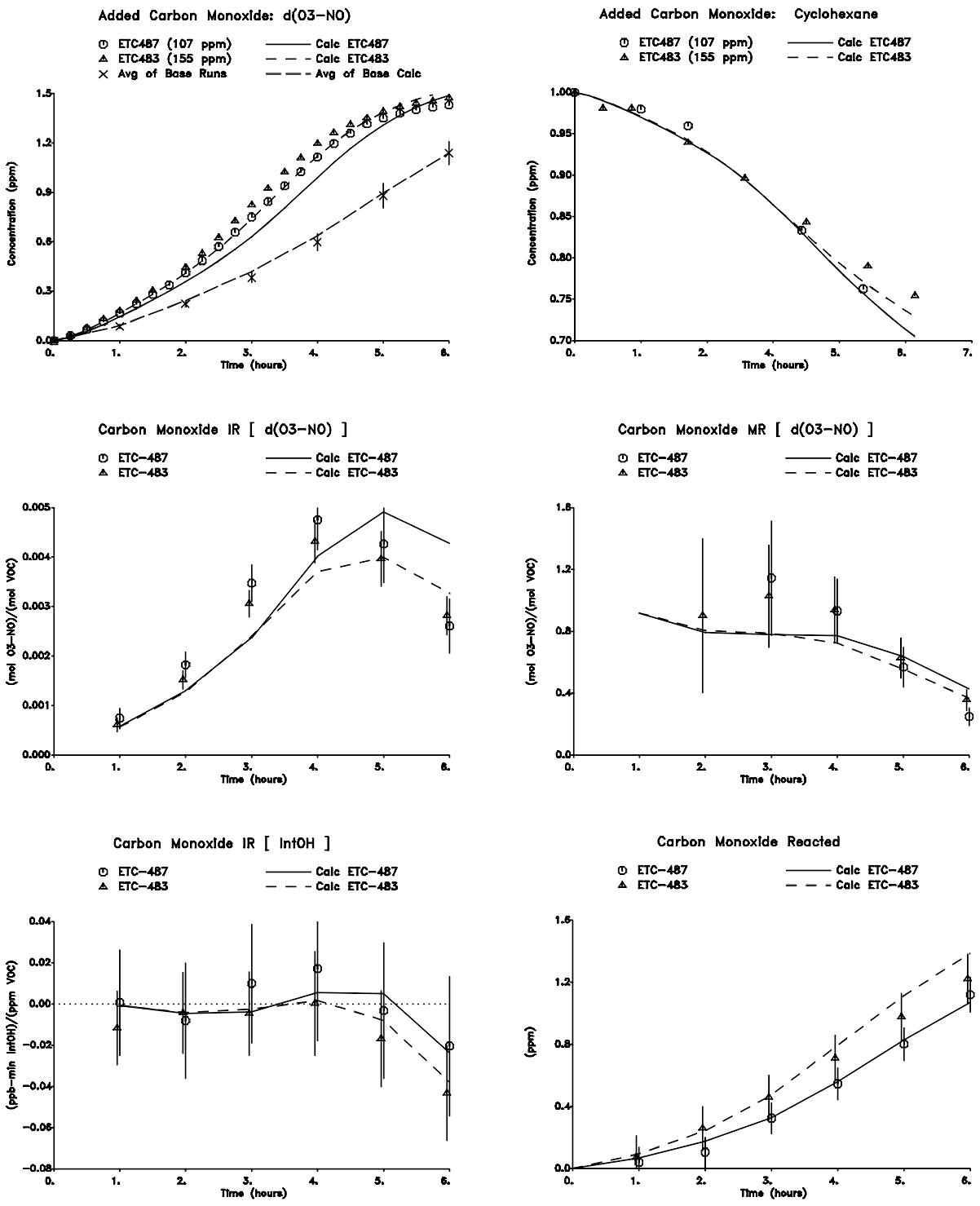

Figure 15. Plots of selected results of ethene surrogate reactivity experiments for **carbon monoxide**

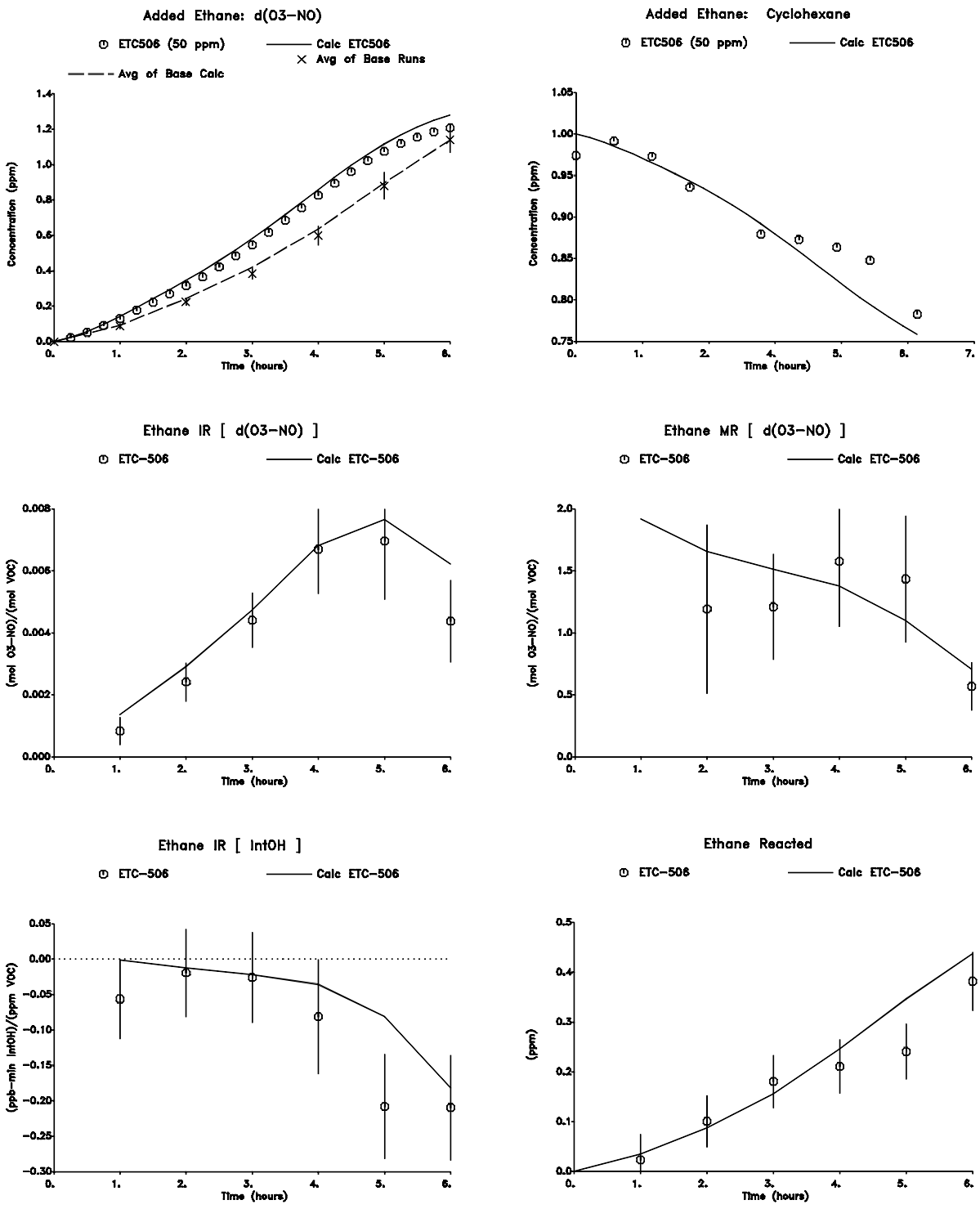

Figure 16. Plots of selected results of ethene surrogate reactivity experiments for **Ethane.**

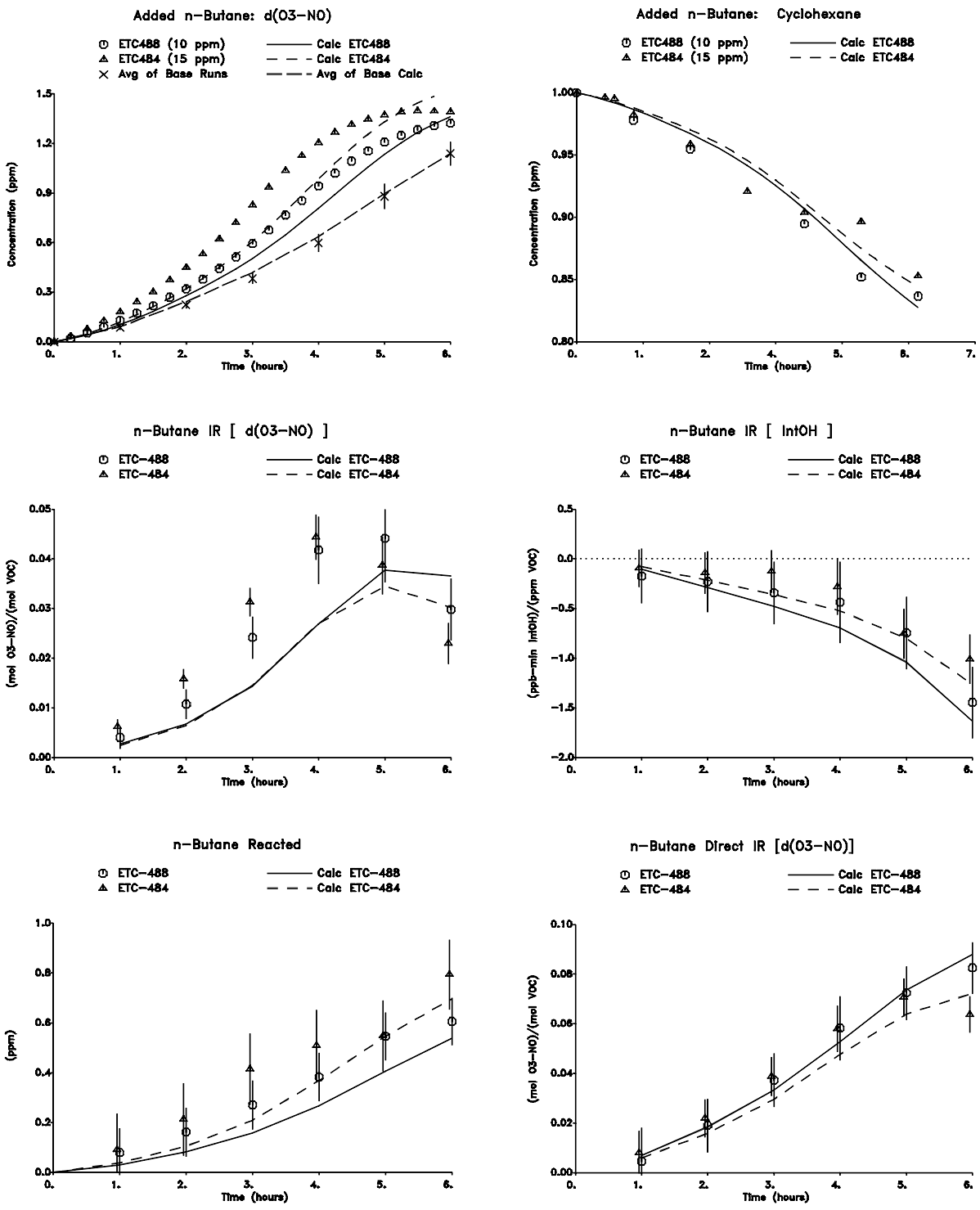

Figure 17. Plots of selected results of ethene surrogate reactivity experiments for **n-Butane**

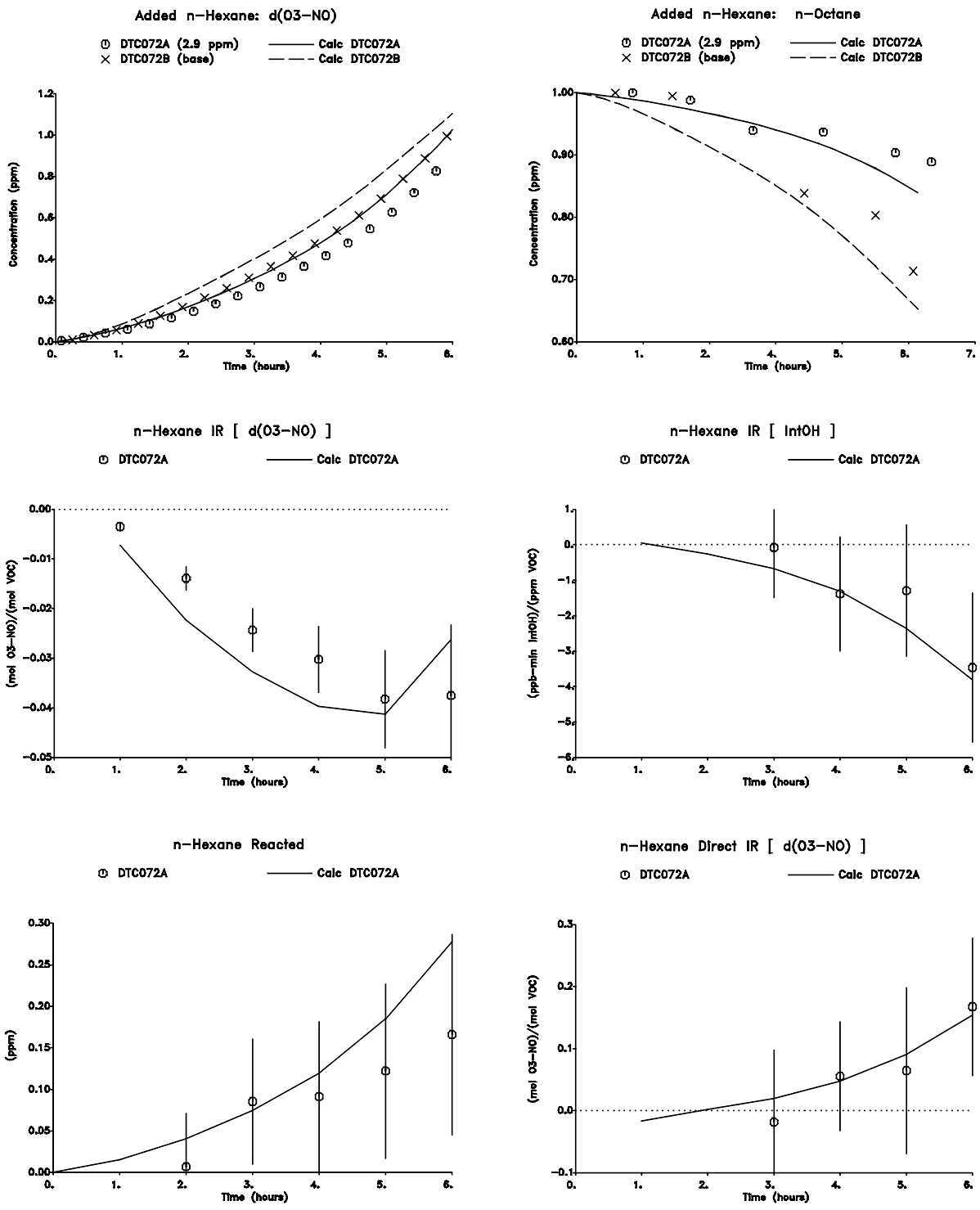

Figure 18. Plots of selected results of ethene surrogate reactivity experiments for **n-Hexane**

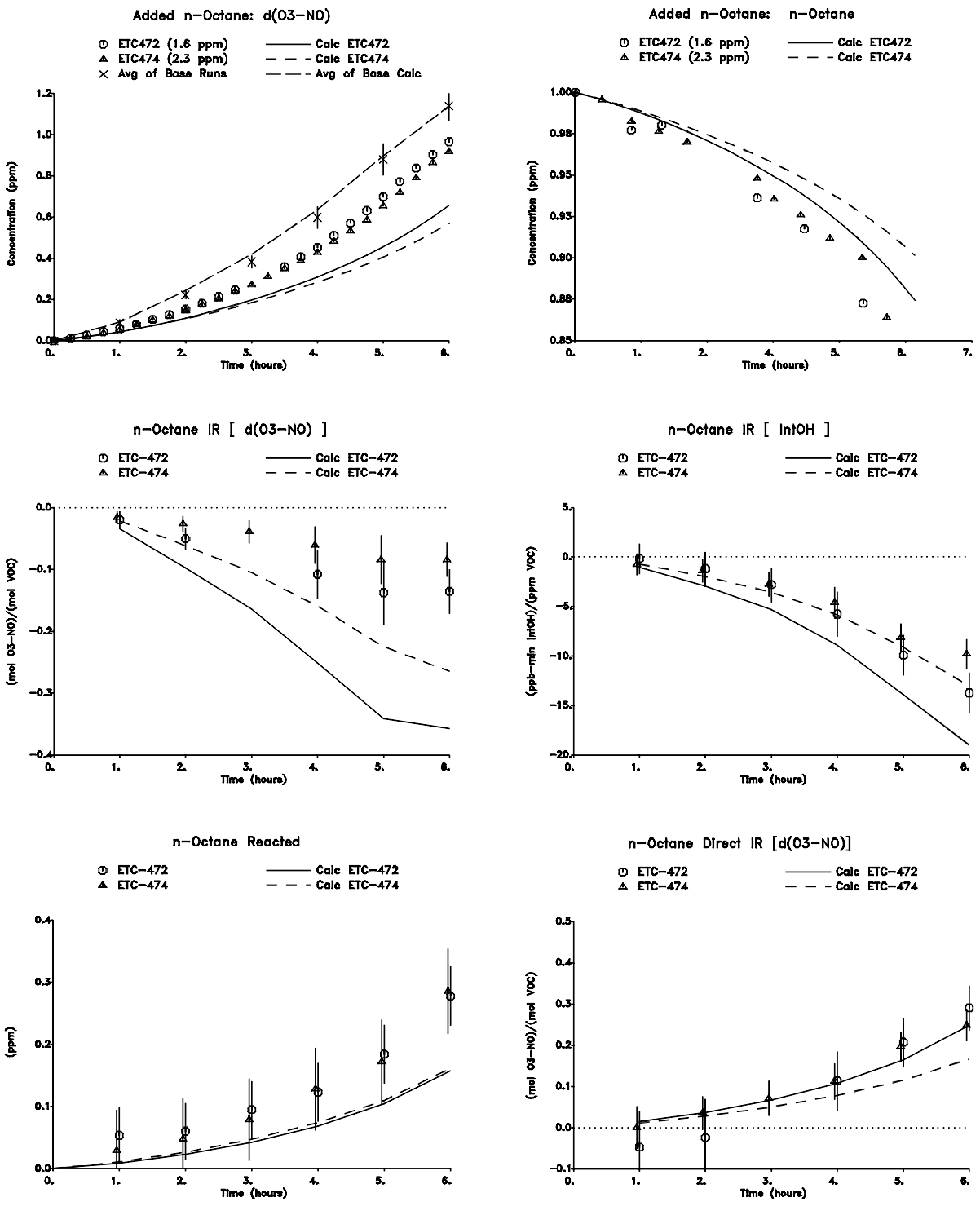

Figure 19. Plots of selected results of ethene surrogate reactivity experiments for **n-Octane**

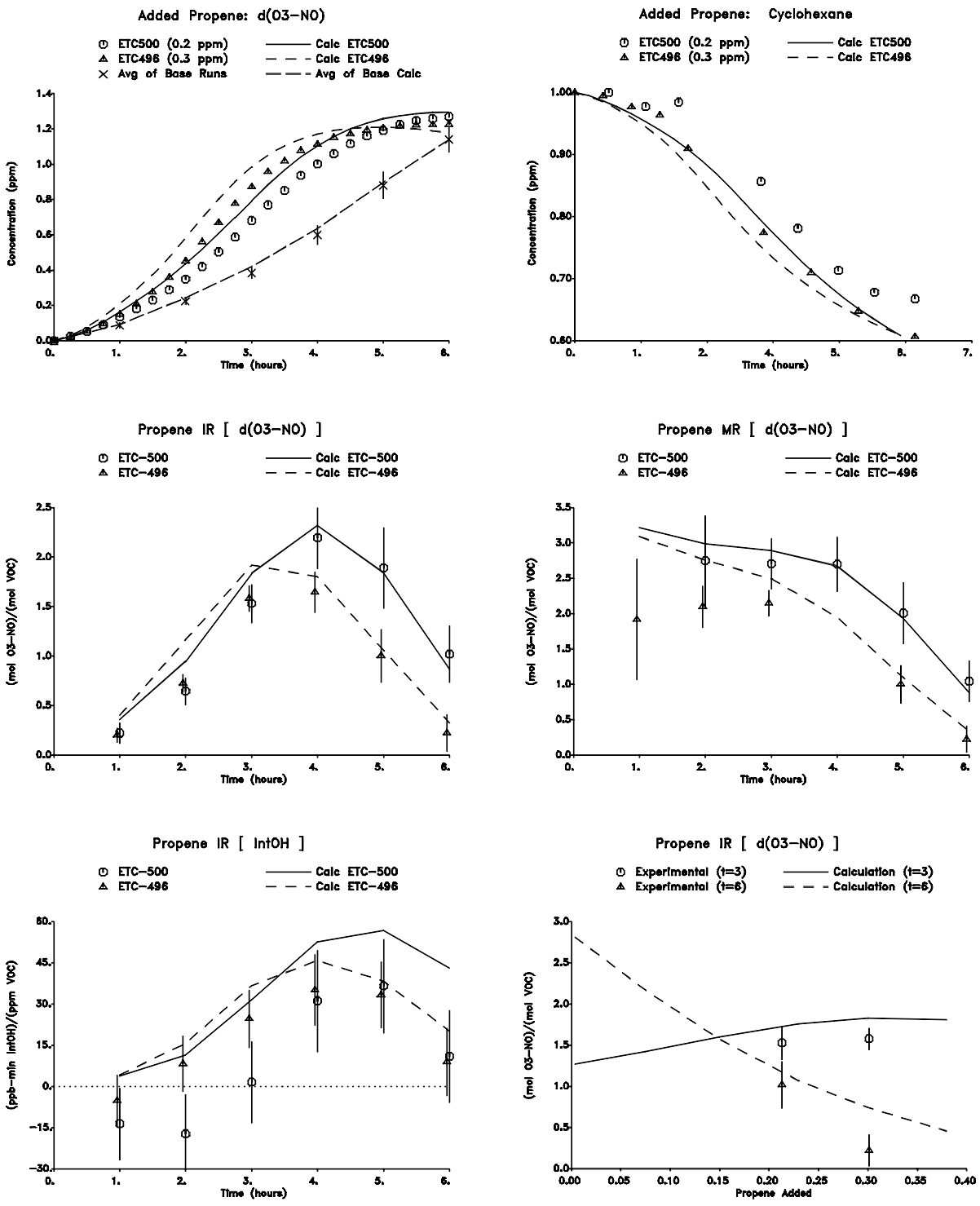

Figure 20. Plots of selected results of ethene surrogate reactivity experiments for **Propene**

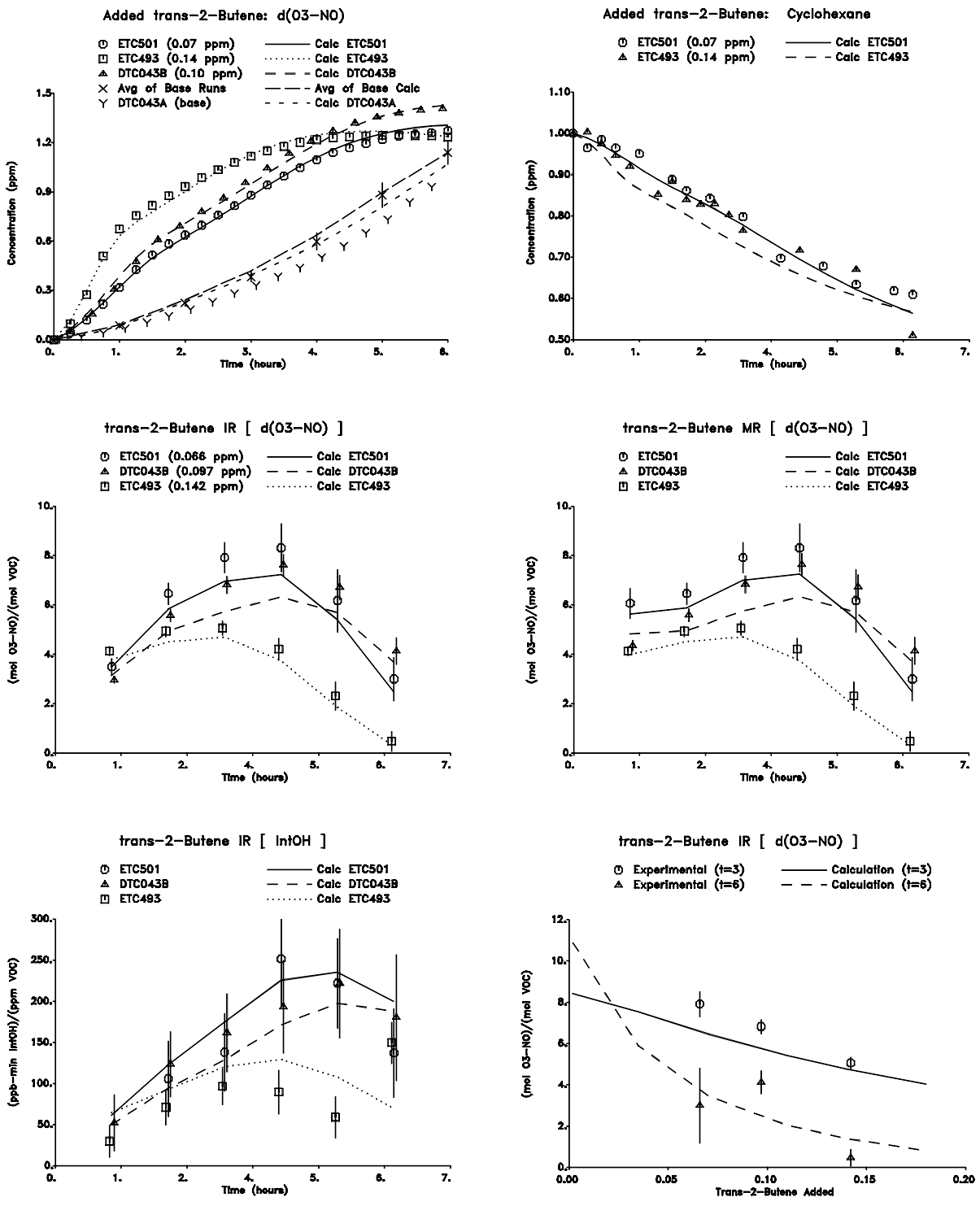

Figure 21. Plots of selected results of ethene surrogate reactivity experiments for **trans-2-Butene**

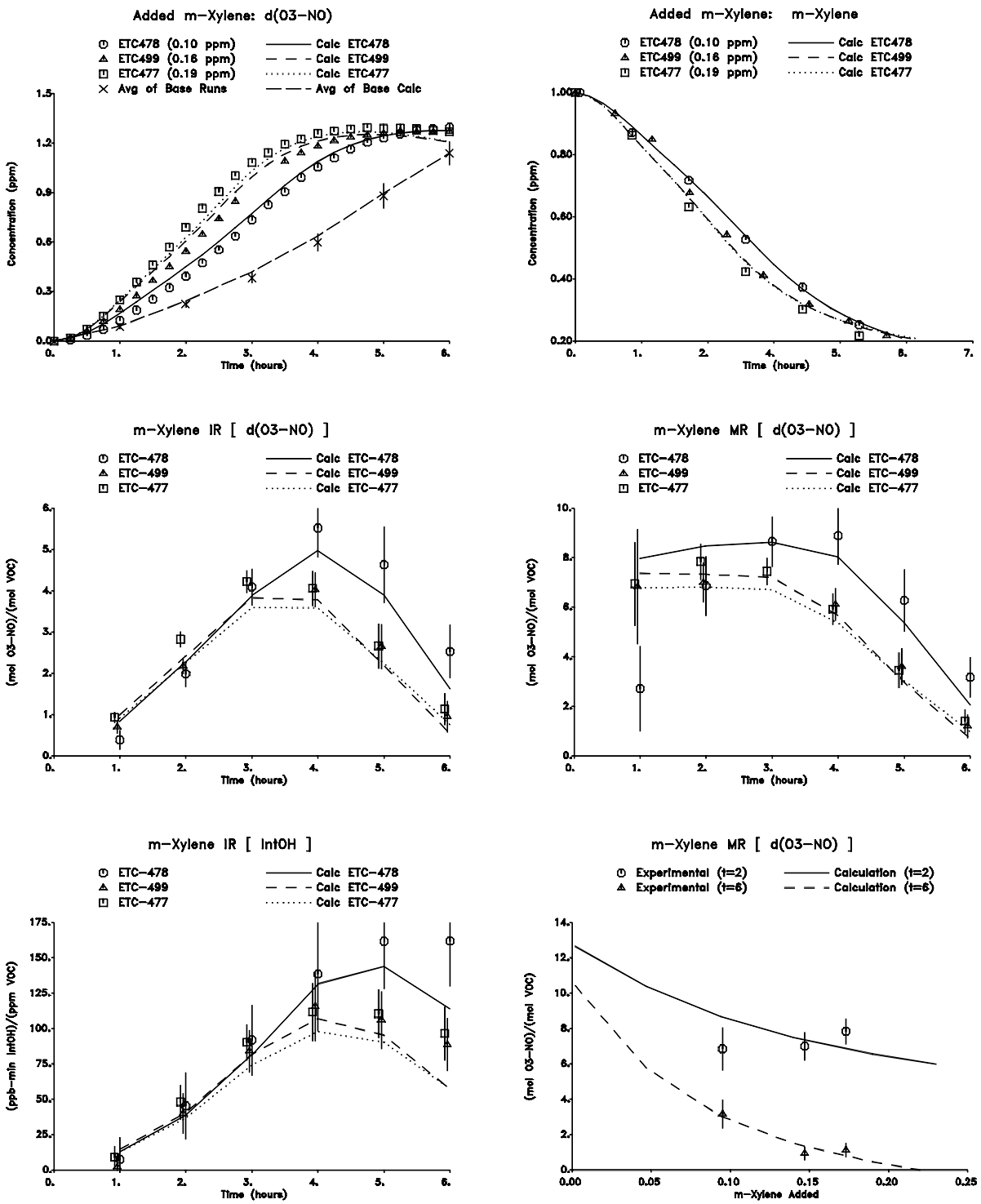

Figure 22. Plots of selected results of ethene surrogate reactivity experiments for **m-Xylene**

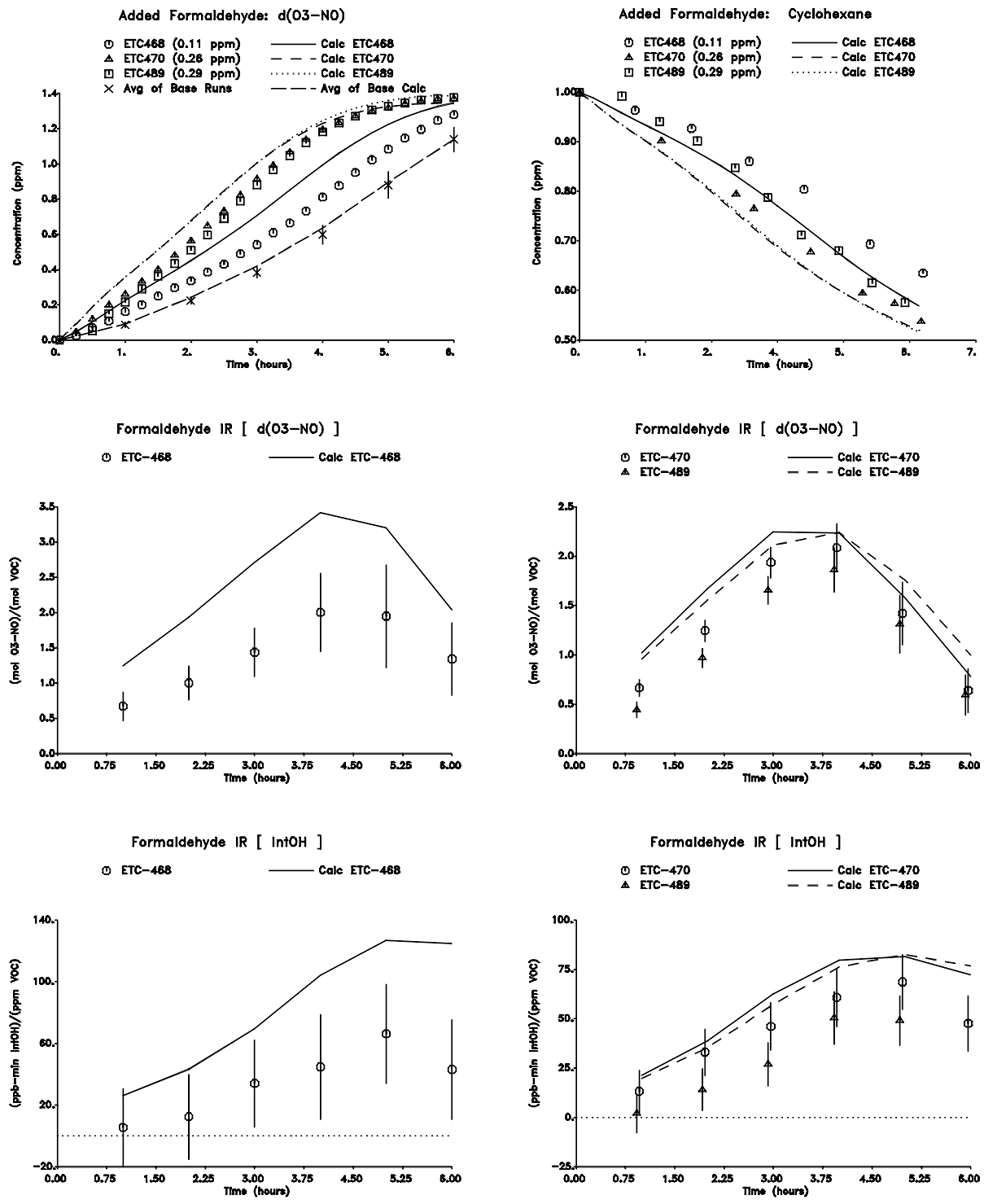

Figure 23. Plots of selected results of ethene surrogate reactivity experiments for **Formaldehyde**

(2) The concentration-time plots of the species (usually cyclohexane) used as the OH tracer for the derivation of IntOH in the added VOC experiments. (These plots are useful for showing how well the model could fit the IntOH data in the individual runs.)
(3) The d(O_3-NO) and IntOH incremental reactivities for each experiment as a function of time.
(4) The d(O_3-NO) mechanistic reactivities for each species as a function of time. This is not shown for n-hexane and n-octane because the amounts reacted could not be determined with sufficient precision, nor for formaldehyde, where the amount reacted could not be determined because it is formed as a product from the reactions of the base ROG components.
(5) The amount of VOC reacted as a function of time for the slower reacting VOCs. These data are not shown for propene, trans-2-butene and m-xylene, which react rapidly and whose amounts reacted are reasonably well predicted by the model, or for formaldehyde, where the amount reacted could not be determined.
(6) For n-hexane and n-octane, the estimates of the direct incremental reactivities are shown as a function of time.
(7) For propene, trans-2-butene, and m-xylene, whose incremental reactivities appeared to depend on the amount of VOC added, plots of the d(O_3-NO) incremental reactivities for selected times against amount of added VOC are also shown.

All the VOCs studied but n-hexane and n-octane were found to have positive effects on d(O_3-NO), with the negative reactivity of the higher alkanes being due to their large negative effect on OH radicals. (Note that because of scatter in the tracer data, combined with the larger amount of dilution uncertainty in the n-hexane reactivity experiment, IntOH and IR (IntOH) could not be determined very precisely in the n-hexane experiments.) Butane also tended to inhibit OH radical levels, though in this case the positive effect of its direct reactivity was more than enough to counteract this, giving it a positive net d(O_3-NO) reactivity. The alkenes, m-xylene, and formaldehyde had positive effects on both IntOH and d(O_3-NO), except perhaps for one of the propene runs at early reaction times, where there may be a problem with the data. CO and ethane did not have a significant effect on OH radicals until around the end of the experiments, when they tended to slightly inhibit radical levels.

Note that in many of the added VOC experiments, particularly the runs with the larger amounts of n-butane, propene, m-xylene and formaldehyde, and in both of the trans-2-butene runs, the rate of ozone formation slowed down significantly or stopped by the end of the experiment. This indicates that O_3 formation in those runs is becoming NO_x-limited by the end of the runs. Not only are the reactivities in those experiments far from the "incremental" limit, their final incremental reactivities no longer represent high NO_x "maximum reactivity" conditions. In such cases, the mechanistic reactivities tended to be relatively constant with time (causing incremental reactivities to increase with time

because of increasing amounts of VOC reacted) up to about t=4 hours, and then decreased. The decrease in reactivities after about t=4 is due to the effect of the system becoming NO_x-limited, which causes VOCs to be less efficient in forming ozone. The d(O_3-NO) plots on Figures 15-23 suggest that the final reactivities may be reflecting either NO_x-limited or near NO_x-limited conditions for almost all of the experiments with positively reactive VOCs (i.e., for all VOCs except n-octane), but that all experiments are still in the excess NO_x regime for up to at least 3 hours. Therefore, reactivity data for up to t=3 hours can be considered to approximate maximum reactivity conditions, and thus can be compared with maximum reactivity data obtained by other methods. However, this is not the case for the t=6 hour reactivity data except for n-octane.

Note that the assumptions behind the derivation of the "direct reactivity" estimates are valid only for conditions where O_3 is not NO_x-limited. For that reason, Table 10 does not show direct reactivity derivations for the latter parts of experiments where O_3 appears to becoming NO_x-limited.

A comparison of these ethene surrogate reactivity results with results using other base ROG surrogates, and the results of model simulations, will be discussed later in this report.

C. Lumped Surrogate Reactivity Results

1. Base Case results

Table 11 gives a summary of the conditions of the reactivity experiments where the 8-component lumped molecule surrogate was used as the base ROG mixture. The initial base case ROG in these experiments averaged 4.0 ppmC (±4%), the initial NO_x levels averaged 0.48 and 0.17 ppm (±3%) in the high and low NO_x experiments, respectively. Concentration-time plots for selected species typical high and low NO_x base case experiments are shown in Figures 24 and 25. Results of model simulations of the experiments, discussed later in this report, are also shown. It can be seen that NO_2 is still being consumed and O_3 is still forming at the end of the high NO_x experiment, indicating that this approximates maximum reactivity conditions. On the other hand, ozone formation stops after about 3 hours in the low NO_x base case run, indicating that the final O_3 is NO_x-limited.

Table 11 shows that the temperature and initial base case reactant concentrations in these DTC surrogate runs were quite reproducible. The base case d(O_3-NO), IntOH, and d(O_3-NO)/IntOH results for the high and low NO_x experiments are shown on Figures 26 and 27. The only variable input which had any apparent effect on the results was the initial base ROG; the temperature variation in the experiments was insufficient for any temperature effects to become apparent. The runs in Figures 26 and 27 are ordered by increasing initial ROG, to show the dependence of the results on this factor.

Table 11. Summary of average temperatures and initial reactant concentrations of the DTC surrogate reactivity experiments.

Run	Test VOC	T	NO	NO_2	NO_x	Surg C	N-C4	N-C8	ETHENE	PROPENE	T-2-BUTE	TOLUENE	M-XYLENE	FORMALD
low NOx Runs														
DTC029A	CO	301.0	0.144	0.030	0.175	4.20	0.390	0.092	0.078	0.058	0.057	0.085	0.081	0.101
DTC029B		301.0	0.144	0.031	0.174	4.27	0.396	0.094	0.079	0.059	0.059	0.087	0.082	0.101
DTC030A		300.4	0.141	0.026	0.167	4.00	0.365	0.088	0.073	0.054	0.054	0.087	0.076	0.096
DTC030B	TOLUENE	300.4	0.140	0.026	0.166		0.363	0.089	0.073	0.052	0.054	[a]	0.079	0.095
DTC031A	N-C4	300.7	0.142	0.030	0.171		[a]	0.095	0.075	0.059	[b]	0.087	0.082	0.100
DTC031B		300.7	0.141	0.031	0.171	4.27	0.394	0.095	0.076	0.059	0.059	0.087	0.083	0.100
DTC032A		300.4	0.142	0.033	0.174	4.21	0.386	0.093	0.077	0.058	0.058	0.086	0.084	0.100
DTC032B	PROPENE	300.4	0.142	0.033	0.175		0.381	0.092	0.073	[a]	0.056	0.084	0.080	0.097
DTC033A	T-2-BUTE	300.3	0.137	0.031	0.168		0.380	0.092	0.073	0.055	[a]	0.084	0.081	0.095
DTC033B		300.3	0.137	0.031	0.168	4.15	0.381	0.093	0.073	0.056	0.056	0.085	0.082	0.096
DTC034A		300.9	0.134	0.030	0.165	3.90	0.365	0.086	0.073	0.054	0.055	0.079	0.073	0.092
DTC034B	A-PINENE	300.9	0.134	0.031	0.165	3.95	0.368	0.087	0.072	0.055	0.054	0.080	0.076	0.090
DTC035A	M-XYLENE	300.6	0.134	0.032	0.166		0.368	0.090	0.074	0.054	0.055	0.082	[a]	0.098
DTC035B		300.6	0.134	0.033	0.167	3.98	0.372	0.089	0.074	0.052	0.055	0.081	0.074	0.096
DTC036A	FORMALD	300.2	0.147	0.035	0.182		0.409	0.098	0.081	0.060	0.060	0.089	0.083	[a]
DTC036B		300.2	0.146	0.035	0.181	4.35	0.408	0.097	0.081	0.059	0.060	0.088	0.080	0.105
DTC037A		300.6	0.143	0.032	0.174	4.25	0.389	0.101	0.076	0.054	0.058	0.084	0.081	0.106
DTC037B	N-C8	300.6	0.143	0.032	0.175		0.388	[a]	0.076	0.057	0.058	0.085	0.080	0.100
DTC038A	ETHENE	300.7	0.138	0.031	0.169		0.357	0.087	[a]	0.052	0.052	0.079	0.073	0.090
DTC038B		300.7	0.138	0.031	0.169	3.91	0.358	0.088	0.072	0.049	0.052	0.081	0.077	0.095
DTC039A		300.9	0.145	0.033	0.178		0.380	0.091	[b]	0.049	0.056	0.084	0.079	0.100
DTC039B	BENZENE	300.9	0.145	0.033	0.178		0.373	0.092	[b]	0.050	0.054	0.085	0.078	0.095
DTC066A		301.6	0.141	0.032	0.173	3.80	0.347	0.086	0.066	0.051	0.050	0.078	0.076	0.083
DTC066B	ACETALD	301.6	0.144	0.031	0.175	3.91	0.365	0.087	0.067	0.053	0.053	0.080	0.075	0.097
DTC067A		301.4	0.139	0.032	0.171	3.84	0.345	0.089	0.065	0.051	0.049	0.081	0.078	0.086
DTC067B	M-XYLENE	301.4	0.138	0.033	0.171		0.336	0.085	0.064	0.051	0.047	0.077	[a]	0.085
DTC071A		301.7	0.146	0.032	0.178	3.97	0.367	0.090	0.070	0.055	0.051	0.081	0.077	0.093
DTC071B	N-C8	301.7	0.146	0.031	0.177		0.354	[a]	0.068	0.054	0.045	0.078	0.076	0.096
Average		**300.8**	**0.141**	**0.032**	**0.172**	**4.06**	**0.373**	**0.091**	**0.073**	**0.054**	**0.054**	**0.083**	**0.079**	**0.096**
St.Dev		**0.5**	**3%**	**6%**	**3%**	**4%**	**5%**	**4%**	**6%**	**6%**	**7%**	**4%**	**4%**	**6%**
High NOx Runs														
DTC014A	CO	300.6	0.374	0.103	0.477	3.96	0.377	0.086	0.075	0.055	0.054	0.079	0.075	0.089
DTC014B		300.6	0.373	0.103	0.477	3.93	0.370	0.086	0.074	0.056	0.052	0.078	0.075	0.088
DTC015A		301.1	0.389	0.114	0.503	4.10	0.385	0.090	0.077	0.057	0.056	0.083	0.079	0.086
DTC015B	CO	301.1	0.390	0.115	0.505	4.11	0.384	0.090	0.078	0.056	0.054	0.083	0.080	0.087
DTC016A	CO	300.2	0.374	0.105	0.479	3.93	0.376	0.086	0.073	0.045	0.053	0.079	0.075	0.092
DTC016B		300.2	0.372	0.103	0.475	3.87	0.371	0.085	0.073	0.042	0.052	0.078	0.073	0.090
DTC017A	ETHENE	300.1	0.374	0.105	0.479		0.370	0.087	[a]	0.043	0.053	0.079	0.074	0.095
DTC017B		300.1	0.374	0.105	0.479	3.89	0.368	0.086	0.071	0.044	0.052	0.079	0.075	0.093
DTC018A	PROPENE	300.6	0.380	0.103	0.482		0.396	0.093	0.077	[a]	0.057	0.085	0.082	0.091
DTC018B		300.6	0.381	0.103	0.484	4.17	0.394	0.092	0.076	0.053	0.056	0.084	0.080	0.088
DTC019A		300.3	0.359	0.100	0.459	4.07	0.384	0.090	0.069	0.050	0.055	0.083	0.079	0.090
DTC019B	N-C4	300.3	0.360	0.100	0.460		[a]	0.089	0.069	0.050	[b]	0.081	0.077	0.091
DTC020A		300.4	0.386	0.115	0.501		0.380	0.093	0.073	0.052	0.057	0.086	0.083	[c]
DTC020B	CO	300.4	0.387	0.115	0.502		0.380	0.092	0.076	0.052	0.057	0.084	0.081	[c]
DTC021A		300.1	0.387	0.106	0.492	4.10	0.378	0.092	0.071	0.051	0.057	0.084	0.078	0.114
DTC021B	T-2-BUTE	300.1	0.386	0.106	0.492		0.374	0.092	0.070	0.052	[a]	0.085	0.080	0.111
DTC022A		300.3	0.399	0.105	0.503	3.95	0.366	0.089	0.070	0.050	0.054	0.081	0.076	0.103
DTC022B	FORMALD	300.3	0.401	0.105	0.505		0.367	0.091	0.070	0.050	0.055	0.083	0.080	[a]
DTC023A	TOLUENE	300.6	0.373	0.096	0.469		0.370	0.090	0.070	0.050	0.055	[a]	0.079	0.100
DTC023B		300.6	0.374	0.098	0.471	4.03	0.372	0.090	0.071	0.051	0.055	0.084	0.078	0.099
DTC024A		300.9	0.397	0.105	0.502	4.03	0.376	0.091	0.075	0.052	0.056	0.081	0.075	0.103
DTC024B	N-C8	300.9	0.397	0.105	0.503		0.377	[a]	0.074	0.053	0.056	0.081	0.076	0.104
DTC025A	M-XYLENE	301.7	0.368	0.099	0.467		0.381	0.093	0.071	0.058	0.057	0.085	[a]	0.099
DTC025B		301.7	0.369	0.097	0.466	4.14	0.382	0.093	0.072	0.057	0.057	0.084	0.080	0.097
DTC028A	ACETONE	300.9	0.381	0.102	0.483	4.09	0.373	0.092	0.076	0.056	0.055	0.084	0.080	0.095
DTC028B		300.9	0.383	0.102	0.485	4.11	0.377	0.092	0.075	0.058	0.056	0.084	0.081	0.096
DTC064A		301.5	0.385	0.101	0.486	3.97	0.365	0.089	0.072	0.054	0.054	0.081	0.077	0.095
DTC064B	ACETONE	301.5	0.385	0.102	0.487	3.80	0.354	0.084	0.069	0.052	0.051	0.077	0.073	0.092
DTC065A	ACETALD	301.3	0.355	0.100	0.455	3.89	0.358	0.088	0.066	0.050	0.052	0.080	0.077	0.096
DTC065B		301.3	0.378	0.099	0.477	3.95	0.357	0.090	0.068	0.053	0.053	0.082	0.079	0.097
DTC068A		301.1	0.384	0.100	0.484	3.80	0.349	0.086	0.065	0.051	0.050	0.079	0.074	0.097
DTC068B	M-XYLENE	301.1	0.383	0.100	0.484		0.339	0.085	0.064	0.051	0.048	0.078	[a]	0.097
TC069A	T-2-BUTE	301.5	0.381	0.097	0.478		0.339	0.086	0.065	0.051	[a]	0.079	0.076	0.094
DTC069B		301.5	0.381	0.097	0.478	3.65	0.328	0.083	0.063	0.049	0.047	0.076	0.073	0.097
DTC070A	N-C8	301.2	0.389	0.099	0.488		0.370	[a]	0.071	0.056	0.054	0.084	0.082	0.094
DTC070B		301.2	0.389	0.098	0.487	4.01	0.364	0.091	0.069	0.055	0.053	0.083	0.080	0.093
Average		**300.8**	**0.381**	**0.102**	**0.483**	**3.99**	**0.367**	**0.090**	**0.070**	**0.053**	**0.054**	**0.082**	**0.078**	**0.098**
St.Dev		**0.5**	**3%**	**5%**	**3%**	**4%**	**4%**	**3%**	**5%**	**5%**	**5%**	**3%**	**4%**	**6%**

[a] Concentration increased for reactivity determinatin
[b] No data or data unreliable
[c] Not added

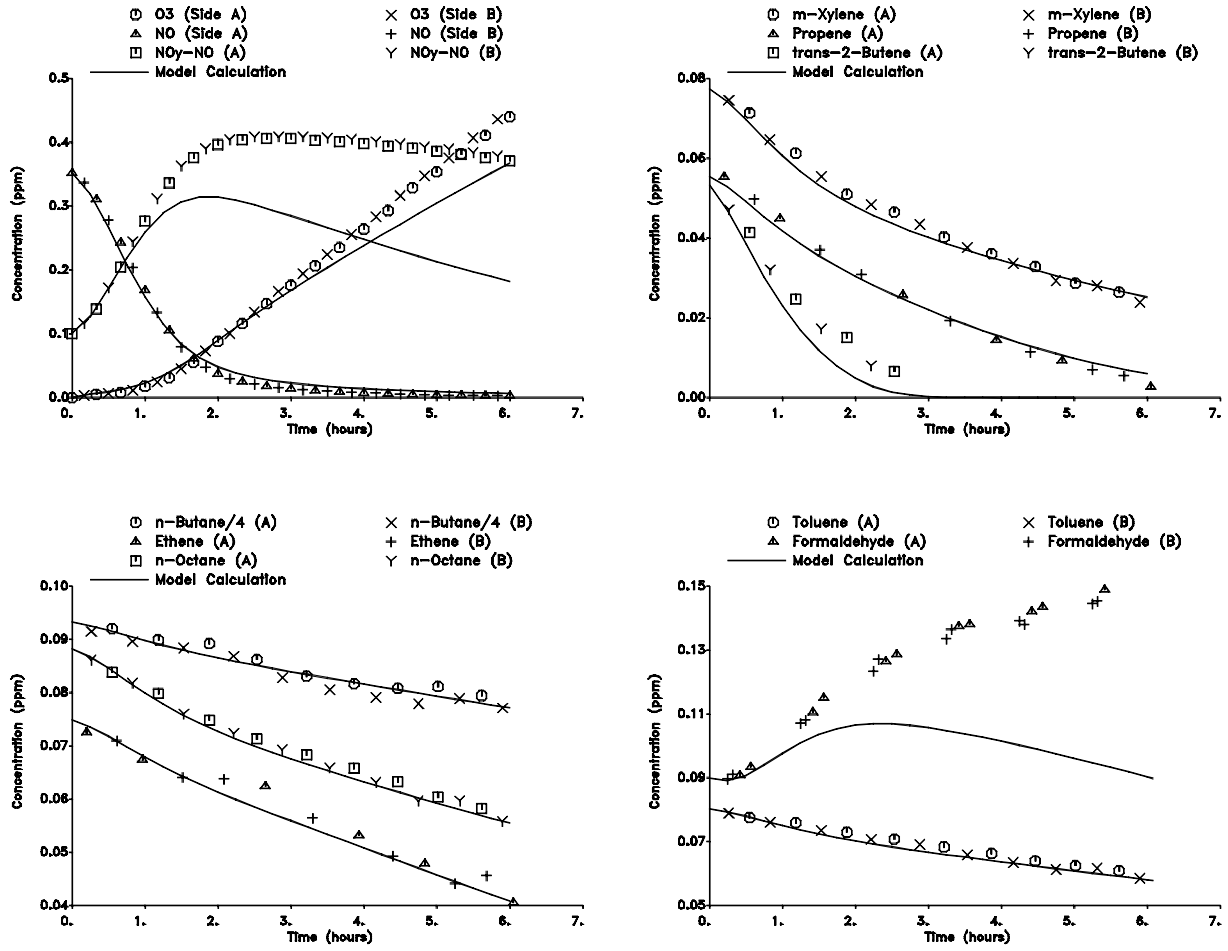

Figure 24. Concentration - time plots for selected species in the base case high NO_x lumped surrogate run DTC013. This run is a side equivalency test with the same mixture irriadiated on both sides. Results of model calculations are also shown.

It is interesting to note that the slight variation in the initial ROG affected d(O_3-NO) primarily through affecting the d(O_3-NO)/IntOH ratio, rather than by affecting IntOH. In other words, slight increases in the initial ROG did not affect the overall radical levels as much as it affects the amount of NO oxidized and O_3 formed at a given radical level. The latter effect is presumably because increasing ROG means that there is more ROG reaction if radical levels are the same. In the low NO_x experiments, all of the initial ROG components were highly correlated to each other, so the relative importance of the components in affecting this variability could not be determined. In the high NO_x experiments, the d(O_3-NO) correlated primarily with the variations in the gas-phase reactants (n-butane, ethene, trans-2-butene, and propene), and had a slightly negative and probably insignificant correlation (-25%) with the initial formaldehyde.

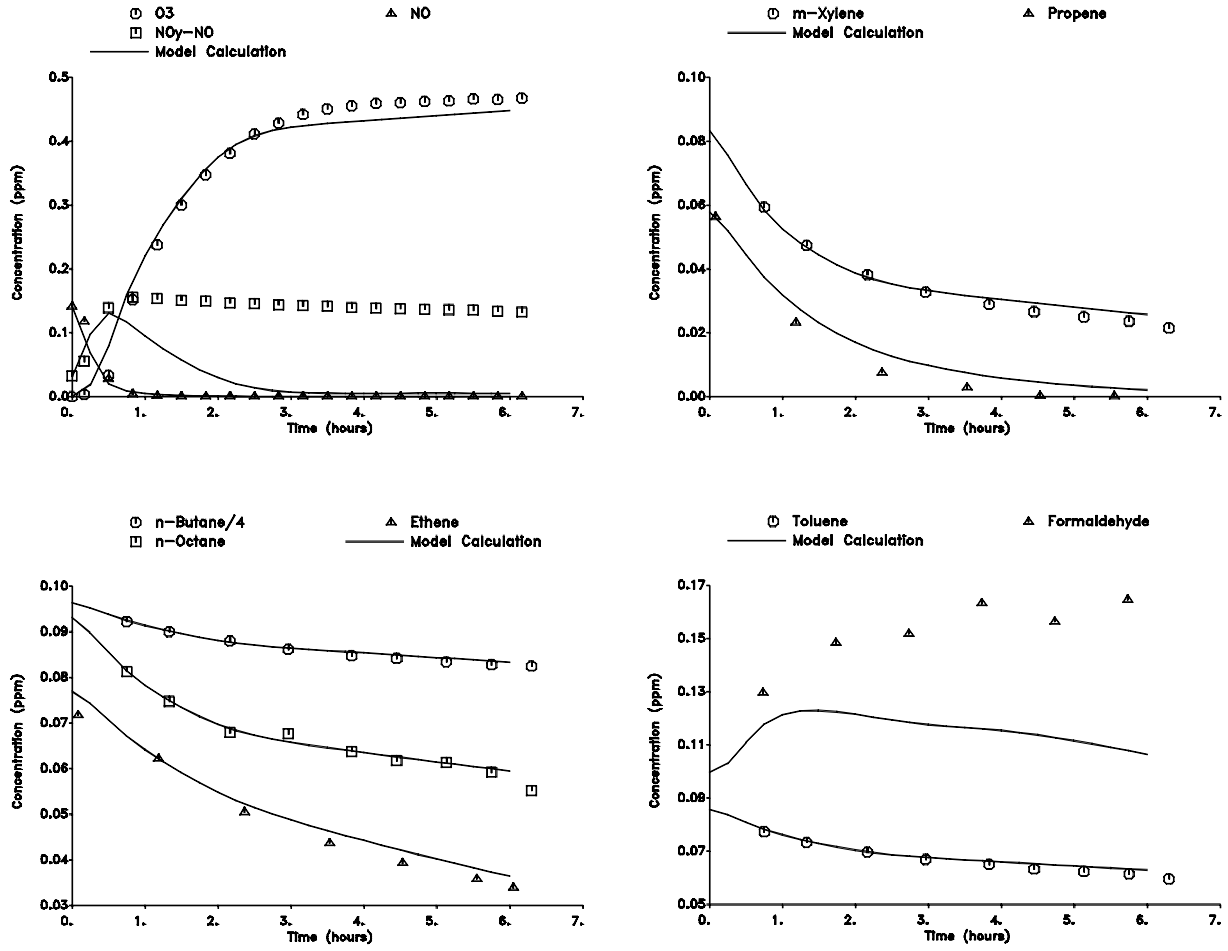

Figure 25. Concentration - time plots for selected species in the base case low NO_x lumped surrogate run DTC032A. Results of model calculations are also shown.

Note that all these runs were divided chamber runs where the base case and the added test VOC irradiations were carried out at the same time, with the base case reactants being mixed in both chamber "sides" before injecting the test compound. As discussed above, the simultaneous base case experiment is assumed to have the same conditions of the test run on the other side, so no regression to account for variability of conditions was carried out. The averages of the side-by-side discrepancies of initial concentrations of the base case reactants were less than 2% in all cases except for formaldehyde, where the average discrepancy was 4%. These differences are in the range of measurement variabilities and do not indicate real differences in initial reactant concentrations.

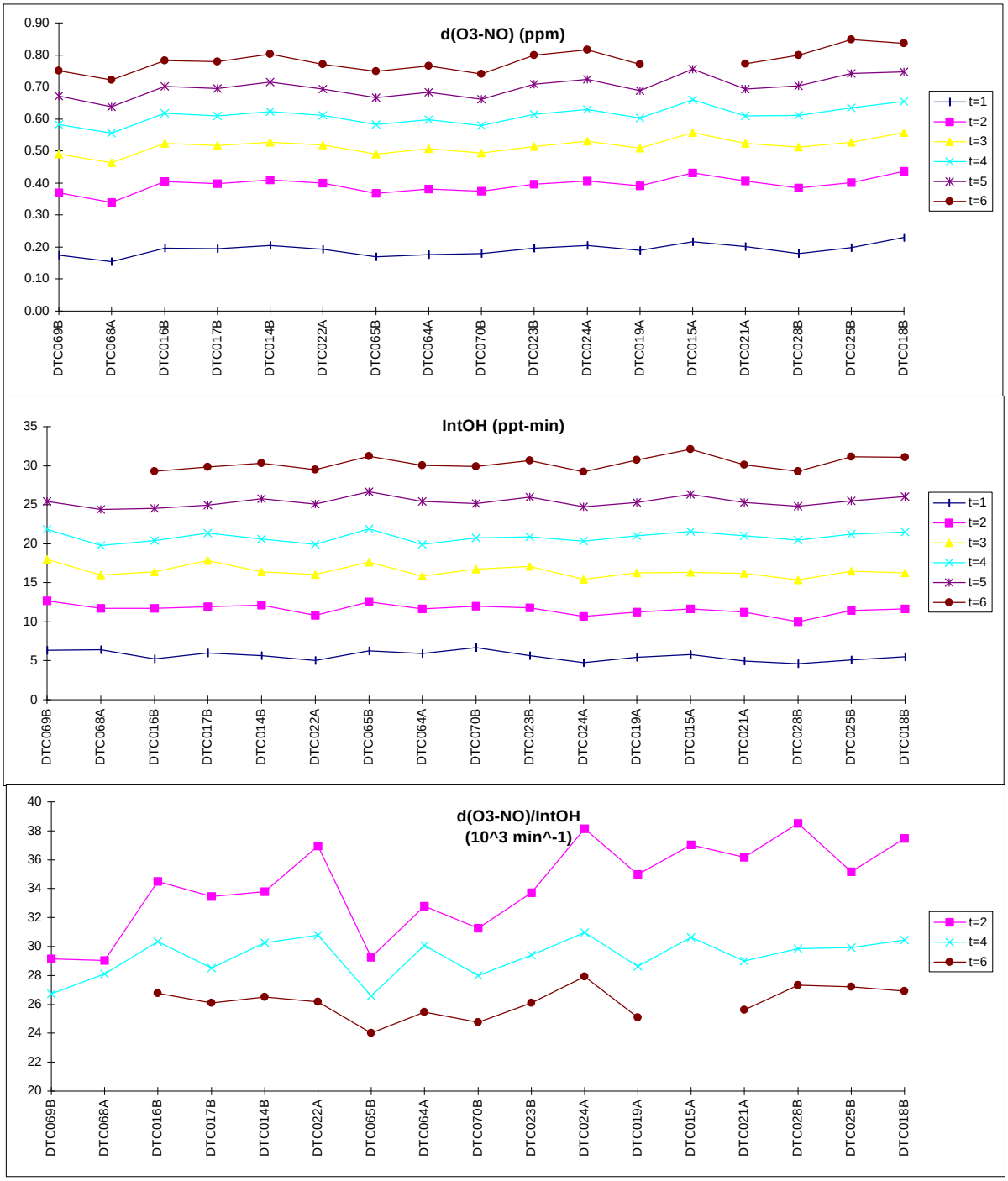

Figure 26. Base case d(O3-NO), IntOH, and d(O3-NO)/IntOH results for the high NOx lumped surrogate runs. Runs are given in order of increasing initial ROG carbon concentrations.

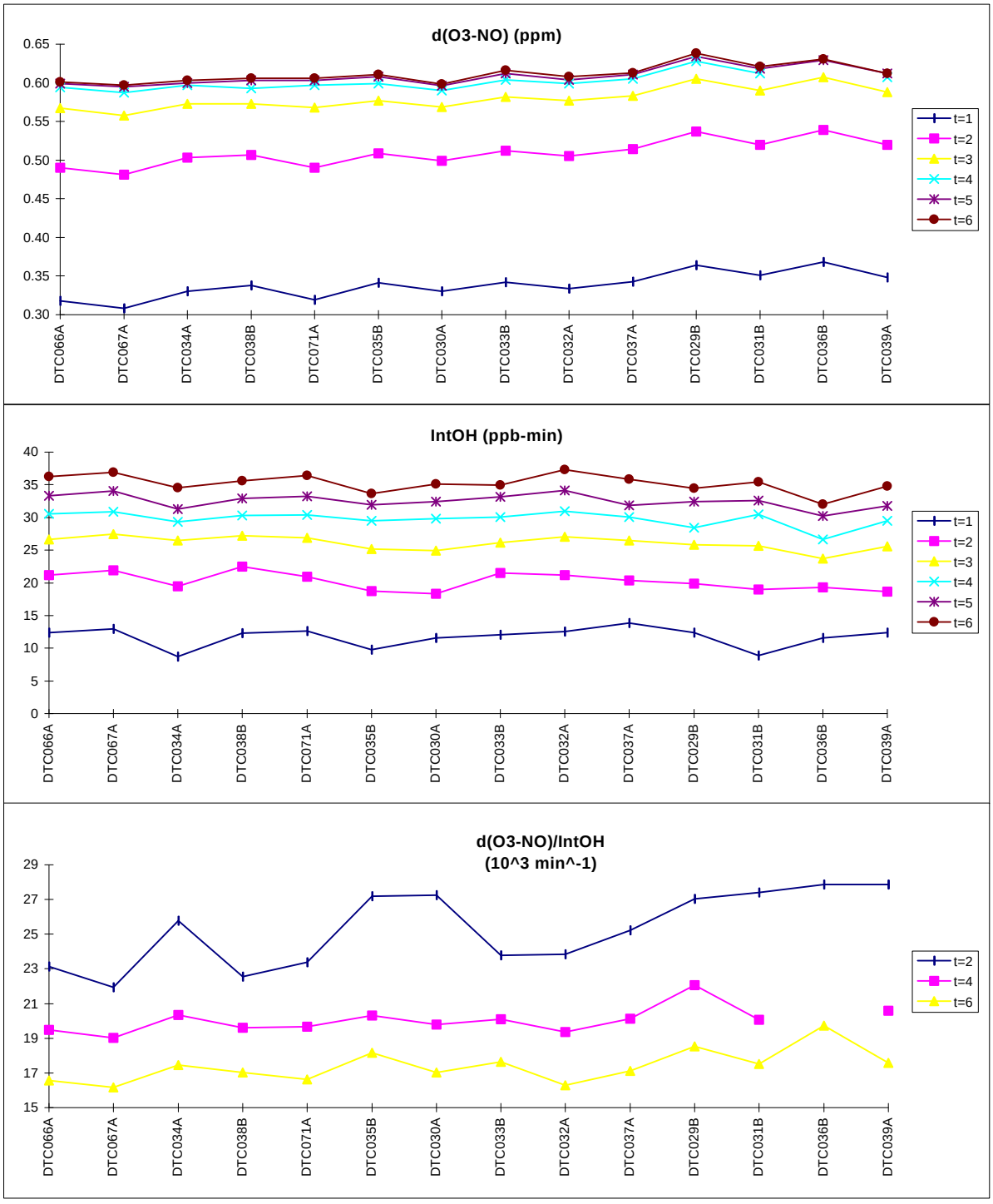

Figure 27. Base case d(O3-NO), IntOH, and d(O3-NO)/IntOH results for the low NOx lumped surrogate runs. Runs are given in order of increasing initial ROG carbon concentrations.

Several experiments were carried out early in the program to test for equivalency of results of irradiations in the two sides of the chamber. The results of one such experiment are shown in Figure 24, above, where it can be seen that the differences between the sides are minor. Figure 28 shows plots of the side differences in d(O_3-NO) and IntOH as a function of time, where the "error bars" are derived in the same manner as used when estimating uncertainties of incremental reactivities. It can be seen that, except for the first hour d(O_3-NO), the inequivalency is well within the estimated minimum uncertainty ranges used in the reactivity derivation. Comparable side equivalency was also seen in replicate propene-NO_x irradiations, which were carried out at various times in this chamber throughout this program.

2. High NO_x Reactivity Results

As indicated in Table 6, high NO_x lumped surrogate reactivity experiments were carried out for each of the 8 surrogate components plus carbon monoxide and acetaldehyde. Three reactivity experiments were carried out for CO and two each were conducted for n-octane, trans-2-butene and m-xylene, and one experiment was carried out for the other VOCs. Because of the good precision and reproducibility in reactivity results (discussed below), it was not considered necessary to repeat reactivity experiments for all the VOCs. The detailed results and reactivity analysis of the DTC surrogate experiments are given in Tables 12-14, and plots of selected reactivity results for the high NO_x experiments are shown on Figures 29-38. Model calculations, discussed later, are also shown.

The format of the data in these tables and figures are similar to those discussed previously for the ethene reactivity experiments. However, the figures also include IntOH mechanistic reactivities and estimated d(O_3-NO) mechanistic reactivities for those VOCs where these could be derived with sufficient precision to be meaningful.

A notable feature of the reactivity results of these experiments, when compared to the ethene surrogate runs discussed above and the mini-surrogate experiments discussed in the Phase I report (Carter et al., 1993a) is the much lower level of estimated uncertainties of the incremental reactivity numbers which were derived. The appropriateness of these lower error estimates are supported by the level of reproducibility in reactivity results observed in the runs with CO, n-octane, and m-xylene, as shown on Figures 27, 31, and 36. (The differences between the two reactivity experiments with trans-2-butene, shown on Figure 34, are more likely due to differences in amount of butene added, rather than imprecisions in the reactivity derivations.) This greater apparent precision can be attributed to the use of the dual chamber system, where the corresponding base case run is conducted simultaneously for each added VOC run. Thus there is much less uncertainty due to the variability in temperature, initial reactant concentrations, and perhaps other conditions, when estimating the base case conditions for each run. The main uncertainty would be due to

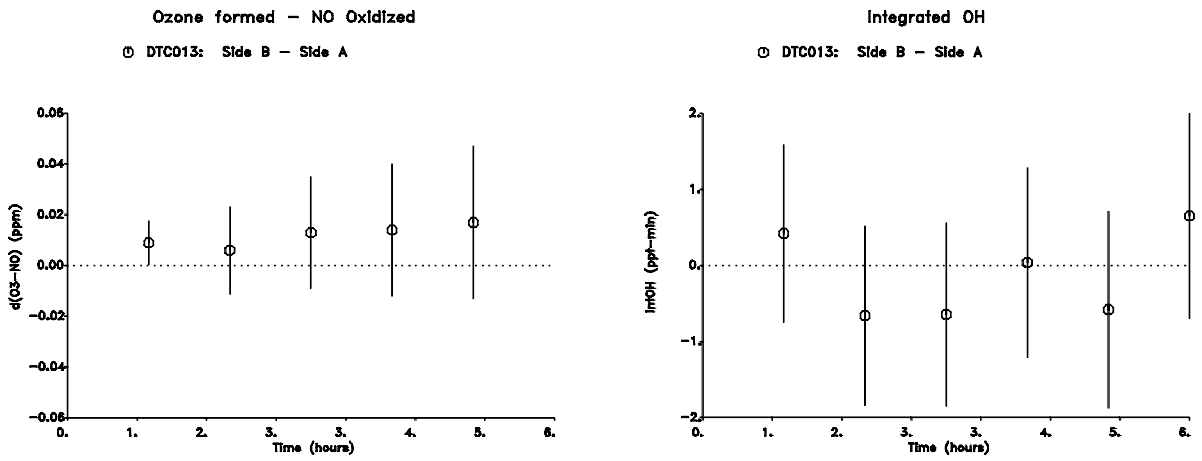

Figure 28. Differences in d(O_3-NO) and IntOH in a DTC side equivalency test experiment. The "error bars" show the uncertainty ranges as used in the incremental reactivity derivations.

inequivalency in conditions in the different chamber sides, which, as shown in Figures 24, appear to be small. Figure 28 suggests that the uncertainty estimates derived with the reactivity data appropriately encompass the uncertainty due to possible side equivalency.

Unlike many of the ethene reactivity experiments, most of the high NO_x added VOC experiments remained out of the NO_x-limited regime throughout the run. The exceptions include the added propene run, the run with the higher amount of added trans-2-butene, and the added toluene run. For those runs, data for times less than 6 hours were used when the results are discussed in terms of maximum reactivity conditions. Note that the "direct reactivity" estimates shown for the latter periods of those runs do not necessarily indicate true direct reactivity. (However, the comparison with the model calculations are still a valid measure of model performance, since they are both derived in the same way.)

All the VOCs studied were found to have positive effects on d(O_3-NO) in these experiments, including n-octane, which had a negative d(O_3-NO) reactivity in the ethene surrogate and mini-surrogate runs. As with the ethene and/or mini-surrogate runs, n-butane, n-octane, and acetaldehyde inhibited OH radical levels, while the alkenes, the aromatics, and formaldehyde enhanced radicals. Because of the greater precision of the data, reasonably precise direct reactivity estimates could be obtained for most of the VOCs studied, except for the aromatics and formaldehyde. These results, and how they vary depending on the ROG surrogate employed, are discussed in more detail later.

Table 12. Derivation of hourly d(O_3-NO) reactivities from the results of the lumped molecule surrogate experiments.

ETC Run No.	Added (ppm)	Time (hr)	Reacted [a] (ppm)	Deriv.	d(O3-NO) (ppm) Test	Base min.Unc	Change	Reactivity (mol/mol) Incremental	Mechanistic
Carbon Monoxide (High NOx)									
14	155.	1	0.363 ±0.045	A	0.548	0.205 ±0.006	0.343 ±0.018	0.0022 ± 5%	0.95 ± 13%
	± 0.	2	0.635 ±0.045	A	0.907	0.409 ±0.012	0.498 ±0.030	0.0032 ± 6%	0.78 ± 9%
		3	0.870 ±0.047	A	1.135	0.528 ±0.016	0.607 ±0.038	0.0039 ± 6%	0.70 ± 8%
		4	0.978 ±0.049	A	1.301	0.623 ±0.019	0.678 ±0.043	0.0044 ± 6%	0.69 ± 8%
		5	1.107 ±0.052	A	1.405	0.716 ±0.021	0.689 ±0.047	0.0044 ± 7%	0.62 ± 8%
		6	1.209 ±0.056	A	1.463	0.803 ±0.024	0.660 ±0.050	0.0043 ± 8%	0.55 ± 9%
15	161.	1	0.396 ±0.046	B	0.637	0.216 ±0.006	0.421 ±0.020	0.0026 ± 5%	1.06 ± 13%
	± 0.	2	0.649 ±0.047	B	1.023	0.432 ±0.013	0.591 ±0.033	0.0037 ± 6%	0.91 ± 9%
		3	0.857 ±0.047	B	1.266	0.558 ±0.017	0.708 ±0.042	0.0044 ± 6%	0.83 ± 8%
		4	1.100 ±0.049	B	1.417	0.660 ±0.020	0.757 ±0.047	0.0047 ± 6%	0.69 ± 8%
		5	1.244 ±0.052	B	1.501	0.755 ±0.023	0.746 ±0.050	0.0046 ± 7%	0.60 ± 8%
		6	1.358 ±0.054	B	1.532		2.532 ±0.055		
16	74.2	1	0.155 ±0.021	A	0.354	0.197 ±0.006	0.157 ±0.012	0.0021 ± 8%	1.01 ± 16%
	±0.0	2	0.297 ±0.021	A	0.654	0.404 ±0.012	0.250 ±0.023	0.0034 ± 9%	0.84 ± 12%
		3	0.400 ±0.022	A	0.835	0.524 ±0.016	0.311 ±0.030	0.0042 ± 10%	0.78 ± 11%
		4	0.496 ±0.023	A	0.992	0.618 ±0.019	0.374 ±0.035	0.0050 ± 9%	0.75 ± 10%
		5	0.606 ±0.024	A	1.121	0.702 ±0.021	0.419 ±0.040	0.0056 ± 9%	0.69 ± 10%
		6	0.684 ±0.025	A	1.223	0.783 ±0.023	0.440 ±0.044	0.0059 ± 10%	0.64 ± 11%
20	103.	1	0.154 ±0.030	B	0.316	0.134 ±0.004	0.182 ±0.010	0.0018 ± 6%	1.18 ± 20%
	± 0.	2	0.306 ±0.030	B	0.656	0.320 ±0.010	0.336 ±0.022	0.0033 ± 7%	1.10 ± 12%
		3	0.455 ±0.030	B	0.837	0.446 ±0.013	0.391 ±0.028	0.0038 ± 7%	0.86 ± 10%
		4	0.622 ±0.031	B	0.999	0.532 ±0.016	0.467 ±0.034	0.0045 ± 7%	0.75 ± 9%
		5	0.738 ±0.032	B	1.140	0.605 ±0.018	0.535 ±0.039	0.0052 ± 7%	0.73 ± 8%
		6	0.869 ±0.034	B	1.251	0.678 ±0.020	0.573 ±0.043	0.0055 ± 7%	0.66 ± 8%
Carbon Monoxide (Low NOx)									
29	85.8	1	0.282 ±0.025	A	0.557	0.364 ±0.011	0.193 ±0.020	0.0022 ± 10%	0.68 ± 14%
	±0.2	2	0.437 ±0.025	A	0.735	0.537 ±0.016	0.198 ±0.027	0.0023 ± 14%	0.45 ± 15%
		3	0.497 ±0.025	A	0.809	0.605 ±0.018	0.204 ±0.030	0.0024 ± 15%	0.41 ± 16%
		4	0.586 ±0.026	A	0.840	0.628 ±0.019	0.212 ±0.031	0.0025 ± 15%	0.36 ± 15%
		5	0.626 ±0.027	A	0.845	0.634 ±0.019	0.211 ±0.032	0.0025 ± 15%	0.34 ± 16%
		6	0.659 ±0.028	A	0.845	0.638 ±0.019	0.207 ±0.032	0.0024 ± 15%	0.31 ± 16%
n-Butane (High NOx)									
19	6.48	1	0.098 ±0.020	B	0.372	0.190 ±0.006	0.182 ±0.013	0.028 ± 7%	1.86 ± 21%
	±0.13	2	0.203 ±0.020	B	0.716	0.392 ±0.012	0.324 ±0.024	0.050 ± 8%	1.60 ± 12%
		3	0.273 ±0.020	B	0.907	0.509 ±0.015	0.398 ±0.031	0.061 ± 8%	1.46 ± 11%
		4	0.333 ±0.021	B	1.073	0.602 ±0.018	0.471 ±0.037	0.073 ± 8%	1.42 ± 10%
		5	0.395 ±0.022	B	1.207	0.688 ±0.021	0.519 ±0.042	0.080 ± 8%	1.32 ± 10%
		6	0.441 ±0.023	B	1.295	0.771 ±0.023	0.524 ±0.045	0.081 ± 9%	1.19 ± 10%
n-Butane (Low NOx)									
31	5.48	1	0.119 ±0.017	A	0.523	0.351 ±0.011	0.172 ±0.019	0.031 ± 11%	1.45 ± 18%
	±0.11	2	0.185 ±0.017	A	0.701	0.520 ±0.016	0.181 ±0.026	0.033 ± 15%	0.98 ± 17%
		3	0.244 ±0.017	A	0.774	0.590 ±0.018	0.184 ±0.029	0.034 ± 16%	0.75 ± 17%
		4	0.270 ±0.018	A	0.801	0.612 ±0.018	0.189 ±0.030	0.034 ± 16%	0.70 ± 17%
		5	0.287 ±0.018	A	0.803	0.618 ±0.019	0.185 ±0.030	0.034 ± 17%	0.64 ± 18%
		6	0.281 ±0.019	A	0.803	0.621 ±0.019	0.182 ±0.030	0.033 ± 17%	0.65 ± 18%
n-Octane (High NOx)									
24	1.102	1	[b]		0.176	0.205 ±0.006	-0.029 ±0.008	-0.026 ± 28%	
	±0.022	2	0.073 ±0.031	B	0.409	0.407 ±0.012	0.002 ±0.017	(0.002 ±0.02)	(0.0 ± 0.2)
		3	0.117 ±0.030	B	0.586	0.530 ±0.016	0.056 ±0.024	0.051 ± 42%	0.48 ± 50%
		4	0.154 ±0.030	B	0.720	0.629 ±0.019	0.091 ±0.029	0.083 ± 32%	0.59 ± 37%
		5	0.179 ±0.031	B	0.857	0.724 ±0.022	0.133 ±0.034	0.121 ± 25%	0.74 ± 31%
		6	0.216 ±0.031	B	0.995	0.816 ±0.024	0.179 ±0.039	0.162 ± 22%	0.83 ± 26%
70	0.746	1	0.039 ±0.021	A	0.160	0.179 ±0.005	-0.019 ±0.007	-0.025 ± 38%	-0.49 ± 66%
	±0.015	2	0.080 ±0.020	A	0.382	0.374 ±0.011	0.008 ±0.016	(0.011 ±0.02)	(0.1 ± 0.2)
		3	0.110 ±0.020	A	0.543	0.494 ±0.015	0.049 ±0.022	0.066 ± 45%	0.44 ± 49%
		4	0.132 ±0.020	A	0.658	0.580 ±0.017	0.078 ±0.026	0.105 ± 34%	0.59 ± 37%
		5	0.157 ±0.020	A	0.765	0.661 ±0.020	0.104 ±0.030	0.139 ± 29%	0.66 ± 32%
		6	0.176 ±0.020	A	0.870	0.740 ±0.022	0.130 ±0.034	0.174 ± 26%	0.74 ± 29%

Table 12 (continued)

ETC Run No.	Added (ppm)	Time (hr)	Reacted [a] (ppm)	Deriv.	d(O3-NO) (ppm) Test	Base min.Unc	Change	Reactivity (mol/mol) Incremental	Mechanistic
n-Octane (Low NOx)									
37	1.126 ±0.023	1	0.065 ±0.031	B	0.326	0.343 ±0.010	-0.017 ±0.014	-0.0151 ± 84%	-0.26 ± 96%
		2	0.128 ±0.031	B	0.543	0.514 ±0.015	0.029 ±0.022	0.026 ± 77%	0.23 ± 81%
		3	0.168 ±0.031	B	0.630	0.583 ±0.017	0.047 ±0.026	0.042 ± 55%	0.28 ± 58%
		4	0.170 ±0.032	B	0.664	0.605 ±0.018	0.059 ±0.027	0.052 ± 46%	0.35 ± 49%
		5	0.180 ±0.033	B	0.672	0.611 ±0.018	0.061 ±0.027	0.054 ± 45%	0.34 ± 48%
		6	0.201 ±0.034	B	0.672	0.613 ±0.018	0.059 ±0.027	0.052 ± 46%	0.29 ± 49%
71	0.647 ±0.013	1	0.057 ±0.007	B	0.299	0.319 ±0.010	-0.020 ±0.013	-0.031 ± 66%	-0.35 ± 67%
		2	0.100 ±0.008	B	0.520	0.490 ±0.015	0.030 ±0.021	0.046 ± 71%	0.30 ± 72%
		3	0.113 ±0.010	B	0.607	0.568 ±0.017	0.039 ±0.025	0.060 ± 64%	0.35 ± 65%
		4	0.128 ±0.012	B	0.645	0.597 ±0.018	0.048 ±0.026	0.074 ± 55%	0.38 ± 56%
		5	0.135 ±0.014	B	0.653	0.603 ±0.018	0.050 ±0.027	0.077 ± 53%	0.37 ± 54%
		6	0.142 ±0.017	B	0.653	0.606 ±0.018	0.047 ±0.027	0.073 ± 57%	0.33 ± 58%
Ethene (High NOx)									
17	0.608 ±0.012	1	0.042 ±0.017	A	0.285	0.195 ±0.006	0.090 ±0.010	0.148 ± 12%	2.12 ± 41%
		2	0.095 ±0.016	A	0.563	0.398 ±0.012	0.165 ±0.021	0.27 ± 13%	1.73 ± 21%
		3	0.155 ±0.016	A	0.755	0.518 ±0.016	0.237 ±0.027	0.39 ± 12%	1.53 ± 15%
		4	0.215 ±0.015	A	0.938	0.610 ±0.018	0.328 ±0.034	0.54 ± 10%	1.52 ± 12%
		5	0.279 ±0.015	A	1.093	0.695 ±0.021	0.398 ±0.039	0.66 ± 10%	1.43 ± 11%
		6	0.340 ±0.015	A	1.188	0.779 ±0.023	0.409 ±0.043	0.67 ± 11%	1.20 ± 11%
Ethene (Low NOx)									
38	0.659 ±0.013	1	0.103 ±0.018	A	0.464	0.338 ±0.010	0.126 ±0.017	0.191 ± 14%	1.22 ± 23%
		2	0.183 ±0.020	A	0.628	0.507 ±0.015	0.121 ±0.024	0.184 ± 20%	0.66 ± 23%
		3	0.240 ±0.022	A	0.663	0.573 ±0.017	0.090 ±0.026	0.137 ± 29%	0.38 ± 31%
		4	0.289 ±0.025	A	0.663	0.593 ±0.018	0.070 ±0.027	0.106 ± 38%	0.24 ± 39%
		5	0.324 ±0.028	A	0.663	0.603 ±0.018	0.060 ±0.027	0.091 ± 45%	0.19 ± 46%
		6	[b]		0.663	0.606 ±0.018	0.057 ±0.027	0.086 ± 47%	
Propene (High NOx)									
18	0.350 ±0.007	1	0.096 ±0.009	A	0.402	0.230 ±0.007	0.172 ±0.014	0.49 ± 8%	1.80 ± 12%
		2	0.211 ±0.008	A	0.728	0.437 ±0.013	0.291 ±0.025	0.83 ± 9%	1.38 ± 9%
		3	0.291 ±0.007	A	0.960	0.557 ±0.017	0.403 ±0.033	1.15 ± 9%	1.38 ± 9%
		4	0.328 ±0.007	A	1.093	0.655 ±0.020	0.438 ±0.038	1.25 ± 9%	1.34 ± 9%
		5	0.347 ±0.007	A	1.157	0.747 ±0.022	0.410 ±0.041	1.17 ± 10%	1.18 ± 10%
		6	0.348 ±0.007	A	1.169	0.837 ±0.025	0.332 ±0.043	0.95 ± 13%	0.95 ± 13%
Propene (Low NOx)									
32	0.305 ±0.006	1	0.099 ±0.007	B	0.510	0.334 ±0.010	0.176 ±0.018	0.58 ± 11%	1.78 ± 13%
		2	0.216 ±0.006	B	0.610	0.505 ±0.015	0.105 ±0.024	0.34 ± 23%	0.49 ± 23%
		3	0.271 ±0.006	B	0.610	0.577 ±0.017	0.033 ±0.025	0.108 ± 76%	0.12 ± 76%
		4	0.289 ±0.006	B	0.610	0.599 ±0.018	0.011 ±0.026	(0.04 ±0.08)	(0.0 ± 0.1)
		5	0.298 ±0.006	B	0.610	0.604 ±0.018	0.006 ±0.026	(0.02 ±0.08)	(0.0 ± 0.1)
		6	0.303 ±0.006	B	0.610	0.608 ±0.018	0.002 ±0.026	(0.007 ±0.08)	(0.0 ± 0.1)
trans-2-Butene (High NOx)									
21	0.324 ±0.007	1	[b]		0.773	0.201 ±0.006	0.572 ±0.024	1.76 ± 5%	
		2	0.320 ±0.007	B	0.901	0.407 ±0.012	0.494 ±0.030	1.52 ± 6%	1.54 ± 6%
		3	0.320 ±0.007	B	0.998	0.524 ±0.016	0.474 ±0.034	1.46 ± 7%	1.48 ± 7%
		4	0.320 ±0.007	B	1.070	0.610 ±0.018	0.460 ±0.037	1.42 ± 8%	1.44 ± 8%
		5	0.320 ±0.007	B	1.110	0.693 ±0.021	0.417 ±0.039	1.29 ± 10%	1.30 ± 10%
		6	0.320 ±0.007	B	1.118	0.772 ±0.023	0.346 ±0.041	1.07 ± 12%	1.08 ± 12%
69	0.190 ±0.004	1	0.157 ±0.004	A	0.503	0.175 ±0.005	0.328 ±0.016	1.73 ± 5%	2.09 ± 5%
		2	0.190 ±0.004	A	0.694	0.370 ±0.011	0.324 ±0.024	1.71 ± 8%	1.71 ± 8%
		3	0.190 ±0.004	A	0.793	0.490 ±0.015	0.303 ±0.028	1.60 ± 9%	1.60 ± 9%
		4	0.190 ±0.004	A	0.894	0.583 ±0.017	0.311 ±0.032	1.64 ± 10%	1.64 ± 10%
		5	0.190 ±0.004	A	0.984	0.671 ±0.020	0.313 ±0.036	1.65 ± 12%	1.65 ± 12%
		6	0.190 ±0.004	A	1.060	0.750 ±0.023	0.310 ±0.039	1.63 ± 13%	1.63 ± 13%
trans-2-Butene (Low NOx)									
33	0.156 ±0.003	1	[b]		0.476	0.342 ±0.010	0.134 ±0.018	0.86 ± 13%	
		2	0.154 ±0.004	A	0.554	0.512 ±0.015	0.042 ±0.023	0.27 ± 54%	0.27 ± 54%
		3	0.154 ±0.004	A	0.572	0.582 ±0.017	-0.010 ±0.024	(-0.06 ± 0.2)	(-0.1 ± 0.2)
		4	0.154 ±0.004	A	0.580	0.604 ±0.018	-0.024 ±0.025	(-0.2 ± 0.2)	(-0.2 ± 0.2)
		5	0.154 ±0.004	A	0.587	0.612 ±0.018	-0.025 ±0.025	(-0.2 ± 0.2)	(-0.2 ± 0.2)
		6	0.154 ±0.004	A	0.594	0.616 ±0.018	-0.022 ±0.026	(-0.14 ± 0.2)	(-0.1 ± 0.2)

Table 12 (continued)

ETC Run No.	Added (ppm)	Time (hr)	Reacted [a] (ppm)	Deriv.	d(O3-NO) (ppm) Test	Base min.Unc	Change	Reactivity (mol/mol) Incremental	Mechanistic
Benzene (Low NOx)									
39	7.39 ±0.15	1	0.147 ±0.012	B	0.486	0.348 ±0.010	0.138 ±0.018	0.0187 ± 13%	0.94 ± 15%
		2	0.213 ±0.012	B	0.531	0.520 ±0.016	0.011 ±0.022	(0.001±0.003)	(0.1 ± 0.1)
		3	0.250 ±0.012	B	0.531	0.588 ±0.018	-0.057 ±0.024	-0.0077 ± 42%	-0.23 ± 42%
		4	0.261 ±0.013	B	0.531	0.607 ±0.018	-0.076 ±0.024	-0.0103 ± 32%	-0.29 ± 32%
		5	0.280 ±0.013	B	0.531	0.612 ±0.018	-0.081 ±0.024	-0.0110 ± 30%	-0.29 ± 30%
		6	0.296 ±0.014	B	0.531	0.612 ±0.018	-0.081 ±0.024	-0.0110 ± 30%	-0.27 ± 30%
Toluene (High NOx)									
23	0.573 ±0.012	1	0.035 ±0.016	A	0.301	0.196 ±0.006	0.105 ±0.011	0.183 ± 10%	2.99 ± 46%
		2	0.077 ±0.015	A	0.599	0.396 ±0.012	0.203 ±0.022	0.35 ± 11%	2.64 ± 23%
		3	0.108 ±0.015	A	0.822	0.513 ±0.015	0.309 ±0.029	0.54 ± 10%	2.85 ± 17%
		4	0.143 ±0.015	A	1.003	0.614 ±0.018	0.389 ±0.035	0.68 ± 9%	2.72 ± 14%
		5	0.167 ±0.015	A	1.080	0.708 ±0.021	0.372 ±0.039	0.65 ± 11%	2.23 ± 14%
		6	0.181 ±0.015	A	1.083	0.800 ±0.024	0.283 ±0.040	0.49 ± 14%	1.56 ± 17%
Toluene (Low NOx)									
30	1.134 ±0.023	1	0.096 ±0.031	B	0.471	0.330 ±0.010	0.141 ±0.017	0.124 ± 12%	1.47 ± 35%
		2	0.145 ±0.031	B	0.507	0.499 ±0.015	0.008 ±0.021	(0.007 ±0.02)	(0.1 ± 0.1)
		3	0.159 ±0.031	B	0.507	0.569 ±0.017	-0.062 ±0.023	-0.055 ± 37%	-0.39 ± 42%
		4	0.176 ±0.031	B	0.507	0.590 ±0.018	-0.083 ±0.023	-0.073 ± 28%	-0.47 ± 33%
		5	0.186 ±0.031	B	0.507	0.596 ±0.018	-0.089 ±0.023	-0.079 ± 26%	-0.48 ± 31%
		6	0.201 ±0.032	B	0.507	0.598 ±0.018	-0.091 ±0.024	-0.080 ± 26%	-0.45 ± 30%
m-Xylene (High NOx)									
25	0.085 ±0.004	1	0.018 ±0.002	A	0.289	0.198 ±0.006	0.091 ±0.011	1.07 ± 12%	5.10 ± 17%
		2	0.034 ±0.002	A	0.566	0.402 ±0.012	0.164 ±0.021	1.94 ± 13%	4.79 ± 14%
		3	0.045 ±0.002	A	0.735	0.528 ±0.016	0.207 ±0.027	2.4 ± 14%	4.61 ± 14%
		4	0.054 ±0.002	A	0.908	0.635 ±0.019	0.273 ±0.033	3.2 ± 13%	5.03 ± 13%
		5	0.060 ±0.002	A	1.051	0.743 ±0.022	0.308 ±0.039	3.6 ± 13%	5.10 ± 13%
		6	0.066 ±0.002	A	1.141	0.848 ±0.025	0.293 ±0.043	3.5 ± 15%	4.43 ± 15%
68	0.064 ±0.003	1	0.014 ±0.002	B	0.217	0.155 ±0.005	0.062 ±0.008	0.96 ± 14%	4.40 ± 17%
		2	0.026 ±0.002	B	0.467	0.340 ±0.010	0.127 ±0.017	1.97 ± 15%	4.87 ± 15%
		3	0.032 ±0.001	B	0.616	0.464 ±0.014	0.152 ±0.023	2.4 ± 16%	4.69 ± 16%
		4	0.038 ±0.001	B	0.749	0.555 ±0.017	0.194 ±0.028	3.0 ± 15%	5.09 ± 15%
		5	0.043 ±0.001	B	0.879	0.638 ±0.019	0.241 ±0.033	3.7 ± 14%	5.56 ± 14%
		6	0.047 ±0.001	B	0.997	0.722 ±0.022	0.275 ±0.037	4.3 ± 14%	5.81 ± 14%
m-Xylene (Low NOx)									
35	0.106 ±0.004	1	0.038 ±0.003	A	0.423	0.341 ±0.010	0.082 ±0.016	0.77 ± 20%	2.15 ± 21%
		2	0.052 ±0.002	A	0.543	0.509 ±0.015	0.034 ±0.022	0.32 ± 66%	0.65 ± 66%
		3	0.059 ±0.002	A	0.556	0.577 ±0.017	-0.021 ±0.024	(-0.2 ± 0.2)	(-0.4 ± 0.4)
		4	0.064 ±0.002	A	0.556	0.599 ±0.018	-0.043 ±0.025	-0.41 ± 57%	-0.67 ± 57%
		5	0.068 ±0.002	A	0.556	0.608 ±0.018	-0.052 ±0.025	-0.49 ± 48%	-0.77 ± 48%
		6	0.069 ±0.002	A	0.557	0.611 ±0.018	-0.054 ±0.025	-0.51 ± 46%	-0.78 ± 46%
67	0.173 ±0.005	1	0.068 ±0.004	B	0.458	0.308 ±0.009	0.150 ±0.017	0.87 ± 11%	2.21 ± 13%
		2	0.088 ±0.005	B	0.535	0.481 ±0.014	0.054 ±0.022	0.31 ± 40%	0.62 ± 40%
		3	0.094 ±0.005	B	0.537	0.558 ±0.017	-0.021 ±0.023	(-0.12 ±0.13)	(-0.2 ± 0.2)
		4	0.099 ±0.006	B	0.537	0.587 ±0.018	-0.050 ±0.024	-0.29 ± 48%	-0.51 ± 48%
		5	0.105 ±0.006	B	0.537	0.595 ±0.018	-0.058 ±0.024	-0.34 ± 42%	-0.55 ± 42%
		6	0.107 ±0.007	B	0.537	0.597 ±0.018	-0.060 ±0.024	-0.35 ± 40%	-0.56 ± 41%
Formaldehyde (High NOx)									
22	0.408 ±0.007	1	[b]		0.393	0.193 ±0.006	0.200 ±0.013	0.49 ± 7%	
		2	[b]		0.616	0.400 ±0.012	0.216 ±0.022	0.53 ± 10%	
		3	[b]		0.762	0.519 ±0.016	0.243 ±0.028	0.60 ± 11%	
		4	[b]		0.891	0.612 ±0.018	0.279 ±0.032	0.68 ± 12%	
		5	[b]		0.997	0.693 ±0.021	0.304 ±0.036	0.74 ± 12%	
		6	[b]		1.079	0.771 ±0.023	0.308 ±0.040	0.75 ± 13%	
Formaldehyde (Low NOx)									
36	0.247 ±0.004	1	[b]		0.452	0.368 ±0.011	0.084 ±0.017	0.34 ± 21%	
		2	[b]		0.598	0.539 ±0.016	0.059 ±0.024	0.24 ± 41%	
		3	[b]		0.638	0.607 ±0.018	0.031 ±0.026	0.125 ± 85%	
		4	[b]		0.643		1.643 ±0.036		
		5	[b]		0.643	0.629 ±0.019	0.014 ±0.027	(0.06 ±0.11)	
		6	[b]		0.643	0.631 ±0.019	0.012 ±0.027	(0.05 ±0.11)	

Table 12 (continued)

ETC Run No.	Added (ppm)	Time (hr)	Reacted [a] (ppm)	Deriv.	d(O3-NO) (ppm) Test	Base min.Unc	Change	Reactivity (mol/mol) Incremental	Mechanistic
Acetaldehyde (High NOx)									
65	1.53 ±0.03	1	[b]		0.353	0.169 ±0.005	0.184 ±0.012	0.120 ± 7%	
		2	0.108 ±0.052	A	0.543	0.368 ±0.011	0.175 ±0.020	0.114 ± 11%	1.63 ± 50%
		3	0.205 ±0.060	A	0.670	0.491 ±0.015	0.179 ±0.025	0.117 ± 14%	0.87 ± 32%
		4	0.242 ±0.070	A	0.786	0.582 ±0.017	0.204 ±0.029	0.133 ± 15%	0.84 ± 32%
		5	0.292 ±0.081	A	0.893	0.667 ±0.020	0.226 ±0.033	0.147 ± 15%	0.77 ± 31%
		6	0.377 ±0.091	A	0.977	0.749 ±0.022	0.228 ±0.037	0.148 ± 16%	0.60 ± 29%
Acetaldehyde (Low NOx)									
66	1.62 ±0.03	1	[b]		0.297	0.318 ±0.010	-0.021 ±0.013	-0.0130 ± 62%	
		2	0.092 ±0.055	B	0.429	0.490 ±0.015	-0.061 ±0.020	-0.038 ± 32%	-0.66 ± 68%
		3	0.131 ±0.065	B	0.481	0.567 ±0.017	-0.086 ±0.022	-0.053 ± 26%	-0.66 ± 56%
		4	0.168 ±0.076	B	0.507	0.594 ±0.018	-0.087 ±0.023	-0.054 ± 27%	-0.52 ± 52%
		5	0.206 ±0.088	B	0.527	0.599 ±0.018	-0.072 ±0.024	-0.044 ± 33%	-0.35 ± 54%
		6	0.247 ±0.100	B	0.545	0.601 ±0.018	-0.056 ±0.024	-0.035 ± 44%	-0.23 ± 59%

[a] Derivation methods: "IntOH" = hourly amounts reacted computed from the experimentally measured IntOH and VOC's OH rate constant; "Direct" = hourly amounts reacted determined by interpolating experimental measurements of the VOC, with a correction for dilution.
[b] Amount reacted could not be determined for this VOC, or amount reacted could not be determined for this time with sufficient precision to be useful.

Table 13. Derivation of hourly IntOH reactivities from the results of the lumped molecule surrogate experiments.

ETC Run No	Added (ppm)	Time (hr)	Reacted (ppm)	IntOH (ppt-min) Test Run	Base Run	Change	Reactivity (ppt-min/ppm) Incremental	Mechanistic
Carbon Monoxide (High NOx)								
14	155.	1	0.363 ±0.045	6.7 ±0.8	5.6 ±0.8	1.0 ±1.2	(0.007 ±0.007)	(3. ± 3.)
		2	0.635 ±0.045	11.8 ±0.8	12.1 ±0.8	-0.3 ±1.2	(-0.002 ±0.008)	(-1. ± 2.)
		3	0.870 ±0.047	16.2 ±0.9	16.4 ±0.8	-0.2 ±1.2	(-0.001 ±0.008)	(0. ± 1.)
		4	0.978 ±0.049	18.3 ±0.9	20.6 ±0.8	-2.3 ±1.2	-0.0148 ± 53%	-2. ± 53%
		5	1.107 ±0.052	20.8 ±0.9	25.8 ±0.9	-4.9 ±1.3	-0.032 ± 25%	-4. ± 26%
		6	1.209 ±0.056	22.8 ±1.0	30.3 ±0.9	-7.5 ±1.3	-0.048 ± 17%	-6. ± 18%
15	161.	1	0.396 ±0.046	7.0 ±0.8	5.8 ±0.8	1.2 ±1.2	0.0077 ± 94%	3. ± 94%
		2	0.649 ±0.047	11.6 ±0.8	11.7 ±0.8	0.0 ±1.2	(-.0003 ±0.007)	(0. ± 2.)
		3	0.857 ±0.047	15.5 ±0.8	16.3 ±0.8	-0.8 ±1.2	(-0.005 ±0.007)	(-1. ± 1.)
		4	1.100 ±0.049	20.0 ±0.9	21.5 ±0.9	-1.5 ±1.2	-0.0095 ± 80%	-1. ± 80%
		5	1.244 ±0.052	22.8 ±0.9	26.3 ±0.9	-3.5 ±1.2	-0.022 ± 36%	-3. ± 36%
		6	1.358 ±0.054	25.1 ±0.9	32.1 ±0.9	-7.0 ±1.3	-0.043 ± 18%	-5. ± 19%
16	74.2	1	0.155 ±0.021	6.0 ±0.8	5.2 ±0.8	0.8 ±1.2	(0.010 ±0.02)	(5. ± 7.)
		2	0.297 ±0.021	11.5 ±0.8	11.7 ±0.8	-0.2 ±1.2	(-0.003 ±0.02)	(-1. ± 4.)
		3	0.400 ±0.022	15.6 ±0.8	16.4 ±0.8	-0.8 ±1.2	(-0.011 ±0.02)	(-2. ± 3.)
		4	0.496 ±0.023	19.4 ±0.9	20.4 ±0.9	-1.0 ±1.2	(-0.013 ±0.02)	(-2. ± 2.)
		5	0.606 ±0.024	23.8 ±0.9	24.5 ±0.9	-0.7 ±1.2	(-0.010 ±0.02)	(-1. ± 2.)
		6	0.684 ±0.025	27.0 ±0.9	29.3 ±0.9	-2.2 ±1.3	-0.030 ± 57%	-3. ± 58%
20	103.	1	0.154 ±0.030	4.3 ±0.8	4.2 ±0.8	0.1 ±1.2	(0.0010 ±0.011)	(1. ± 8.)
		2	0.306 ±0.030	8.5 ±0.8	9.0 ±0.8	-0.6 ±1.2	(-0.005 ±0.011)	(-2. ± 4.)
		3	0.455 ±0.030	12.6 ±0.8	14.6 ±0.8	-1.9 ±1.2	-0.0187 ± 61%	-4. ± 62%
		4	0.622 ±0.031	17.3 ±0.8	18.2 ±0.9	-0.9 ±1.2	(-0.009 ±0.012)	(-1. ± 2.)
		5	0.738 ±0.032	20.5 ±0.9	22.9 ±0.9	-2.4 ±1.2	-0.023 ± 52%	-3. ± 52%
		6	0.869 ±0.034	24.3 ±0.9	25.7 ±0.9	-1.4 ±1.3	-0.0141 ± 87%	-2. ± 87%
Carbon Monoxide (Low NOx)								
29	85.8	1	0.282 ±0.025	9.4 ±0.8	12.4 ±0.8	-3.0 ±1.2	-0.035 ± 38%	-11. ± 39%
		2	0.437 ±0.025	14.5 ±0.8	19.9 ±0.8	-5.4 ±1.2	-0.062 ± 22%	-12. ± 23%
		3	0.497 ±0.025	16.5 ±0.8	25.9 ±0.8	-9.3 ±1.2	-0.109 ± 13%	-19. ± 14%
		4	0.586 ±0.026	19.5 ±0.8	28.5 ±0.8	-9.0 ±1.2	-0.104 ± 13%	-15. ± 14%
		5	0.626 ±0.027	20.9 ±0.9	32.4 ±0.9	-11.6 ±1.2	-0.135 ± 11%	-18. ± 11%
		6	0.659 ±0.028	22.0 ±0.9	34.4 ±0.9	-12.4 ±1.3	-0.145 ± 10%	-19. ± 11%

Table 13 (continued)

ETC Run No	Added (ppm)	Time (hr)	Reacted (ppm)	IntOH (ppt-min) Test Run	IntOH (ppt-min) Base Run	IntOH (ppt-min) Change	Reactivity (ppt-min/ppm) Incremental	Reactivity (ppt-min/ppm) Mechanistic
n-Butane (High NOx)								
19	6.48	1	0.098 ±0.020	4.0 ±0.8	5.5 ±0.8	-1.4 ±1.2	-0.22 ± 81%	-15. ± 83%
		2	0.203 ±0.020	8.5 ±0.8	11.2 ±0.8	-2.7 ±1.2	-0.42 ± 43%	-14. ± 44%
		3	0.273 ±0.020	11.4 ±0.8	16.3 ±0.8	-4.8 ±1.2	-0.75 ± 24%	-18. ± 26%
		4	0.333 ±0.021	14.0 ±0.8	21.0 ±0.8	-7.0 ±1.2	-1.08 ± 17%	-21. ± 18%
		5	0.395 ±0.022	16.8 ±0.9	25.3 ±0.9	-8.5 ±1.2	-1.31 ± 15%	-22. ± 15%
		6	0.441 ±0.023	18.8 ±0.9	30.7 ±0.9	-11.9 ±1.3	-1.84 ± 11%	-27. ± 12%
n-Butane (Low NOx)								
31	5.48	1	0.119 ±0.017	5.8 ±0.8	8.8 ±0.8	-3.0 ±1.2	-0.55 ± 39%	-25. ± 41%
		2	0.185 ±0.017	9.2 ±0.8	19.0 ±0.8	-9.8 ±1.2	-1.79 ± 12%	-53. ± 15%
		3	0.244 ±0.017	12.2 ±0.8	25.7 ±0.8	-13.5 ±1.2	-2.5 ± 9%	-55. ± 11%
		4	0.270 ±0.018	13.6 ±0.8	30.5 ±0.8	-16.9 ±1.2	-3.1 ± 7%	-63. ± 10%
		5	0.287 ±0.018	14.5 ±0.9	32.6 ±0.9	-18.1 ±1.2	-3.3 ± 7%	-63. ± 9%
		6	0.281 ±0.019	14.2 ±0.9	35.4 ±0.9	-21.2 ±1.3	-3.9 ± 6%	-75. ± 9%
n-Octane (High NOx)								
24	1.102	1	[b]	2.1 ±0.8	4.8 ±0.8	-2.6 ±1.2	-2.4 ± 44%	
		2	0.073 ±0.031	4.9 ±0.8	10.7 ±0.8	-5.8 ±1.2	-5.3 ± 20%	-79. ± 47%
		3	0.117 ±0.030	7.9 ±0.8	15.4 ±0.8	-7.5 ±1.2	-6.8 ± 16%	-64. ± 30%
		4	0.154 ±0.030	10.7 ±0.8	20.3 ±0.8	-9.6 ±1.2	-8.7 ± 13%	-62. ± 23%
		5	0.179 ±0.031	13.1 ±0.9	24.7 ±0.9	-11.6 ±1.2	-10.5 ± 11%	-65. ± 20%
		6	0.216 ±0.031	16.1 ±0.9	29.2 ±0.9	-13.1 ±1.3	-11.9 ± 10%	-61. ± 17%
70	0.746	1	0.039 ±0.021	4.2 ±0.8	6.7 ±0.8	-2.5 ±1.2	-3.4 ± 46%	-66. ± 71%
		2	0.080 ±0.020	8.1 ±0.8	12.0 ±0.8	-3.9 ±1.2	-5.2 ± 30%	-49. ± 40%
		3	0.110 ±0.020	11.5 ±0.8	16.7 ±0.8	-5.2 ±1.2	-7.0 ± 23%	-47. ± 29%
		4	0.132 ±0.020	14.0 ±0.8	20.7 ±0.9	-6.7 ±1.2	-9.0 ± 18%	-51. ± 24%
		5	0.157 ±0.020	17.3 ±0.9	25.1 ±0.9	-7.9 ±1.2	-10.5 ± 16%	-50. ± 20%
		6	0.176 ±0.020	19.7 ±0.9	29.9 ±0.9	-10.2 ±1.3	-13.6 ± 13%	-58. ± 17%
n-Octane (Low NOx)								
37	1.126	1	0.065 ±0.031	4.8 ±0.8	13.8 ±0.9	-9.0 ±1.2	-8.0 ± 13%	-138. ± 50%
		2	0.128 ±0.031	9.5 ±0.8	20.4 ±1.0	-10.9 ±1.3	-9.7 ± 12%	-85. ± 27%
		3	0.168 ±0.031	12.5 ±0.9	26.5 ±1.2	-14.0 ±1.5	-12.4 ± 11%	-83. ± 21%
		4	0.170 ±0.032	12.4 ±0.9	30.0 ±1.4	-17.7 ±1.7	-15.7 ± 10%	-104. ± 21%
		5	0.180 ±0.033	13.3 ±0.9	31.8 ±1.7	-18.5 ±1.9	-16.4 ± 11%	-103. ± 21%
		6	0.201 ±0.034	14.8 ±1.0	35.8 ±1.9	-21.0 ±2.2	-18.7 ± 11%	-105. ± 20%
71	0.647	1	0.057 ±0.007	7.1 ±0.9	12.6 ±0.9	-5.5 ±1.2	-8.5 ± 22%	-97. ± 25%
		2	0.100 ±0.008	13.0 ±1.0	21.0 ±1.0	-8.0 ±1.4	-12.3 ± 18%	-80. ± 20%
		3	0.113 ±0.010	15.0 ±1.2	26.9 ±1.2	-11.9 ±1.7	-18.4 ± 14%	-105. ± 17%
		4	0.128 ±0.012	17.2 ±1.4	30.4 ±1.4	-13.2 ±2.0	-20. ± 16%	-103. ± 18%
		5	0.135 ±0.014	18.4 ±1.7	33.2 ±1.7	-14.9 ±2.4	-23. ± 16%	-110. ± 19%
		6	0.142 ±0.017	19.4 ±1.9	36.4 ±1.9	-17.1 ±2.8	-26. ± 16%	-121. ± 20%
Ethene (High NOx)								
17	0.608	1	0.042 ±0.017	5.7 ±0.8	6.0 ±0.8	-0.4 ±1.2	(-0.6 ± 2.)	(-8. ± 28.)
		2	0.095 ±0.016	12.0 ±0.8	11.9 ±0.8	0.1 ±1.2	(0.2 ± 2.)	(1. ± 12.)
		3	0.155 ±0.016	19.4 ±0.8	17.8 ±0.8	1.6 ±1.2	2.6 ± 76%	10. ± 76%
		4	0.215 ±0.015	26.8 ±0.9	21.4 ±0.8	5.4 ±1.2	8.8 ± 23%	25. ± 24%
		5	0.279 ±0.015	34.0 ±0.9	24.9 ±0.9	9.1 ±1.2	14.9 ± 14%	33. ± 15%
		6	0.340 ±0.015	41.5 ±0.9	29.9 ±0.9	11.7 ±1.3	19.3 ± 11%	34. ± 12%
Ethene (Low NOx)								
38	0.659	1	0.103 ±0.018	12.6 ±0.9	12.3 ±0.9	0.2 ±1.2	(0.4 ± 2.)	(2. ± 12.)
		2	0.183 ±0.020	18.9 ±1.0	22.5 ±1.0	-3.5 ±1.4	-5.4 ± 40%	-19. ± 42%
		3	0.240 ±0.022	23.7 ±1.2	27.2 ±1.2	-3.5 ±1.7	-5.3 ± 49%	-14. ± 50%
		4	0.289 ±0.025	26.3 ±1.4	30.3 ±1.4	-4.0 ±2.0	-6.1 ± 51%	-14. ± 51%
		5	0.324 ±0.028	28.8 ±1.7	32.9 ±1.7	-4.1 ±2.4	-6.2 ± 58%	-13. ± 59%
		6	[b]	30.5 ±1.9	35.6 ±1.9	-5.1 ±2.8	-7.7 ± 54%	
Propene (High NOx)								
18	0.350	1	0.096 ±0.009	6.6 ±0.8	5.5 ±0.8	1.0 ±1.2	(3. ± 3.)	(11. ± 12.)
		2	0.211 ±0.008	15.6 ±0.8	11.7 ±0.8	3.9 ±1.2	11.2 ± 30%	19. ± 30%
		3	0.291 ±0.007	23.6 ±0.8	16.3 ±0.8	7.3 ±1.2	21. ± 16%	25. ± 16%
		4	0.328 ±0.007	31.4 ±0.9	21.5 ±0.8	9.9 ±1.2	28. ± 12%	30. ± 12%
		5	0.347 ±0.007	36.6 ±0.9	26.0 ±0.9	10.5 ±1.2	30. ± 12%	30. ± 12%
		6	0.348 ±0.007	41.0 ±0.9	31.1 ±0.9	9.9 ±1.3	28. ± 13%	28. ± 13%

Table 13 (continued)

ETC Run No	Added (ppm)	Time (hr)	Reacted (ppm)	IntOH (ppt-min) Test Run	IntOH (ppt-min) Base Run	IntOH (ppt-min) Change	Reactivity (ppt-min/ppm) Incremental	Reactivity (ppt-min/ppm) Mechanistic
Propene (Low NOx)								
32	0.305	1	0.099 ±0.007	10.5 ±0.8	12.6 ±0.8	-2.1 ±1.2	-6.8 ± 56%	-21. ± 57%
		2	0.216 ±0.006	18.0 ±0.8	21.2 ±0.8	-3.2 ±1.2	-10.4 ± 37%	-15. ± 37%
		3	0.271 ±0.006	20.9 ±0.8	27.0 ±0.8	-6.1 ±1.2	-20. ± 19%	-23. ± 19%
		4	0.289 ±0.006	23.2 ±0.8	30.9 ±0.8	-7.7 ±1.2	-25. ± 16%	-27. ± 16%
		5	0.298 ±0.006	25.8 ±0.9	34.2 ±0.9	-8.4 ±1.2	-27. ± 15%	-28. ± 15%
		6	0.303 ±0.006	27.5 ±0.9	37.3 ±0.9	-9.9 ±1.3	-32. ± 13%	-33. ± 13%
trans-2-Butene (High NOx)								
21	0.324	1	[b]	14.0 ±0.8	5.0 ±0.8	9.0 ±1.2	28. ± 13%	
		2	0.320 ±0.007	19.9 ±0.8	11.3 ±0.8	8.6 ±1.2	27. ± 14%	27. ± 14%
		3	0.320 ±0.007	23.6 ±0.8	16.2 ±0.8	7.4 ±1.2	23. ± 16%	23. ± 16%
		4	0.320 ±0.007	27.7 ±0.8	21.0 ±0.8	6.6 ±1.2	20. ± 18%	21. ± 18%
		5	0.320 ±0.007	31.6 ±0.9	25.3 ±0.9	6.3 ±1.2	19.5 ± 19%	20. ± 19%
		6	0.320 ±0.007	35.1 ±0.9	30.1 ±0.9	5.0 ±1.3	15.4 ± 25%	16. ± 25%
69	0.190	1	0.157 ±0.004	11.7 ±0.8	6.4 ±0.8	5.4 ±1.2	28. ± 22%	34. ± 22%
		2	0.190 ±0.004	19.6 ±0.8	12.7 ±0.8	7.0 ±1.2	37. ± 17%	37. ± 17%
		3	0.190 ±0.004	24.0 ±0.8	18.0 ±0.9	6.0 ±1.2	32. ± 20%	32. ± 20%
		4	0.190 ±0.004	29.3 ±0.9	21.8 ±0.9	7.4 ±1.2	39. ± 17%	39. ± 17%
		5	0.190 ±0.004	32.7 ±0.9	25.4 ±0.9	7.3 ±1.3	38. ± 18%	38. ± 18%
		6	0.190 ±0.004	37.0 ±0.9	-75.8 ±1.0	112.8 ±1.3	0.0 ± 0%	0. ± 0%
trans-2-Butene (Low NOx)								
33	0.156	1	[b]	15.5 ±0.8	12.1 ±0.8	3.4 ±1.2	22. ± 34%	
		2	0.154 ±0.004	20.7 ±0.8	21.5 ±0.8	-0.8 ±1.2	(-5. ± 8.)	(-5. ± 8.)
		3	0.154 ±0.004	22.7 ±0.8	26.1 ±0.8	-3.4 ±1.2	-22. ± 34%	-22. ± 34%
		4	0.154 ±0.004	25.7 ±0.8	30.0 ±0.8	-4.4 ±1.2	-28. ± 27%	-29. ± 27%
		5	0.154 ±0.004	27.5 ±0.9	33.2 ±0.9	-5.7 ±1.2	-37. ± 22%	-37. ± 22%
		6	0.154 ±0.004	29.6 ±0.9	34.9 ±0.9	-5.3 ±1.3	-34. ± 24%	-34. ± 24%
Benzene (Low NOx)								
39	7.39	1	0.147 ±0.012	10.7 ±0.8	12.4 ±0.8	-1.7 ±1.2	-0.24 ± 67%	-12. ± 67%
		2	0.213 ±0.012	15.5 ±0.8	18.7 ±0.8	-3.1 ±1.2	-0.42 ± 37%	-15. ± 38%
		3	0.250 ±0.012	18.3 ±0.8	25.5 ±0.8	-7.3 ±1.2	-0.98 ± 16%	-29. ± 17%
		4	0.261 ±0.013	19.1 ±0.8	29.5 ±0.8	-10.4 ±1.2	-1.41 ± 12%	-40. ± 13%
		5	0.280 ±0.013	20.5 ±0.9	31.8 ±0.9	-11.3 ±1.2	-1.52 ± 11%	-40. ± 12%
		6	0.296 ±0.014	21.8 ±0.9	34.8 ±0.9	-13.0 ±1.3	-1.76 ± 10%	-44. ± 11%
Toluene (High NOx)								
23	0.573	1	0.035 ±0.016	7.1 ±0.8	5.6 ±0.8	1.5 ±1.2	2.6 ± 78%	42. ± 90%
		2	0.077 ±0.015	16.4 ±0.8	11.8 ±0.8	4.6 ±1.2	8.1 ± 25%	60. ± 32%
		3	0.108 ±0.015	23.8 ±0.8	17.1 ±0.8	6.8 ±1.2	11.8 ± 18%	62. ± 22%
		4	0.143 ±0.015	33.0 ±0.8	20.9 ±0.8	12.2 ±1.2	21. ± 10%	85. ± 14%
		5	0.167 ±0.015	39.8 ±0.9	25.9 ±0.9	13.9 ±1.2	24. ± 9%	83. ± 13%
		6	0.181 ±0.015	44.3 ±0.9	30.6 ±0.9	13.6 ±1.3	24. ± 9%	75. ± 12%
Toluene (Low NOx)								
30	1.134	1	0.096 ±0.031	10.7 ±0.8	11.6 ±0.8	-0.9 ±1.2	(-0.8 ± 1.0)	(-9. ± 12.)
		2	0.145 ±0.031	16.4 ±0.8	18.3 ±0.8	-2.0 ±1.2	-1.73 ± 60%	-14. ± 63%
		3	0.159 ±0.031	18.5 ±0.8	24.9 ±0.8	-6.4 ±1.2	-5.7 ± 19%	-40. ± 27%
		4	0.176 ±0.031	20.5 ±0.8	29.8 ±0.8	-9.3 ±1.2	-8.2 ± 13%	-53. ± 22%
		5	0.186 ±0.031	21.7 ±0.9	32.4 ±0.9	-10.7 ±1.2	-9.4 ± 12%	-57. ± 20%
		6	0.201 ±0.032	23.3 ±0.9	35.1 ±0.9	-11.8 ±1.3	-10.4 ± 11%	-59. ± 19%
m-Xylene (High NOx)								
25	0.085	1	0.018 ±0.002	6.8 ±0.8	5.1 ±0.8	1.7 ±1.2	20. ± 67%	97. ± 68%
		2	0.034 ±0.002	15.0 ±0.8	11.4 ±0.8	3.6 ±1.2	42. ± 33%	105. ± 33%
		3	0.045 ±0.002	21.9 ±0.8	16.5 ±0.8	5.5 ±1.2	64. ± 22%	122. ± 22%
		4	0.054 ±0.002	29.8 ±0.8	21.2 ±0.8	8.6 ±1.2	102. ± 15%	158. ± 14%
		5	0.060 ±0.002	36.4 ±0.9	25.5 ±0.9	10.9 ±1.2	129. ± 12%	180. ± 12%
		6	0.066 ±0.002	44.4 ±0.9	31.1 ±0.9	13.2 ±1.3	156. ± 10%	200. ± 10%
68	0.064	1	0.014 ±0.002	7.2 ±0.8	6.4 ±0.8	0.8 ±1.2	(12. ± 18.)	(55. ± 82.)
		2	0.026 ±0.002	15.1 ±0.8	11.7 ±0.8	3.4 ±1.2	52. ± 35%	128. ± 35%
		3	0.032 ±0.001	20.3 ±0.8	16.0 ±0.8	4.3 ±1.2	67. ± 28%	134. ± 28%
		4	0.038 ±0.001	26.1 ±0.8	19.8 ±0.8	6.4 ±1.2	99. ± 20%	166. ± 19%
		5	0.043 ±0.001	32.6 ±0.9	24.4 ±0.9	8.2 ±1.2	128. ± 16%	190. ± 15%
		6	0.047 ±0.001	38.9 ±0.9	-75.9 ±0.9	114.8 ±1.3	0.0 ± 0%	0. ± 0%

Table 13 (continued)

ETC Run No	Added (ppm)	Time (hr)	Reacted (ppm)	IntOH (ppt-min) Test Run	IntOH (ppt-min) Base Run	IntOH (ppt-min) Change	Reactivity (ppt-min/ppm) Incremental	Reactivity (ppt-min/ppm) Mechanistic
m-Xylene (Low NOx)								
35	0.106	1	0.038 ±0.003	12.9 ±0.8	9.7 ±0.8	3.2 ±1.2	30. ± 37%	84. ± 37%
		2	0.052 ±0.002	19.6 ±0.8	18.7 ±0.8	0.9 ±1.2	(9. ± 11.)	(18. ± 22.)
		3	0.059 ±0.002	23.5 ±0.8	25.2 ±0.8	-1.7 ±1.2	-16.2 ± 69%	-29. ± 69%
		4	0.064 ±0.002	27.2 ±0.8	29.5 ±0.8	-2.3 ±1.2	-22. ± 53%	-35. ± 53%
		5	0.068 ±0.002	29.6 ±0.9	31.9 ±0.9	-2.3 ±1.2	-21. ± 54%	-34. ± 54%
		6	0.069 ±0.002	30.9 ±0.9	33.6 ±0.9	-2.7 ±1.3	-25. ± 47%	-39. ± 47%
67	0.173	1	0.068 ±0.004	14.4 ±0.9	12.9 ±0.9	1.5 ±1.2	8.7 ± 81%	22. ± 81%
		2	0.088 ±0.005	20.5 ±1.0	21.9 ±1.0	-1.5 ±1.4	-8.5 ± 96%	-17. ± 96%
		3	0.094 ±0.005	22.7 ±1.2	27.5 ±1.2	-4.7 ±1.7	-27. ± 36%	-50. ± 36%
		4	0.099 ±0.006	24.6 ±1.4	30.9 ±1.4	-6.3 ±2.0	-36. ± 33%	-63. ± 33%
		5	0.105 ±0.006	27.4 ±1.7	34.1 ±1.7	-6.7 ±2.4	-39. ± 36%	-64. ± 36%
		6	0.107 ±0.007	28.2 ±1.9	36.9 ±1.9	-8.7 ±2.8	-50. ± 32%	-81. ± 32%
Formaldehyde (High NOx)								
22	0.408	1	[b]	9.5 ±0.8	5.1 ±0.8	4.4 ±1.2	10.8 ± 26%	
		2	[b]	18.6 ±0.8	10.8 ±0.8	7.8 ±1.2	19.1 ± 15%	
		3	[b]	24.4 ±0.8	16.1 ±0.8	8.3 ±1.2	20. ± 14%	
		4	[b]	30.9 ±0.8	19.9 ±0.8	11.0 ±1.2	27. ± 11%	
		5	[b]	36.7 ±0.9	25.0 ±0.9	11.7 ±1.2	29. ± 11%	
		6	[b]	43.7 ±0.9	29.5 ±0.9	14.3 ±1.3	35. ± 9%	
Formaldehyde (Low NOx)								
36	0.247	1	[b]	13.6 ±0.8	11.6 ±0.8	2.1 ±1.2	8.4 ± 56%	
		2	[b]	22.0 ±0.8	19.3 ±0.8	2.6 ±1.2	10.7 ± 44%	
		3	[b]	26.3 ±0.8	23.7 ±0.8	2.6 ±1.2	10.7 ± 45%	
		4	[b]	28.6 ±0.8	26.6 ±0.8	1.9 ±1.2	7.9 ± 62%	
		5	[b]	32.0 ±0.9	30.2 ±0.9	1.8 ±1.2	7.4 ± 67%	
		6	[b]	33.5 ±0.9	32.0 ±0.9	1.6 ±1.3	6.3 ± 81%	
Acetaldehyde (High NOx)								
65	1.53	1	[b]	3.5 ±0.9	6.3 ±0.8	-2.8 ±1.2	-1.81 ± 43%	
		2	0.108 ±0.052	6.3 ±1.0	12.6 ±0.8	-6.2 ±1.3	-4.1 ± 21%	-58. ± 53%
		3	0.205 ±0.060	7.8 ±1.2	17.6 ±0.8	-9.8 ±1.5	-6.4 ± 15%	-48. ± 33%
		4	0.242 ±0.070	10.0 ±1.4	21.9 ±0.8	-11.9 ±1.7	-7.8 ± 14%	-49. ± 32%
		5	0.292 ±0.081	11.5 ±1.7	26.6 ±0.9	-15.1 ±1.9	-9.8 ± 13%	-52. ± 30%
		6	0.377 ±0.091	14.6 ±1.9	31.2 ±0.9	-16.6 ±2.1	-10.8 ± 13%	-44. ± 27%
Acetaldehyde (Low NOx)								
66	1.62	1	[b]	2.6 ±0.9	12.4 ±0.9	-9.8 ±1.2	-6.1 ± 13%	
		2	0.092 ±0.055	3.9 ±1.0	21.2 ±1.0	-17.3 ±1.4	-10.7 ± 8%	-188. ± 60%
		3	0.131 ±0.065	5.3 ±1.2	26.7 ±1.2	-21.4 ±1.7	-13.2 ± 8%	-164. ± 50%
		4	0.168 ±0.076	6.0 ±1.4	30.5 ±1.4	-24.5 ±2.0	-15.1 ± 9%	-146. ± 46%
		5	0.206 ±0.088	6.7 ±1.7	33.3 ±1.7	-26.6 ±2.4	-16.4 ± 9%	-129. ± 43%
		6	0.247 ±0.100	7.8 ±1.9	36.3 ±1.9	-28.5 ±2.8	-17.6 ± 10%	-115. ± 42%

[a] Amount reacted could not be determined for this VOC, or amount reacted could not be determined for this time with sufficient precision to be useful.

3. Low NO_x Reactivity Results

Low NO_x lumped surrogate reactivity experiments were carried out for each of the 8 surrogate components plus carbon monoxide, benzene, and acetaldehyde. Two reactivity experiments were carried out for n-octane and m-xylene, and one experiment was carried out for the other VOCs. The detailed results and reactivity analysis of the low NO_x surrogate experiments are given with the other DTC surrogate reactivity experiments in Tables 12-14, and plots of selected reactivity results for the low NO_x runs are shown on Figures 39-49. Model calculations, discussed later, are also shown.

Table 14. Derivation of the hourly direct reactivities from the results of the lumped molecule surrogate reactivity experiments. [a]

ETC Run No.	Added (ppm)	Time (hr)	Reacted (ppm)	IntOH (ppt-min)	d(O3-NO)/ IntOH (base) (10^3 min-1)	d(O3-NO) (ppm) Total	d(O3-NO) (ppm) From Base ROG	Direct d(O3-NO) Reactivity (mol d(O3-NO)/mol VOC) Incremental	Direct d(O3-NO) Reactivity (mol d(O3-NO)/mol VOC) Mechanistic
Carbon Monoxide (High NOx)									
14	155.	1	0.363+12%	6.7+0.8	36.3+ 5.3	0.548	0.242+0.046	0.0020 + 15%	0.8 +19%
		2	0.635+ 7%	11.8+0.8	33.8+ 2.3	0.907	0.398+0.039	0.0033 + 8%	0.8 +10%
		3	0.870+ 5%	16.2+0.9	32.2+ 1.6	1.135	0.521+0.038	0.0040 + 6%	0.7 + 8%
		4	0.978+ 5%	18.3+0.9	30.3+ 1.2	1.301	0.553+0.035	0.0048 + 5%	0.8 + 7%
		5	1.107+ 5%	20.8+0.9	27.8+ 0.9	1.405	0.579+0.032	0.0053 + 4%	0.7 + 6%
		6	1.209+ 5%	22.8+1.0	26.5+ 0.8	1.463	0.605+0.031	0.0055 + 4%	0.7 + 6%
15	161.	1	0.396+12%	7.0+0.8	37.2+ 5.3	0.637	0.262+0.048	0.0023 + 13%	0.9 +17%
		2	0.649+ 7%	11.6+0.8	37.0+ 2.6	1.023	0.431+0.043	0.0037 + 7%	0.9 +10%
		3	0.857+ 6%	15.5+0.8	34.2+ 1.8	1.266	0.529+0.040	0.0046 + 5%	0.9 + 8%
		4	1.100+ 4%	20.0+0.9	30.6+ 1.2	1.417	0.613+0.036	0.0050 + 4%	0.7 + 6%
		5	1.244+ 4%	22.8+0.9	28.7+ 1.0	1.501	0.655+0.034	0.0052 + 4%	0.7 + 6%
16	74.2	1	0.155+14%	6.0+0.8	37.8+ 6.0	0.354	0.226+0.047	0.0017 + 37%	0.8 +39%
		2	0.297+ 7%	11.5+0.8	34.5+ 2.4	0.654	0.397+0.040	0.0035 + 16%	0.9 +17%
		3	0.400+ 5%	15.6+0.8	32.0+ 1.6	0.835	0.498+0.037	0.0045 + 11%	0.8 +12%
		4	0.496+ 5%	19.4+0.9	30.3+ 1.3	0.992	0.589+0.036	0.0054 + 9%	0.8 +10%
		5	0.606+ 4%	23.8+0.9	28.6+ 1.0	1.121	0.681+0.035	0.0059 + 8%	0.7 + 9%
		6	0.684+ 4%	27.0+0.9	26.8+ 0.8	1.223	0.723+0.033	0.0067 + 7%	0.7 + 8%
20	103.	1	0.154+19%	4.3+0.8	32.3+ 6.4	0.316	0.137+0.038	0.0017 + 21%	1.2 +29%
		2	0.306+10%	8.5+0.8	35.5+ 3.3	0.656	0.300+0.040	0.0034 + 11%	1.2 +15%
		3	0.455+ 7%	12.6+0.8	30.7+ 1.8	0.837	0.387+0.034	0.0044 + 8%	1.0 +10%
		4	0.622+ 5%	17.3+0.8	29.2+ 1.4	0.999	0.505+0.034	0.0048 + 7%	0.8 + 9%
		5	0.738+ 4%	20.5+0.9	26.4+ 1.0	1.140	0.543+0.031	0.0058 + 5%	0.8 + 7%
		6	0.869+ 4%	24.3+0.9	26.3+ 0.9	1.251	0.640+0.032	0.0059 + 5%	0.7 + 7%
Carbon Monoxide (Low NOx)									
29	85.8	1	0.282+ 9%	9.4+0.8	29.4+ 1.9	0.557	0.275+0.030	0.0033 + 11%	1.0 +14%
		2	0.437+ 6%	14.5+0.8	27.0+ 1.1	0.735	0.392+0.028	0.0040 + 8%	0.8 +10%
n-Butane (High NOx)									
19	6.48	1	0.098+20%	4.0+0.8	34.7+ 5.2	0.372	0.140+0.035	0.036 + 15%	2.4 +25%
		2	0.203+10%	8.5+0.8	35.0+ 2.6	0.716	0.296+0.036	0.065 + 9%	2.1 +13%
		3	0.273+ 7%	11.4+0.8	31.3+ 1.6	0.907	0.358+0.032	0.085 + 6%	2.0 + 9%
		4	0.333+ 6%	14.0+0.8	28.6+ 1.2	1.073	0.402+0.029	0.104 + 5%	2.0 + 8%
		5	0.395+ 6%	16.8+0.9	27.2+ 0.9	1.207	0.456+0.028	0.116 + 4%	1.9 + 7%
		6	0.441+ 5%	18.8+0.9	25.1+ 0.7	1.295	0.472+0.026	0.127 + 4%	1.9 + 6%
n-Butane (Low NOx)									
31	5.48	1	0.119+14%	5.8+0.8	39.7+ 3.7	0.523	0.232+0.039	0.053 + 14%	2.5 +19%
		2	0.185+ 9%	9.2+0.8	27.4+ 1.2	0.701	0.251+0.025	0.082 + 6%	2.4 +11%
n-Octane (High NOx)									
24	1.102	1	[c]	2.1+0.8	43.1+ 7.4	0.176	0.091+0.039	0.077 + 46%	
		2	0.073+42%	4.9+0.8	38.1+ 3.0	0.409	0.186+0.035	0.20 + 16%	3.1 +45%
		3	0.117+26%	7.9+0.8	34.4+ 1.9	0.586	0.271+0.032	0.29 + 10%	2.7 +28%
		4	0.154+20%	10.7+0.8	31.0+ 1.3	0.720	0.331+0.030	0.35 + 8%	2.5 +21%
		5	0.179+17%	13.1+0.9	29.3+ 1.0	0.857	0.384+0.029	0.43 + 6%	2.6 +18%
		6	0.216+14%	16.1+0.9	27.9+ 0.8	0.995	0.450+0.028	0.49 + 6%	2.5 +15%
70	0.746	1	0.039+54%	4.2+0.8	26.7+ 3.3	0.160	0.111+0.026	0.066 + 53%	1.3 +75%
		2	0.080+26%	8.1+0.8	31.3+ 2.2	0.382	0.253+0.031	0.173 + 24%	1.6 +35%
		3	0.110+18%	11.5+0.8	29.6+ 1.5	0.543	0.340+0.030	0.27 + 15%	1.8 +24%
		4	0.132+15%	14.0+0.8	28.0+ 1.2	0.658	0.391+0.029	0.36 + 11%	2.0 +19%
		5	0.157+13%	17.3+0.9	26.3+ 0.9	0.765	0.454+0.028	0.42 + 9%	2.0 +16%
		6	0.176+12%	19.7+0.9	24.8+ 0.7	0.870	0.488+0.026	0.51 + 7%	2.2 +13%
n-Octane (Low NOx)									
37	1.126	1	0.065+48%	4.8+0.8	24.8+ 1.6	0.326	0.119+0.022	0.183 + 11%	3.2 +49%
		2	0.128+24%	9.5+0.8	25.2+ 1.2	0.543	0.239+0.024	0.27 + 8%	2.4 +25%
71	0.647	1	0.057+12%	7.1+0.9	25.2+ 1.7	0.299	0.180+0.025	0.184 + 21%	2.1 +24%
		2	0.100+ 8%	13.0+1.0	23.4+ 1.1	0.520	0.304+0.028	0.33 + 13%	2.2 +15%
Ethene (High NOx)									
17	0.608	1	0.042+40%	5.7+0.8	32.5+ 4.4	0.285	0.184+0.037	0.167 + 36%	2.4 +54%
		2	0.095+17%	12.0+0.8	33.5+ 2.3	0.563	0.401+0.039	0.27 + 24%	1.7 +30%
		3	0.155+10%	19.4+0.8	29.0+ 1.4	0.755	0.564+0.036	0.31 + 19%	1.2 +21%
		4	0.215+ 7%	26.8+0.9	28.5+ 1.1	0.938	0.763+0.039	0.29 + 22%	0.8 +23%
		5	0.279+ 5%	34.0+0.9	27.9+ 1.0	1.093	0.948+0.041	0.24 + 29%	0.5 +29%
		6	0.340+ 4%	41.5+0.9	26.1+ 0.8	1.188	1.084+0.040	0.171 + 39%	0.3 +39%

Table 14 (continued)

ETC Run No.	Added (ppm)	Time (hr)	Reacted (ppm)	IntOH (ppt-min)	d(O3-NO)/ IntOH (base) (10^3 min-1)	d(O3-NO) (ppm) Total	d(O3-NO) (ppm) From Base ROG	Direct d(O3-NO) Reactivity (mol d(O3-NO)/mol VOC) Incremental	Direct d(O3-NO) Reactivity (mol d(O3-NO)/mol VOC) Mechanistic
Ethene (Low NOx)									
38	0.659	1	0.103+18%	12.6+0.9	27.4+ 1.9	0.464	0.345+0.034	0.181 + 29%	1.2 +34%
Propene (High NOx)									
18	0.350	1	0.096+ 9%	6.6+0.8	41.5+ 6.1	0.402	0.272+0.053	0.37 + 41%	1.4 +42%
		2	0.211+ 4%	15.6+0.8	37.5+ 2.7	0.728	0.584+0.052	0.41 + 36%	0.7 +36%
		3	0.291+ 3%	23.6+0.8	34.2+ 1.8	0.960	0.807+0.051	0.44 + 33%	0.5 +33%
		4	0.328+ 2%	31.4+0.9	30.5+ 1.2	1.093	0.956+0.046	0.39 + 34%	0.4 +34%
		5	0.347+ 2%	36.6+0.9	28.7+ 1.0	1.157	1.050+0.043	0.31 + 40%	0.3 +40%
		6	0.348+ 2%	41.0+0.9	26.9+ 0.8	1.169	1.103+0.040	0.190 + 60%	0.2 +60%
Propene (Low NOx)									
32	0.305	1	0.099+ 8%	10.5+0.8	26.6+ 1.7	0.510	0.279+0.028	0.76 + 12%	2.3 +14%
trans-2-Butene (High NOx)									
21	0.324	1	[c]	14.0+0.8	40.4+ 6.7	0.773	0.566+0.099	0.64 + 48%	
	+0.007	2	0.320+ 2%	19.9+0.8	36.2+ 2.7	0.901	0.718+0.061	0.56 + 33%	0.6 +33%
		3	0.320+ 2%	23.6+0.8	32.3+ 1.7	0.998	0.763+0.048	0.72 + 20%	0.7 +20%
		4	0.320+ 2%	27.7+0.8	29.0+ 1.2	1.070	0.802+0.041	0.83 + 15%	0.8 +15%
		5	0.320+ 2%	31.6+0.9	27.4+ 0.9	1.110	0.867+0.038	0.75 + 16%	0.8 +16%
		6	0.320+ 2%	35.1+0.9	25.6+ 0.8	1.118	0.900+0.035	0.67 + 16%	0.7 +16%
69	0.190	1	0.157+ 2%	11.7+0.8	27.5+ 3.6	0.503	0.322+0.047	0.95 + 26%	1.1 +26%
		2	0.190+ 2%	19.6+0.8	29.2+ 1.9	0.694	0.573+0.045	0.64 + 37%	0.6 +37%
		3	0.190+ 2%	24.0+0.8	27.3+ 1.3	0.793	0.655+0.039	0.73 + 28%	0.7 +28%
		4	0.190+ 2%	29.3+0.9	26.7+ 1.1	0.894	0.781+0.039	0.59 + 35%	0.6 +35%
		5	0.190+ 2%	32.7+0.9	26.4+ 1.0	0.984	0.863+0.039	0.64 + 32%	0.6 +32%
trans-2-Butene (Low NOx)									
33	0.156	1	[c]	15.5+0.8	28.4+ 1.9	0.476	0.440+0.038	(0.2 + 0.2)	
Benzene (Low NOx)									
39	7.39	1	0.147+ 8%	10.7+0.8	28.0+ 1.9	0.486	0.299+0.030	0.025 + 16%	1.3 +18%
Toluene (High NOx)									
23	0.573	3	0.108+14%	23.8+0.8	30.0+ 1.5	0.822	0.716+0.043	0.185 + 41%	1.0 +43%
		4	0.143+10%	33.0+0.8	29.4+ 1.2	1.003	0.971+0.047	(0.06 +0.08)	(0.2 +0.3)
		5	0.167+ 9%	39.8+0.9	27.3+ 0.9	1.080	1.087+0.043	(-0.013 +0.08)	(0.0 +0.3)
		6	0.181+ 8%	44.3+0.9	26.1+ 0.8	1.083	1.156+0.041	-0.128 + 55%	-0.4 +56%
Toluene (Low NOx)									
30	1.134	1	0.096+32%	10.7+0.8	28.5+ 2.0	0.471	0.305+0.032	0.147 + 19%	1.7 +38%
Acetaldehyde (High NOx)									
65	1.53	1	[c]	3.5+0.9	26.9+ 3.5	0.353	0.094+0.026	0.169 + 10%	
		2	0.108+48%	6.3+1.0	29.3+ 1.9	0.543	0.185+0.032	0.23 + 9%	3.3 +49%
		3	0.205+29%	7.8+1.2	27.9+ 1.3	0.670	0.218+0.035	0.29 + 8%	2.2 +30%
		4	0.242+29%	10.0+1.4	26.6+ 1.0	0.786	0.265+0.039	0.34 + 8%	2.1 +30%
		5	0.292+28%	11.5+1.7	25.0+ 0.8	0.893	0.289+0.043	0.39 + 7%	2.1 +29%
		6	0.377+24%	14.6+1.9	24.0+ 0.7	0.977	0.351+0.048	0.41 + 8%	1.7 +25%
Acetaldehyde (Low NOx)									
66	1.62	1	[c]	2.6+0.9	25.6+ 1.8	0.297	0.066+0.023	0.143 + 10%	
	+0.03	2	0.092+60%	3.9+1.0	23.1+ 1.1	0.429	0.090+0.024	0.21 + 7%	3.7 +60%

[a] Data are not shown for times in runs where it appears that O_3 formation is becoming NO_x-limited, because the assumptions behind the derivation of direct reactivities are not valid for such conditions. Data are also not shown when the uncertainties of the direct reactivity estimates are too high to provide meaningful data.
[b] Amount reacted could not be determined for this time with sufficient precision to be useful.
[c] This is a DTC run. "Base fit" data is from base case run carried out in the other side of the chamber.

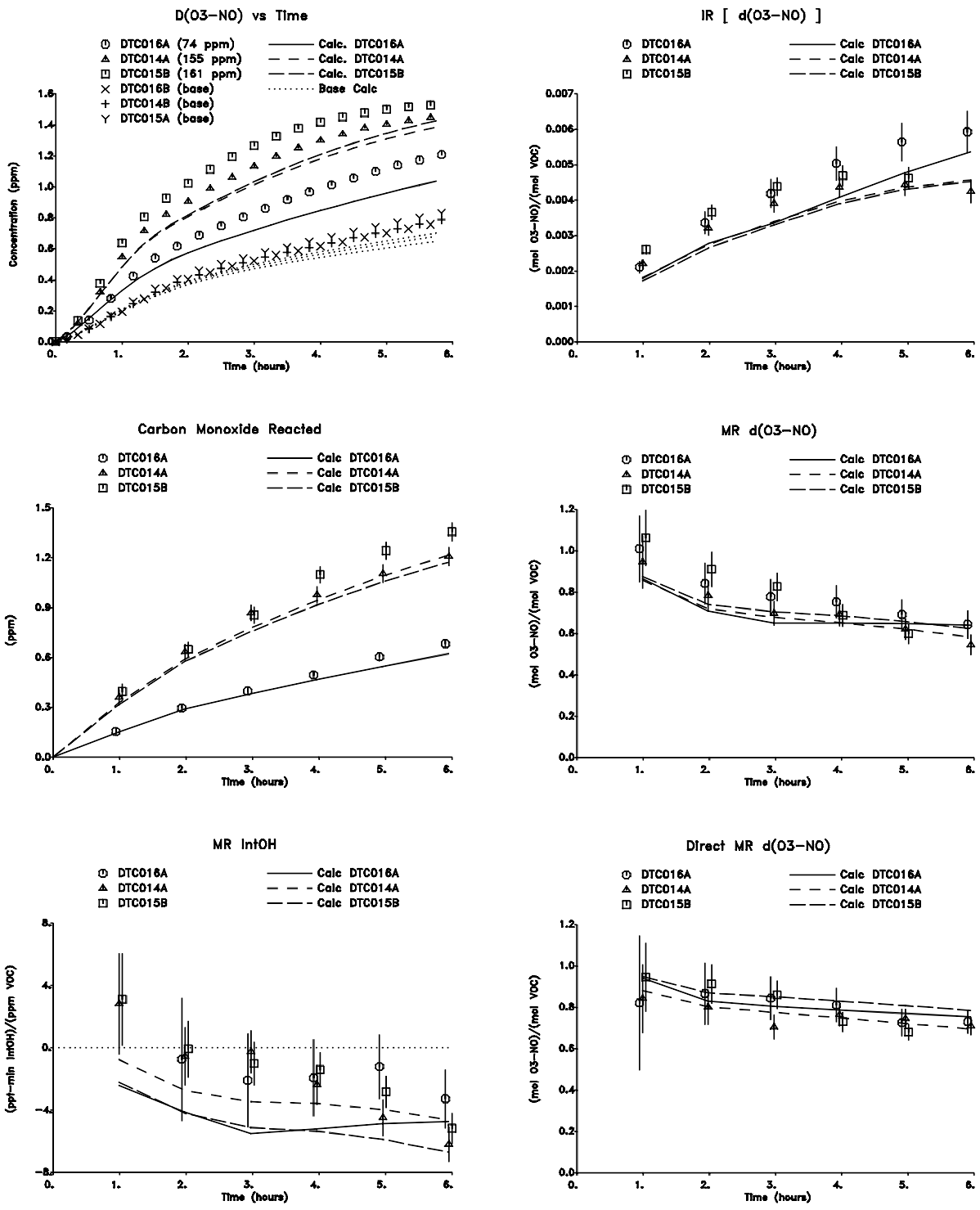

Figure 29. Plots of selected results of the high NO_x lumped molecule surrogate reactivity experiments for **carbon monoxide**

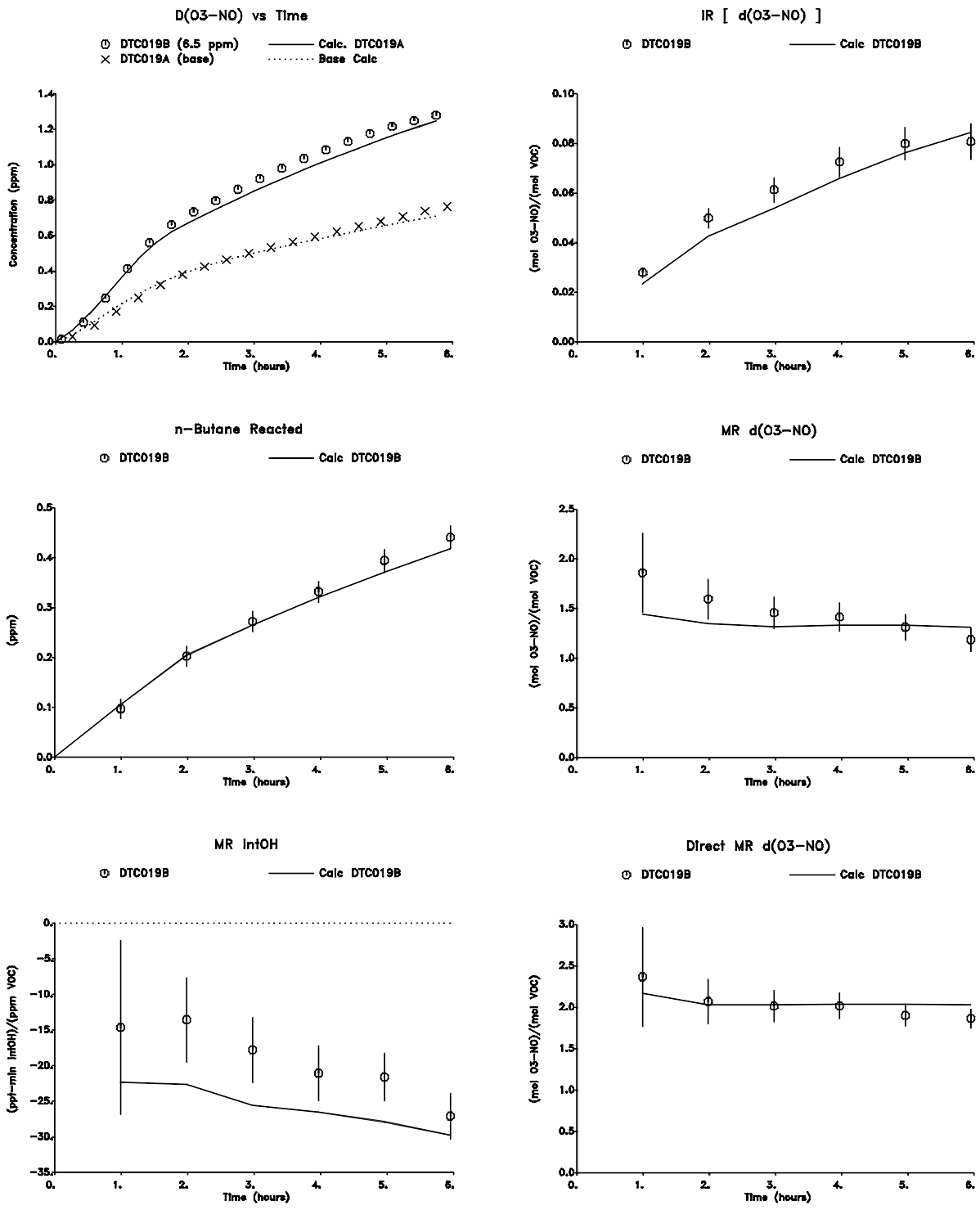

Figure 30. Plots of selected results of the high NO_x lumped molecule surrogate reactivity experiment for **n-butane**

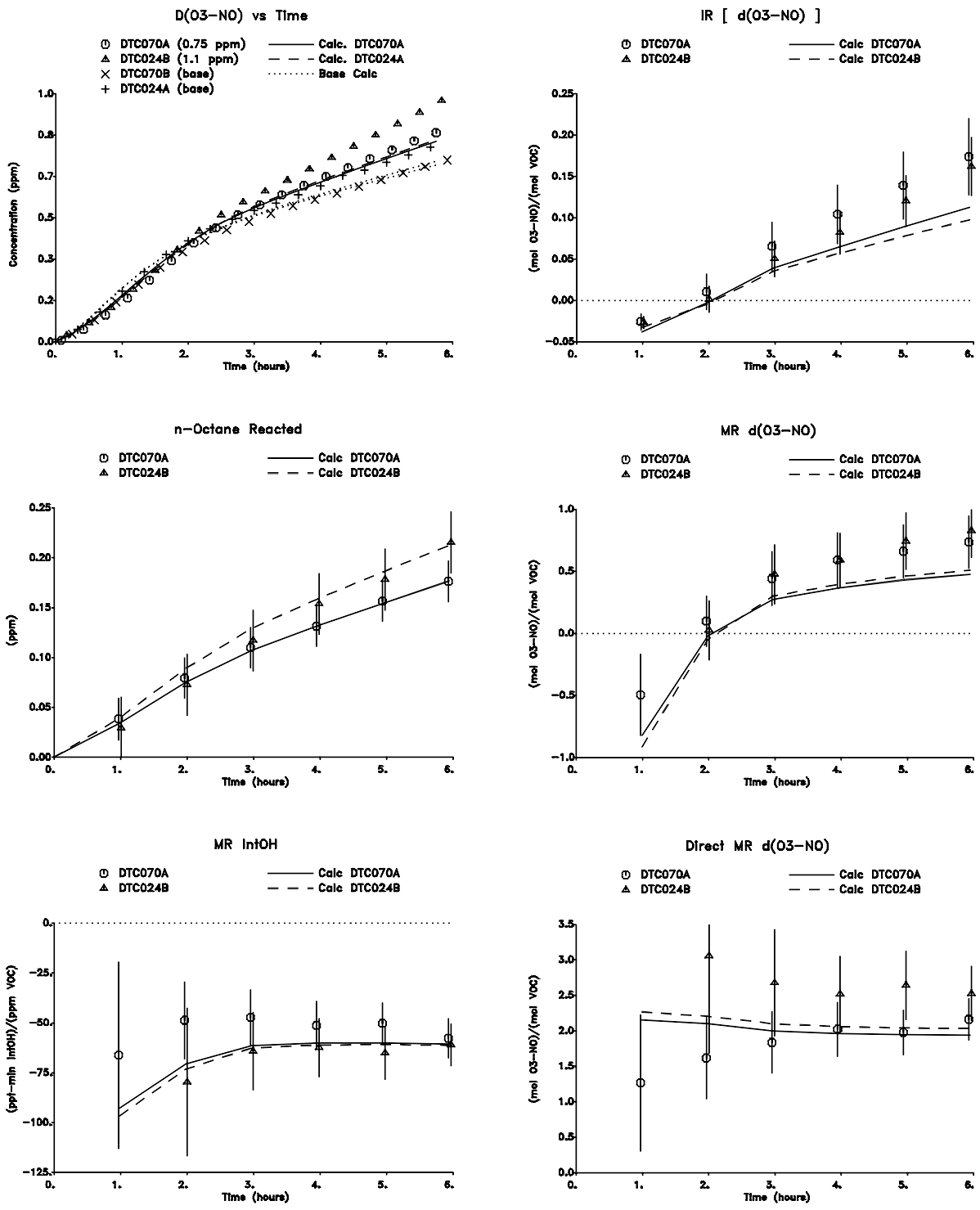

Figure 31. Plots of selected results of the high NO_x lumped molecule surrogate reactivity experiments for **n-octane**

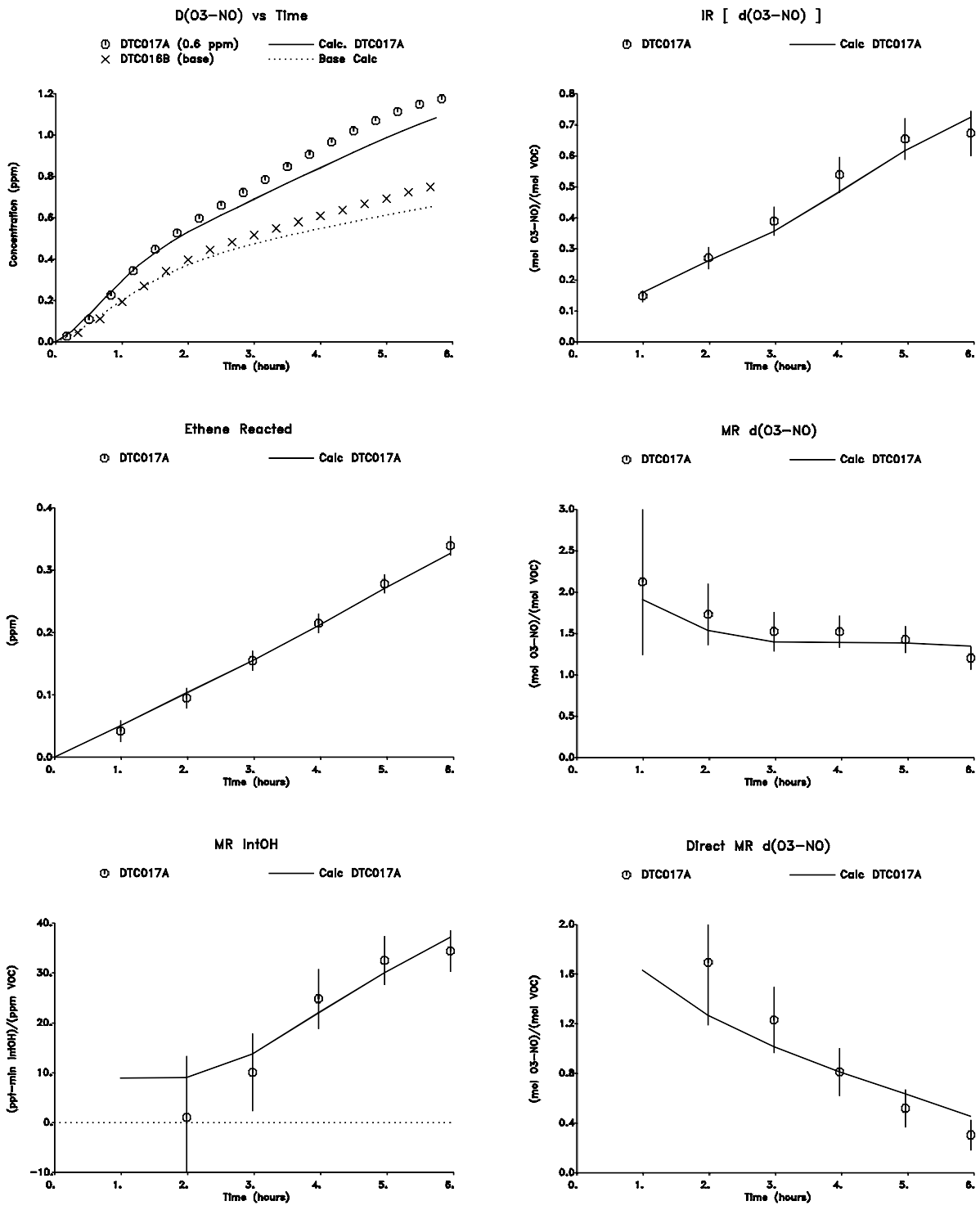

Figure 32. Plots of selected results of the high NO_x lumped molecule surrogate reactivity experiment for **ethene**

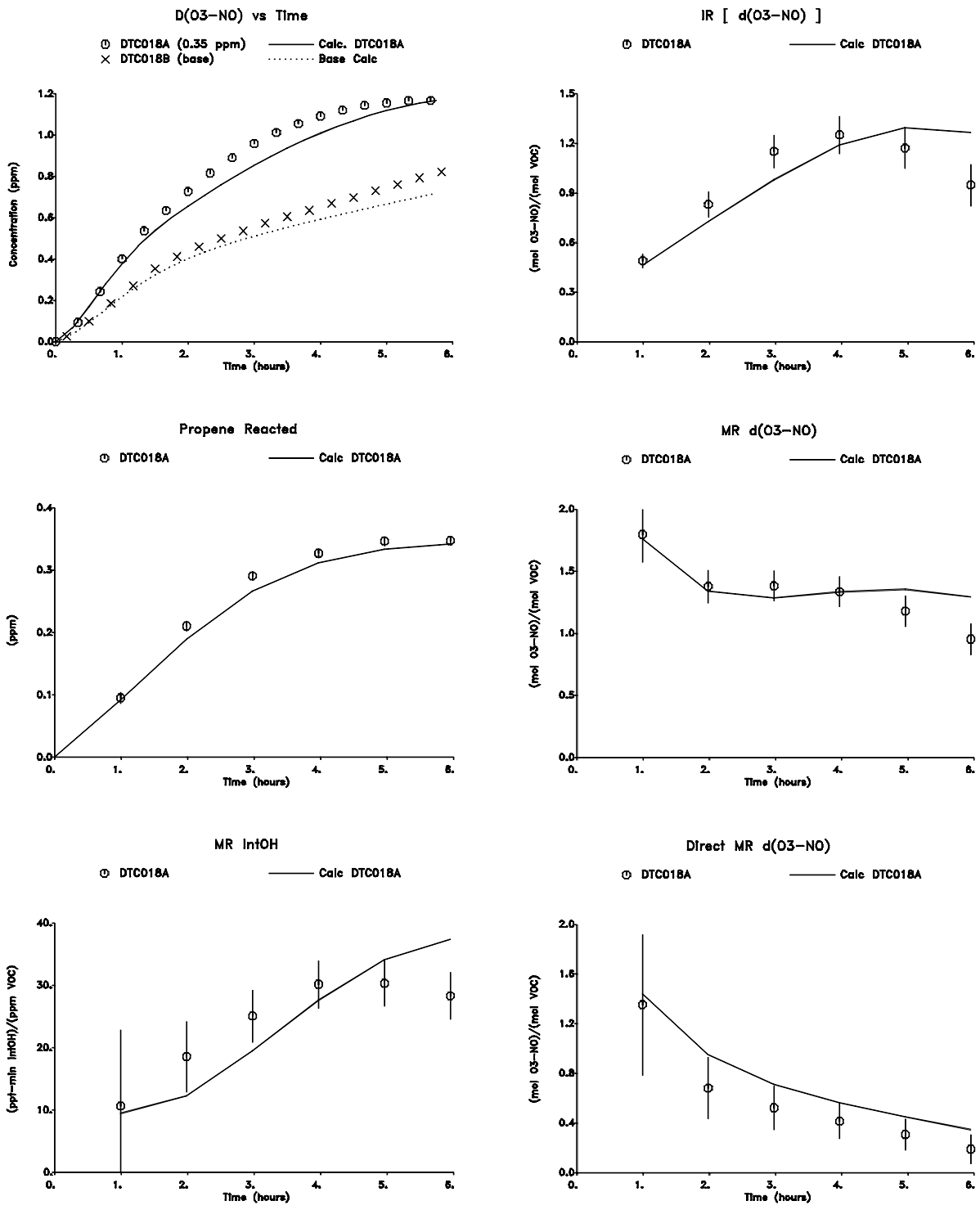

Figure 33. Plots of selected results of the high NO_x lumped molecule surrogate reactivity experiment for **propene**

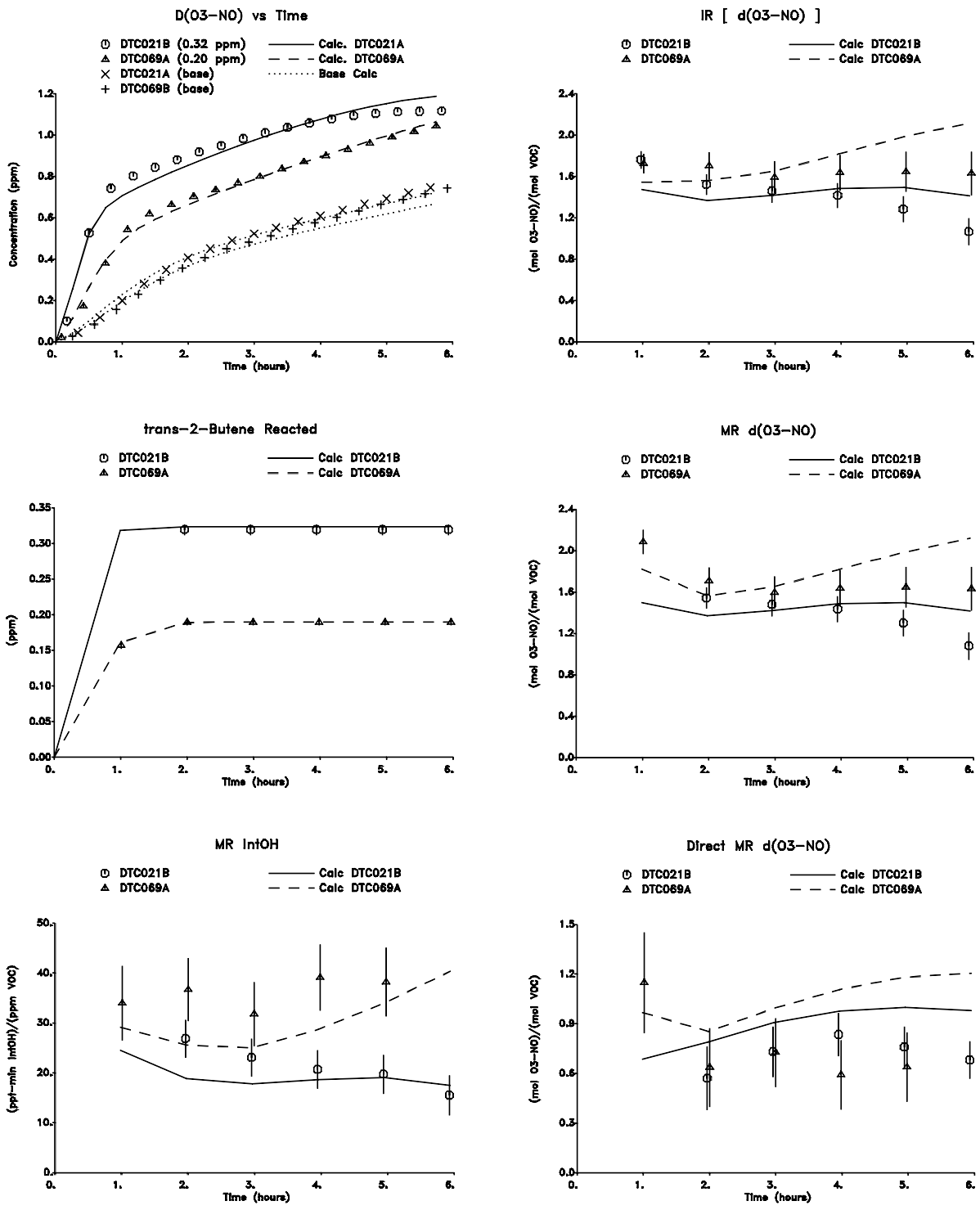

Figure 34. Plots of selected results of the high NO_x lumped molecule surrogate reactivity experiments for **trans-2-Butene**

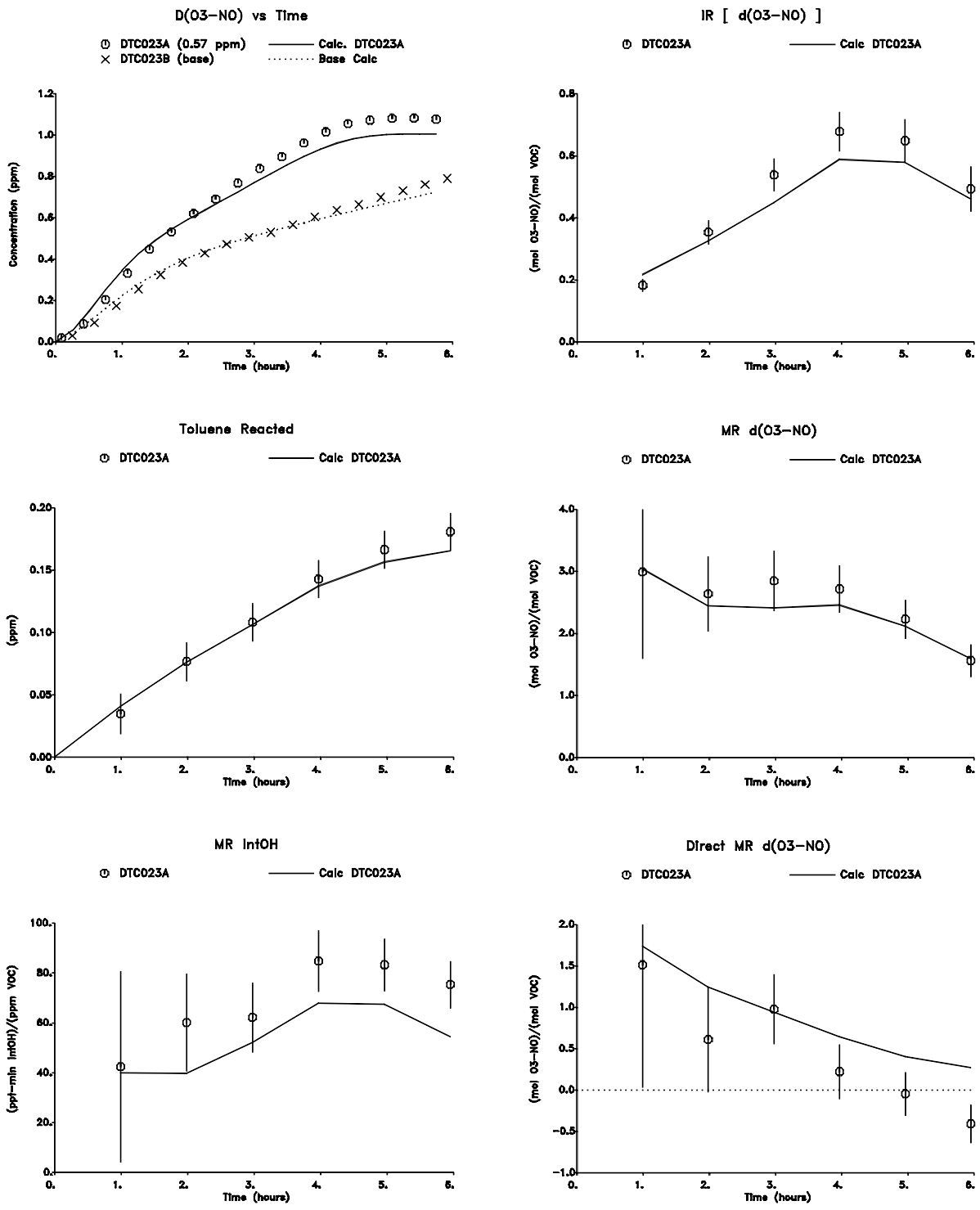

Figure 35. Plots of selected results of the high NO_x lumped molecule surrogate reactivity experiment for **toluene**