# APPENDIX A

## PLOTS OF RESULTS OF CHAMBER EXPERIMENTS AND MODEL SIMULATIONS

In this appendix, the concentration-time plots for the major species monitored in the surrogate-$NO_x$-air experiments and selected types of control runs carried out in this program are given. Table A-1 gives a list of the specific runs whose data are plotted, together with an indication of the type of run, in the order in which the plots can be found. The runs are ordered according to the type of run and the order in which their results are discussed in Section IV.

Model simulations of all of the control runs, and of most of the surrogate runs listed in Table A-1, have been carried out, and the results of the model simulations are plotted with the experimental results. The only runs for which model simulations were not carried out were the side equivalency tests carried out in the outdoor chamber, and runs OTC-219, 225 and 231, which were considered to have too many experimental problems to be useful for model testing.

For the surrogate-$NO_x$-air irradiations, the following notation is employed in Table A-1 and in the figure captions to indicate the type of experiment: For runs carried out in the indoor chamber, the notation "n-S", is employed, where "n" is the approximate nominal initial ROG/$NO_x$ ratio, and "S" refers to the surrogate type, which is either "B" for the base case surrogate, "MF" for the methanol + formaldehyde substitution surrogate, "M" for the methanol-only substitution surrogate, "BL" for the blank substitution surrogate, and "X" for surrogate mixtures which correspond to none of the above. For the outdoor chamber runs, the analogous notation "n-S1-S2" is employed, where "S1" refers to the surrogate type on side 1, and "S2" refers to the surrogate type on side 2.

Table A-1. List of Chamber Experiments for which Concentration-Time Plots are Given in this Appendix

| Figure | Run | Type of Run |
|---|---|---|
| A-1 | OTC-211 | n-Butane-$NO_x$-air runs |
| A-2 | OTC-246 | |
| A-3 | OTC-252 | |
| A-4 | ITC-860 | Propene-$NO_x$-air runs |
| A-5 | OTC-210 | |
| A-6 | OTC-233 | |
| A-7 | OTC-236 | |
| A-8 | OTC-244 | |
| A-9 | OTC-251 | |
| A-10 | ITC-864 | Tracer-$NO_x$-air runs , with formaldehyde |
| A-11 | OTC-235 | added at t = 2 hours. |
| A-12 | ITC-863 | Tracer-$NO_x$-air runs , with methanol |
| A-13 | ITC-887 | added at t = 2 hours. |
| | | ITC surrogate-$NO_x$-air runs: |
| A-14 | ITC-865 | 15-B |
| A-15 | ITC-891 | 15-B |
| A-16 | ITC-867 | 15-MF |
| A-17 | ITC-888 | 15-M |
| A-18 | ITC-868 | 15-BL |
| A-19 | ITC-871 | 6-B |
| A-20 | ITC-872 | 6-MF |
| A-21 | ITC-877 | 6-MF |
| A-22 | ITC-874 | 6-M |
| A-23 | ITC-873 | 6-BL |
| A-24 | ITC-880 | 3-B |
| A-25 | ITC-881 | 3-MF |
| A-26 | ITC-886 | 3-M |
| A-27 | ITC-885 | 3-BL |
| | | OTC Surrogate-$NO_x$-air runs. |
| A-28 | OTC-241 | 13-B-MF |
| A-29 | OTC-224 | 13-M-B |

(continued)

Table A-1 (concluded) - 2

| Figure | Run | Type of Run | |
|---|---|---|---|
| A-30 | OTC-215 | 10-B-MF | |
| A-31 | OTC-249 | 10-B-MF | |
| A-32 | OTC-243 | 10-B-MF | |
| A-33 | OTC-217 | 10-M-B | |
| A-34 | OTC-237 | 10-B-M | |
| A-35 | OTC-222 | 10-M-MF | |
| A-36 | OTC-223 | 10-B-BL | |
| A-37 | OTC-238 | 10-BL-MF | |
| A-38 | OTC-214 | 10-MF-MF | (side equivalency test) |
| A-39 | OTC-250 | 10-MF-MF | (side equivalency test) |
| A-40 | OTC-221 | 7-MF-B | |
| A-41 | OTC-248 | 7-B-MF | |
| A-42 | OTC-242 | 7-M-B | |
| A-43 | OTC-219 | 7-MF-M | (not modeled) |
| A-44 | OTC-239 | 7-MF-M | |
| A-45 | OTC-230 | 7-B-BL | |
| A-46 | OTC-229 | 7-M-BL | |
| A-47 | OTC-226 | 7-B-B | (side equivalency test) |
| A-48 | OTC-228 | 5-B-MF | |
| A-49 | OTC-225 | 5-B-MF | (not modeled) |
| A-50 | OTC-240 | 5-M-B | |
| A-51 | OTC-231 | 5-X-MF | (not modeled) |

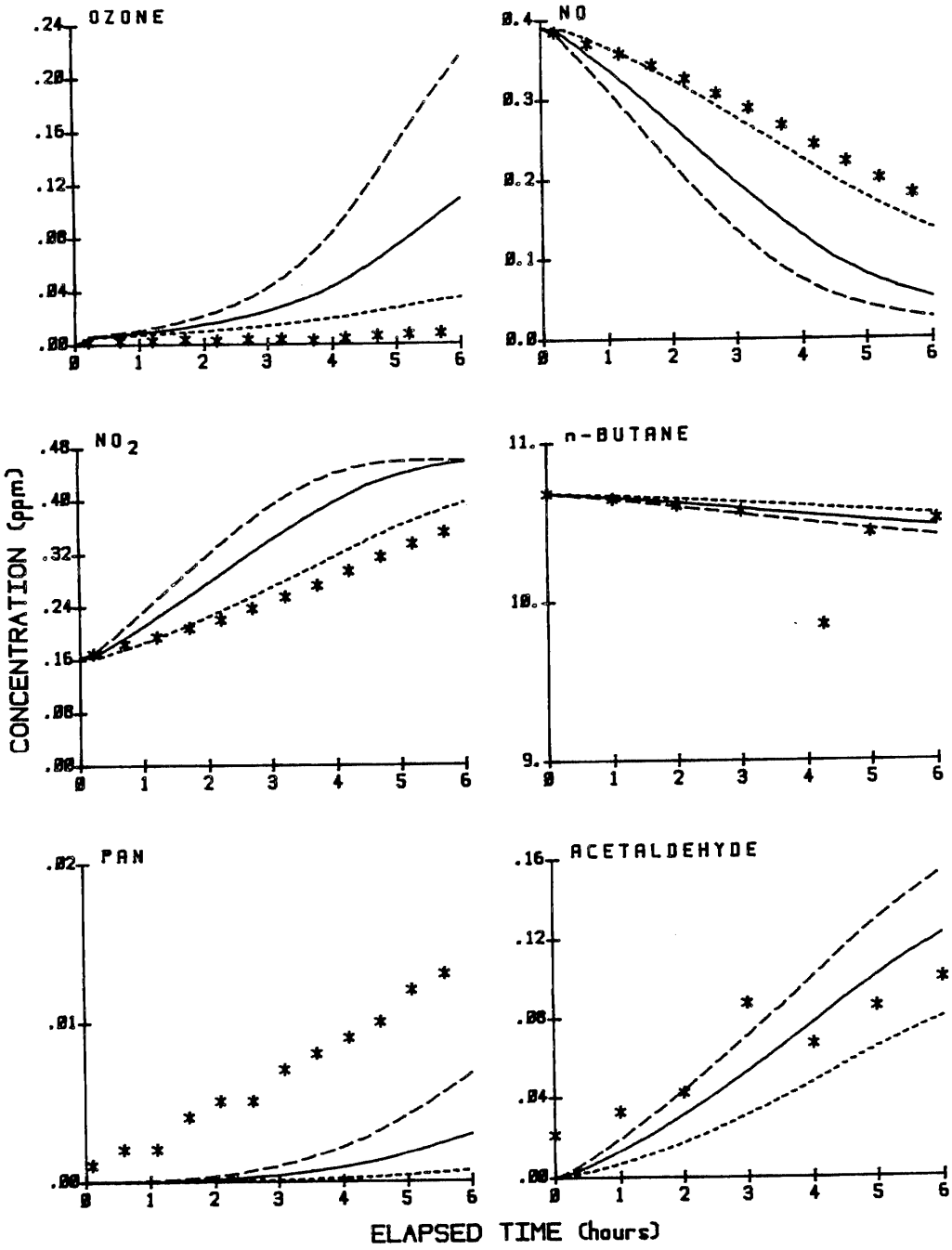


Figure A-1. Experimental and calculated concentration-time plots for selected species observed in the n-butane-$NO_x$-air run OTC-211.

* = experimental data
..... = model calculation, $k_{RS}$ = 0.1 ppb
——— = model calculation, $k_{RS}$ = 0.2 ppb
- - - = model calculation, $k_{RS}$ = 0.3 ppb

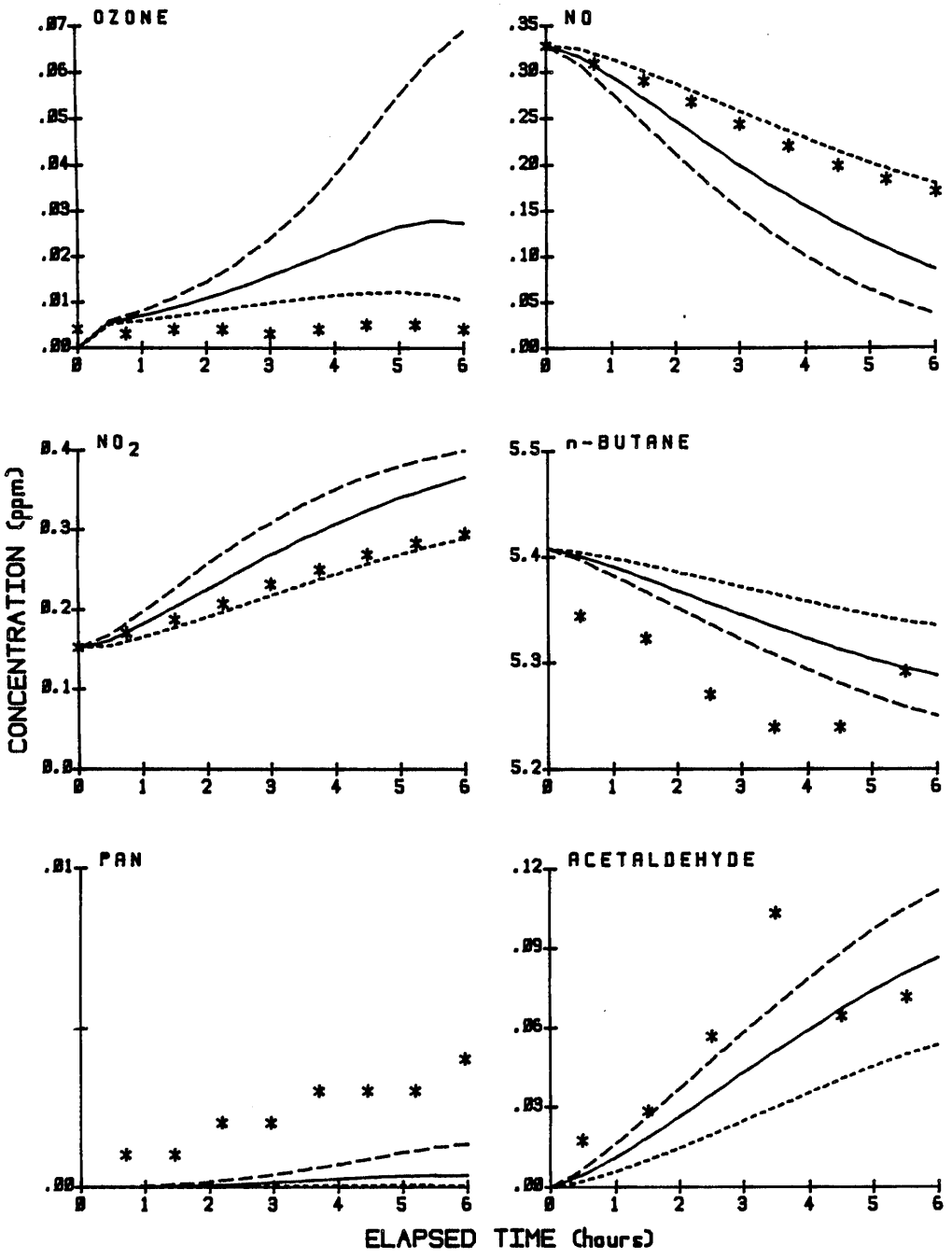


Figure A-2. Experimental and calculated concentration-time plots for selected species observed in the n-butane-$NO_x$-air run OTC-246.

* = experimental data, side A
X = experimental data, side B
..... = model calculation, $k_{RS}$ = 0.1 ppb
——— = model calculation, $k_{RS}$ = 0.2 ppb
- - - = model calculation, $k_{RS}$ = 0.3 ppb

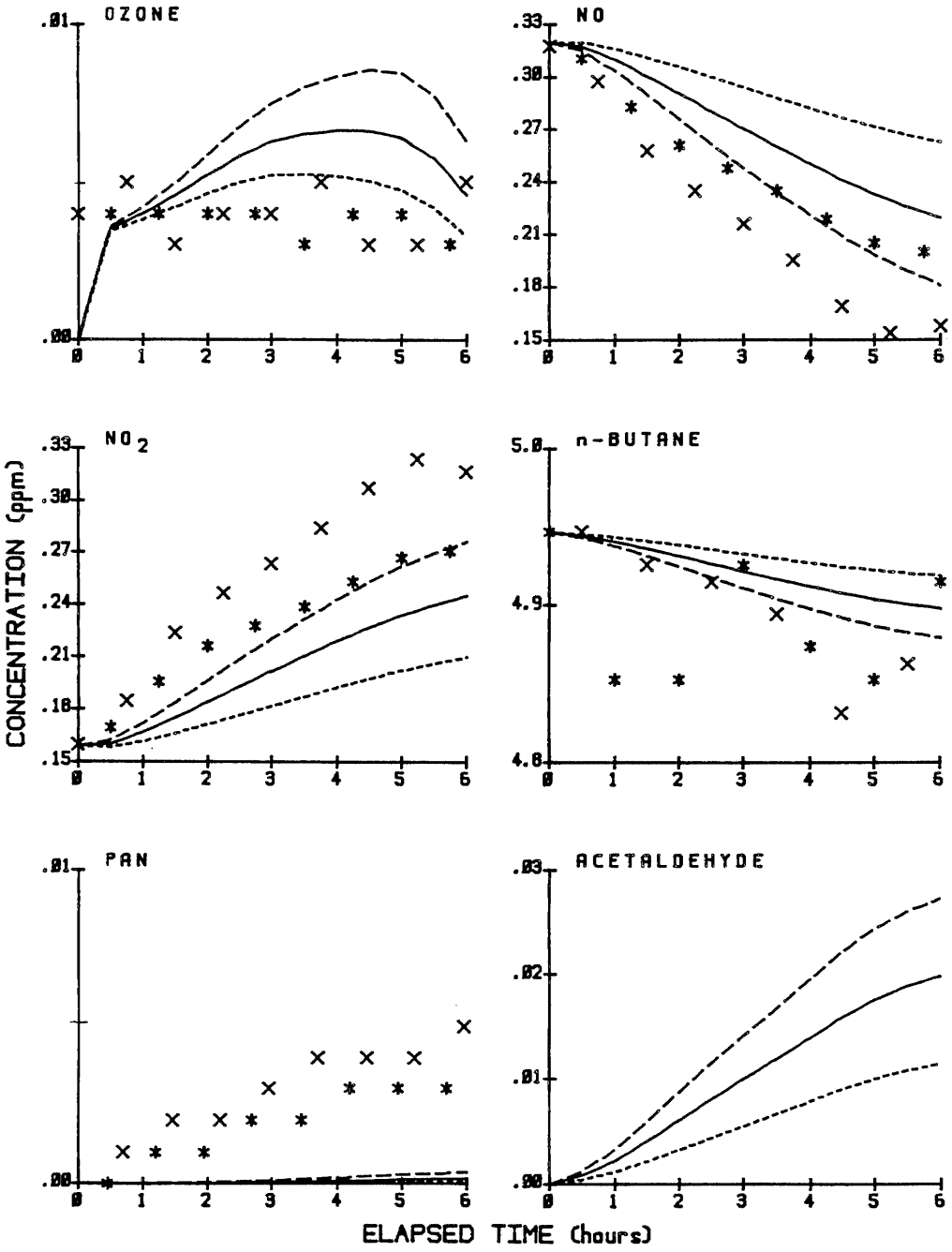


Figure A-3. Experimental and calculated concentration-time plots for selected species observed in the n-butane-$NO_x$-air run OTC-252.

* = experimental data, side A
X = experimental data, side B
..... = model calculation, $k_{RS}$ = 0.1 ppb
——— = model calculation, $k_{RS}$ = 0.2 ppb
- - - = model calculation, $k_{RS}$ = 0.3 ppb

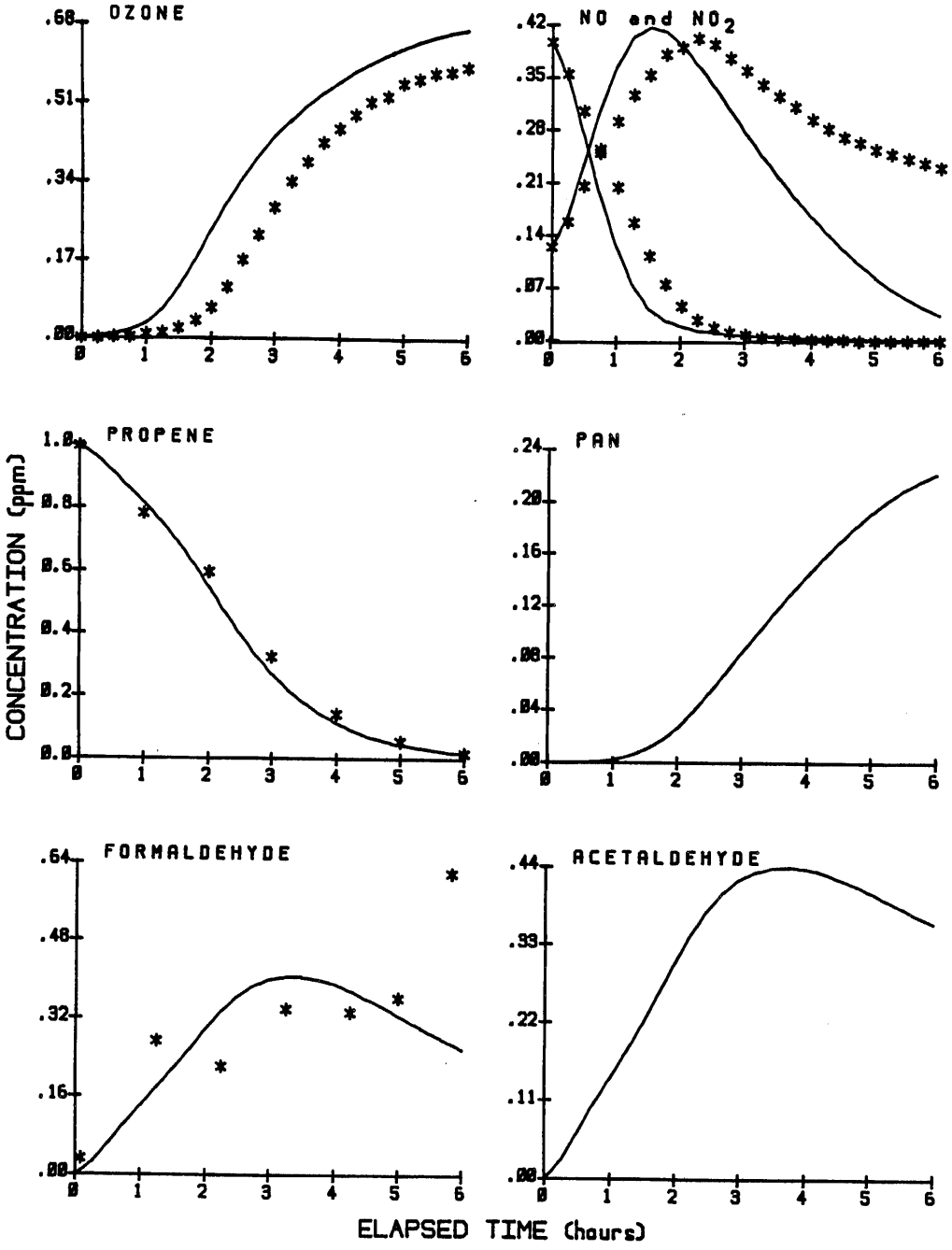


Figure A-4. Experimental and calculated concentration-time plots for selected species observed in the propene-$NO_x$-air run ITC-860.

* = experimental data
——— = model calculation

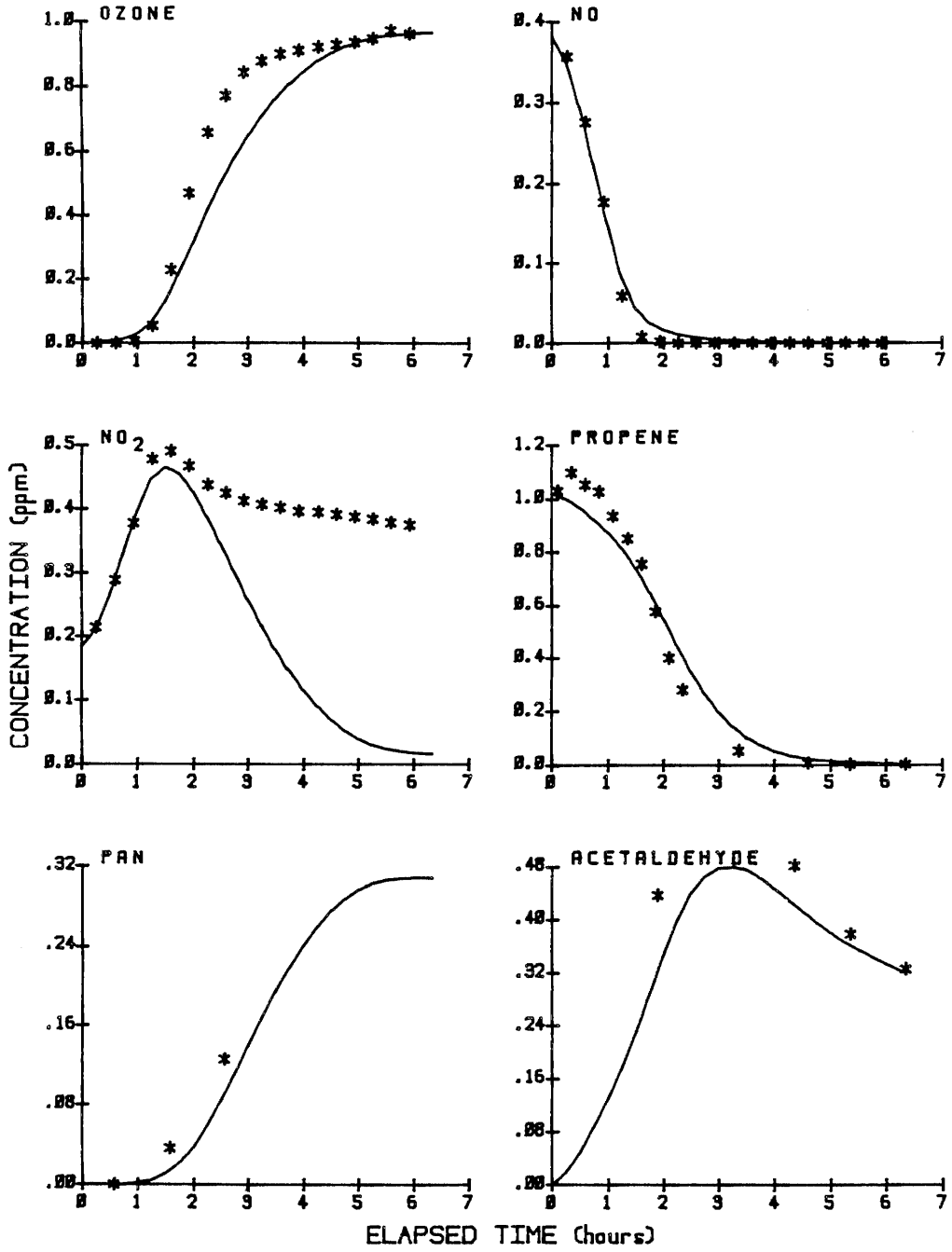


Figure A-5. Experimental and calculated concentration-time plots for selected species observed in the propene-$NO_x$-air run OTC-210.

* = experimental data
——— = model calculation

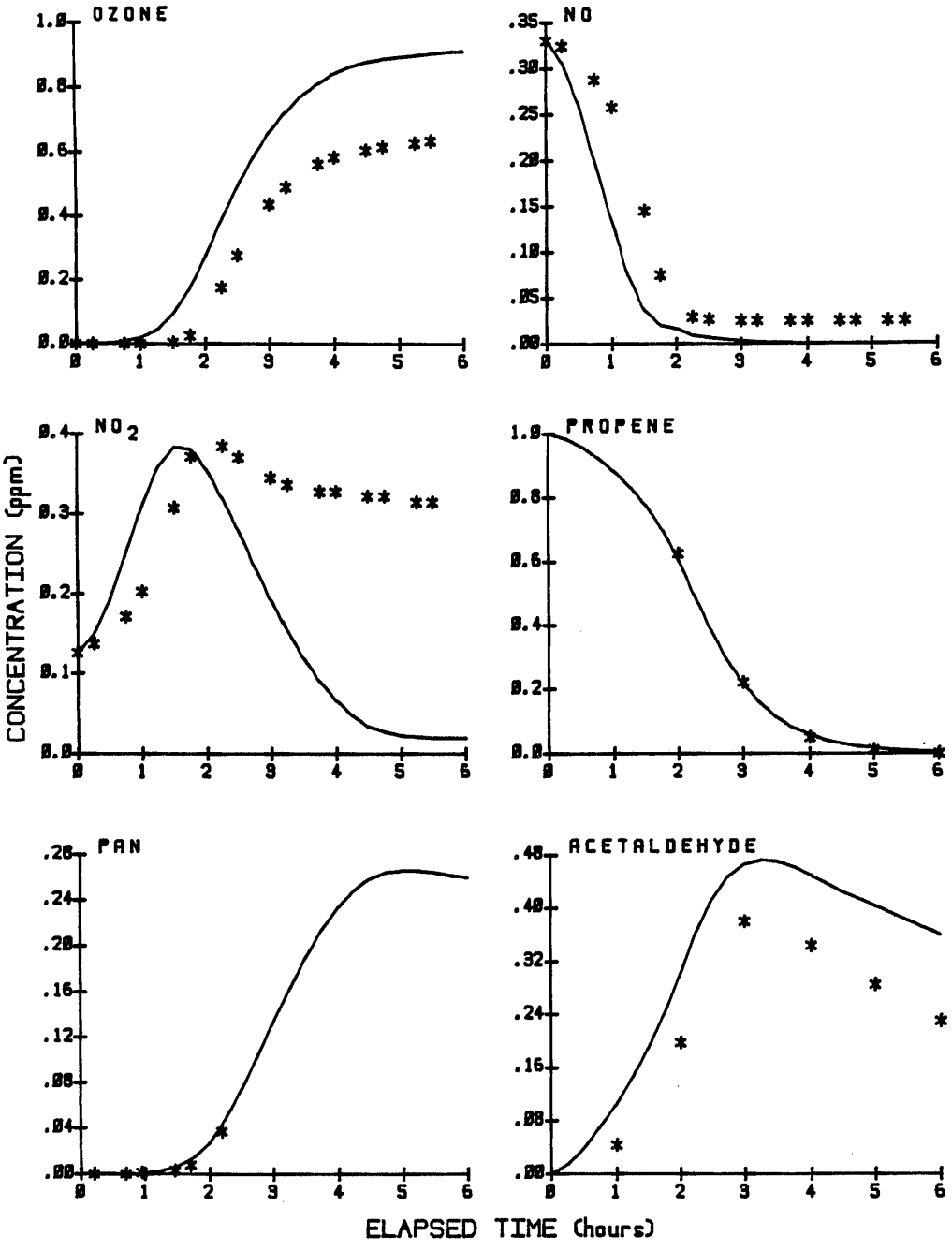


Figure A-6. Experimental and calculated concentration-time plots for selected species observed in the propene-$NO_x$-air run OTC-233.

* = experimental data
——— = model calculation

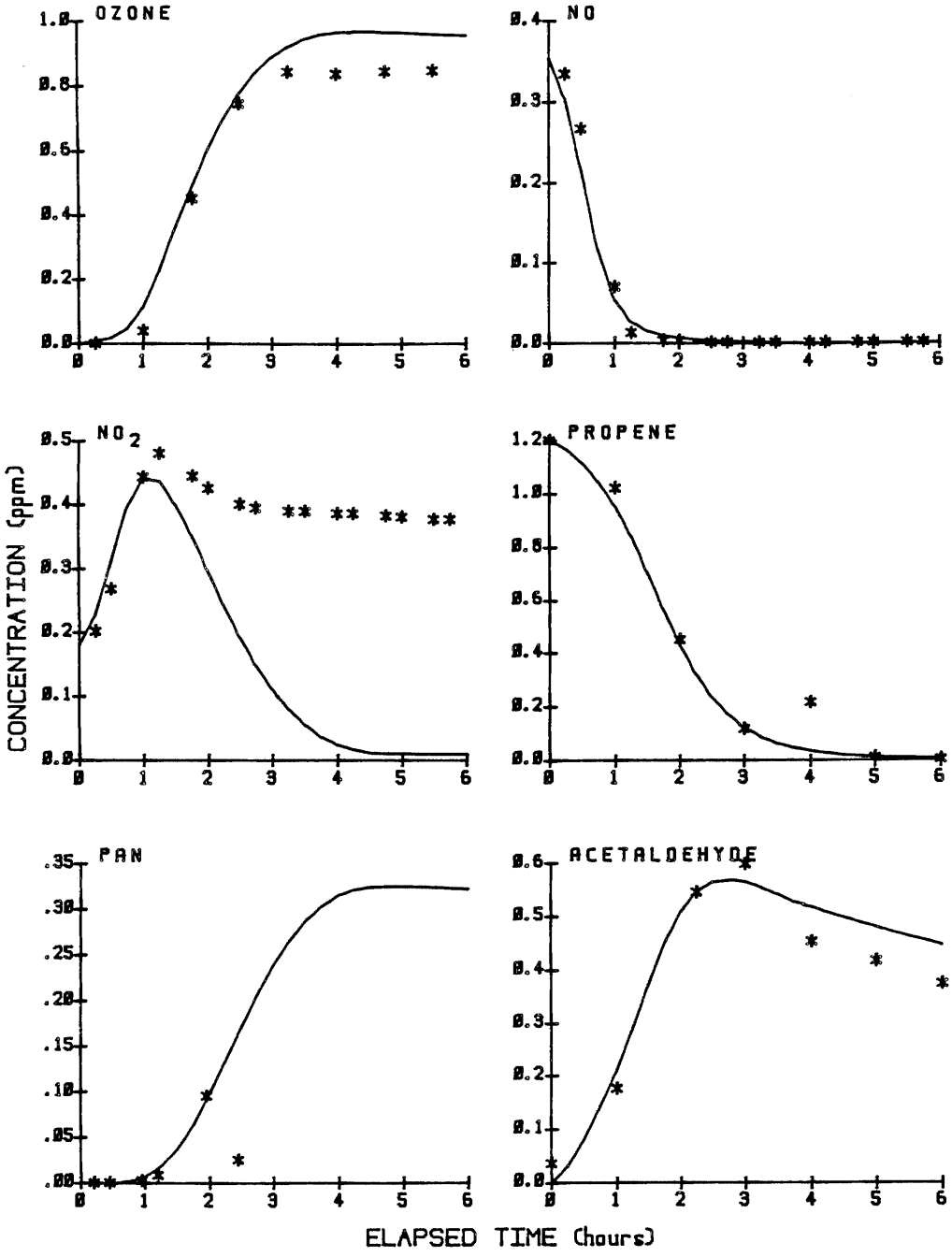


Figure A-7. Experimental and calculated concentration-time plots for selected species observed in the propene-$NO_x$-air run OTC-236.

* = experimental data
——— = model calculation

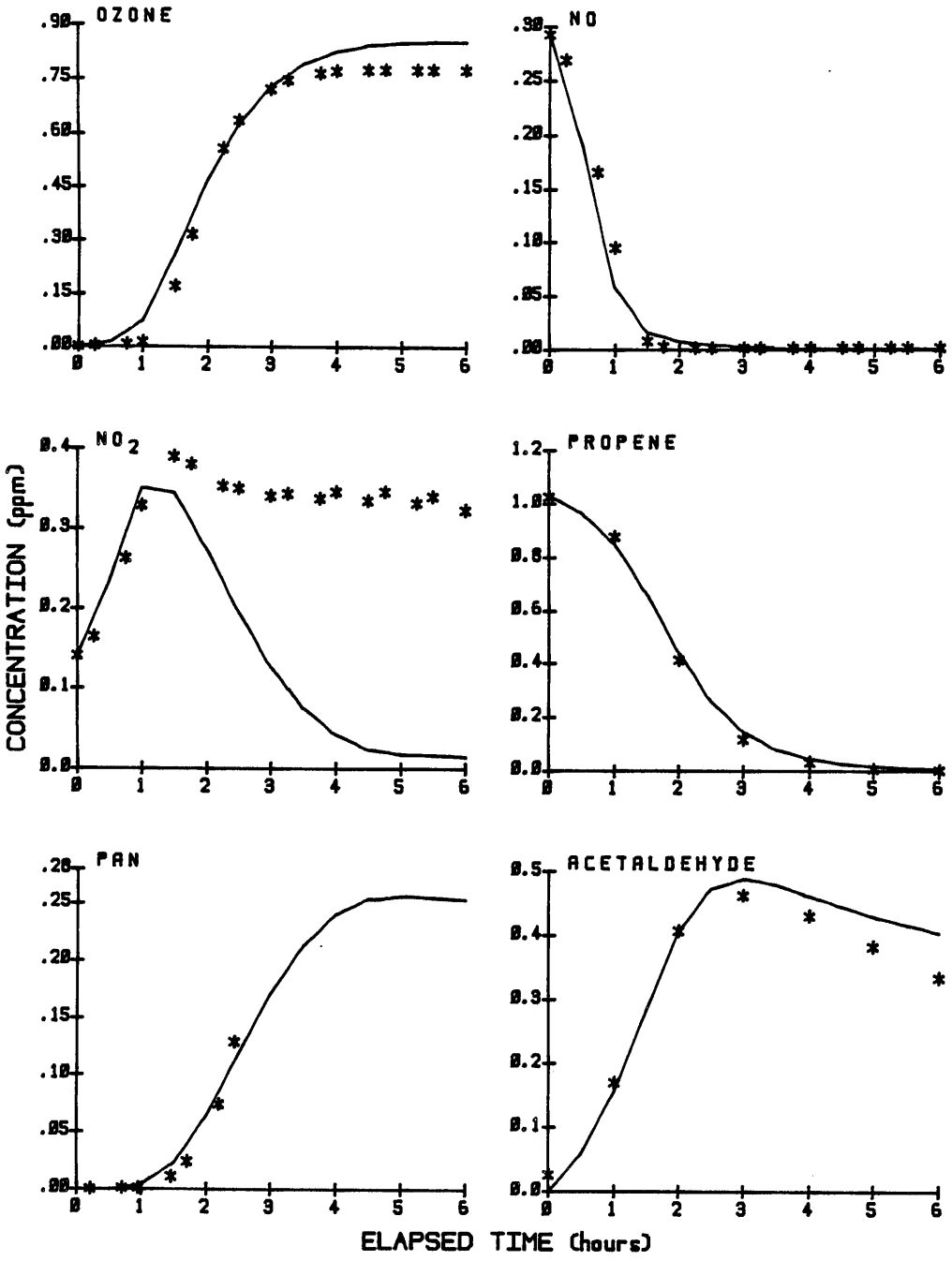


Figure A-8. Experimental and calculated concentration-time plots for selected species observed in the propene-$NO_x$-air run OTC-244.

* = experimental data
——— = model calculation

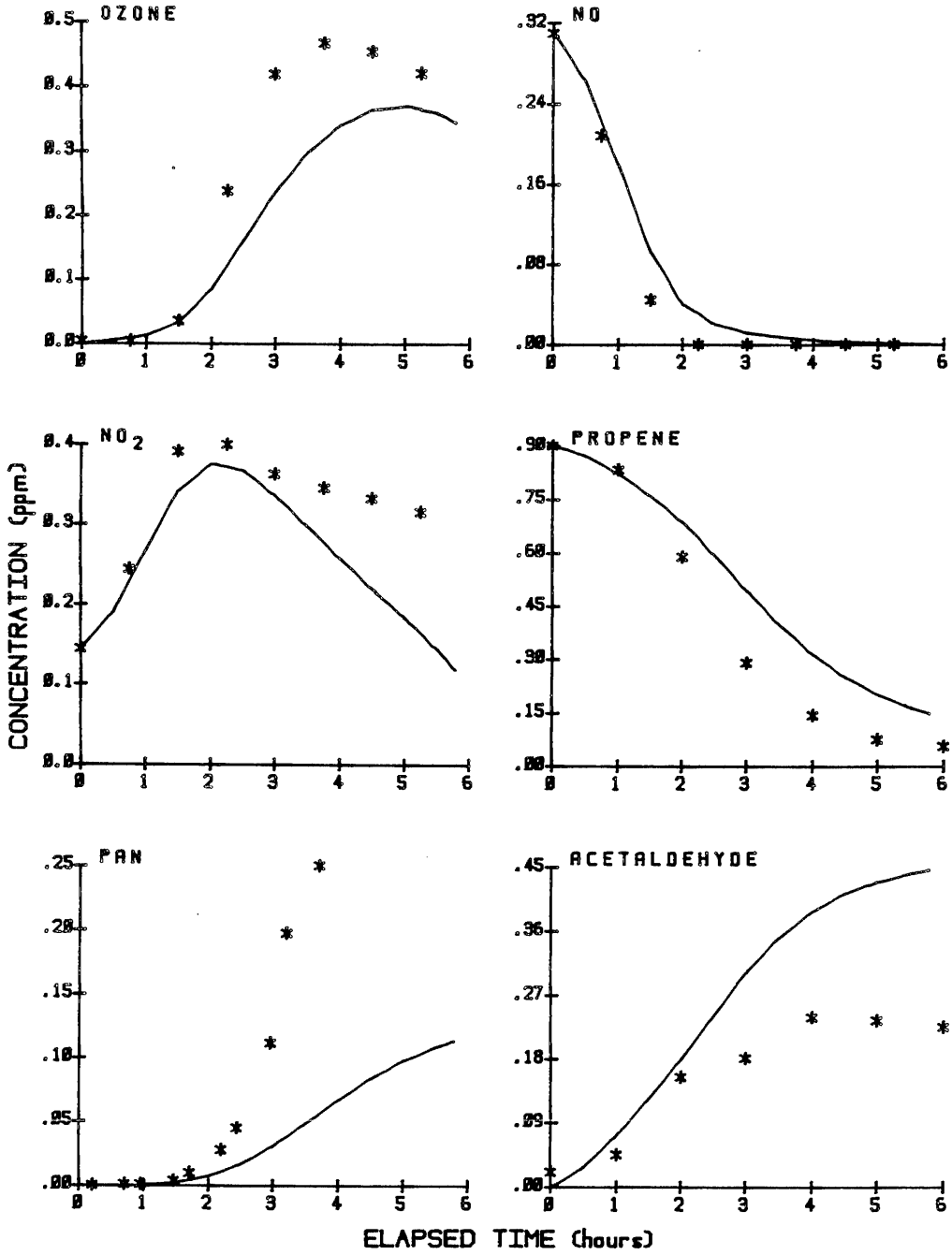


Figure A-9. Experimental and calculated concentration-time plots for selected species observed in the propene-$NO_x$-air run OTC-251.

* = experimental data
——— = model calculation

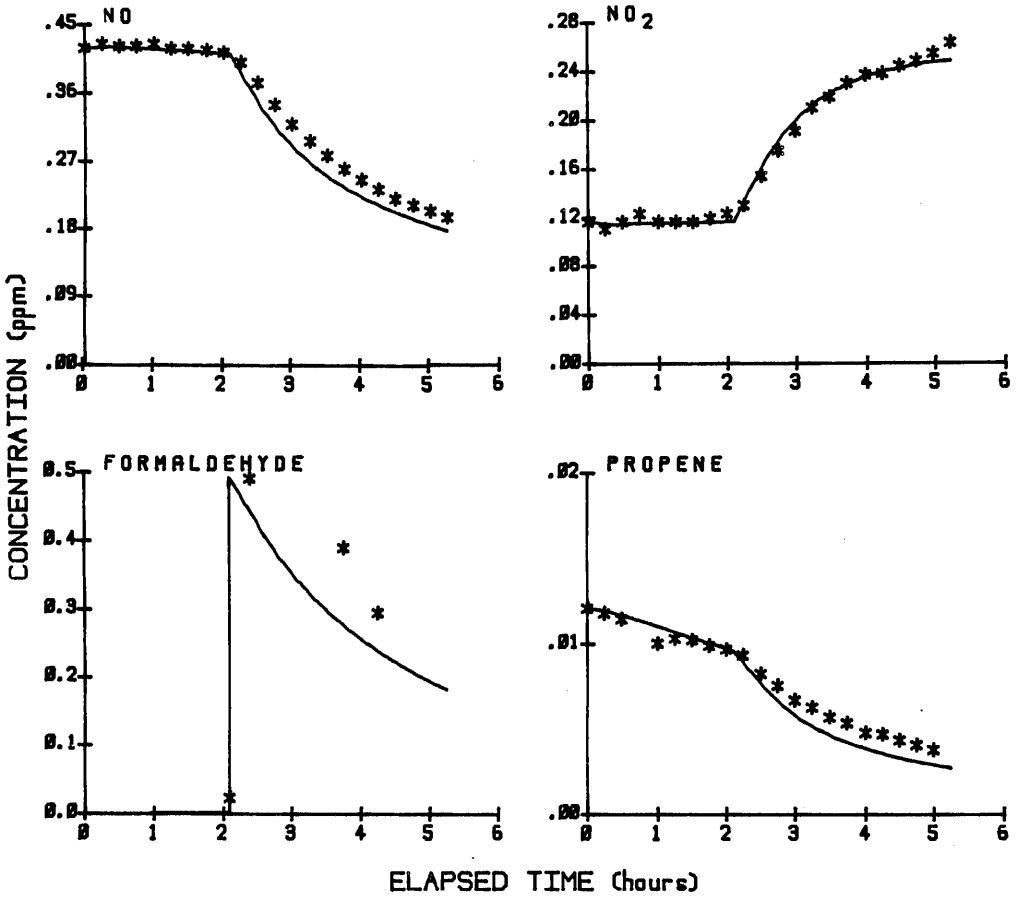


Figure A-10. Experimental and calculated concentration-time plots for selected species observed in the tracer-$NO_x$-air, with added formaldehyde, run ITC-864.

* = experimental data
——— = model calculation

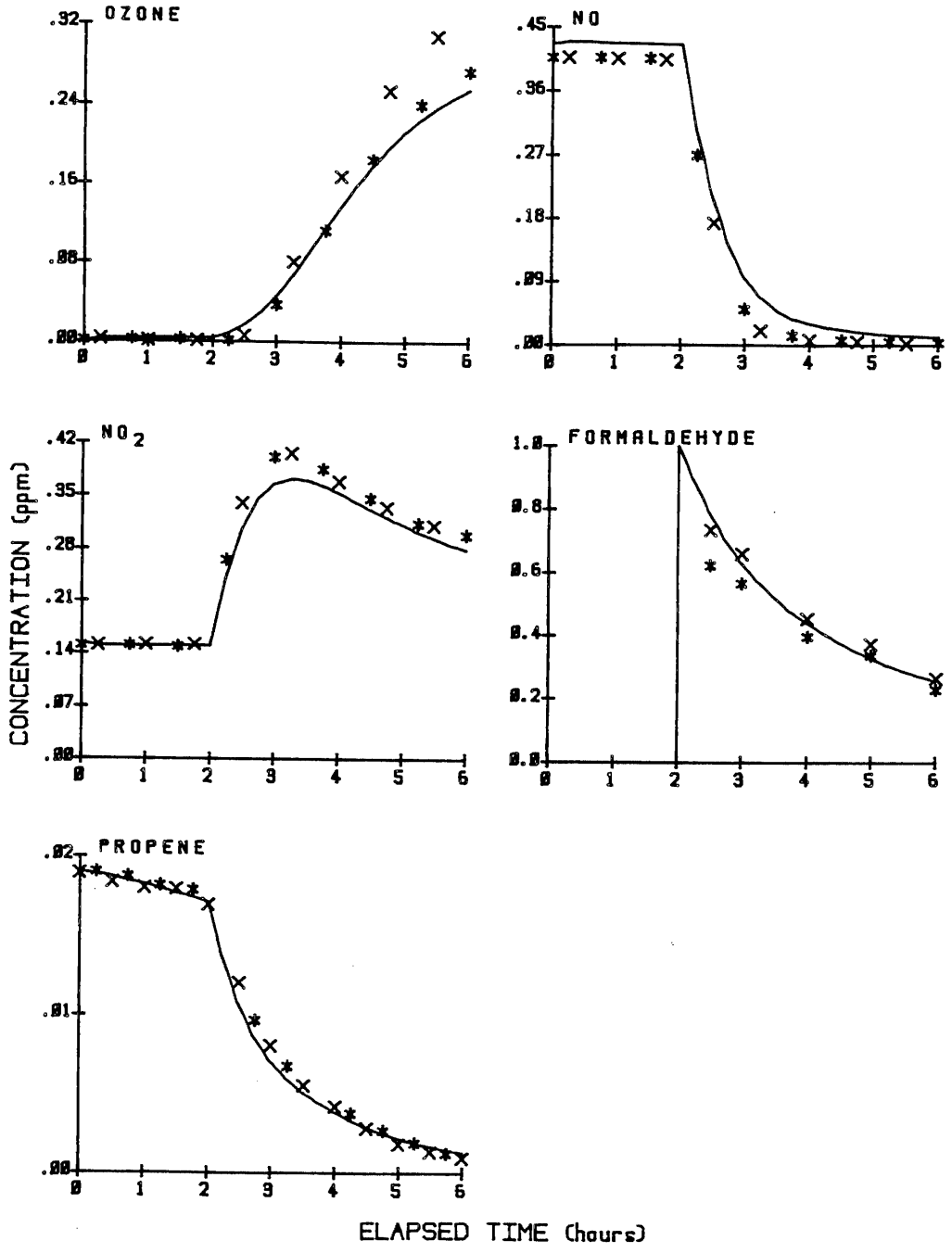


Figure A-11. Experimental and calculated concentration-time plots for selected species observed in the tracer-$NO_x$-air, with added formaldehyde, run OTC-235.

* = experimental data, side A
X = experimental data, side B
——— = model calculation

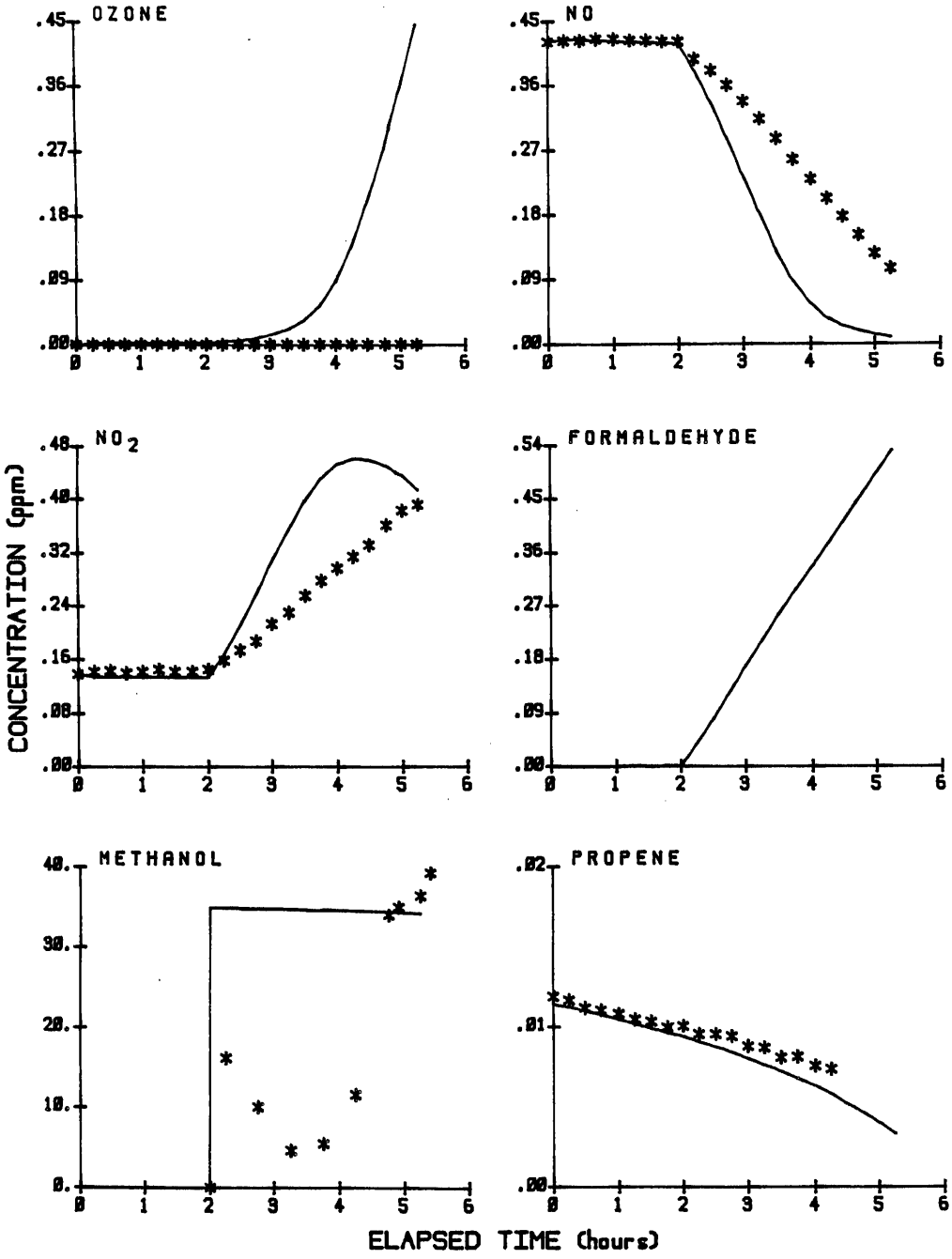


Figure A-12. Experimental and calculated concentration-time plots for selected species observed in the tracer-$NO_x$-air, with added methanol, run ITC-863.

* = experimental data
——— = model calculation

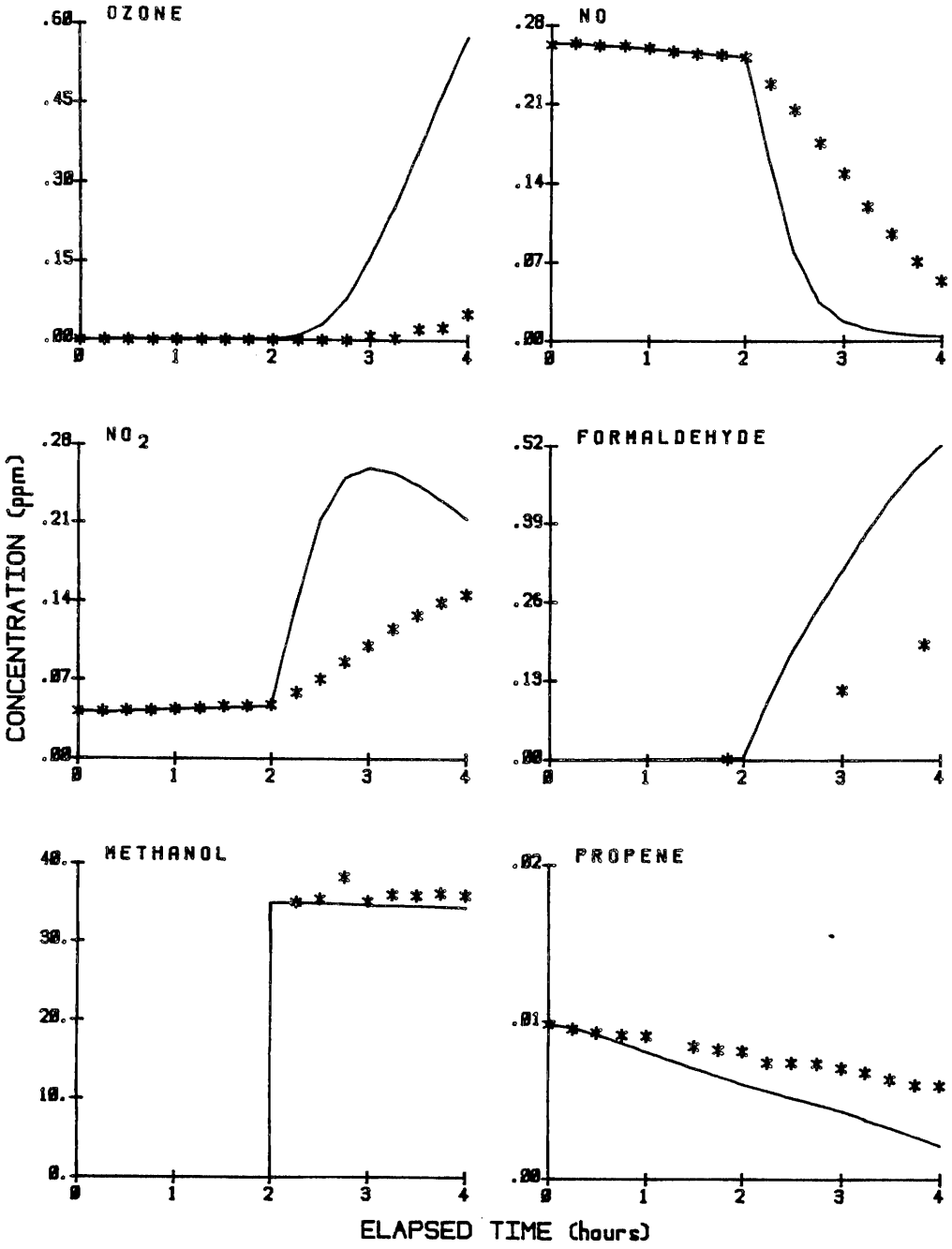


Figure A-13. Experimental and calculated concentration-time plots for selected species observed in the tracer-$NO_x$-air, with added methanol, run ITC-887.

* = experimental data
——— = model calculation

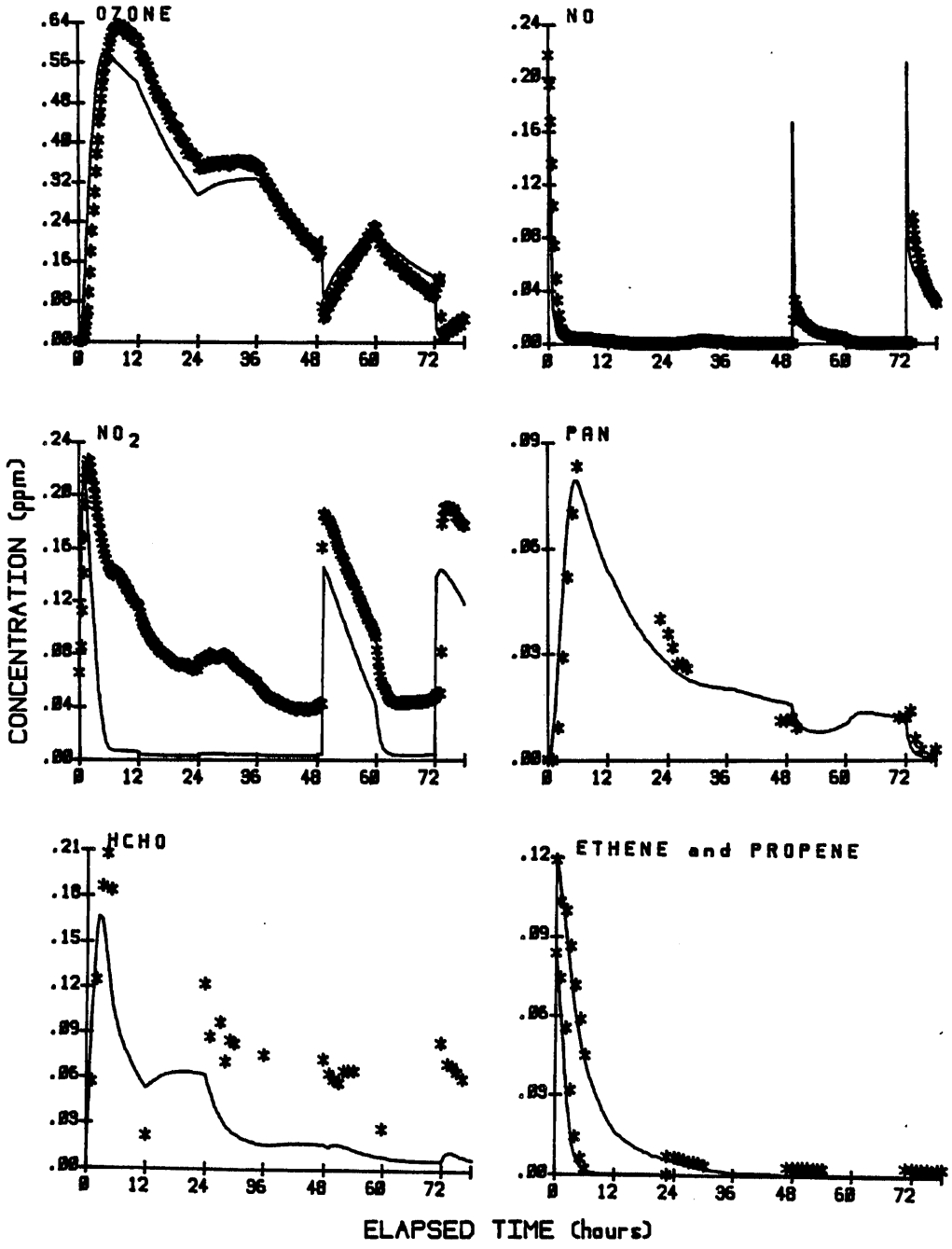


Figure A-14a. Experimental and calculated concentration-time plots for selected species observed in the 15-B surrogate-$NO_x$-air run ITC-865. (Page 1 of 2).

* = experimental data
——— = model calculation

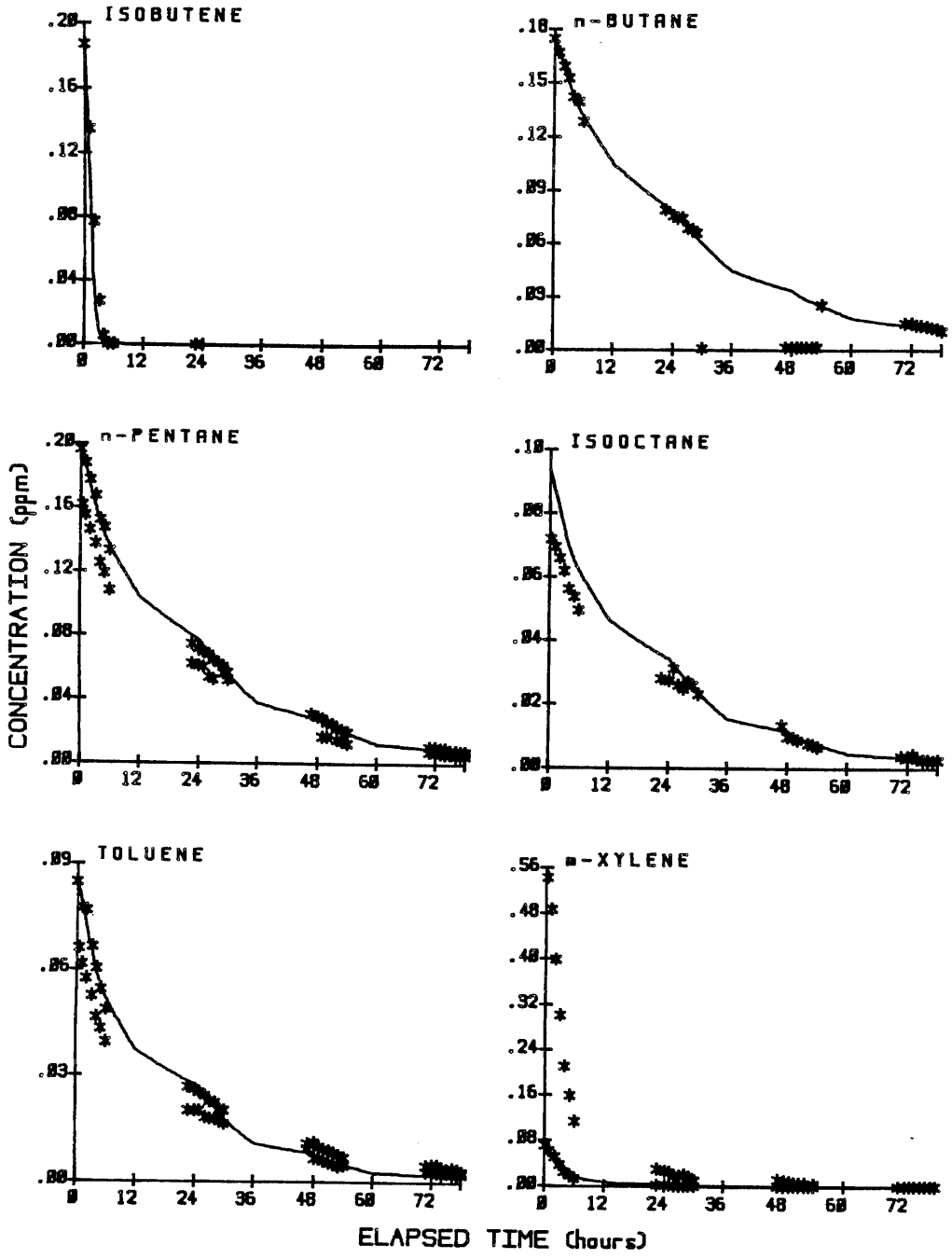


Figure A-14b. Experimental and calculated concentration-time plots for selected species observed in the 15-B surrogate-$NO_x$-air run ITC-865. (Page 2 of 2).

* = experimental data
——— = model calculation

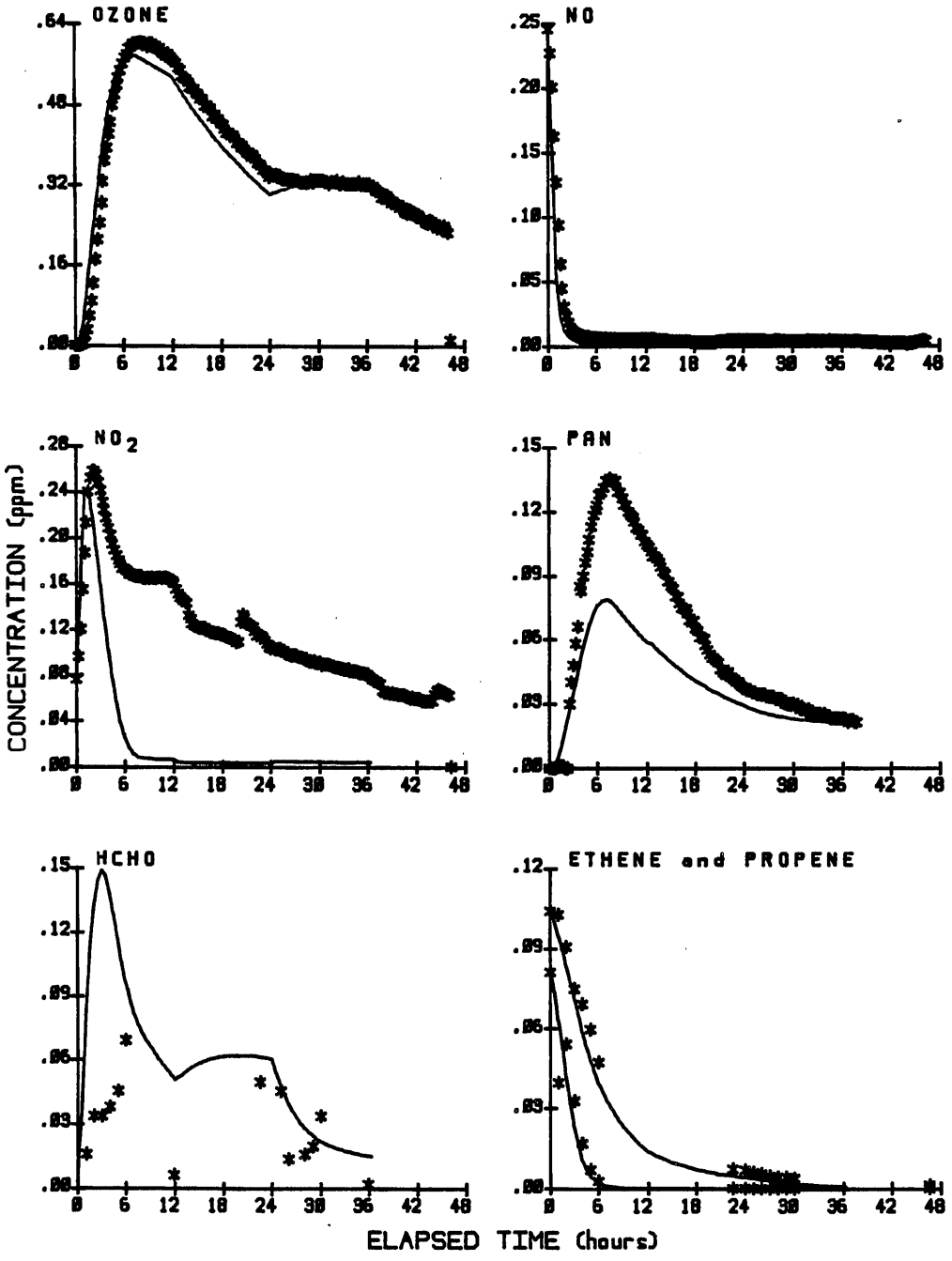


Figure A-15a. Experimental and calculated concentration-time plots for selected species observed in the 15-B surrogate-$NO_x$-air run ITC-891. (Page 1 of 2).

* = experimental data
——— = model calculation

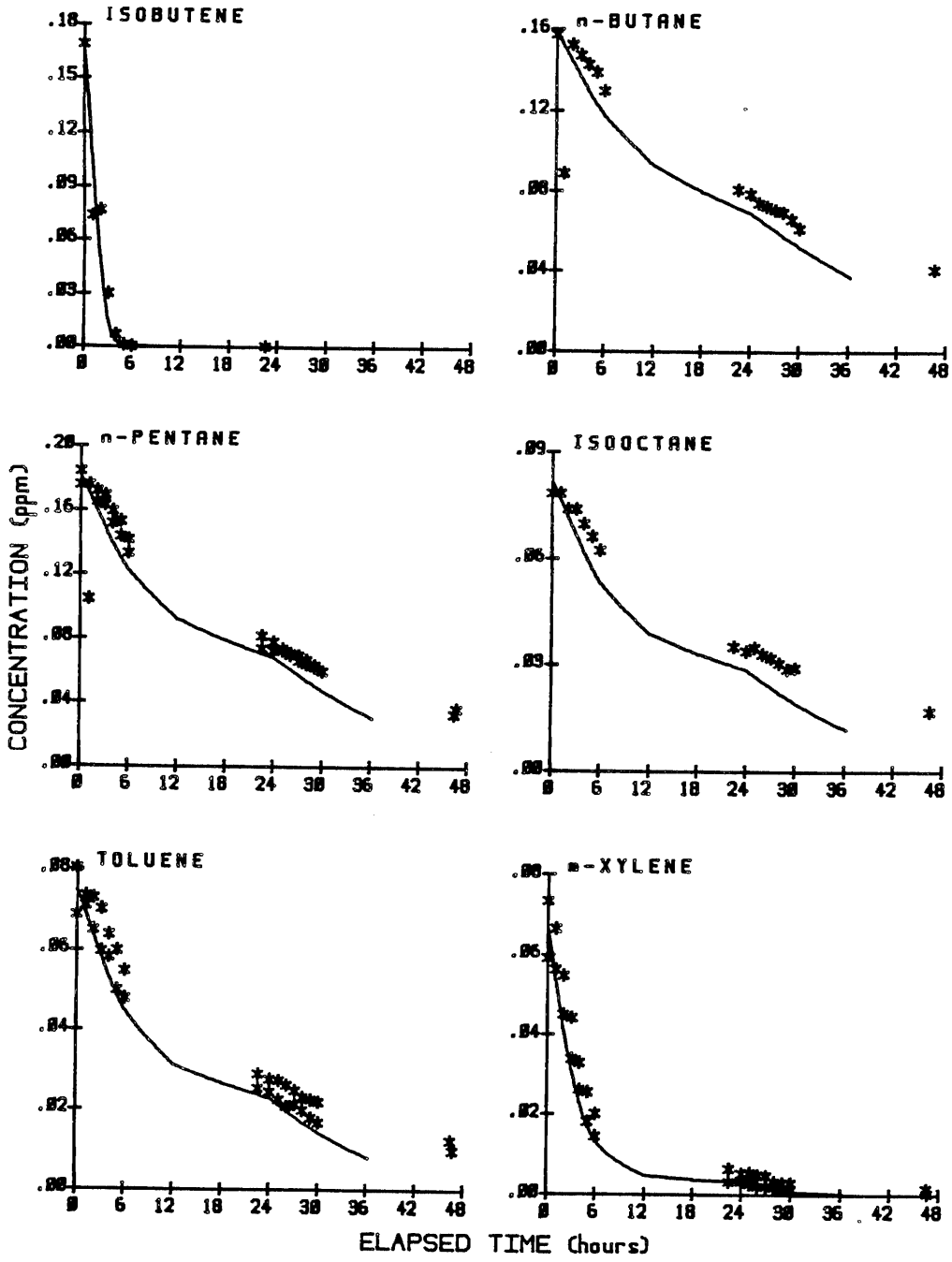


Figure A-15b. Experimental and calculated concentration-time plots for selected species observed in the 15-B surrogate-$NO_x$-air run ITC-891. (Page 2 of 2).

* = experimental data
——— = model calculation

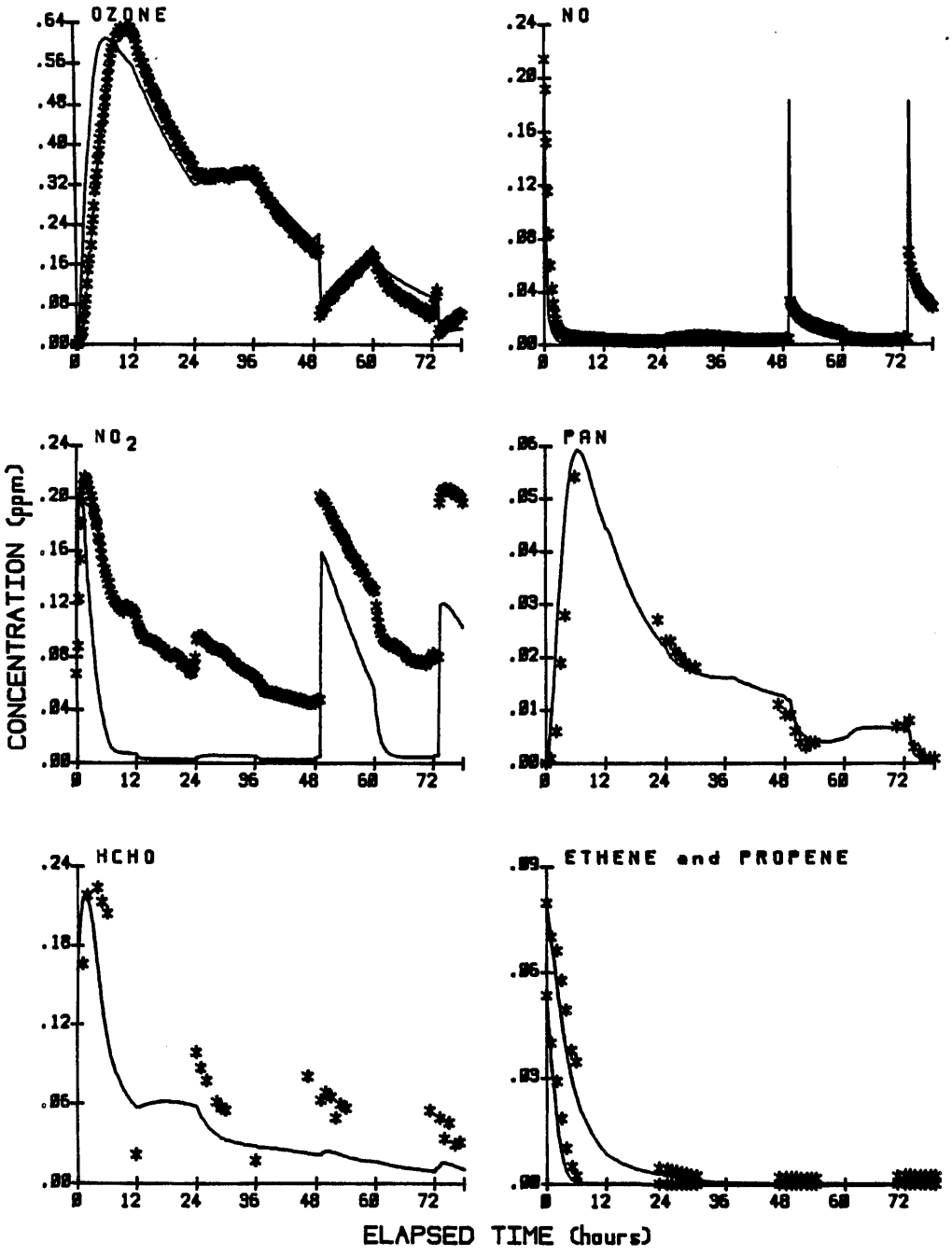


Figure A-16a. Experimental and calculated concentration-time plots for selected species observed in the 15-MF surrogate-$NO_x$-air run ITC-867. (Page 1 of 2).

* = experimental data
——— = model calculation

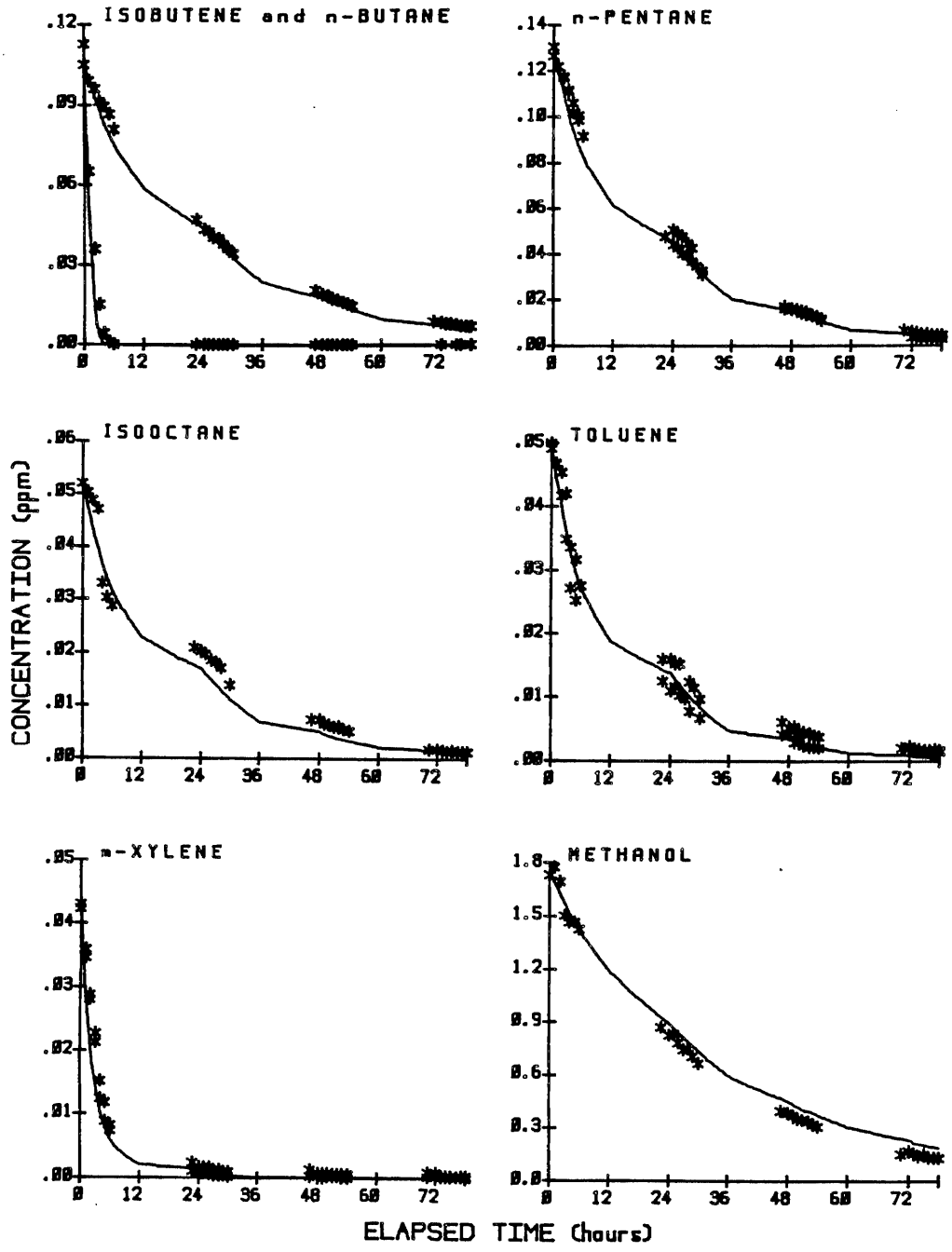


Figure A-16b. Experimental and calculated concentration-time plots for selected species observed in the 15-MF surrogate-$NO_x$-air run ITC-867. (Page 2 of 2).

* = experimental data
——— = model calculation

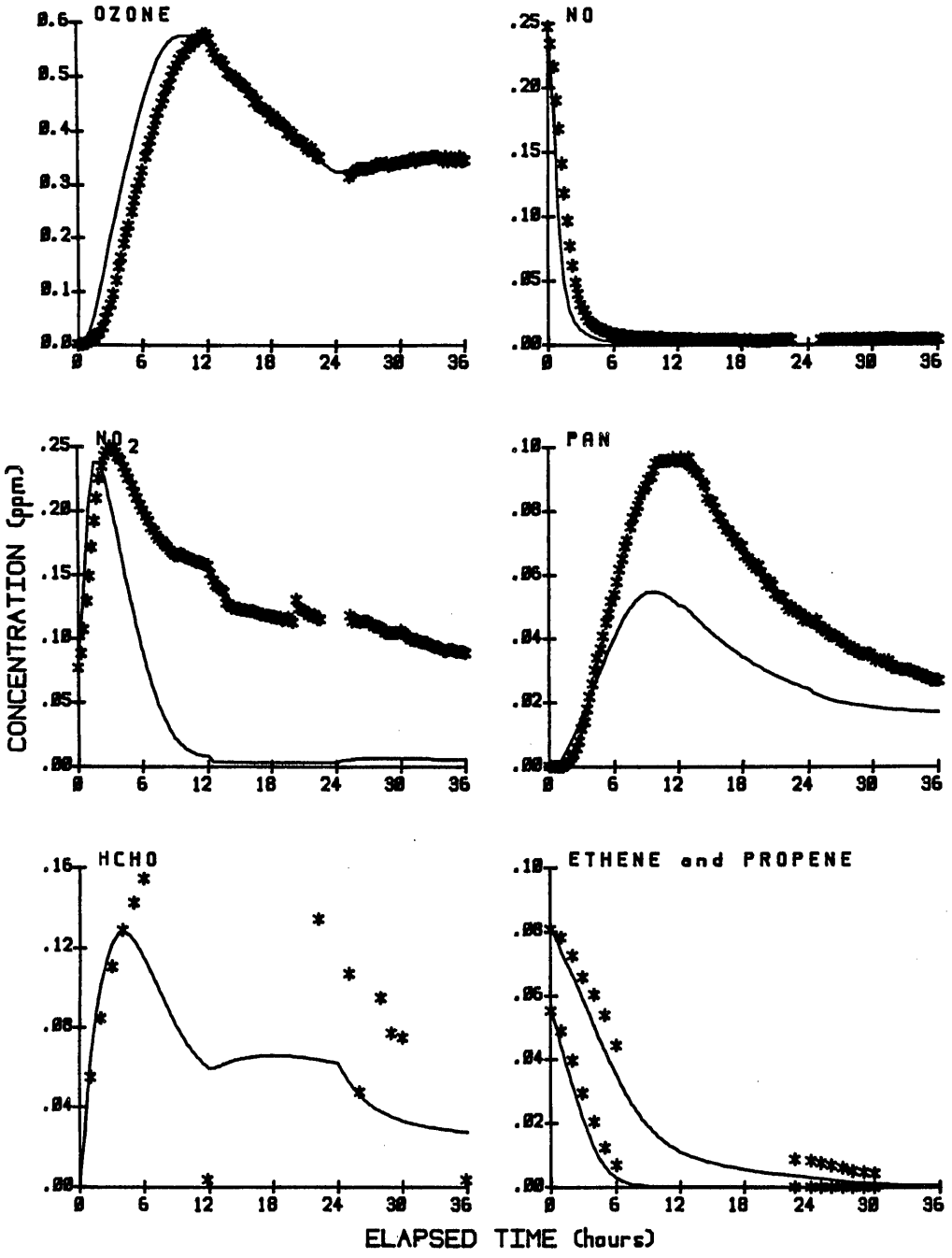


Figure A-17a. Experimental and calculated concentration-time plots for selected species observed in the 15-M surrogate-$NO_x$-air run ITC-888. (Page 1 of 2).

* = experimental data
——— = model calculation

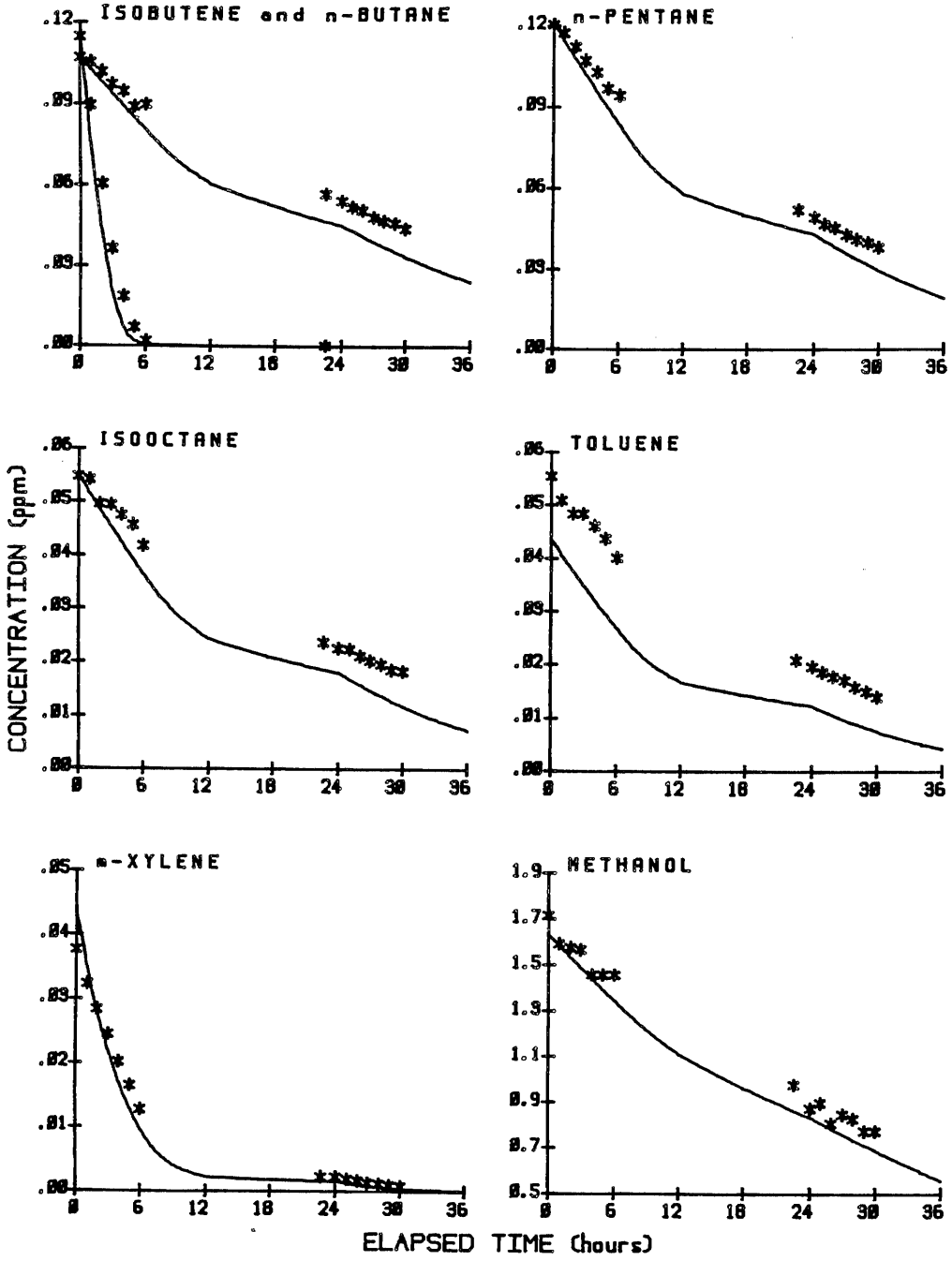


Figure A-17b. Experimental and calculated concentration-time plots for selected species observed in the 15-M surrogate-$NO_x$-air run ITC-888. (Page 2 of 2).

* = experimental data

——— = model calculation

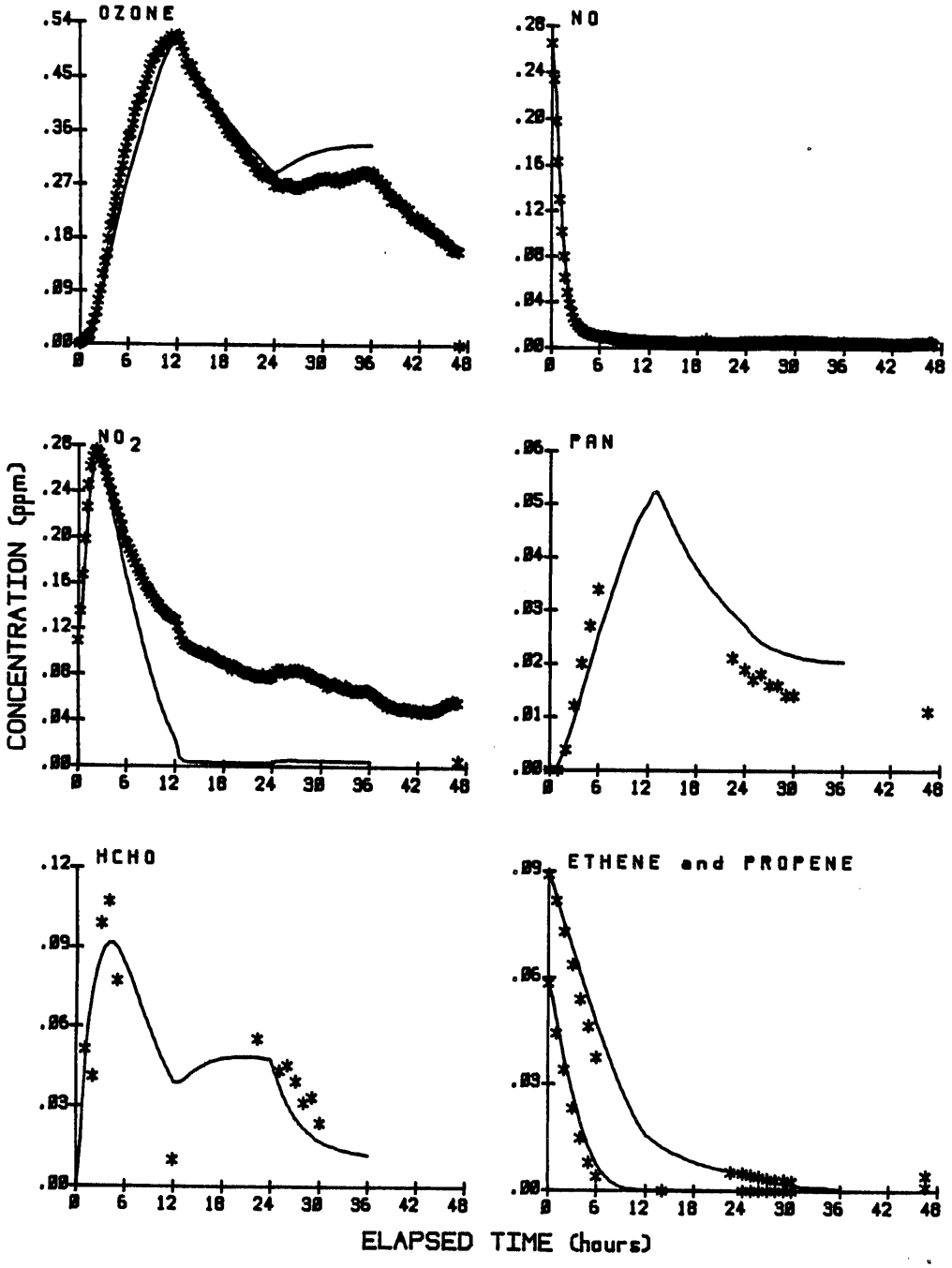


Figure A-18a. Experimental and calculated concentration-time plots for selected species observed in the 15-BL surrogate-$NO_x$-air run ITC-868. (Page 1 of 2).

* = experimental data
——— = model calculation

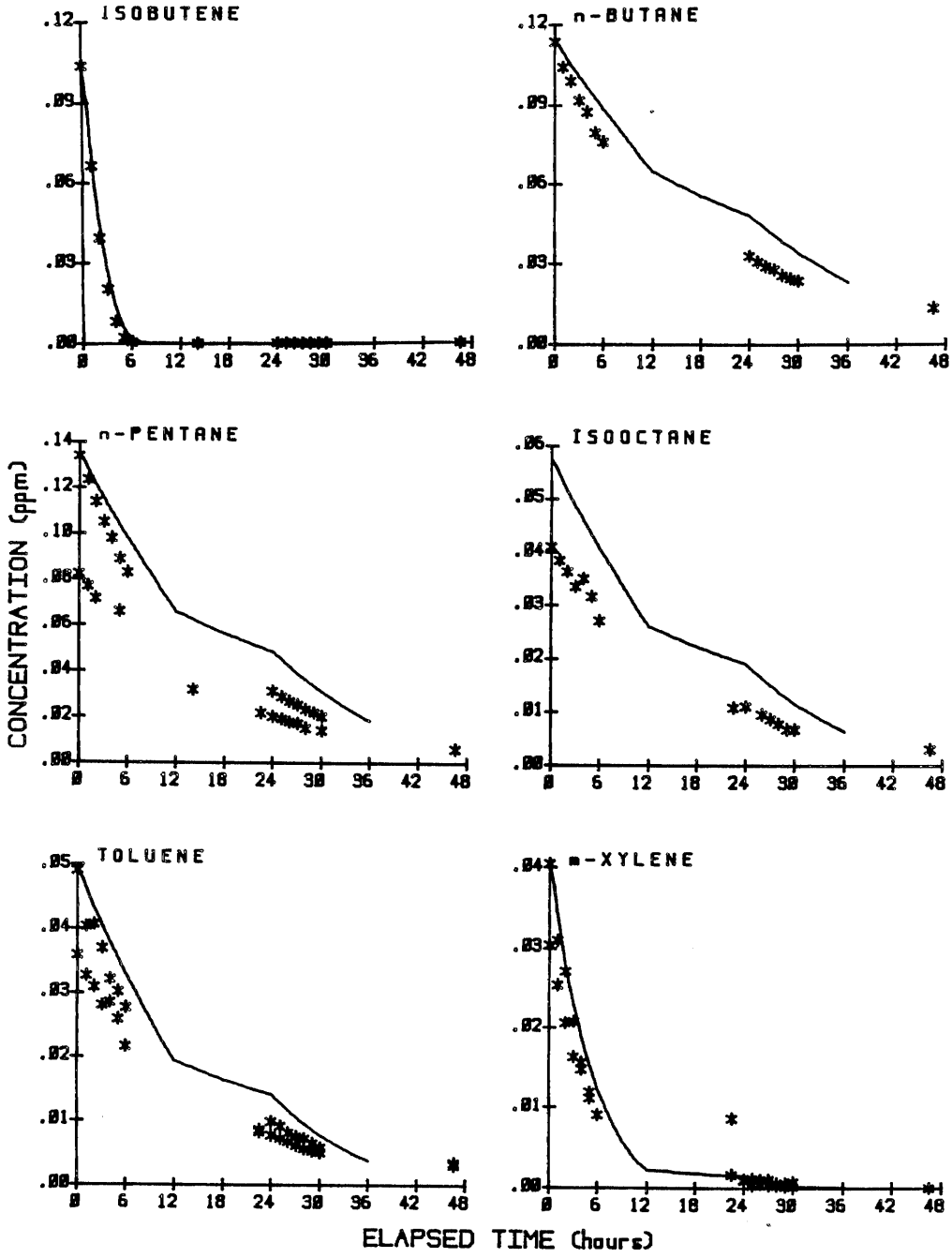


Figure A-18b. Experimental and calculated concentration-time plots for selected species observed in the 15-BL surrogate-$NO_x$-air run ITC-868. (Page 2 of 2).

* = experimental data

——— = model calculation

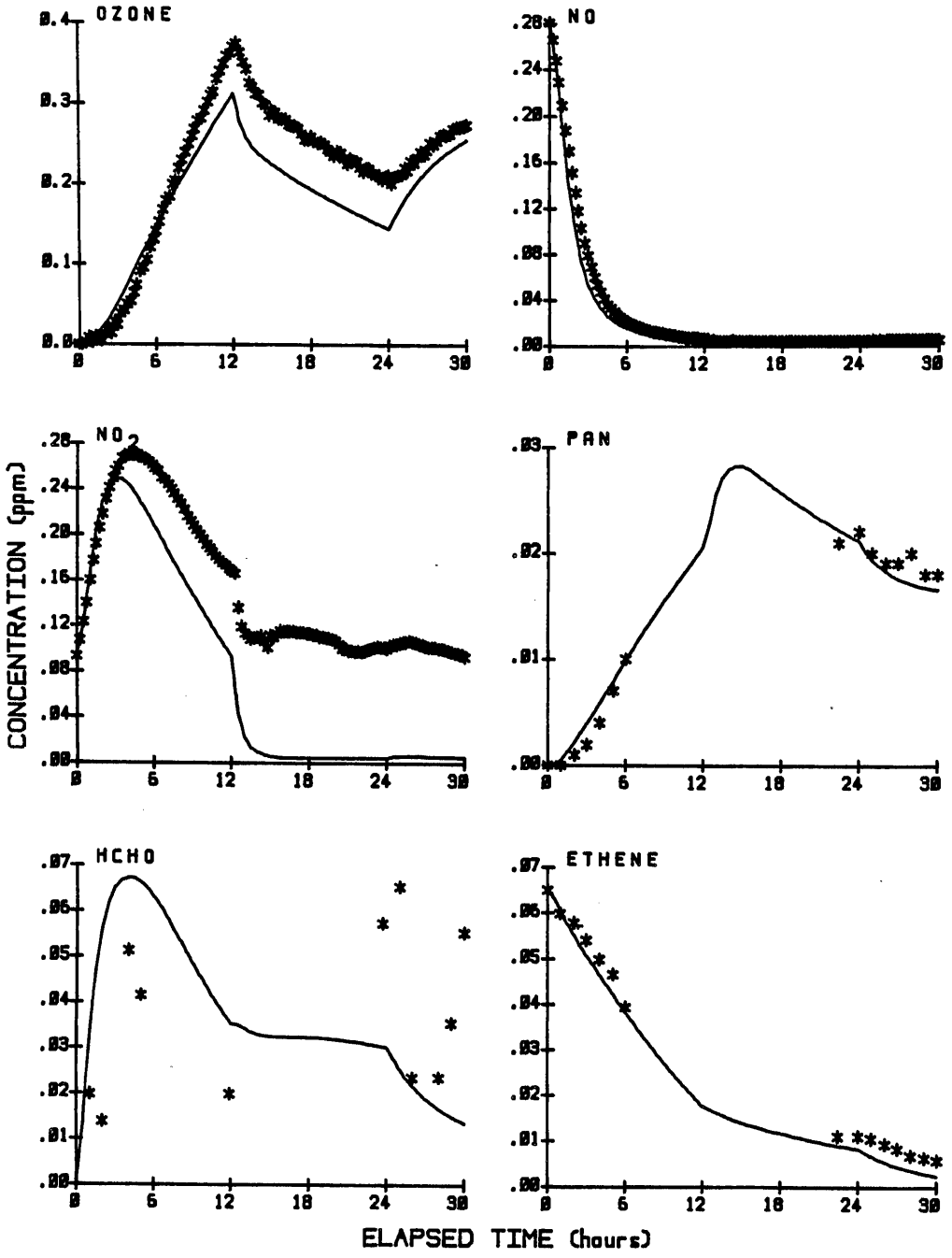


Figure A-19a. Experimental and calculated concentration-time plots for selected species observed in the 6-B surrogate-$NO_x$-air run ITC-871. Page 1 of 2.

* = experimental data
——— = model calculation

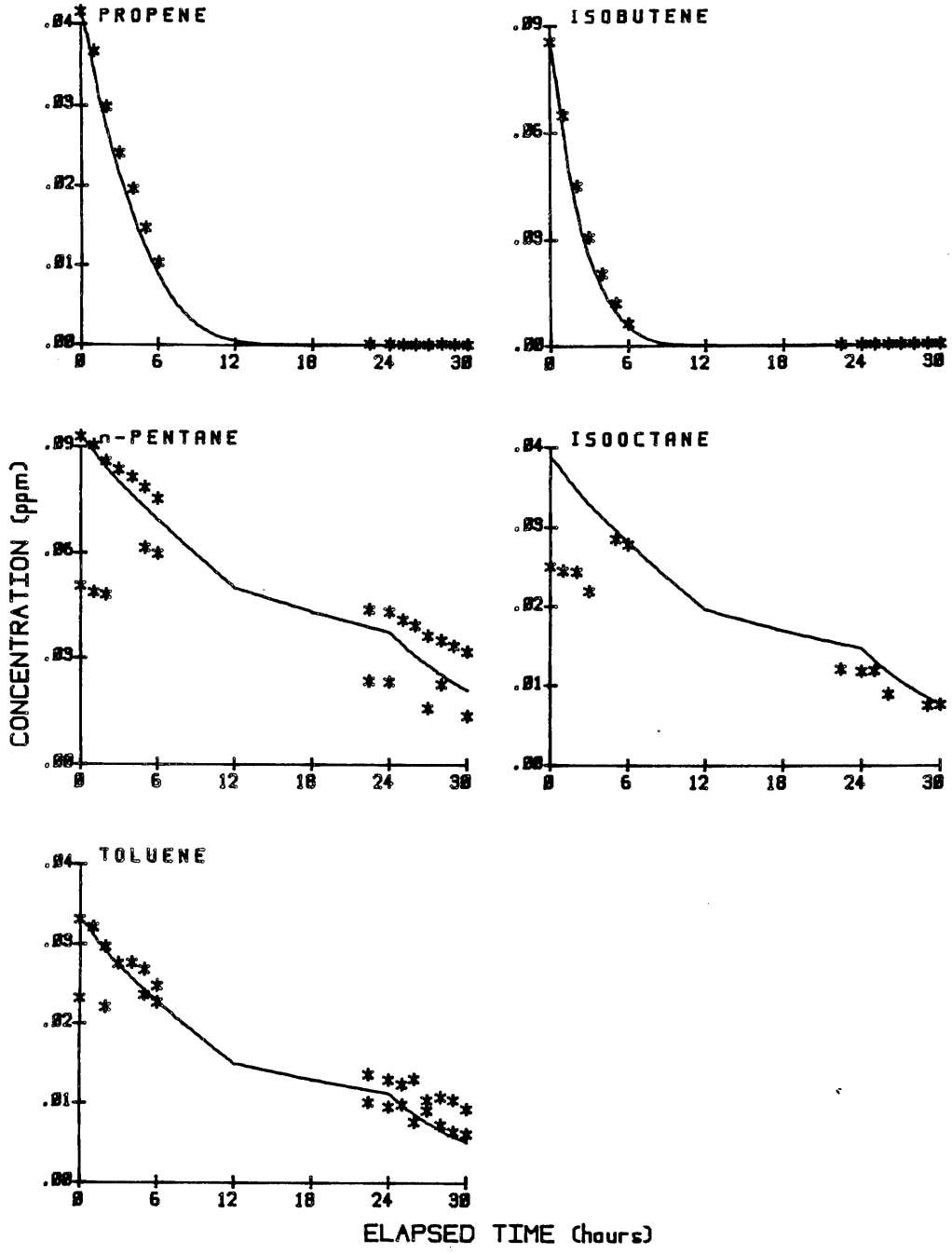


Figure A-19b. Experimental and calculated concentration-time plots for selected species observed in the 6-B surrogate-$NO_x$-air run ITC-871. (Page 2 of 2).

* = experimental data
——— = model calculation

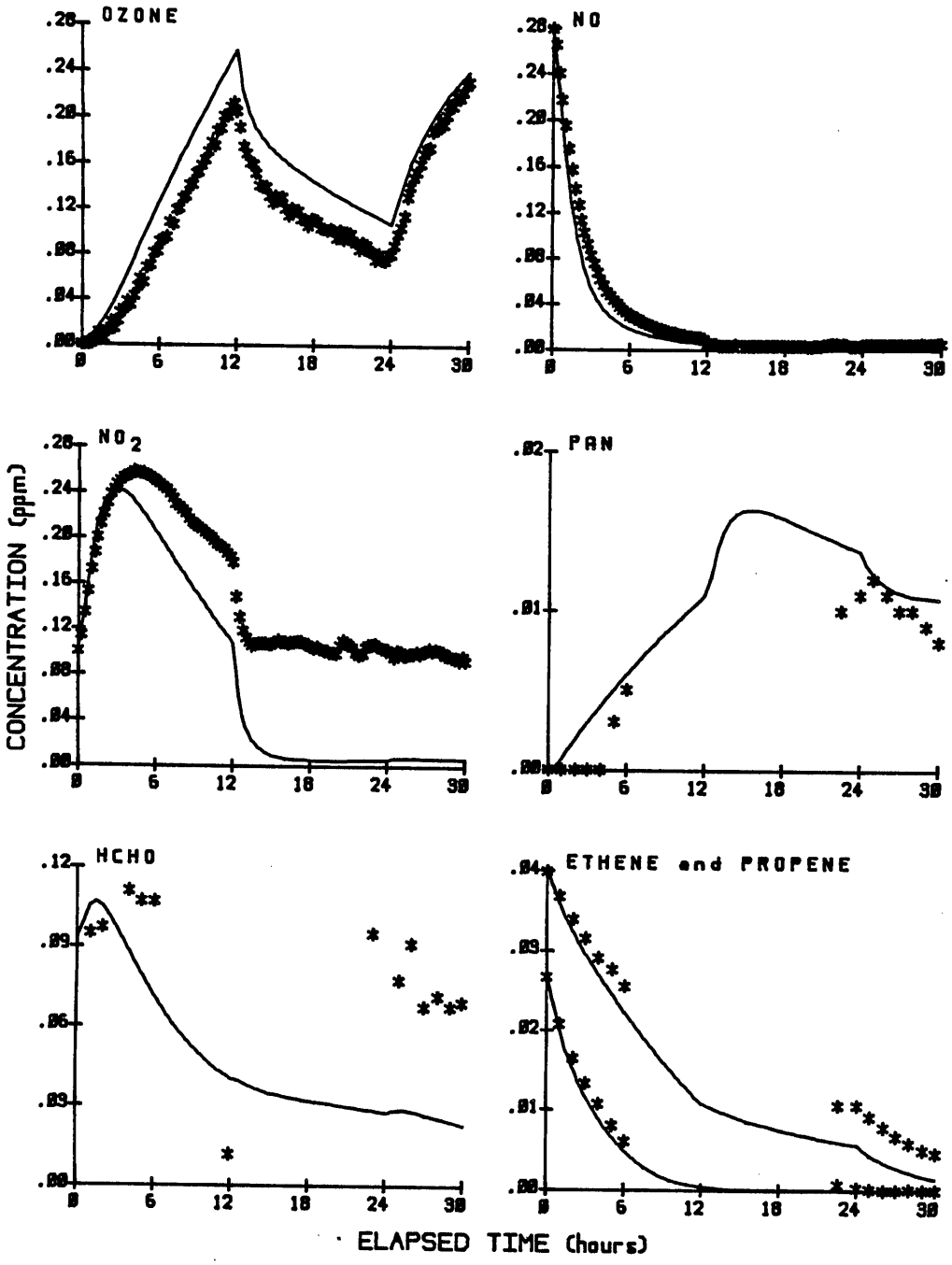


Figure A-20a. Experimental and calculated concentration-time plots for selected species observed in the 6-MF surrogate-$NO_x$-air run ITC-872. (Page 1 of 2).

* = experimental data
——— = model calculation

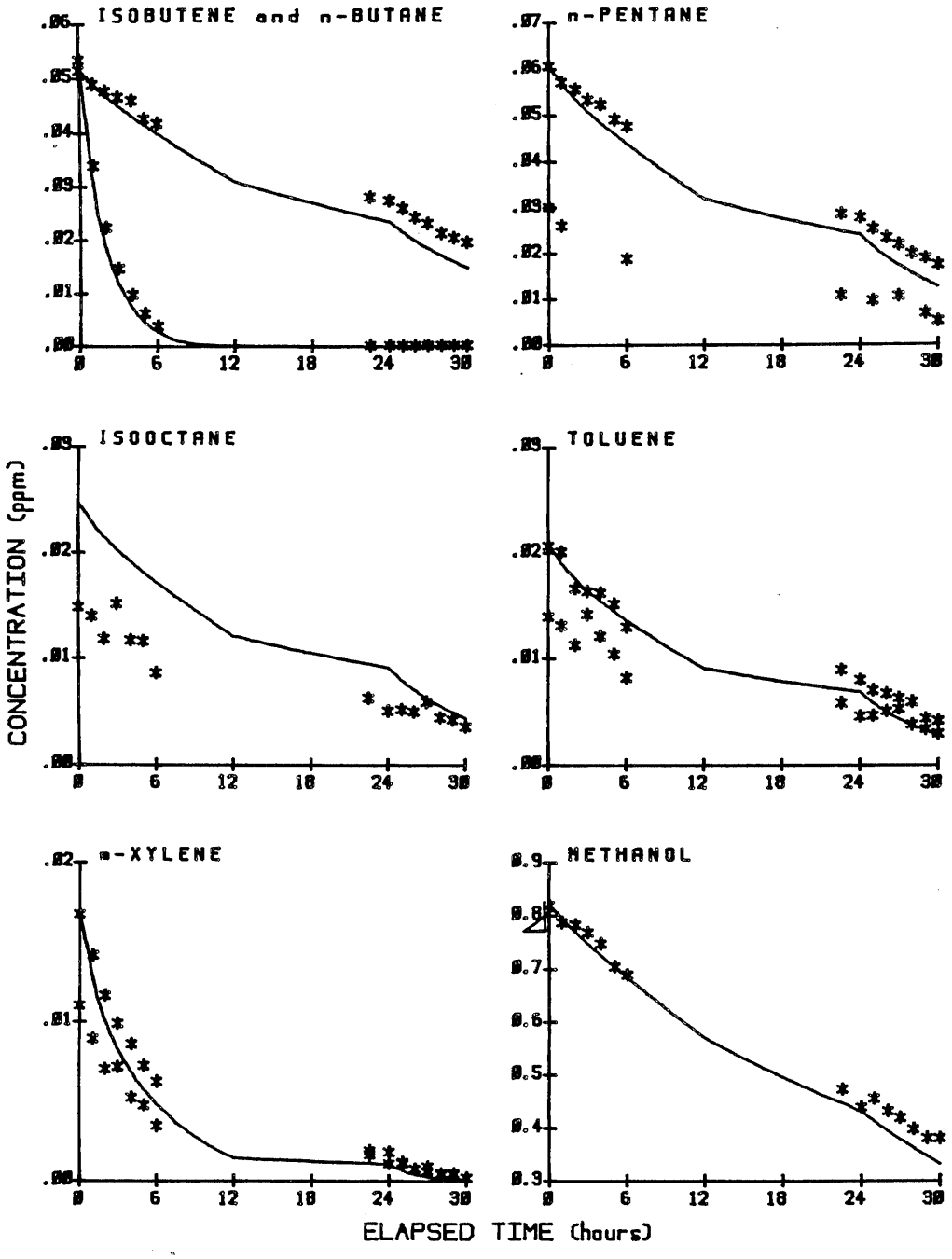


Figure A-20b. Experimental and calculated concentration-time plots for selected species observed in the 6-MF surrogate-$NO_x$-air run ITC-872. (Page 2 of 2).

* = experimental data
——— = model calculation

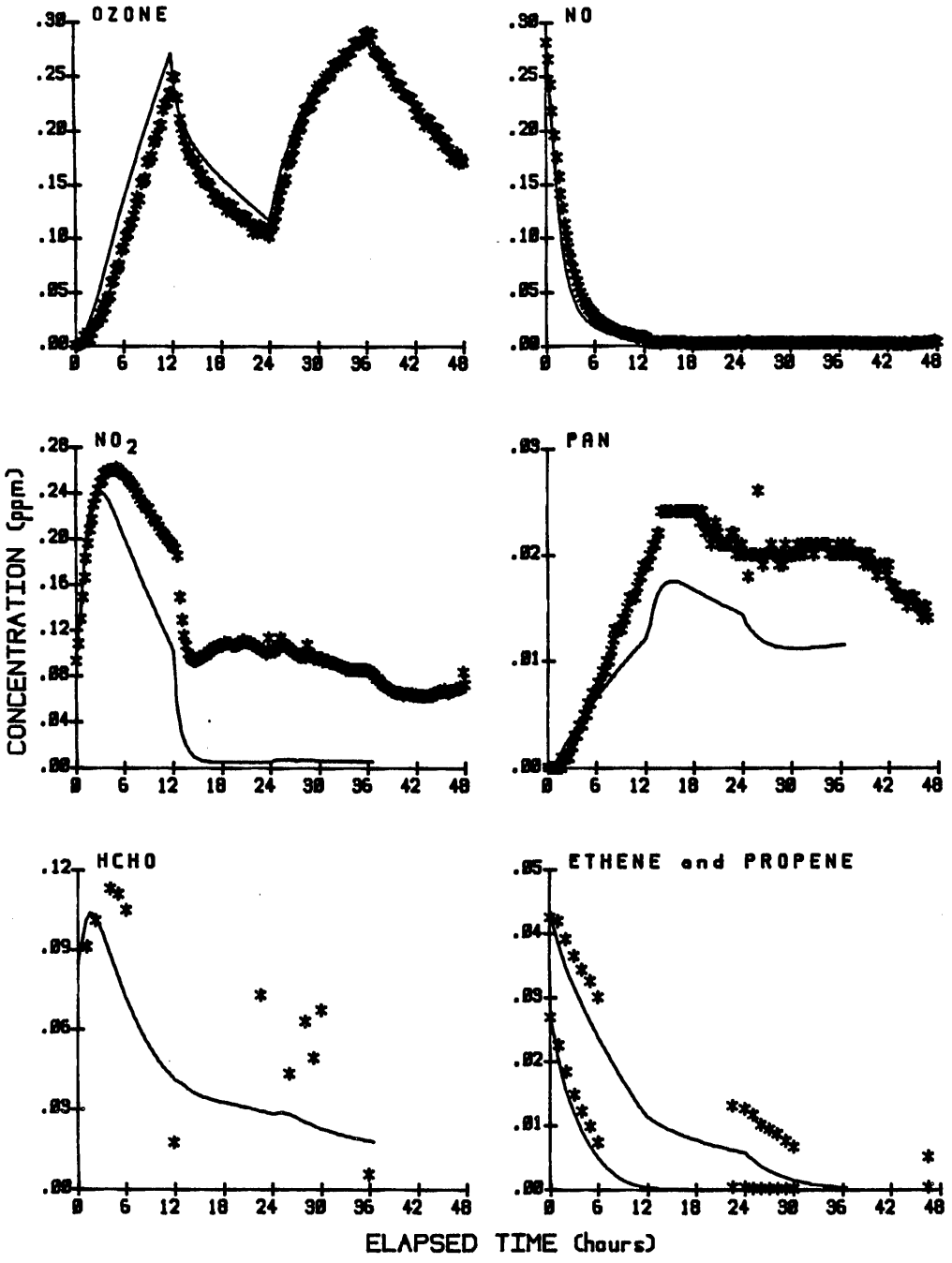


Figure A-21a. Experimental and calculated concentration-time plots for selected species observed in the 6-MF surrogate-$NO_x$-air run ITC-877. (Page 1 of 2).

* = experimental data
——— = model calculation

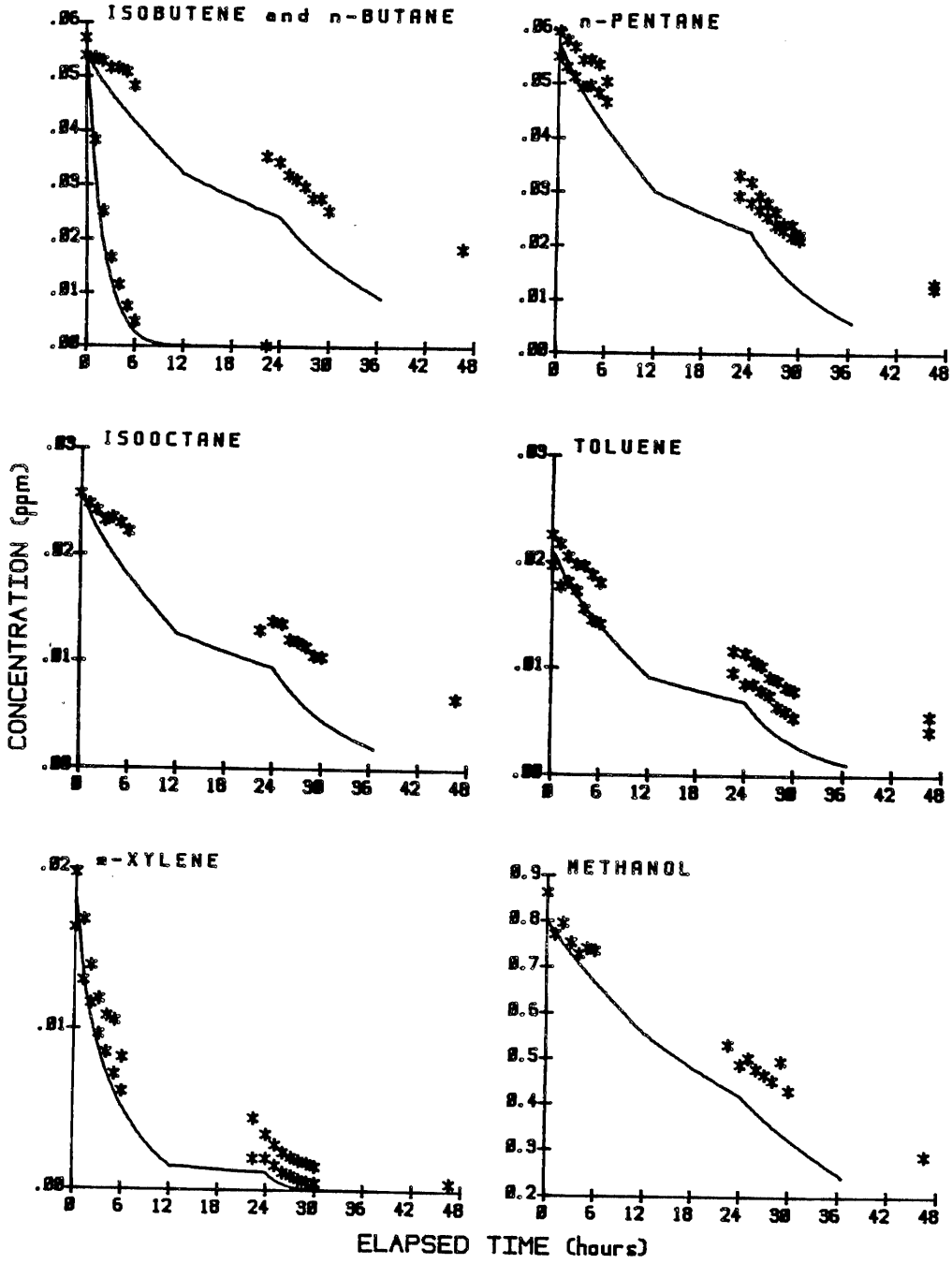


Figure A-21b. Experimental and calculated concentration-time plots for selected species observed in the 6-MF surrogate-$NO_x$-air run ITC-877. (Page 2 of 2).

* = experimental data
——— = model calculation

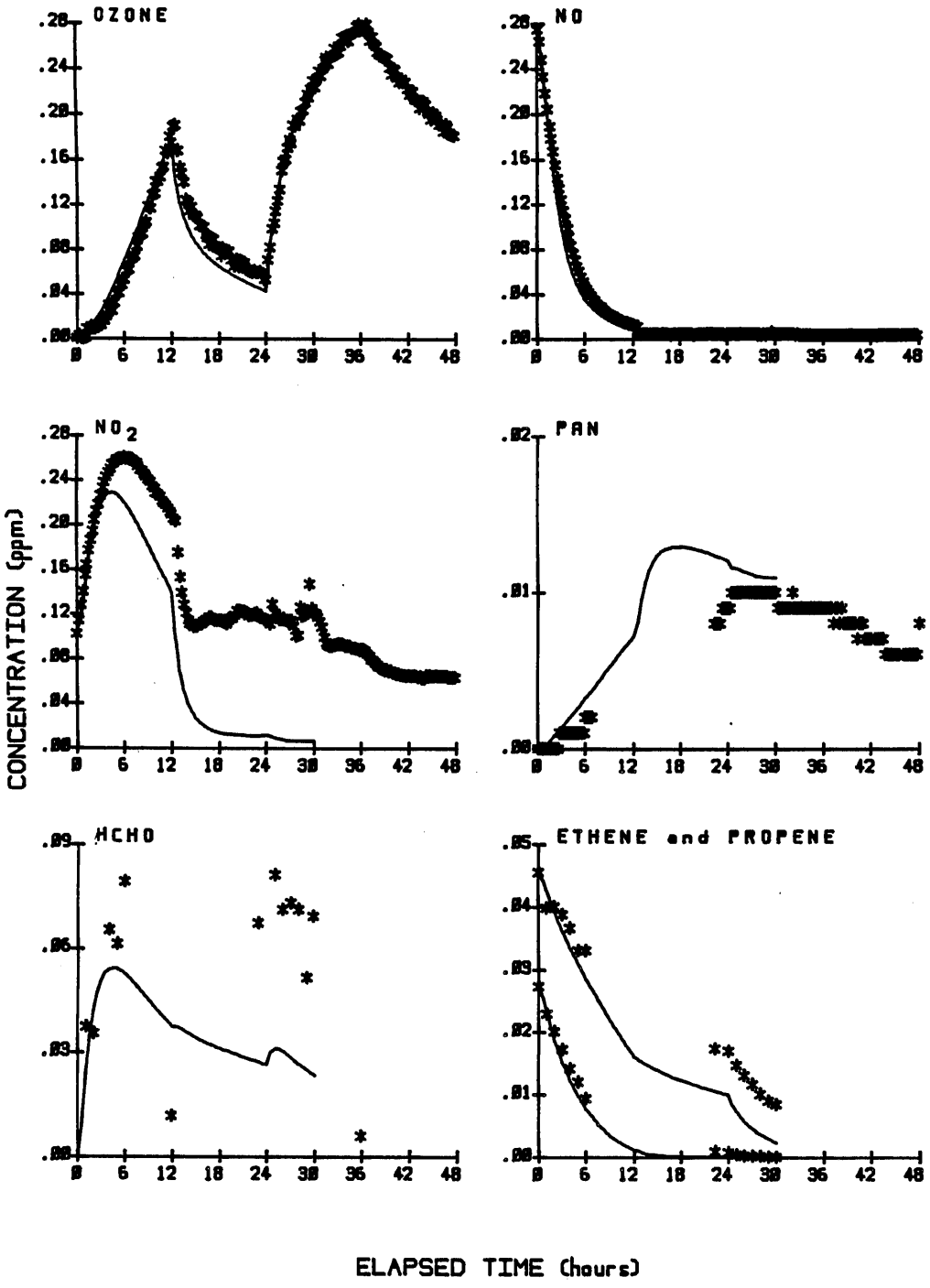


Figure A-22a. Experimental and calculated concentration-time plots for selected species observed in the 6-M surrogate-$NO_x$-air run ITC-874. (Page 1 of 2).

* = experimental data
——— = model calculation

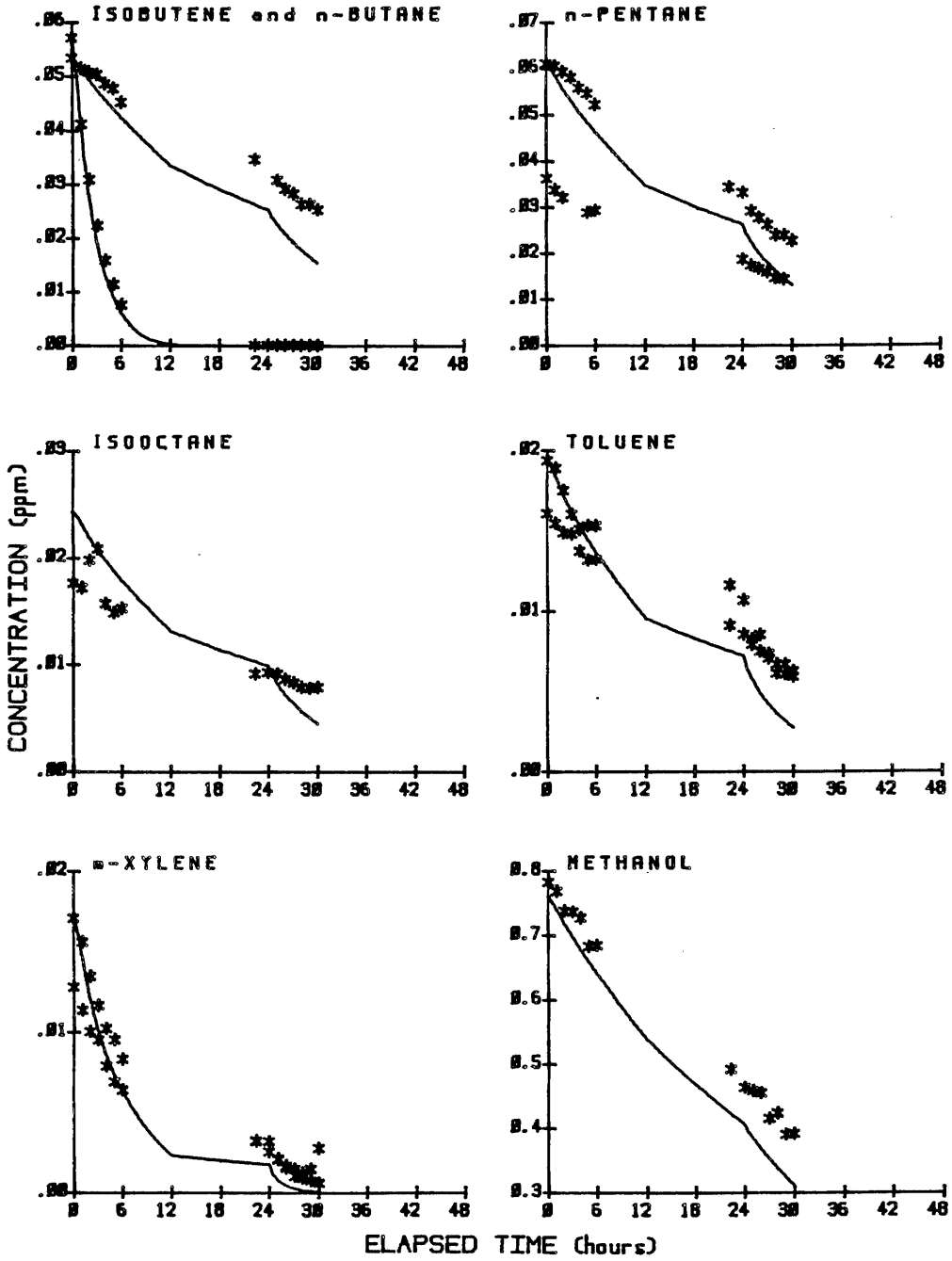


Figure A-22b. Experimental and calculated concentration-time plots for selected species observed in the 6-M surrogate-$NO_x$-air run ITC-874. (Page 2 of 2).

* = experimental data
——— = model calculation

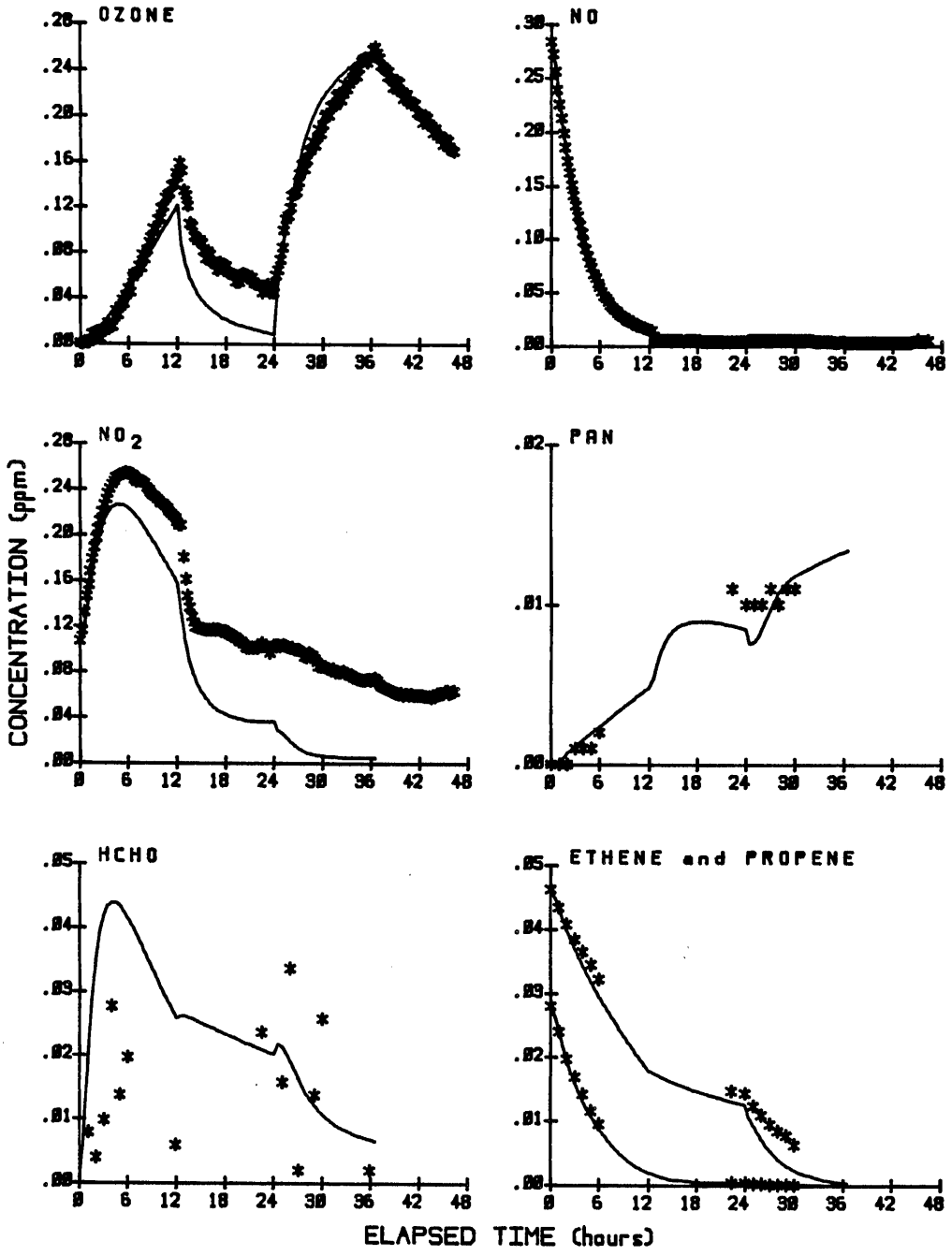


Figure A-23a. Experimental and calculated concentration-time plots for selected species observed in the 6-BL surrogate-$NO_x$-air run ITC-873. (Page 1 of 2).

* = experimental data
——— = model calculation

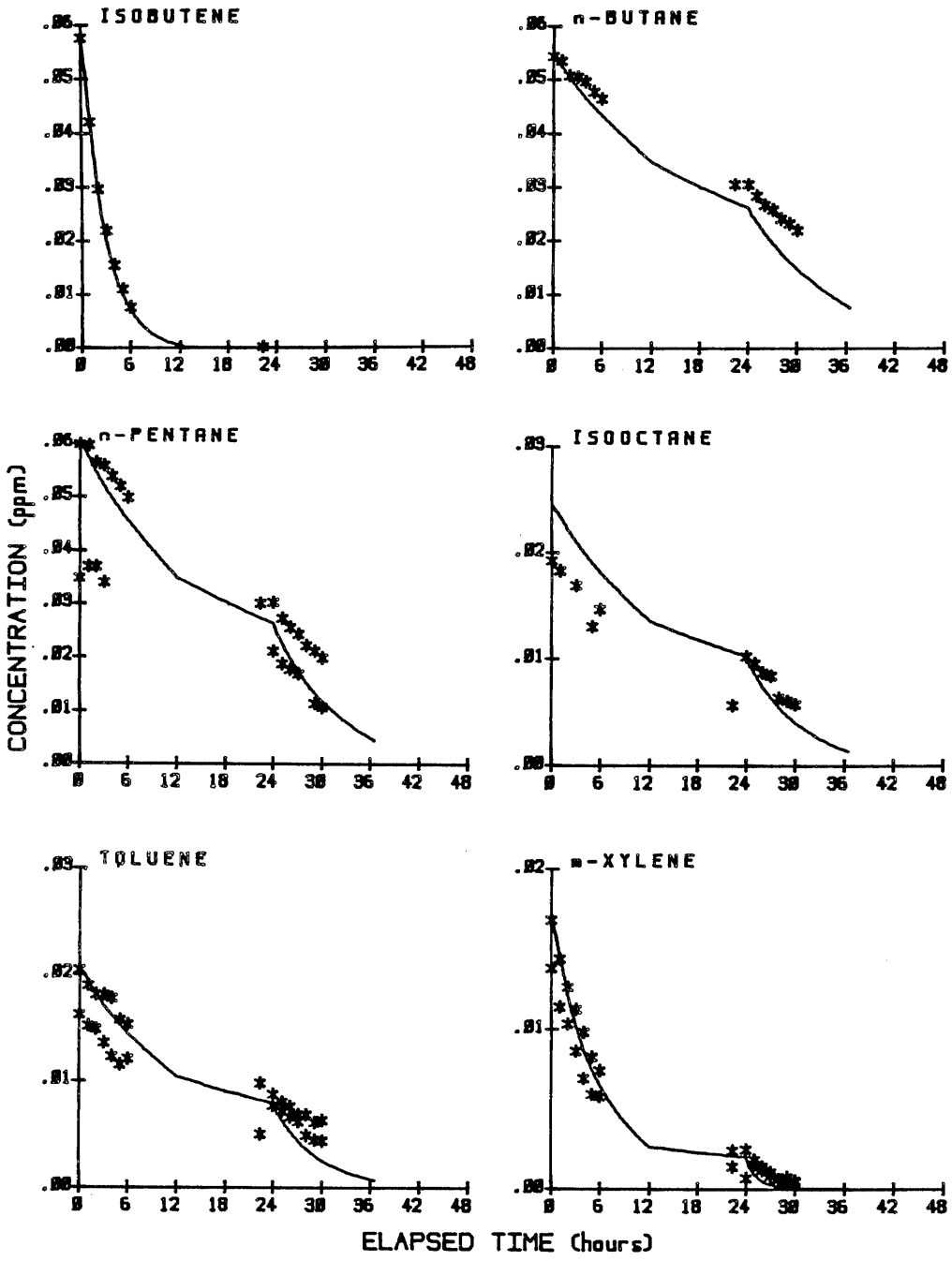


Figure A-23b. Experimental and calculated concentration-time plots for selected species observed in the 6-BL surrogate-$NO_x$-air run ITC-873. (Page 2 of 2).

* = experimental data
——— = model calculation

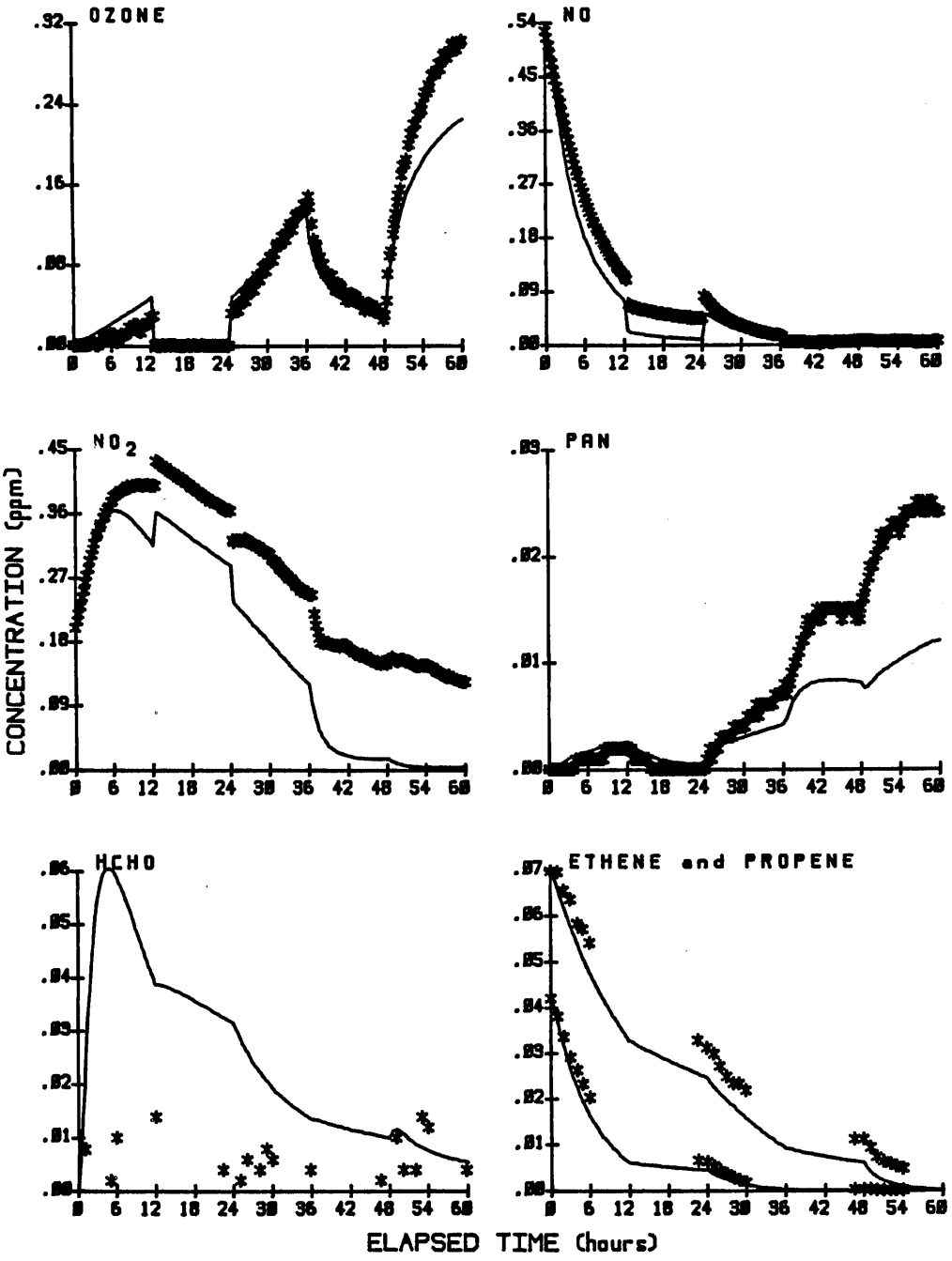


Figure A-24a. Experimental and calculated concentration-time plots for selected species observed in the 3-B surrogate-$NO_x$-air run ITC-880. (Page 1 of 2).

* = experimental data
_____ = model calculation

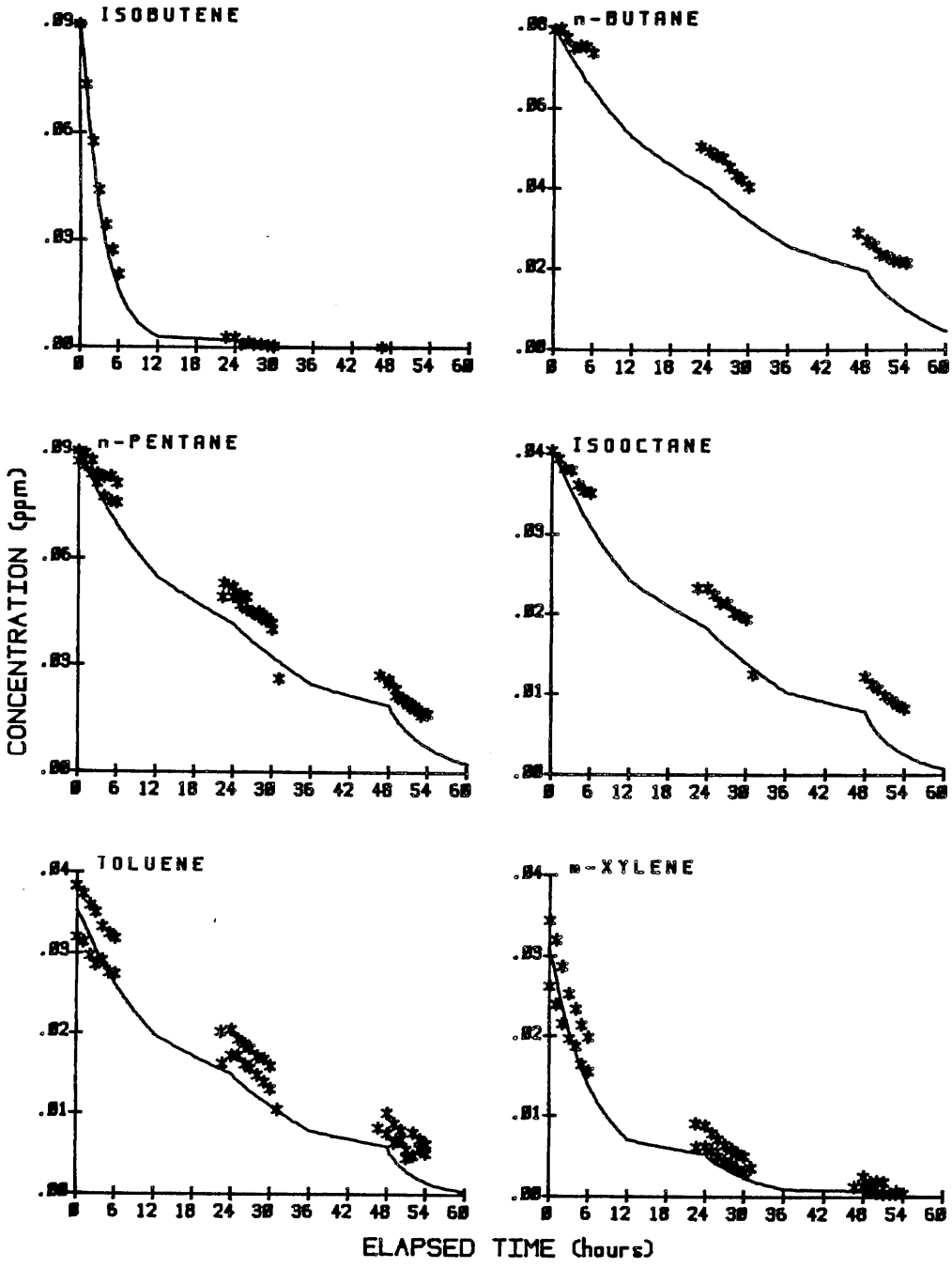


Figure A-24b. Experimental and calculated concentration-time plots for selected species observed in the 3-B surrogate-$NO_x$-air run ITC-880. (Page 2 of 2).

* = experimental data
——— = model calculation

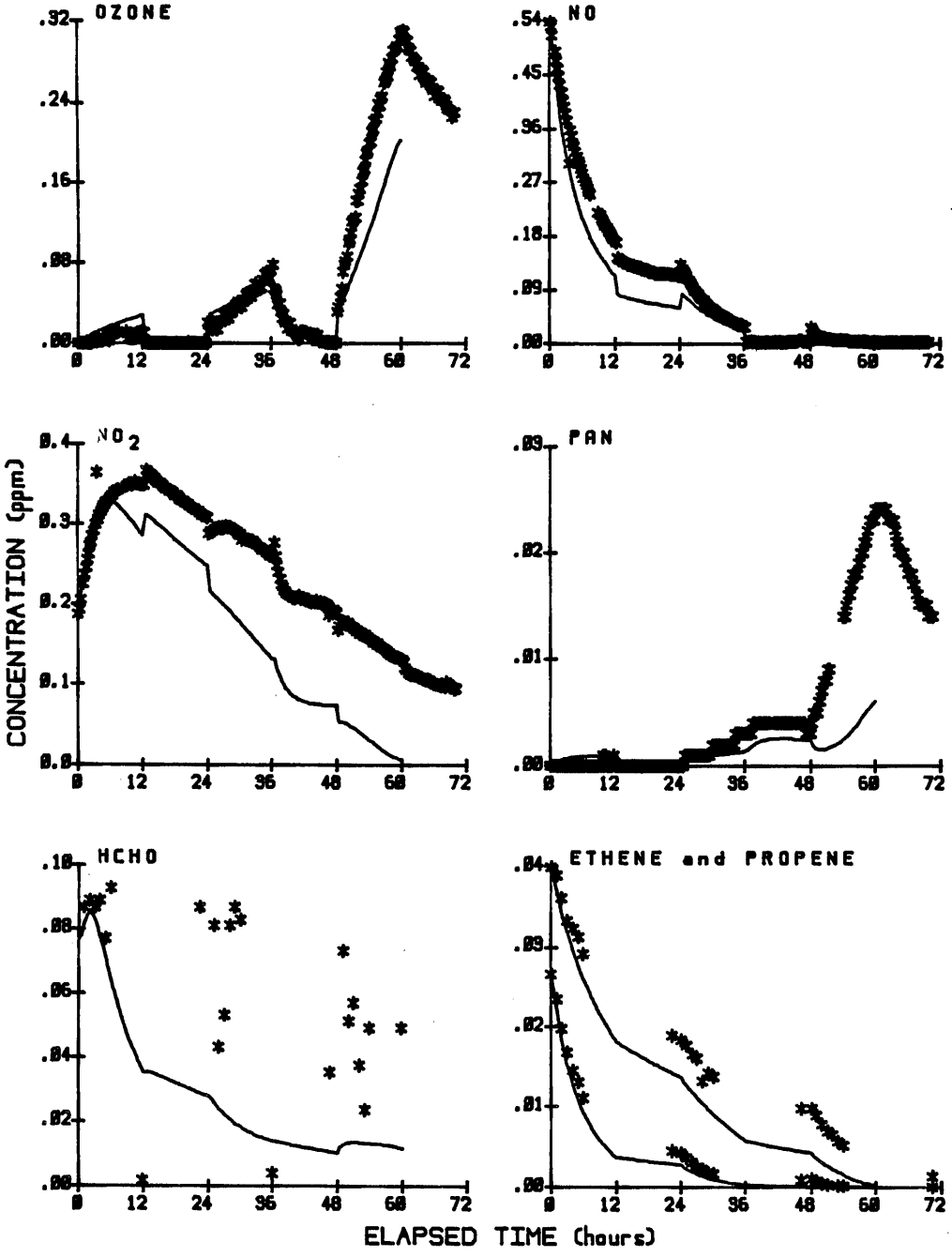


Figure A-25a. Experimental and calculated concentration-time plots for selected species observed in the 3-MF surrogate-$NO_x$-air run ITC-881. (Page 1 of 2).

* = experimental data
——— = model calculation

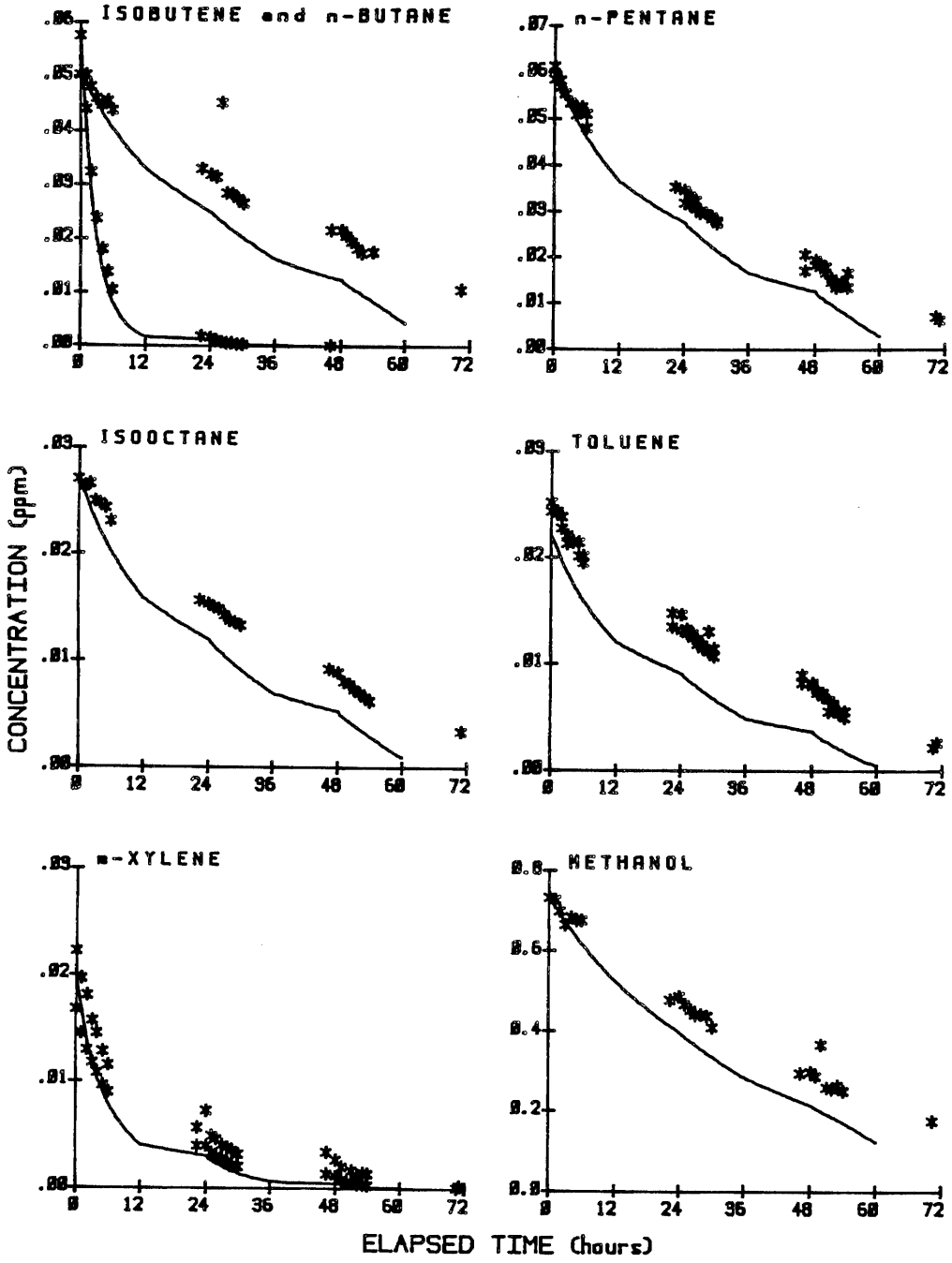


Figure A-25b. Experimental and calculated concentration-time plots for selected species observed in the 3-MF surrogate-$NO_x$-air run ITC-881. (Page 2 of 2).

* = experimental data
——— = model calculation

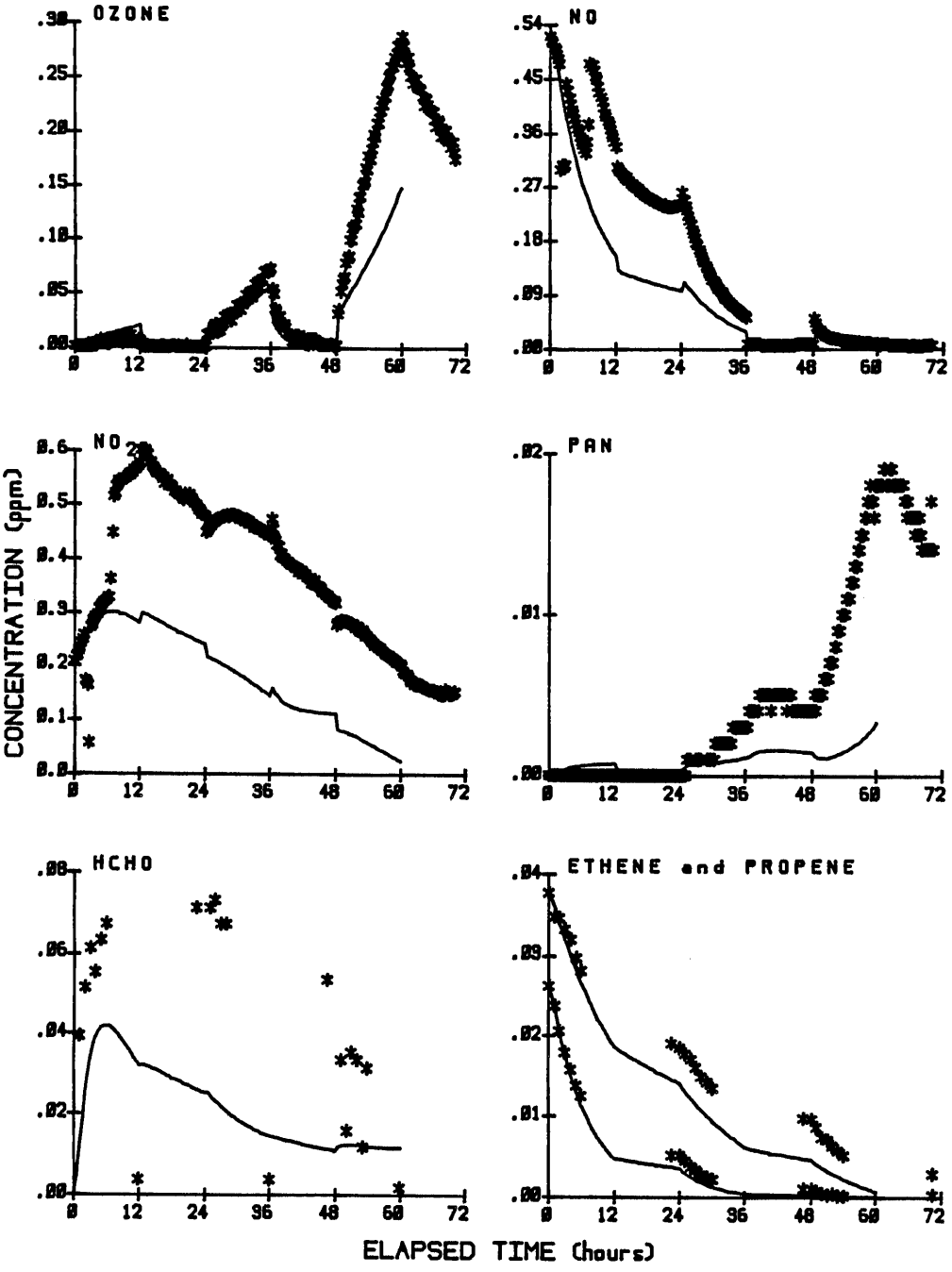


Figure A-26a. Experimental and calculated concentration-time plots for selected species observed in the 3-M surrogate-$NO_x$-air run ITC-886. (Page 1 of 2).

* = experimental data

——— = model calculation

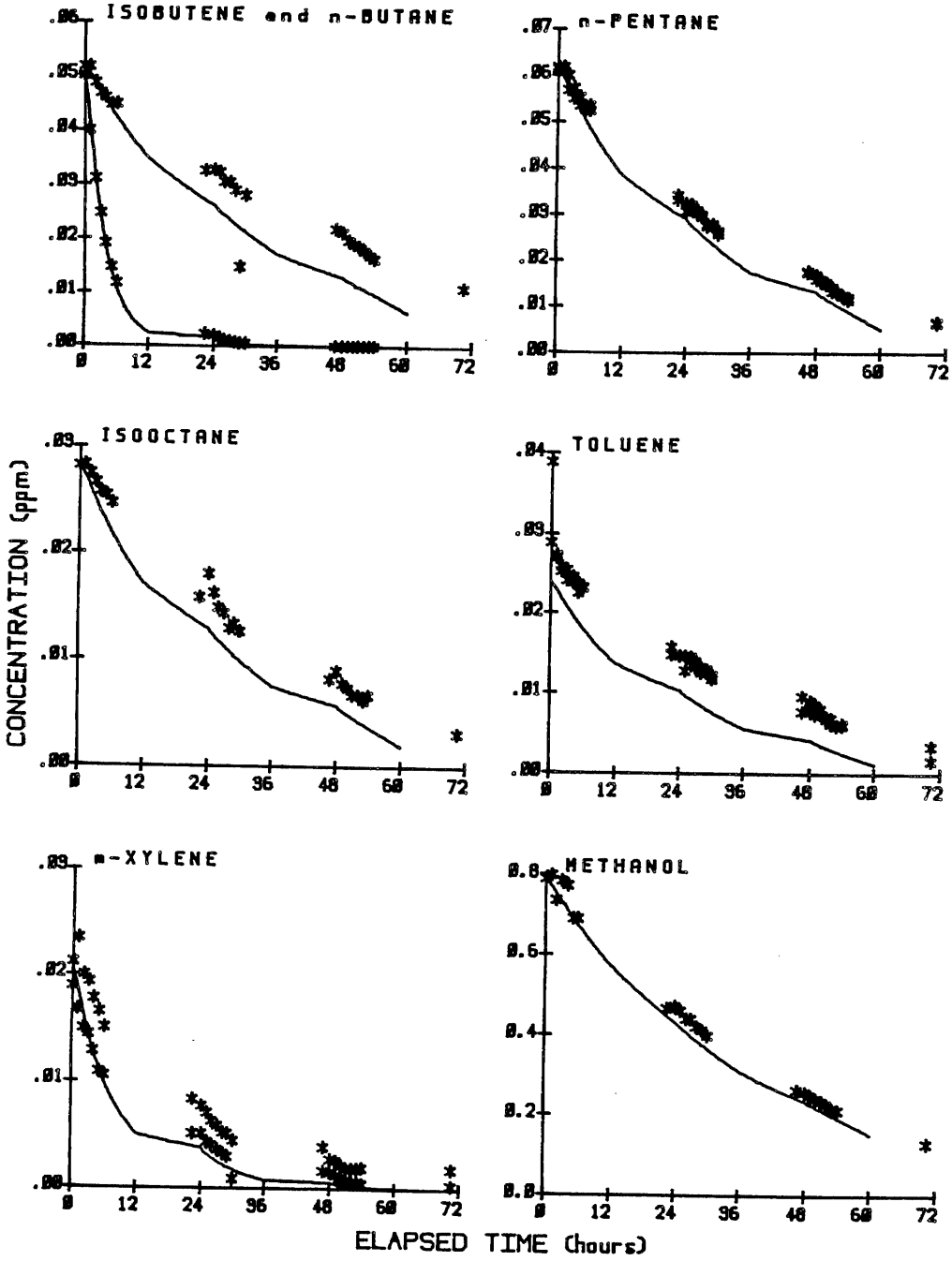


Figure A-26b. Experimental and calculated concentration-time plots for selected species observed in the 3-M surrogate-$NO_x$-air run ITC-886. (Page 2 of 2).

* = experimental data
——— = model calculation

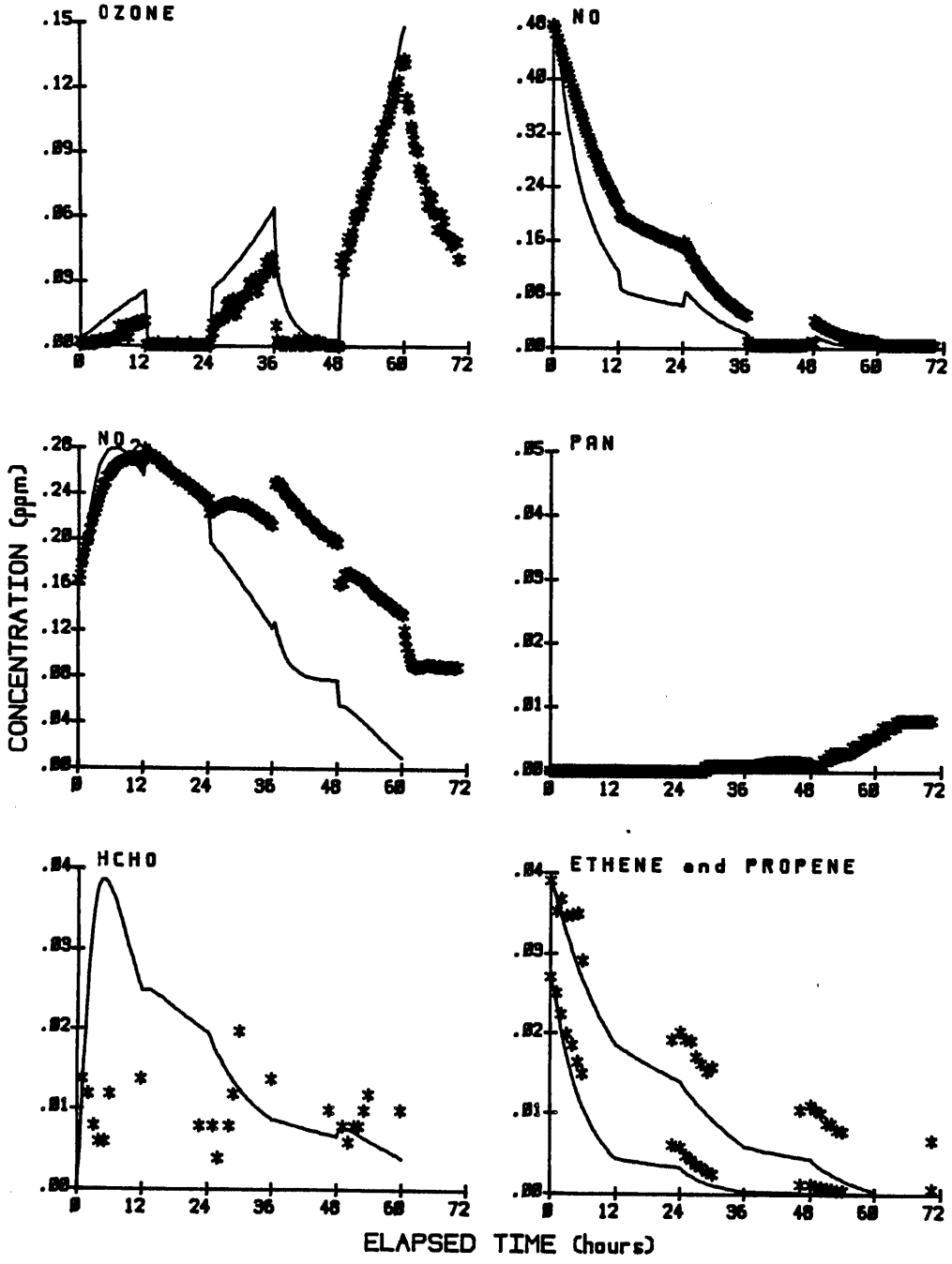


Figure A-27a. Experimental and calculated concentration-time plots for selected species observed in the 3-BL surrogate-$NO_x$-air run ITC-885. (Page 1 of 2).

* = experimental data
——— = model calculation

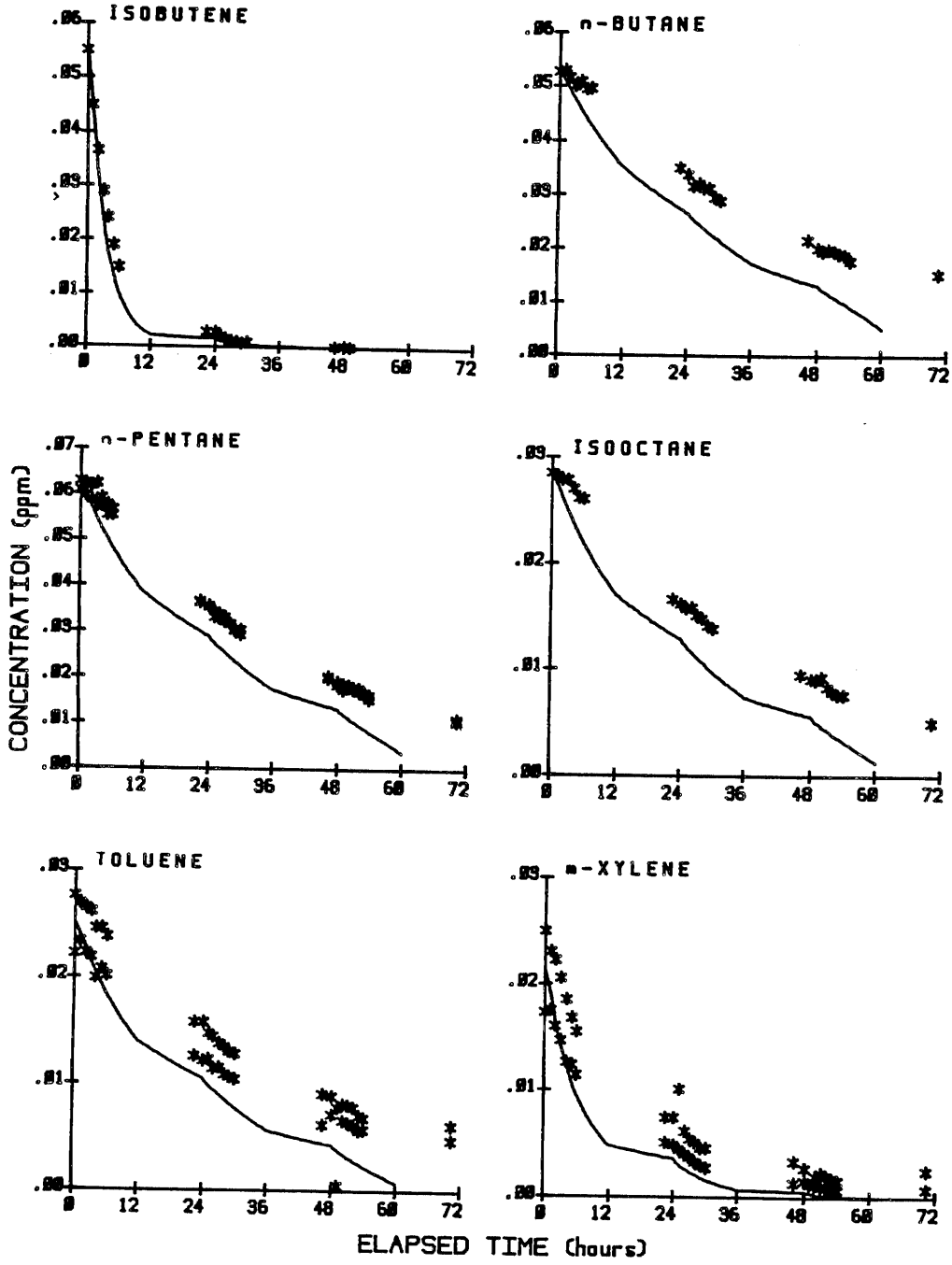


Figure A-27b. Experimental and calculated concentration-time plots for selected species observed in the 3-BL surrogate-$NO_x$-air run ITC-885. (Page 2 of 2).

* = experimental data
——— = model calculation

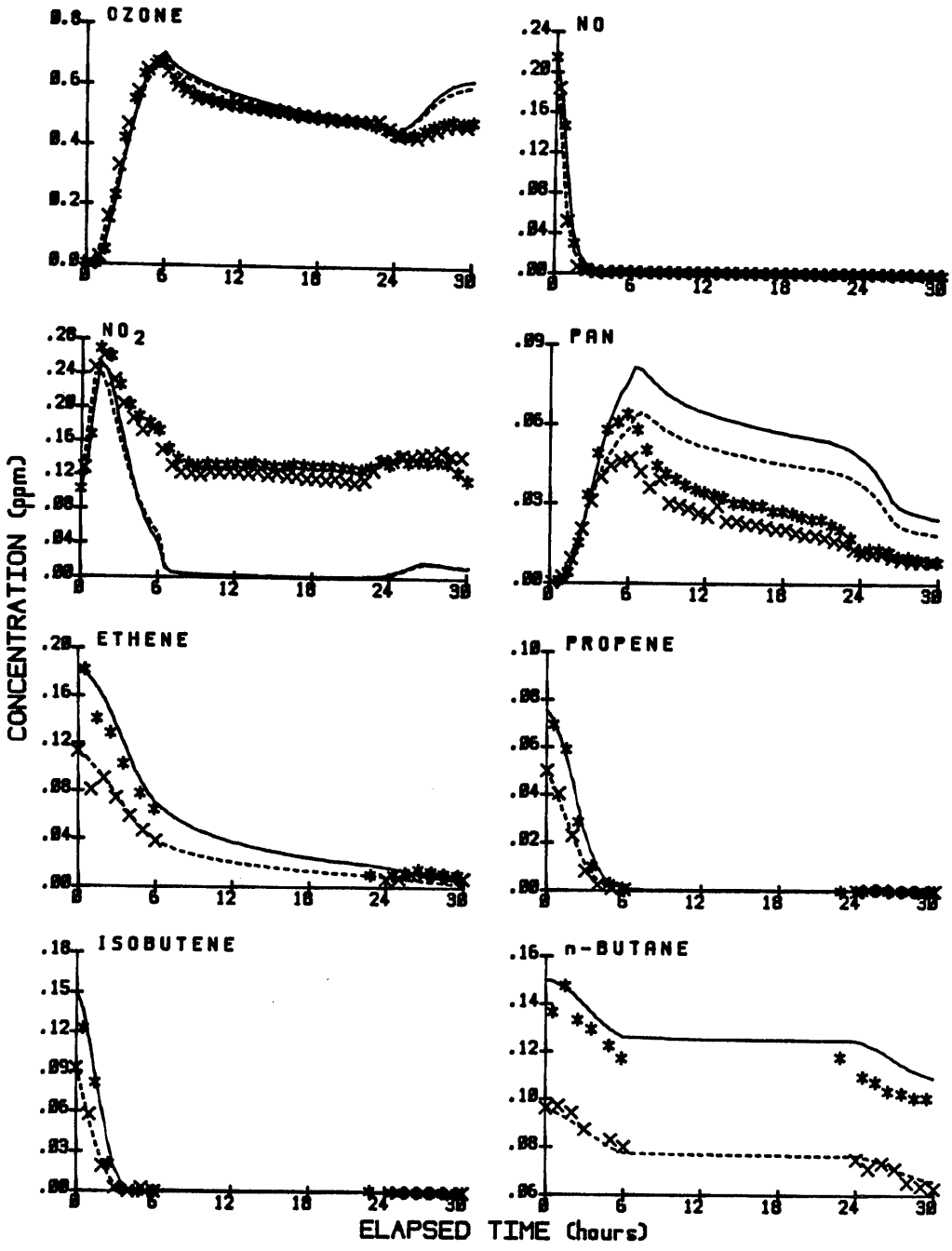


Figure A-28a. Experimental and calculated concentration-time plots for selected species observed in the 13-B-MF surrogate-$NO_x$-air run OTC-241. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

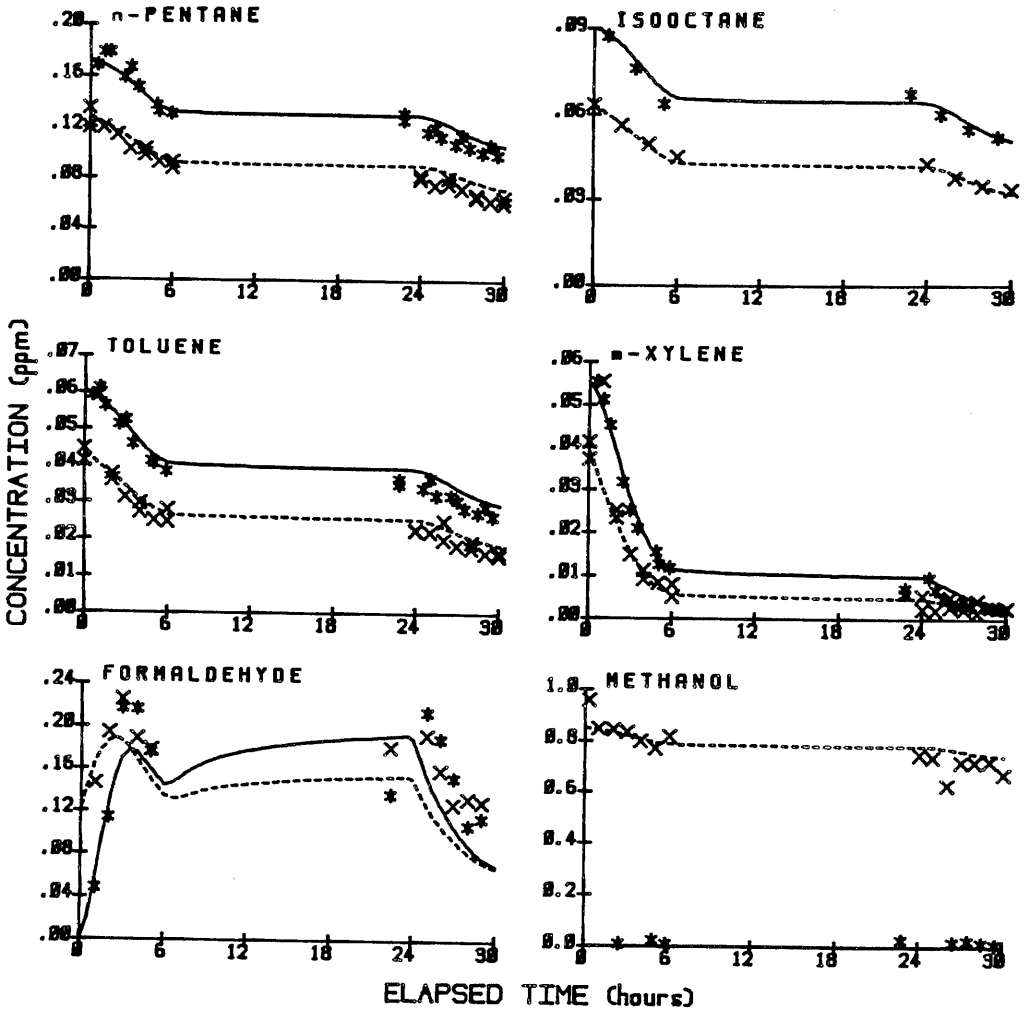


Figure A-28b. Experimental and calculated concentration-time plots for selected species observed in the 13-B-MF surrogate-$NO_x$-air run OTC-241. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

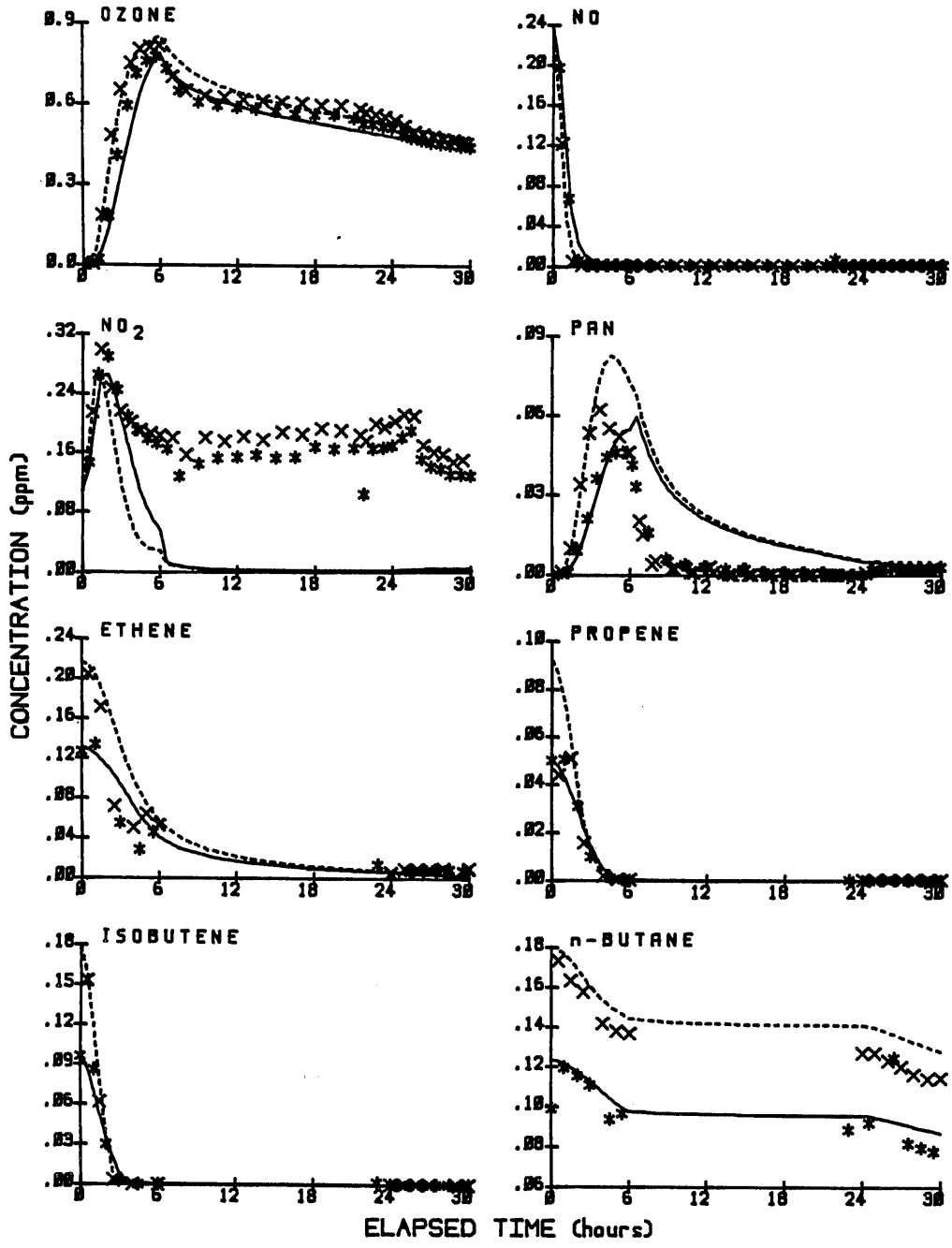


Figure A-29a. Experimental and calculated concentration-time plots for selected species observed in the 14-M-B surrogate-$NO_x$-air run OTC-224. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

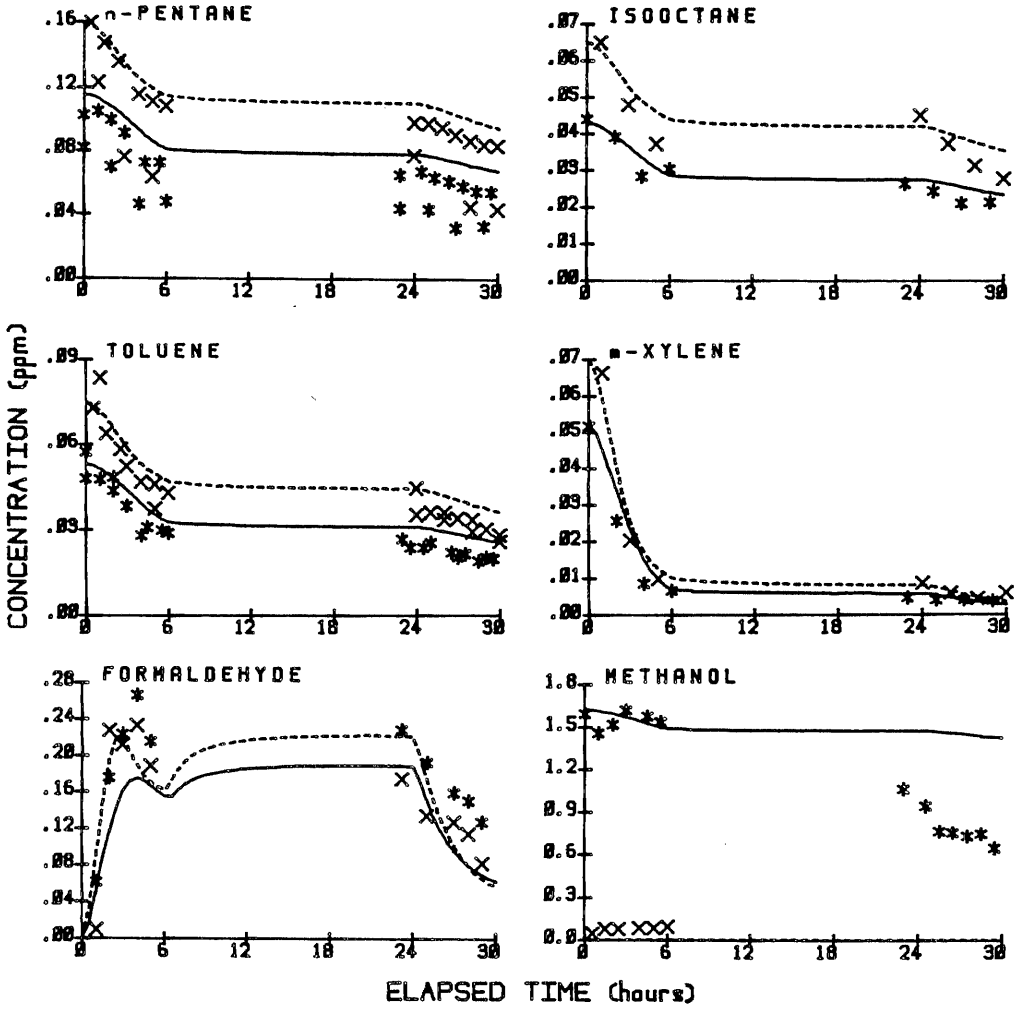


Figure A-29b. Experimental and calculated concentration-time plots for selected species observed in the 14-M-B surrogate-$NO_x$-air run OTC-224. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

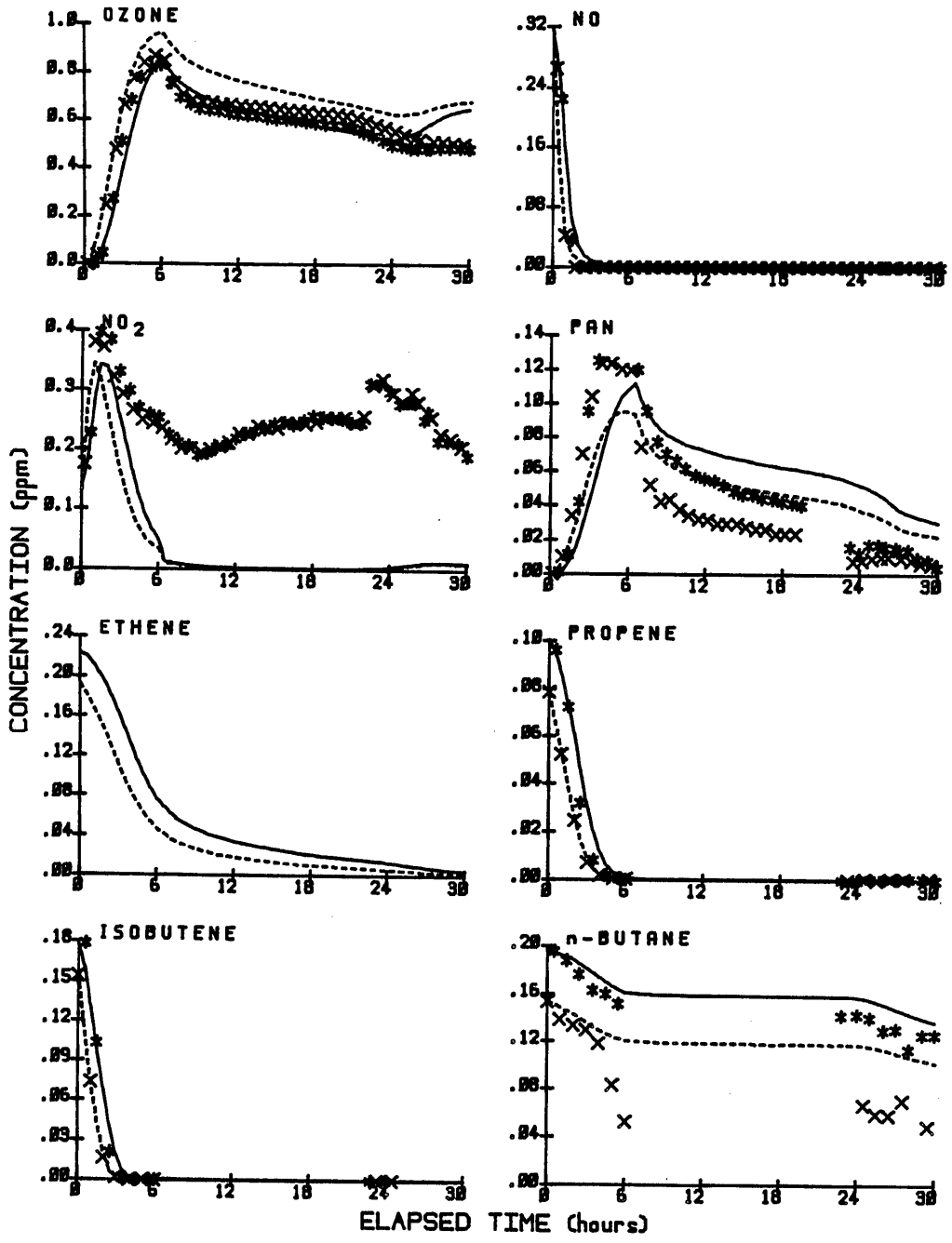


Figure A-30a. Experimental and calculated concentration-time plots for selected species observed in the 10-B-MF surrogate-$NO_x$-air run OTC-215. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

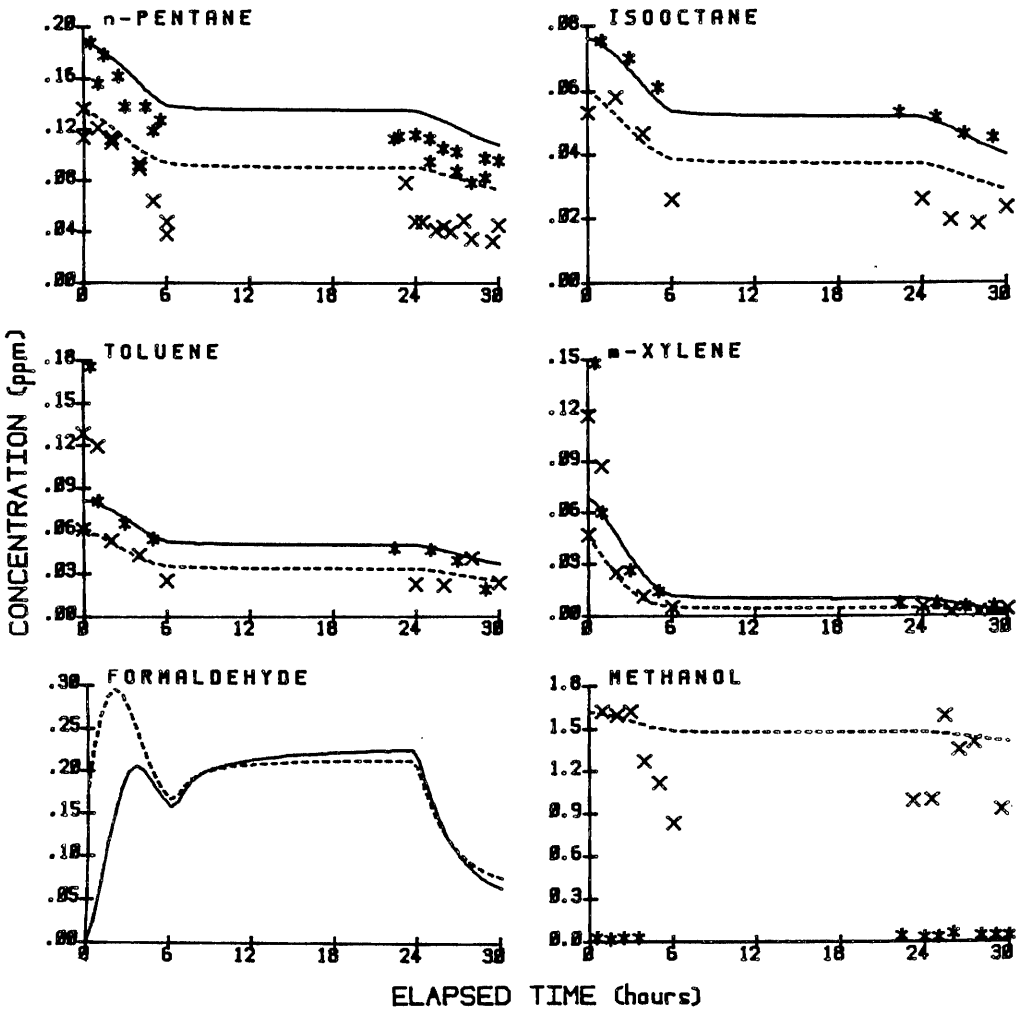


Figure A-30b. Experimental and calculated concentration-time plots for selected species observed in the 10-B-MF surrogate-$NO_x$-air run OTC-215. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

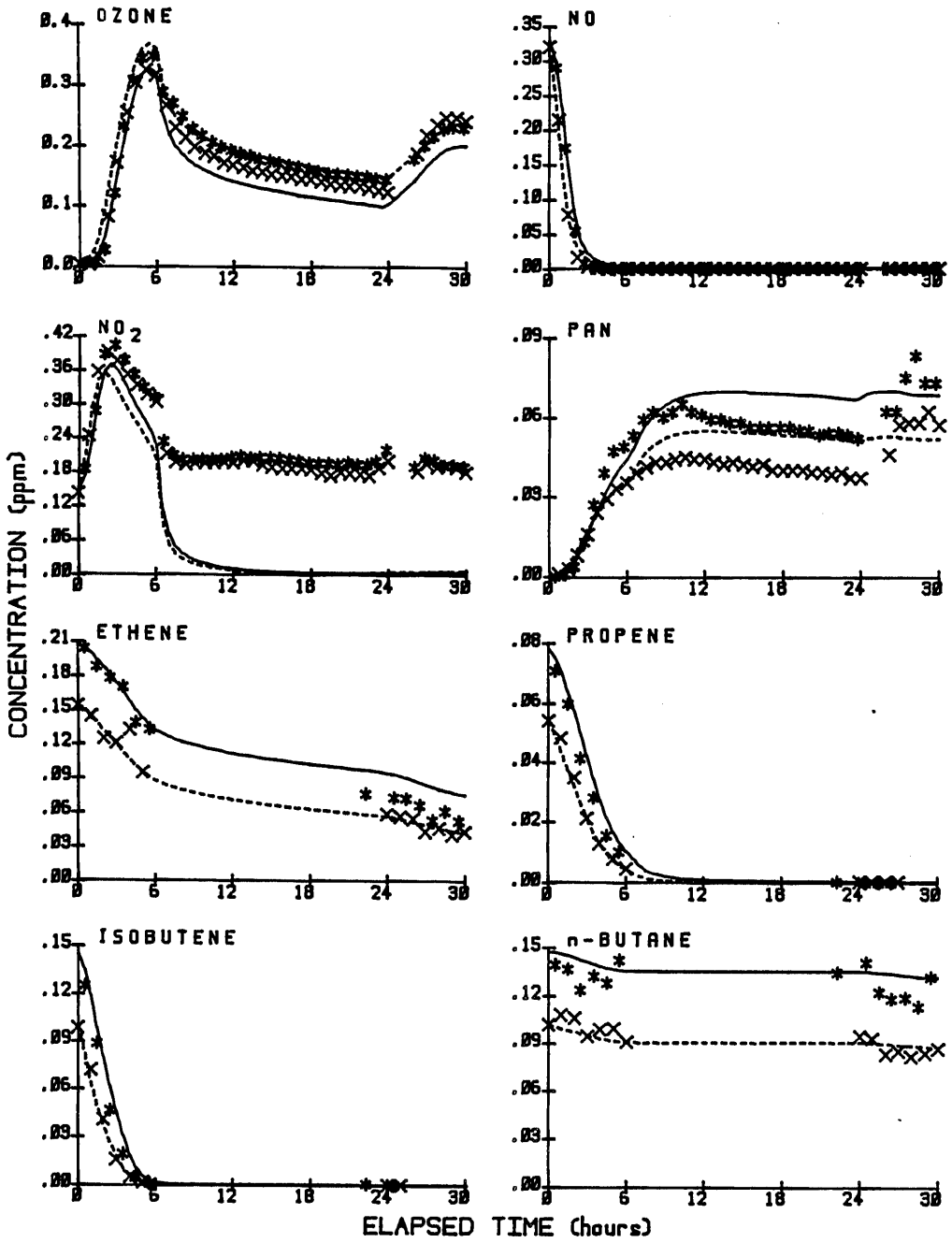


Figure A-31a. Experimental and calculated concentration-time plots for selected species observed in the 10-B-MF surrogate-$NO_x$-air run OTC-249. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

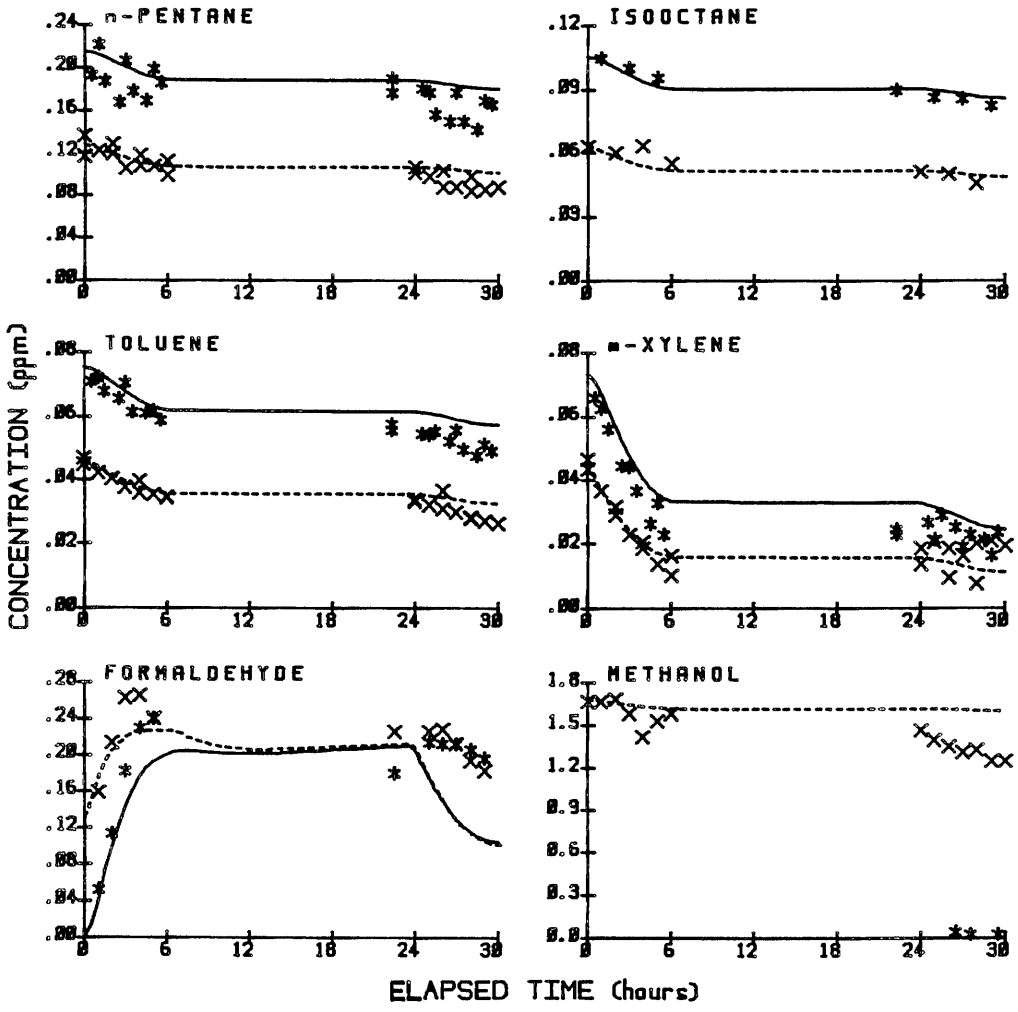


Figure A-31b. Experimental and calculated concentration-time plots for selected species observed in the 10-B-MF surrogate-$NO_x$-air run OTC-249. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

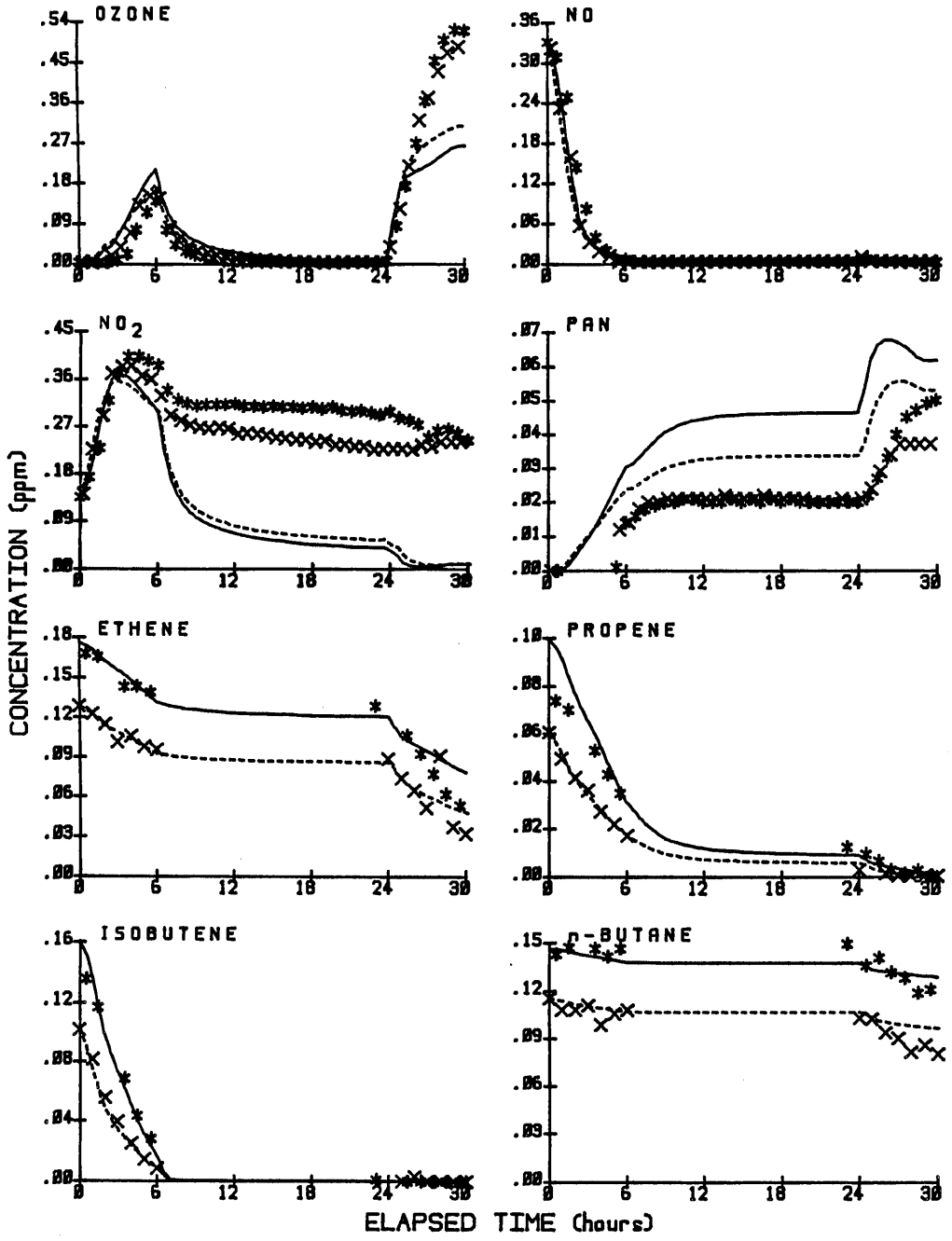


Figure A-32a. Experimental and calculated concentration-time plots for selected species observed in the 10-B-MF surrogate-$NO_x$-air run OTC-243. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

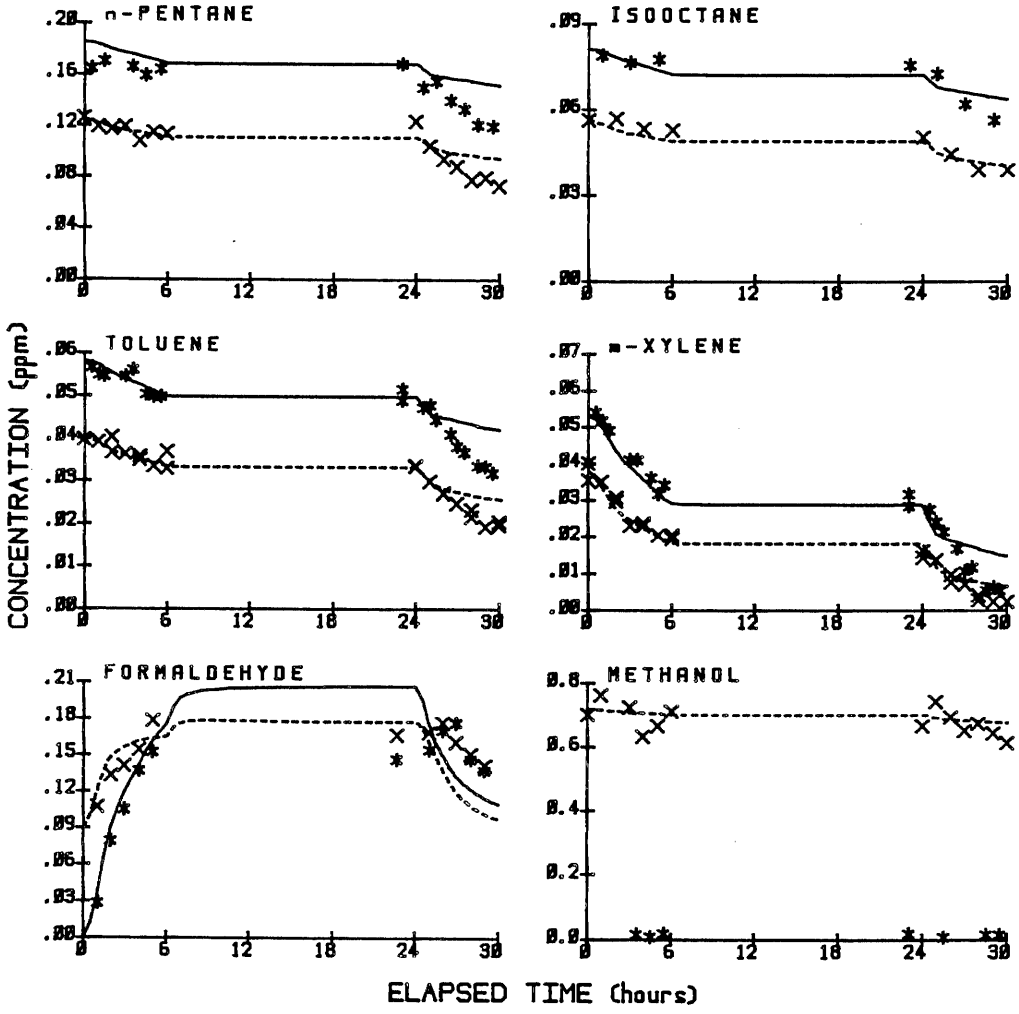


Figure A-32b. Experimental and calculated concentration-time plots for selected species observed in the 10-B-MF surrogate-$NO_x$-air run OTC-243. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

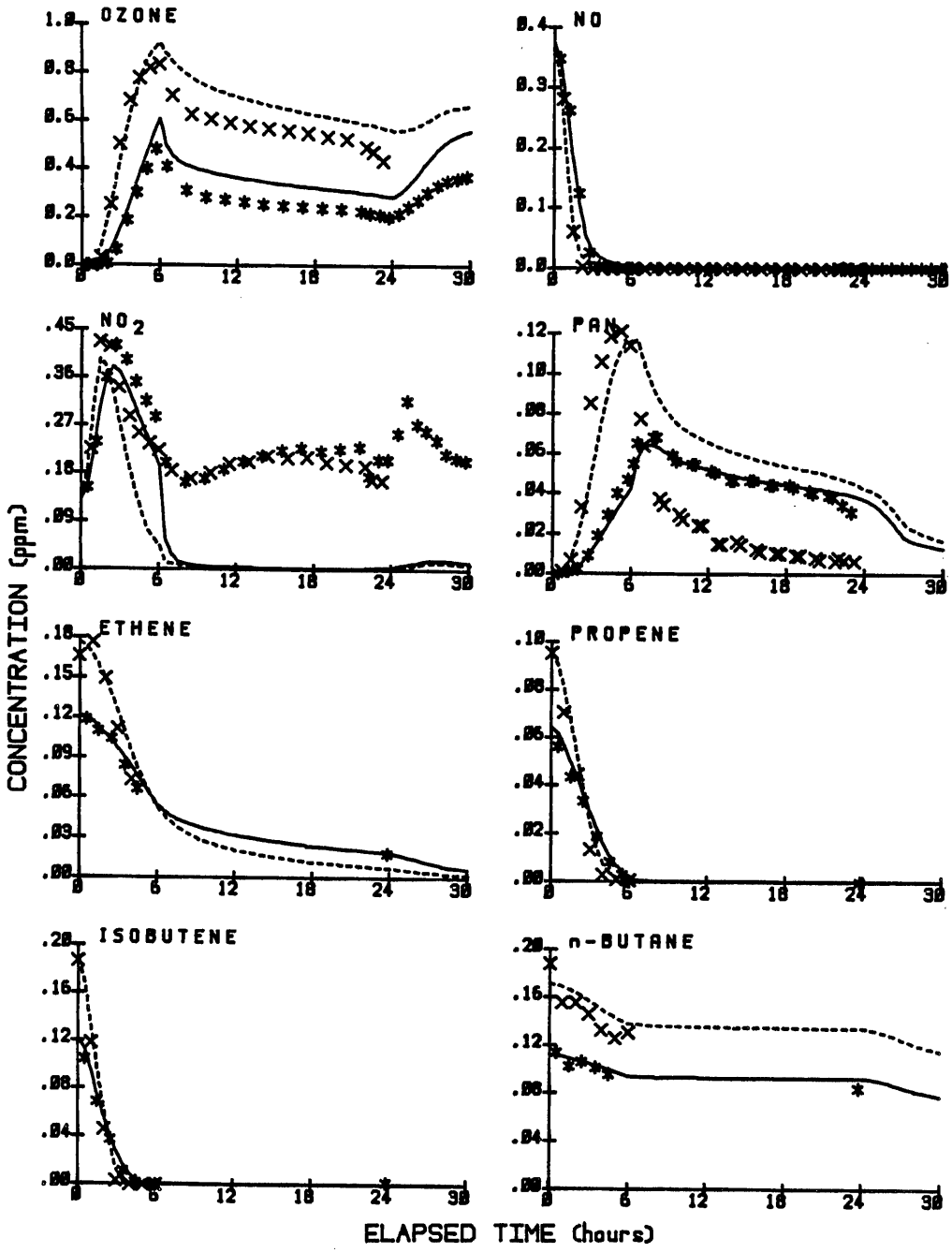


Figure A-33a. Experimental and calculated concentration-time plots for selected species observed in the 10-M-B surrogate-$NO_x$-air run OTC-217. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

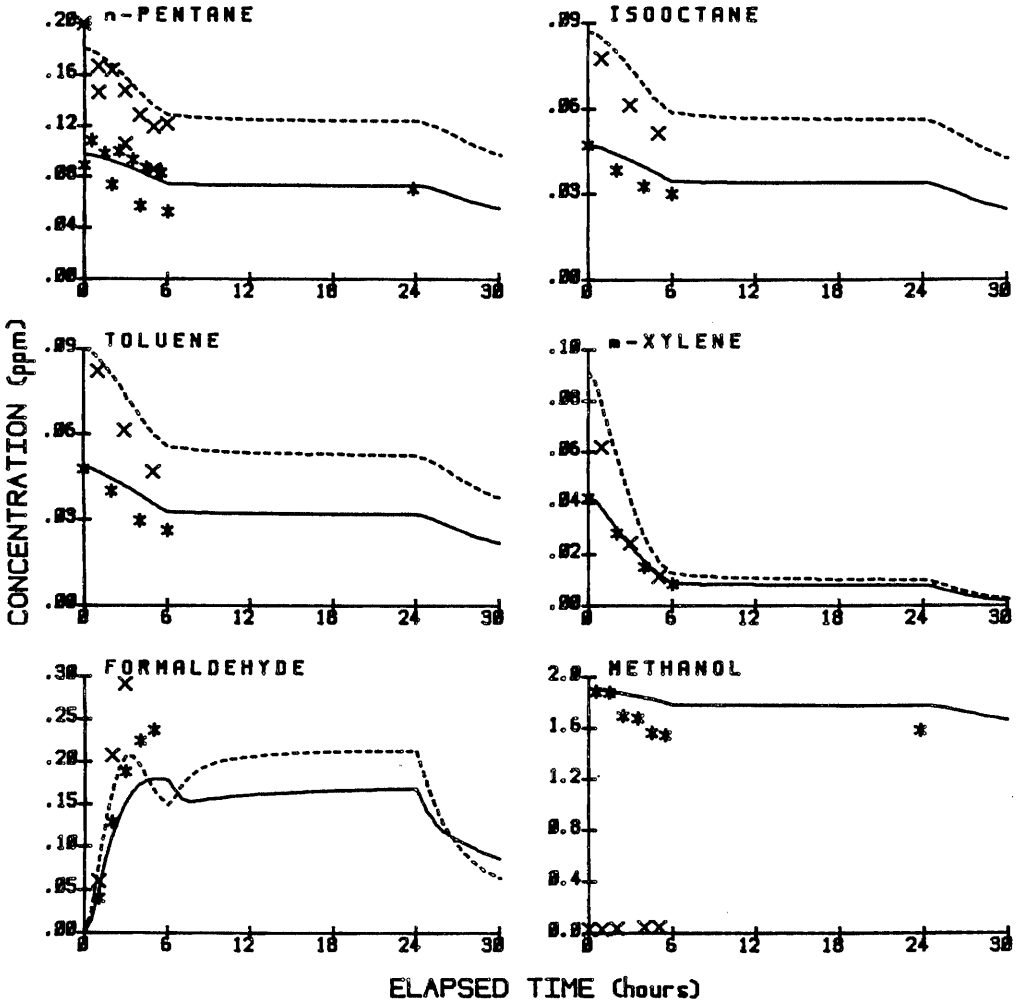


Figure A-33b. Experimental and calculated concentration-time plots for selected species observed in the 10-M-B surrogate-$NO_x$-air run OTC-217. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

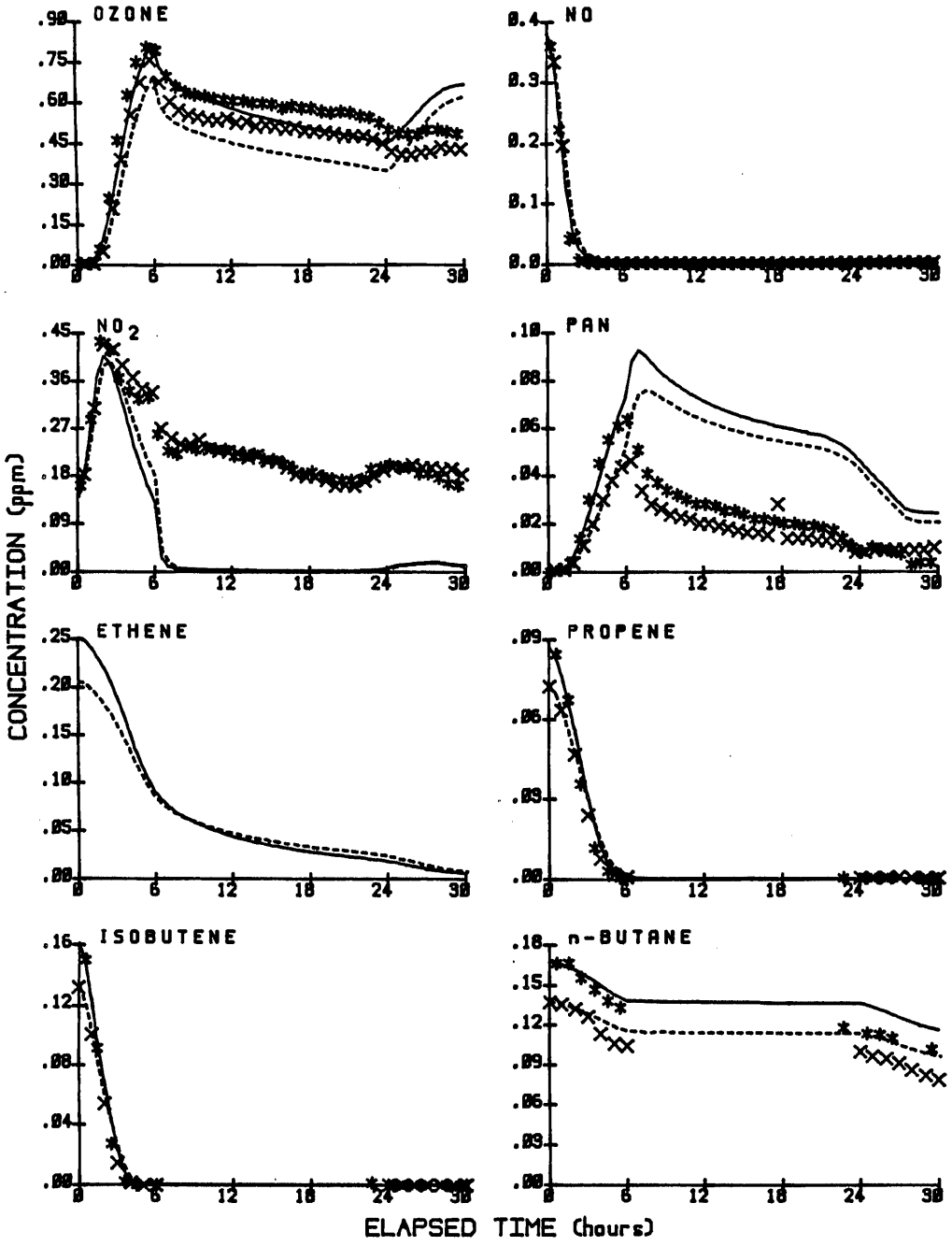


Figure A-34a. Experimental and calculated concentration-time plots for selected species observed in the 10-B-M surrogate-$NO_x$-air run OTC-237. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

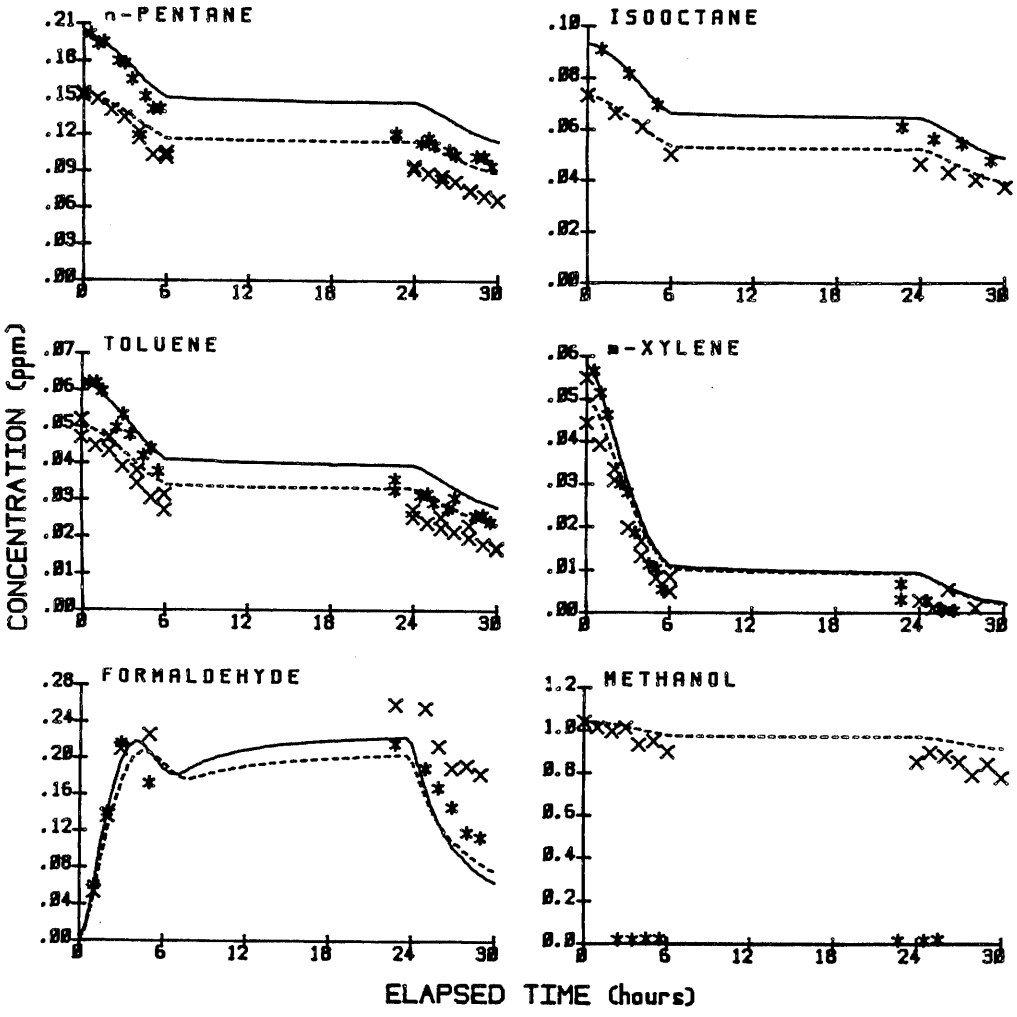


Figure A-34b. Experimental and calculated concentration-time plots for selected species observed in the 10-B-M surrogate-$NO_x$-air run OTC-237. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

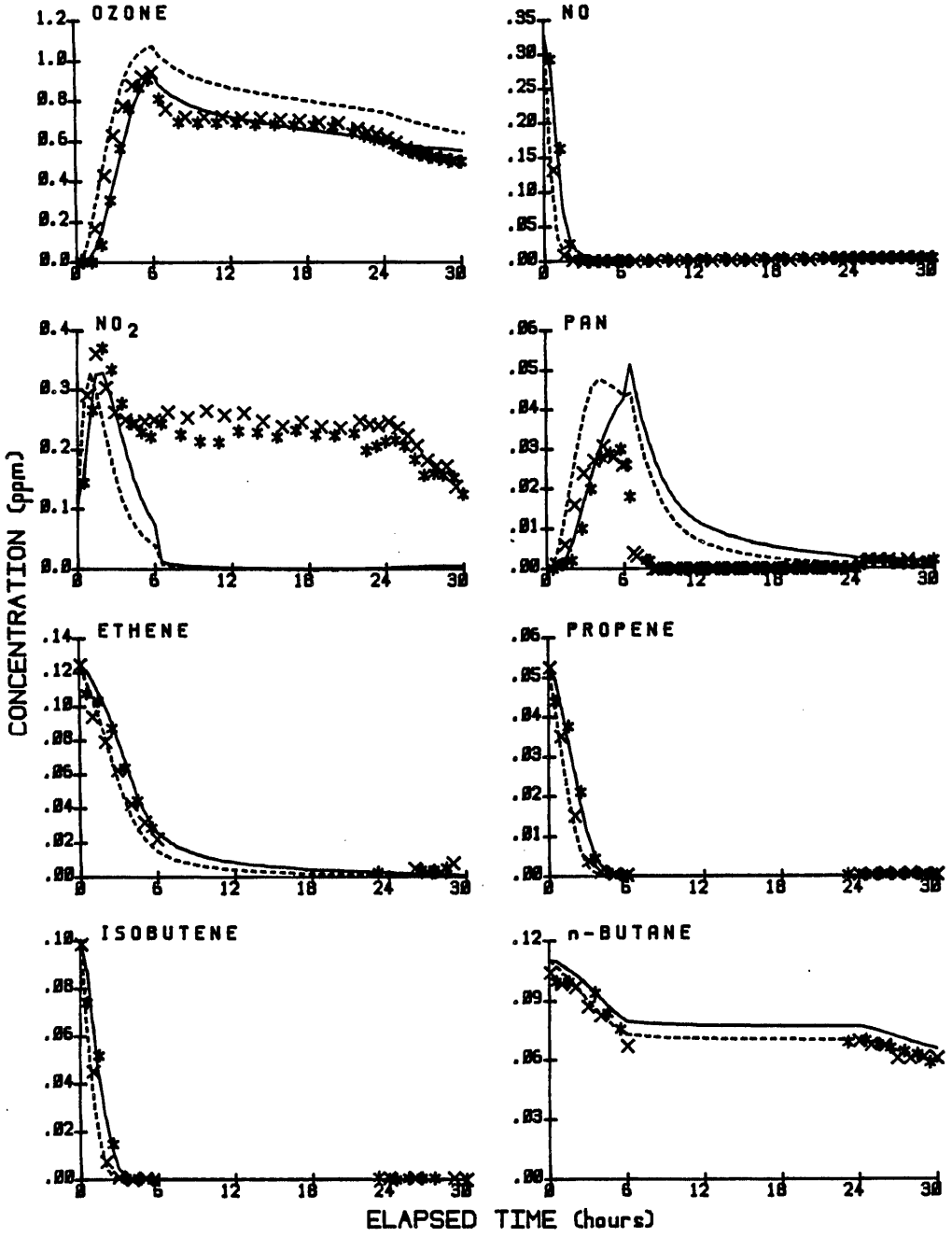


Figure A-35a. Experimental and calculated concentration-time plots for selected species observed in the 10-M-MF surrogate-$NO_x$-air run OTC-222. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

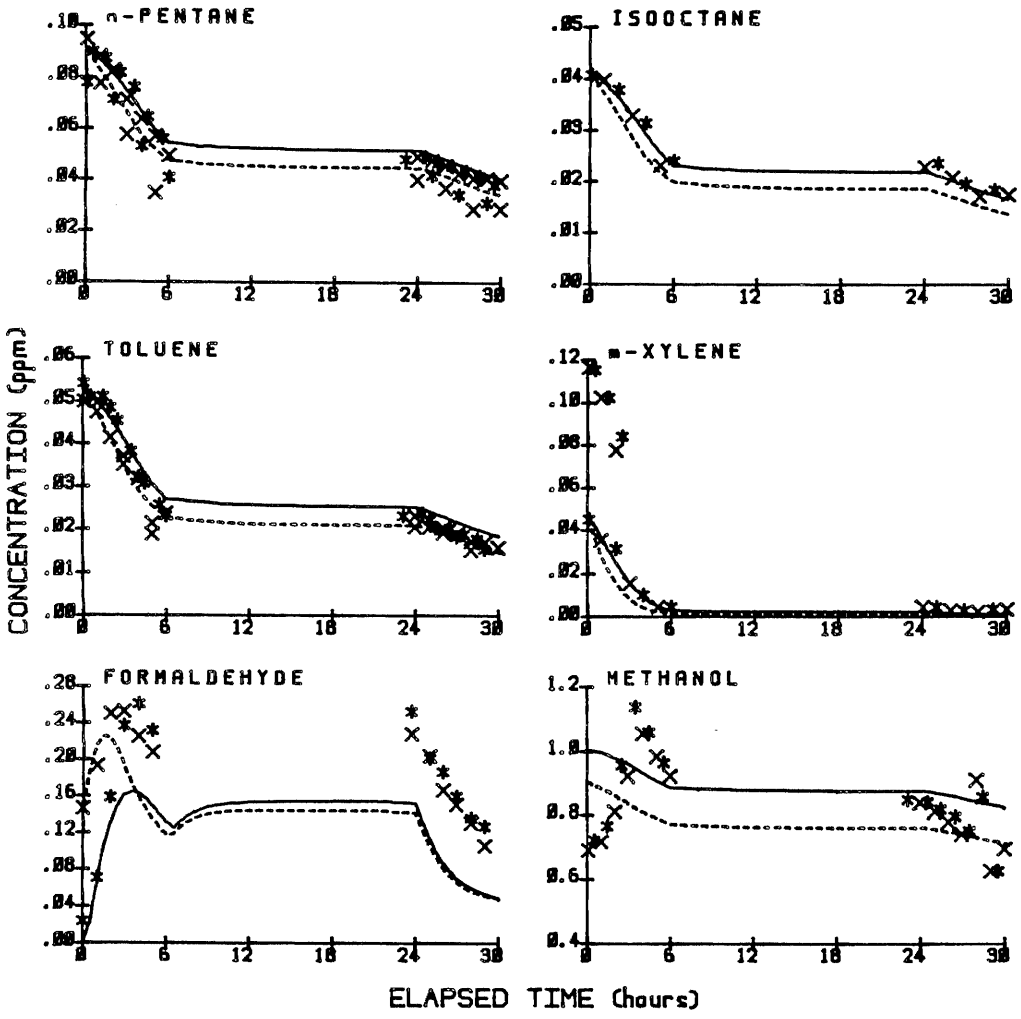


Figure A-35b. Experimental and calculated concentration-time plots for selected species observed in the 10-M-MF surrogate-$NO_x$-air run OTC-222. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

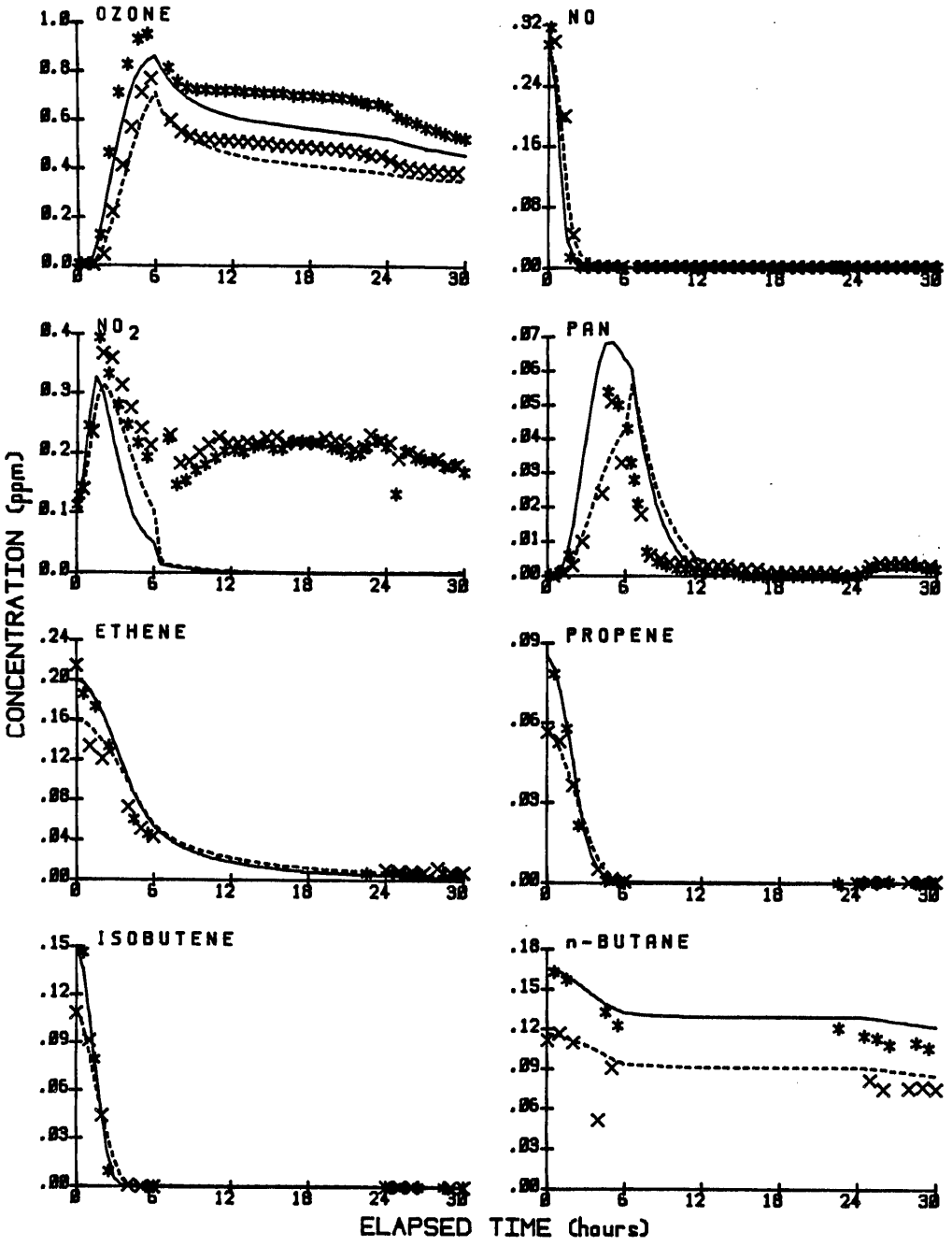


Figure A-36a. Experimental and calculated concentration-time plots for selected species observed in the 10-B-BL surrogate-$NO_x$-air run OTC-223. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

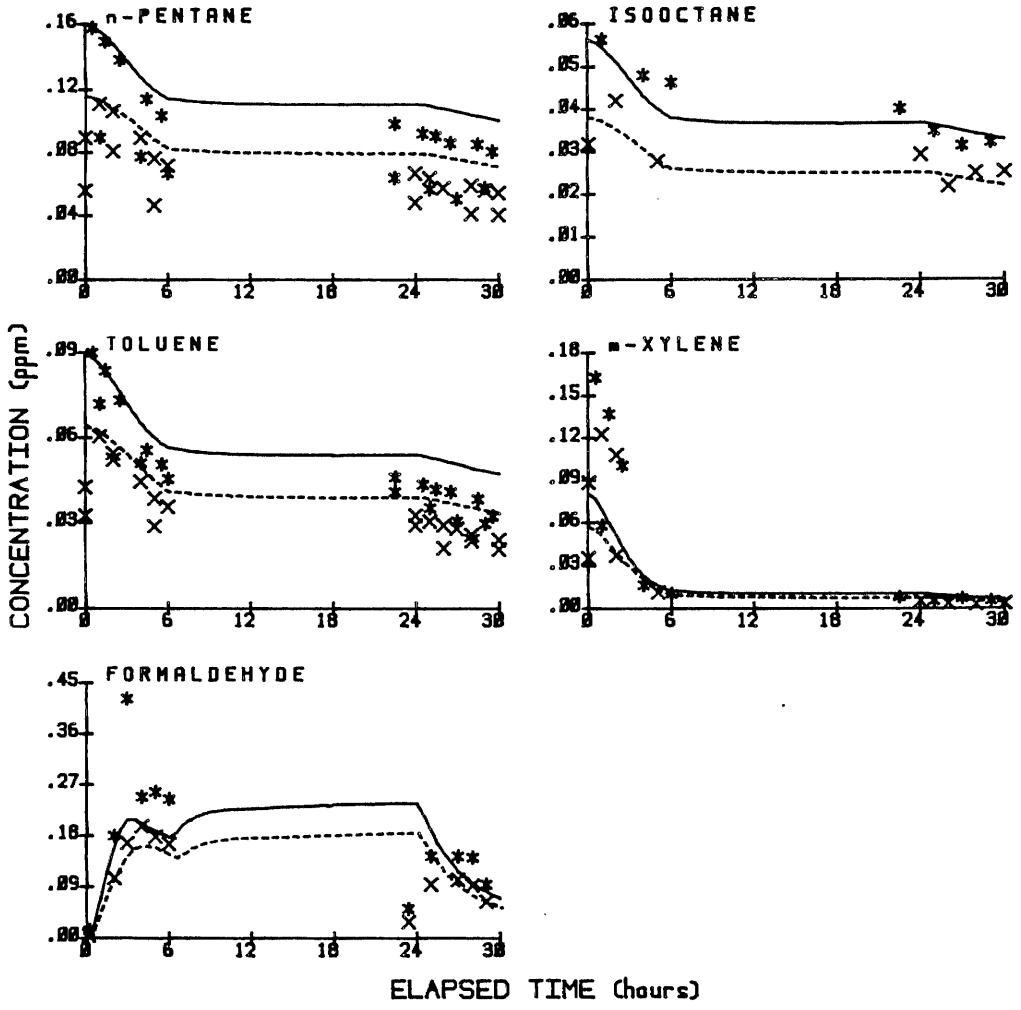


Figure A-36b. Experimental and calculated concentration-time plots for selected species observed in the 10-B-BL surrogate-$NO_x$-air run OTC-223. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

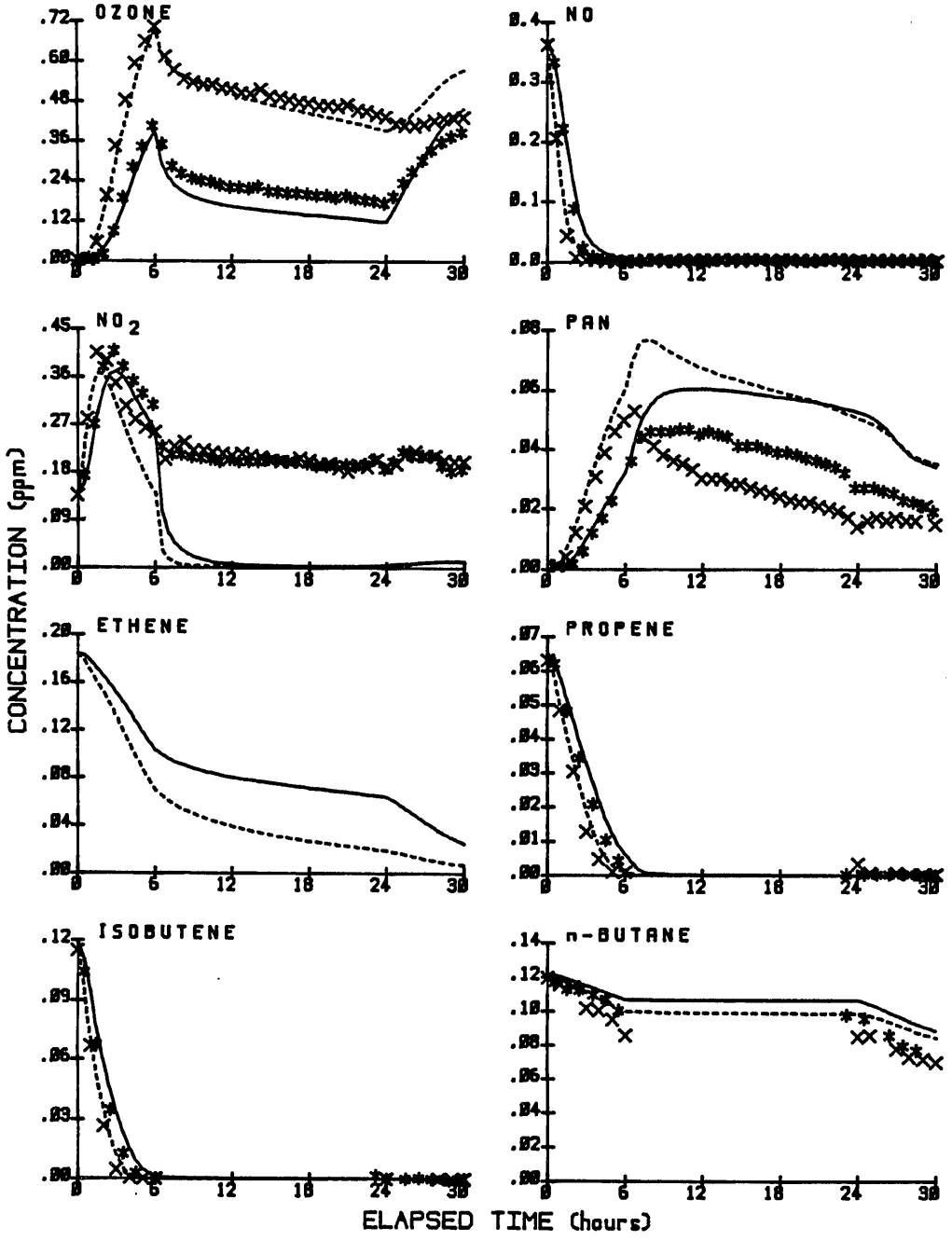


Figure A-37a. Experimental and calculated concentration-time plots for selected species observed in the 10-BL-MF surrogate-$NO_x$-air run OTC-238. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

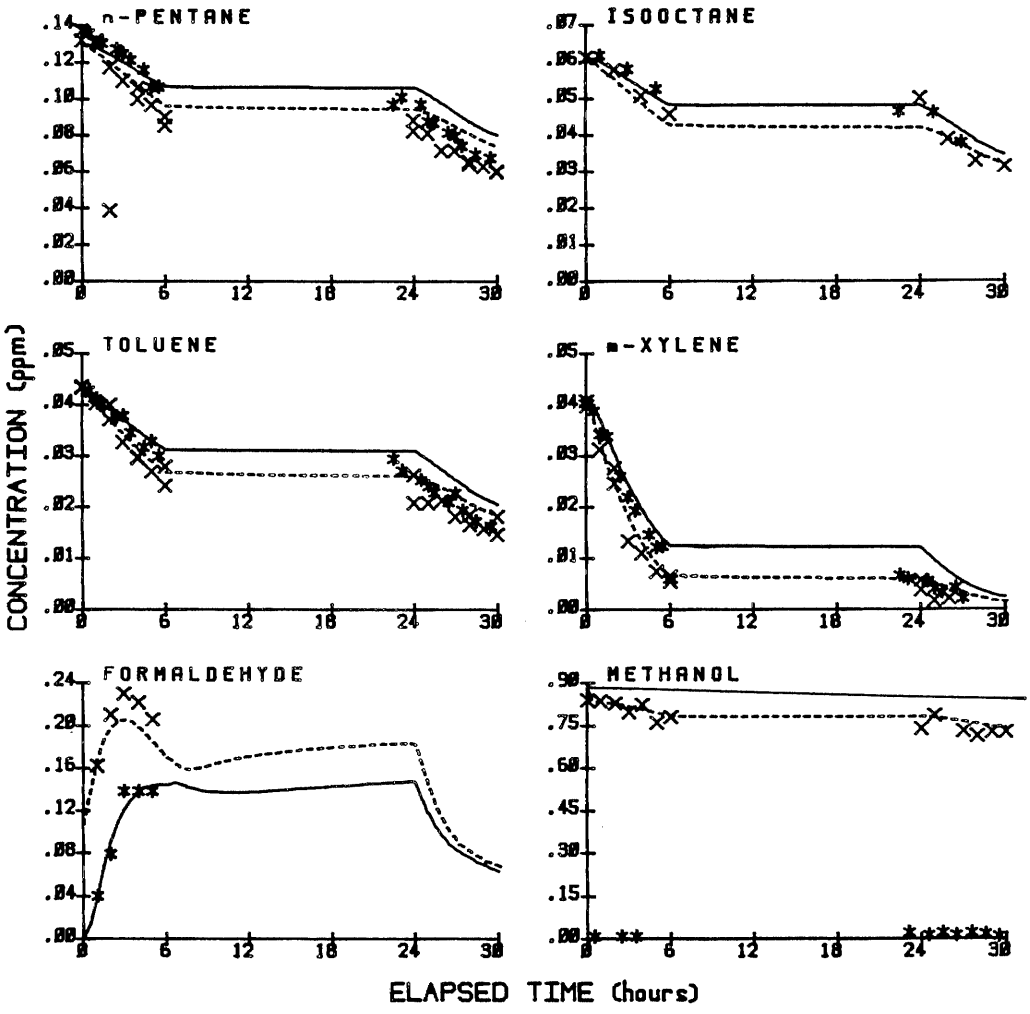


Figure A-37b. Experimental and calculated concentration-time plots for selected species observed in the 10-BL-MF surrogate-$NO_x$-air run OTC-238. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

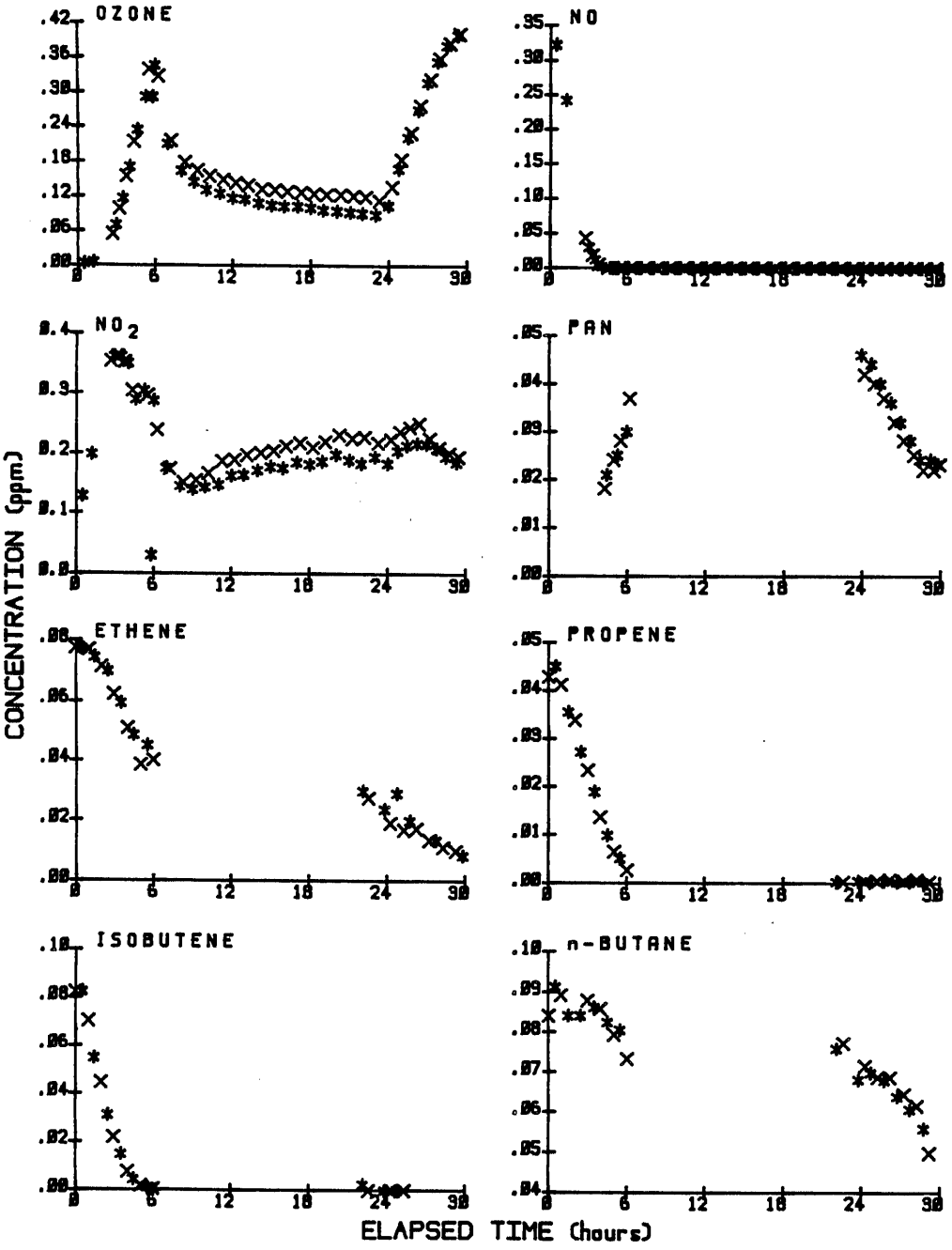


Figure A-38a. Experimental concentration-time plots for selected species observed in the 10-MF-MF surrogate-$NO_x$-air side equivalency test run OTC-214. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B

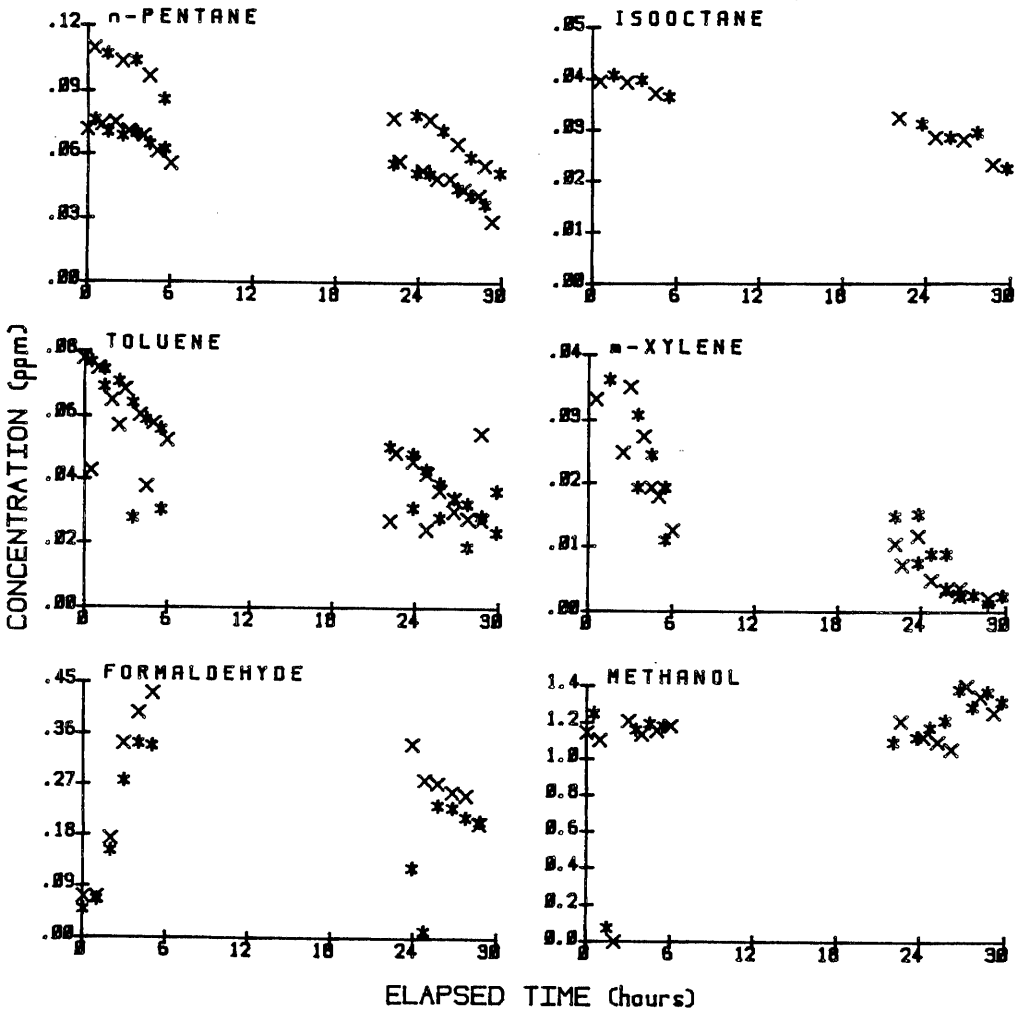


Figure A-38b. Experimental concentration-time plots for selected species observed in the 10-MF-MF surrogate-$NO_x$-air side equivalency test run OTC-214. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B

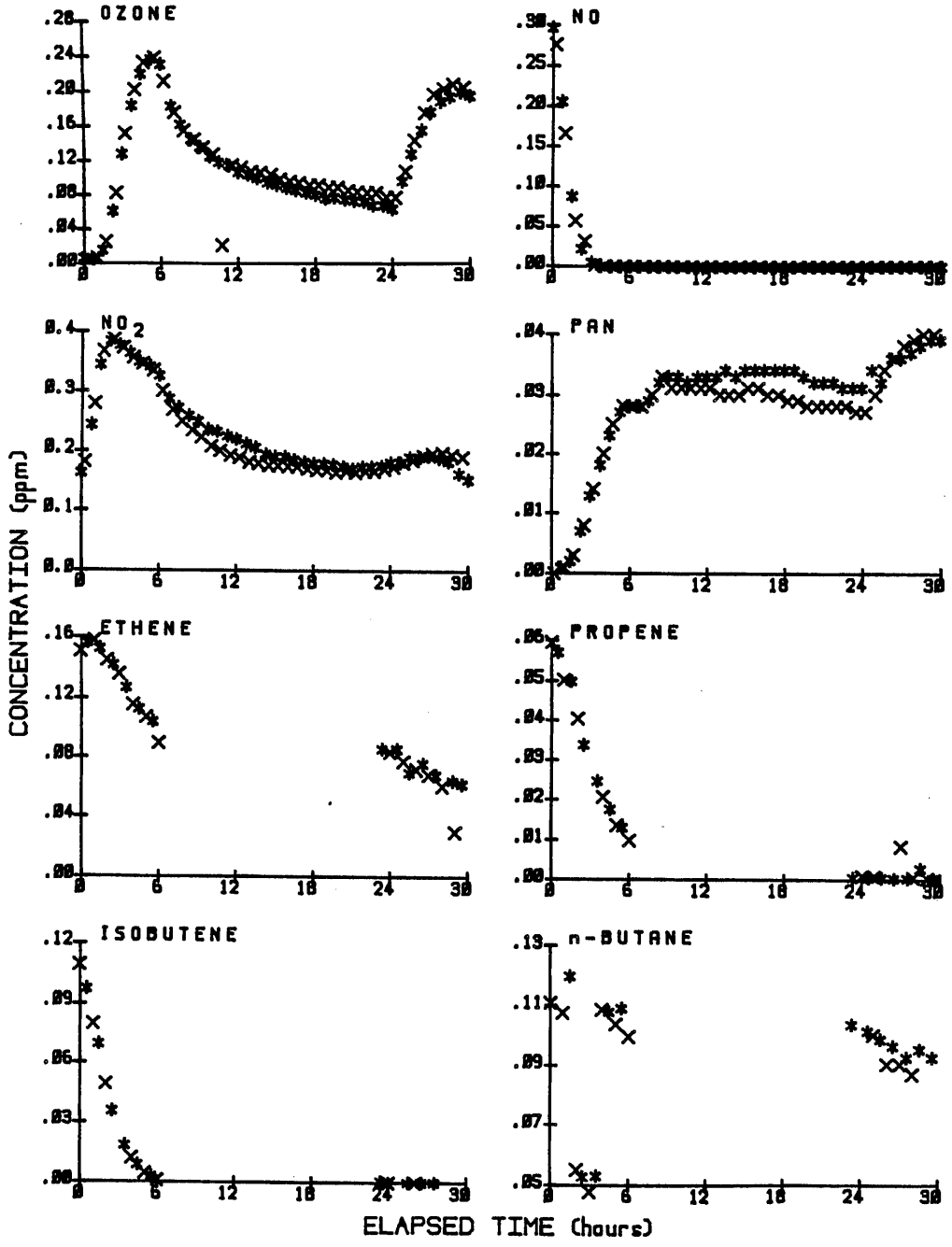


Figure A-39a. Experimental concentration-time plots for selected species observed in the 10-MF-MF surrogate-$NO_x$-air side equivalency test run OTC-250. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B

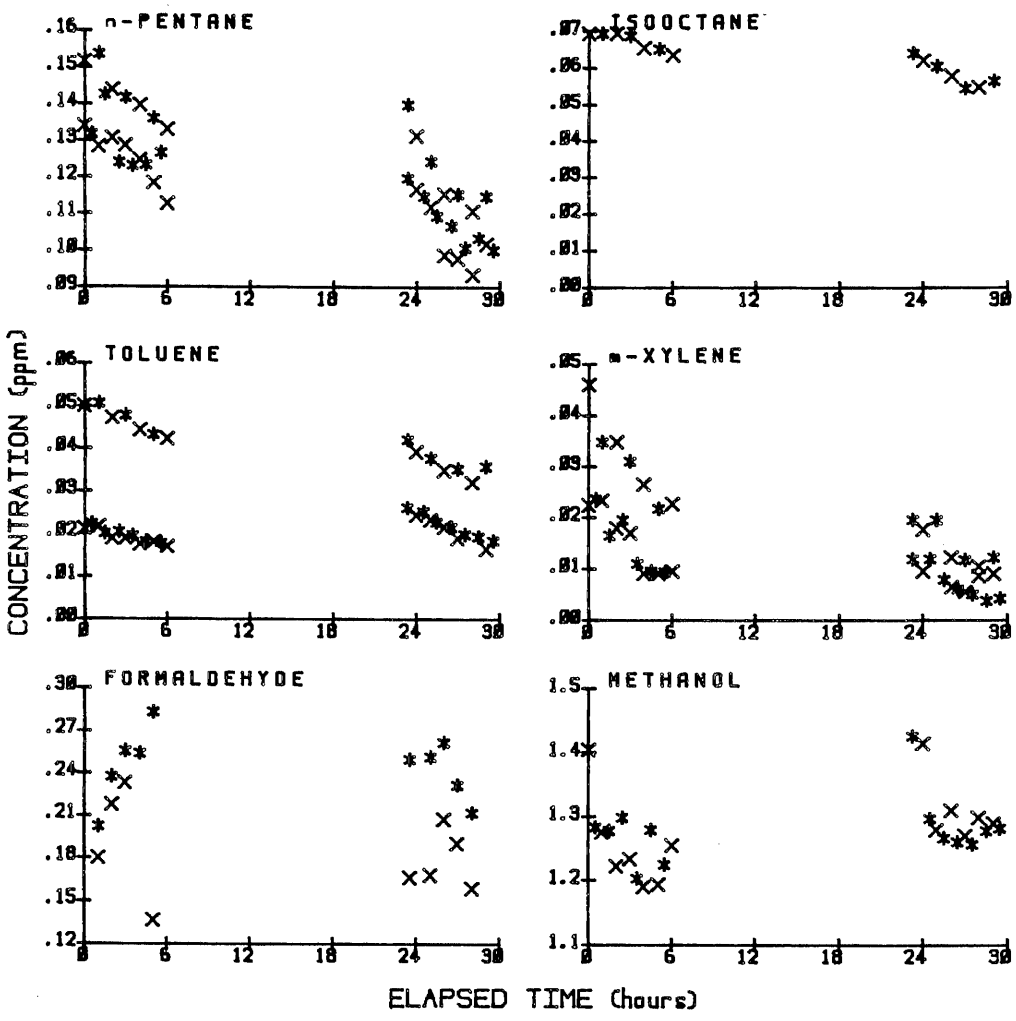


Figure A-39b. Experimental concentration-time plots for selected species observed in the 10-MF-MF surrogate-$NO_x$-air side equivalency test run OTC-250. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B

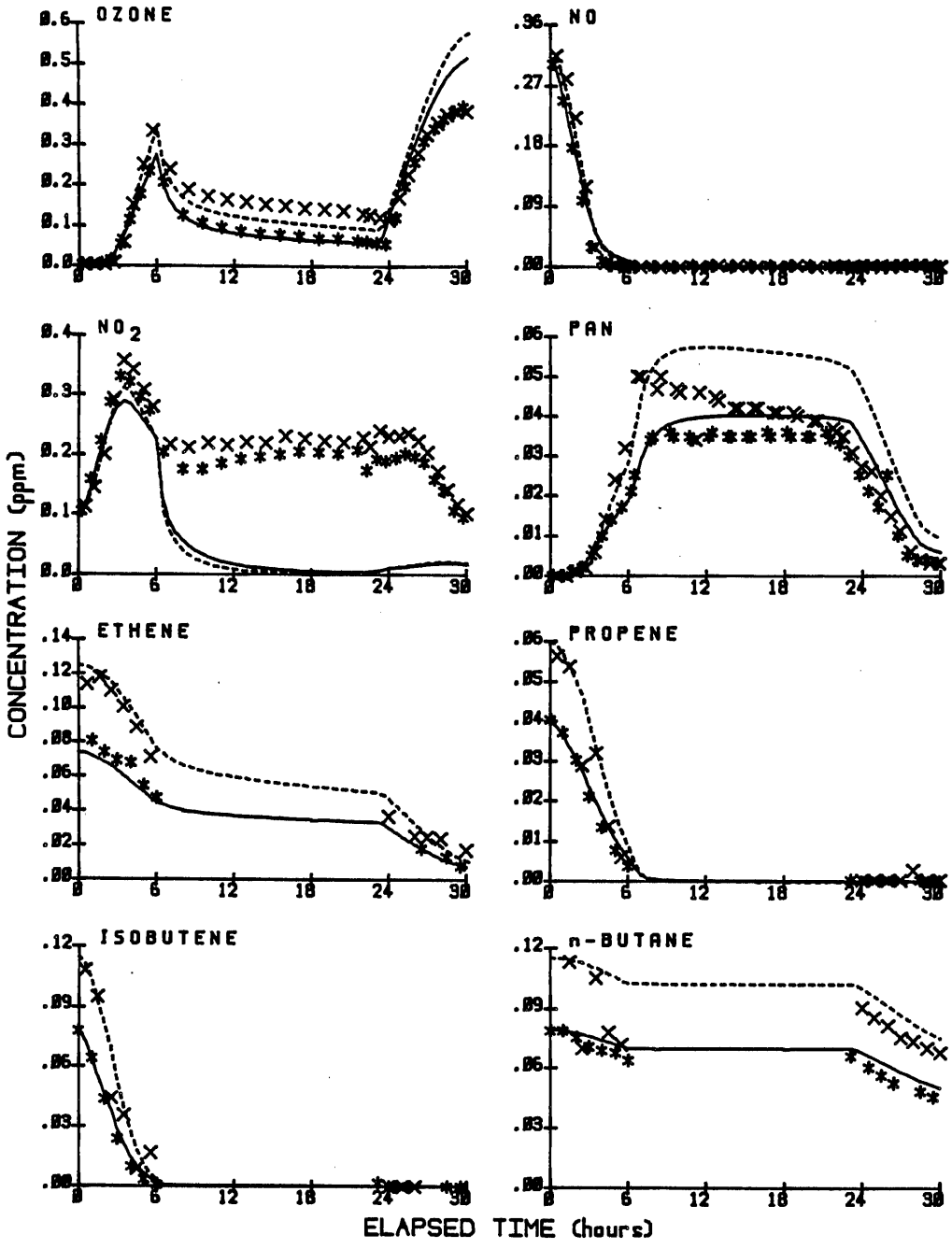


Figure A-40a. Experimental and calculated concentration-time plots for selected species observed in the 7-MF-B surrogate-$NO_x$-air run OTC-221. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

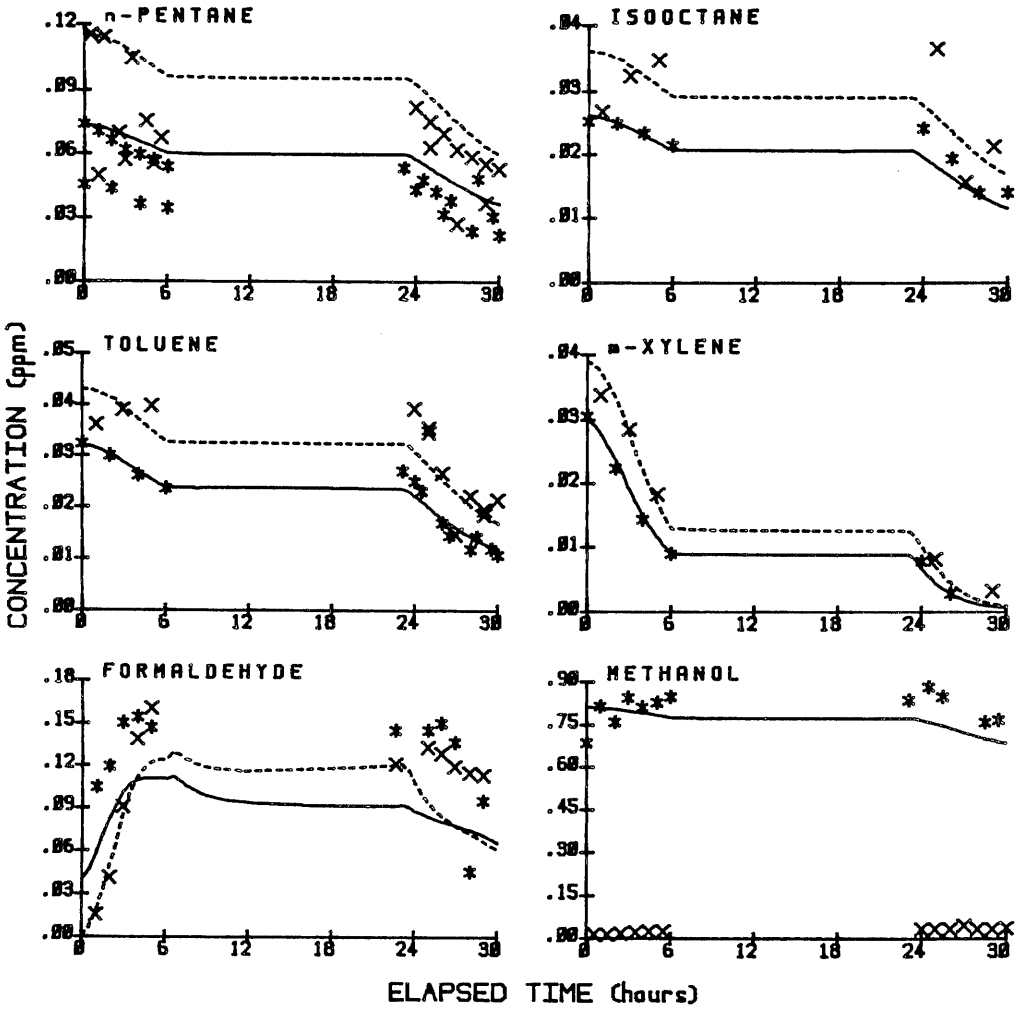


Figure A-40b. Experimental and calculated concentration-time plots for selected species observed in the 7-MF-B surrogate-$NO_x$-air run OTC-221. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

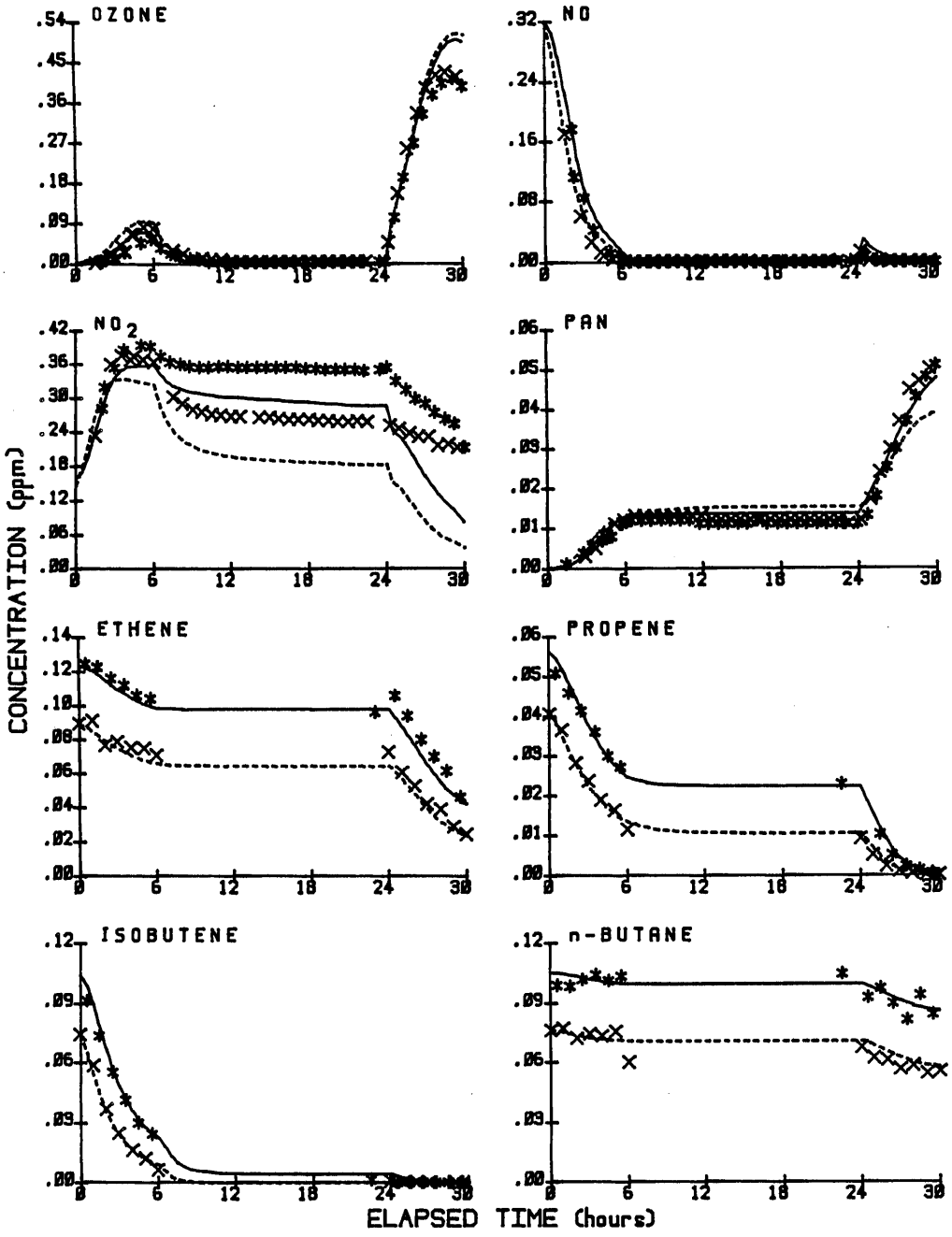


Figure A-41a. Experimental and calculated concentration-time plots for selected species observed in the 7-B-MF surrogate-$NO_x$-air run OTC-248. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

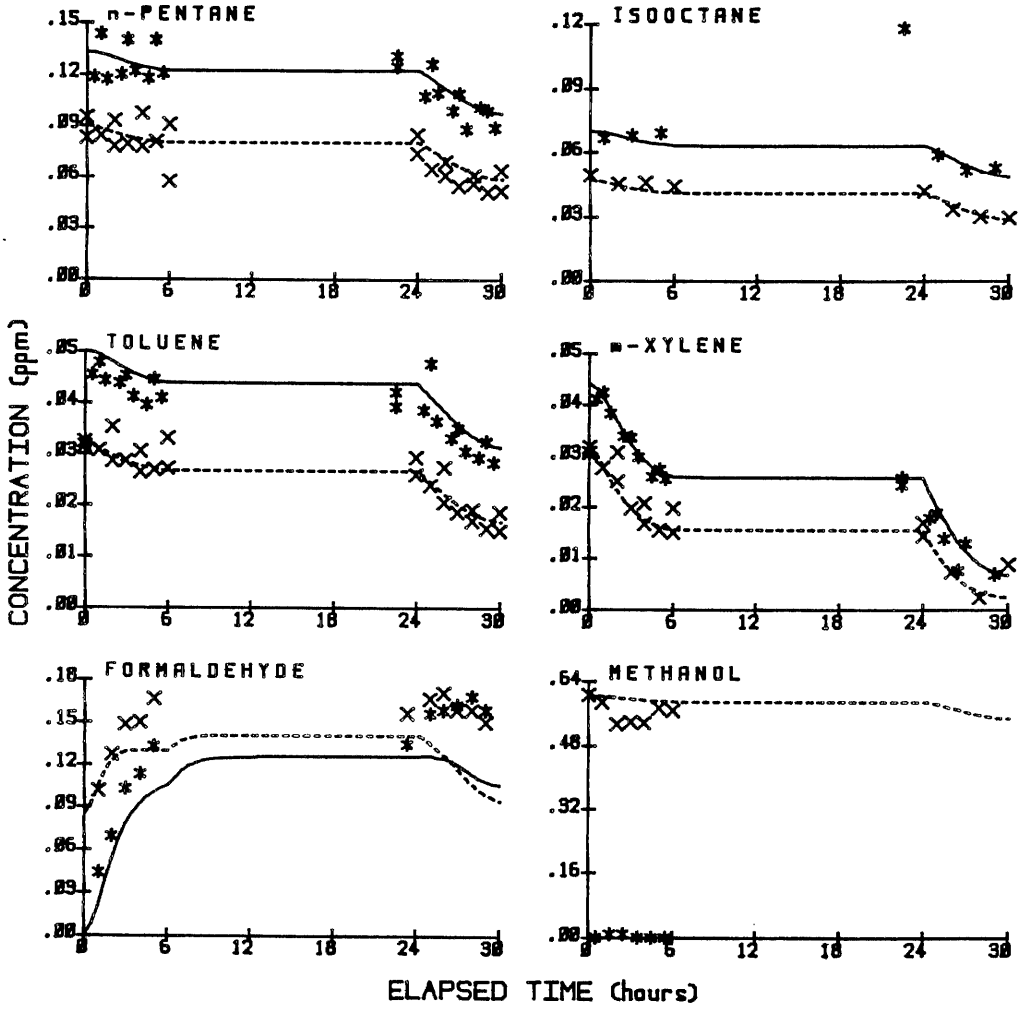


Figure A-41b. Experimental and calculated concentration-time plots for selected species observed in the 7-B-MF surrogate-$NO_x$-air run OTC-248. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

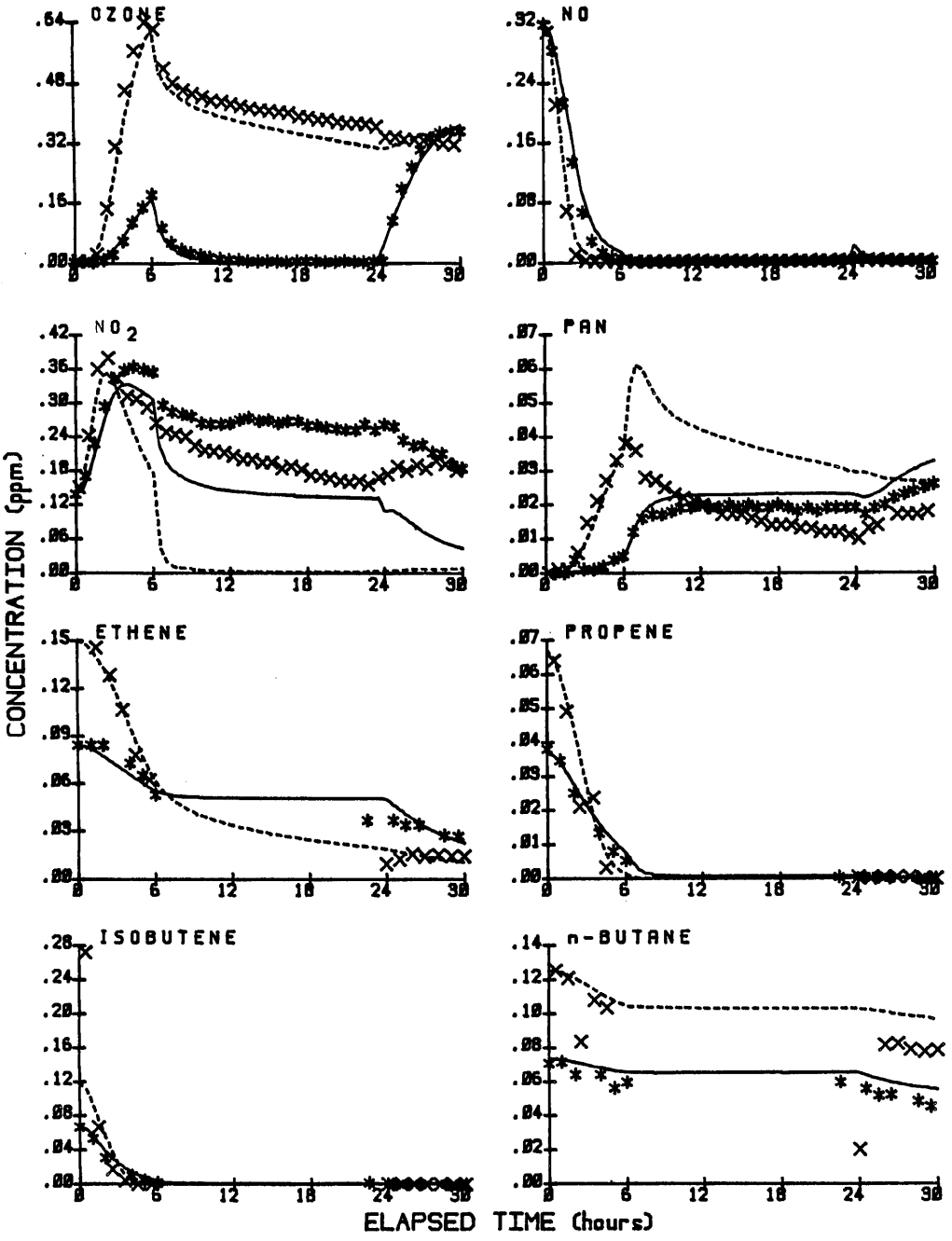


Figure A-42a. Experimental and calculated concentration-time plots for selected species observed in the 7-M-B surrogate-$NO_x$-air run OTC-242. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

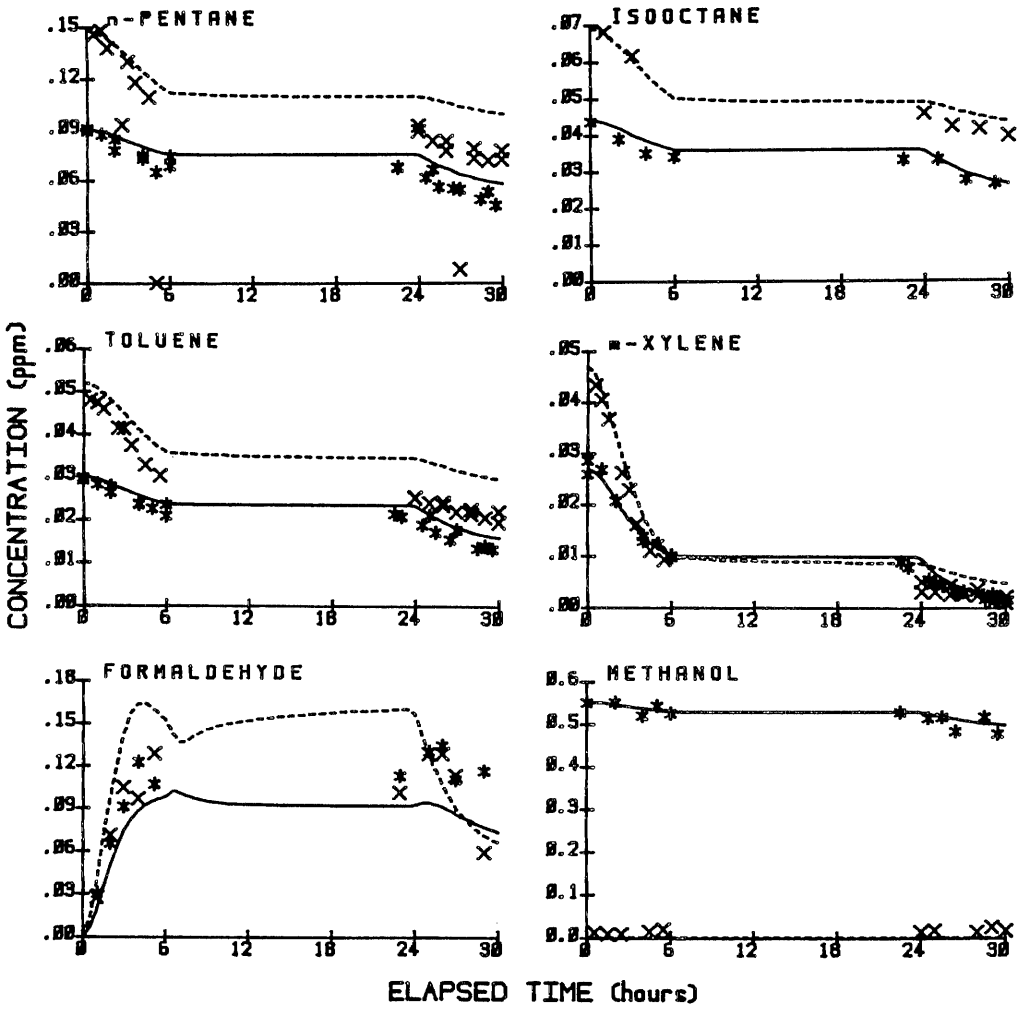


Figure A-42b. Experimental and calculated concentration-time plots for selected species observed in the 7-M-B surrogate-$NO_x$-air run OTC-242. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

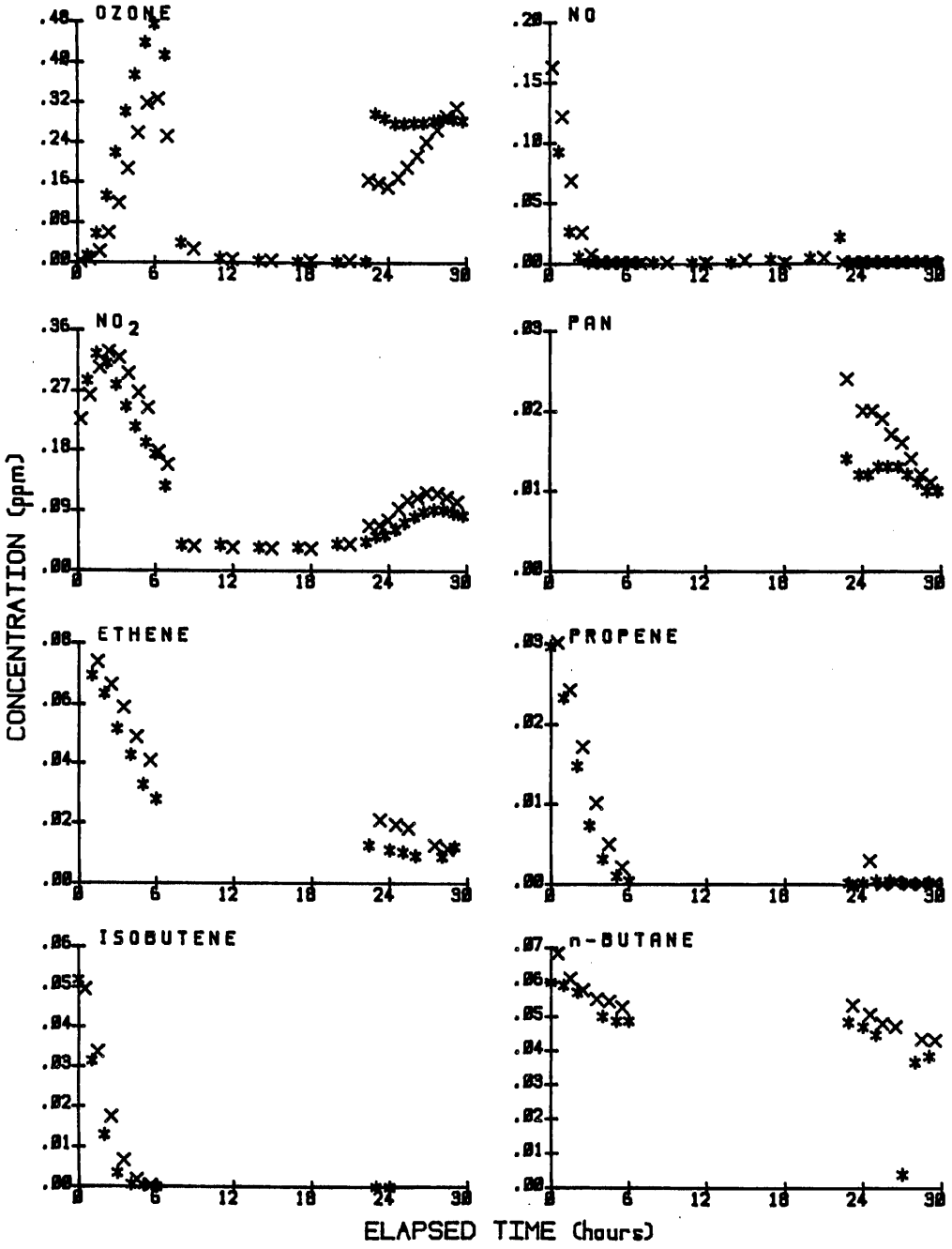


Figure A-43a. Experimental concentration-time plots for selected species observed in the 7-MF-M surrogate-$NO_x$-air run OTC-219. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B

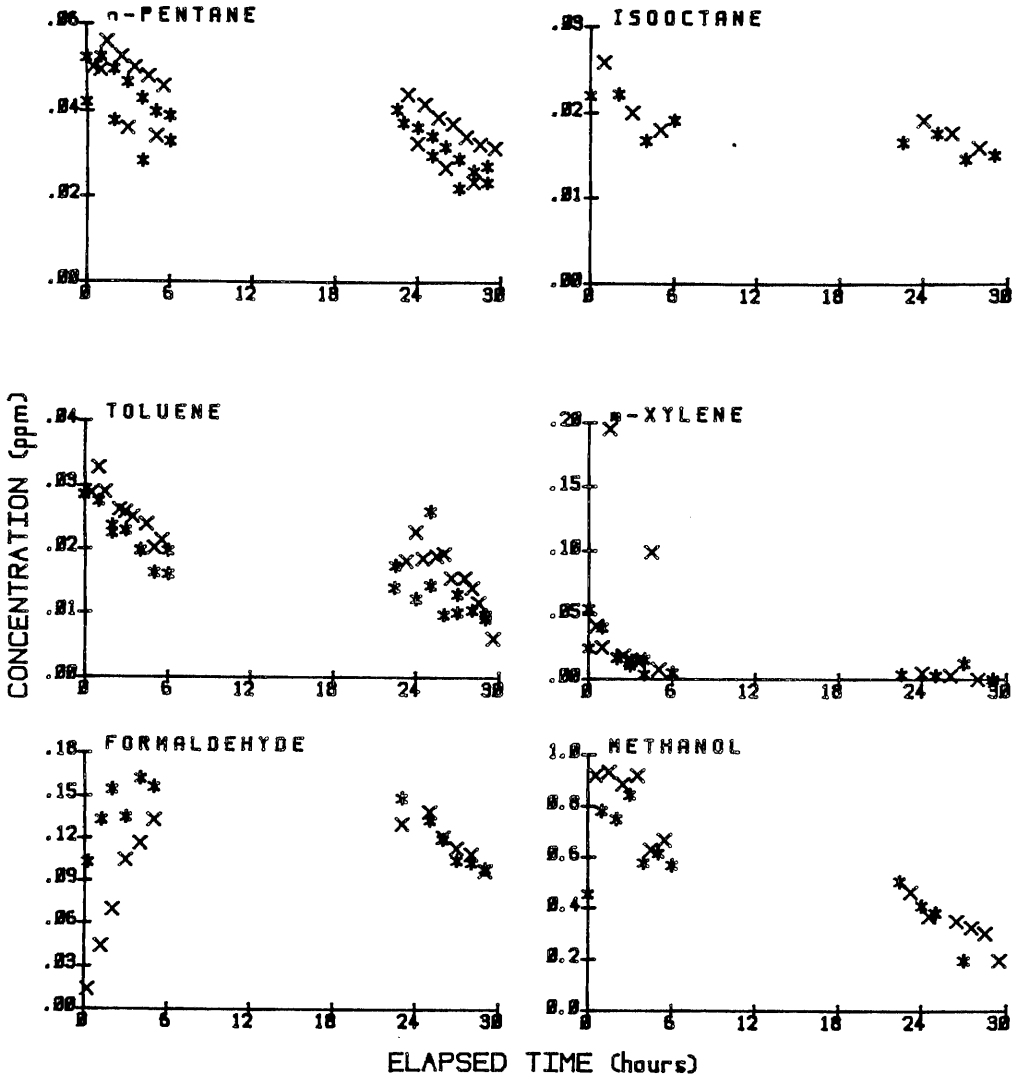


Figure A-43b. Experimental concentration-time plots for selected species observed in the 7-MF-M surrogate-$NO_x$-air run OTC-219. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B

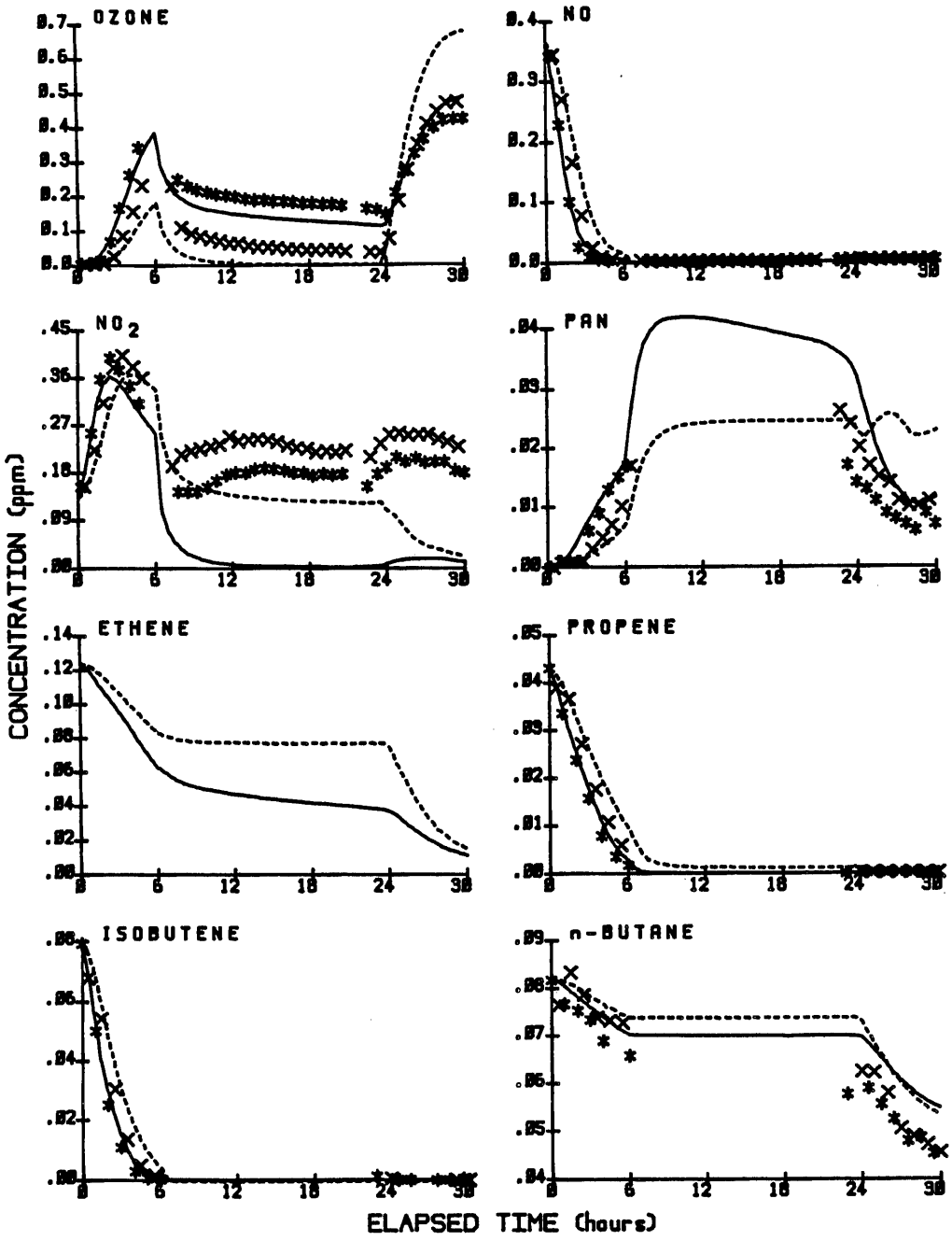


Figure A-44a. Experimental and calculated concentration-time plots for selected species observed in the 7-MF-M surrogate-$NO_x$-air run OTC-239. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

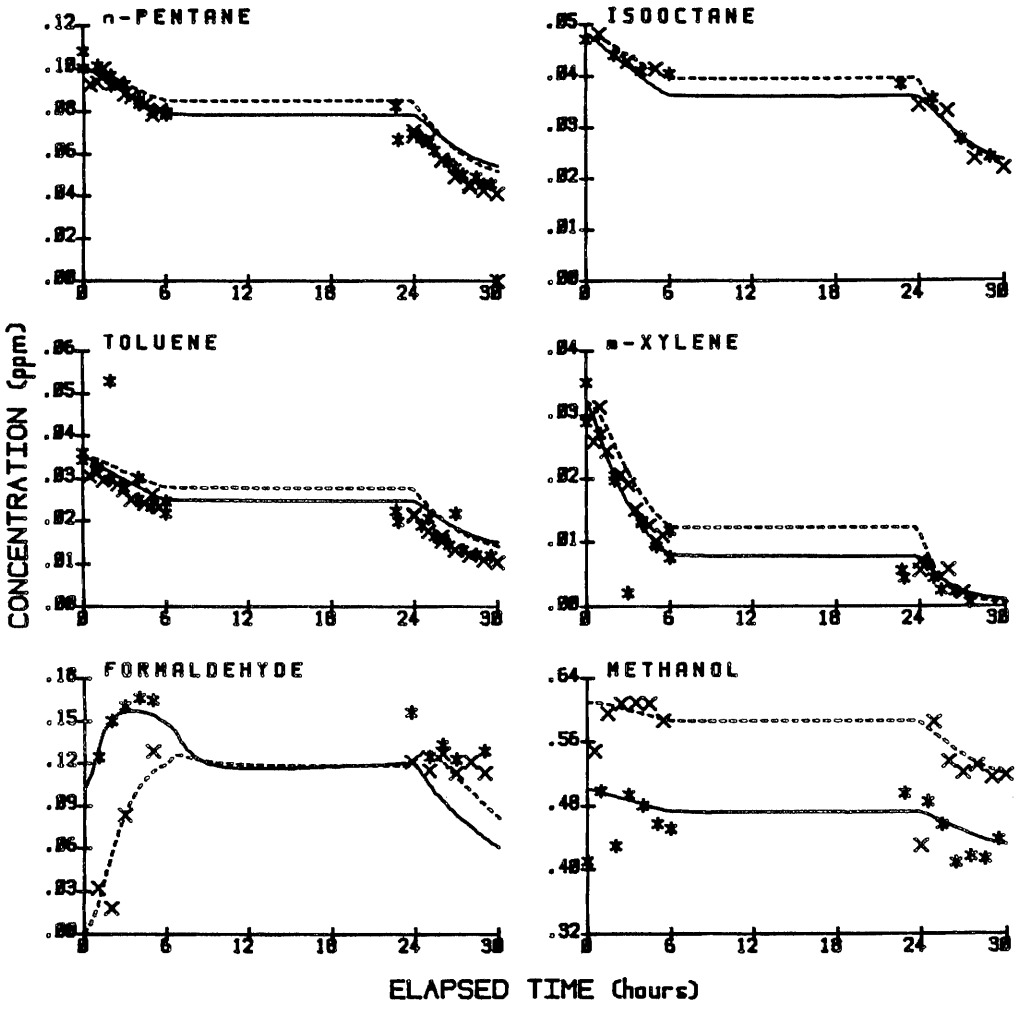


Figure A-44b. Experimental and calculated concentration-time plots for selected species observed in the 7-MF-M surrogate-$NO_x$-air run OTC-239. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

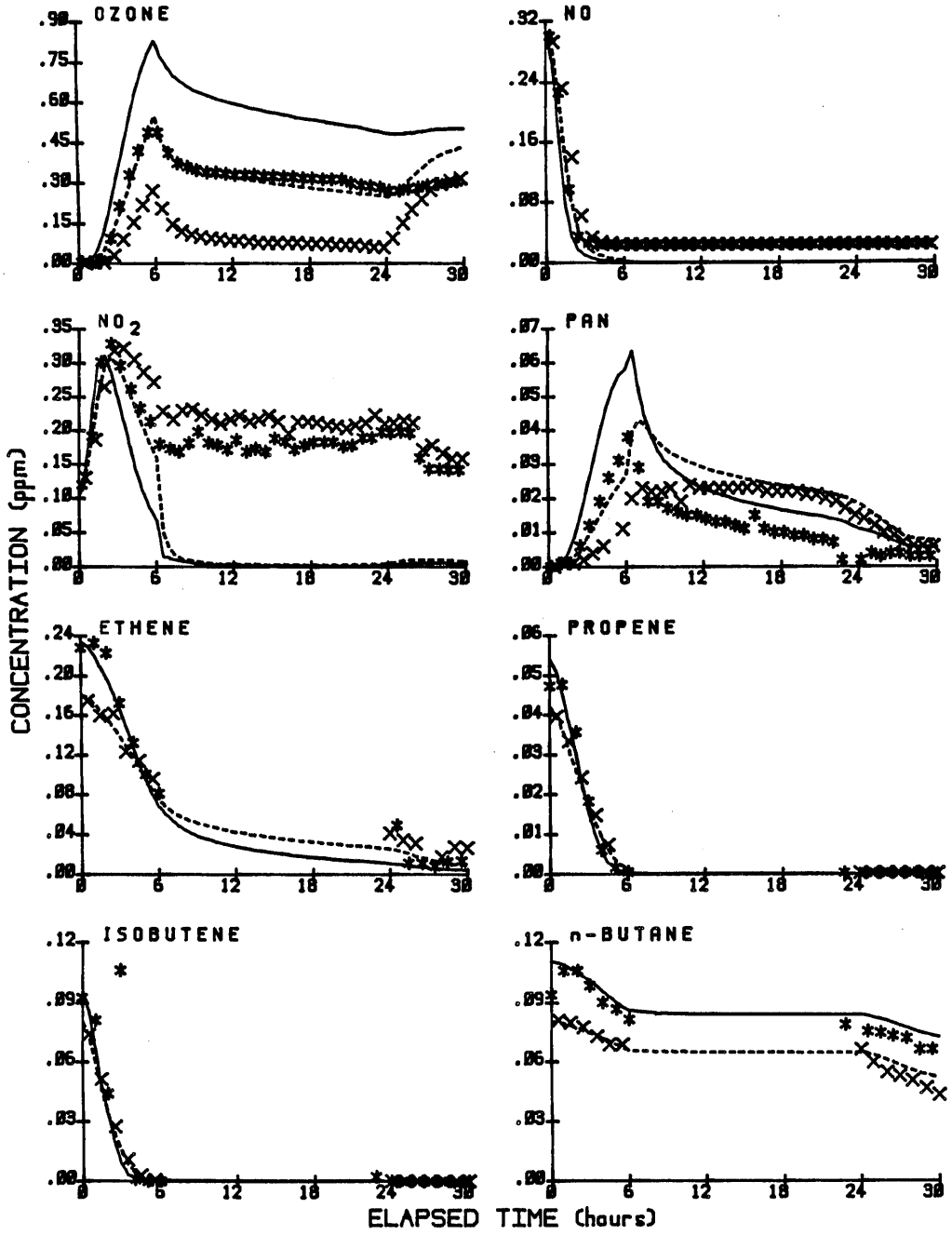


Figure A-45a. Experimental and calculated concentration-time plots for selected species observed in the 7-B-BL surrogate-$NO_x$-air run OTC-230. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

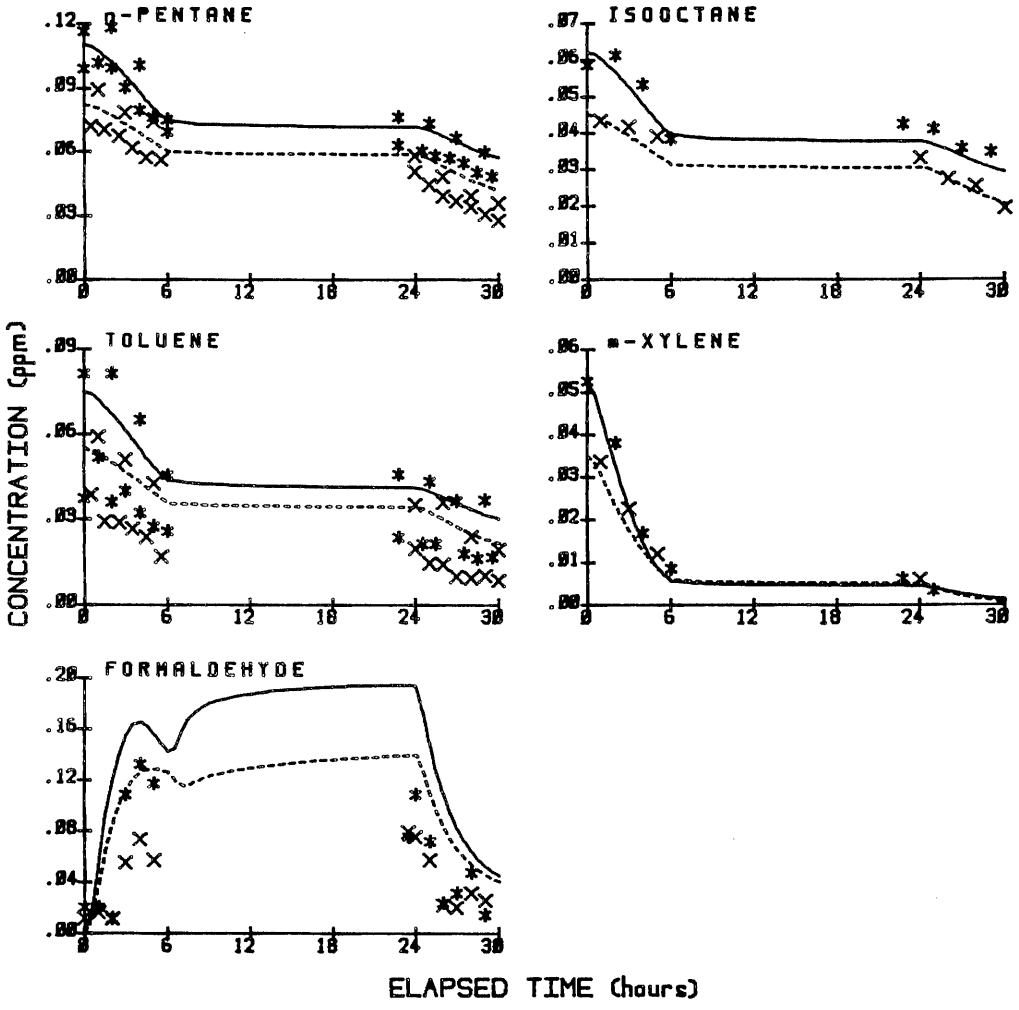


Figure A-45b. Experimental and calculated concentration-time plots for selected species observed in the 7-B-BL surrogate-$NO_x$-air run OTC-230. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

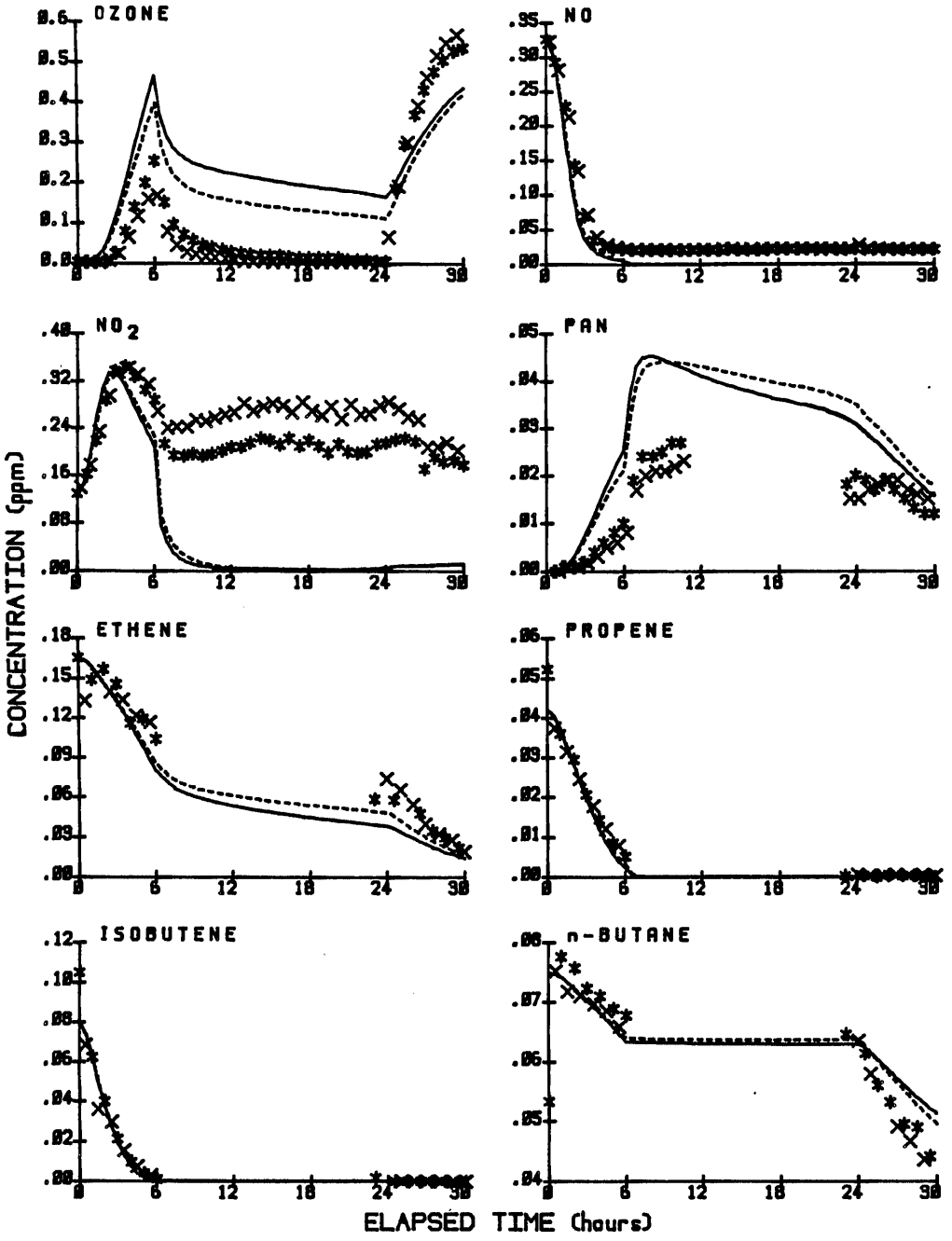


Figure A-46a. Experimental and calculated concentration-time plots for selected species observed in the 7-M-BL surrogate-$NO_x$-air run OTC-229. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

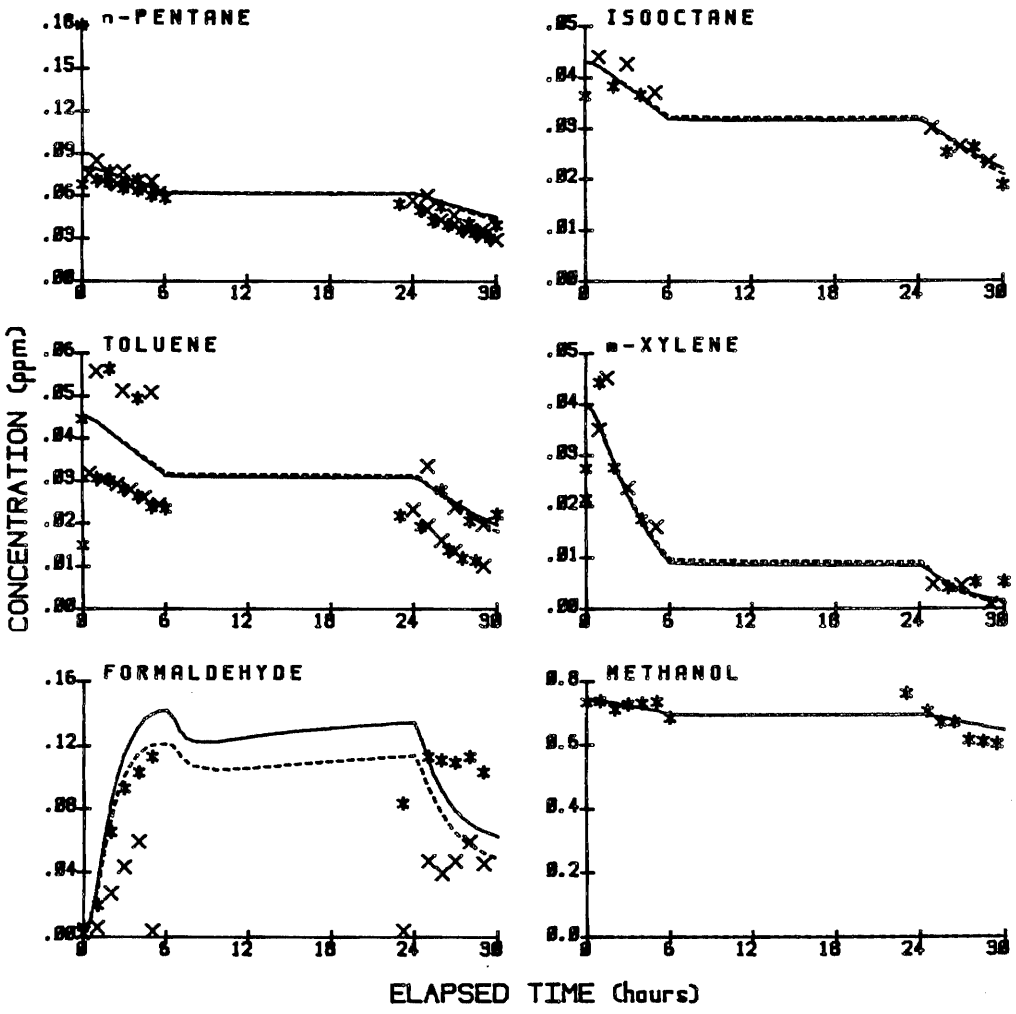


Figure A-46b. Experimental and calculated concentration-time plots for selected species observed in the 7-M-BL surrogate-$NO_x$-air run OTC-229. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

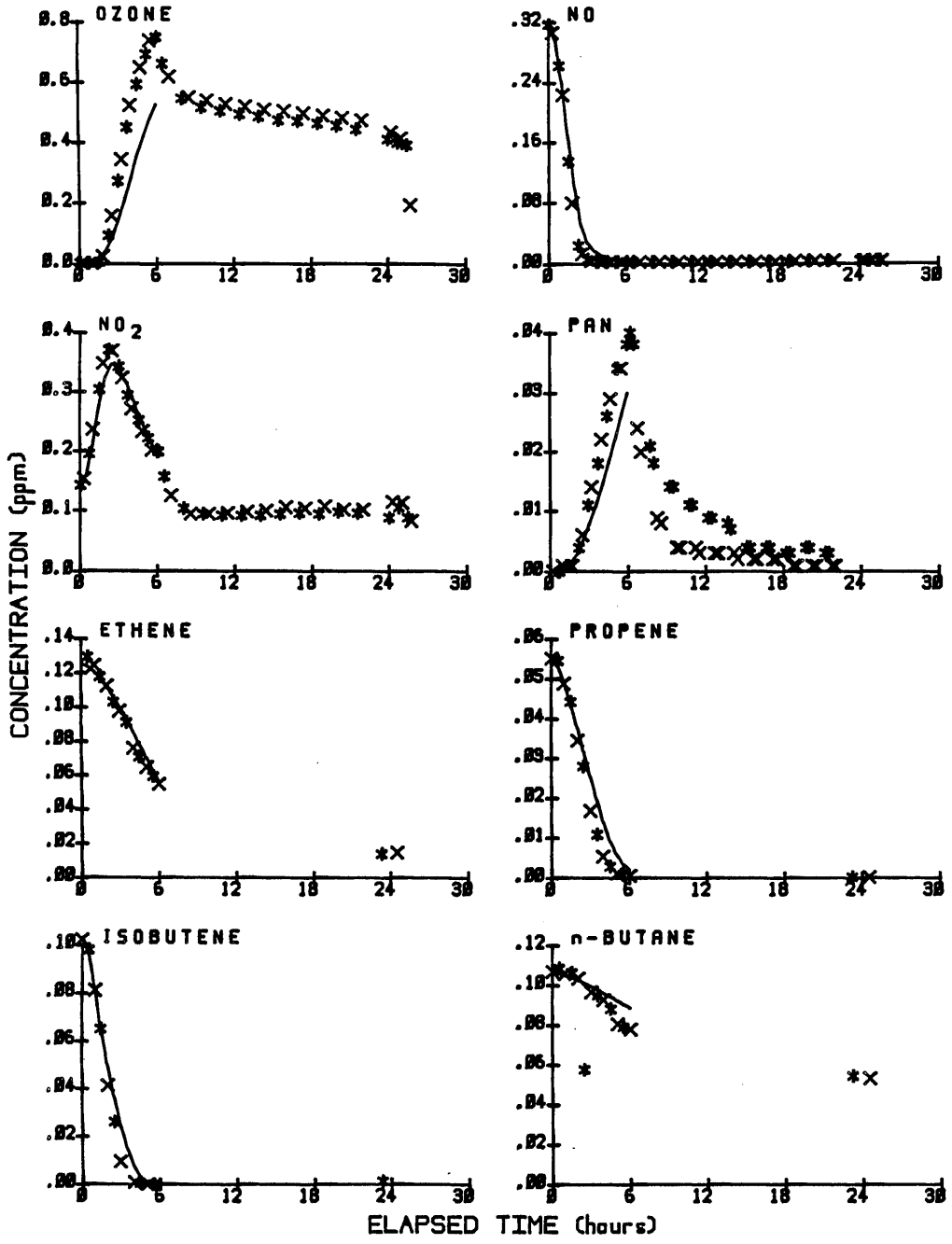


Figure A-47a. Experimental and calculated concentration-time plots for selected species observed in the 7-B-B surrogate-$NO_x$-air side equivalency test run OTC-226. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation

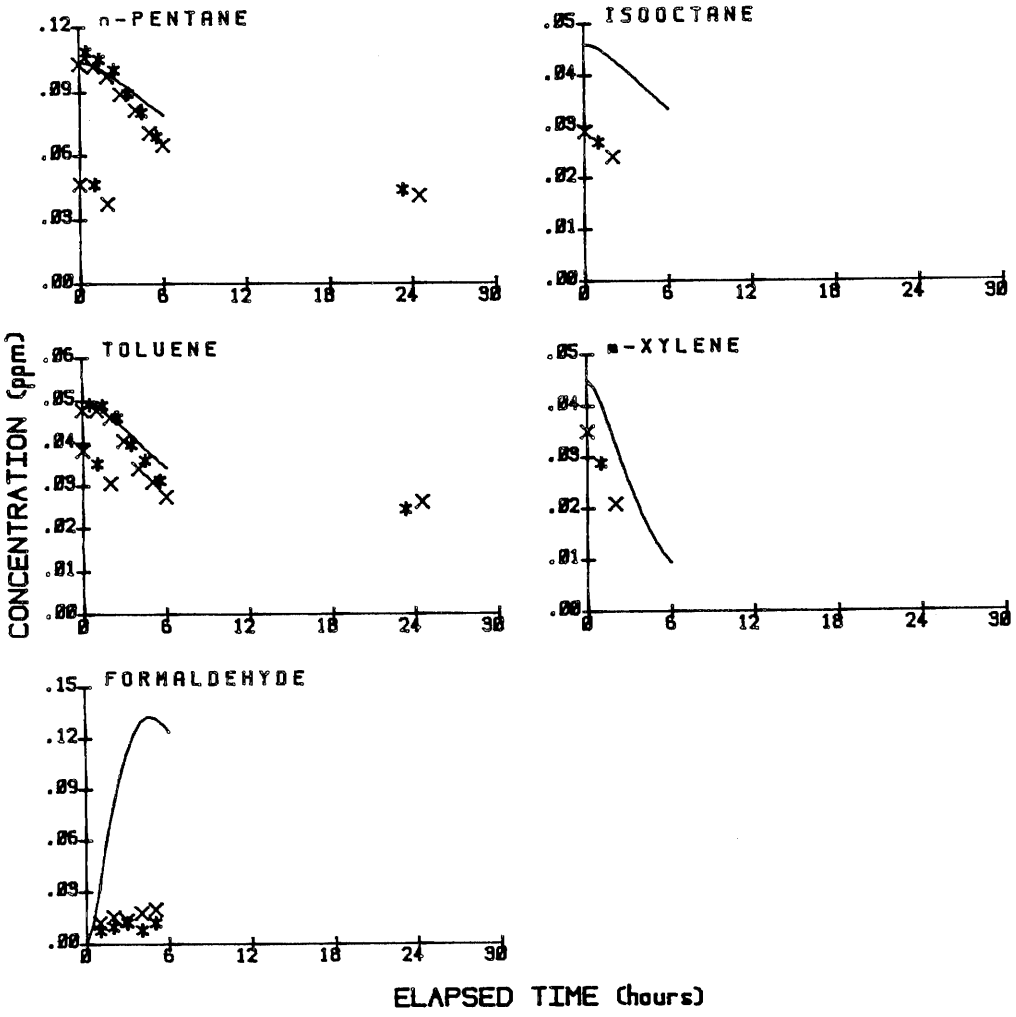


Figure A-47b. Experimental and calculated concentration-time plots for selected species observed in the 7-B-B surrogate-$NO_x$-air side equivalency test run OTC-226. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation

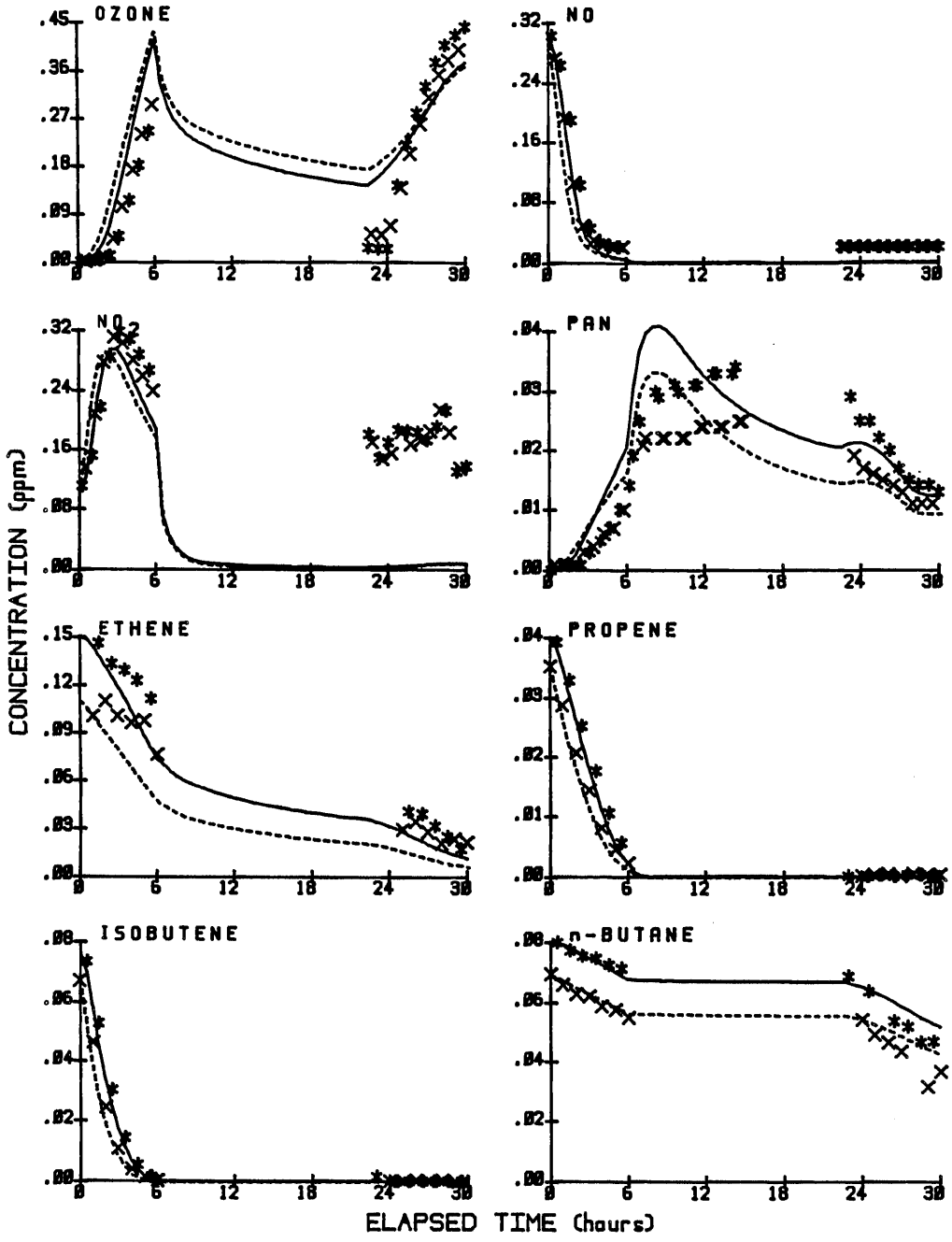


Figure A-48a. Experimental and calculated concentration-time plots for selected species observed in the 5-B-MF surrogate-$NO_x$-air run OTC-228. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

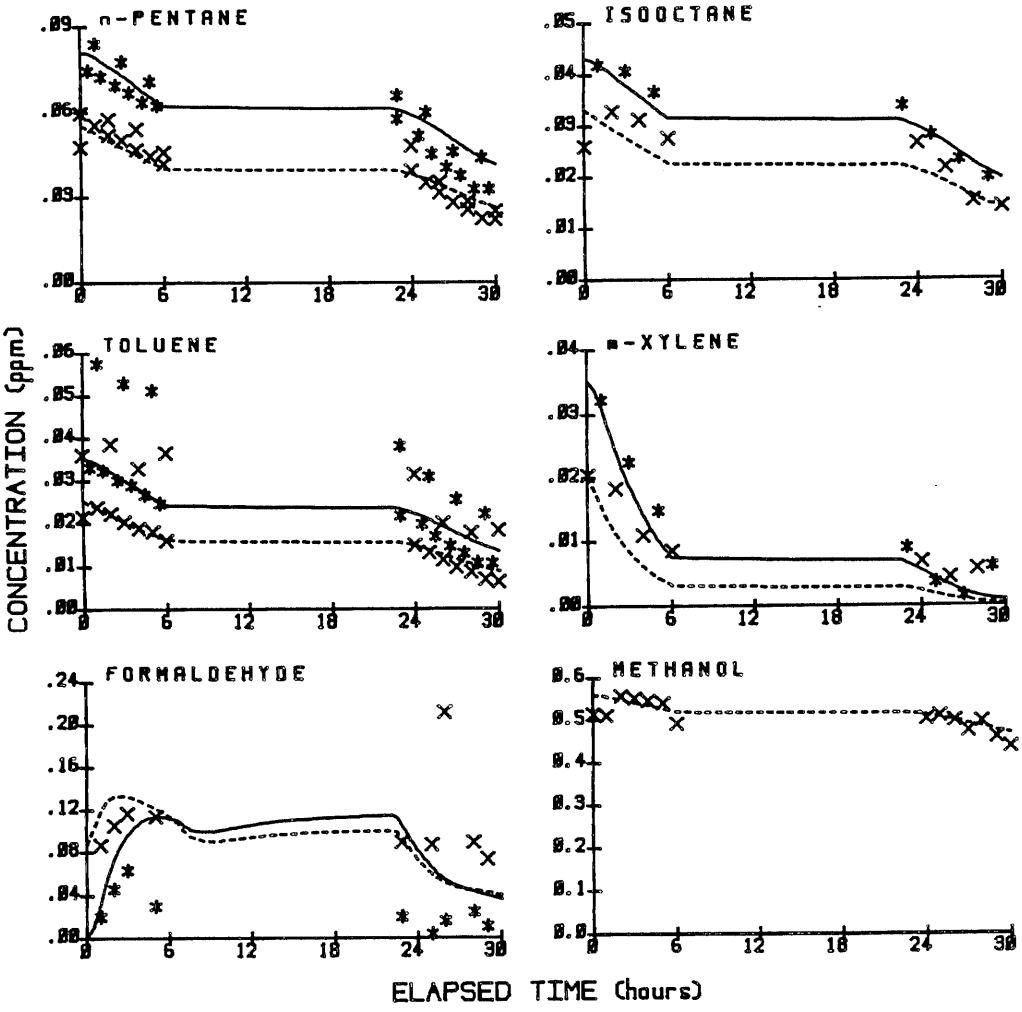


Figure A-48b. Experimental and calculated concentration-time plots for selected species observed in the 5-B-MF surrogate-$NO_x$-air run OTC-228. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

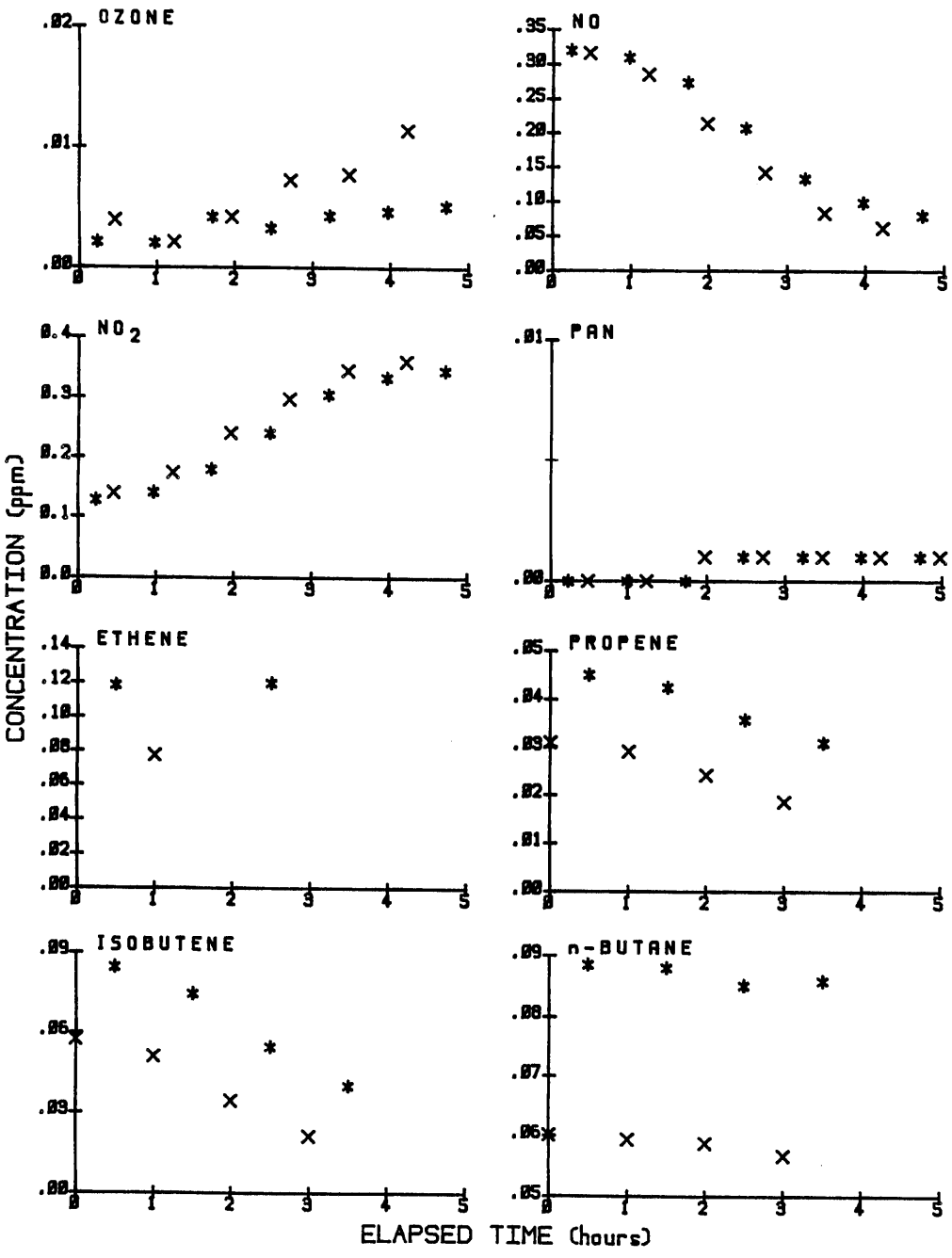


Figure A-49a. Experimental concentration-time plots for selected species observed in the 5-B-MF surrogate-$NO_x$-air run OTC-225. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B

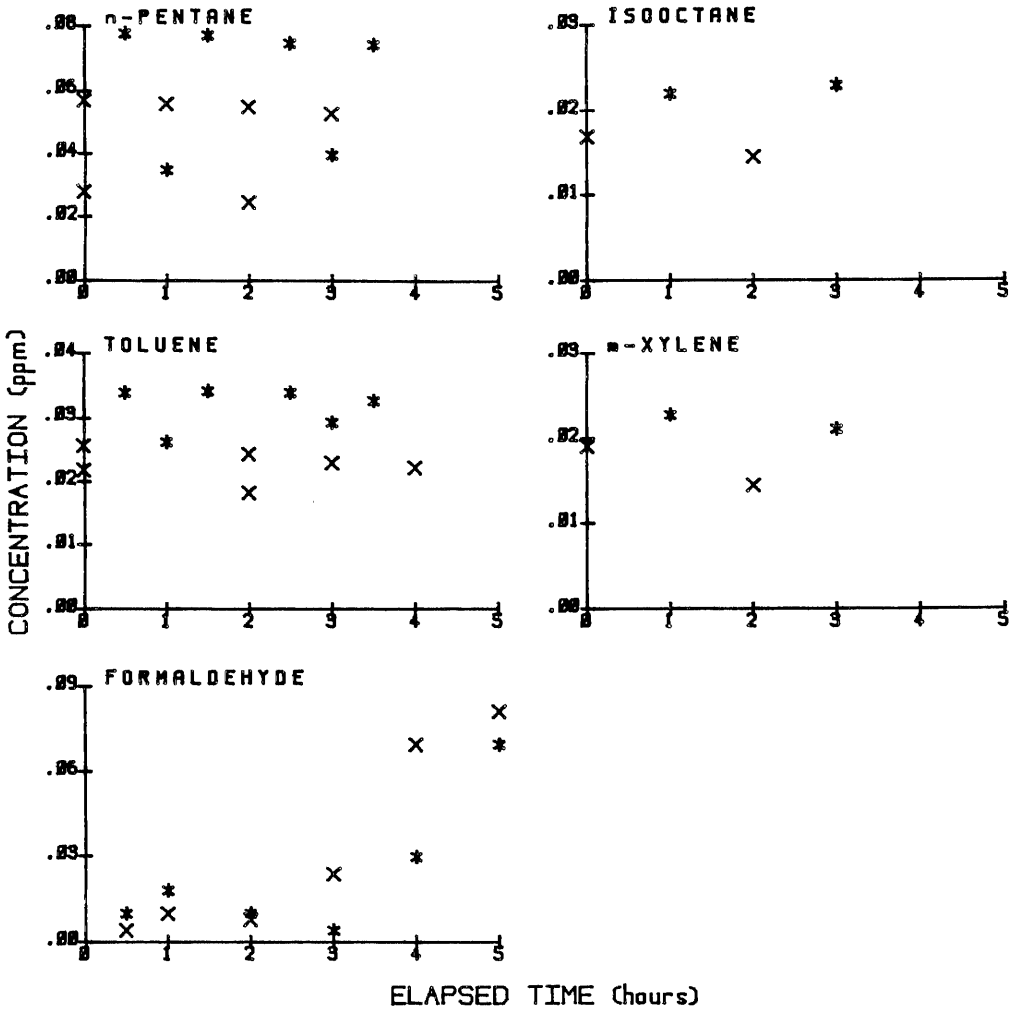


Figure A-49b. Experimental concentration-time plots for selected species observed in the 5-B-MF surrogate-$NO_x$-air run OTC-225. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B

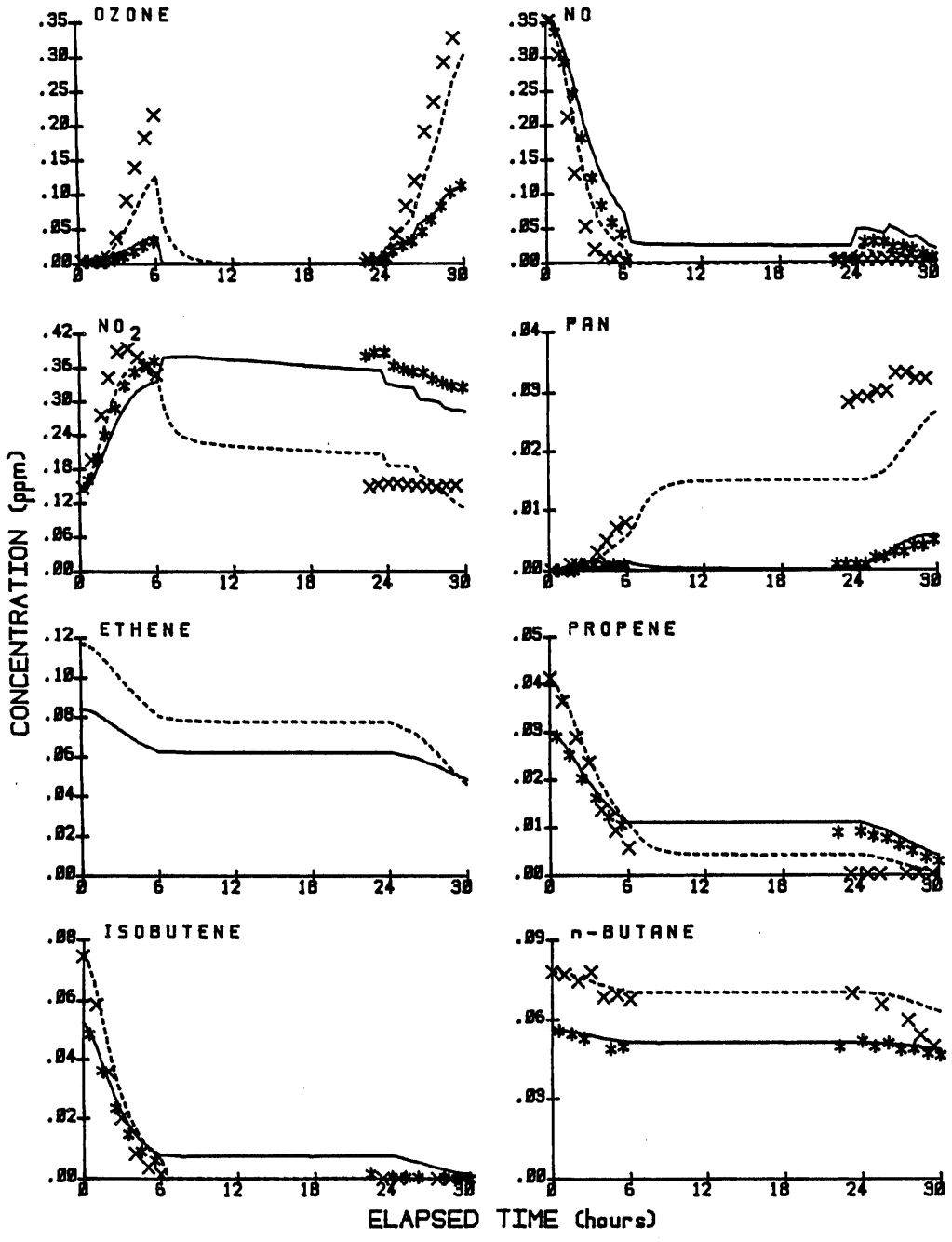


Figure A-50a. Experimental and calculated concentration-time plots for selected species observed in the 5-M-B surrogate-$NO_x$-air run OTC-240. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

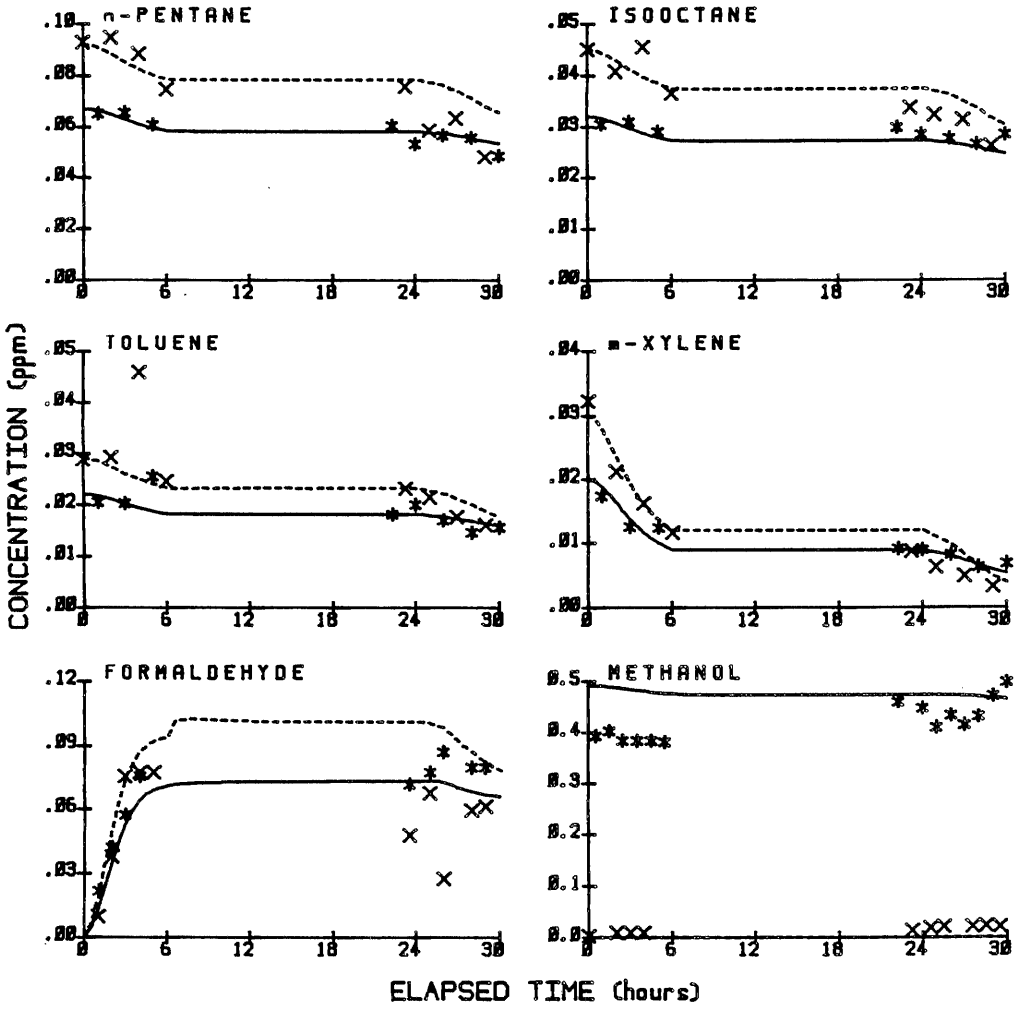


Figure A-50b. Experimental and calculated concentration-time plots for selected species observed in the 5-M-B surrogate-$NO_x$-air run OTC-240. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B
——— = model calculation, side A
- - - = model calculation, side B

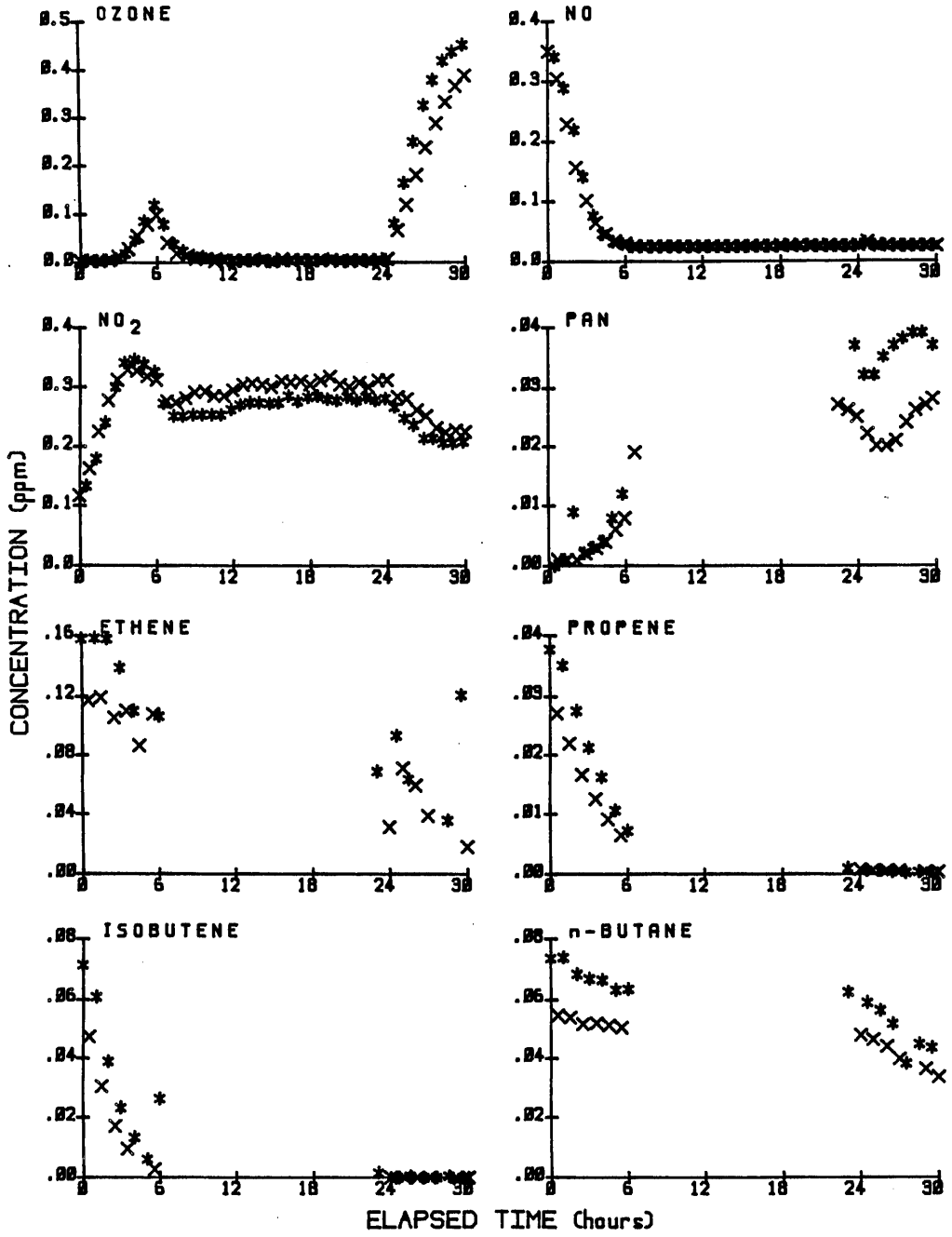


Figure A-51a. Experimental concentration-time plots for selected species observed in the 5-X-MF surrogate-$NO_x$-air run OTC-231. (Page 1 of 2).

* = experimental data, side A
X = experimental data, side B

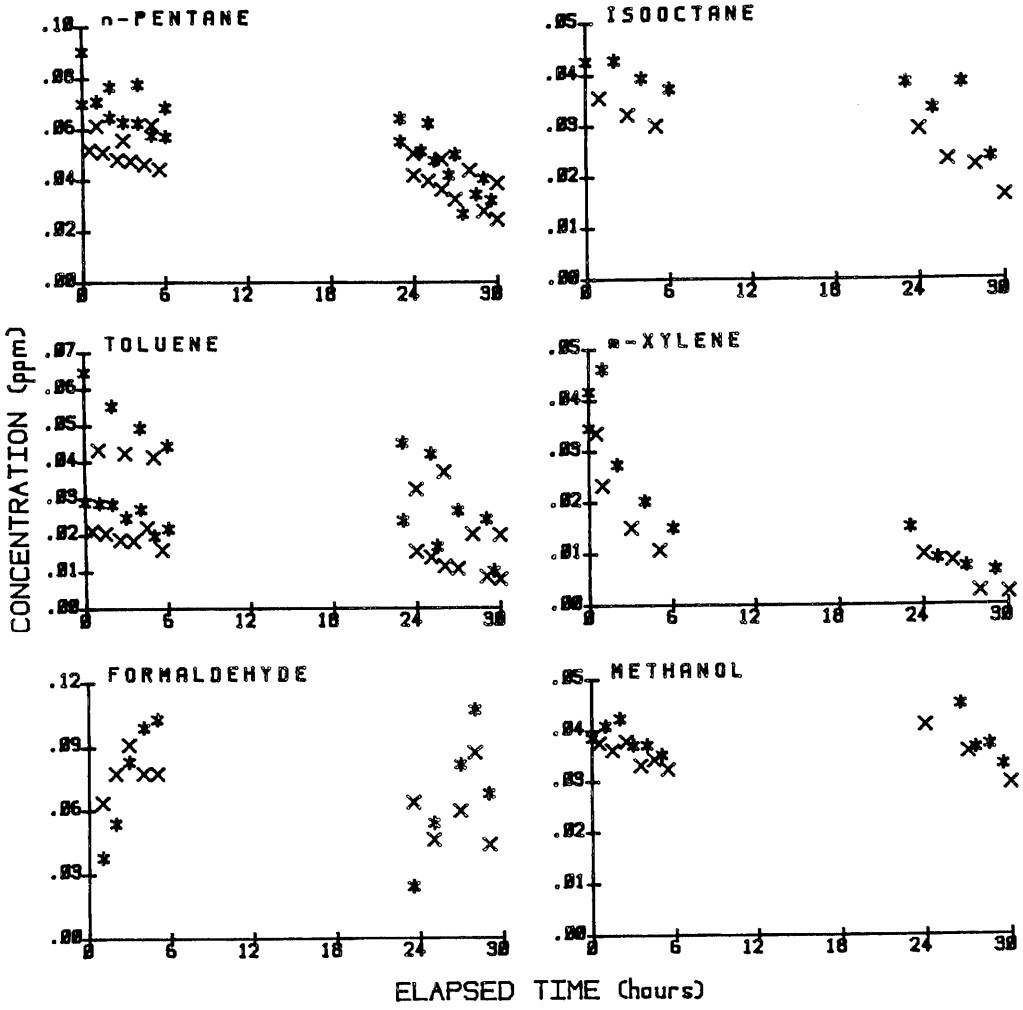


Figure A-51b. Experimental concentration-time plots for selected species observed in the 5-X-MF surrogate-$NO_x$-air run OTC-231. (Page 2 of 2).

* = experimental data, side A
X = experimental data, side B

# APPENDIX B

## CHEMICAL MECHANISM AND PARAMETERS USED IN MODEL SIMULATIONS

In this Appendix, the reactions and kinetic and mechanistic parameters used in the model simulations of the surrogate-$NO_x$-air irradiations are given. The reactions and kinetic parameters used are given in Table B-1; Table B-2 gives a list of the species used in the mechanism; Table B-3 gives the values of the temperature-dependent mechanistic coefficients at 270, 300, and 330 K (with values at intermediate temperatures being determined by linear interpolation); and Table B-4 gives the values of the chamber-dependent rate constants and coefficients used in the model simulations of the experiments carried out in the two chambers used in this program. The rate constants for photolysis reactions were obtained as indicated below.

Rate constants for photolysis reactions are calculated from the products of the absorption coefficients and quantum yields, given as a function of wavelength for each type of photolysis reaction in Table B-5, and the intensity and spectral distribution of the light source. For the indoor chamber experiments, the intensity and spectral distribution of the light source was constant (see Section IV-A-8), and the rate constants for each type of photolysis reaction is given in Table B-6. For the outdoor chamber runs, the photolysis rate constants were calculated as described in detail by Carter et al. (1986). Briefly, the photolysis rate constants for the outdoor chamber experiments were calculated theoretically as a function of zenith angle using their absorption coefficients x quantum yield products given in Table B-5, and the actinic irradiances given by Peterson (1976) for his "best estimate" surface albitos, and then adjusted by a wavelength-independent, but time-varying, factor derived such that the theoretically calculated UV intensities were consistent with the experimental UV radiometer measurements. The theoretical, clear-sky photolysis rate constants for zenith angles of 0, 40, and 70 degrees are given in Table B-6, where they can be compared with the values for the indoor chamber. The only difference between the way outdoor chamber photolysis rates were calculated in this work compared to that described by Carter et al. (1986) is that in this work it was assumed that walls of the SAPRC outdoor chamber suppresses the light intensity by a factor of

1.2 at all wavelengths, based on the analysis of the $k_1$ and UV data given in Section IV-A-9 of this report; which differs by the suppression factor of 1.1 used by Carter et al. (1986), based on an analysis of previous data.

References

Carter, W. P. L., Lurmann, F. W., Atkinson, R. and Lloyd, A. C. (1986): Development and testing of a surrogate species chemical reaction mechanism. Final Report, U. S. Environmental Protection Agency Contract No. 68-02-4104, Atmospheric Chemistry and Physics Division, Atmospheric Sciences Research Laboratory, Research Triangle Park, NC 27711.

Peterson, J. T. (1976): Calculated actinic fluxes (290-700 nm) for air pollution photochemistry applications. EPA-600/4-76-025, June.

Table B-1. Reactions and Rate Constants Used in the Model Simulations of the Surrogate-$NO_x$-Air Irradiations

| Reaction label[a] | Kinetic Parameters[b] | | | Reaction[c] |
|---|---|---|---|---|
| | | | | Inorganic Reactions |
| 1 ) | PHOT. = NO2 | | | NO2 + HV = NO + O |
| 2 ) | 2.155E-05 | 0.00 | -4.300 | O + O2 + M = O3 + M |
| 3A ) | 1.365E+04 | 0.00 | -1.000 | O + NO2 = NO + O2 |
| 3B ) | 3.232E-03 | 0.00 | -4.000 | O + NO2 + M = NO3 + M |
| 4 ) | 2.642E+03 | 2.72 | -1.000 | O3 + NO = NO2 + O2 |
| 5 ) | 1.761E+02 | 4.87 | -1.000 | O3 + NO2 = O2 + NO3 |
| 6 ) | 1.174E+04 | -0.50 | -1.000 | NO + NO3 = #2 NO2 |
| 7 ) | 1.185E-10 | -1.05 | -2.000 | NO + NO + O2 = #2 NO2 |
| 8 ) | FALLOFF F= 0.600, N= 0.972 | | | NO2 + NO3 = N2O5 |
| KO: | 7.182E-02 | 0.00 | -6.300 | |
| KI: | 2.055E+03 | 0.00 | -1.500 | |
| 9 ) | 4.333E+13 | 22.55 | 0.000 | N2O5 + #RCON8 = NO2 + NO3 |
| 10 ) | 1.468E-06 | 0.00 | -1.000 | N2O5 + H2O = #2 HONO2 |
| 11 ) | 3.670E+01 | 2.44 | -1.000 | NO2 + NO3 = NO + NO2 + O2 |
| 12A ) | PHOT. = NO3NO | | | NO3 + HV = NO + O2 |
| 12B ) | PHOT. = NO3NO2 | | | NO3 + HV = NO2 + O |
| 13A ) | PHOT. = O3O3P | | | O3 + HV = O + O2 |
| 13BL) | PHOT. = O3T270 | | | O3 + HV + #T270 = O*1D2 + O2 |
| 13BM) | PHOT. = O3T300 | | | O3 + HV + #T300 = O*1D2 + O2 |
| 13BH) | PHOT. = O3T330 | | | O3 + HV + #T330 = O*1D2 + O2 |
| 14 ) | 3.229E+05 | 0.00 | -1.000 | O*1D2 + H2O = #2 HO. |
| 15 ) | 4.257E+04 | 0.00 | -1.000 | O*1D2 + M = O + M |
| 16 ) | FALLOFF F= 0.600, N= 1.000 | | | HO. + NO = HONO |
| KO: | 2.406E-02 | 0.00 | -5.300 | |
| KI: | 4.404E+04 | 0.00 | -2.000 | |
| 17 ) | PHOT. = HONO | | | HONO + HV = HO. + NO |
| 18 ) | FALLOFF F= 0.600, N= 1.000 | | | HO. + NO2 = HONO2 |
| KO: | 9.337E-02 | 0.00 | -5.200 | |
| KI: | 3.523E+04 | 0.00 | -2.300 | |
| 19 ) | 1.380E+01 | -1.55 | -1.000 | HO. + HONO2 = H2O + NO3 |
| 21 ) | 3.200E+02 | 0.00 | -1.000 | HO. + CO = HO2. + CO2 |
| 22 ) | 2.349E+03 | 1.87 | -1.000 | HO. + O3 = HO2. + O2 |
| 23 ) | 5.431E+03 | -0.48 | -1.000 | HO2. + NO = HO. + NO2 |
| 24 ) | FALLOFF F= 0.560, N= 1.000 | | | HO2. + NO2 = HO2NO2 |
| KO: | 8.260E-03 | 0.00 | -6.600 | |
| KI: | 6.165E+03 | 0.00 | -0.800 | |
| 25 ) | 1.754E+13 | 21.60 | 1.000 | HO2NO2 + #RCON24 = HO2. + NO2 |
| 27 ) | 5.872E+03 | 0.00 | -1.000 | HO2NO2 + HO. = H2O + NO2 + O2 |
| 28 ) | 2.055E+01 | 1.15 | -1.000 | HO2. + O3 = HO. + #2 O2 |
| 29A ) | 3.229E+02 | -1.23 | -1.000 | HO2. + HO2. = HO2H + O2 |
| 29B ) | 6.823E-05 | -1.95 | -2.000 | HO2. + HO2. + M = HO2H + O2 |
| 29C ) | 1.113E-05 | -5.60 | -2.000 | HO2. + HO2. + H2O = HO2H + O2 + H2O |

(continued)

Table B-1 (continued) - 2

| Reaction label[a] | Kinetic Parameters[b] | Reaction[c] |
|---|---|---|
| 29D ) | 2.370E-06 -6.32 -2.000 | HO2. + HO2. + H2O = HO2H + O2 + H2O |
| 30A ) | SAME K AS 29A | NO3 + HO2. = HONO2 + O2 |
| 30B ) | SAME K AS 29B | NO3 + HO2. + M = HONO2 + O2 |
| 30C ) | SAME K AS 29C | NO3 + HO2. + H2O = HONO2 + O2 + H2O |
| 30A ) | SAME K AS 29D | NO3 + HO2. + H2O = HONO2 + O2 + H2O |
| 31 ) | PHOT. = H2O2 | HO2H + HV = #2 HO. |
| 32 ) | 4.550E+03 0.37 -1.000 | HO2H + HO. = HO2. + H2O |
| | | General Peroxy Radical Reactions[d] |
| B1 ) | 6.165E+03 -0.36 -1.000 | RO2. + NO = NO |
| B2 ) | 6.165E+03 -0.36 -1.000 | RCO3. + NO = NO |
| B4 ) | 4.110E+03 -0.36 -1.000 | RCO3. + NO2 = NO2 |
| B5 ) | 4.404E+03 0.00 -1.000 | RO2. + HO2. = HO2. |
| B6 ) | 4.404E+03 0.00 -1.000 | RCO3. + HO2. = HO2. |
| B7 ) | PHOT. = CO2H | -OOH + HV = HO2. + HO. |
| B8 ) | 1.468E+00 0.00 -1.000 | RO2. + RO2. = |
| B9 ) | 4.404E+03 0.00 -1.000 | RO2. + RCO3. = |
| B10 ) | 3.670E+03 0.00 -1.000 | RCO3. + RCO3. = |
| F7 ) | SAME K AS B1 | R2O2. + NO = NO2 |
| F8 ) | SAME K AS B5 | R2O2. + HO2. = |
| F9 ) | SAME K AS B8 | R2O2. + RO2. = RO2. |
| F10 ) | SAME K AS B9 | R2O2. + RCO3. = RCO3. |
| | | Reactions of Formaldehyde |
| C1 ) | PHOT. = HCHOR | HCHO + HV = #2 HO2. + CO |
| C2 ) | PHOT. = HCHOM | HCHO + HV = H2 + CO |
| C3 ) | 1.321E+04 0.00 -1.000 | HCHO + HO. = HO2. + CO + H2O |
| C4 ) | 1.468E+01 0.00 -1.000 | HCHO + HO2. = HOC-O2. + RO2. |
| C5 ) | SAME K AS B1 | HOC-O2. + NO = NO2 + HO2. + -C !(HCO-OH) |
| C6 ) | SAME K AS B5 | HOC-O2. + HO2. = -OOH + -C |
| C7 ) | SAME K AS B8 | HOC-O2. + RO2. = RO2. + #.5 HO2. + RO2. + -C |
| C8 ) | SAME K AS B9 | HOC-O2. + RCO3. = RCO3. + #.5 HO2. + RCO3. + -C |
| C9 ) | 8.807E+02 4.09 -1.000 | HCHO + NO3 = HONO2 + HO2. + CO |
| | | Reactions of Acetaldehyde and PAN |
| C10 ) | 1.013E+04 -0.50 -1.000 | CCHO + HO. = CCO-O2. + H2O + RCO3. |
| C11A) | PHOT. = CCHOR | CCHO + HV = CO + C-O2. + HO2. + RO2. |
| C12 ) | 4.404E+02 2.84 -1.000 | CCHO + NO3 = HONO2 + CCO-O2. + RCO3. |
| C13 ) | SAME K AS B2 | CCO-O2. + NO = C-O2. + CO2 + NO2 + RO2. |
| C14 ) | SAME K AS B4 | CCO-O2. + NO2 = C-PAN |

(continued)

Table B-1 (continued) - 3

| Reaction label[a] | Kinetic Parameters[b] | | | Reaction[c] |
|---|---|---|---|---|
| C15 ) | SAME K AS B6 | | | CCO-O2. + HO2. = -OOH + CO2 + HCHO |
| C16 ) | SAME K AS B9 | | | CCO-O2. + RO2. = RO2. + #.5 HO2. + CO2 + HCHO |
| C17 ) | SAME K AS B10 | | | CCO-O2. + RCO3. = RCO3. + HO2. + CO2 + HCHO |
| C18 ) | 1.200E+18 | 26.91 | 0.000 | C-PAN = CCO-O2. + NO2 + RCO3. |
| C19 ) | SAME K AS B1 | | | C-O2. + NO = C-O. + NO2 |
| C20 ) | SAME K AS B5 | | | C-O2. + HO2. = -OOH + HCHO |
| C21 ) | SAME K AS B8 | | | C-O2. + RO2. = RO2. + #.5 HO2. + HCHO |
| C22 ) | SAME K AS B9 | | | C-O2. + RCO3. = RCO3. + #.5 HO2. + HCHO |
| C23 ) | 8.073E+01 | 1.99 | -1.000 | C-O. + O2 = HCHO + HO2. |
| C24 ) | 2.202E+04 | 0.00 | -1.000 | C-O. + NO2 = CONO2 |
| | | | | Reactions of Propionaldehyde and the Higher Alaphatic Aldehydes |
| C25 ) | 1.248E+04 | -0.50 | -1.000 | RCHO + HO. = C2CO-O2. + RCO3. |
| C26 ) | PHOT. = RCHO | | | RCHO + HV + #.2 = C2-O2. + RO2. + CO + HO2. |
| C27 ) | 4.404E+02 | 2.84 | -1.000 | NO3 + RCHO = C2CO-O2. + RCO3. |
| C28 ) | SAME K AS B2 | | | C2CO-O2. + NO = C2-O2. + CO2 + NO2 + RO2. |
| C29 ) | SAME K AS B4 | | | C2CO-O2. + NO2 = C2-PAN |
| C30 ) | SAME K AS B6 | | | C2CO-O2. + HO2. = -OOH + CCHO + CO2 |
| C31 ) | SAME K AS B9 | | | C2CO-O2. + RO2. = RO2. + #.5 HO2. + CCHO + CO2 |
| C32 ) | SAME K AS B10 | | | C2CO-O2. + RCO3. = RCO3. + HO2. + CCHO + CO2 |
| C33 ) | 1.200E+18 | 26.91 | 0.000 | C2-PAN = C2CO-O2. + NO2 + RCO3. |
| C34 ) | SAME K AS B1 | | | C2-O2. + NO = NO2 + CCHO + HO2. |
| C35 ) | SAME K AS B5 | | | C2-O2. + HO2. = -OOH + CCHO |
| C36 ) | SAME K AS B8 | | | C2-O2. + RO2. = RO2. + #.5 HO2. + CCHO |
| C37 ) | SAME K AS B9 | | | C2-O2. + RCO3. = RCO3. + #.5 HO2. + CCHO |
| | | | | Reactions of Acetone |
| C38 ) | 1.468E+04 | 2.23 | -1.000 | C-CO-C + HO. = C-CO-C-O2. + RO2. |
| C39 ) | PHOT. = KETONE | | | C-CO-C + HV + #.07 = CCO-O2. + C-O2. + RCO3. & + RO2. |
| C40 ) | SAME K AS B1 | | | C-CO-C-O2. + NO = NO2 + CCOCHO + HO2. |
| C41 ) | SAME K AS B5 | | | C-CO-C-O2. + HO2. = -OOH + CCOCHO |
| C42 ) | SAME K AS B8 | | | C-CO-C-O2. + RO2. = RO2. + #.5 HO2. + CCOCHO |
| C43 ) | SAME K AS B9 | | | C-CO-C-O2. + RCO3. = RCO3. + #.5 HO2. + CCOCHO |
| | | | | Reactions of Methyl Ethyl Ketone and the Higher Ketones |
| C44 ) | 1.761E+04 | 1.48 | -1.000 | MEK + HO. = H2O + MEK-O2. + RO2. |
| C45') | SAME K AS B1 | | | MEK-O2. + NO = NO2 + #.5 "CCO-O2. + CCHO + & MEK(2)-O2. + RCO3. + RO2." |
| C46') | SAME K AS B5 | | | MEK-O2. + HO2. = -OOH + CO2 + HCHO + CCHO |

(continued)

Table B-1 (continued) - 4

| Reaction label[a] | Kinetic Parameters[b] | Reaction[c] |
|---|---|---|
| C47') | SAME K AS B8 | MEK-O2. + RO2. = RO2. + #.5 HO2. + CO2 + & HCHO + CCHO |
| C48') | SAME K AS B9 | MEK-O2. + RCO3. = RCO3. + #.5 HO2. + CO2 + & HCHO + CCHO |
| C50 ) | SAME K AS B1 | MEK(2)-O2. + NO = NO2 + HCHO + C2CO-O2. |
| C54 ) | SAME K AS B5 | MEK(2)-O2. + HO2. = -OOH + CO2 + HCHO + CCHO |
| C55 ) | SAME K AS B8 | MEK(2)-O2. + RO2. = RO2. + #.5 HO2. + CO2 + & HCHO + CCHO |
| C56 ) | SAME K AS B9 | MEK(2)-O2. + RCO3. = RCO3. + #.5 HO2. + CO2 + & HCHO + CCHO |
| C57 ) | PHOT. = KETONE | MEK + HV + #.1 = CCO-O2. + C2-O2. + RCO3. + & RO2. |
| | | Reactions of the Lumped Higher Alcohol (used to represent the reactions at the -OH group for the isomerization products of the higher alkanes) |
| C111) | 2.055E+04 0.00 -1.000 | ROH + HO. = #.2 "ROH-O2. + RO2." + #.8 "MEK & + HO2. + -C" |
| C112) | SAME K AS B1 | ROH-O2. + NO = NO2 + #2 RCHO + HO2. + #-1 -C |
| C113) | SAME K AS B5 | ROH-O2. + HO2. = -OOH + #2 RCHO + #-1 -C |
| C114) | SAME K AS B8 | ROH-O2. + RO2. = RO2. + #.5 HO2. + #2 RCHO + & #-1 -C |
| C115) | SAME K AS B9 | ROH-O2. + RCO3. = RCO3. + #.5 HO2. + #2 RCHO & + #-1 -C |
| | | Reactions of Glyoxal |
| C58 ) | PHOT. = GLYOXAL | HCOCHO + HV + #.029 = #.13 HCHO + #.87 H2 + & #1.87 CO |
| C59 ) | 1.688E+04 0.00 -1.000 | HCOCHO + HO. = HCOCO. |
| C60 ) | 8.807E+02 4.09 -1.000 | HCOCHO + NO3 = HONO2 + HCOCO. |
| C61 ) | 6.000E+01 | HCOCO. = #.63 HO2. + #1.26 CO + #.37 & "HCOCO-O2. + RCO3." |
| C62 ) | SAME K AS B2 | HCOCO-O2. + NO = NO2 + CO2 + CO + HO2. |
| C63 ) | SAME K AS B4 | HCOCO-O2. + NO2 = HCO-PAN |
| C64 ) | 1.200E+18 26.91 0.000 | HCO-PAN = HCOCO-O2. + NO2 + RCO3. |
| C65 ) | SAME K AS B6 | HCOCO-O2. + HO2. = -OOH + CO2 + CO |
| C66 ) | SAME K AS B9 | HCOCO-O2. + RO2. = RO2. + #.5 HO2. + CO2 + CO |
| C67 ) | SAME K AS B10 | HCOCO-O2. + RCO3. = RCO3. + HO2. + CO2 + CO |
| | | Reactions of Methylglyoxal |
| C68 ) | PHOT. = MEGLYOX | CCOCHO + HV + #.107 = HO2. + CO + CCO-O2. + & RCO3. |

(continued)

Table B-1 (continued) - 5

| Reaction label[a] | Kinetic Parameters[b] | | | Reaction[c] |
|---|---|---|---|---|
| C69 ) | 2.495E+04 | 0.00 | -1.000 | CCOCHO + HO. = CO + CCO-O2. + RCO3. |
| C70 ) | 4.404E+03 | 2.84 | -1.000 | CCOCHO + NO3 = HONO2 + CO + CCO-O2. + RCO3. |
| | | | | Reactions of Glycolaldehyde |
| C72 ) | 3.376E+04 | 0.00 | -1.000 | HOCCHO + HO. = HOCCO-O2. + H2O + RCO3. |
| C73 ) | SAME K AS B2 | | | HOCCO-O2. + NO = NO2 + CO2 + HCHO + HO2. |
| C74 ) | SAME K AS B4 | | | HOCCO-O2. + NO2 = HOC-PAN |
| C75 ) | 1.200E+18 | 26.91 | 0.000 | HOC-PAN = HOCCO-O2. + NO2 + RCO3. |
| C76 ) | SAME K AS B6 | | | HOCCO-O2. + HO2. = -OOH + CO2 + HCHO |
| C77 ) | SAME K AS B9 | | | HOCCO-O2. + RO2. = RO2. + #.5 HO2. + CO2 + HCHO |
| C78 ) | SAME K AS B10 | | | HOCCO-O2. + RCO3. = RCO3. + HO2. + CO2 + HCHO |
| C79 ) | PHOT. = CCHOR | | | HOCCHO + HV = CO + HCHO + #2 HO2. |
| C80 ) | 4.404E+02 | 2.84 | -1.000 | HOCCHO + NO3 = HONO2 + HOCCO-O2. + RCO3. |
| | | | | Reactions of the $\geq C_4$ Alkyl Nitrates |
| C81 ) | 2.936E+04 | 2.02 | -1.000 | C4ONO2 + HO. = #.2 "NO2 + MEK" + #.8 & "C4ONO2-O2. + RO2." |
| C82') | SAME K AS B1 | | | C4ONO2-O2. + NO = #1.6 NO2 + #.6 "CCHO + & C2-O2." + #.4 C4ONO2(2)-O2. + RO2. |
| C84 ) | SAME K AS B1 | | | C4ONO2(2)-O2. + NO = #2 NO2 + HCHO + RCHO |
| C85') | SAME K AS B5 | | | C4ONO2-O2. + HO2. = -OOH + NO2 + #1.2 CCHO + & #.4 "HCHO + RCHO" |
| C87 ) | SAME K AS B5 | | | C4ONO2(2)-O2. + HO2. = -OOH + NO2 + HCHO + RCHO |
| C88') | SAME K AS B8 | | | C4ONO2-O2. + RO2. = RO2. + #.5 HO2. + NO2 + & #1.2 CCHO + #.4 "HCHO + RCHO" |
| C90 ) | SAME K AS B8 | | | C4ONO2(2)-O2. + RO2. = RO2. + #.5 HO2. + NO2 & + HCHO + RCHO |
| C91') | SAME K AS B9 | | | C4ONO2-O2. + RCO3. = RCO3. + #.5 HO2. + NO2 + & #1.2 CCHO + #.4 "HCHO + RCHO" |
| C93 ) | SAME K AS B9 | | | C4ONO2(2)-O2. + RCO3. = RCO3. + #.5 HO2. + & NO2 + HCHO + RCHO |
| C94 ) | 4.404E+04 | 1.29 | -1.000 | C7ONO2 + HO. = C7ONO2-O2. + RO2. |
| C95') | SAME K AS B1 | | | C7ONO2-O2. + NO = #1.34 NO2 + #.11 MEK + & #.66 C7ONO2(2)-O2. + #.46 RCHO + #.56 -C |
| C98 ) | SAME K AS B1 | | | C7ONO2(2)-O2. + NO = #2 NO2 + #2 RCHO + -C |
| C99') | SAME K AS B5 | | | C7ONO2-O2. + HO2. = -OOH + NO2 + #.11 MEK + & #1.78 RCHO + #1.22 -C |
| C102) | SAME K AS B5 | | | C7ONO2(2)-O2. + HO2. = -OOH + NO2 + #2 RCHO & + -C |
| C103) | SAME K AS B8 | | | C7ONO2-O2. + RO2. = RO2. + #.5 HO2. + NO2 + & #.11 MEK + #1.78 RCHO + #1.22 -C |
| C106) | SAME K AS B8 | | | C7ONO2(2)-O2. + RO2. = RO2. + #.5 HO2. + NO2 & + & #2 RCHO + -C |

(continued)

Table B-1 (continued) - 6

| Reaction label[a] | Kinetic Parameters[b] | | | Reaction[c] |
|---|---|---|---|---|
| C107) | SAME K AS B9 | | | C7ONO2-O2. + RCO3. = RCO3. + #.5 HO2. + NO2 + & #.11 MEK + #1.78 RCHO + #1.22 -C |
| C110) | SAME K AS B9 | | | C7ONO2(2)-O2. + RCO3. = RCO3. + #.5 HO2. + & NO2 + #2 RCHO + -C |
| | | | | Reactions of Ethene |
| D1 ) | 3.156E+03 | -0.82 | -1.000 | C:C + HO. = HOC2-O2. + RO2. |
| D2 ) | SAME K AS B1 | | | HOC2-O2. + NO = NO2 + #.22 HOCCHO + #1.56 & HCHO + HO2. |
| D3 ) | SAME K AS B5 | | | HOC2-O2. + HO2. = -OOH + #.22 HOCCHO + #1.56 & HCHO |
| D4 ) | SAME K AS B8 | | | HOC2-O2. + RO2. = RO2. + #.5 HO2. + #.22 & HOCCHO + #1.56 HCHO |
| D5 ) | SAME K AS B9 | | | HOC2-O2. + RCO3. = RCO3. + #.5 HO2. + #.22 & HOCCHO + #1.56 HCHO |
| D6 ) | 1.761E+01 | 5.23 | -1.000 | C:C + O3 = HCHO + (HCHO2) |
| D8 ) | 1.527E+04 | 1.57 | -1.000 | C:C + O = C-O2. + HO2. + CO + RO2. |
| D9 ) | 2.936E+03 | 5.81 | -1.000 | C:C + NO3 = C:C-N-O2. + RO2. |
| D10 ) | SAME K AS B1 | | | C:C-N-O2. + NO = #2 NO2 + #2 HCHO |
| D11 ) | SAME K AS B5 | | | C:C-N-O2. + HO2. = -OOH + NO2 + #2 HCHO |
| D12 ) | SAME K AS B8 | | | C:C-N-O2. + RO2. = RO2. + #.5 HO2. + NO2 + & #2 HCHO |
| D13 ) | SAME K AS B9 | | | C:C-N-O2. + RCO3. = RCO3. + #.5 HO2. + NO2 + & #2 HCHO |
| D7 ) | (fast) | | | (HCHO2) = #.4 HCHO2 + #.18 CO2 + #.42 CO + & #.12 H2 + #.42 H2O + #.12 HO2. |
| D65 ) | 7.927E-03 | 0.00 | -1.000 | HCHO2 + H2O = -C |
| | | | | Reactions of Propene |
| D14 ) | 7.119E+03 | -1.00 | -1.000 | C:CC + HO. = C:CC-O2. + RO2. |
| D15 ) | SAME K AS B1 | | | C:CC-O2. + NO = NO2 + HCHO + CCHO + HO2. |
| D16 ) | SAME K AS B5 | | | C:CC-O2. + HO2. = -OOH + HCHO + CCHO |
| D17 ) | SAME K AS B8 | | | C:CC-O2. + RO2. = RO2. + #.5 HO2. + HCHO + CCHO |
| D18 ) | SAME K AS B9 | | | C:CC-O2. + RCO3. = RCO3. + #.5 HO2. + HCHO + & CCHO |
| D19 ) | 1.938E+01 | 4.18 | -1.000 | C:CC + O3 = #.5 "CCHO + (HCHO2) + HCHO + & (CCHO2)" |
| D21 ) | 1.732E+04 | 0.64 | -1.000 | C:CC +O = #.6 C-CO-C + #.4 CO + #.4 C-O2. + & #.2 C2-O2. + #.2 HO2. + #.6 RO2. |
| D22 ) | 7.340E+03 | 3.84 | -1.000 | C:CC + NO3 = C:CC-N-O2. + RO2. |
| D23 ) | SAME K AS B1 | | | C:CC-N-O2. + NO = #2 NO2 + CCHO + HCHO |
| D24 ) | SAME K AS B5 | | | C:CC-N-O2. + HO2. = -OOH + NO2 + CCHO + HCHO |
| D25 ) | SAME K AS B8 | | | C:CC-N-O2. + RO2. = RO2. + #.5 HO2. + NO2 + & CCHO + HCHO |

(continued)

Table B-1 (continued) - 7

| Reaction label[a] | Kinetic Parameters[b] | | | Reaction[c] |
|---|---|---|---|---|
| D26 ) | SAME K AS B9 | | | C:CC-N-O2. + RCO3. = RCO3. + #.5 HO2. + NO2 + & CCHO + HCHO |
| D20 ) | (fast) | | | (CCHO2) = #.2 CCHO2 + #.14 CH4 + #.29 CO2 + & #.15 CO + #.03 HCHO + #.27 "C-O2. + RO2." + & #.21 HO2. + #.12 HO. + #.72 -C |
| D66 ) | 7.927E-03 | 0.00 | -1.000 | CCHO2 + H2O = #2 -C |
| | | | | Reactions of Isobutene |
| D52 ) | 1.396E+04 | -1.00 | -1.000 | ISOBUTEN + HO. = ISOBUTEN-O2. + RO2. |
| D53 ) | SAME K AS B1 | | | ISOBUTEN-O2. + NO = NO2 + HO2. + HCHO + C-CO-C |
| D54 ) | SAME K AS B5 | | | ISOBUTEN-O2. + HO2. = -OOH + HCHO + C-CO-C |
| D55 ) | SAME K AS B8 | | | ISOBUTEN-O2. + RO2. = RO2. + #.5 HO2. + HCHO & + C-CO-C |
| D56 ) | SAME K AS B9 | | | ISOBUTEN-O2. + RCO3. = RCO3. + #.5 HO2. + & HCHO + C-CO-C |
| D57 ) | 5.211E+00 | 3.36 | -1.000 | ISOBUTEN + O3 = #.5 "C-CO-C + (HCHO2) + HCHO & + (C(C)CO2)" |
| D59 ) | 2.584E+04 | 0.09 | -1.000 | ISOBUTEN + O = #.5 "MEK + RCHO + -C" + #.4 HO2. |
| D60 ) | 1.468E+04 | 2.14 | -1.000 | ISOBUTEN + NO3 = ISOBUTEN-N-O2. + RO2. |
| D61 ) | SAME K AS B1 | | | ISOBUTEN-N-O2. + NO = #2 NO2 + C-CO-C + HCHO |
| D62 ) | SAME K AS B5 | | | ISOBUTEN-N-O2. + HO2. = -OOH + NO2 + C-CO-C & + HCHO |
| D63 ) | SAME K AS B8 | | | ISOBUTEN-N-O2. + RO2. = RO2. + #.5 HO2. + & NO2 + C-CO-C + HCHO |
| D64 ) | SAME K AS B9 | | | ISOBUTEN-N-O2. + RCO3. = RCO3. + #.5 HO2. + & NO2 + C-CO-C + HCHO |
| D58 ) | (fast) | | | (C(C)CO2) = #.2 "HO. + C-CO-C-O2. + RO2." + & #.8 MEK + #-.8 -C |
| | | | | Reactions of n-Butane |
| E11 ) | 2.275E+04 | 1.07 | -1.000 | C4 + HO. = #YE11A C4-O2. + #1-YE11A & C3(C)-O2. + RO2. |
| E12 ) | SAME K AS B1 | | | C4-O2. + NO = #YE12A C4ONO2 + #1-YE12A NO2 + & #E12P1 "HOC4-O2. + RO2." + #E12P2 "RCHO + & -C + HO2." |
| E13 ) | SAME K AS B1 | | | C3(C)-O2. + NO = #YE13A C4ONO2 + #1-YE13A & NO2 + #E13P1 "MEK + HO2." + #E13P2 "CCHO + & C2-O2. + RO2." |
| E14 ) | SAME K AS B1 | | | HOC4-O2. + NO = NO2 + HO2. + RCHO + -C |
| E15 ) | SAME K AS B5 | | | C4-O2. + HO2. = -OOH + RCHO + -C |
| E16 ) | SAME K AS B5 | | | C3(C)-O2. + HO2. = -OOH + #YE13B MEK + & #1-YE13B "CCHO + CCHO" |
| E17 ) | SAME K AS B5 | | | HOC4-O2. + HO2. = -OOH + RCHO + -C |
| E18 ) | SAME K AS B8 | | | C4-O2. + RO2. = RO2. + #.5 HO2. + RCHO + -C |

(continued)

Table B-1 (continued) - 8

| Reaction label[a] | Kinetic Parameters[b] | Reaction[c] |
|---|---|---|
| E19 ) | SAME K AS B8 | C3(C)-O2. + RO2. = RO2. + #.5 HO2. + #YE13B & MEK + #1-YE13B "CCHO + CCHO" |
| E20 ) | SAME K AS B8 | HOC4-O2. + RO2. = RO2. + #.5 HO2. + RCHO + -C |
| E12 ) | SAME K AS B9 | C4-O2. + RCO3. = RCO3. + #.5 HO2. + RCHO + -C |
| E22 ) | SAME K AS B9 | C3(C)-O2. + RCO3. = RCO3. + #.5 HO2. + & #YE13B MEK + #1-YE13B "CCHO + CCHO" |
| E23 ) | SAME K AS B9 | HOC4-O2. + RCO3. = RCO3. + #.5 HO2. + RCHO + -C |
| | | Reactions of n-Pentane |
| C5F1) | 2.950E+04 0.97 -1.000 | HO. + C5 = C5-RO2. + RO2. |
| C5F2) | SAME K AS B1 | C5-RO2. + NO = #C5P1 C4ONO2 + #C5P2 C7ONO2 + & #C5P4 "HO2. + NO2" + #C5P5 "R2O2. + RO2." + & #C5P6 HCHO + #C5P7 CCHO + #C6P9 RCHO + & #C5PA MEK + #C5PB ROH |
| C5F3) | SAME K AS B5 | C5-RO2. + HO2. = -OOH + C5-PROD |
| C5F4) | SAME K AS B8 | C5-RO2. + RO2. = RO2. + #.5 HO2. + C5-PROD |
| C5F5) | SAME K AS B9 | C5-RO2. + RCO3. = RCO3. + #.5 HO2. + C5-PROD |
| C5F6) | (fast) | C5-PROD = #C5XP6 HCHO + #C5XP7 CCHO + #C5XP9 & RCHO + #C5XPA MEK + #C5XPB ROH |
| | | Reactions of iso-Octane |
| I8F1) | 1.596E+04 0.50 -1.000 | HO. + ISO-C8 = I8-RO2. + RO2. |
| I8F2) | SAME K AS B1 | I8-RO2. + NO = #I8P1 C4ONO2 + #I8P2 C7ONO2 + & #I8P3 -N + #I8P4 "HO2. + NO2" + #I8P5 & "R2O2. + RO2." + #I8P6 HCHO + #I8P7 CCHO + & #I8P8 C-CO-C + #I8P9 RCHO + #I8PA MEK + & #I8PB ROH + #I8PC -C |
| I8F3) | SAME K AS B5 | I8-RO2. + HO2. = -OOH + I8-PROD |
| I8F4) | SAME K AS B8 | I8-RO2. + RO2. = RO2. + #.5 HO2. + I8-PROD |
| I8F5) | SAME K AS B9 | I8-RO2. + RCO3. = RCO3. + #.5 HO2. + I8-PROD |
| I8F6) | (fast) | I8-PROD = #I8XP6 HCHO + #I8XP7 CCHO + #I8XP8 & C-CO-C + #I8XP9 RCHO + #I8XPA MEK + #I8XPB & ROH + #I8XPC -C |
| | | Reactions of Toluene (and its uncharacterized ring-opening products) |
| G6 ) | 3.083E+03 -0.64 -1.000 | HO. + TOLU = #.16 "CRES + HO2." + #.08 & BZ-C-O2. + #.76 HO-TOLU-O2. + #.84 RO2. |
| G7 ) | SAME K AS B1 | BZ-C-O2. + NO = NO2 + HO2. + BZ-CHO |
| G8 ) | SAME K AS B5 | BZ-C-O2. + HO2. = -OOH + BZ-CHO |
| G9 ) | SAME K AS B8 | BZ-C-O2. + RO2. = RO2. + #.5 HO2. + BZ-CHO |
| G10 ) | SAME K AS B9 | BZ-C-O2. + RCO3. = RCO3. + #.5 HO2. + BZ-CHO |

(continued)

Table B-1 (continued) - 9

| Reaction label[a] | Kinetic Parameters[b] | Reaction[c] |
|---|---|---|
| G11 ) | SAME K AS B1 | HO-TOLU-O2. + NO = NO2 + HO2. + #.15 HCOCHO + & #.19 CCOCHO + TOLU-UNKN |
| G12 ) | SAME K AS B5 | HO-TOLU-O2. + HO2. = -OOH + #.15 HCOCHO + & #.19 CCOCHO + TOLU-UNKN |
| G13 ) | SAME K AS B8 | HO-TOLU-O2. + RO2. = RO2. + #.5 HO2. + #.15 & HCOCHO + #.19 CCOCHO + TOLU-UNKN |
| G14 ) | SAME K AS B9 | HO-TOLU-O2. + RCO3. = RCO3. + #.5 HO2. + & #.15 HCOCHO + #.19 CCOCHO + TOLU-UNKN |
| G622) | 4.404E+04 0.00 -1.000 | HO. + TOLU-UNKN = TOLU-RCO3. + RCO3. |
| G632) | SAME K AS B2 | TOLU-RCO3. + NO = NO2 + CO2 + TOLU-R1O2. + RO2. |
| G642) | SAME K AS B4 | TOLU-RCO3. + NO2 = TOLU-PAN |
| G652) | 1.200E+18 26.91 0.000 | TOLU-PAN = TOLU-RCO3. + RCO3. + NO2 |
| G662) | SAME K AS B1 | TOLU-R1O2. + NO = NO2 + TOLU-R2O2. + RO2. |
| G672) | SAME K AS B1 | TOLU-R2O2. + NO = NO2 + #.73 "CO + HO2." + & #1.12 HCOCHO + #.54 CCOCHO + #.27 "CCO-O2. & + RCO3." |
| G682) | SAME K AS B6 | TOLU-RCO3. + HO2. = -OOH + CO2 + #.73 CO + & #1.12 HCOCHO + #.54 CCOCHO + #.27 "HCHO + CO2" |
| G692) | SAME K AS B9 | TOLU-RCO3. + RO2. = RO2. + #.5 HO2. + CO2 + & #.73 CO + #1.12 HCOCHO + #.54 CCOCHO + #.27 & "HCHO + CO2" |
| G702) | SAME K AS B10 | TOLU-RCO3. + RCO3. = RCO3. + HO2. + CO2 + & #.73 CO + #1.12 HCOCHO + #.54 CCOCHO + #.27 & "HCHO + CO2" |
| G712) | SAME K AS B5 | TOLU-R1O2. + HO2. = -OOH + #.73 CO + #1.12 & HCOCHO + #.54 CCOCHO + #.27 "HCHO + CO2" |
| G722) | SAME K AS B8 | TOLU-R1O2. + RO2. = RO2. + #.5 HO2. + #.73 & CO + #1.12 HCOCHO + #.54 CCOCHO + #.27 & "HCHO + CO2" |
| G732) | SAME K AS B9 | TOLU-R1O2. + RCO3. = RCO3. + #.5 HO2. + #.73 & CO + #1.12 HCOCHO + #.54 CCOCHO + #.27 & "HCHO + CO2" |
| G742) | SAME K AS B5 | TOLU-R2O2. + HO2. = -OOH + #.73 CO + #1.12 & HCOCHO + #.54 CCOCHO + #.27 "HCHO + CO2" |
| G752) | SAME K AS B8 | TOLU-R2O2. + RO2. = RO2. + #.5 HO2. + #.73 & CO + #1.12 HCOCHO + #.54 CCOCHO + #.27 & "HCHO + CO2" |
| G762) | SAME K AS B9 | TOLU-R2O2. + RCO3. = RCO3. + #.5 HO2. + & #.73 CO + #1.12 HCOCHO + #.54 CCOCHO + #.27 & "HCHO + CO2" |
| G772) | PHOT. = AROMUNKN | TOLU-UNKN + HV = #1.66 HCOCHO + #.81 & "CCO-O2. + RCO3." + #1.19 "HO2. + CO" |
| | | Reactions of m-Xylene (and its uncharacterized ring-opening products) |

(continued)

Table B-1 (continued) - 10

| Reaction label[a] | Kinetic Parameters[b] | Reaction[c] |
|---|---|---|
| G15 ) | 2.437E+04 -0.23 -1.000 | HO. + M-XYEN = #.04 BZ-C-O2. + #.17 "CRES + & HO2." + #.79 HO-MXYL-O2. + #.83 RO2. + #.21 -C |
| G16 ) | SAME K AS B1 | HO-MXYL-O2. + NO = NO2 + HO2. + #.12 HCOCHO + & #.40 CCOCHO + MXYL-UNKN |
| G17 ) | SAME K AS B5 | HO-MXYL-O2. + HO2. = -OOH + #.12 HCOCHO + & #.40 CCOCHO + MXYL-UNKN |
| G18 ) | SAME K AS B8 | HO-MXYL-O2. + RO2. = RO2. + #.5 HO2. + #.12 & HCOCHO + #.40 CCOCHO + MXYL-UNKN |
| G19 ) | SAME K AS B9 | HO-MXYL-O2. + RCO3. = RCO3. + #.5 HO2. + & #.12 HCOCHO + #.40 CCOCHO + MXYL-UNKN |
| G623) | 4.404E+04 0.00 -1.000 | HO. + MXYL-UNKN = MXYL-RCO3. + RCO3. |
| G633) | SAME K AS B2 | MXYL-RCO3. + NO = NO2 + CO2 + MXYL-R1O2. + RO2. |
| G643) | SAME K AS B4 | MXYL-RCO3. + NO2 = MXYL-PAN |
| G653) | 1.200E+18 26.91 0.000 | MXYL-PAN = MXYL-RCO3. + RCO3. + NO2 |
| G663) | SAME K AS B1 | MXYL-R1O2. + NO = NO2 + MXYL-R2O2. + RO2. |
| G673) | SAME K AS B1 | MXYL-R2O2. + NO = NO2 + #.47 "CO + HO2." + & #.41 HCOCHO + #1.07 CCOCHO + #.53 "CCO-O2. + & RCO3." |
| G683) | SAME K AS B6 | MXYL-RCO3. + HO2. = -OOH + CO2 + #.47 CO + & #.41 HCOCHO + #1.07 CCOCHO + #.53 "HCHO + CO2" |
| G693) | SAME K AS B9 | MXYL-RCO3. + RO2. = RO2. + #.5 HO2. + CO2 + & #.47 CO + #.41 HCOCHO + #1.07 CCOCHO + #.53 & "HCHO + CO2" |
| G703) | SAME K AS B10 | MXYL-RCO3. + RCO3. = RCO3. + HO2. + CO2 + & #.47 CO + #.41 HCOCHO + #1.07 CCOCHO + #.53 & "HCHO + CO2" |
| G713) | SAME K AS B5 | MXYL-R1O2. + HO2. = -OOH + #.47 CO + #.41 & HCOCHO + #1.07 CCOCHO + #.53 "HCHO + CO2" |
| G723) | SAME K AS B8 | MXYL-R1O2. + RO2. = RO2. + #.5 HO2. + #.47 & CO + #.41 HCOCHO + #1.07 CCOCHO + #.53 & "HCHO + CO2" |
| G733) | SAME K AS B9 | MXYL-R1O2. + RCO3. = RCO3. + #.5 HO2. + #.47 & CO + #.41 HCOCHO + #1.07 CCOCHO + #.53 & "HCHO + CO2" |
| G743) | SAME K AS B5 | MXYL-R2O2. + HO2. = -OOH + #.47 CO + #.41 & HCOCHO + #1.07 CCOCHO + #.53 "HCHO + CO2" |
| G753) | SAME K AS B8 | MXYL-R2O2. + RO2. = RO2. + #.5 HO2. + #.47 & CO + #.41 HCOCHO + #1.07 CCOCHO + #.53 & "HCHO + CO2" |
| G763) | SAME K AS B9 | MXYL-R2O2. + RCO3. = RCO3. + #.5 HO2. + #.47 & CO + #.41 HCOCHO + #1.07 CCOCHO + #.53 & "HCHO + CO2" |
| G773) | PHOT. = AROMUNKN | MXYL-UNKN + HV + #2 = #1.48 HCOCHO + & #1.68 "CCO-O2. + RCO3." + #.32 "HO2. + CO" |

(continued)

Table B-1 (continued) - 11

| Reaction label[a] | Kinetic Parameters[b] | | | Reaction[c] |
|---|---|---|---|---|
| | | | | Reactions of Benzaldehyde |
| G30 ) | 1.761E+04 | 0.00 | -1.000 | BZ-CHO + HO. = BZ-CO-O2. + RCO3. |
| G31 ) | PHOT. = BZCHO | | | BZ-CHO + HV + #.05 = #7 -C |
| G32 ) | 4.404E+02 | 2.97 | -1.000 | BZ-CHO + NO3 = HONO2 + BZ-CO-O2. |
| G33 ) | SAME K AS B2 | | | BZ-CO-O2. + NO = BZ-O2. + CO2 + NO2 + RO2. |
| G34 ) | SAME K AS B4 | | | BZ-CO-O2. + NO2 = BZ-PAN |
| G35 ) | 9.600E+16 | 25.90 | 0.000 | BZ-PAN = BZ-CO-O2. + NO2 + RCO3. |
| G36 ) | SAME K AS B6 | | | BZ-CO-O2. + HO2. = -OOH + CO2 + PHENOL |
| G37 ) | SAME K AS B9 | | | BZ-CO-O2. + RO2. = RO2. + #.5 HO2. + CO2 + & PHENOL |
| G38 ) | SAME K AS B10 | | | BZ-CO-O2. + RCO3. = RCO3. + HO2. + CO2 + PHENOL |
| G39 ) | SAME K AS B1 | | | BZ-O2. + NO = BZ-O. + NO2 |
| G40 ) | SAME K AS B5 | | | BZ-O2. + HO2. = -OOH + PHENOL |
| G41 ) | SAME K AS B8 | | | BZ-O2. + RO2. = RO2. + #.5 HO2. + PHENOL |
| G42 ) | SAME K AS B9 | | | BZ-O2. + RCO3. = RCO3. + HO2. + PHENOL |
| G43 ) | 2.202E+04 | 0.00 | -1.000 | BZ-O. + NO2 = NITROPHEN |
| G44 ) | 4.404E+03 | 0.00 | -1.000 | BZ-O. + HO2. = PHENOL |
| G45 ) | 6.000E-02 | 0.00 | 0.000 | BZ-O. = PHENOL |
| | | | | Reactions of Phenol |
| G46 ) | 4.154E+04 | 0.00 | -1.000 | HO. + PHENOL = HO-PHEN-O2. + RO2. |
| G47 ) | SAME K AS B1 | | | HO-PHEN-O2. + NO = #.15 NITROPHEN + #.2 & HCOCHO + #.85 "NO2 + HO2." + #4.7 -C |
| G48 ) | SAME K AS B5 | | | HO-PHEN-O2. + HO2. = -OOH + #.24 HCOCHO + & #5.52 -C |
| G49 ) | SAME K AS B8 | | | HO-PHEN-O2. + RO2. = RO2. + #.24 HCOCHO + & #5.52 -C |
| G50 ) | SAME K AS B9 | | | HO-PHEN-O2. + RCO3. = RCO3. + #.5 HO2. + & #.24 HCOCHO + #5.52 -C |
| G51 ) | 5.578E+03 | 0.00 | -1.000 | NO3 + PHENOL = HONO2 + BZ-O. |
| | | | | Reactions of Alkyl-Substituted Phenols |
| G52 ) | 6.018E+04 | 0.00 | -1.000 | HO. + CRES = HO-CRES-O2. + RO2. |
| G53 ) | SAME K AS B1 | | | HO-CRES-O2. + NO = #.15 NITROPHEN + #.2 & CCOCHO + #.85 "NO2 + HO2." + #5.5 -C |
| G54 ) | SAME K AS B5 | | | HO-CRES-O2. + HO2. = -OOH + #.24 CCOCHO + & #6.28 -C |
| G55 ) | SAME K AS B8 | | | HO-CRES-O2. + RO2. = RO2. + #.24 CCOCHO + & #6.28 -C |
| G56 ) | SAME K AS B9 | | | HO-CRES-O2. + RCO3. = RCO3. + #.5 HO2. + & #.24 CCOCHO + #6.28 -C |
| G57 ) | 3.229E+04 | 0.00 | -1.000 | NO3 + CRES = HONO2 + BZ-O. + -C |

(continued)

Table B-1 (continued) - 12

| Reaction label[a] | Kinetic Parameters[b] | | | Reaction[c] |
|---|---|---|---|---|
| | | | | Reactions of Nitrophenol |
| G58 ) | 5.578E+03 | 0.00 | -1.000 | NITROPHEN + NO3 = HONO2 + BZ(NO2)-O. |
| G59 ) | 2.202E+04 | 0.00 | -1.000 | BZ(NO2)-O. + NO2 = -N + #6 -C ! DINITROPHENOL |
| G60 ) | 4.404E+03 | 0.00 | -1.000 | BZ(NO2)-O. + HO2. = NITROPHEN |
| G61 ) | 6.000E-02 | 0.00 | 0.000 | BZ(NO2)-O. = NITROPHEN |
| | | | | Reactions of Methanol |
| H1 ) | 1.967E+04 | 1.60 | -1.000 | MEOH + HO. = H2O + HCHO + HO2. |
| | | | | Chamber-Dependent Reactions (See Table B-4 for rate constants and parameters used) |
| O3W ) | 0.000E-01 | 0.00 | 0.000 | O3 = |
| N25I) | 0.000E-01 | 0.00 | 0.000 | N2O5 = #2 NOX-WALL |
| N25S) | 0.000E-01 | 0.00 | -1.000 | N2O5 + H2O = #2 NOX-WALL |
| NO2W) | 0.000E-01 | 0.00 | 0.000 | NO2 = #YHONO HONO + #1-YHONO NOX-WALL |
| RSI ) | PHOT. = NO2 | | | HV + #RS-I = HO. |
| RSS ) | PHOT. = NO2 | | | NO2 + HV + #RS-S = #.5 HONO + #.5 NOX-WALL |
| ONO2) | PHOT. = NO2 | | | #E-NO2/K1 = NO2 + #-1 NOX-WALL |

[a]Reaction label notation of Carter et al. (1986).

[b]The kinetic parameters in this mechanism, which are used by the computer modeling software to define the rate constants as a function of temperature, light intensity and spectral distribution, or rate constants for other reactions, are specified in one of four ways:

1. Simple thermal reactions:

   If the kinetic parameters are given as three numbers without any additional notation, then the numbers given are (in order) A, Ea, and B, and the rate constant, k, is calculated by the modified Arrhenius expression.

   $$k = A \times (T/300)^{B} \times \exp [-Ea / (0.0019872 \times T)]$$

   where T is the temperature in K, Ea is given in kcal $mole^{-1}$, and the units of k and A are $min^{-1}$ for first order reactions, $ppm^{-1}$ $min^{-1}$ for second order reactions, or $ppm^{-2}$ $min^{-1}$ for third order reactions. (The order of the reaction is determined by the number of non-coefficient reactants; see note c, below.)

   (If a reaction has the symbol "#RCONxxxx as one of the "reactants", [where "xxxx" is the reaction label of some previously input reaction which should be the reverse of this reaction] then the "k" calculated as given above is actually an equilibrium constant, since the rate constant for this reaction is given by "k" times the rate constant for reaction "xxxx". See Footnote c for a discussion of coefficients as reactants.)

(continued)

2. "Falloff" Thermal Reactions:

If the kinetic parameters are given as seven numbers in the following format,

```
          FALLOFF F= f,    N= n
KO:  A0,       Ea0,       B0
KI:  AI,       EaI,       BI
```

then the rate constant, k is calculated by

$$k = [(k_0 \times M)/(1 + [k_0 \times M / k_I] ) ] \times f^{\,1/[1 + (\log_{10} [k_0 \times M / k_I] / n)^2]}$$

where

$$k_0 = A_0 \times (T/300)^{B_0} \times \exp(-Ea_0 / [0.0019872 \times T]),$$
$$k_I = A_I \times (T/300)^{B_I} \times \exp(-Ea_I / [0.0019872 \times T]),$$

T is the temperature in K and M is the concentration of the constant species "M", which is the the total pressure in ppm. In these calculations, M is always $10^6$ ppm.

Reactions of this type are always second order, so the units of k, $k_I$ and $A_I$ are $ppm^{-1}$ $min^{-1}$, and the units of $k_0$ and $A_0$ are $ppm^{-2}$ $min^{-2}$. The units of $Ea_0$ and $Ea_I$ are kcal/mole,

3. Reactions with same rate constants as other reactions.

The notation "SAME K AS xxxx", where "xxxx" is the reaction label for some other reaction, means that the reaction always has the same rate constant as reaction "xxxx".

4. Photolysis reactions.

Photolysis reactions are indicated by the notation "PHOT. = filename", where "filename" refers to a "photolysis file", which gives the absorption coefficients and quantum yields, as a function of wavelength, which are used to calculate the photolysis rate constants for this photolysis reaction, given the spectral distribution of the light source. The contents of the photolysis files used in this mechanism are given in Table B-5.

[c]The following examples indicate the notation used to define the reactants, products, and (where applicable) coefficients involved in the reactions in the mechanism:

```
reactant1 + reactant2 + ... = product1 + product2 + ...
reactant1 + ... = #coefficient2 product1 + ...
reactant1 + ... = #coefficient3 "product1 + product2 + ..." + ...
reactant1 + #coefficient1 + ... = product1 + ...
```

(continued)

The first example is a simple reaction without any coefficients. The second and third have product coefficients which give the yield of the products. The notation in the third reaction is used to indicate that both "product1" and "product2" have the same coefficient, and thus that reaction is equivalent to

reactant1 + ... = #coefficient3 product1 + #coefficient3 product2 + ....

When a coefficient is shown as a "reactant", as in the fourth example, the coefficient is multiplied by the rate constant calculated from the kinetic parameters (as described in footnote b, above), to give the rate constant of the reaction. For example, one of the reactions used to represent the chamber radical source is

RSI) PHOT. = NO2 HV + #RS-I = HO.,

and for this reaction, the rate constant, defining the rate of OH generation, is given by the photolysis rate of NO2 multiplied by the value of the coefficient RS-I, which depends on the chamber. A special kind of reactant coefficient is that of the form "#RCONxxxx", whose value is the rate constant for the reaction labeled "xxxx".

Regardless of how the coefficients are used, they can be either constant, as indicated by their "name" being a number, or variable, as indicated by their names being non-numeric. The values of the variable coefficients, which in general depend on temperature, are given in Table B-3.

If the list of reactants, products, and coefficients do not fit on one line, the symbol "&" is used to indicate that the reaction continues on the following line.

[d]The pseudo-species "RO2" and "RCO3" are used to keep track of the total concentrations of all peroxy and acyl peroxy radicals, respectively, which are used to calculate the rates of peroxy + peroxy radical reactions. These are calculated by including "RO2" as a "product" for each reaction which forms peroxy radicals, with the same yield as the total peroxy radical yield in that reaction, (and likewise for "RCO3" and acyl peroxy radicals), and by including reactions B1 through B10 to represent their consumption processes. Note that reactions B1 - B10 are the only reactions which represent a net sink for these pseudo species; in the reactions used to represent the reaction of a given peroxy radical with all others (e.g., reactions C7, C8, C16, and C17, etc.), these are given as products as well as reactants. See the discussion of representation of peroxy radical reactions in Carter et al. (1986).

The pseudo-species R2O2 is used to represent the additional oxidation of NO to NO2 caused by reactions of subsequently formed peroxy radicals in the alkane photooxidation mechanisms.

Table B-2. List of Species used in the Model Simulations of the Surrogate-$NO_x$-Air Irradiations

| Species Name | Compound or Meaning |
|---|---|
| **1. Species Integrated Explicitly** | |
| O3 | Ozone |
| NO | Nitric Oxide |
| NO2 | Nitrogen Dioxide |
| NO3 | Nitrate Radical |
| N2O5 | $N_2O_5$ |
| HONO2 | Nitric Acid |
| HONO | Nitrous Acid |
| HO2. | $HO_2$ Radicals |
| HO2NO2 | Peroxy Nitric Acid |
| HO2H | Hydrogen Peroxide |
| CO | Carbon Monoxide |
| RO2. | Lumped Alkyl Peroxy Radicals (sum of all alkyl peroxy radicals) |
| RCO3. | Lumped Acyl Peroxy Radicals (sum off all acyl peroxy radicals) |
| -OOH | Lumped Hydroperoxide Group (used to represent photolizable hydroperoxide groups formed when peroxy radicals react with $HO_2$) |
| HCHO | Formaldehyde |
| CCHO | Acetaldehyde |
| C-PAN | PAN |
| RCHO | Propionaldehyde and Lumped Higher Aldehydes |
| C2-PAN | PPN (and PAN analogues formed from higher aldehydes) |
| C-CO-C | Acetone |
| CCOCHO | Methyl Glyoxal |
| MEK | Methyl Ethyl Ketone and Lumped Higher Ketones |
| ROH | 3-Pentanol (used in part to represent OH-substituted bi- and poly-functional compounds formed following the isomerization of long-chain alkoxy radicals formed in the photooxidations of the higher alkanes |
| HCOCHO | Glyoxal |
| HCO-PAN | $HCO-CO-OONO_2$ (PAN analogue formed from glyoxal) |
| HOCCHO | Glycolaldehyde |
| HOC-PAN | $HOCH_2-CO-OONO_2$ (PAN analogue formed from glycol-aldehyde) |
| C4ONO2 | 2-Butyl Nitrate (used with 4-heptyl nitrate to represent $\geq C_4$ alkyl nitrates) |
| C7ONO2 | 4-Heptyl Nitrate |
| C:C | Ethene |
| C:CC | Propene |
| ISOBUTEN | Isobutene |
| C4 | n-Butane |

(continued)

Table B-2 (continued) - 2

| Species Name | Compound or Meaning |
|---|---|
| C5 | n-Pentane |
| ISO-C8 | 2,2,4-Trimethylpentane (iso-Octane) |
| TOLU | Toluene |
| M-XYEN | m-Xylene |
| BZ-CHO | Benzaldehyde |
| BZ-PAN | PBzN (Peroxy penzoyl nitrate) |
| PHENOL | Phenol |
| NITROPHEN | Nitrophenols |
| CRES | Cresols and Other Alkyl Phenols |
| TOLU-UNKN | Unknown Product(s) Formed in the Ring Opening Reactions of Toluene |
| TOLU-PAN | Pan Analogue(s) Assumed to be Formed in the Reactions of TOLU-UNKN |
| MXYL-UNKN | Unknown Product(s) Formed in the Ring Opening Reactions of m-Xylene |
| MXYL-PAN | Pan Analogue(s) Assumed to be Formed in the Reactions of MXYL-UNKN |
| MEOH | Methanol |

2. Constant Species (concentrations held constant during the calculations)

| | |
|---|---|
| HV | Total Light Intensity (either 1.0 or 0.0 in indoor chamber simulations, depending on whether lights are on or off. Varies for outdoor chamber simulations such that HV = 1.0 corresponds to clear sky conditions, and HV < 1 corresponds to overcast or partly overcast conditions.) |
| O2 | Oxygen in Air (always 2.090E+05 PPM) |
| M | Total Pressure (always 1.000E+06 PPM) |
| H2O | Water Concentration (concentration varies from run-to-run. If no humidity or dew point data are available, then the default is used. Default for indoor chamber runs is 2.0E+04 PPM; default for outdoor chamber runs is 5.0E+3 PPM.) |

3. Product-Only and Counter Species (species which are formed, but which do not react, or pseudo-species used to keep track of carbon, nitrogen, etc.)

| | |
|---|---|
| -C | "Lost" or Unreactive Product Carbon (used to check for carbon balance, and to determine the extent of species whose reactions are ignored) |
| NOX-WALL | $NO_x$ Absorbed on the Walls (used primarily to check for nitrogen balance) |
| CO2 | Carbon Dioxide |

(continued)

Table B-2 (continued) - 3

| Species Name | Compound or Meaning |
|---|---|
| CH4 | Methane (reactions ignored) |
| H2 | Hydrogen (reactions ignored) |

4. Species for which the Steady State Approximation is Applied

| | |
|---|---|
| O | $O(^3P)$ Atoms |
| O*1D2 | $O(^1D)$ Atoms |
| HO. | Hydroxyl Radicals |
| HOC-O2. | $HOCH_2OO.$ (peroxy radical formed from $HO_2$ + HCHO) |
| CCO-O2. | Acetyl Peroxy Radicals |
| C-O2. | Methyl Peroxy Radicals |
| C-O. | Methoxy Radicals |
| C2CO-O2. | Propionyl Peroxy Radicals |
| C2-O2. | Ethyl Peroxy Radicals |
| C-CO-C-O2. | $CH_3-CO-CH_2OO.$ (peroxy radical formed in the OH + acetone reaction) |
| MEK-O2. | 50% $CH_3-CO-CH(OO.)CH_3$ + 50% $CH_3-CO-CH_2CH_2OO.$ (formed initially in the OH + methyl ethyl ketone reaction) |
| MEK(2)-O2. | $HOCH_2CH_2-CO-CH_2OO.$ (formed in the OH + MEK reaction) |
| ROH-O2. | Lumped Peroxy Species Used to Represent Species in the OH + Pentanol Reactions |
| HCOCO. | H-CO-CO. (radical initially formed in the OH + glyoxal reaction) |
| HCOCO-O2. | Acyl Peroxy Radical Formed when $O_2$ Reacts with HCOCO. |
| HOCCO-O2. | $HOCH_2-CO-OO.$ (acyl peroxy radical formed from glycolaldehyde) |
| C4ONO2-O2. | 60% $CH_3CH(ONO_2)CH(OO.)CH_3$ + 40% $CH_3CH(ONO_2)CH_2CH_2OO.$ (formed in the OH + 2-butyl nitrate reaction) |
| C4ONO2(2)-O2. | $CH_3C(OO.)(ONO_2)CH_2CH_2OH$ (formed in the OH + 2-butyl nitrate reaction) |
| C7ONO2-O2. | 11% $.OOC_3H_6CH(ONO_2)C_3H_7$ + 66% $CH_3CH(OO.)CH_2CH(ONO2)C_3H_7$ + 23% $C_2H_5CH(OO.)CH(ONO_2)C_3H_7$ (formed in the OH + 4-heptyl nitrate reaction) |
| C7ONO2(2)-O2. | $CH_3CH(OH)CH_2CH(ONO_2)CH(OO.)C_2H_5$ (formed in the OH + 4-heptyl nitrate reaction) |
| HOC2-O2. | $HOCH_2CH_2OO.$ (OH-ethene-$O_2$ adduct) |
| (HCHO2) | "Hot" Criegee Biradical Formed in the Reactions of Ozone with Alkenes with $=CH_2$ Groups |
| HCHO2 | Stabilized Criegee Biradical Formed in the Reactions of Ozone with Alkenes with $=CH_2$ Groups |
| C:C-N-O2. | $.OOCH_2CH_2ONO2$ ($NO_3$-ethene-$O_2$ adduct) |
| C:CC-O2. | $CH_3CH(OH)CH_2OO.$ + $CH_3CH(OO.)CH_2OH$ (OH-propene-$O_2$ adducts) |

(continued)

Table B-2 (continued) - 4

| Species Name | Compound or Meaning |
|---|---|
| (CCHO2) | "Hot" Criegee Biradical Formed in the Reactions of Ozone with Alkenes with $=CHCH_3$ Groups |
| C:CC-N-O2. | $CH_3CH(ONO_2)CH_2OO\cdot$ + $CH_3CH(OO\cdot)CH_2ONO_2$ ($NO_3$-propene-$O_2$ adducts) |
| CCHO2 | Stabilized Criegee Biradical Formed in the Reactions of Ozone with Alkenes with $=CHCH_3$ Groups |
| ISOBUTEN-O2. | $(CH_3)_2(OO\cdot)CH_2OH$ (OH-isobutene-$O_2$ adduct) |
| (C(C)CO2) | "Hot" Criegee Biradical Formed in the Reactions of Ozone with Alkenes with $=C(CH_3)_2$ Groups |
| ISOBUTEN-N-O2. | $(CH_3)_2(OO\cdot)CH_2ONO_2$ ($NO_3$-isobutene-$O_2$ adduct) |
| C4-O2. | $CH_3(CH_2)_3OO\cdot$ (formed in the OH + n-butane reactions) |
| C3(C)-O2. | $CH_3CH(OO\cdot)CH_2CH_3$ (formed in the OH + n-butane reactions) |
| HOC4-O2. | $HO(CH_2)_4OO\cdot$ (formed in the OH + n-butane reactions) |
| C5-RO2. | Lumped Species Representing All Peroxy Radicals Formed in the OH + n-Pentane Reactions |
| R2O2. | Psuedo-Specie (used to account for NO to $NO_2$ conversions caused by subsequently formed peroxy radicals in the reactions of the $\geq C_5$ alkanes) |
| C5-PROD | Temporary Pseudo-Specie (used in the n-pentane mechanism to represent the set of organic products formed. Immediately "reacts" to form those products) |
| I8-RO2. | Lumped Species Representing All Peroxy Radicals Formed in the OH + iso-Octane Reactions |
| I8-PROD | Temporary Pseudo-Specie (used in the iso-octane mechanism to represent the set of organic products formed. Immediately "reacts" to form those products) |
| HO-TOLU-O2. | Used to Represent the Peroxy Radical Intermediates Which Lead to Ring Opening in the OH + Toluene Reactions. |
| BZ-C-O2. | Benzyl Peroxy Radicals |
| TOLU-RCO3. | Used to Represent the Acyl Peroxy Radicals Assumed to be Initially Formed in the Reactions of OH Radicals with the Uncharacterized Toluene Ring-Opening Products. (Assumed to be an analogue of H-CO-CH=CH-CO-OO.) |
| TOLU-RIO2. | Used to Represent the Peroxy Radicals Initially Formed from TOLU-RCO3. (Assumed to be an analogue of H-CO-CH=CHOO.) |
| TOLU-R2O2. | Used to Represent the Peroxy Radicals Formed from TOLU-RIO2. (Assumed to be an analogue of H-CO-CH(OO.)CHO.) |

(continued)

Table B-2 (concluded) - 5

| Species Name | Compound or Meaning |
|---|---|
| MXYL-RCO3. | Used to Represent the Acyl Peroxy Radicals Assumed to be Initially Formed in the Reactions of OH Radicals with the Uncharacterized m-Xylene Ring-Opening Products. (Assumed to be an analogue of H-CO-CH=CH-CO-OO.) |
| MXYL-R1O2. | Used to Represent the Peroxy Radicals Initially Formed from MXYL-RCO3. (Assumed to be an analogue of H-CO-CH=CHOO.) |
| MXYL-R2O2. | Used to Represent the Peroxy Radicals Formed from MXYL-R1O2. (Assumed to be an analogue of H-CO-CH(OO.)CHO.) |
| BZ-CO-O2. | Benzoyl Peroxy Radical |
| BZ-O2. | Phenyl Peroxy Radical |
| BZ-O. | Phenoxy Radical |
| BZ(NO2)-O. | Nitro-Substituted Phenoxy Radicals |
| HO-PHEN-O2. | Lumped Peroxy Radical Used in the Empirical Representation of the OH + Phenol Reactions |
| HO-CRES-O2. | Lumped Peroxy Radical Used in the Empirical Representation of the OH + Cresol Reactions |

Table B-3. Values of Temperature-Dependent Coefficients Used in the Model Simulations of the Surrogate-$NO_x$-Air Irradiations (See Table B-1 for the reactions in which these coefficients appear)

| Name | Values | | |
|---|---|---|---|
| | 270 K | 300 K | 330 K |
| T270 | 1.00 | 0.000 | 0.000 |
| T300 | 0.000 | 1.00 | 0.000 |
| T330 | 0.000 | 0.000 | 1.00 |
| YE11A | 0.130 | 0.150 | 0.160 |
| 1-YE11A | 0.870 | 0.850 | 0.840 |
| YE12A | 5.000E-02 | 3.000E-02 | 2.000E-02 |
| 1-YE12A | 0.950 | 0.970 | 0.980 |
| YE12B | 0.460 | 0.780 | 0.920 |
| E12P1 | 0.437 | 0.757 | 0.902 |
| E12P2 | 0.513 | 0.213 | 7.840E-02 |
| YE13A | 0.130 | 8.000E-02 | 5.000E-02 |
| 1-YE13A | 0.870 | 0.920 | 0.950 |
| YE13B | 0.970 | 0.630 | 0.150 |
| 1-YE13B | 3.000E-02 | 0.370 | 0.850 |
| E13P1 | 0.844 | 0.580 | 0.143 |
| E13P2 | 2.610E-02 | 0.340 | 0.808 |
| C5P1 | 0.135 | 8.490E-02 | 5.600E-02 |
| C5P2 | 6.740E-02 | 4.230E-02 | 2.770E-02 |
| C5P4 | 0.798 | 0.873 | 0.916 |
| C5P5 | 0.240 | 0.515 | 0.807 |
| C5P6 | 0.000 | 6.500E-03 | 1.380E-02 |
| C5P7 | 0.000 | 7.350E-02 | 0.281 |
| C5P9 | 5.980E-02 | 0.163 | 0.385 |
| C5PA | 0.706 | 0.584 | 0.352 |
| C5PB | 0.197 | 0.277 | 0.289 |
| C5XP6 | 0.000 | 7.500E-03 | 1.510E-02 |
| C5XP7 | 0.000 | 8.490E-02 | 0.308 |
| C5XP9 | 6.540E-02 | 0.181 | 0.417 |
| C5XPA | 0.897 | 0.675 | 0.387 |
| C5XPB | 0.243 | 0.316 | 0.314 |
| I8P1 | 2.600E-03 | 5.400E-03 | 6.400E-03 |
| I8P2 | 0.264 | 0.171 | 0.114 |
| I8P3 | 1.000E-04 | 8.000E-04 | 1.100E-03 |
| I8P4 | 0.733 | 0.823 | 0.878 |
| I8P5 | 0.659 | 0.956 | 1.33 |
| I8P6 | 1.200E-02 | 0.117 | 0.292 |
| I8P7 | 0.000 | 0.000 | 9.000E-04 |
| I8P8 | 6.170E-02 | 0.260 | 0.536 |
| I8P9 | 0.620 | 0.747 | 0.816 |
| I8PA | 0.114 | 7.760E-02 | 3.730E-02 |

(continued)

Table B-3 (concluded)

| Name | Values | | |
|---|---|---|---|
| | 270 K | 300 K | 330 K |
| I8PB | 0.585 | 0.578 | 0.511 |
| I8PC | 0.704 | 0.446 | 0.116 |
| I8XP6 | 2.720E-02 | 0.175 | 0.357 |
| I8XP7 | 0.000 | 0.000 | 1.200E-03 |
| I8XP8 | 8.680E-02 | 0.339 | 0.623 |
| I8XP9 | 0.750 | 0.883 | 0.925 |
| I8XPA | 0.250 | 0.115 | 4.350E-02 |
| I8XPB | 0.694 | 0.644 | 0.564 |
| I8XPC | 0.994 | 0.476 | 0.000 |

Table B-4. Chamber-Dependent Parameters and Rate Constants Used in the Model Simulations of the Experiments Carried Out in the SAPRC Indoor Teflon Chamber (ITC) and in the SAPRC Outdoor Teflon Chamber (OTC). [See Table B-1 for chamber-dependent reactions and use of chamber-dependent parameters. Unless indicated otherwise, values from Carter et al. (1986)]

| Parameter or Reaction Label | Value | |
|---|---|---|
| | ITC | OTC |
| **Parameters** | | |
| RS-I | 3.0E-4 | 2.0E-4[a] |
| RS-S | 0.0 | 0.0 |
| YHONO | 0.2 | 0.2 |
| 1-YHONO | 0.8 | 0.8 |
| E-NO2/K1 | 1.5E-4 | 1.0E-4 |
| **First Order Rate Constants ($min^{-1}$)** | | |
| O3W | 1.3E-4 | 1.67E-4 |
| N25I | 2.5E-3 | 1.6E-3 |
| NO2W | 1.4E-4 | 9.0E-5 |
| **Second Order Rate Constants ($ppm^{-1}$ $min^{-1}$)** | | |
| N25S | 5.0E-8 | 3.0E-8 |
| **Dilution Rate ($min^{-1}$)** | | |
| Dilution | 3.9E-4[b] | 0.0 |

[a] Carter et al. (1986) used RS-I = $3.0 \times 10^{-4}$. This lower value is more consistent with the results of the tracer-$NO_x$-air irradiations carried out in this program (see Section IV-A-1).

[b] Adjusted to fit concentration-time profiles for n-butane in the ITC surrogate-$NO_x$-air runs. Carter et al. (1986) assumed no dilution in the ITC.

Table B-5. Absorption Coefficient x Quantum Yield Products used to Calculate the Rate Constants for Photolysis Reactions in Table B-1 (From Carter et al. 1986)

| PHOT. Name | (Wavelength, Absorption Coefficient x Quantum Yield) (microns) ($cm^2$ $molec^{-1}$, base e) | | |
|---|---|---|---|
| NO2 | (0.250 2.830E-20) | (0.255 1.450E-20) | (0.260 1.900E-20) |
| | (0.265 2.010E-20) | (0.270 3.130E-20) | (0.275 4.020E-20) |
| | (0.280 5.540E-20) | (0.285 6.990E-20) | (0.290 8.180E-20) |
| | (0.295 6.970E-20) | (0.300 1.156E-19) | (0.305 1.619E-19) |
| | (0.310 1.695E-19) | (0.315 2.137E-19) | (0.320 2.383E-19) |
| | (0.325 2.581E-19) | (0.330 2.730E-19) | (0.335 3.105E-19) |
| | (0.340 3.445E-19) | (0.345 3.561E-19) | (0.350 3.538E-19) |
| | (0.355 4.361E-19) | (0.360 3.779E-19) | (0.365 4.768E-19) |
| | (0.370 4.406E-19) | (0.375 3.906E-19) | (0.380 4.852E-19) |
| | (0.385 4.158E-19) | (0.390 4.440E-19) | (0.395 4.771E-19) |
| | (0.400 4.394E-19) | (0.405 2.022E-19) | (0.410 8.078E-20) |
| | (0.415 4.221E-20) | (0.420 1.433E-20) | (0.425 0.000E-01) |
| NO3NO | (0.585 0.000E-01) | (0.590 1.285E-18) | (0.595 1.632E-18) |
| | (0.600 7.075E-19) | (0.605 6.900E-19) | (0.610 2.960E-19) |
| | (0.615 1.960E-19) | (0.620 3.580E-19) | (0.625 4.625E-19) |
| | (0.630 2.830E-19) | (0.635 4.350E-20) | (0.640 0.000E-01) |
| NO3NO2 | (0.400 0.000E-01) | (0.405 3.000E-20) | (0.410 4.000E-20) |
| | (0.415 5.000E-20) | (0.420 8.000E-20) | (0.425 1.000E-19) |
| | (0.430 1.300E-19) | (0.435 1.800E-19) | (0.440 1.900E-19) |
| | (0.445 2.200E-19) | (0.450 2.800E-19) | (0.455 3.300E-19) |
| | (0.460 3.700E-19) | (0.465 4.300E-19) | (0.470 5.100E-19) |
| | (0.475 6.000E-19) | (0.480 6.400E-19) | (0.485 6.900E-19) |
| | (0.490 8.800E-19) | (0.495 9.500E-19) | (0.500 1.010E-18) |
| | (0.505 1.100E-18) | (0.510 1.320E-18) | (0.515 1.400E-18) |
| | (0.520 1.450E-18) | (0.525 1.480E-18) | (0.530 1.940E-18) |
| | (0.535 2.040E-18) | (0.540 1.810E-18) | (0.545 1.810E-18) |
| | (0.550 2.360E-18) | (0.555 2.680E-18) | (0.560 3.070E-18) |
| | (0.565 2.530E-18) | (0.570 2.540E-18) | (0.575 2.740E-18) |
| | (0.580 3.050E-18) | (0.585 2.770E-18) | (0.590 3.855E-18) |
| | (0.595 2.448E-18) | (0.600 1.556E-18) | (0.605 1.380E-18) |
| | (0.610 4.350E-19) | (0.615 4.900E-19) | (0.620 7.160E-19) |
| | (0.625 1.388E-18) | (0.630 2.830E-19) | (0.635 0.000E-01) |
| O3O3P | (0.260 1.070E-08) | (0.270 7.740E-19) | (0.280 3.790E-19) |
| | (0.290 1.340E-19) | (0.300 3.160E-20) | (0.310 4.341E-20) |
| | (0.320 2.600E-20) | (0.330 6.700E-21) | (0.340 1.700E-21) |
| | (0.350 4.000E-22) | (0.355 0.000E-01) | (0.400 0.000E-01) |
| | (0.450 1.600E-22) | (0.500 1.340E-21) | (0.550 3.320E-21) |
| | (0.600 5.060E-21) | (0.650 2.450E-21) | (0.700 8.700E-22) |
| | (0.750 3.200E-22) | (0.800 1.600E-22) | (0.900 0.000E-01) |

(continued)

Table B-5 (continued) - 2

| PHOT. Name | (Wavelength, (microns) | Absorption Coefficient x Quantum Yield) ($cm^2$ $molec^{-1}$, base e) | |
|---|---|---|---|
| O3T270 | (0.260 9.630E-18) | (0.270 6.966E-18) | (0.280 3.411E-18) |
| | (0.290 1.206E-18) | (0.300 3.420E-19) | (0.305 1.617E-19) |
| | (0.310 4.508E-20) | (0.313 1.200E-20) | (0.315 3.640E-21) |
| | (0.317 1.248E-21) | (0.320 0.000E-01) | |
| O3T300 | (0.260 9.630E-18) | (0.270 6.966E-18) | (0.280 3.411E-18) |
| | (0.290 1.206E-18) | (0.300 3.420E-19) | (0.305 1.673E-19) |
| | (0.310 5.488E-20) | (0.313 1.950E-20) | (0.315 6.760E-21) |
| | (0.317 2.080E-21) | (0.320 0.000E-01) | |
| O3T330 | (0.260 9.630E-18) | (0.270 6.966E-18) | (0.280 3.411E-18) |
| | (0.290 1.206E-18) | (0.300 3.420E-19) | (0.305 1.692E-19) |
| | (0.310 6.174E-20) | (0.313 2.700E-20) | (0.315 1.144E-20) |
| | (0.317 4.992E-21) | (0.320 7.800E-22) | (0.322 0.000E-01) |
| HONO | (0.311 0.000E-01) | (0.312 2.000E-21) | (0.313 4.200E-21) |
| | (0.314 4.600E-21) | (0.315 4.200E-21) | (0.316 3.000E-21) |
| | (0.317 4.600E-21) | (0.318 3.600E-20) | (0.319 6.100E-20) |
| | (0.320 2.100E-20) | (0.321 4.270E-20) | (0.322 4.010E-20) |
| | (0.323 3.930E-20) | (0.324 4.010E-20) | (0.325 4.040E-20) |
| | (0.326 3.130E-20) | (0.327 4.120E-20) | (0.328 7.550E-20) |
| | (0.329 6.640E-20) | (0.330 7.290E-20) | (0.331 8.700E-20) |
| | (0.332 1.380E-19) | (0.333 5.910E-20) | (0.334 5.910E-20) |
| | (0.335 6.450E-20) | (0.336 5.910E-20) | (0.337 4.580E-20) |
| | (0.338 1.910E-19) | (0.339 1.630E-19) | (0.340 1.050E-19) |
| | (0.341 8.700E-20) | (0.342 3.350E-19) | (0.343 2.010E-19) |
| | (0.344 1.020E-19) | (0.345 8.540E-20) | (0.346 8.320E-20) |
| | (0.347 8.200E-20) | (0.348 7.490E-20) | (0.349 7.130E-20) |
| | (0.350 6.830E-20) | (0.351 1.740E-19) | (0.352 1.140E-19) |
| | (0.353 3.710E-19) | (0.354 4.960E-19) | (0.355 2.460E-19) |
| | (0.356 1.190E-19) | (0.357 9.350E-20) | (0.358 7.780E-20) |
| | (0.359 7.290E-20) | (0.360 6.830E-20) | (0.361 6.900E-20) |
| | (0.362 7.320E-20) | (0.363 9.000E-20) | (0.364 1.210E-19) |
| | (0.365 1.330E-19) | (0.366 2.130E-19) | (0.367 3.520E-19) |
| | (0.368 4.500E-19) | (0.369 2.930E-19) | (0.370 1.190E-19) |
| | (0.371 9.460E-20) | (0.372 8.850E-20) | (0.373 7.440E-20) |
| | (0.374 4.770E-20) | (0.375 2.700E-20) | (0.376 1.900E-20) |
| | (0.377 1.500E-20) | (0.378 1.900E-20) | (0.379 5.800E-20) |
| | (0.380 7.780E-20) | (0.381 1.140E-19) | (0.382 1.400E-19) |
| | (0.383 1.720E-19) | (0.384 1.990E-19) | (0.385 1.900E-19) |
| | (0.386 1.190E-19) | (0.387 5.650E-20) | (0.388 3.200E-20) |
| | (0.389 1.900E-20) | (0.390 1.200E-20) | (0.391 5.000E-21) |
| | (0.392 0.000E-01) | | |

(continued)

Table B-5 (continued) - 3

| PHOT. Name | (Wavelength, (microns) | Absorption Coefficient x Quantum Yield) ($cm^2$ $molec^{-1}$, base e) | |
|---|---|---|---|
| H2O2 | (0.250 8.300E-20) | (0.255 6.700E-20) | (0.260 5.200E-20) |
| | (0.265 4.200E-20) | (0.270 3.200E-20) | (0.275 2.500E-20) |
| | (0.280 2.000E-20) | (0.285 1.500E-20) | (0.290 1.130E-20) |
| | (0.295 8.700E-21) | (0.300 6.600E-21) | (0.305 4.900E-21) |
| | (0.310 3.700E-21) | (0.315 2.800E-21) | (0.320 2.000E-21) |
| | (0.325 1.500E-21) | (0.330 1.200E-21) | (0.335 9.000E-22) |
| | (0.340 7.000E-22) | (0.345 5.000E-22) | (0.350 3.000E-22) |
| | (0.355 0.000E-01) | | |
| CO2H | (0.210 3.750E-19) | (0.220 2.200E-19) | (0.230 1.380E-19) |
| | (0.240 8.800E-20) | (0.250 5.800E-20) | (0.260 3.800E-20) |
| | (0.270 2.500E-20) | (0.280 1.500E-20) | (0.290 9.000E-21) |
| | (0.300 5.800E-21) | (0.310 3.400E-21) | (0.320 1.900E-21) |
| | (0.330 1.100E-21) | (0.340 6.000E-22) | (0.350 4.000E-22) |
| | (0.360 0.000E-01) | | |
| HCHOR | (0.240 6.300E-23) | (0.250 3.120E-22) | (0.260 1.410E-21) |
| | (0.270 3.440E-21) | (0.280 1.097E-20) | (0.290 1.782E-20) |
| | (0.300 2.044E-20) | (0.310 1.886E-20) | (0.320 1.147E-20) |
| | (0.330 5.456E-21) | (0.340 0.000E-01) | |
| HCHOM | (0.240 1.260E-22) | (0.250 5.980E-22) | (0.260 2.256E-21) |
| | (0.270 3.956E-21) | (0.280 6.510E-21) | (0.290 6.526E-21) |
| | (0.300 5.764E-21) | (0.310 5.635E-21) | (0.320 7.030E-21) |
| | (0.330 1.214E-20) | (0.340 8.142E-21) | (0.350 1.680E-21) |
| | (0.360 7.200E-23) | (0.370 0.000E-01) | |
| CCHOR | (0.260 6.696E-21) | (0.270 1.315E-20) | (0.280 2.549E-20) |
| | (0.290 2.618E-20) | (0.295 2.181E-20) | (0.300 1.672E-20) |
| | (0.305 1.111E-20) | (0.310 6.392E-21) | (0.315 3.135E-21) |
| | (0.320 1.200E-21) | (0.325 3.390E-22) | (0.330 0.000E-01) |
| RCHO | (0.280 5.260E-20) | (0.290 5.770E-20) | (0.300 5.050E-20) |
| | (0.310 3.680E-20) | (0.320 1.660E-20) | (0.330 6.490E-21) |
| | (0.340 1.440E-21) | (0.345 0.000E-01) | |
| KETONE | (0.210 1.100E-21) | (0.220 1.200E-21) | (0.230 4.600E-21) |
| | (0.240 1.300E-20) | (0.250 2.680E-20) | (0.260 4.210E-20) |
| | (0.270 5.540E-20) | (0.280 5.920E-20) | (0.290 5.160E-20) |
| | (0.300 3.440E-20) | (0.310 1.530E-20) | (0.320 4.600E-21) |
| | (0.330 1.100E-21) | (0.340 0.000E-01) | |

(continued)

Table B-5 (continued) - 4

| PHOT. Name | (Wavelength, (microns) | Absorption Coefficient x Quantum Yield) ($cm^2$ $molec^{-1}$, base e) | |
|---|---|---|---|
| GLYOXAL | (0.230 2.867E-21) | (0.235 2.867E-21) | (0.240 4.301E-21) |
| | (0.245 5.735E-21) | (0.250 8.602E-21) | (0.255 1.147E-20) |
| | (0.260 1.434E-20) | (0.265 1.864E-20) | (0.270 2.294E-20) |
| | (0.275 2.581E-20) | (0.280 2.867E-20) | (0.285 3.298E-20) |
| | (0.290 3.154E-20) | (0.295 3.298E-20) | (0.300 3.584E-20) |
| | (0.305 2.724E-20) | (0.310 2.724E-20) | (0.312 2.867E-20) |
| | (0.315 2.294E-20) | (0.320 1.434E-20) | (0.325 1.147E-20) |
| | (0.327 1.434E-20) | (0.330 1.147E-20) | (0.335 2.867E-21) |
| | (0.340 0.000E-01) | (0.355 0.000E-01) | (0.360 2.294E-21) |
| | (0.365 2.867E-21) | (0.370 8.029E-21) | (0.375 1.004E-20) |
| | (0.380 1.720E-20) | (0.382 1.577E-20) | (0.384 1.491E-20) |
| | (0.386 1.491E-20) | (0.388 2.867E-20) | (0.390 3.154E-20) |
| | (0.391 3.242E-20) | (0.392 3.040E-20) | (0.393 2.229E-20) |
| | (0.394 2.634E-20) | (0.395 3.040E-20) | (0.396 2.634E-20) |
| | (0.397 2.432E-20) | (0.398 3.242E-20) | (0.399 3.040E-20) |
| | (0.400 2.837E-20) | (0.401 3.242E-20) | (0.402 4.458E-20) |
| | (0.403 5.269E-20) | (0.404 4.255E-20) | (0.405 3.040E-20) |
| | (0.406 3.040E-20) | (0.407 2.837E-20) | (0.408 2.432E-20) |
| | (0.409 2.837E-20) | (0.410 6.079E-20) | (0.411 5.066E-20) |
| | (0.412 6.079E-20) | (0.412 4.863E-20) | (0.413 8.308E-20) |
| | (0.414 6.484E-20) | (0.414 7.497E-20) | (0.414 8.105E-20) |
| | (0.415 8.105E-20) | (0.415 6.890E-20) | (0.416 4.255E-20) |
| | (0.417 4.863E-20) | (0.418 5.876E-20) | (0.419 6.687E-20) |
| | (0.420 3.850E-20) | (0.421 5.674E-20) | (0.421 4.458E-20) |
| | (0.422 5.269E-20) | (0.423 1.054E-19) | (0.423 8.511E-20) |
| | (0.424 6.079E-20) | (0.425 7.295E-20) | (0.426 1.175E-19) |
| | (0.426 1.297E-19) | (0.427 1.074E-19) | (0.428 1.662E-19) |
| | (0.429 4.053E-20) | (0.430 5.066E-20) | (0.431 4.863E-20) |
| | (0.432 4.053E-20) | (0.433 3.647E-20) | (0.434 4.053E-20) |
| | (0.435 6.079E-20) | (0.435 5.066E-20) | (0.436 8.105E-20) |
| | (0.437 1.135E-19) | (0.437 5.269E-20) | (0.438 1.013E-19) |
| | (0.438 1.378E-19) | (0.439 7.700E-20) | (0.440 2.472E-19) |
| | (0.441 8.105E-20) | (0.442 6.079E-20) | (0.443 7.497E-20) |
| | (0.444 9.321E-20) | (0.445 1.135E-19) | (0.446 5.269E-20) |
| | (0.447 2.432E-20) | (0.448 2.837E-20) | (0.449 3.850E-20) |
| | (0.450 6.079E-20) | (0.451 1.094E-19) | (0.451 9.321E-20) |
| | (0.452 1.216E-19) | (0.453 2.391E-19) | (0.454 1.702E-19) |
| | (0.455 3.404E-19) | (0.456 4.053E-19) | (0.456 1.013E-19) |
| | (0.457 1.621E-20) | (0.458 1.216E-20) | (0.458 1.418E-20) |
| | (0.459 4.053E-21) | (0.460 4.053E-21) | (0.461 6.079E-21) |
| | (0.461 2.026E-21) | (0.462 0.000E-01) | |

(continued)

Table B-5 (concluded) - 5

| PHOT. Name | (Wavelength, (microns) | Absorption Coefficient x Quantum Yield) ($cm^2$ $molec^{-1}$, base e) | |
|---|---|---|---|
| MEGLYOX | (0.220 2.103E-21) | (0.225 2.103E-21) | (0.230 4.206E-21) |
| | (0.235 7.570E-21) | (0.240 9.252E-21) | (0.245 8.411E-21) |
| | (0.250 9.252E-21) | (0.255 9.252E-21) | (0.260 9.673E-21) |
| | (0.265 1.051E-20) | (0.270 1.262E-20) | (0.275 1.430E-20) |
| | (0.280 1.514E-20) | (0.285 1.430E-20) | (0.290 1.472E-20) |
| | (0.295 1.178E-20) | (0.300 1.136E-20) | (0.305 9.252E-21) |
| | (0.310 6.308E-21) | (0.315 5.467E-21) | (0.320 3.365E-21) |
| | (0.325 1.682E-21) | (0.330 8.411E-22) | (0.335 0.000E-01) |
| | (0.350 0.000E-01) | (0.354 4.206E-22) | (0.358 1.262E-21) |
| | (0.360 2.103E-21) | (0.362 2.103E-21) | (0.364 2.944E-21) |
| | (0.366 3.365E-21) | (0.368 4.206E-21) | (0.370 5.467E-21) |
| | (0.372 5.888E-21) | (0.374 7.570E-21) | (0.376 7.991E-21) |
| | (0.378 8.832E-21) | (0.380 1.009E-20) | (0.382 1.093E-20) |
| | (0.384 1.346E-20) | (0.386 1.514E-20) | (0.388 1.724E-20) |
| | (0.390 2.061E-20) | (0.392 2.103E-20) | (0.394 2.313E-20) |
| | (0.396 2.481E-20) | (0.398 2.607E-20) | (0.400 2.776E-20) |
| | (0.402 2.986E-20) | (0.404 3.196E-20) | (0.406 3.785E-20) |
| | (0.408 3.953E-20) | (0.410 4.332E-20) | (0.412 4.710E-20) |
| | (0.414 4.794E-20) | (0.416 4.879E-20) | (0.418 5.047E-20) |
| | (0.420 5.215E-20) | (0.422 5.299E-20) | (0.424 5.173E-20) |
| | (0.426 5.299E-20) | (0.428 5.215E-20) | (0.430 5.551E-20) |
| | (0.432 5.131E-20) | (0.434 5.678E-20) | (0.436 6.224E-20) |
| | (0.438 6.056E-20) | (0.440 5.467E-20) | (0.441 6.140E-20) |
| | (0.442 5.467E-20) | (0.443 5.551E-20) | (0.433 6.813E-20) |
| | (0.444 5.972E-20) | (0.445 5.131E-20) | (0.446 4.879E-20) |
| | (0.447 5.720E-20) | (0.448 5.467E-20) | (0.449 6.561E-20) |
| | (0.450 5.047E-20) | (0.451 3.028E-20) | (0.452 4.290E-20) |
| | (0.453 2.776E-20) | (0.454 2.271E-20) | (0.456 1.766E-20) |
| | (0.458 8.411E-21) | (0.460 4.206E-21) | (0.464 1.682E-21) |
| | (0.468 0.000E-01) | | |
| BZCHO | (0.299 1.776E-19) | (0.304 7.400E-20) | (0.306 6.910E-20) |
| | (0.309 6.410E-20) | (0.313 6.910E-20) | (0.314 6.910E-20) |
| | (0.318 6.410E-20) | (0.325 8.390E-20) | (0.332 7.650E-20) |
| | (0.338 8.880E-20) | (0.342 8.880E-20) | (0.346 7.890E-20) |
| | (0.349 7.890E-20) | (0.354 9.130E-20) | (0.355 8.140E-20) |
| | (0.364 5.670E-20) | (0.368 6.660E-20) | (0.369 8.390E-20) |
| | (0.370 8.390E-20) | (0.372 3.450E-20) | (0.374 3.210E-20) |
| | (0.376 2.470E-20) | (0.377 2.470E-20) | (0.380 3.580E-20) |
| | (0.382 9.900E-21) | (0.386 0.000E-01) | |
| AROMUNKN | (0.200 3.950E-20) | (0.350 3.950E-20) | (0.360 0.000E-01) |

Table B-6. Photolysis Rate Constants (in $min^{-1}$) Calculated for the Indoor Teflon Chamber (ITC), and for Sunlight at Zenith Angles of 0, 40, and 70 Degrees. Solar Photolysis Rate Constants are Calculated Theoretically for Ground Level and Clear Sky Conditions Using the Actinic Irradiances Given by Peterson (1976) Based on his "Best Estimate" Surface Albitos. (See Table B-1 for the reactions which correspond to these "PHOT. Names")

| PHOT. Name | ITC | Z=0 | Z=40 | Z=70 |
|---|---|---|---|---|
| NO2 | 0.3260 | 0.4619 | 0.3946 | 0.1855 |
| NO3NO | 0.0000 | 1.118 | 1.029 | 0.6644 |
| NO3NO2 | 1.1776E-02 | 10.14 | 9.311 | 5.915 |
| O3O3P | 1.6373E-03 | 2.9380E-02 | 2.6338E-02 | 1.6042E-02 |
| O3T270 | 3.4314E-04 | 2.0321E-03 | 1.0628E-03 | 9.5582E-05 |
| O3T300 | 3.9694E-04 | 2.2697E-03 | 1.2161E-03 | 1.1924E-04 |
| O3T330 | 4.6054E-04 | 2.5105E-03 | 1.3787E-03 | 1.4906E-04 |
| HONO | 0.1055 | 9.7642E-02 | 8.2603E-02 | 3.6946E-02 |
| H2O2 | 2.8281E-04 | 4.5195E-04 | 3.3642E-04 | 1.0193E-04 |
| CO2H | 2.9522E-04 | 4.4349E-04 | 3.3226E-04 | 1.0283E-04 |
| HCHOR | 7.5997E-04 | 1.8149E-03 | 1.3221E-03 | 3.5913E-04 |
| HCHOM | 2.4099E-03 | 2.7772E-03 | 2.2047E-03 | 7.9088E-04 |
| CCHOR | 7.0030E-05 | 2.9228E-04 | 1.8542E-04 | 3.2337E-05 |
| RCHO | 1.2148E-03 | 2.9553E-03 | 2.1135E-03 | 5.4935E-04 |
| KETONE | 3.0027E-04 | 9.5019E-04 | 6.4249E-04 | 1.4140E-04 |
| GLYOXAL1 | 1.1788E-03 | 2.7739E-03 | 2.0258E-03 | 5.5661E-04 |
| GLYOXAL2 | 1.0652E-02 | 0.1334 | 0.1199 | 6.8909E-02 |
| MEGLYOX | 7.7464E-03 | 7.9919E-02 | 7.1566E-02 | 4.0538E-02 |
| BZCHO | 5.5070E-02 | 5.1595E-02 | 4.2403E-02 | 1.7385E-02 |
| AROMUNKN | 1.6263E-02 | 1.5856E-02 | 1.2659E-02 | 4.6825E-03 |

# APPENDIX C

## COMPUTER TAPE CONTAINING RESULTS OF THE CHAMBER EXPERIMENTS

The results of all of the indoor and outdoor environmental chamber experiments successfully completed in this program are available on magnetic tape in computer-readable format. The format of the data on this tape, and descriptions of the data sets on the tape are given in this Appendix. This tape was submitted to the California Air Resources Board along with this report, and copies of this tape are available from SAPRC for handling and distribution costs. Requests for copies of this tape should be addressed to:

Dr. William P. L. Carter
Statewide Air Pollution Research Center
University of California
Riverside, CA 92521

The computer tape has a data density of 1600 BPI, uses ASCII character format, and has a maximum blocksize of 5280 bytes. The tape contains a total of 149 files, of three different types. File 1, which has a logical record length of 80 bytes, is the same as Table C-1 in this Appendix, which contains the complete list of run numbers, run types, and file numbers for the chamber runs carried out in this program. Files 2 through 75, which have logical record lengths of 132 bytes, consist of "printout images" of the tabulated data formatted in a manner most suitable for obtaining hard copy printouts for manual inspection. A description of the data contained in these "printout" files is given in Section 1, below. Files 76 through 149, which have logical record lengths of 80 bytes, contain the data in a compressed format which is more suitable for being read by computer programs for purposes of, for example, data manipulation or plotting. The format of these compressed data sets is described in Section 2. The data set numbers for the printout and the compressed data sets for each of the runs included on the tape are given in Table C-1.

Table C-1. Run Numbers, Run Types, and File Numbers for all Chamber Runs on the Data Tape

| Chamber and Run No. | Run Type | File Numbers[a] | |
|---|---|---|---|
| | | Printout Format | Compressed Format |
| 1. Indoor Chamber Runs | | | |
| ITC-859 | $NO_x$-Air | 2 | 76 |
| ITC-860 | Propene-$NO_x$-Air Conditioning | 3 | 77 |
| ITC-861 | $NO_x$-Air | 4 | 78 |
| ITC-862 | $NO_2$ Actinometry | (b) | |
| ITC-863 | $NO_x$-Air + Methanol | 5 | 79 |
| ITC-864 | $NO_x$-Air + Formaldehyde | 6 | 80 |
| ITC-865 | 15-B Surrogate | 7 | 81 |
| ITC-866 | $NO_x$-Air | 8 | 82 |
| ITC-867 | 15-MF Surrogate | 9 | 83 |
| ITC-868 | 15-BL Surrogate | 10 | 84 |
| ITC-869 | $NO_2$ Actinometry | (b) | |
| ITC-870 | $NO_x$-Air | 11 | 85 |
| ITC-871 | 6-B Surrogate | 12 | 86 |
| ITC-872 | 6-MF Surrogate | 13 | 87 |
| ITC-873 | 6-BL Surrogate | 14 | 88 |
| ITC-874 | 6-M Surrogate | 15 | 89 |
| ITC-875 | $NO_x$-Air | 16 | 90 |
| ITC-876 | $NO_2$ Actinometry | (b) | |
| ITC-877 | 6-MF Surrogate | 17 | 91 |
| ITC-878 | $NO_x$-Air | 18 | 92 |

(continued)

Table C-1 (continued) - 2

| Chamber and Run No. | Run Type | File Numbers[a] | |
|---|---|---|---|
| | | Printout Format | Compressed Format |
| ITC-879 | Surrogate Attempt | (c) | |
| ITC-880 | 3-B Surrogate | 19 | 93 |
| ITC-881 | 3-MF Surrogate | 20 | 94 |
| ITC-882 | $NO_x$-Air | 21 | 95 |
| ITC-883 | $NO_2$ Actinometry | (b) | |
| ITC-884 | $NO_x$-Air | 22 | 96 |
| ITC-885 | 3-BL Surrogate | 23 | 97 |
| ITC-886 | 3-MF Surrogate | 24 | 98 |
| ITC-887 | $NO_x$-Air + Methanol | 25 | 99 |
| ITC-888 | 15-M Surrogate | 26 | 100 |
| ITC-889 | $NO_x$-Air | 27 | 101 |
| ITC-890 | $NO_2$ Actinometry | (b) | |
| ITC-891 | 15-B Surrogate | 28 | 102 |
| ITC-892 | Acetaldehyde-Air | 29 | 103 |
| ITC-893 | $NO_x$-Air | 30 | 104 |
| ITC-869 | $NO_2$ Actinometry | (b) | |
| 2. Outdoor Chamber Runs | | | |
| OTC-209 | Ozone Dark Decay | 31 | 105 |
| OTC-210 | Propene-$NO_x$-Air, Undivided | 32 | 106 |
| OTC-211 | n-Butane-$NO_x$-Air, Undivided | 33 | 107 |
| OTC-212 | $NO_x$-Air, Undivided | 34 | 108 |

(continued)

Table C-1 (continued) - 3

| Chamber and Run No. | Run Type | File Numbers[a] | |
|---|---|---|---|
| | | Printout Format | Compressed Format |
| OTC-213 | Surrogate-$NO_x$-Air Conditioning | 35 | 109 |
| OTC-214 | Surrogate-$NO_x$-Air Side Equivalency Test | 36 | 110 |
| OTC-215 | 10-B-MF Surrogate | 37 | 111 |
| OTC-216 | Formaldehyde-$NO_x$-Air | 38 | 112 |
| OTC-217 | 10-B-M Surrogate | 39 | 113 |
| OTC-218 | Acetaldehyde-Air, Divided | 40 | 114 |
| OTC-219 | 7-MF-M Surrogate | 41 | 115 |
| OTC-220 | 7-MF-B Surrogate (aborted) | 42 | 116 |
| OTC-221 | 7-MF-B Surrogate | 43 | 117 |
| OTC-222 | 10-M-MF Surrogate | 44 | 118 |
| OTC-223 | 10-B-BL Surrogate | 45 | 119 |
| OTC-224 | 13-M-B Surrogate | 46 | 120 |
| OTC-225 | 5-B-MF Surrogate | 47 | 121 |
| OTC-226 | 7-B-B (side equivalency test) | 48 | 122 |
| OTC-227 | $NO_x$-Air, Divided | 49 | 123 |
| OTC-228 | 5-B-MF Surrogate | 50 | 124 |
| OTC-229 | 7-M-BL Surrogate | 51 | 125 |
| OTC-230 | 7-B-BL Surrogate | 52 | 126 |

(continued)

Table C-1 (continued) - 4

| Chamber and Run No. | Run Type | File Numbers[a] | |
|---|---|---|---|
| | | Printout Format | Compressed Format |
| OTC-231 | 7-X-MF Surrogate | 53 | 127 |
| OTC-232 | $NO_x$-Air, Divided | 54 | 128 |
| OTC-233 | Propene-$NO_x$-Air, Undivided | 55 | 129 |
| OTC-234 | Acetaldehyde-Air, Divided | 56 | 130 |
| OTC-235 | $NO_x$-Air + Formaldehyde, Divided | 57 | 131 |
| OTC-236 | Propene-$NO_x$-Air, Undivided | 58 | 132 |
| OTC-237 | 10-B-M Surrogate | 59 | 133 |
| OTC-238 | 10-BL-MF Surrogate | 60 | 134 |
| OTC-239 | 7-MF-M Surrogate | 61 | 135 |
| OTC-240 | 5-M-B Surrogate | 62 | 136 |
| OTC-241 | 13-B-MF Surrogate | 63 | 137 |
| OTC-242 | 7-M-B Surrogate | 64 | 138 |
| OTC-243 | 10-B-MF Surrogate | 65 | 139 |
| OTC-244 | Propene-$NO_x$-Air, Undivided | 66 | 140 |
| OTC-245 | $NO_x$-Air, Divided | 67 | 141 |
| OTC-246 | n-Butane-$NO_x$-Air, Divided | 68 | 142 |
| OTC-247 | Acetaldehyde-Air, Divided | 69 | 143 |
| OTC-248 | 7-B-MF Surrogate | 70 | 144 |

(continued)

Table C-1 (concluded) - 5

| Chamber and Run No. | Run Type | File Numbers[a] | |
|---|---|---|---|
| | | Printout Format | Compressed Format |
| OTC-249 | 10-B-MF Surrogate | 71 | 145 |
| OTC-250 | 10-MF-MF Surrogate | 72 | 146 |
| OTC-251 | Propene-$NO_x$-Air, Undivided | 73 | 147 |
| OTC-252 | n-Butane-$NO_x$-Air, Divided | 74 | 148 |
| OTC-253 | Ozone Dark Decay | 75 | 149 |

[a]File no. 1 consists of this table.
[b]Data for $NO_2$ actinometry runs not on tape. Results of these runs are tabulated in Table IV-8 in Section IV-A-8.
[c]Data from this aborted run was not processed.

1. Data Sets in "Printout" Format

These data sets contain tabulations of the results of the chamber experiments in a format suitable for manual inspection. If hard copies of these data sets are required, these can be printed out on any printer which can print 132 columns, has a page length of 60 lines or more, and which recognizes the "form feed" (ASCII code 12) character. Each of these "printouts" contains the following information (where applicable).

- The indoor Teflon chamber (ITC) or the outdoor Teflon chamber (OTC) run number.
- A brief run description.
- The date the run was carried out (given below the run description).
- The date the printout files was created (given in right hand corner on each page).
- Comments for the run, including experimental operations and operator's comments taken from the log book, problems encountered (if any), observations made by the operators concerning the weather (for outdoor runs), etc.
- The initial concentrations of injected reactants which were monitored.
- Lists of all instruments used in these runs. For each instrument, this list indicates the ID number (used internally at SAPRC), the label identifying the instrument on the data tabulation, and a brief description giving information identifying the instrument and/or technique.
- The data tabulations. The tabulations indicate the compound or parameter measured, the units in which the measurements are reported, and the instrument. Because of space and format limitations, the compound names frequently had to be abbreviated on the tabulations. The meanings of representative abbreviations which may not be obvious are listed in Table C-2. For each data point, the clock time and (in most cases) the elapsed time (in minutes) since the irradiation began (or since the first measurement for dark runs) are indicated.

- If any of the data are flagged (indicated by an "A", or "B", etc., immediately to the right of the value), footnotes giving the reason it is flagged appear at the end of the tabulation for the run.

Table C-2. Representative Abbreviations Used in the Data Tabulations

| Abbreviation | Meaning |
|---|---|
| NO2-UNC | $NO_2$ readings, uncorrected for interferences by organic nitrates and $HNO_3$ |
| N-C4 | n-Butane |
| I-C4 | Isobutane |
| ISO-C8 | Iso-Octane (2,2,4-trimethylpentane) |
| I-C4= | Isobutene |
| M-XYL | m-Xylene |
| C5-K-3 | 3-Pentanone (diethyl ketone) |
| C5-N-2 | 2-Pentyl nitrate |
| ACETALD | Acetaldehyde[a] |
| MEK | Methyl ethyl ketone[a] |
| PROX | Propene oxide[a] |
| BUTYRAL | Butyraldehyde[a] |
| LN C4/C3= | ln([n-butane]/[propene]), whose rate of change is used to derive OH radical concentrations[b] |
| DEW PT | Dew point (units of degrees C) |
| K1 | $k_1$, the $NO_2$ photolysis rate (units of $min^{-1}$) |
| UV RAD | UV radiometer readings (units of mW $cm^{-2}$) |

[a] Or some other compound with the same retention time on the gas chromatographic system employed.
[b] Concentration units are arbitrary; only the slope of the log is of interest.

2. Data Sets in Compressed Format

If it is desired to use the data from these experiments as input to computer programs, for purposes such as data analysis, plotting, etc, then the data sets in the "compressed" format would be more useful. These data sets consist of records in card image format, and are organized as described in Table C-3. The following points should be noted regarding these data sets:

- Because this data format is used for a number of different types of experiments at SAPRC, the records contain provisions for data values which are not used in these particular runs. These should be ignored; usually (but not always) they are zero.

- The types of data on the data sets can be categorized by (a) general information data, such as run title, date, number of instruments, comments, chambers, etc., (b) comments, (c) instrument descriptions, (d) channel parameters and (e) channel data. By "channel" we mean the set of experimental measurements which depend on time, such as ozone concentrations, temperature readings, etc.

- Channels which have data have associated with them a "time set," which is an array of the times at which the measurements for that channel were made. The time sets are stored separately from the channel data because in general more than one channel may have the same time set.

- For outdoor chamber runs, data taken when sampling the air from outside the chamber are always designated as "side 3," even if the chamber was not divided. "Side 1" and "side 2" refer to the chamber side from which the air for sampling was withdrawn, regardless of whether the chamber was divided. If no side number is given for a particular channel, the data applies to both sides (e.g., light intensity data, background measurements, etc.).

- T = 0 refers to the clock time at which the irradiation began; or, for dark runs, the time the first measurement was made.

- Some data points are "flagged" with a non-blank character (as indicated by the values in the "LFLGS" and "FLGS arrays in group 3 of Table C-3), which associates it with a comment which has the same character as its associated flag ("FLGCOM" in group 5 of Table C-3). These comments indicate problems, etc., with the "flagged" data point, or set of data points starting with the one which is flagged. If a comment

has FLGCOM = "N," the comment line is a continuation of the previous flagged comment, and the character "N" does not appear on the printouts in Volume II.

Table C-3. Organization of the Compressed Data Files for Chamber Runs

| Record | Column | Format[a] | Name | Description |
|---|---|---|---|---|
| Group 1. Four Records. General Information | | | | |
| 1 | 1-7 | (1X,I6) | IRUNID | Run number + 10000 x chamber number (chamber numbers: 2 = ITC, 4 = OTC) |
| | 8-13 | (I6) | FORM | File format; always 1. |
| | 14-29 | (A16) | UPDRUN | Date of last update (internal SAPRC use) |
| | 30-69 | (A40) | TITLE | Run title |
| | 70-77 | (A8) | DATE(1) | First half of run date |
| 2 | 1-9 | (1X,A8) | DATE(2) | Second half of run date |
| | 10-25 | (I6) | TZERO | Clock time at T = 0 |
| | 16-21 | (I6) | PSTPDT | 1 for PST, 2 for PDT |
| | 22-39 | (3I6) | - | (Ignore) |
| | 40-45 | (I6) | BAGNO | ITC or OTC reaction bag number (If zero, bag number is not specified) |
| | 46-78 | (3G11.4) | - | (Ignore) |
| 3 | 1-57 | (1X,6E11.4) | - | (Ignore) |
| | 50-64 | (I7) | - | (Ignore - should be zero) |
| | 65-70 | (I6) | NSIDES | Number of sides if chamber is divided (Note: "Side 3" always refers to ambient air outside chamber.) |
| 4 | 1-7 | (1X,I6) | NTS | Number of time sets |
| | 8-13 | (I6) | NCHN | Number of channels |
| | 14-19 | (I6) | - | (Ignore - should be zero) |
| | 20-25 | (I6) | NINS | Number or instruments |
| | 26-31 | (I6) | NCOMS | Number of comments |
| | 32-37 | (I6) | - | (Ignore) |
| | 38-48 | (E11.4) | - | (Ignore) |
| | 49-54 | (I6) | - | (Ignore) |
| Group 2. One Set of One or More Records for Each of the NTS Time Sets | | | | |
| 1 | 1-7 | (1X,I6) | NPTS | Number of points in this time set |
| | 8-73 | (11I6) | TIMES | Clock times + 10000 x day number. (Day number: 0 = first day, 1 = second day, etc. E.G., 10930 = 9:30 AM on day 2 of the run.) |

(continued)

Table C-3 (continued) - 2

| Record | Column | Format[a] | Name | Description |
|---|---|---|---|---|
| 2+ | 1-73 | (1X,12I6) | TIMES | Rest of clock times. (No records of this type if NPTS ≤11.) |
| Group 3. | One Set of Three or More Records for Each of the NCHN Data Channels | | | |
| 1 | 1-7 | (1X,I6) | ID1 | Data type identification number (internal SAPRC use). |
| | 8-13 | (I6) | INST | Instrument number - i.e., record number in group 4 that describes the instrument used for this channel. (0 = instrument undefined) |
| | 14-19 | (I6) | SIDE | Side number (3 = outside). Ignore if NSIDES = 0 or 1. |
| | 20-25 | (I6) | TIMSET | Time set number. (If TIMSET = 0, there are no data for this channel.) |
| | 26-31 | (I6) | NP | Number of data points (ignore if TIMSET = 0) |
| | 32-37 | (I6) | NF | Number of flagged data points (Ignore if TIMSET = 0) |
| | 38-67 | (5I6) | - | (Ignore) |
| | 68-73 | (I6) | PRTORD | If >0, determines order channel appears on printouts - lower number printed first. If PRTORD = -1, channel is not printed. If PRTORD is -2, the data for this channel are printed out separately at the end. |
| | 74-79 | (I6) | DIG | (DIG-2) = number of digits to the right of the decimal point that appears on printouts. If DIG = ≥0 or ≤7, data prints out in exponential notation. |
| 2 | 1-7 | (1X,I6) | UNTS | Code number for units of data: 1 = ppm, 2 = degree C, 7 = $mw\text{-}cm^{-2}$, 8 = blank (no units), 9 = ppmC, 10 = ppb, 11 = degree F, 14 = "raw data," 17 = $min^{-1}$. |
| | 8-19 | (2I6) | - | (Ignore) |

(continued)

Table C-3 (continued) - 3

| Record | Column | Format[a] | Name | Description |
|---|---|---|---|---|
| | 20-41 | (2E11.4) | FAC,ZERO | Factor and zero corrections. Data values = factor x (raw data - zero) (Note however that data values stored on the data sets are already calculated, so these quantities can be ignored.) |
| | 42-52 | (E11.4) | - | (Ignore) |
| | 53-63 | (E11.4) | CONCØ | Initial concentration (if SDEV, below, <0) or average (if SDEV ≥0) to appear at the start of the printouts. If CONCØ = -9.9999E+9, initial concentration or average is not used. If CONCØ = -9.9999E+9, it needs to be calculated from the data. |
| | 64-74 | (E11.4) | SDEV | If SDEV <0, CONCØ is an initial concentration. If SDEV = -1, the initial concentration was assigned; if SDEV = -9.9999E+9, the data value at T = 0 is used as the initial concentration. If SDEV ≥0, CONCØ is the average of the data, and SDEV is the (1σ) standard deviation. If SDEV = 9.999E+9, the standard deviation is unknown. |
| 3 | 1-9 | (1X,A8) | NAME | Channel name |
| 4+ | 1-78 | (1X,7E11.4) | DATA | The data values. As many records as needed for the NP values. A data value of 9.9999E+9 means no data is available for that time point. No records if TIMSET = 0. |
| 5+ | 1-73 | (1X,9(I6,A2)) | LFLCS, FLGS | For each of the NF flagged data points, LFLGS is the index number for the point, and the first byte of FLGS is the flag character. As many records as needed for the NF values; no record if NF = 0. |

(continued)

Table C-3 (concluded) - 4

| Record | Column | Format[a] | Name | Description |
|---|---|---|---|---|
| Group 4. One Record for Each of the NINS Instruments | | | | |
| 1 | 1-7 | (1X,I6) | INSCOD | Instrument code number |
| | 7-19 | (6A2) | - | (Ignore) |
| | 20-27 | (A8) | INSLBL | Instrument label |
| | 28-67 | (A40) | INSDSC | Instrument description |
| | 68-78 | (E11.4) | - | (Ignore) |
| Group 5. One Record for Each of the NCOMS Comments | | | | |
| 1 | 1-3 | (2X,A1) | FLGCOM | If blank, the comment appears on the first page of the printouts. If not blank, the comment is a footnote which is printed along with the first byte of FLGCOM at the end of the printout. |
| | 4-80 | (A77) | COMENT | The comment line |

[a]FORTRAN format code.