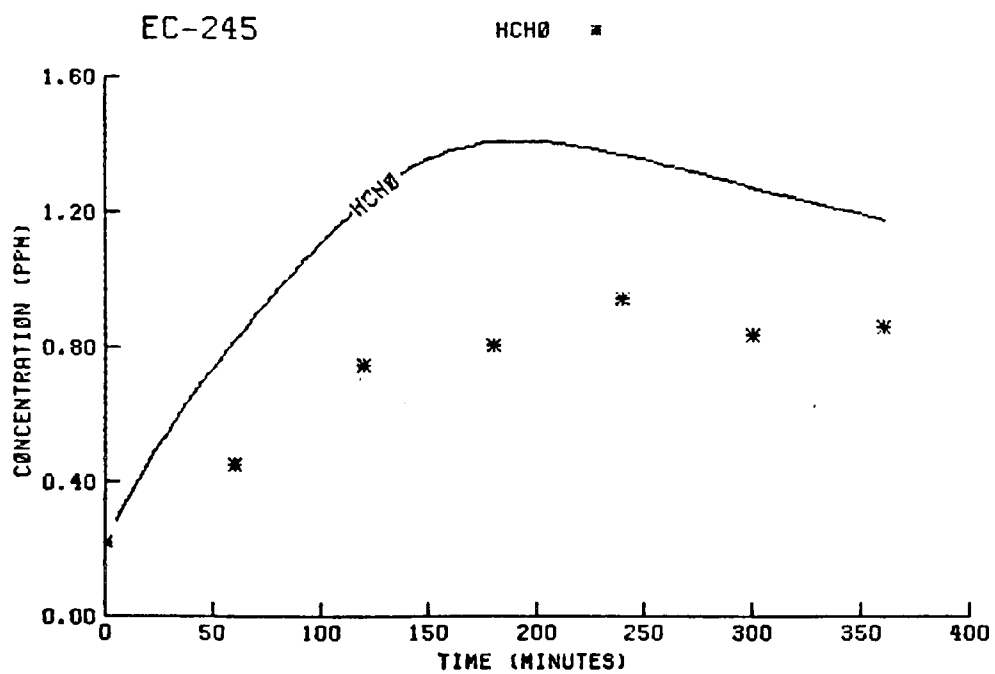


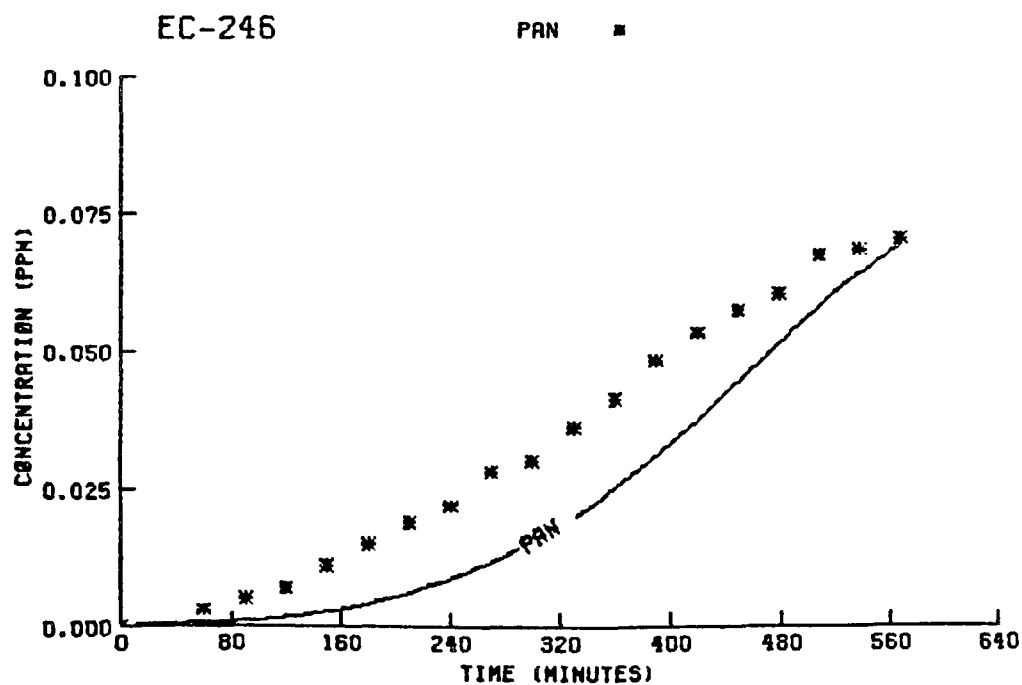
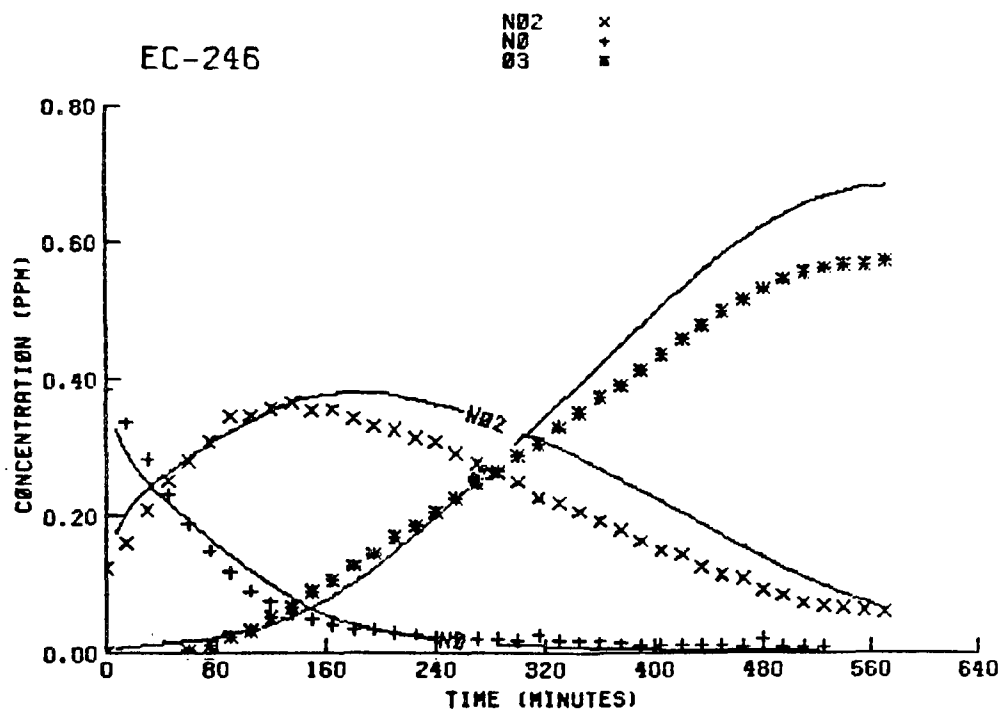
EC-245

PAR *



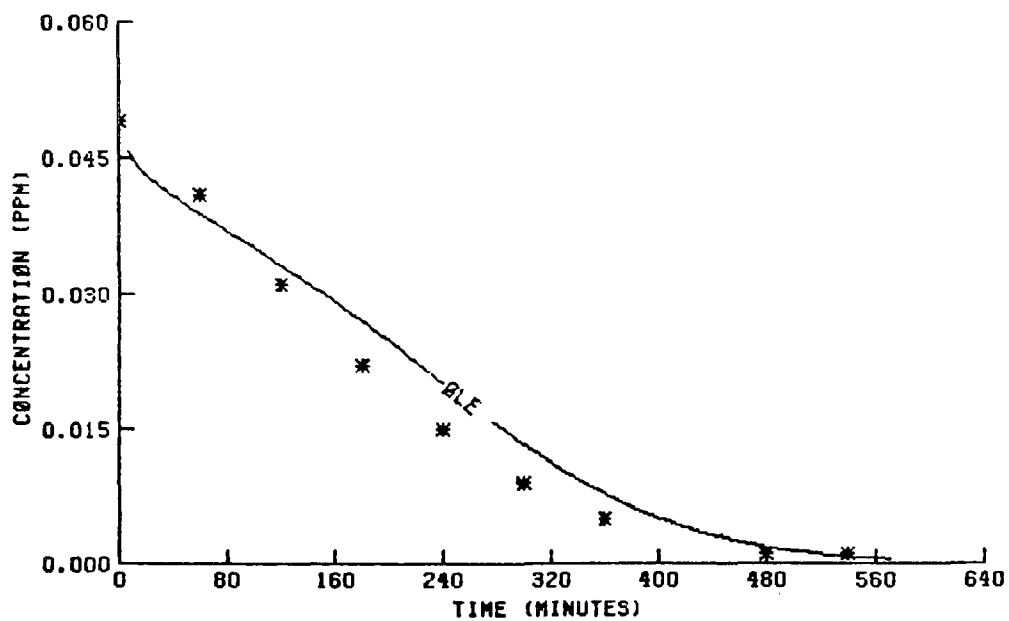






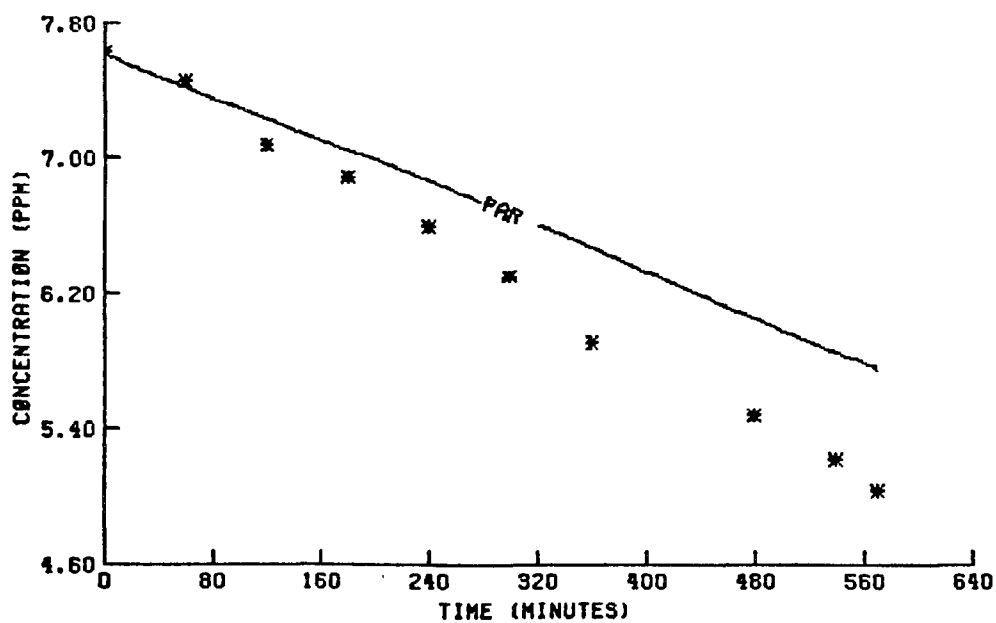
EC-246

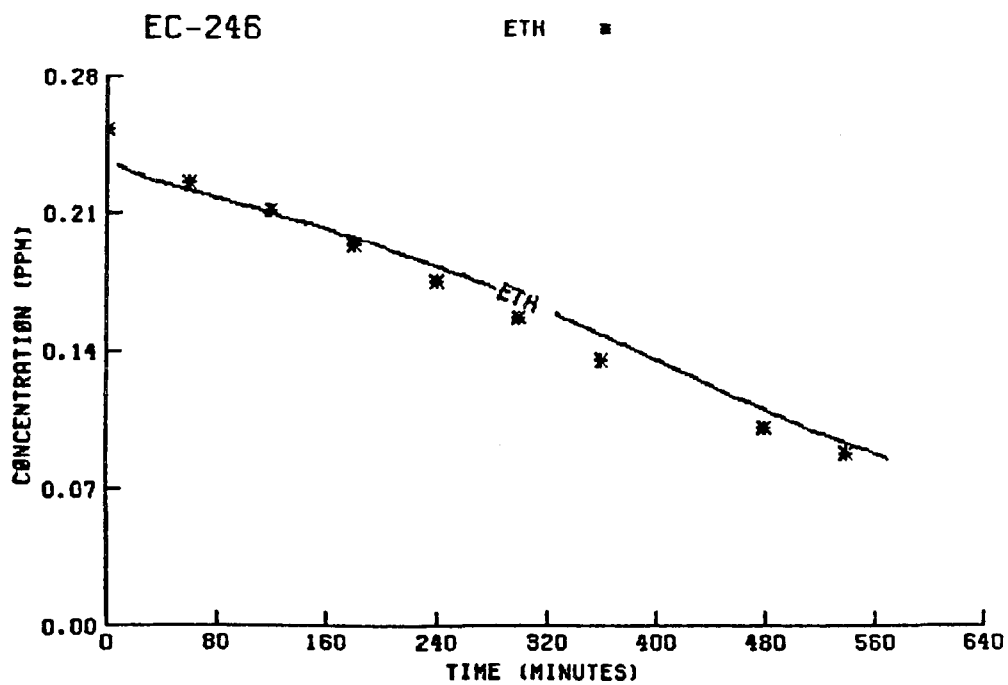
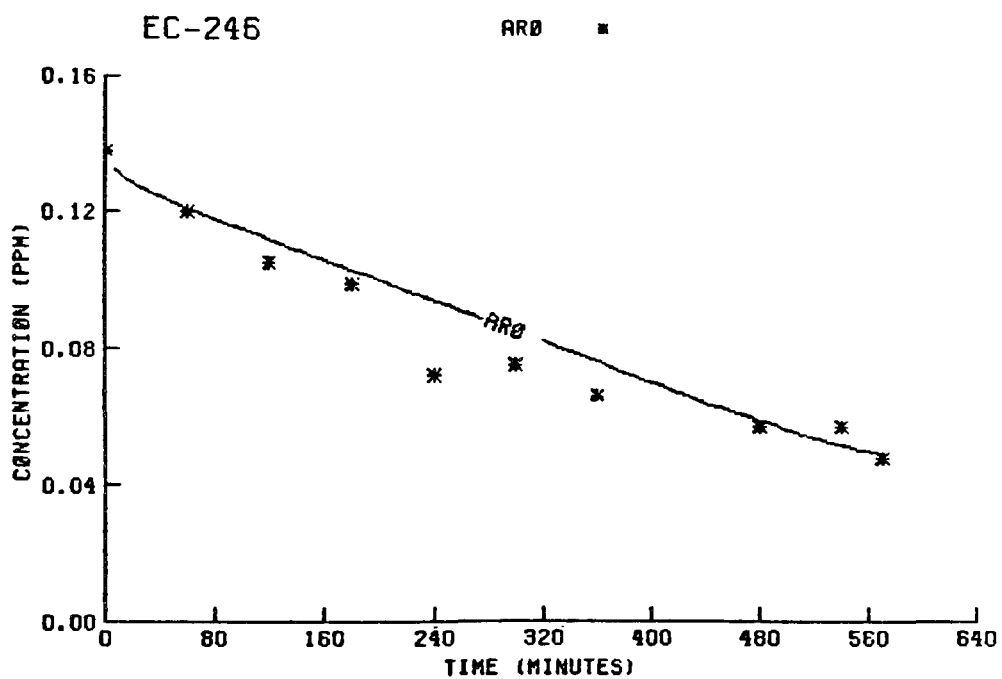
BLE *



EC-246

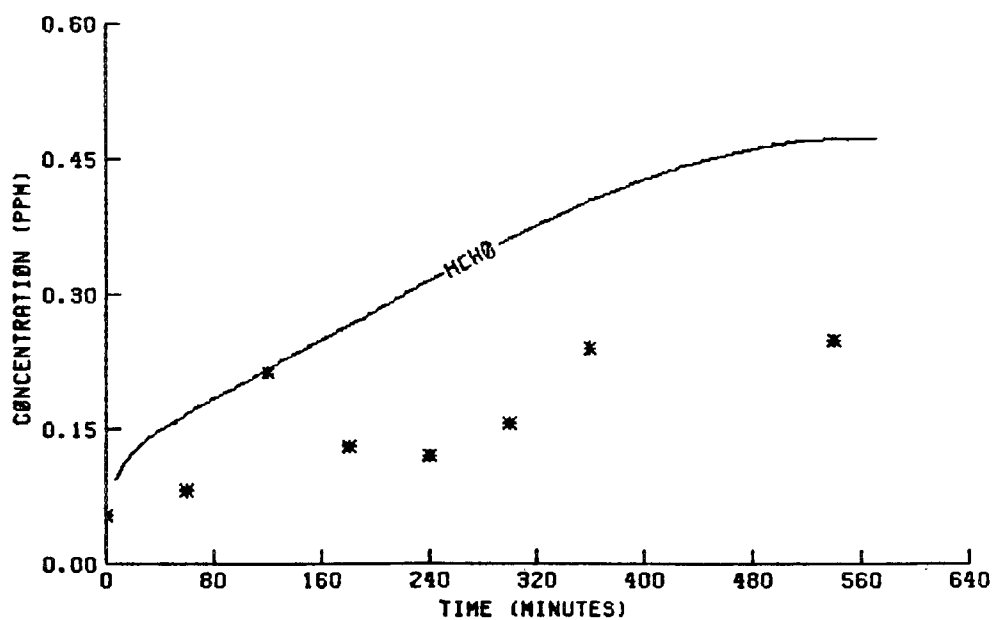
PAR *

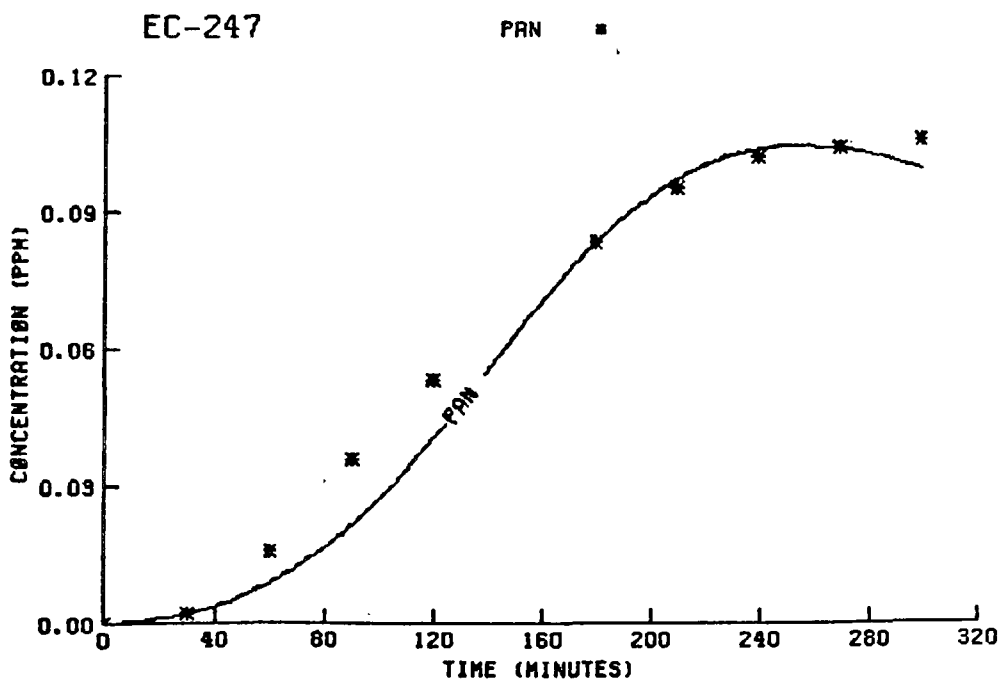
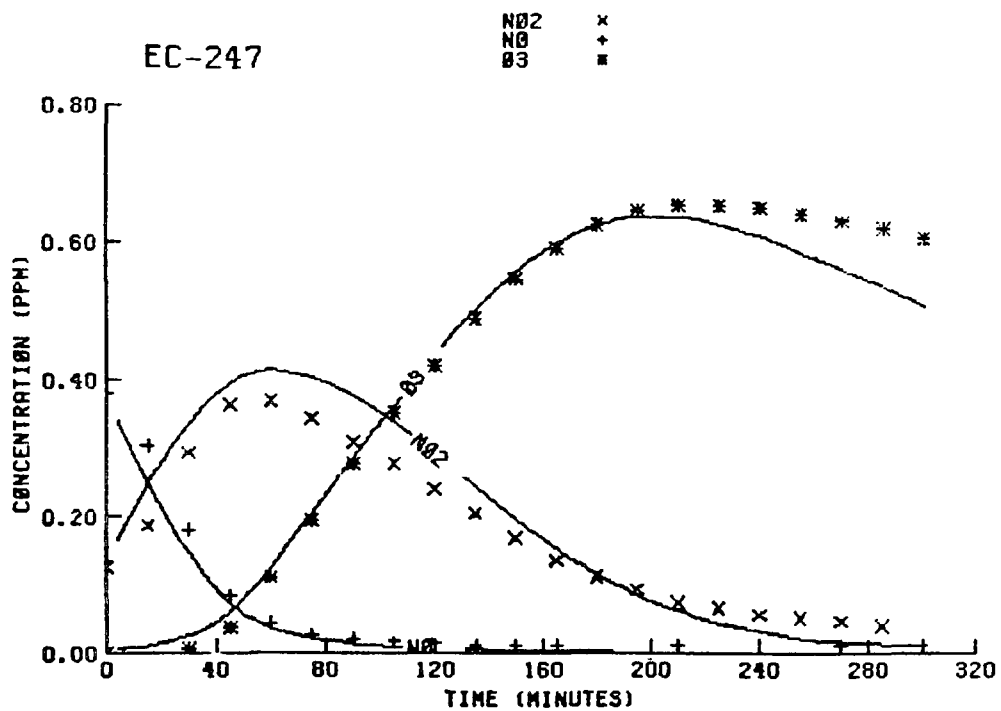


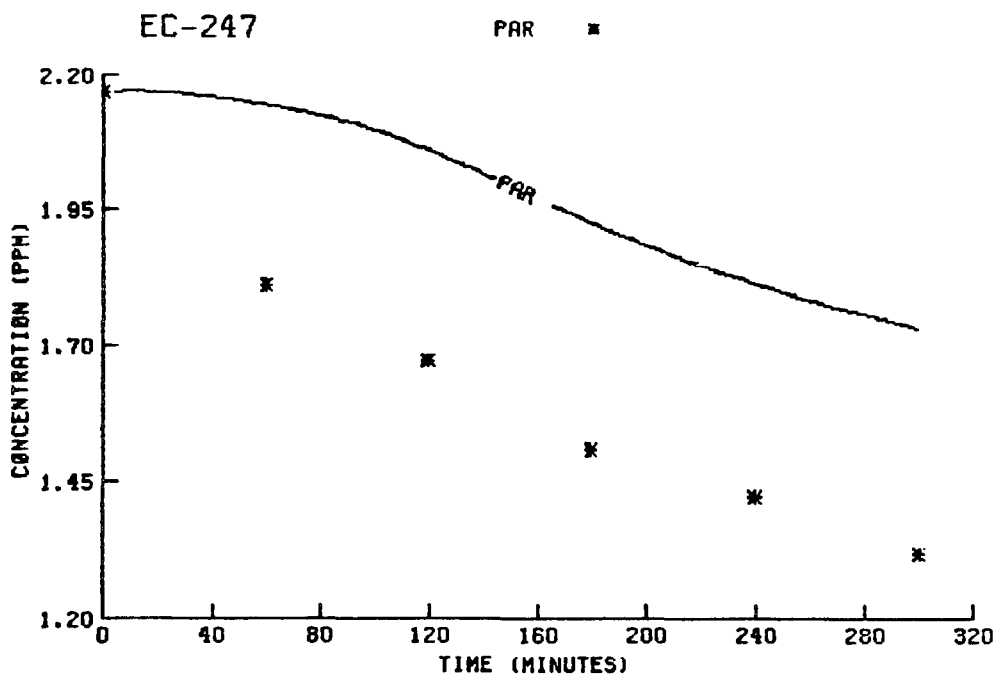
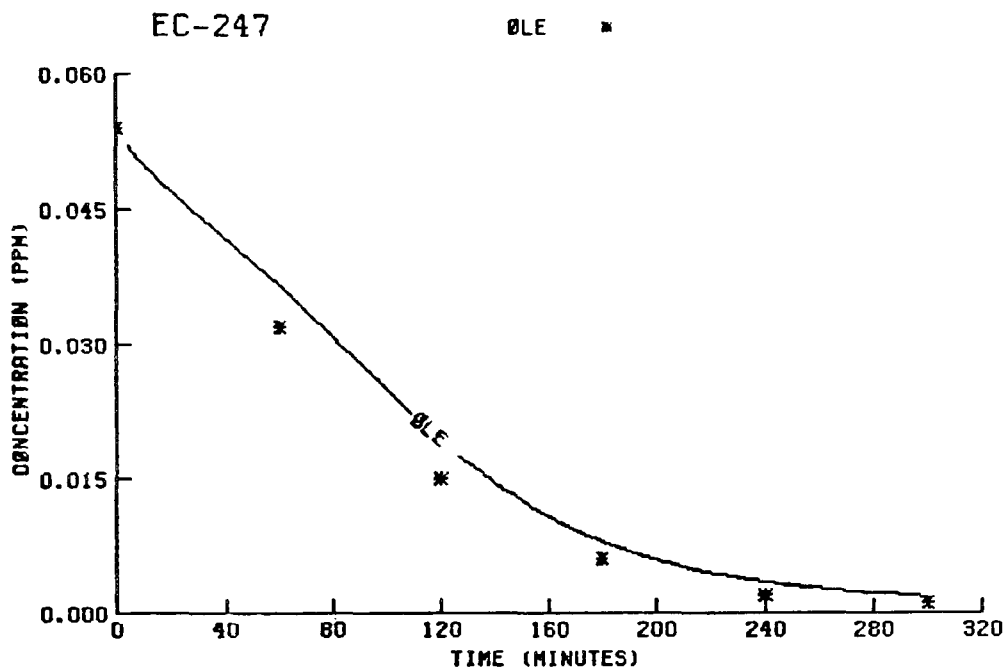


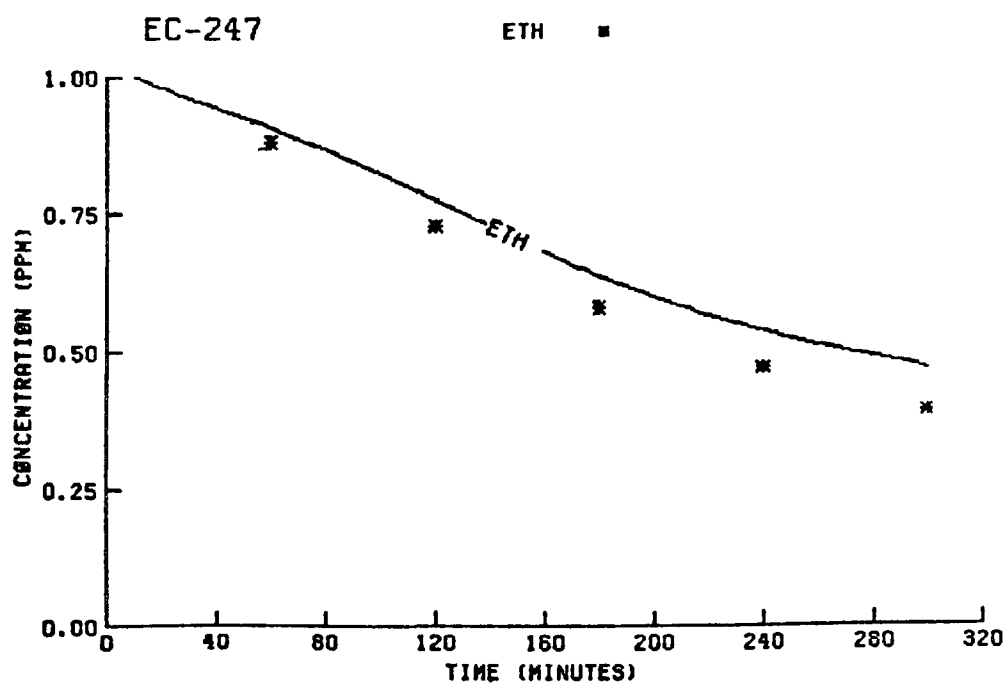
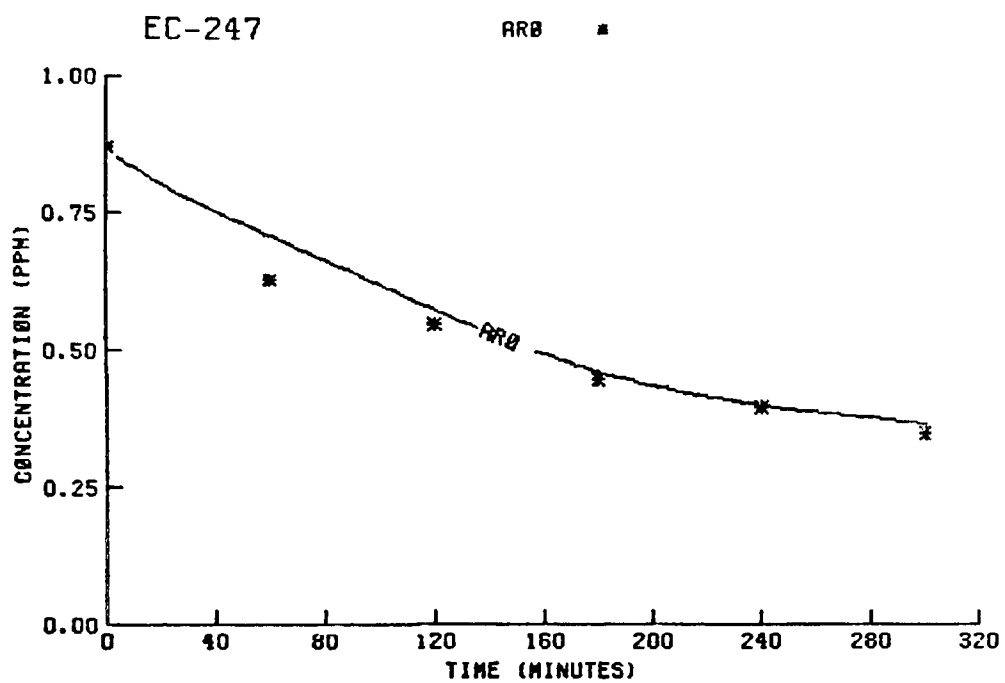
EC-246

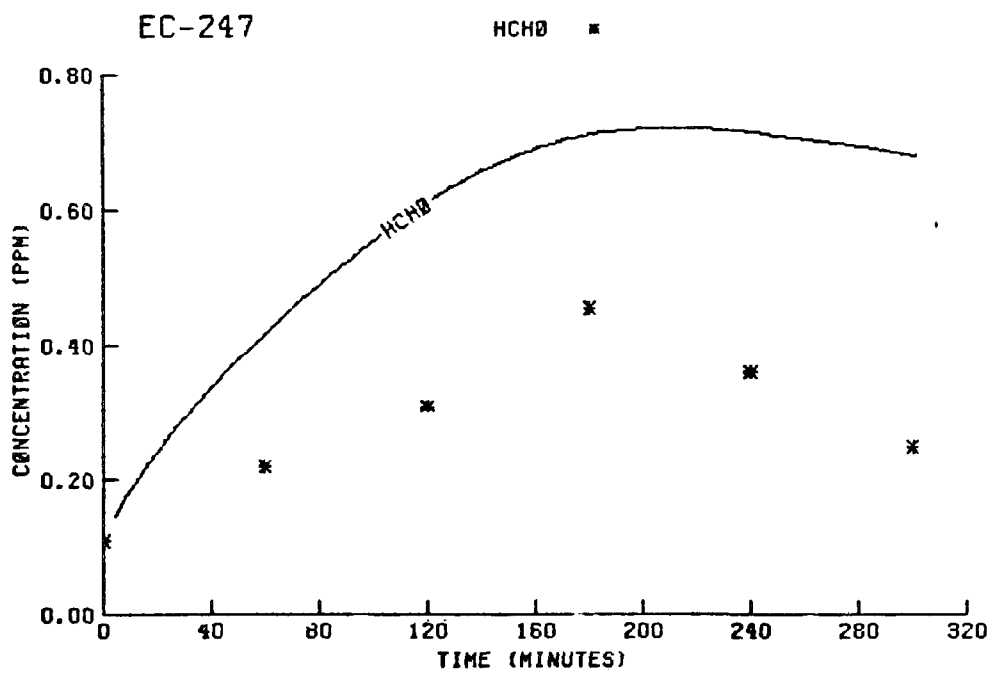
HCHO *











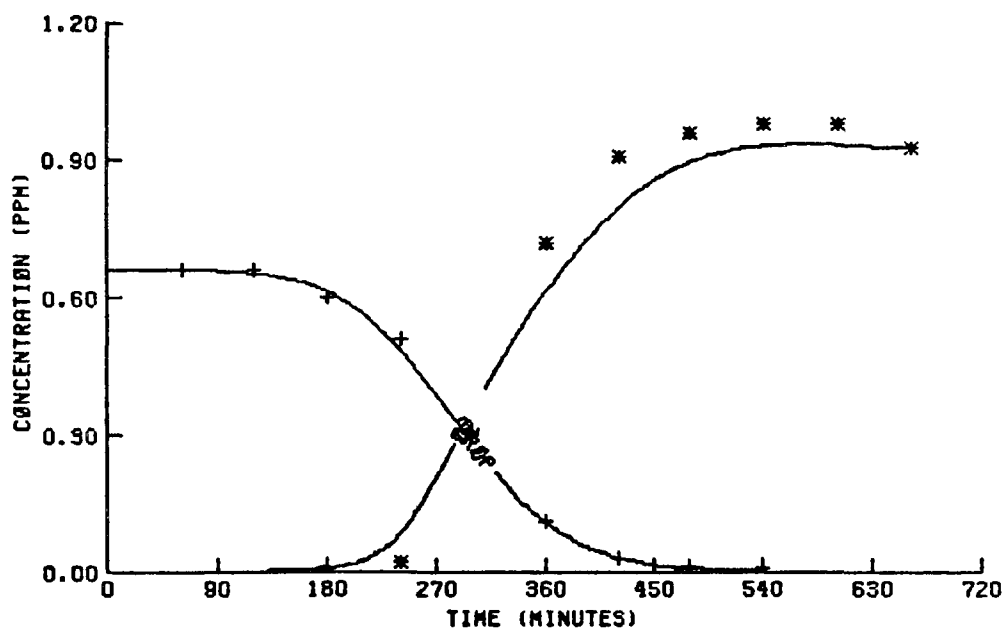
Part C

Simulation Results of Propylene Experiments
Performed at Various Chambers

UNC CHAMBER EXPERIMENTS

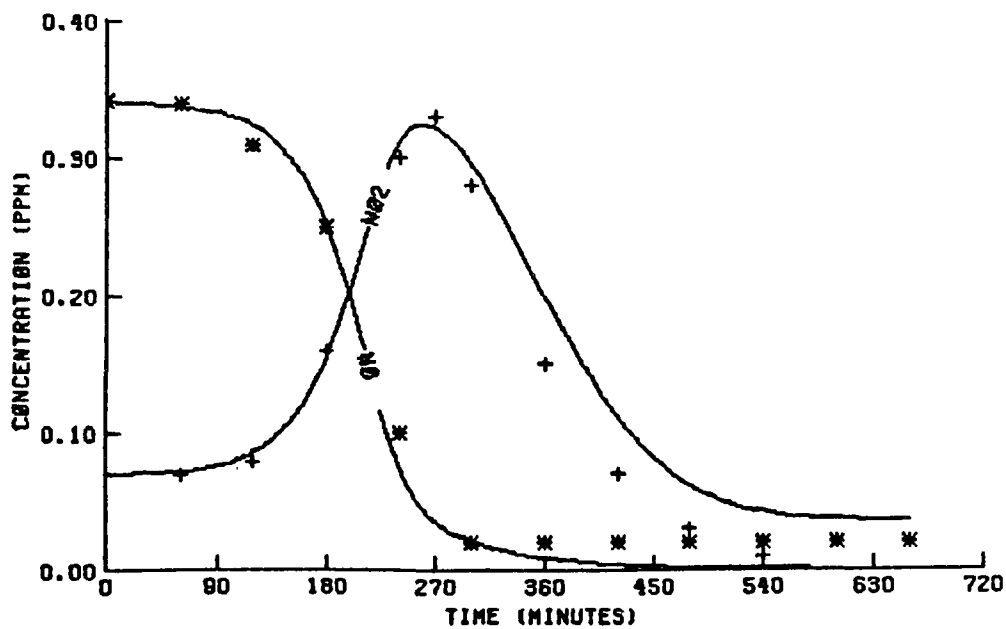
UNCB 8/9/75

PROP +
O3 *



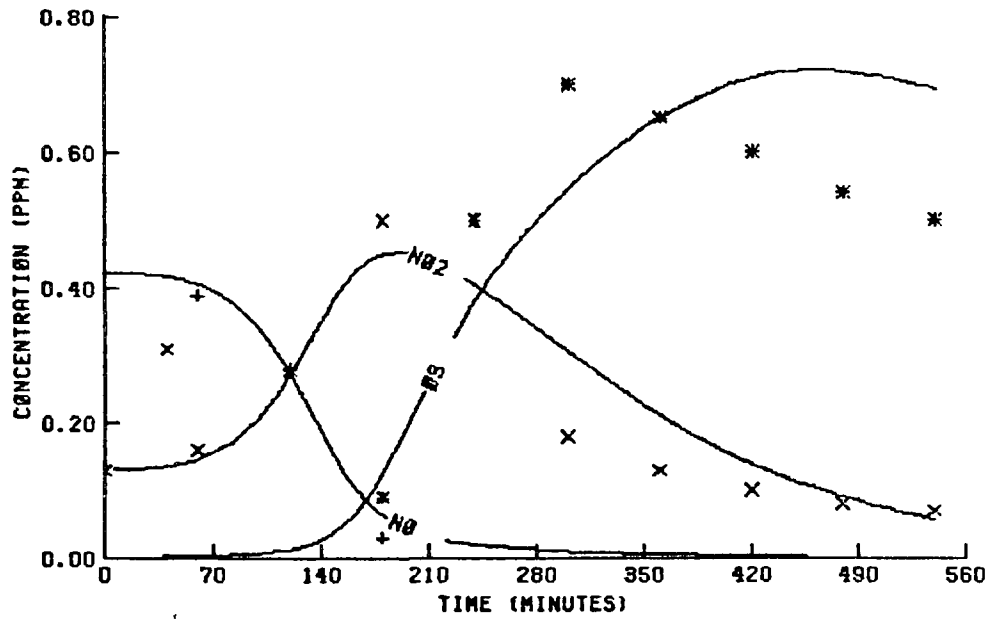
UNCB 8/9/75

NO2 +
NO *



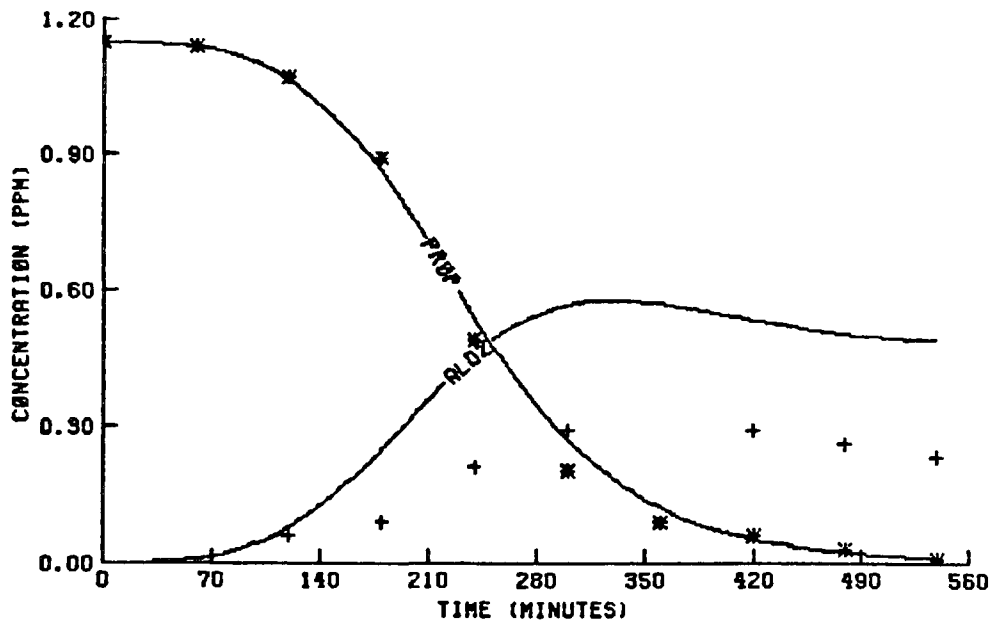
UNCB 11/5/76

NO2 x
NO +
O3 *



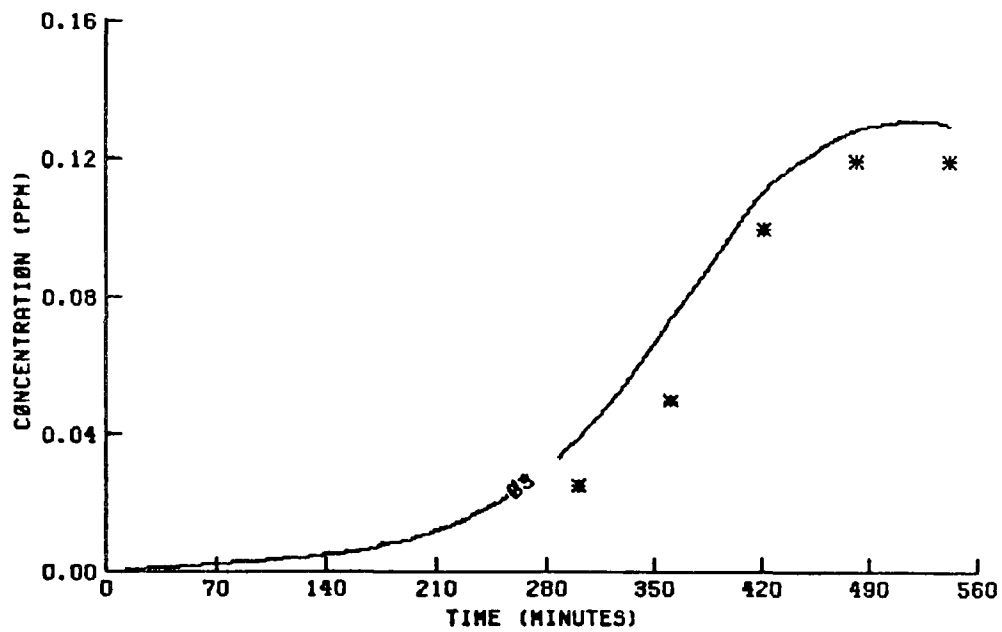
UNCB 11/5/76

ALD2 +
PRDP *



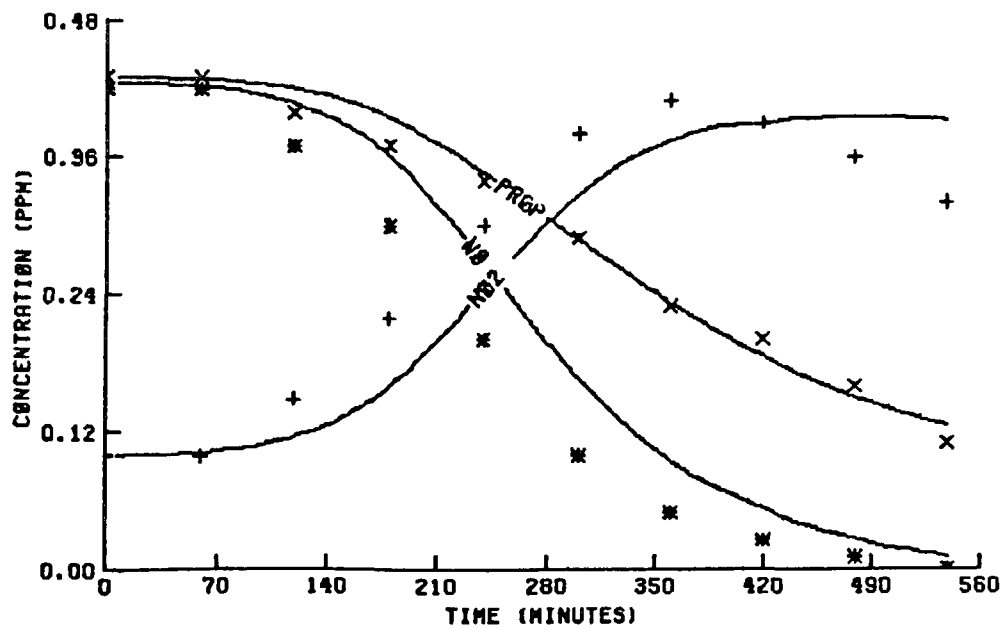
UNCR 11/5/76

03 *



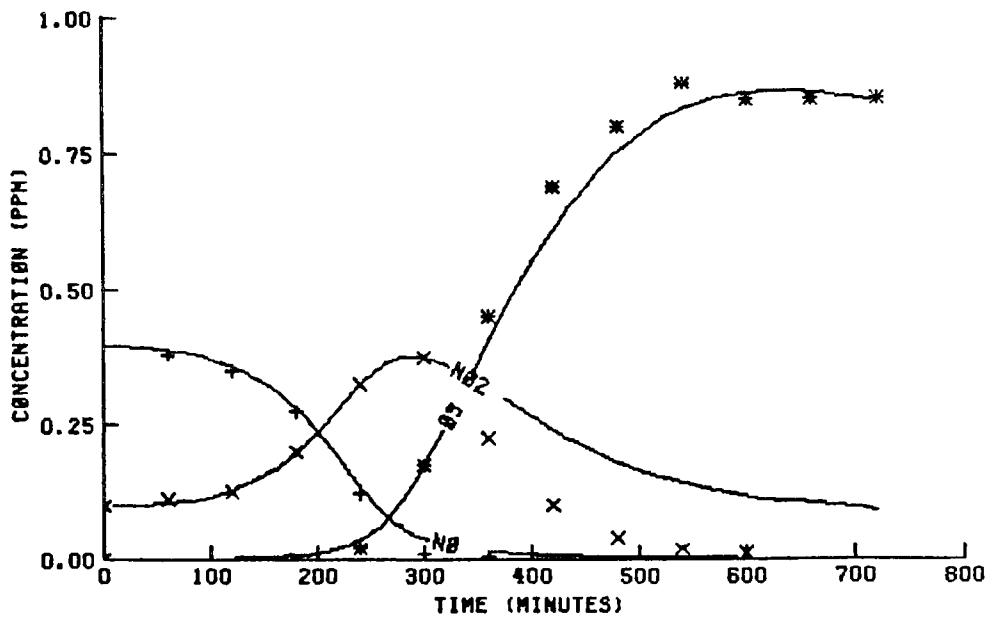
UNCR 11/5/76

PRBP *
N02 +
NB *



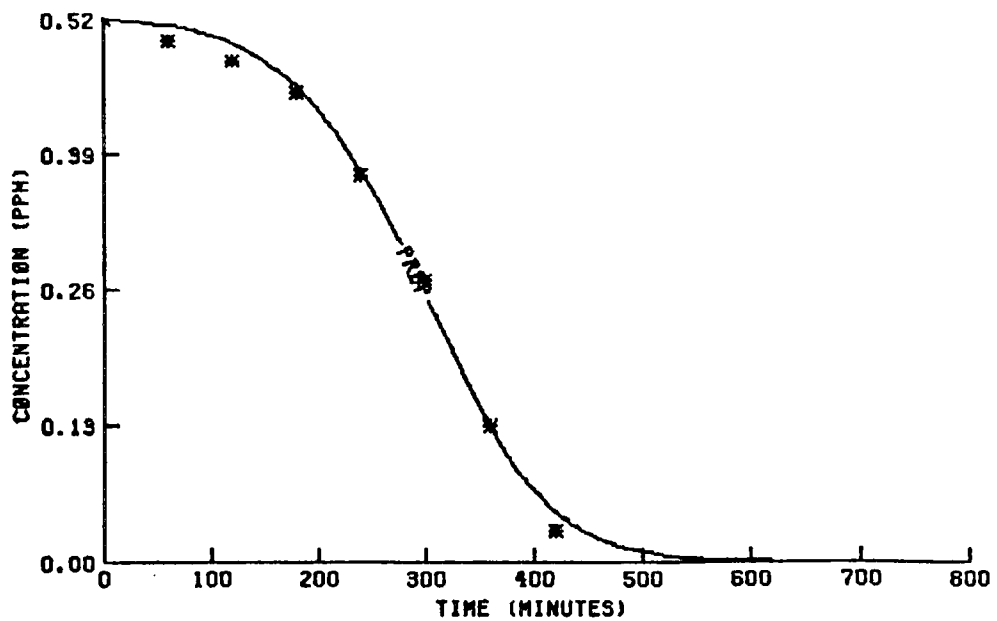
UNCB 8AUG77

NO2 x
NO +
O3 *



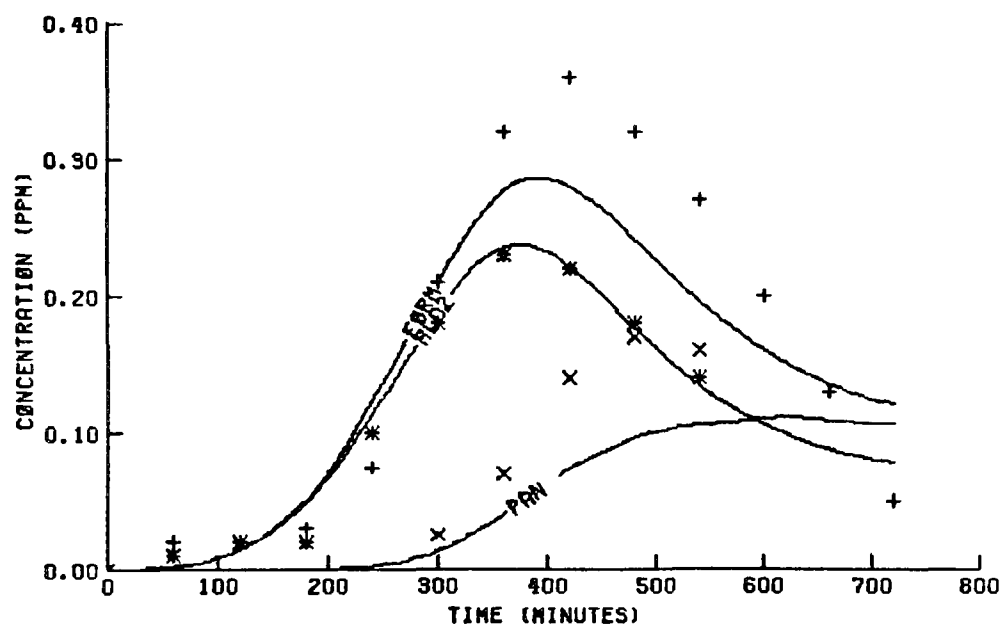
UNCB 8AUG77

PR0P *



UNCB 8AUG77

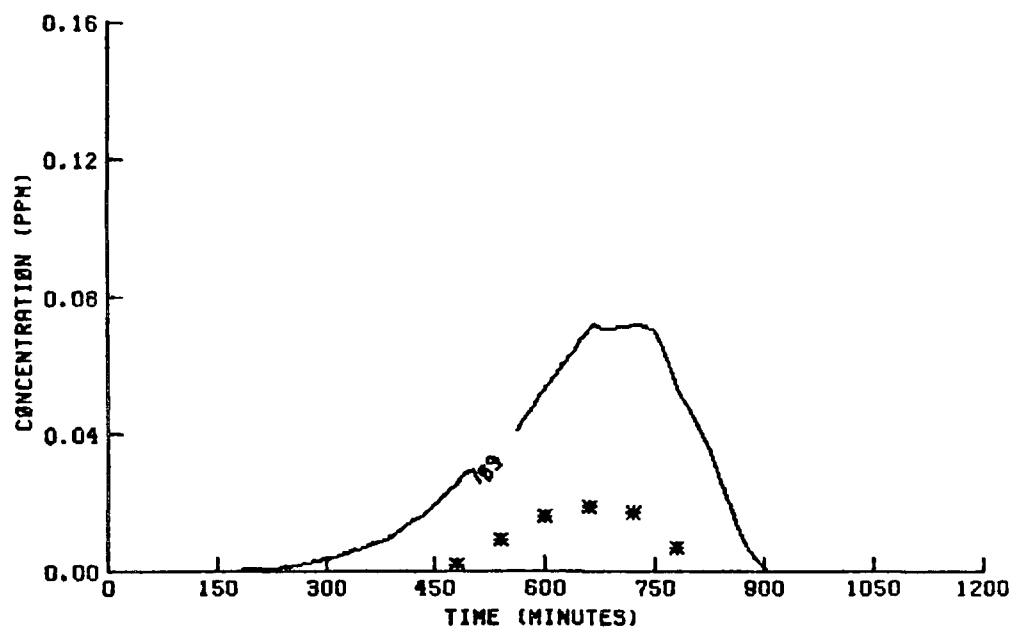
PAN x
F0RM +
ALD2 ■



RTI CHAMBER EXPERIMENTS

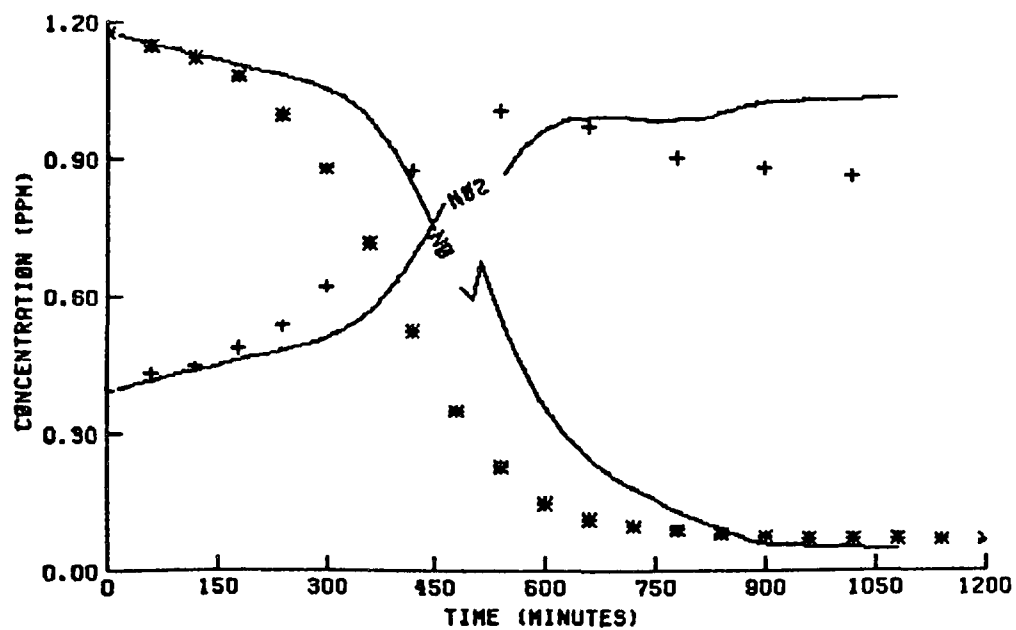
RT12 110CT76

03 *



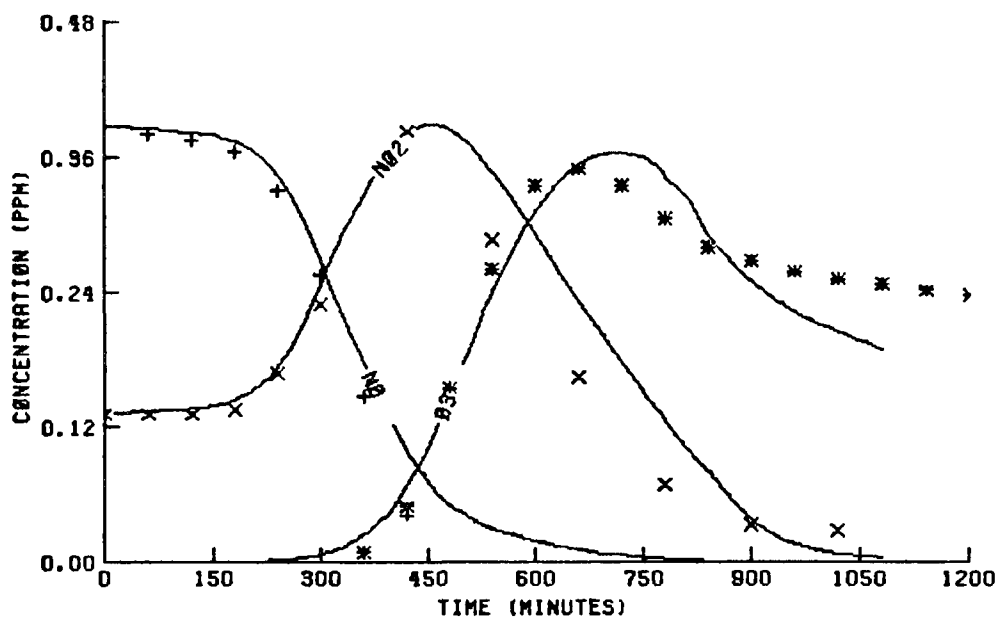
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N02 +
N0 *



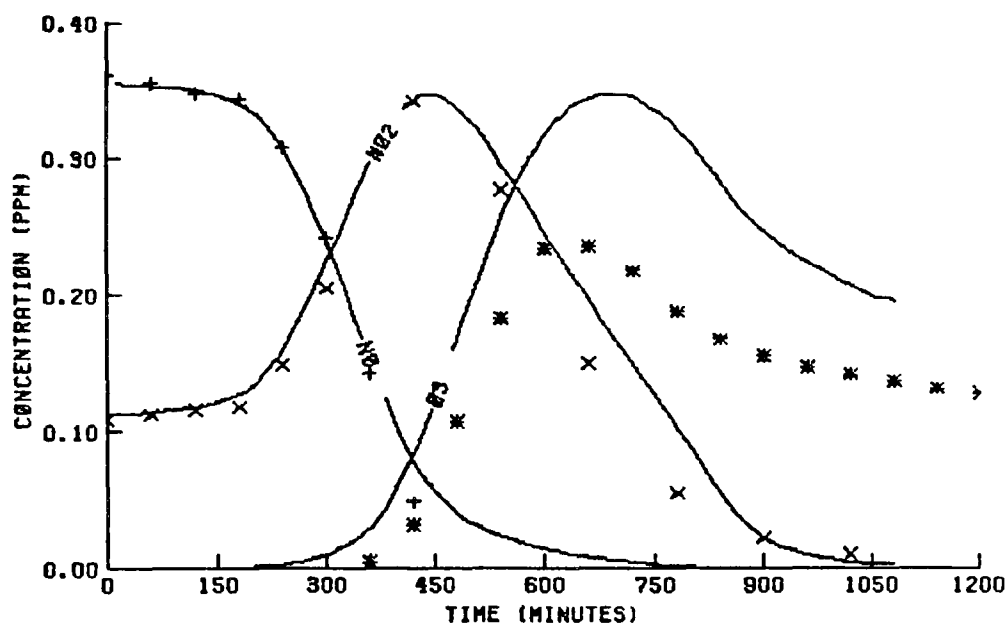
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N0 +
03 *

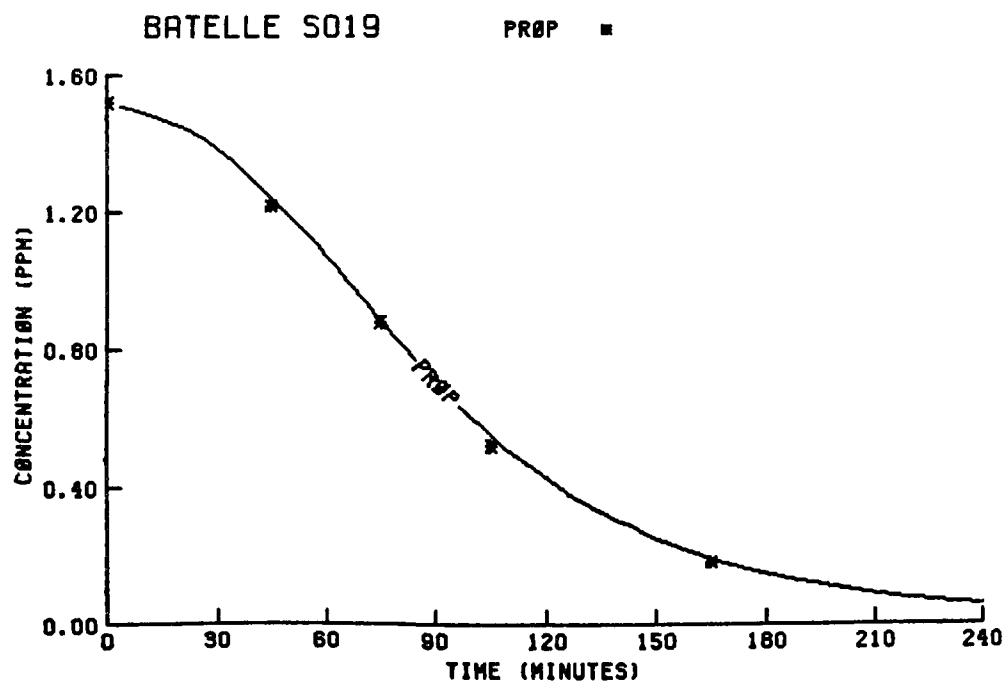
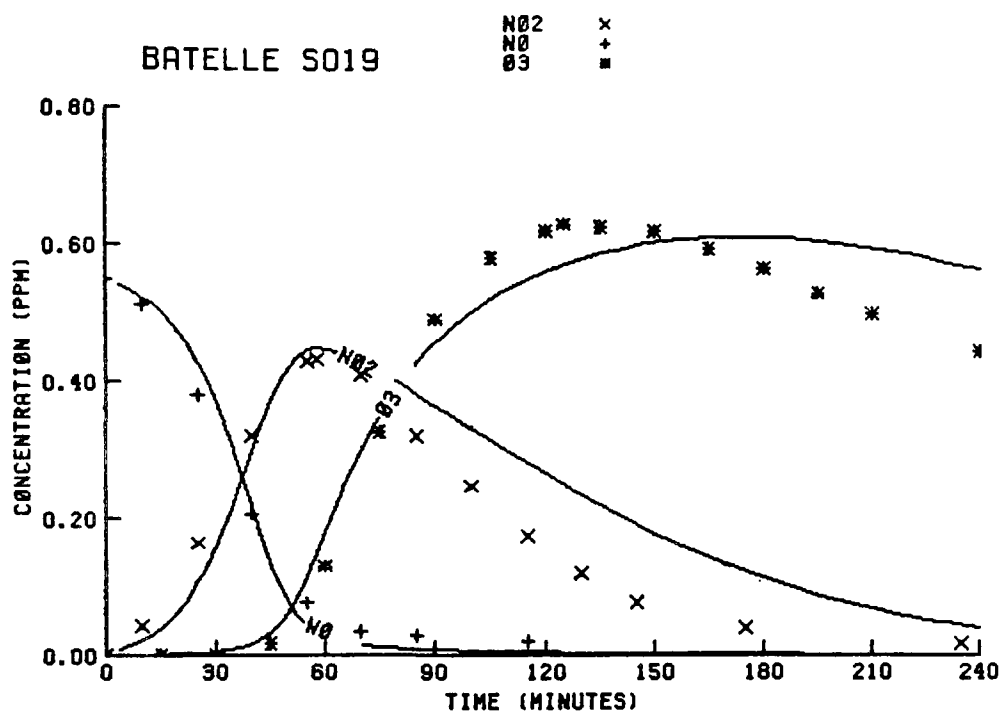


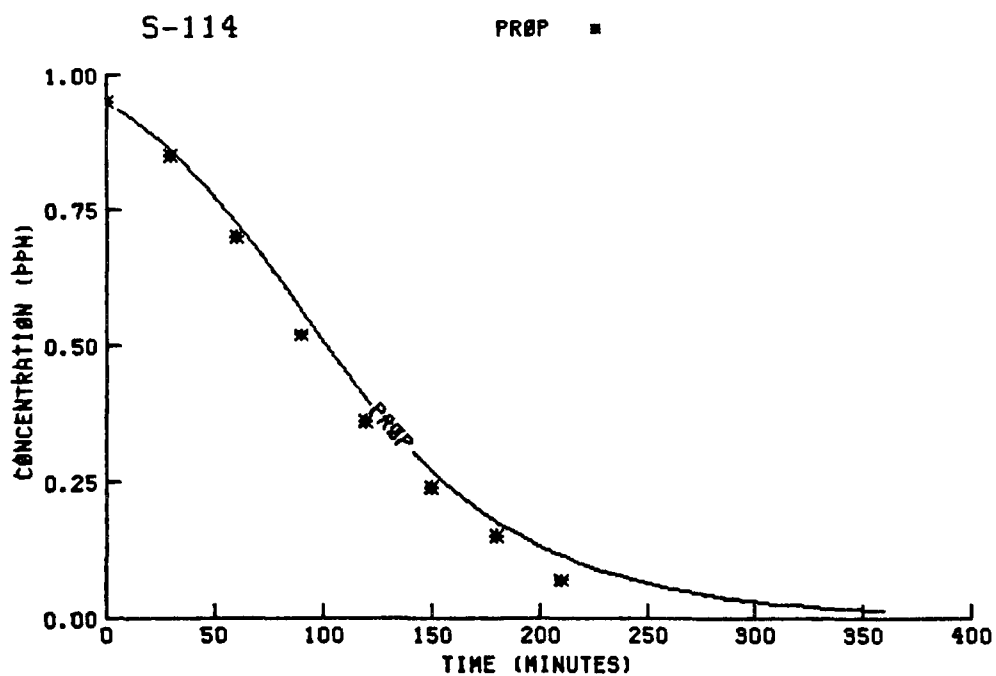
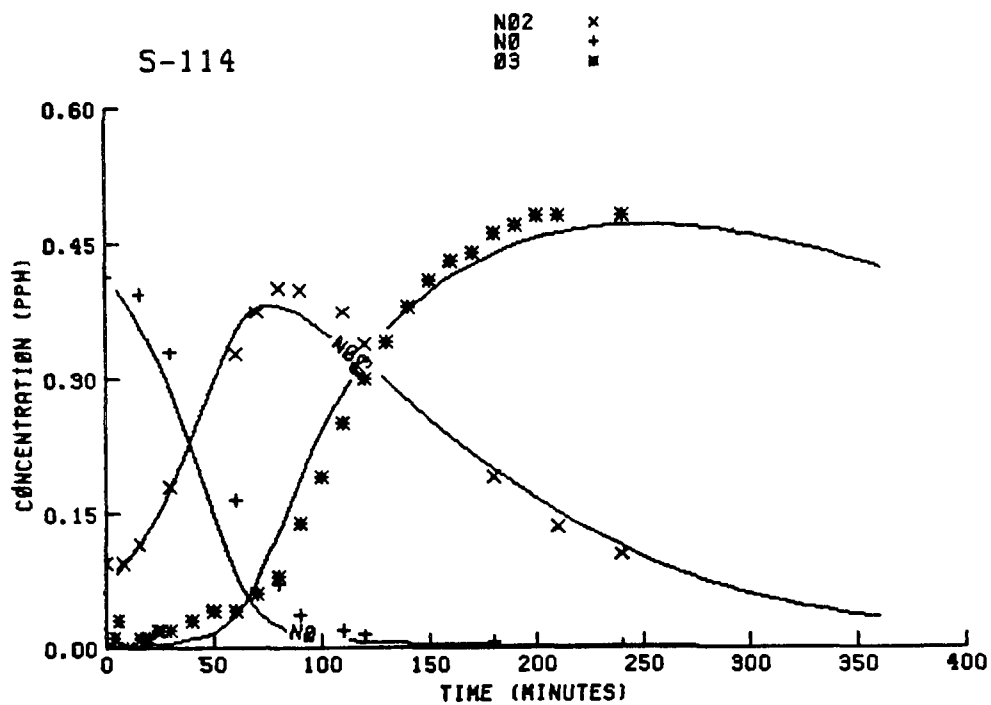
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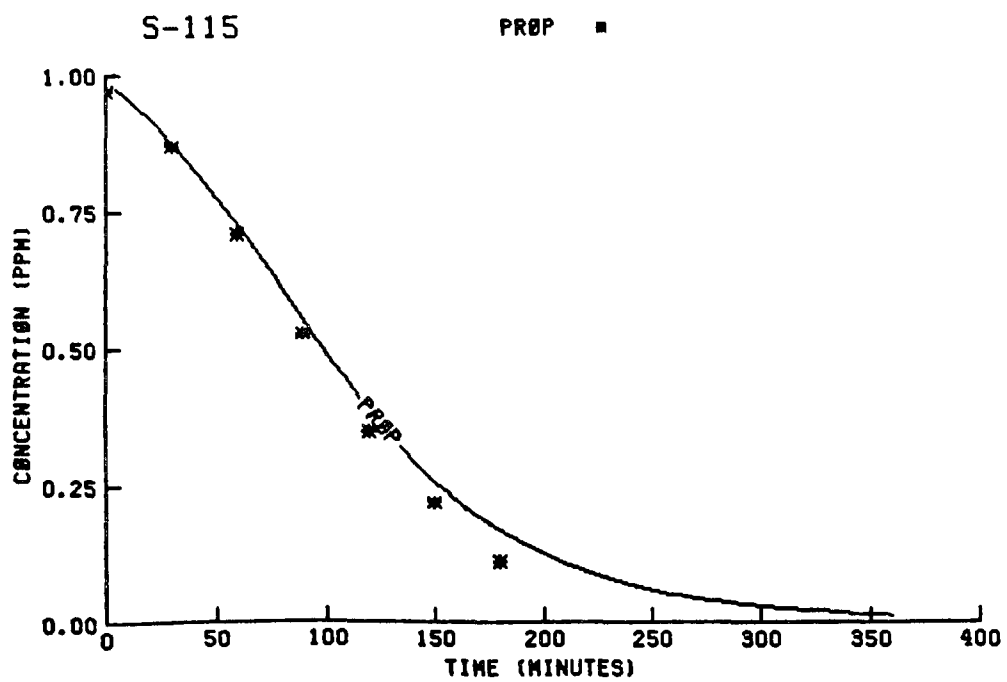
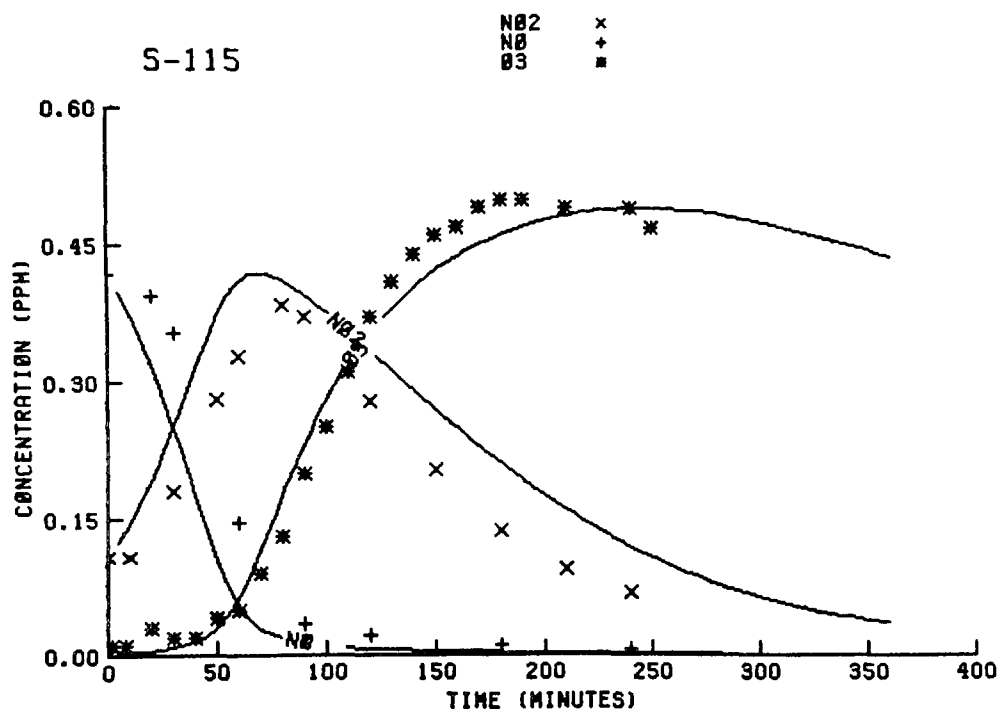
NO2 x
NO +
O3 *



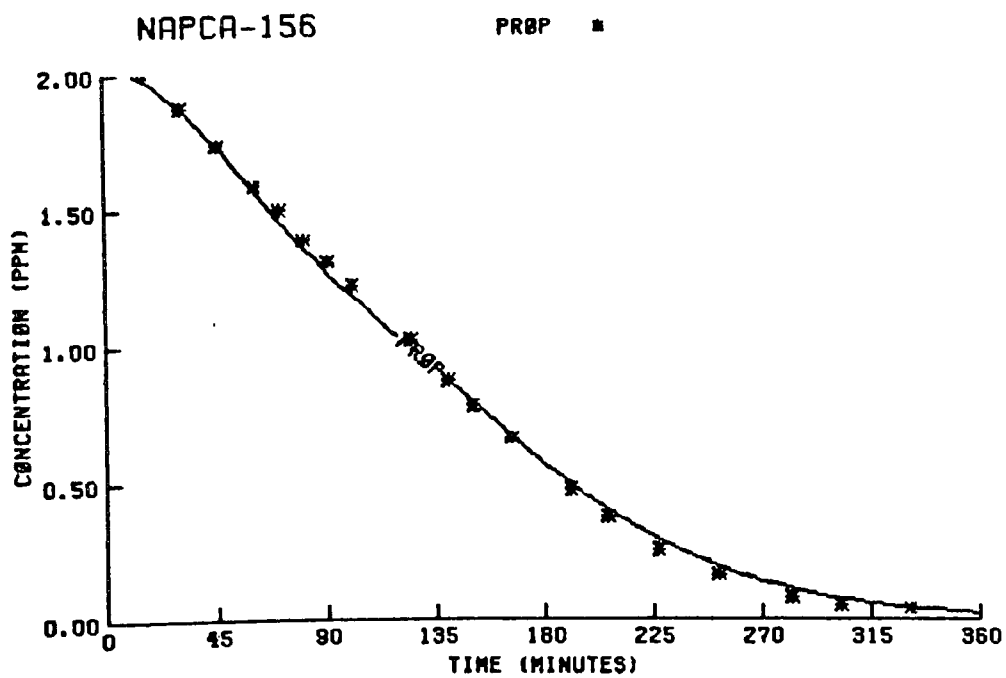
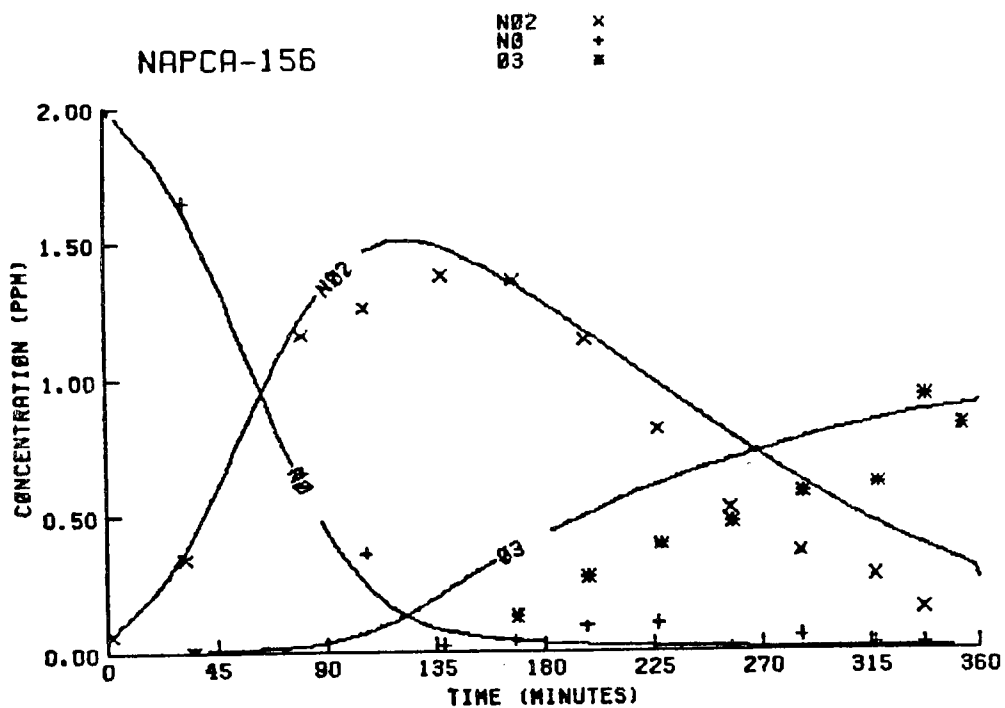
BATTELLE CHAMBER EXPERIMENTS





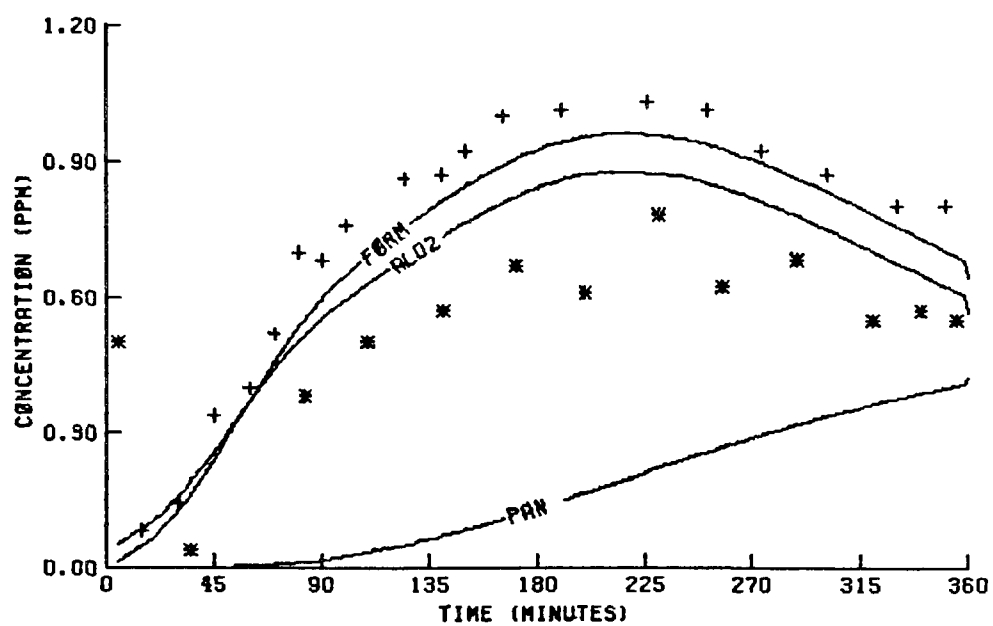


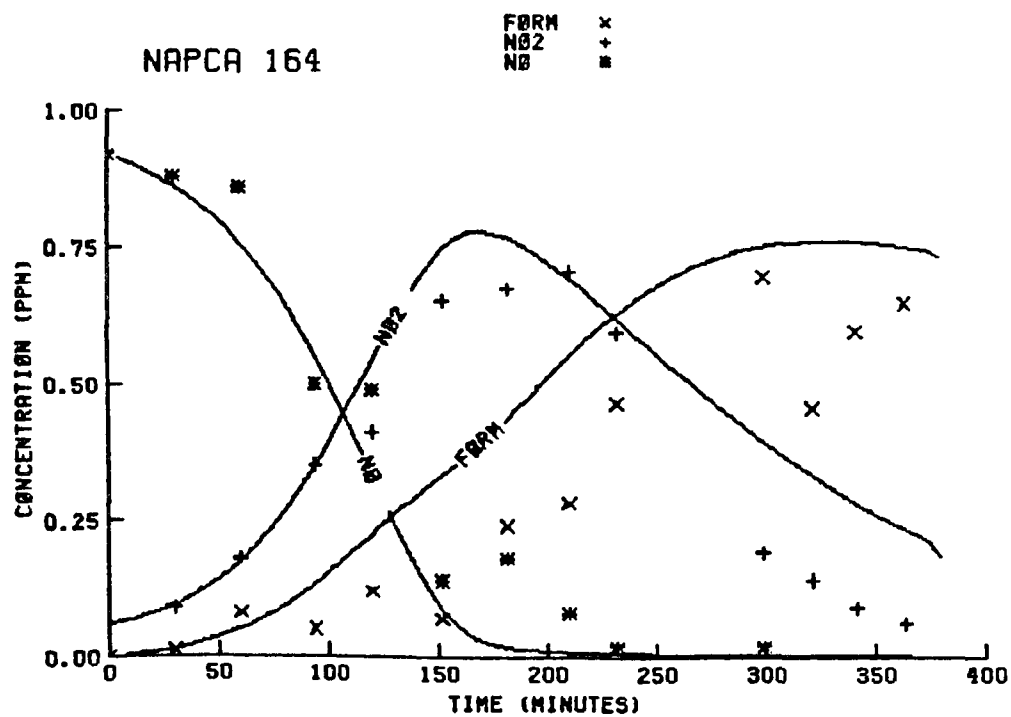
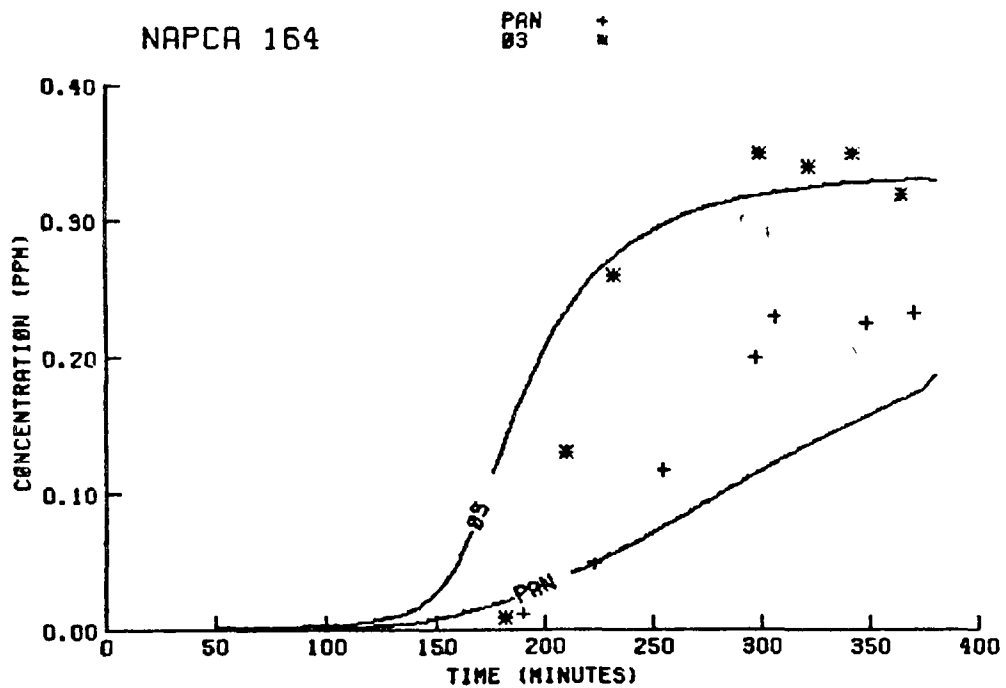
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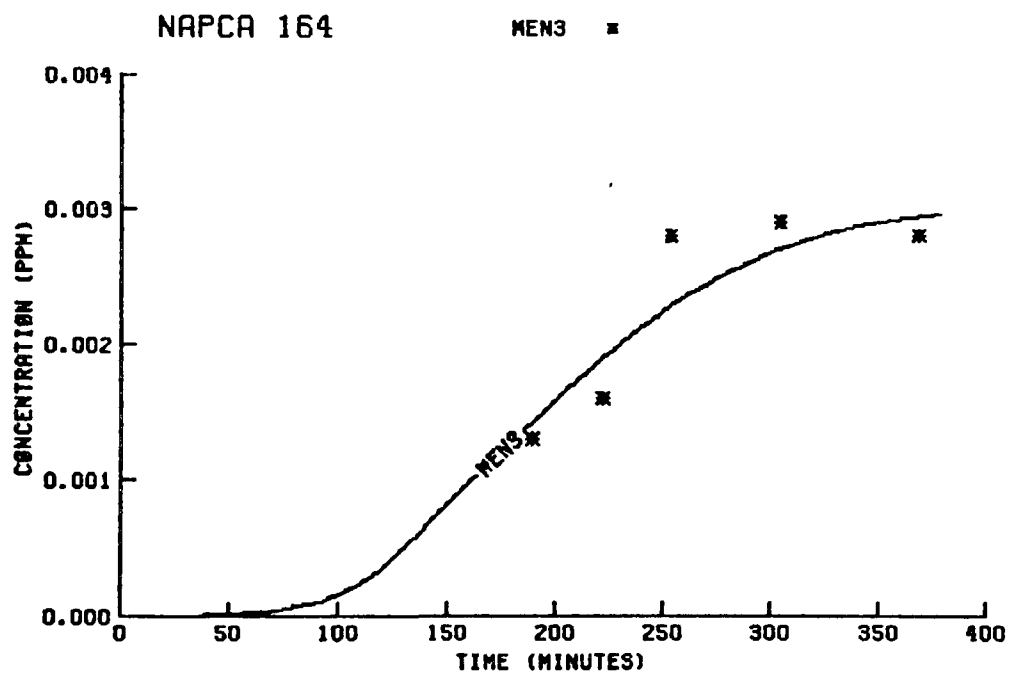
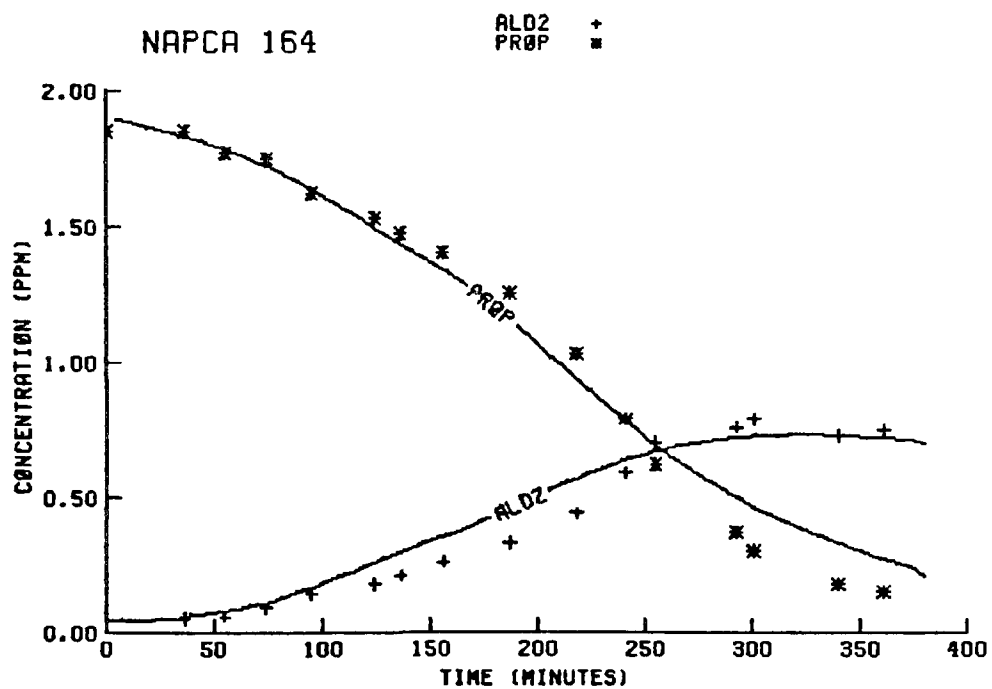


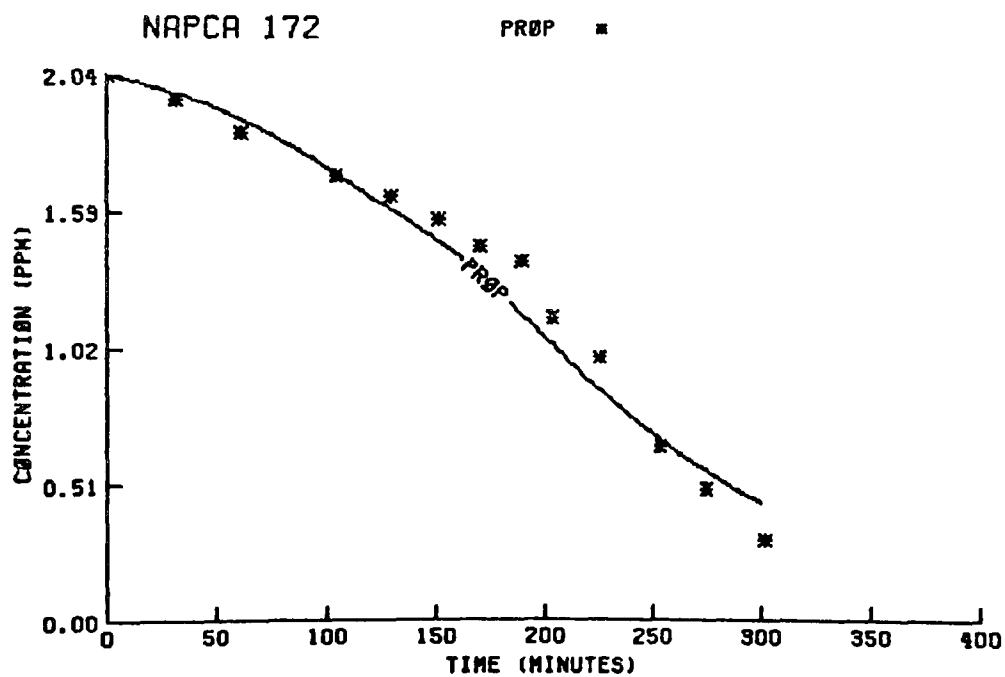
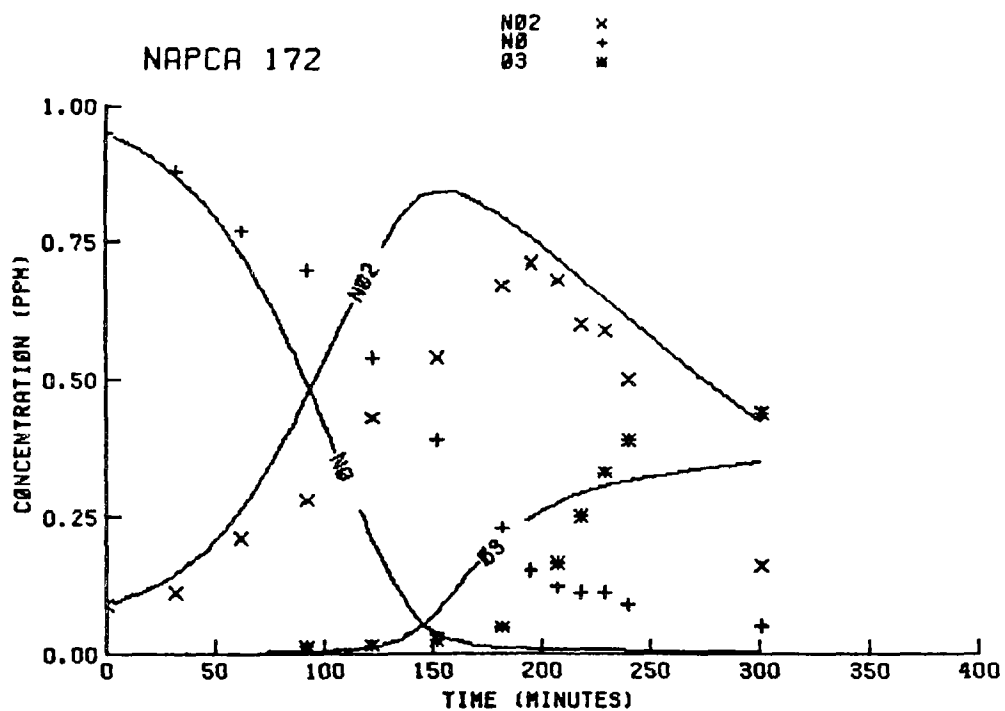
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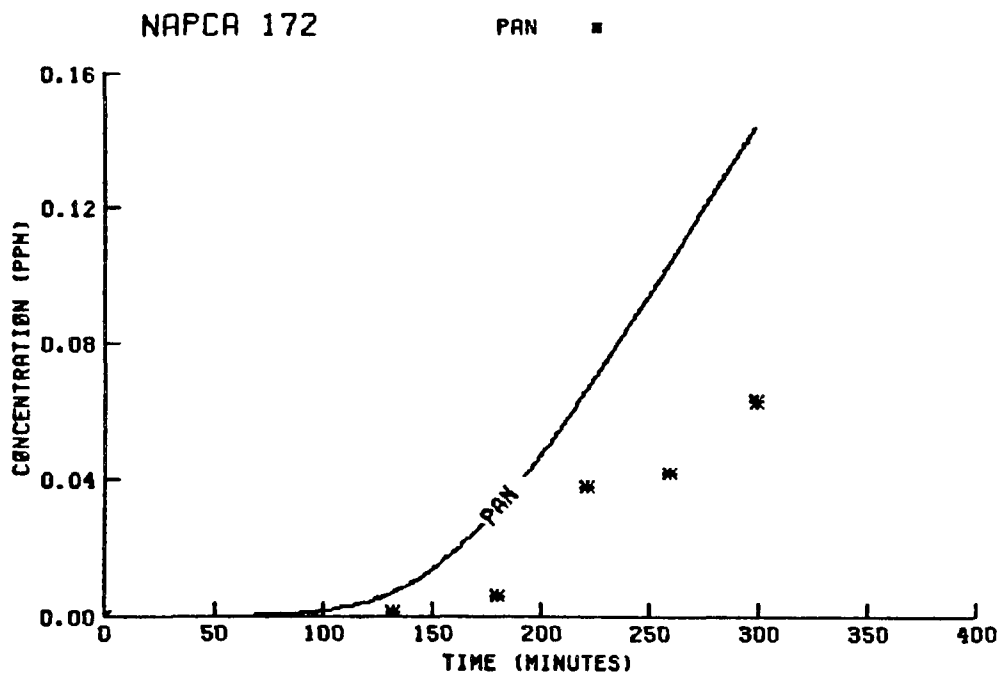
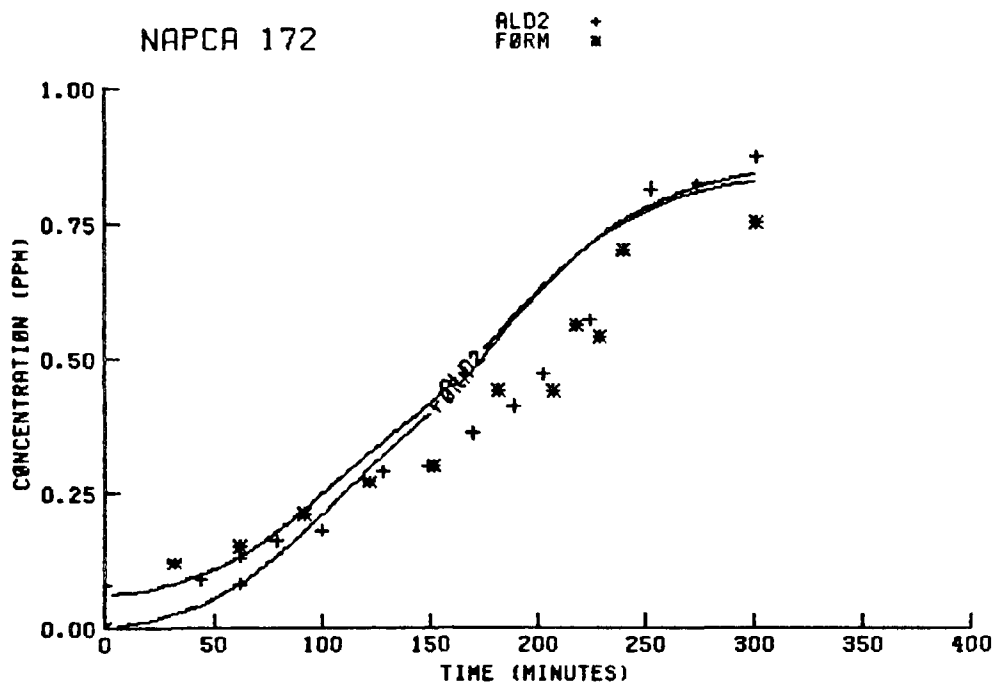
PAN x
ALD2 +
FORM *





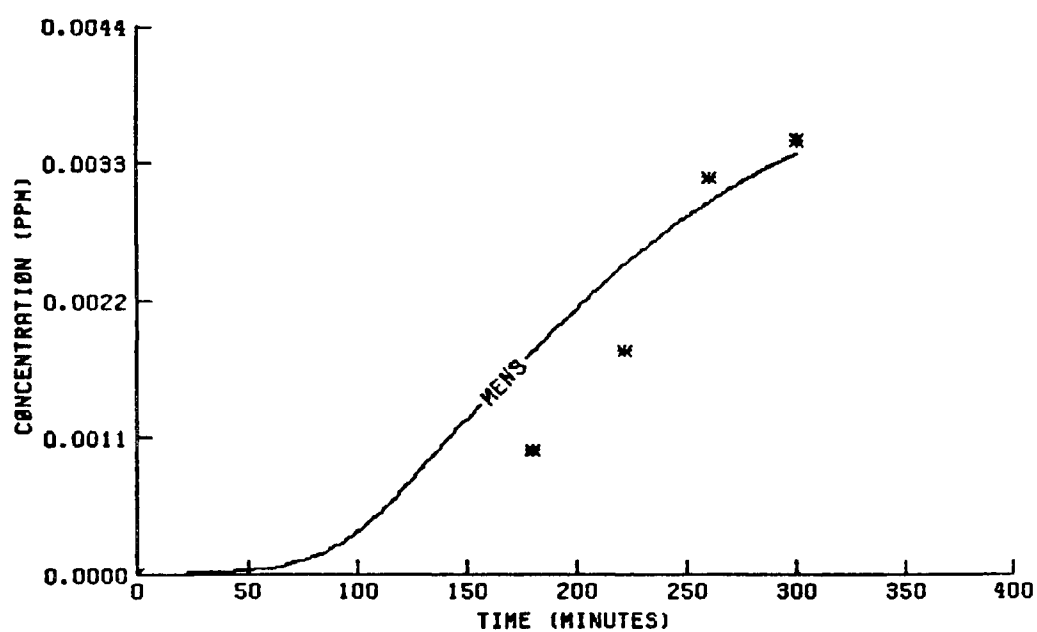




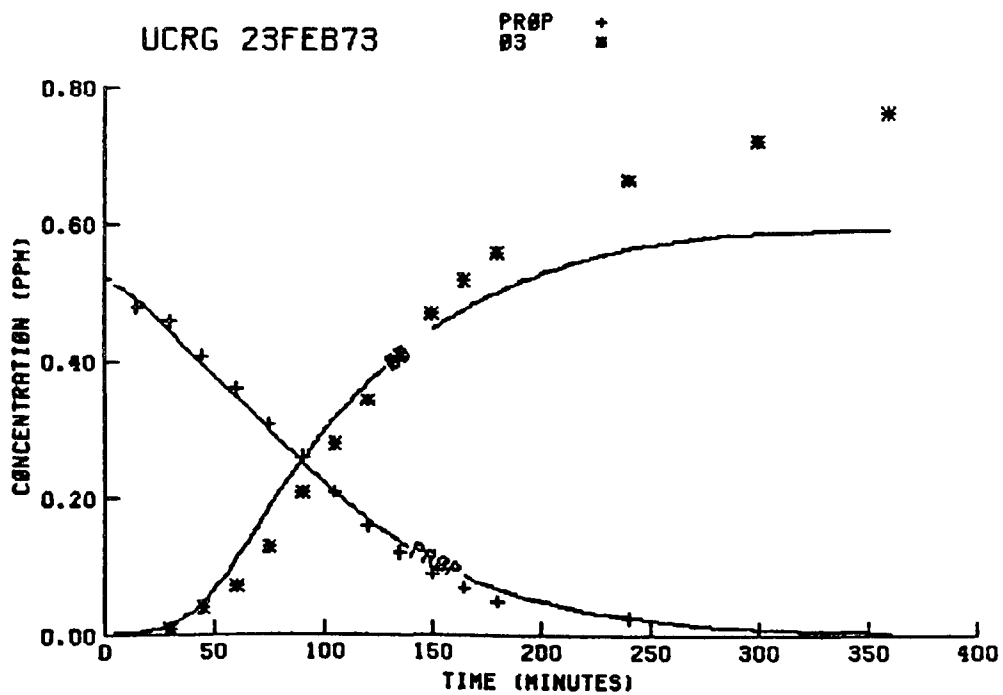
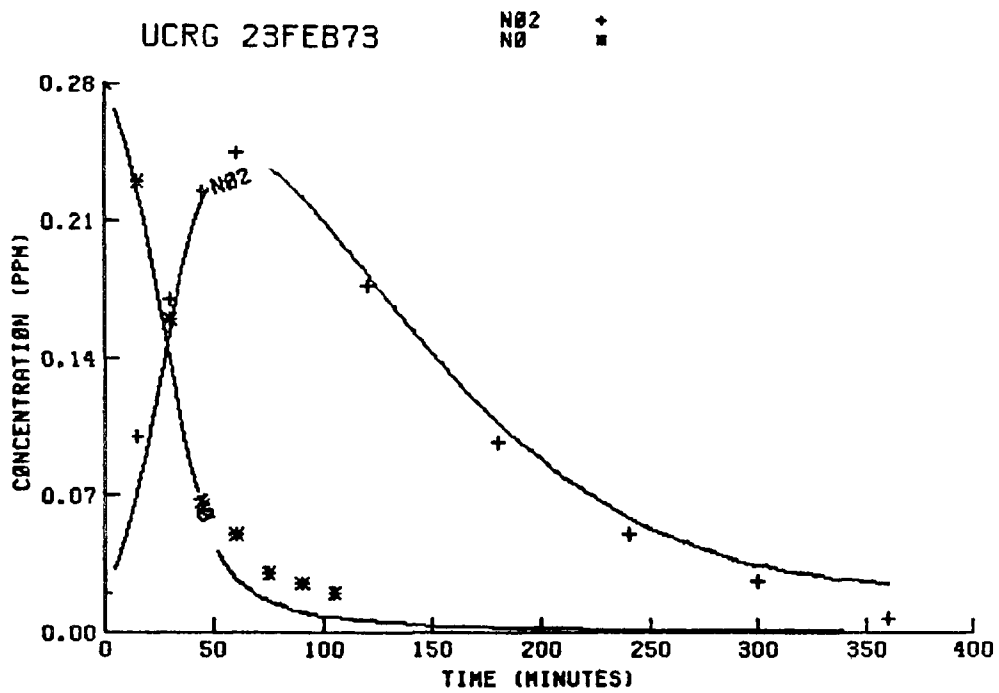


NAPCA 172

MEN3

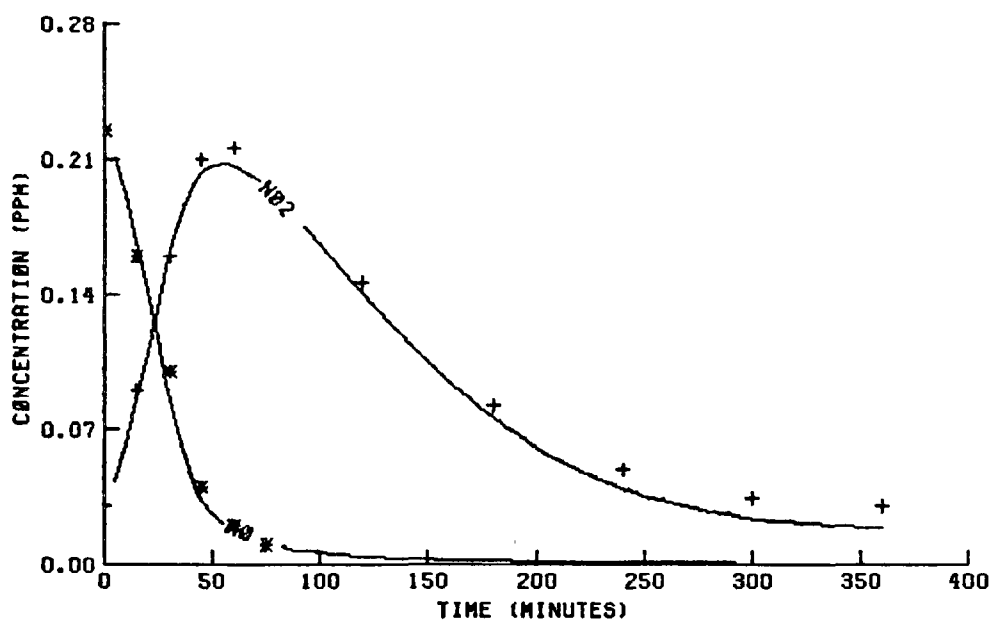


UCR-AGC CHAMBER EXPERIMENTS



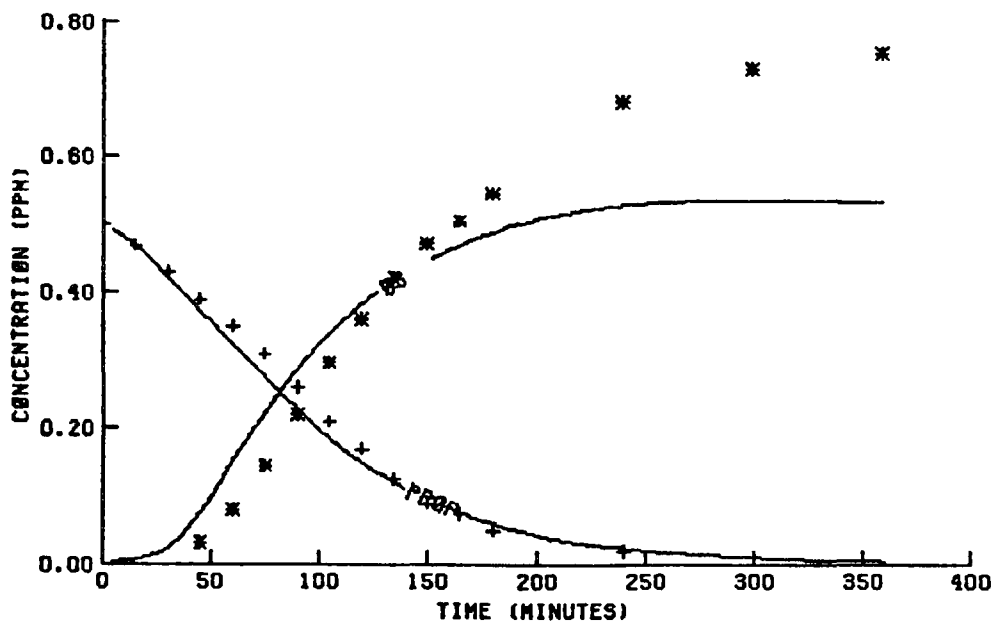
UCRG 5MAR73

N02 +
N0 *



UCRG 5MAR73

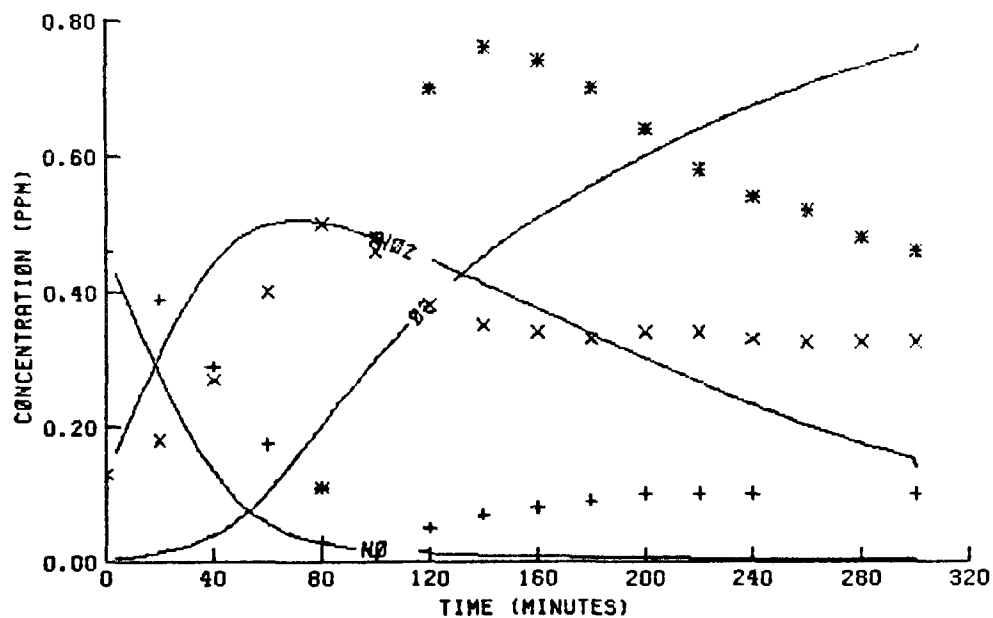
PR0P +
03 *

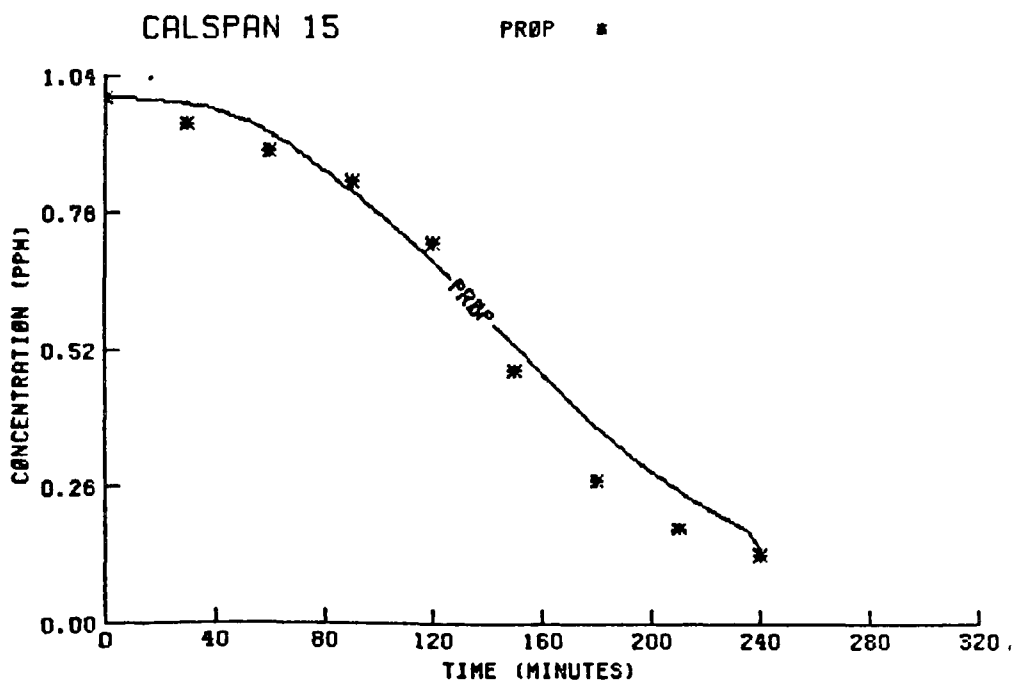
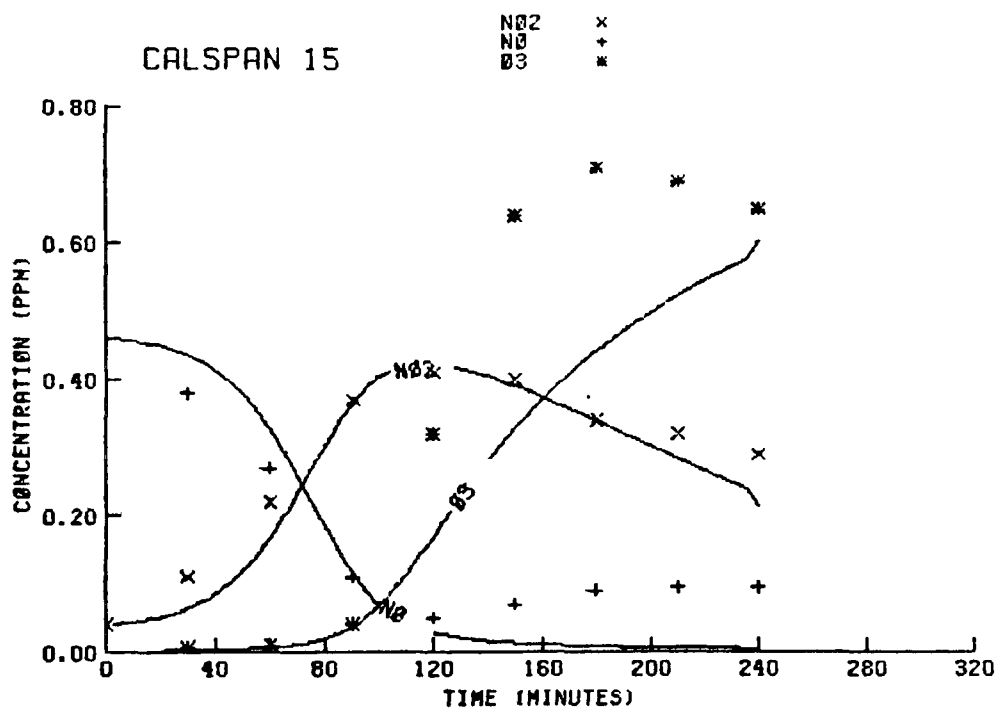


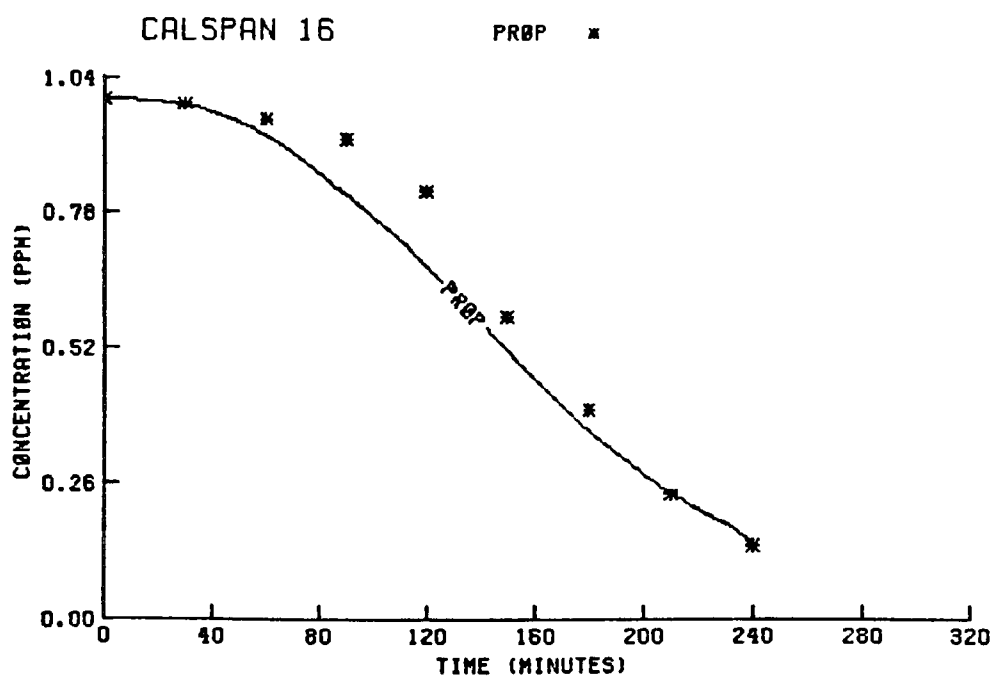
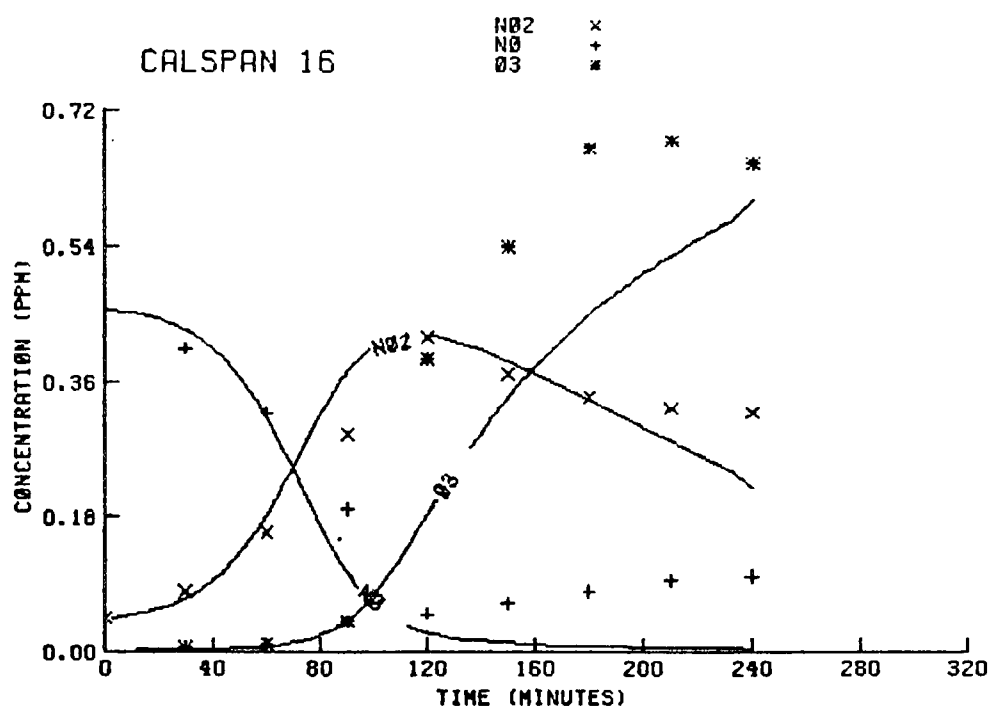
CALSPAN CHAMBER EXPERIMENTS

CALSPAN 11

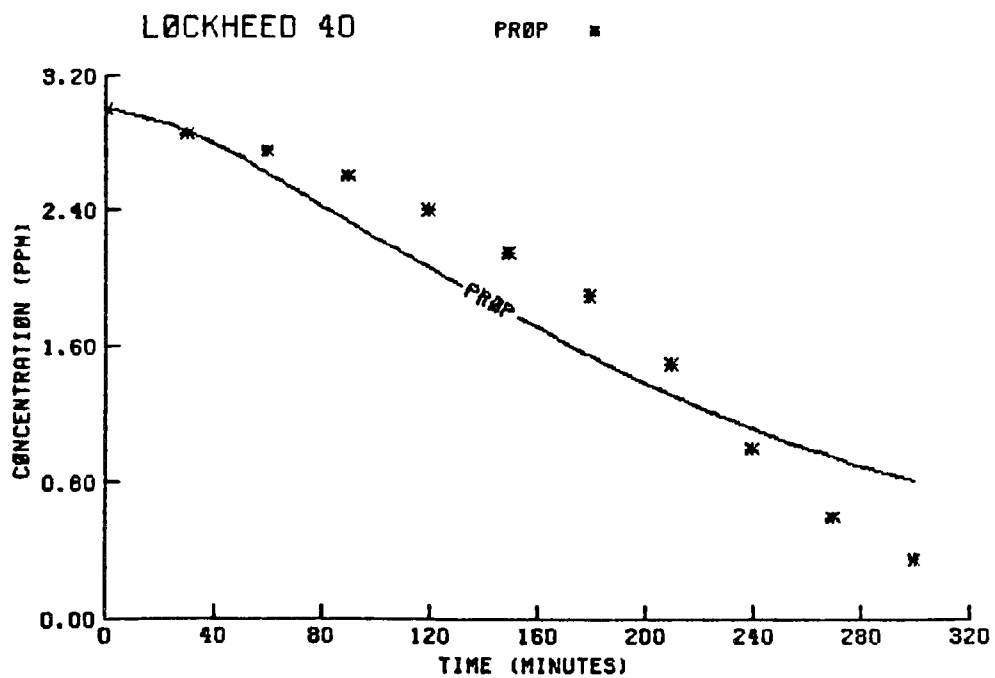
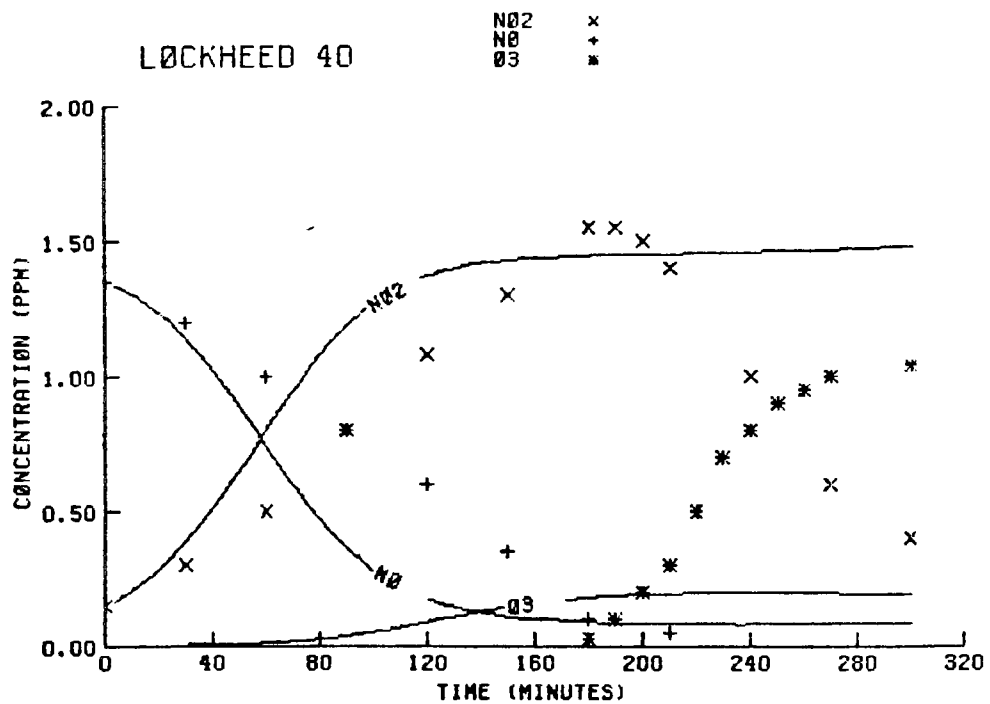
NO₂ x
NO +
O₃ *

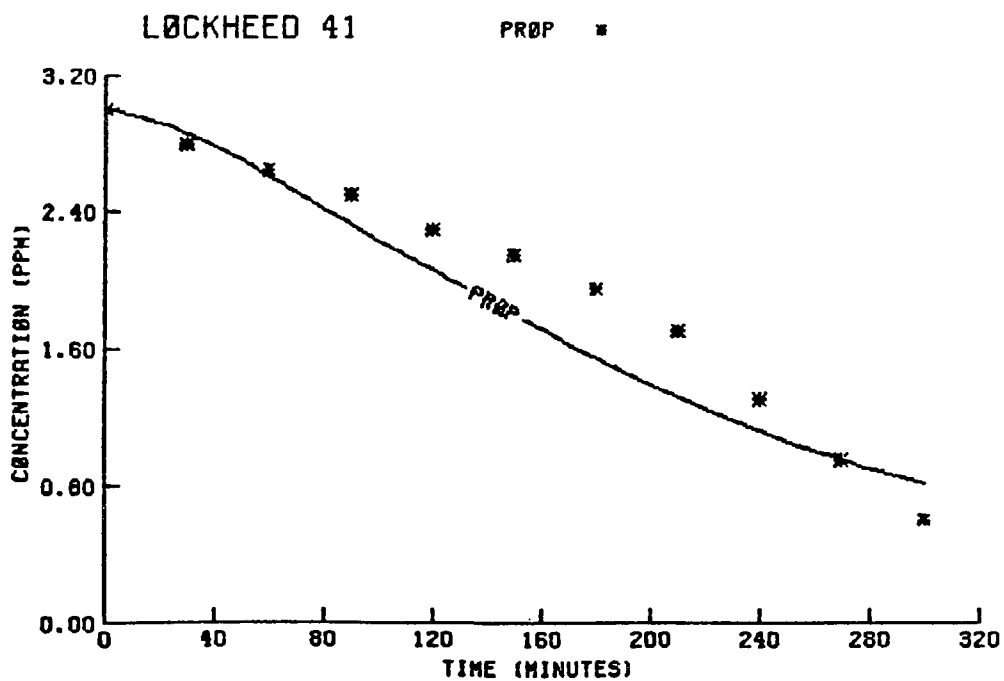
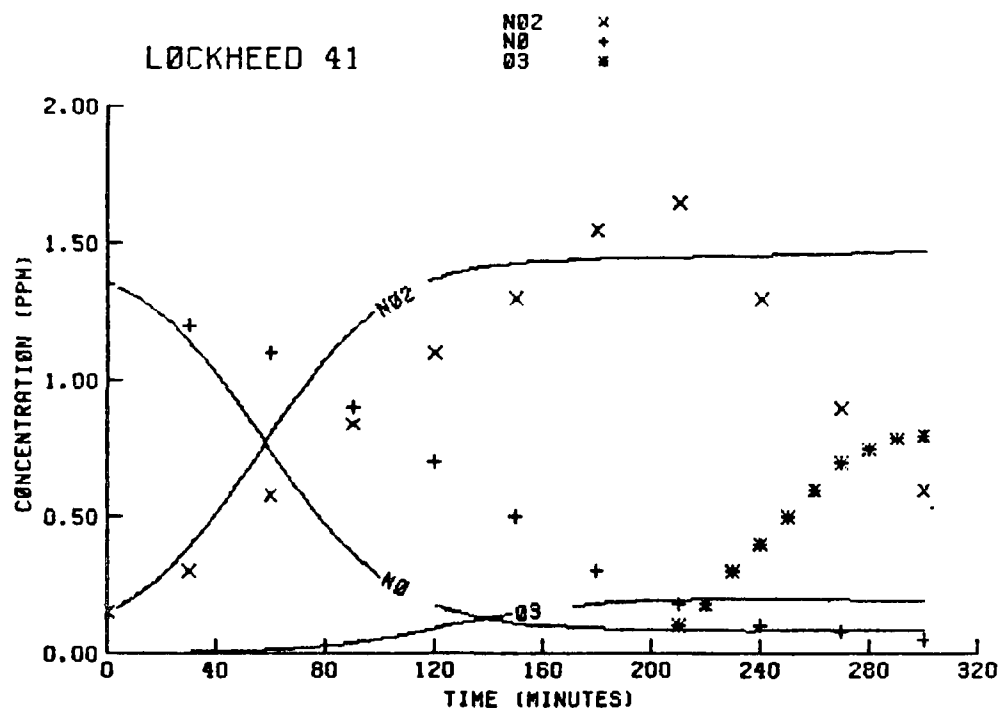


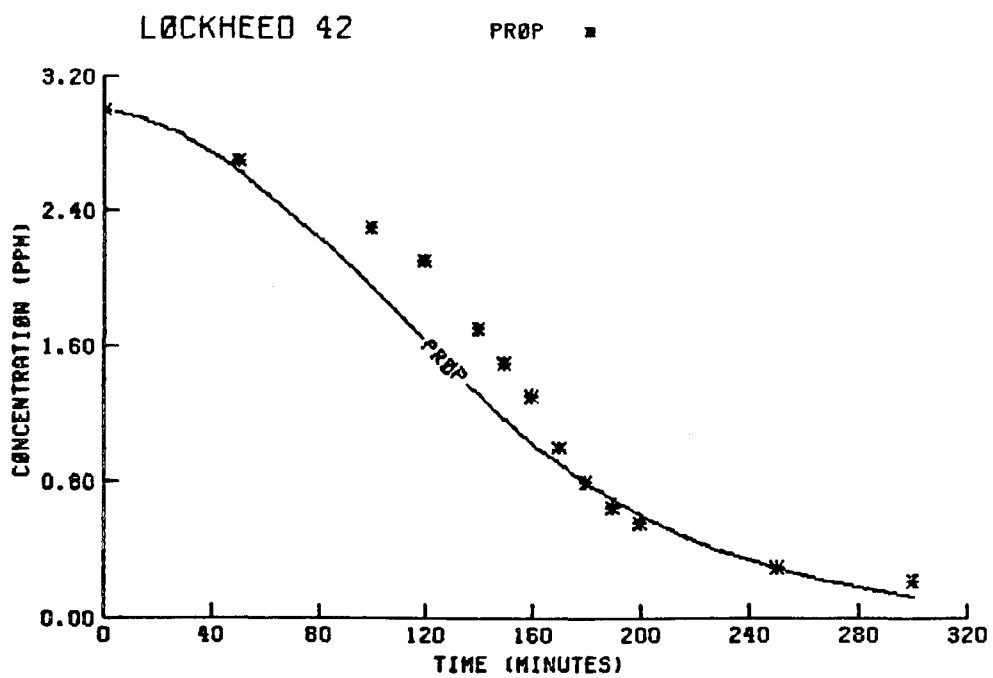
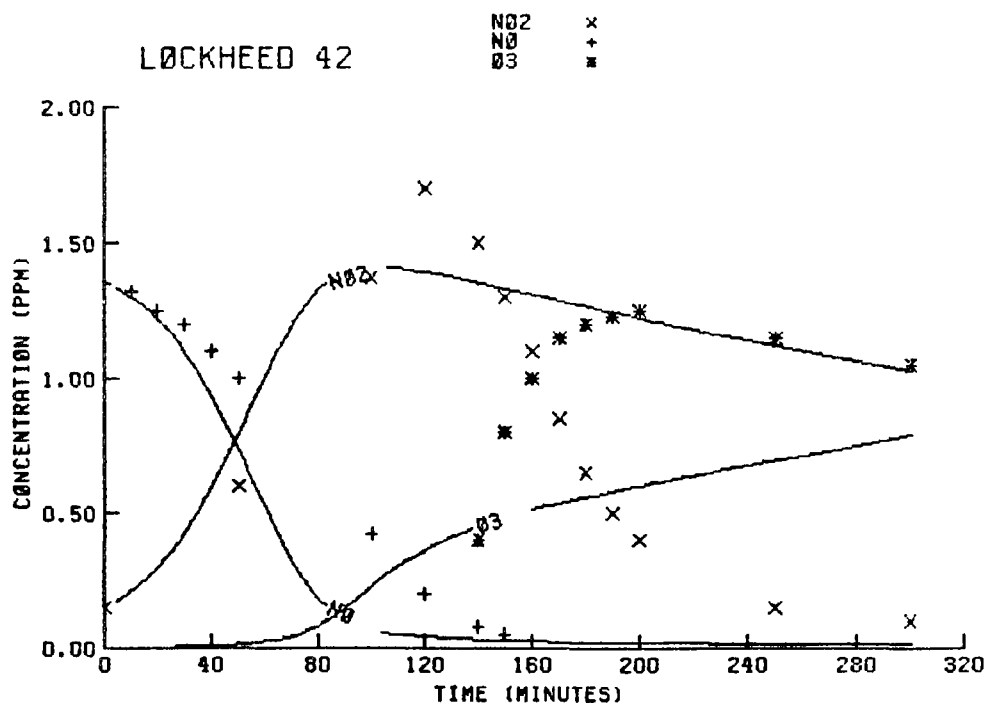


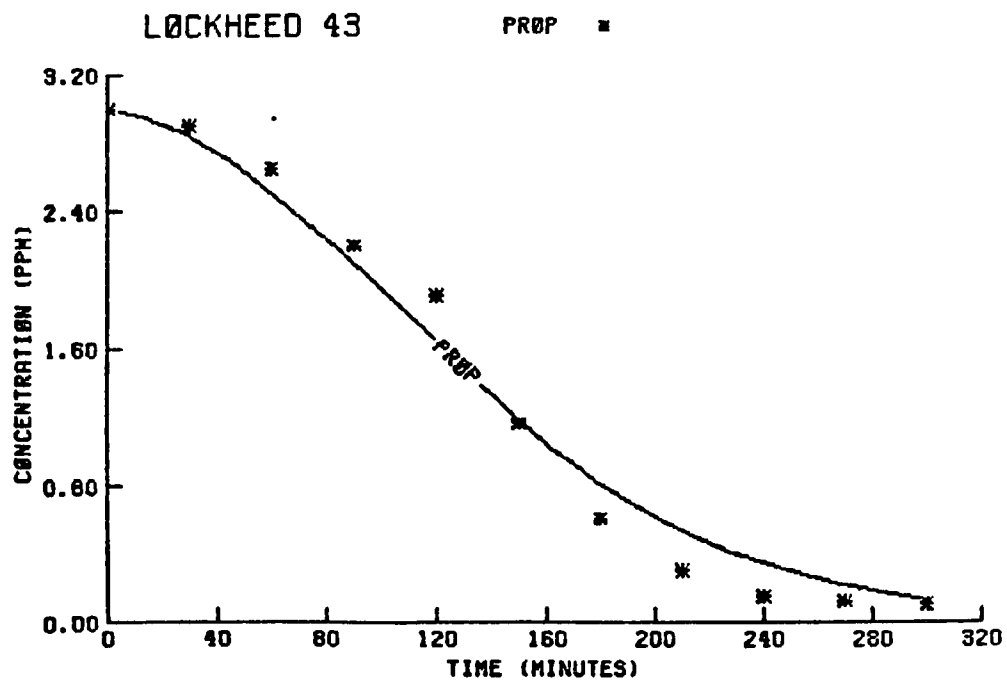
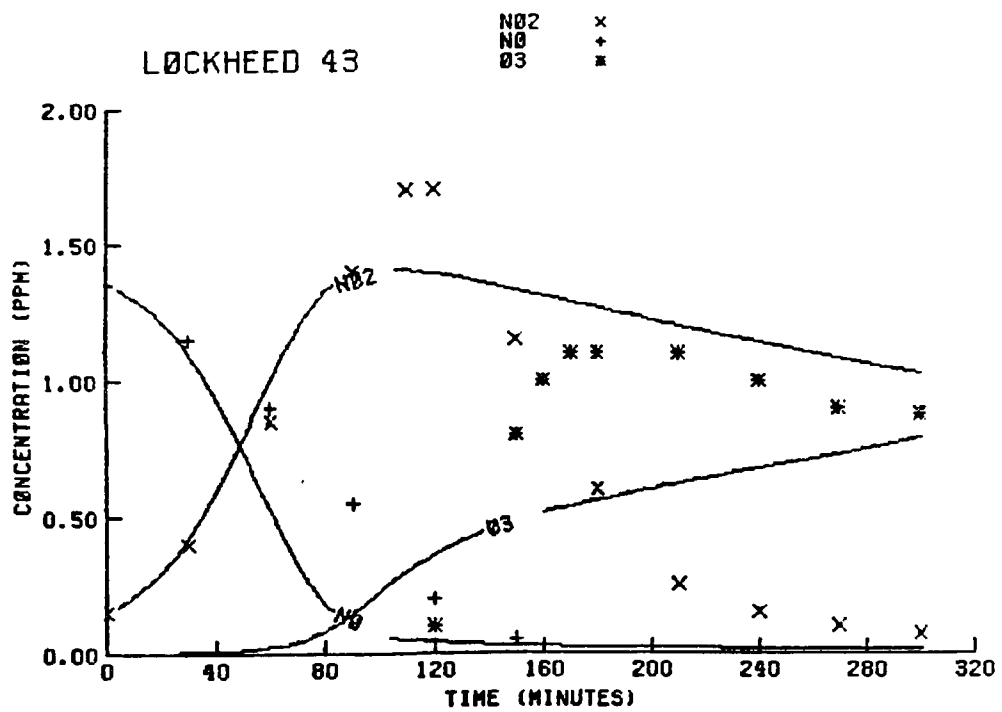


LOCKHEED CHAMBER EXPERIMENTS









TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

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16. ABSTRACT Computer modeling of smog chamber data is discussed in three parts. First, a series of detailed chemical mechanisms were developed to describe the photochemical formation of ozone from nitrogen oxides and the following organic compounds (alone and in various combinations): formaldehyde, acetaldehyde, ethylene, propylene, butane, 1-butene, trans-2-butene, and 2,3-dimethylbutane. Second, a generalized kinetic scheme intended for use in models simulating the formation of ozone in urban atmospheres was refined. The generalized mechanism includes a condensed version of the detailed mechanisms developed in the first part plus a semi-empirical scheme to describe the oxidation of aromatic hydrocarbons. Third, the effects of smog chambers on ozone formation were examined. For this part of the study, similar experiments using nitrogen oxides and propylene in eight different smog chambers were simulated using the detailed propylene mechanism. The main chamber effects identified thus far are apparently due to nitrogen oxides degassing from the walls during experiments and differences between chambers in the spectral distribution of ultraviolet irradiation. Volume 1 contains all textual material. Volume 2 contains graphs of measured and simulated pollutant concentrations for many smog chamber experiments.					
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