

Diagnostic Testing in the Evaluation of CMAQ Against Observations from SOS Field Intensives

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Problem Background

[O₃] in a model cell or from an observation is a **nonunique resultant from complex interactions of multiple processes** :

- emissions
- horizontal and vertical advection and diffusion
- chemical production and loss
- deposition

Compensating errors can lead to cases of **“right for the wrong reasons”**

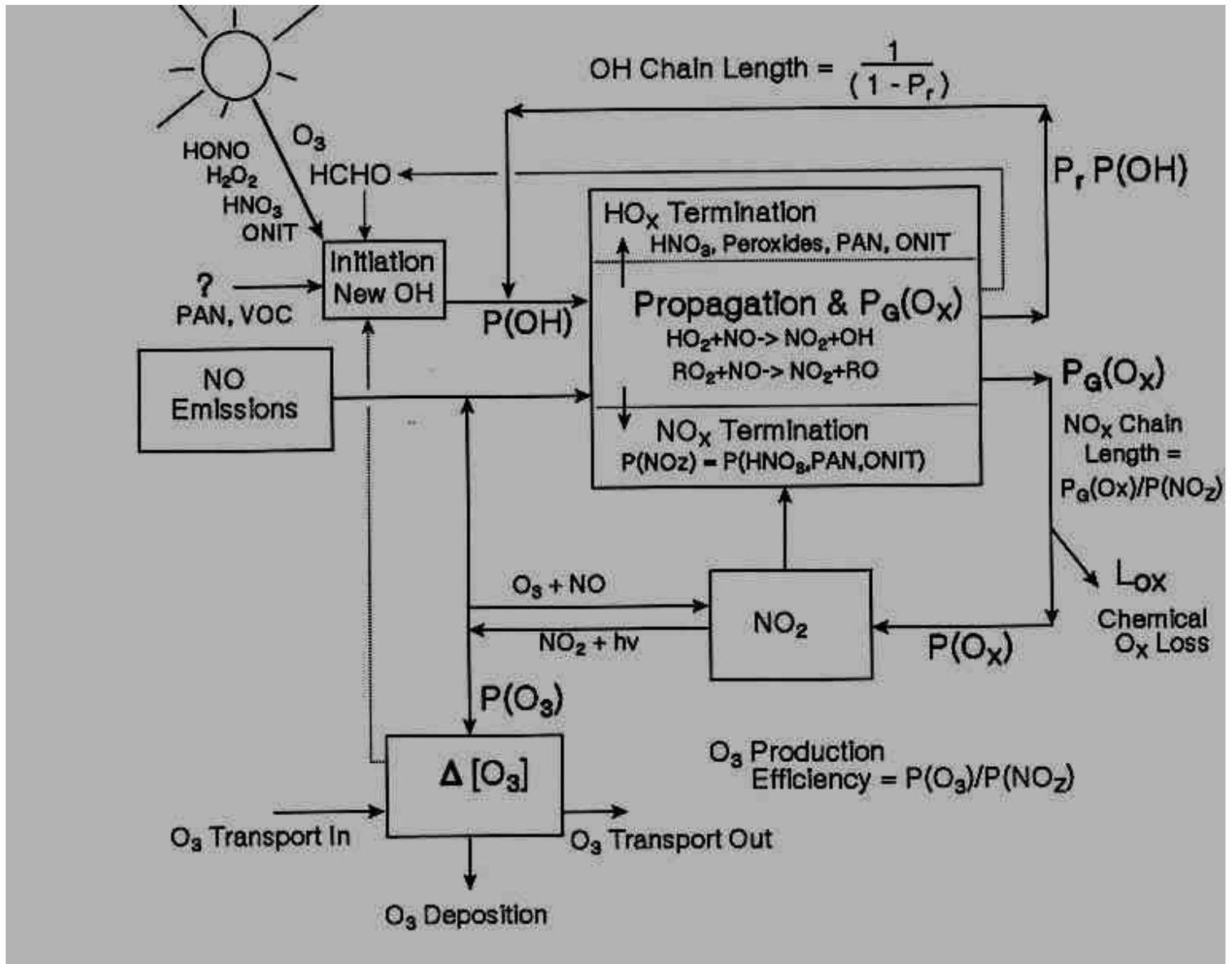
- historical performance evaluation statistics on bias, gross error, and peak prediction accuracy for [O₃] **cannot distinguish these cases**

Regulatory use of the models for predicting control strategy effects means there are **no direct tests for most applications**

- we wish to avoid potentially costly errors in predicting effects, so we must have an **accurate appraisal of the type and size of controls**

Thus, model credibility and user confidence are established by **diagnostically probing process and mechanism representations in the model, checking where possible against analogous tests of photochemical dynamics in ambient atmospheres**

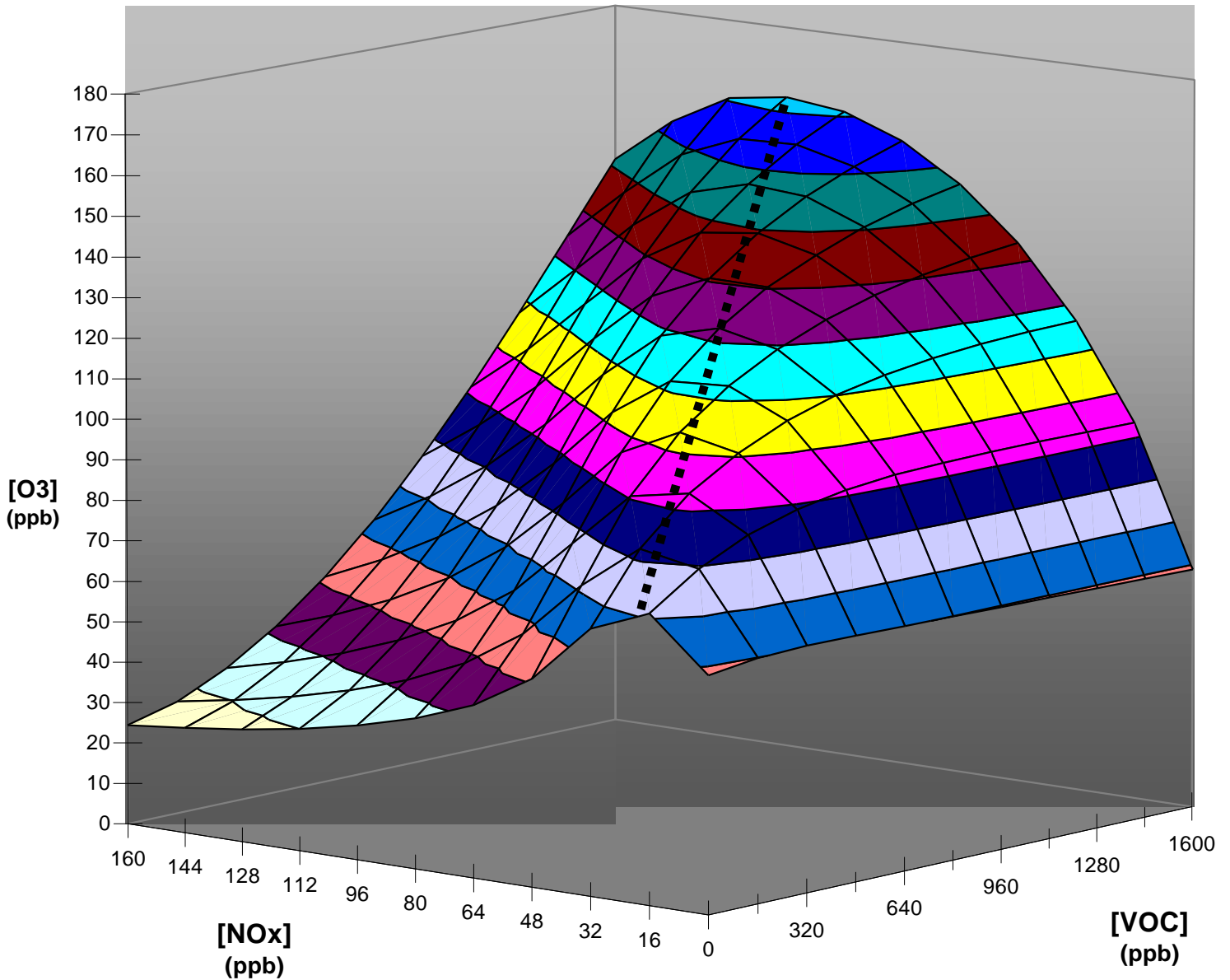
Conceptual Model of Photochemical Dynamics



Key concepts :

- HO_x initiation, propagation, termination
- OH chain length
- **NO_x termination**
- NO_x chain length
- **O_x and O₃ production efficiencies**

Ozone Response Surface



Key concepts :

- daily peak $[O_3]$ from varying initial VOC and NO_x
- nonlinear O_3 response
- **ridgeline of maximum peak $[O_3]$**

Taxonomy of Diagnostic Probes of Photochemical Dynamics

Individual Component Aspects :

- HO_x initiation
- HO_x termination
- Termination pathway competition
- Air mass aging

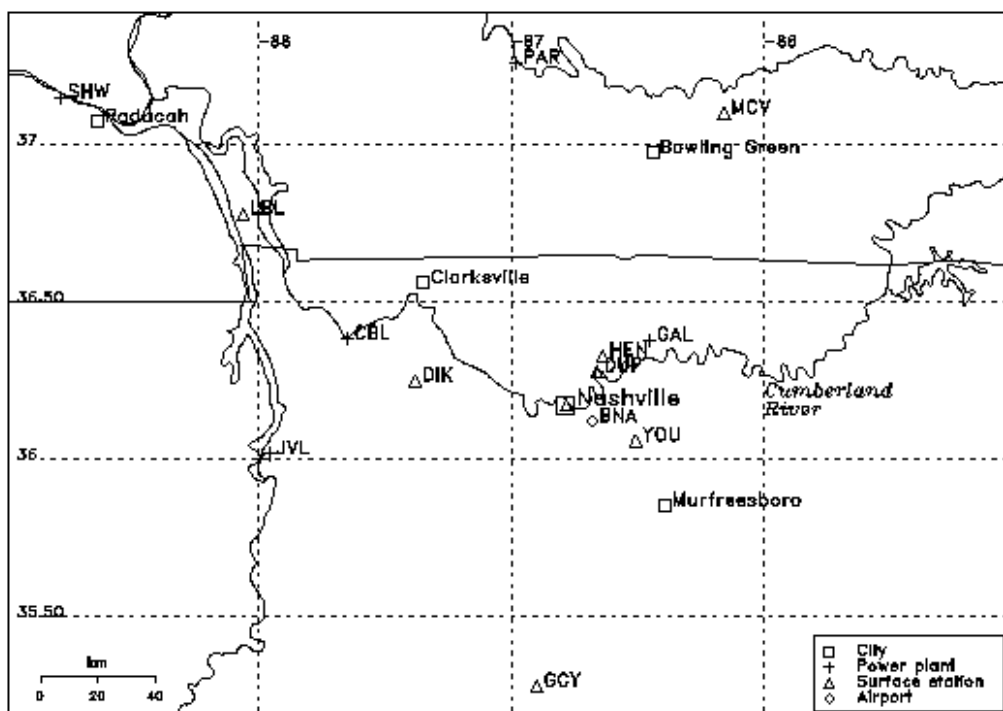
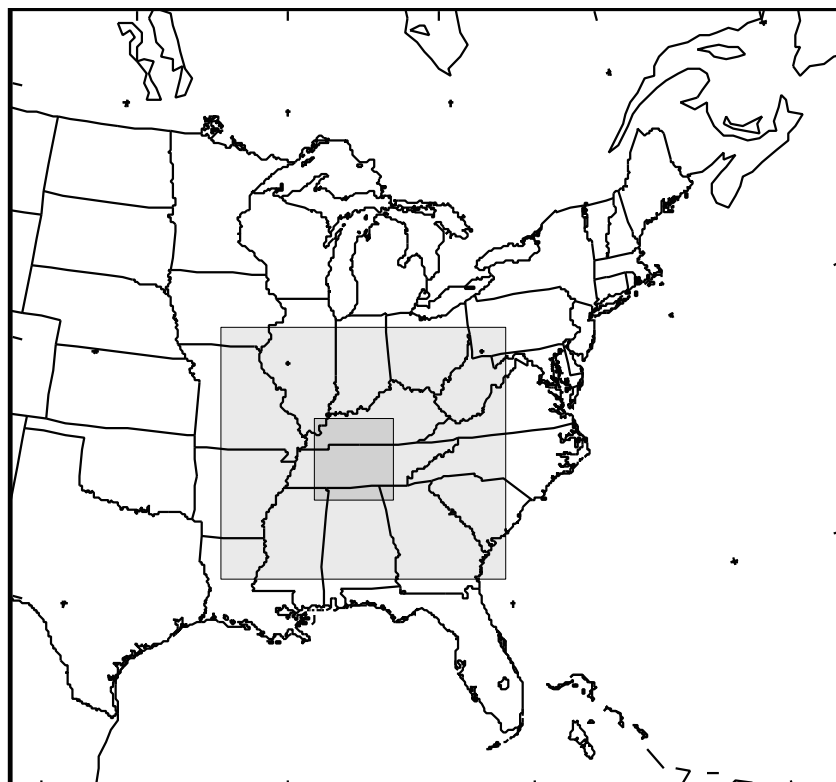
Process Aspects :

- OH production
- HO_x propagation
- OH propagation efficiency, Pr(OH)
- OH chain length
- NO_x chain length
- P(O₃) efficiency per NO_x terminated

Response Surface Aspects :

- Location of the ridgeline in the response surface
- System state relative to the response surface ridgeline
- Slope of the radical-limited response surface domain
- Slope of the NO_x-limited response surface domain

CMAQ Model Domains and SOS 95 Sites

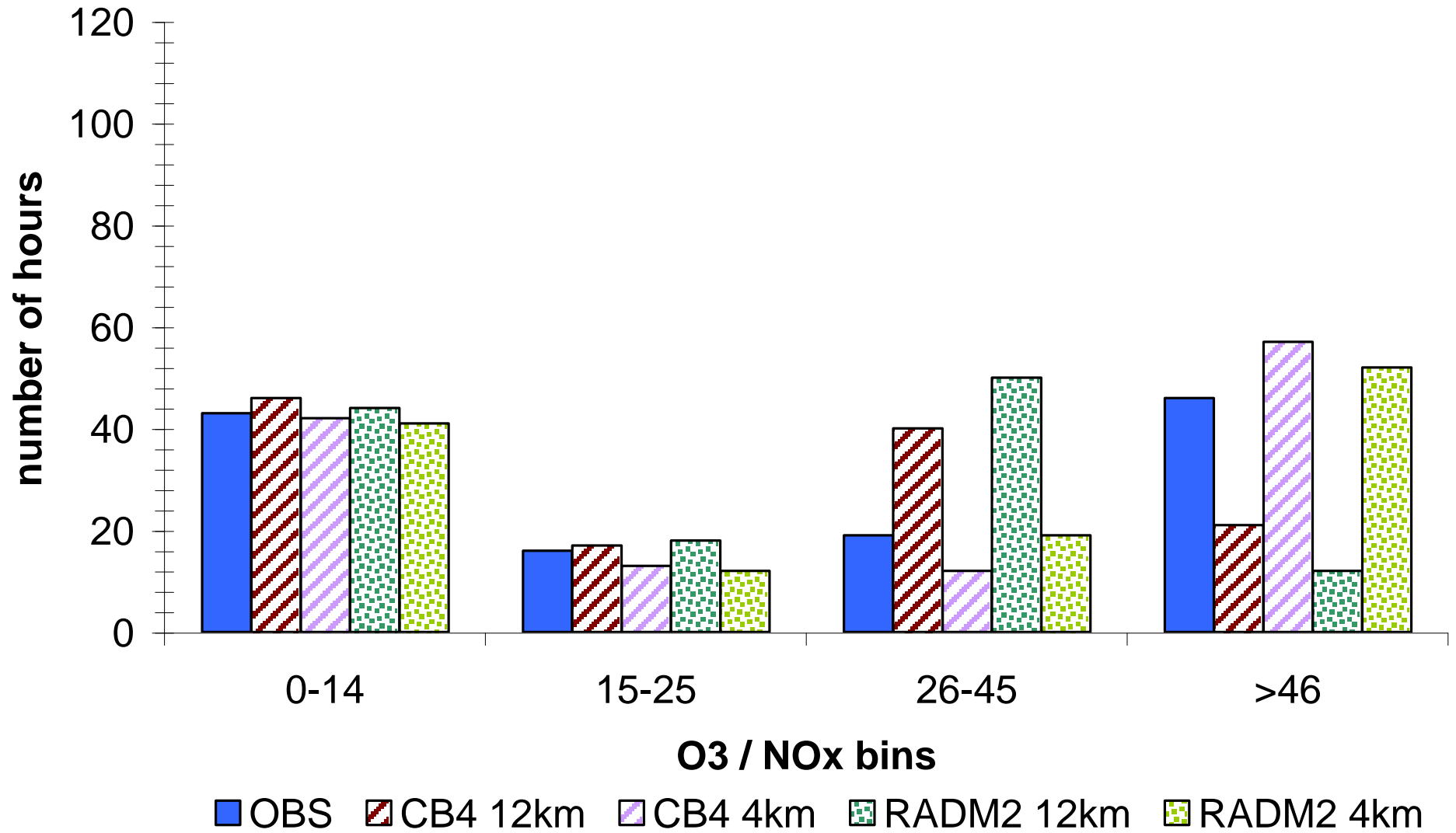


Response Surface Diagnostic Probe

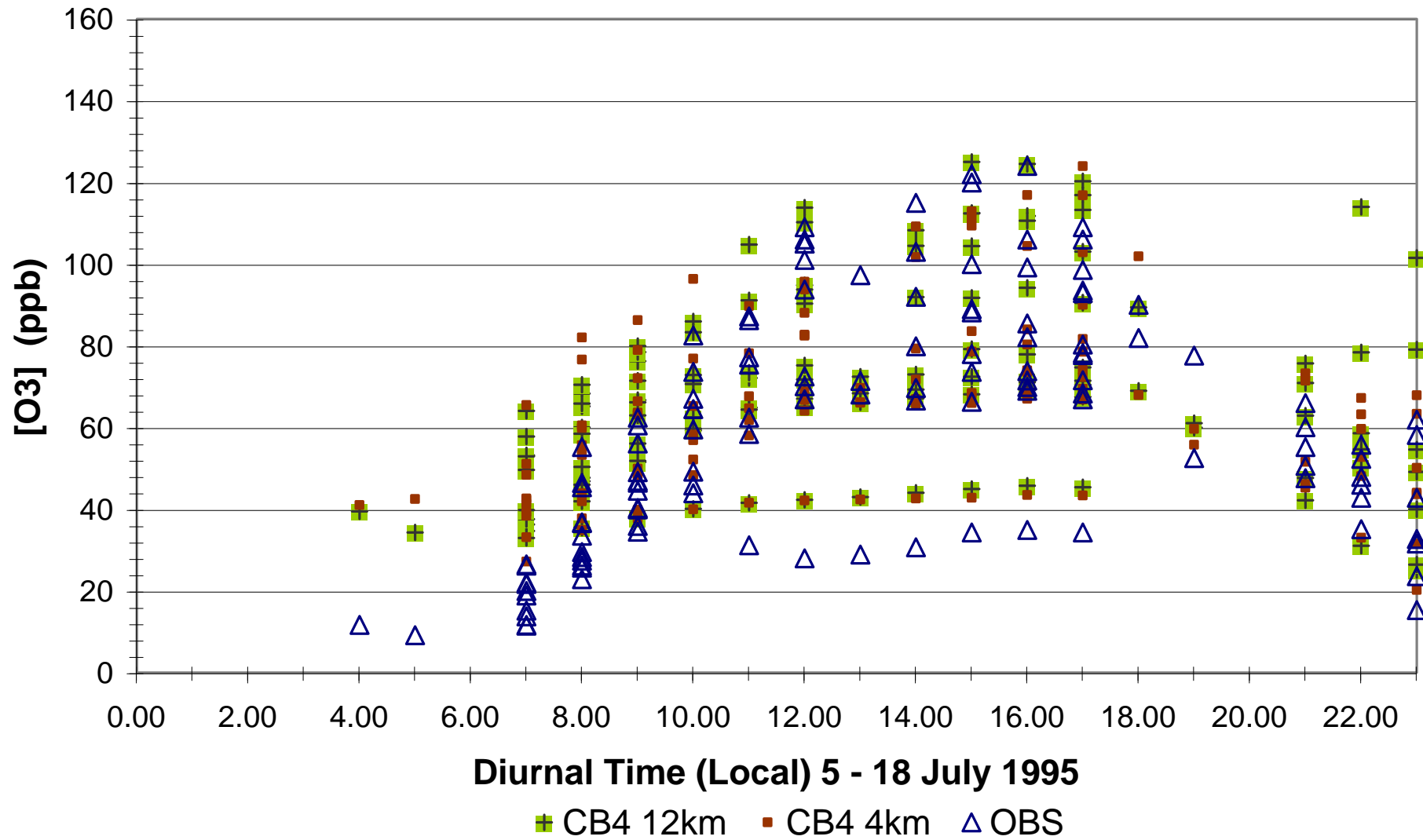
Ridgeline Indicator : $[O_3] / [NO_x]$

- the ratio $[O_3] / [NO_x]$ has proved to be a reliable indicator of the O_3 sensitivity of a photochemical regime by characterizing its position on the $[O_3]$ response surface
 - values of the ratio less than 14 indicate the strongly radical-limited and NO_x -inhibited conditions often prevalent overnight at the surface or in fresh power plant plumes
 - values of the ratio greater than 46 indicate a position across the $[O_3]$ response surface ridgeline well into the NO_x -sensitive region
 - for the observations at the Nashville 95 sites Dickson, Giles, and Youth the ridgeline generally falls in a range between 15 and 25, although it does vary somewhat day-to-day and site-to-site

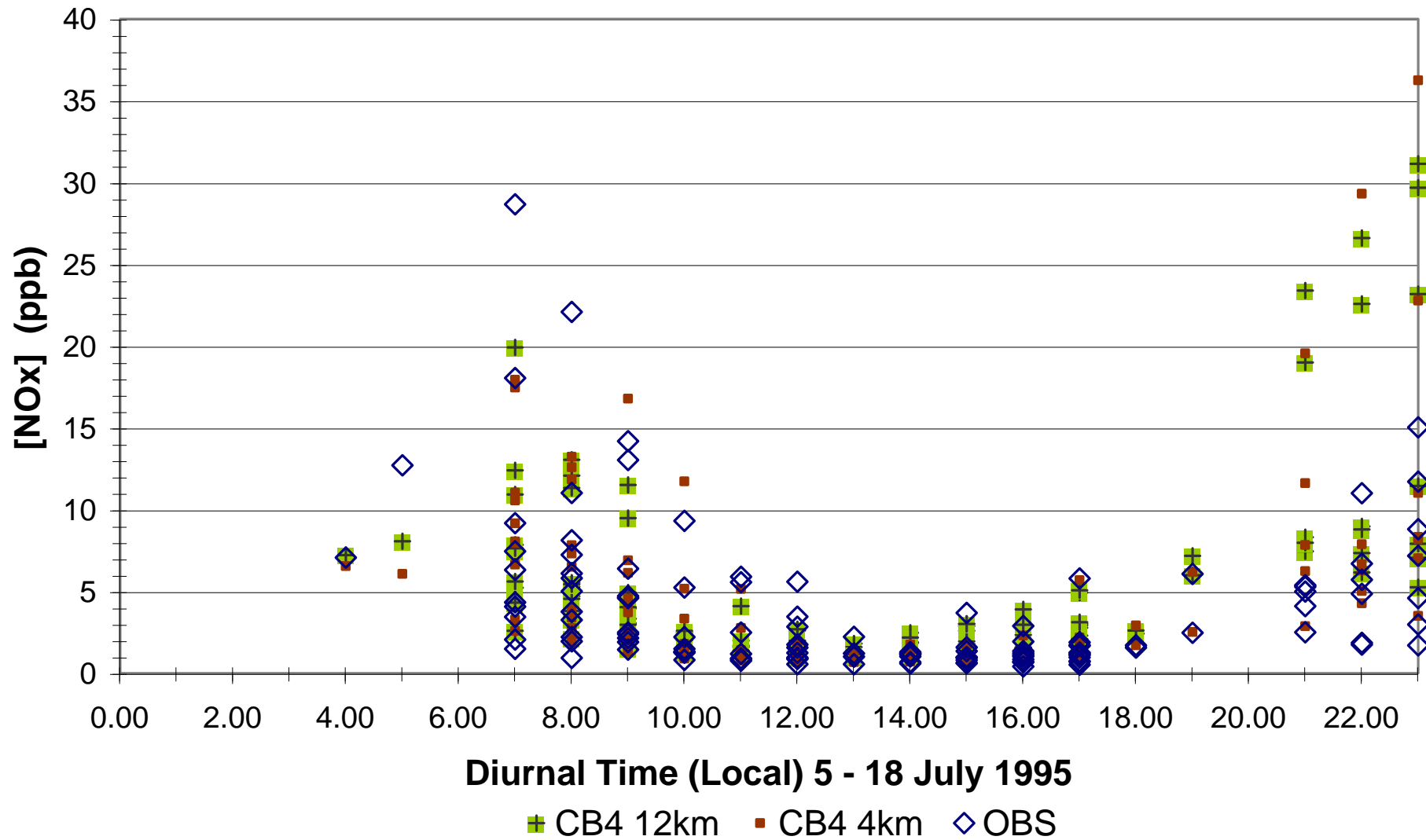
SOS site Youth
O3 / NOx Distributions by Bins
OBS-limited Hours 5 - 18 July 1995 (124 hours)



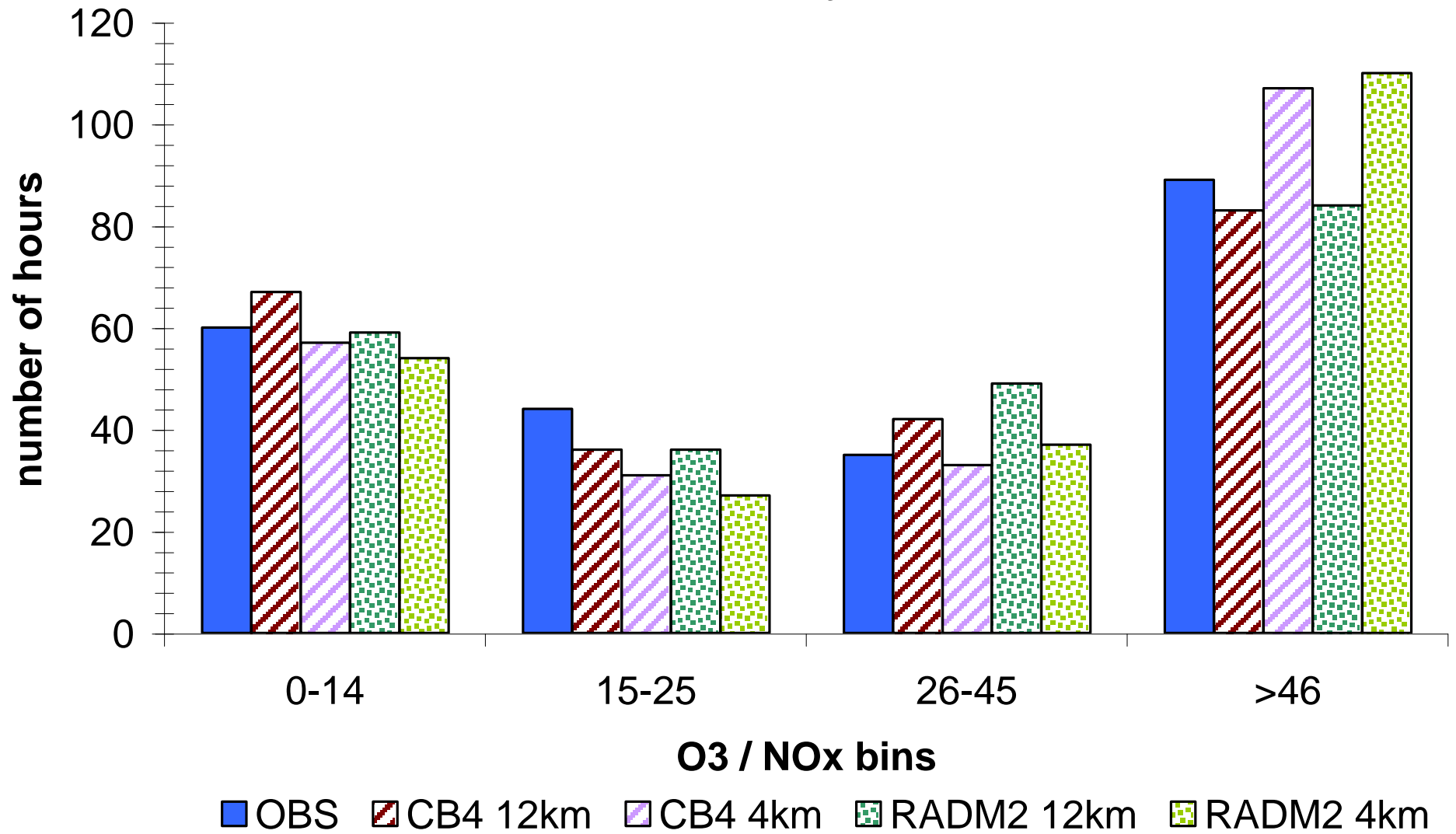
SOS site Youth
OBS & CMAQ CB4 O3 Distributions by Time of Day
All OBS-limited Hours



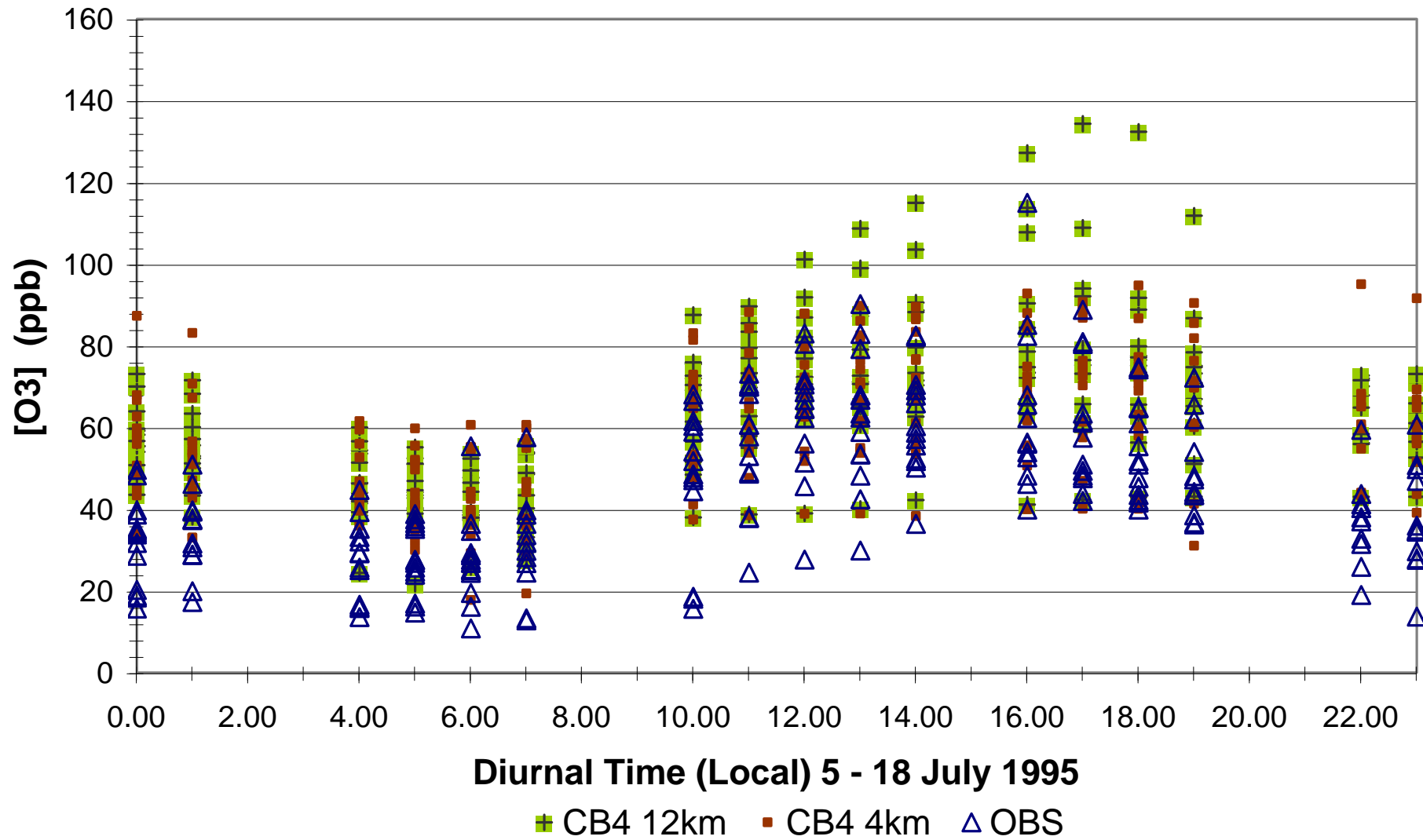
SOS site Youth
OBS & CMAQ CB4 NOx Distributions by Time of Day
All OBS-limited Hours



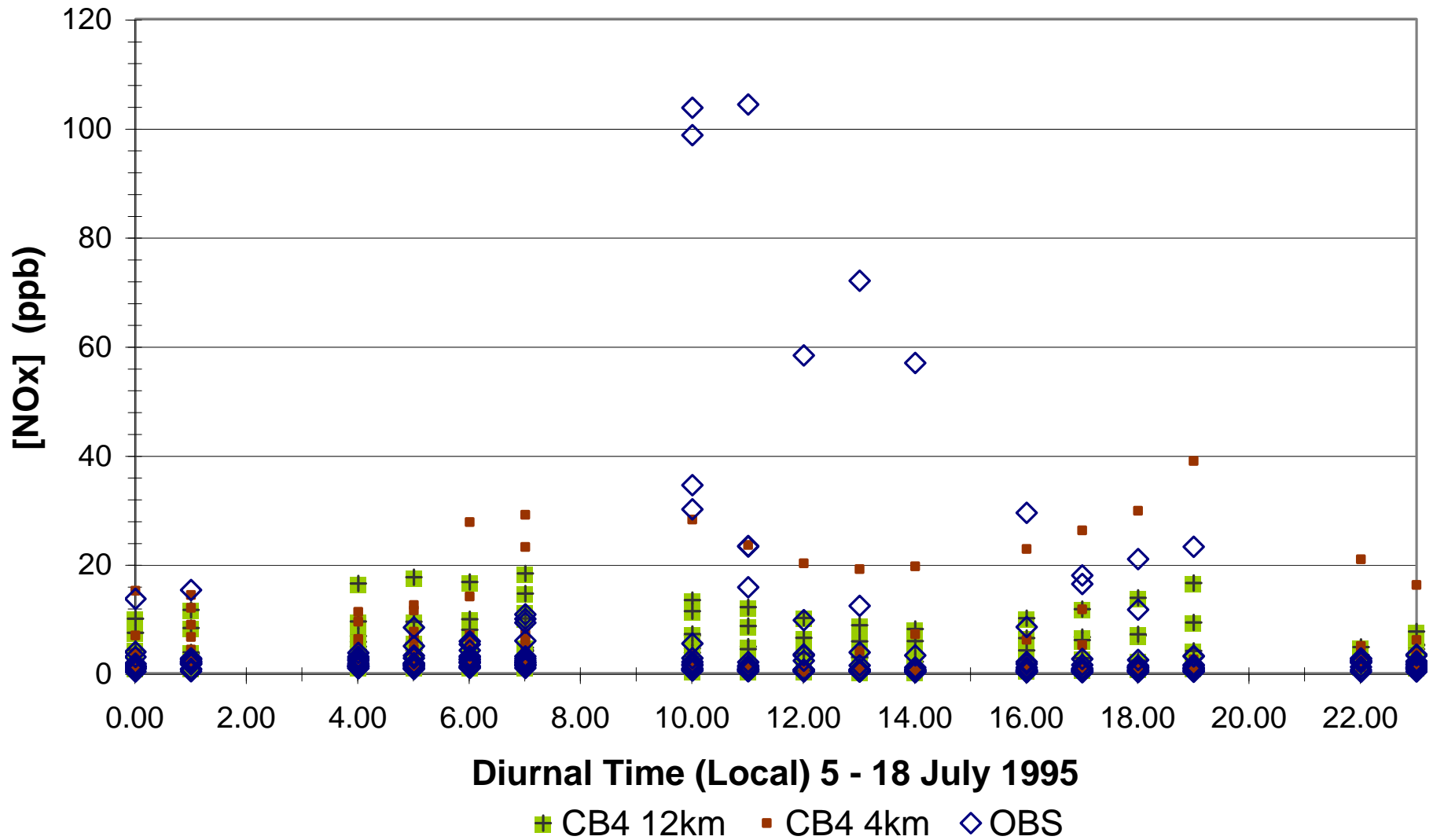
SOS site Dickson
O3 / NOx Distributions by Bins
OBS-limited Hours 5 - 18 July 1995 (228 hours)



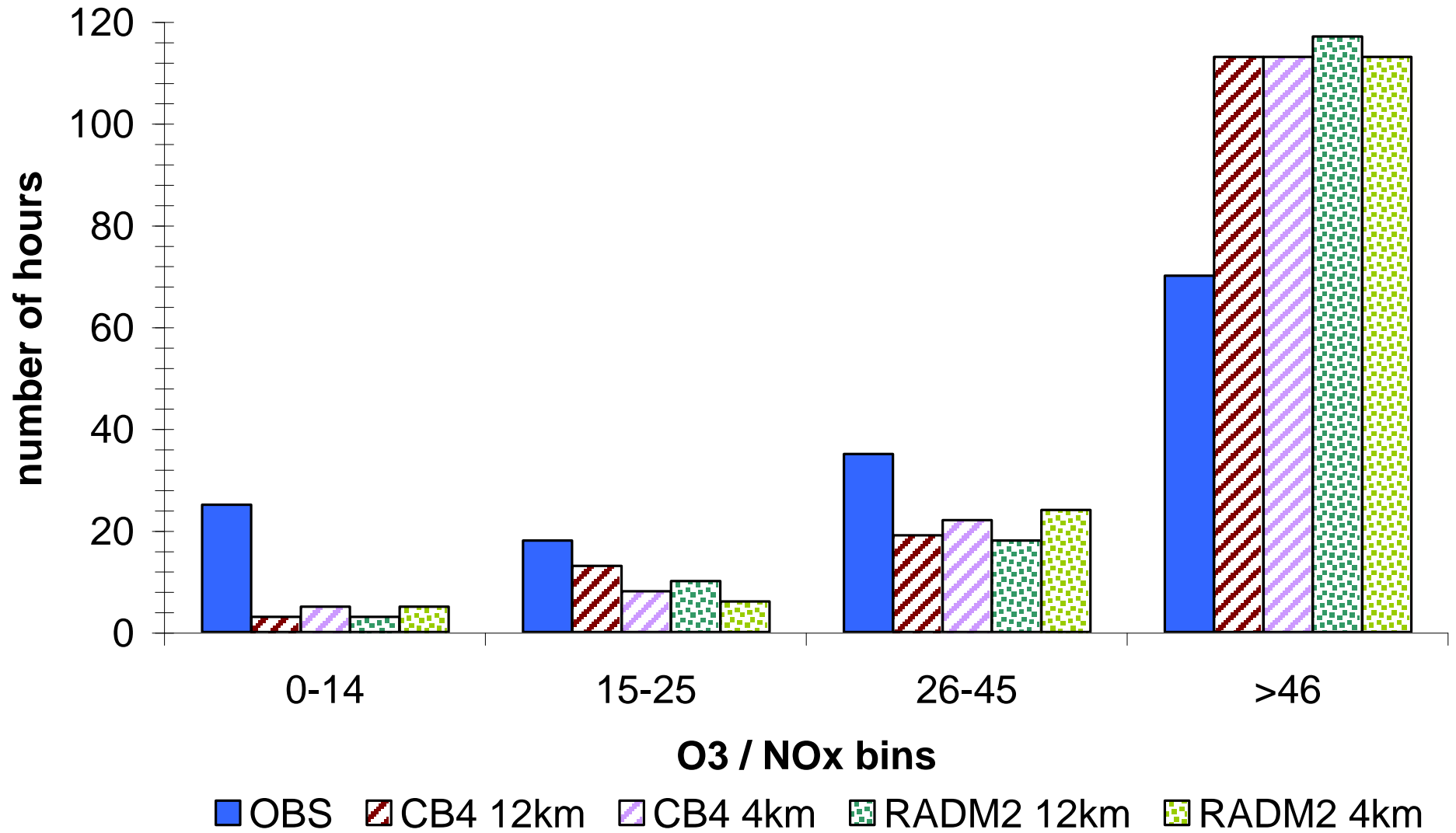
SOS site Dickson
OBS & CMAQ CB4 O3 Distributions by Time of Day
All OBS-limited Hours



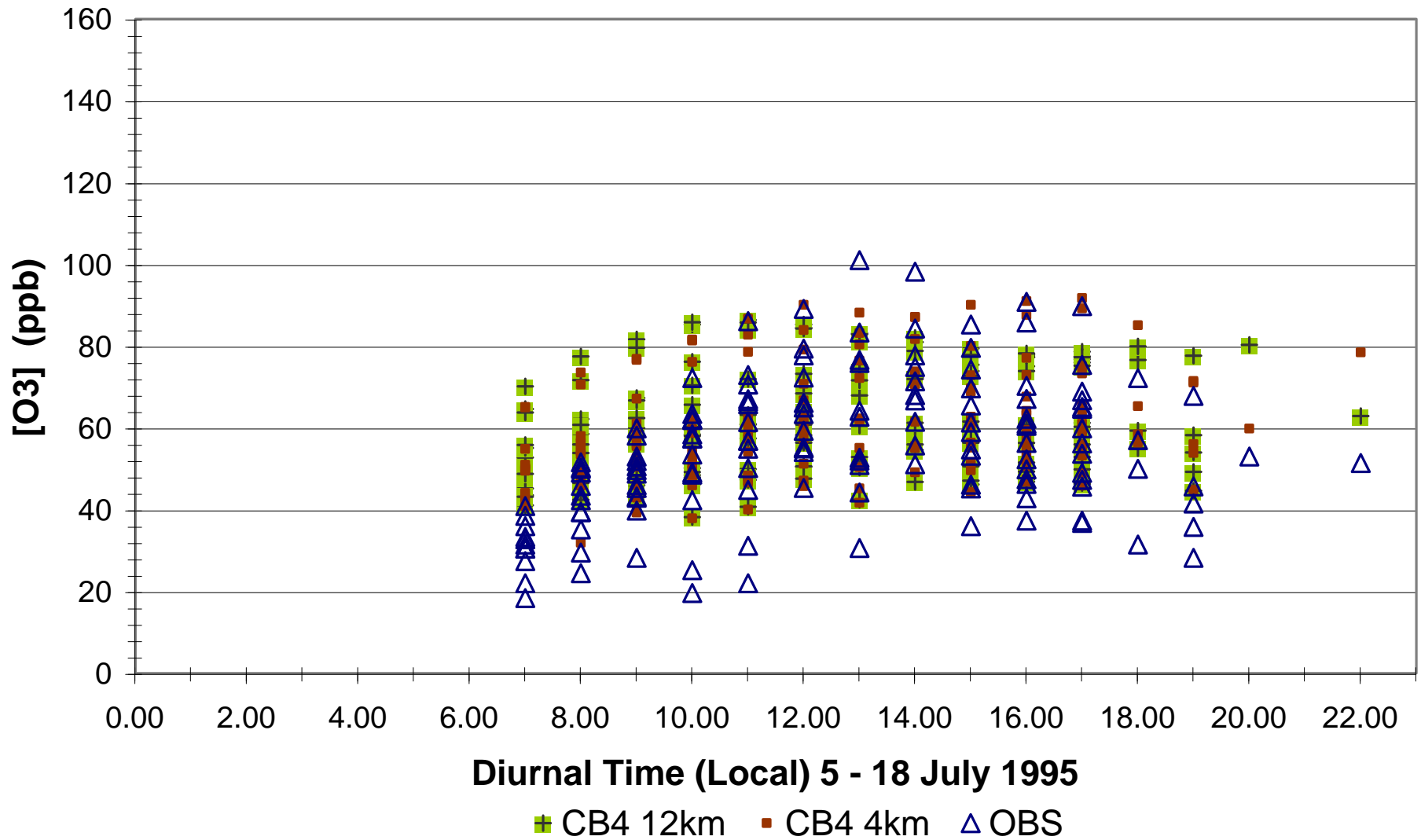
SOS site Dickson
OBS & CMAQ CB4 NOx Distributions by Time of Day
All OBS-limited Hours



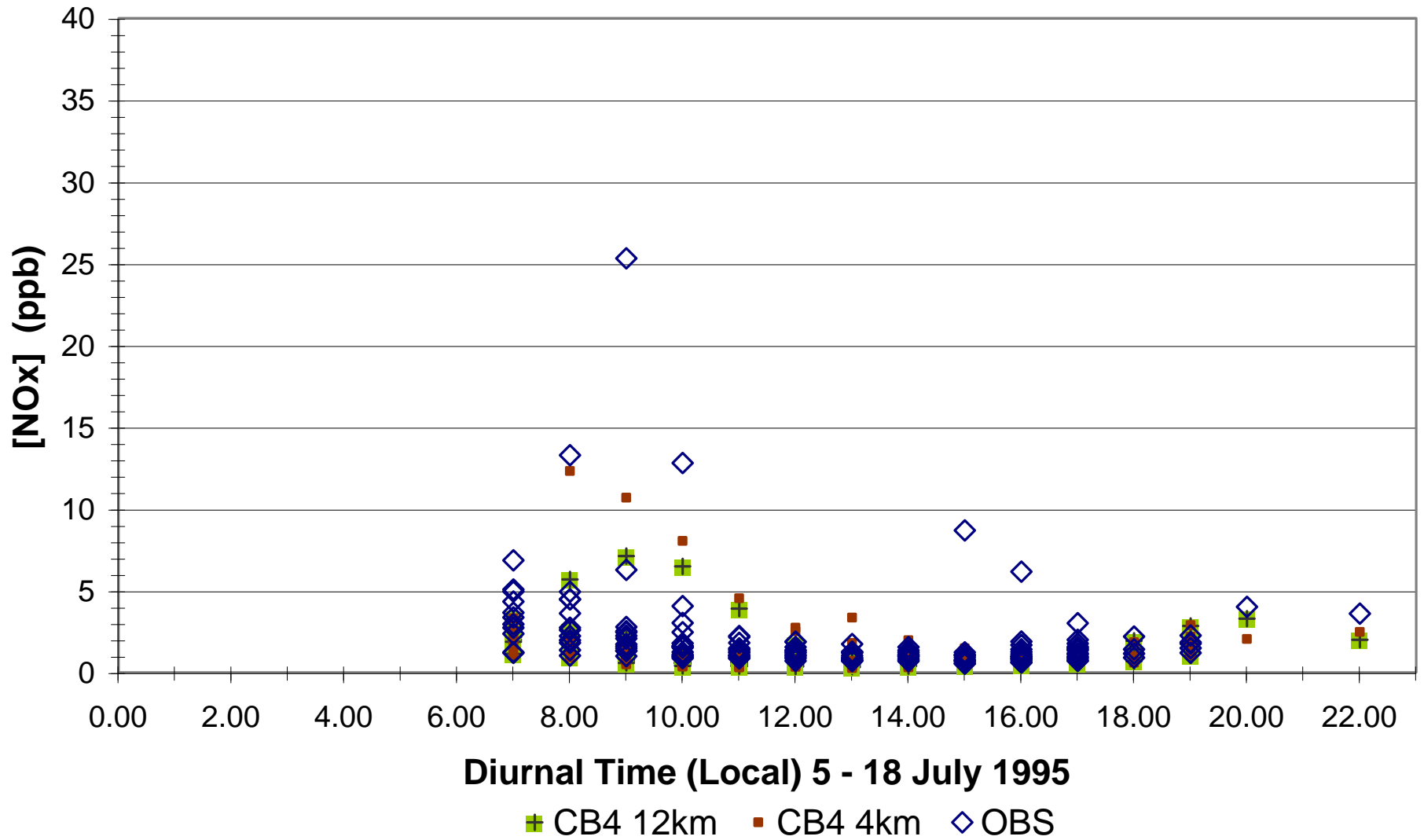
SOS site Giles
O3 / NOx Distributions by Bins
OBS-limited Hours 5 - 18 July 1995 (148 hours)



SOS site Giles
OBS & CMAQ CB4 O3 Distributions by Time of Day
All OBS-limited Hours



SOS site Giles
OBS & CMAQ CB4 NOx Distributions by Time of Day
All OBS-limited Hours



Response Surface Diagnostic Probe (*cont'd*)

Ridgeline Indicator Results

For the most part, CMAQ **correctly reproduces the relevant distributions of observed O₃ / NO_x values** in ranges that separate radical-limited (<14), NO_x-limited (>46), and near ridgeline (~15 to ~25) conditions

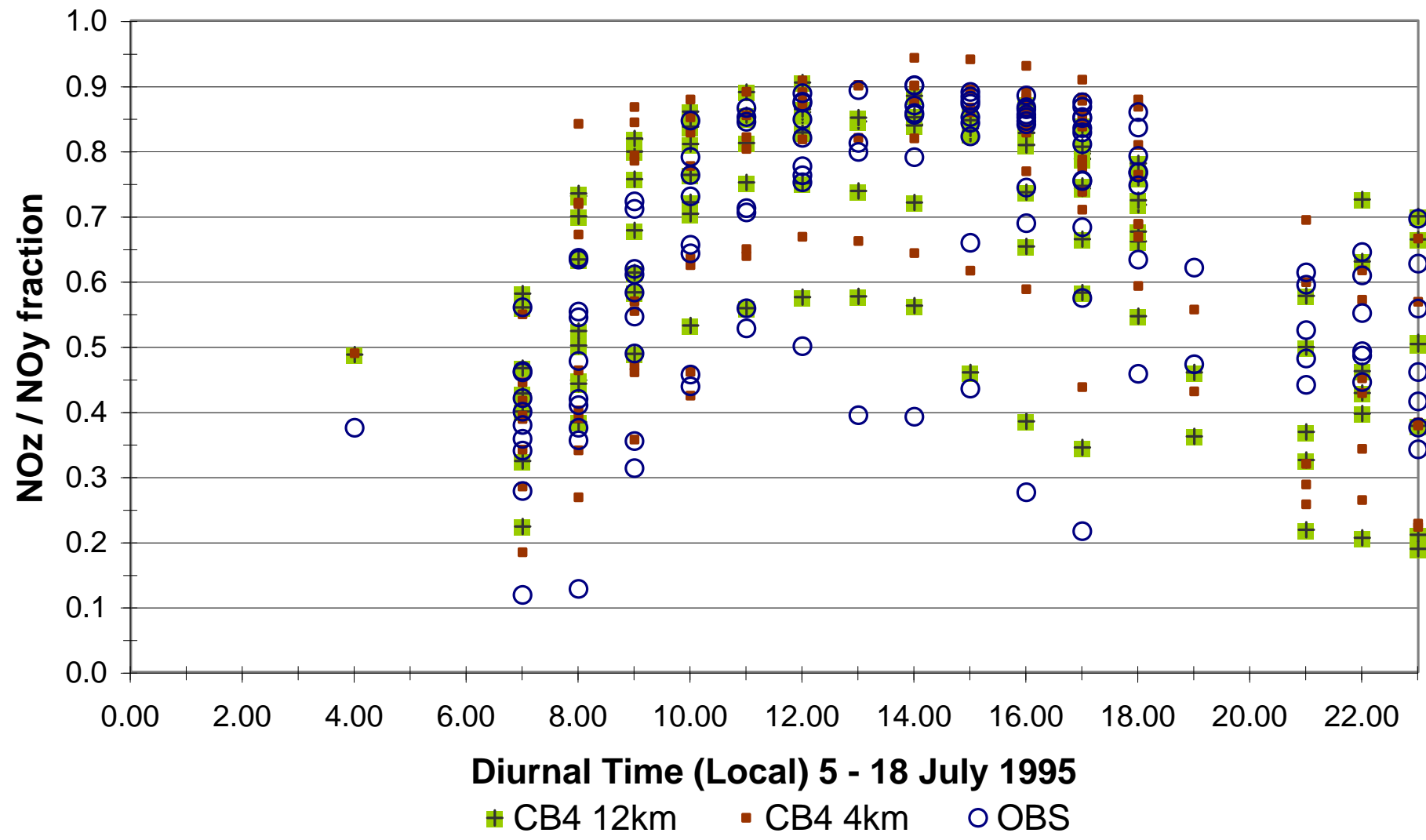
- discrepancies in the >46 ranges at Youth are **improved with the 4km models relative to the 12km models, ratio values for which appear to have a ceiling related to excessive NO_x retained in the larger grid scale model**
- some discrepancies at Dickson appear due to **excessive NO_y retained in the grid model from the Cumberland power plant plumes touching down at this surface site; preliminary results (not shown) from PinG modeling for Dickson demonstrate improvement here**
- some discrepancies across all indicator ranges at Giles appear due to a very **local fresh NO_x source not accounted for in CMAQ input emissions**

Individual Components Diagnostic Probe

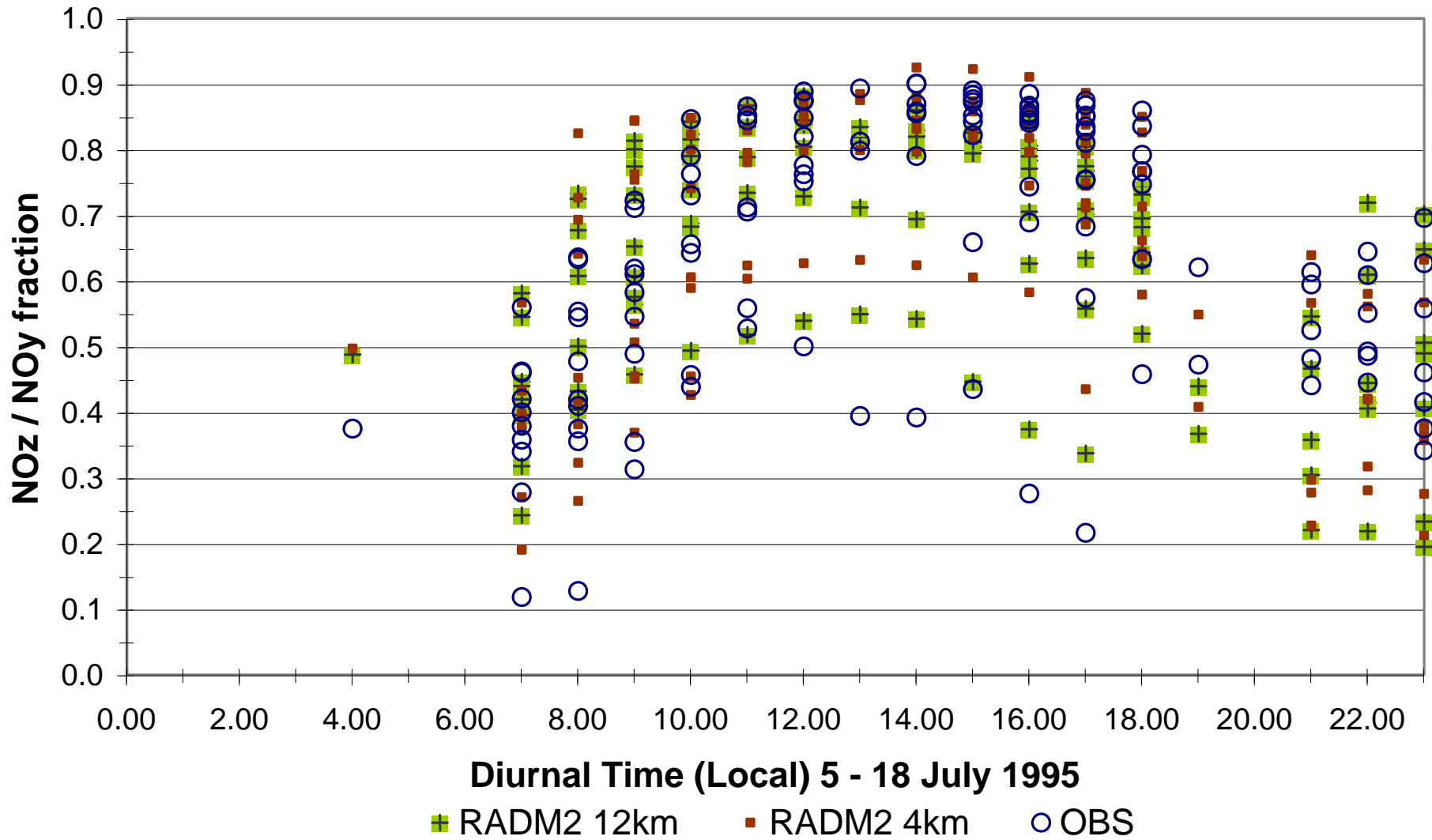
Air Mass Aging : $[\text{NO}_z] / [\text{NO}_y]$

Values less than ~0.6 indicate a fresh NO_x plume with an increased potential for O_3 production or loss – conditional on radical availability, *i.e.*, on the position of the photochemical regime on the response surface – relative to higher values of the ratio in an aged plume

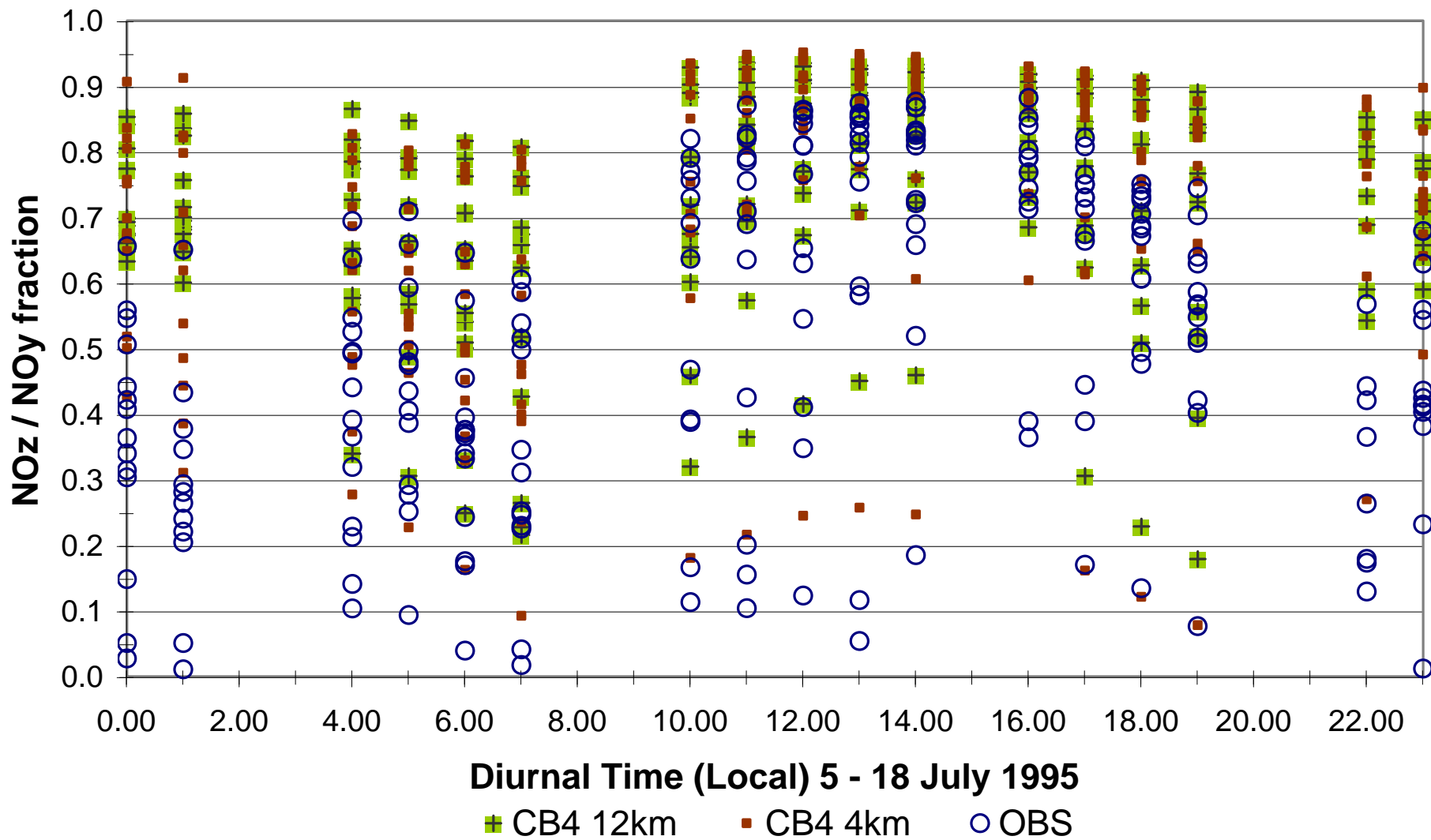
SOS site Youth
OBS & CMAQ CB4 NO_z / NO_y Distributions by Time of Day
All OBS-limited Hours



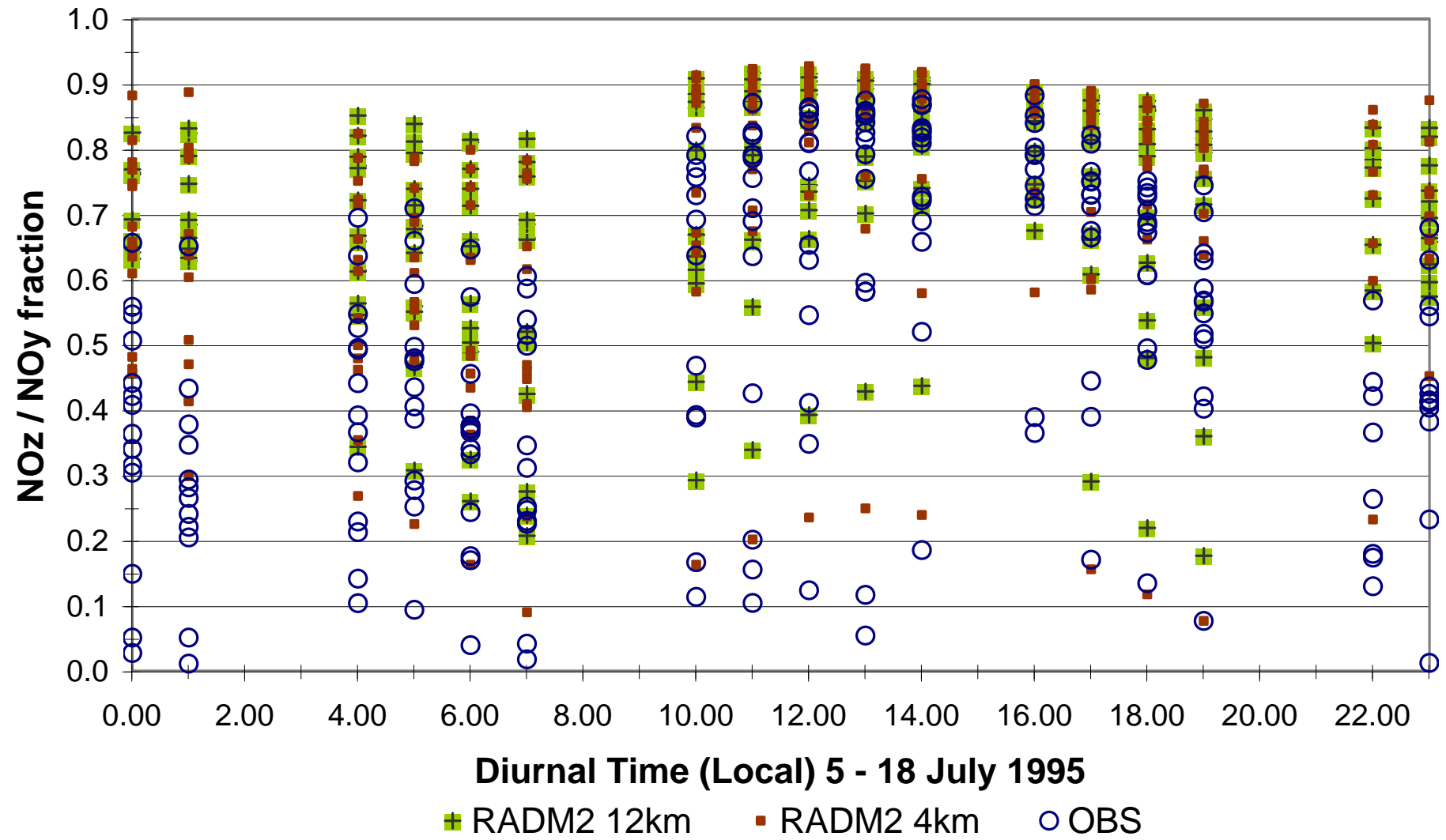
SOS site Youth
OBS & CMAQ RADM2 NO_z / NO_y Distributions by Time of Day
All OBS-limited Hours



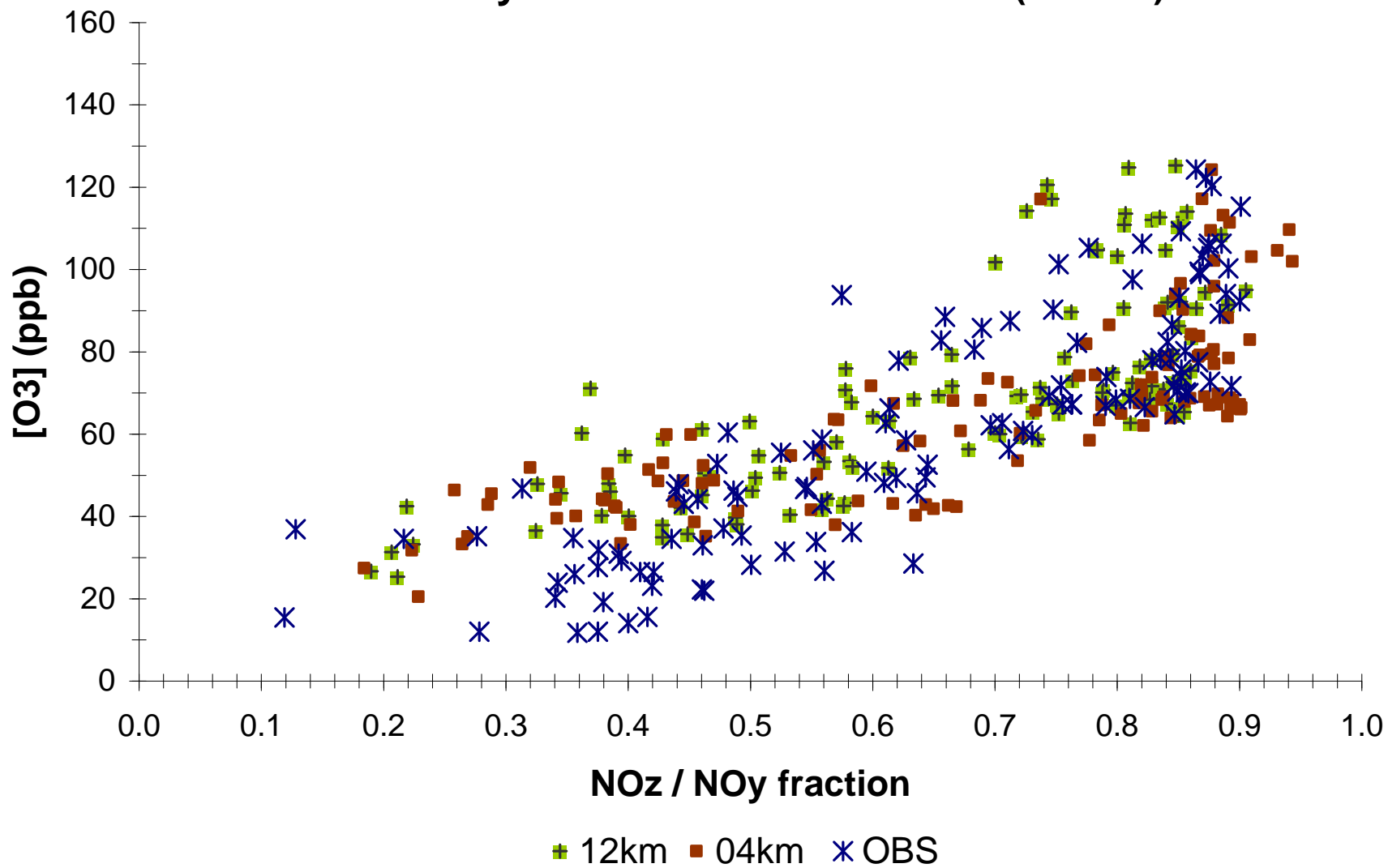
SOS site Dickson
OBS and CMAQ CB4 NO_z / NO_y Distributions by Time of Day
All OBS-limited Hours



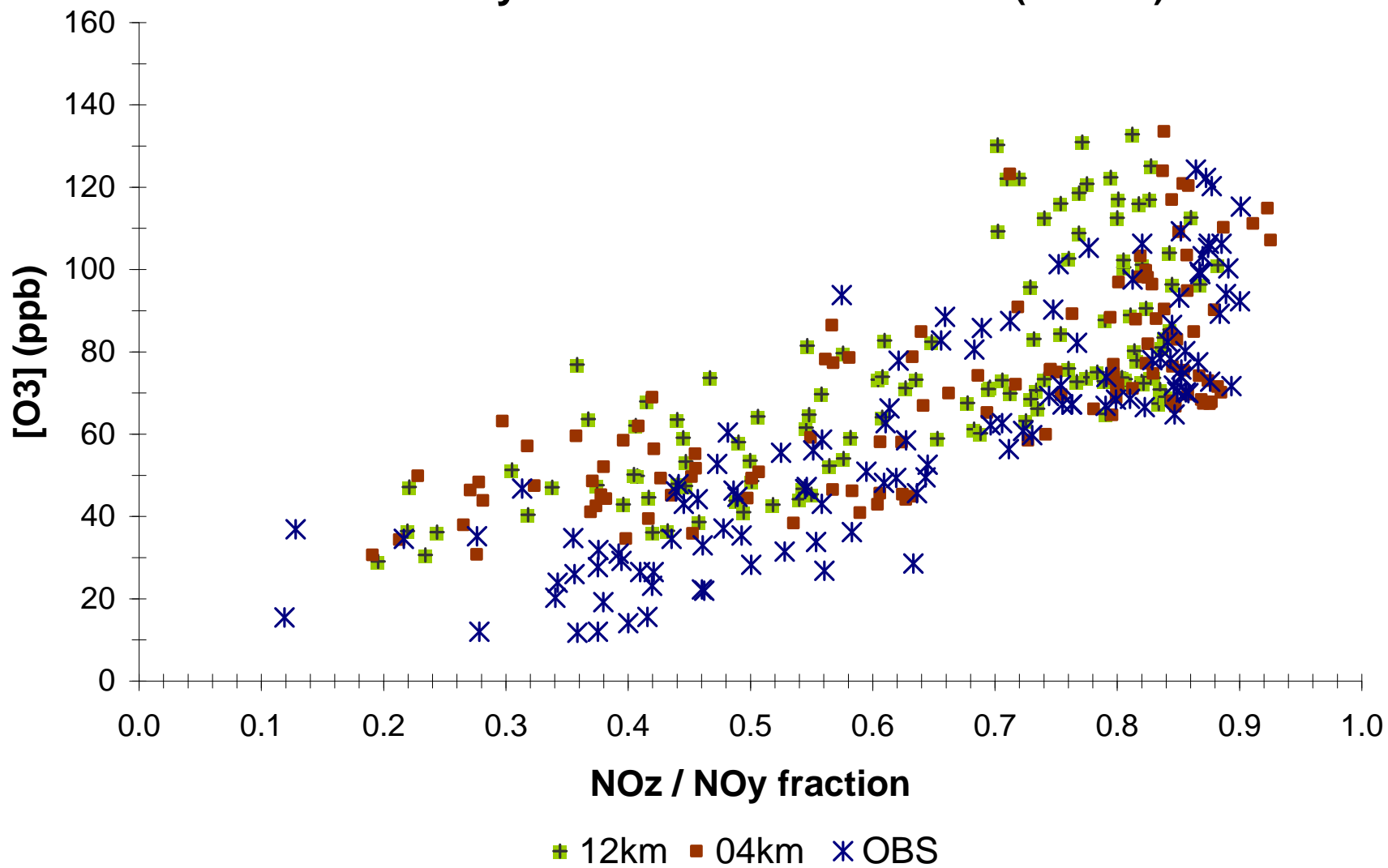
SOS site Dickson
OBS and CMAQ RADM2 NO_z / NO_y
Distributions by Time of Day All OBS-limited Hours



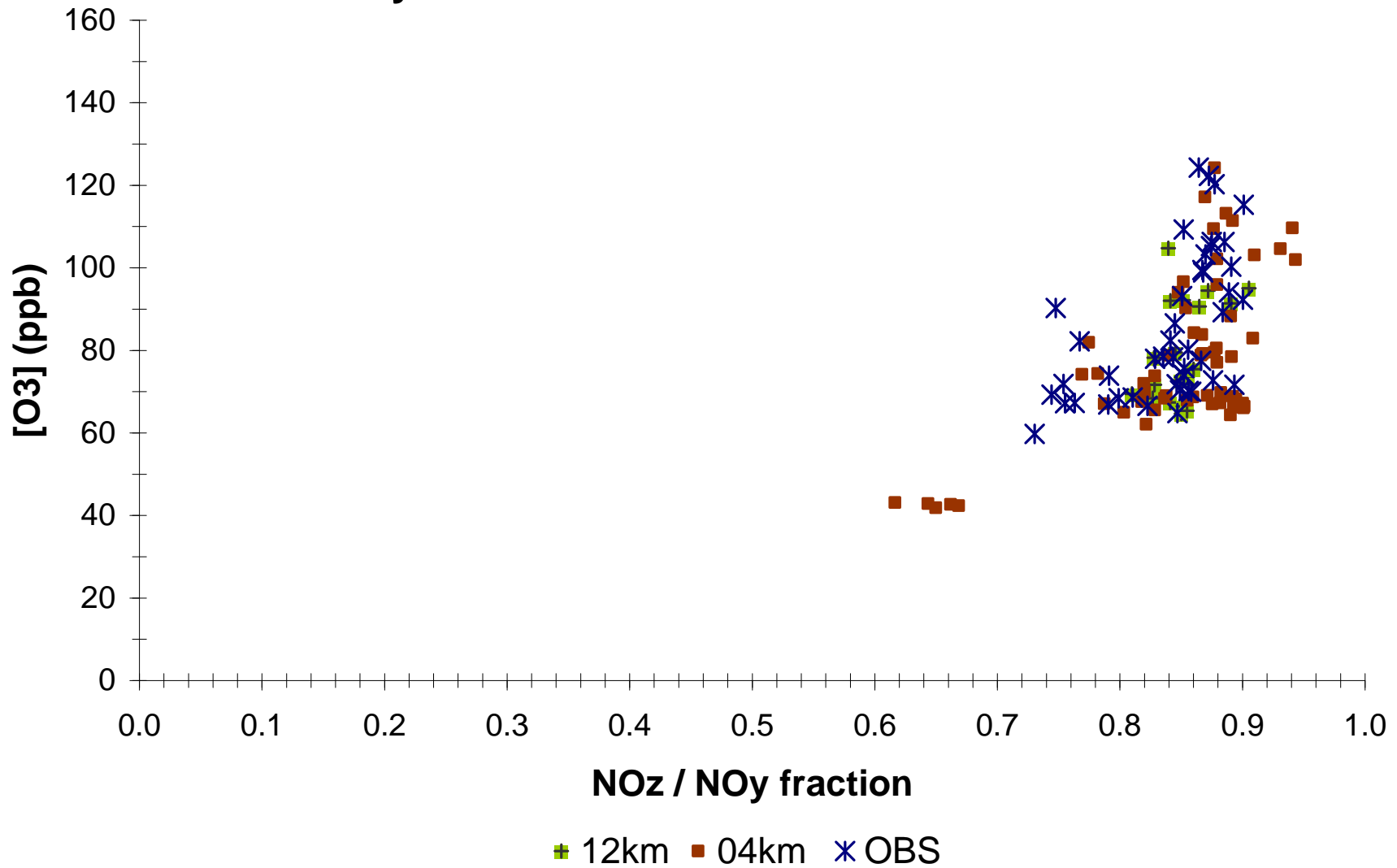
SOS site Youth
CMAQ CB4 vs. OBS
5 - 18 July 1995 OBS-limited Hours (124 hrs)



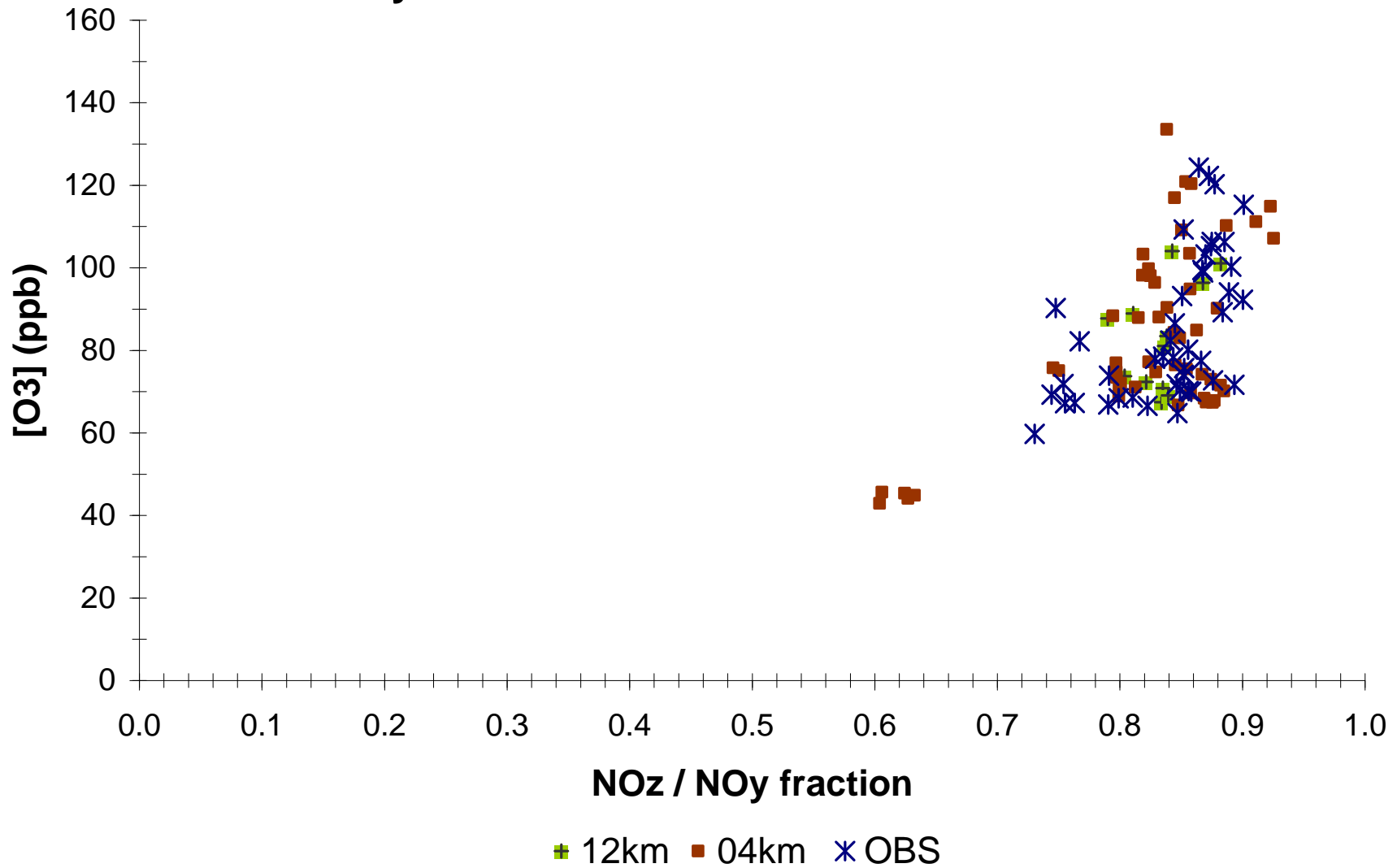
SOS site Youth
CMAQ RADM2 vs. OBS
5 - 18 July 1995 OBS-limited Hours (124 hrs)



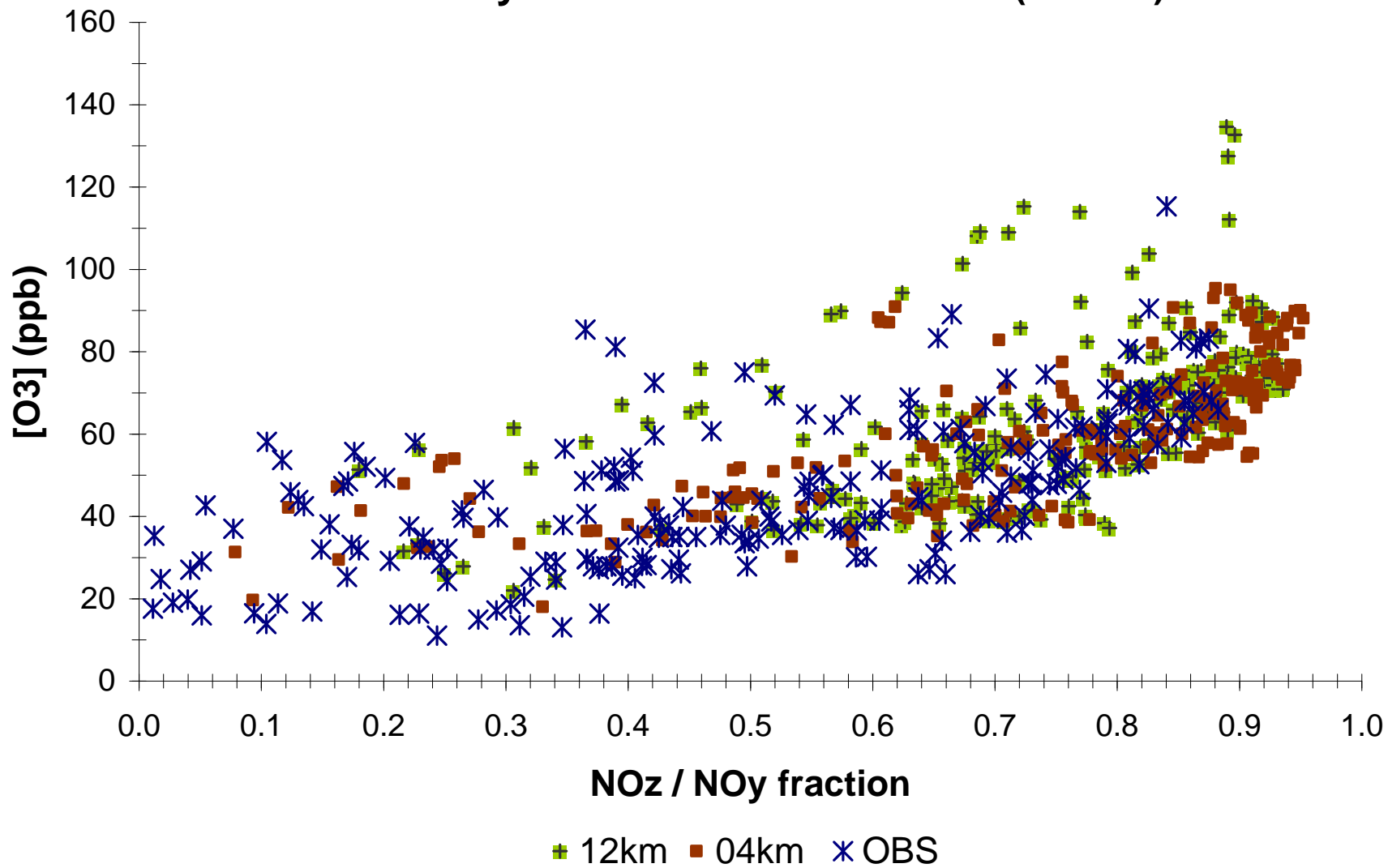
SOS site Youth
CMAQ CB4 vs. OBS
5 - 18 July 1995 OBS-limited Hours with O3 / NOx >46



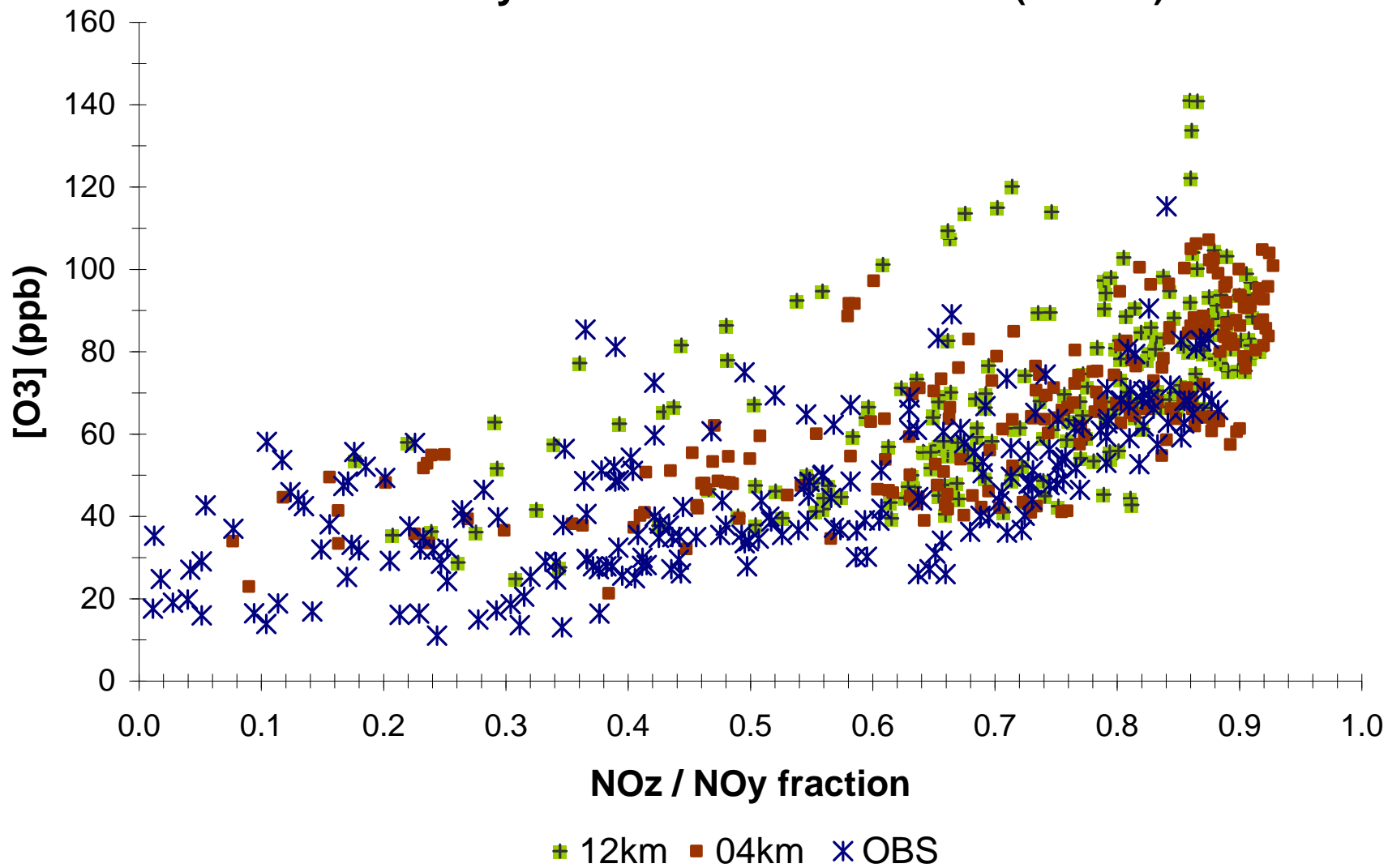
SOS site Youth
CMAQ RADM2 vs. OBS
5 - 18 July 1995 OBS-limited Hours with O3 / NOx >46



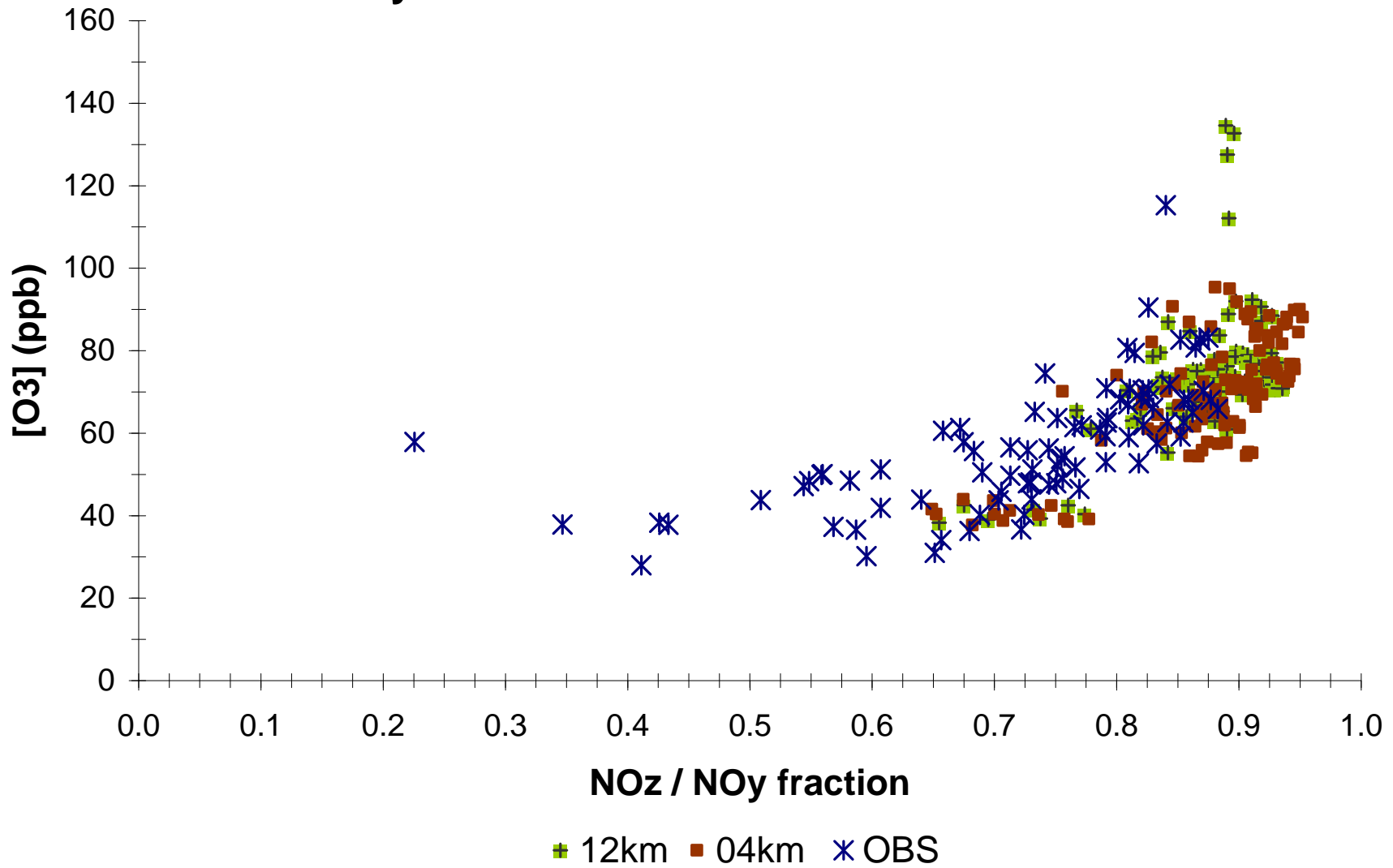
SOS site Dickson
CMAQ Re-eval CB4 vs OBS
5 - 18 July 1995 OBS-limited Hours (217 hrs)



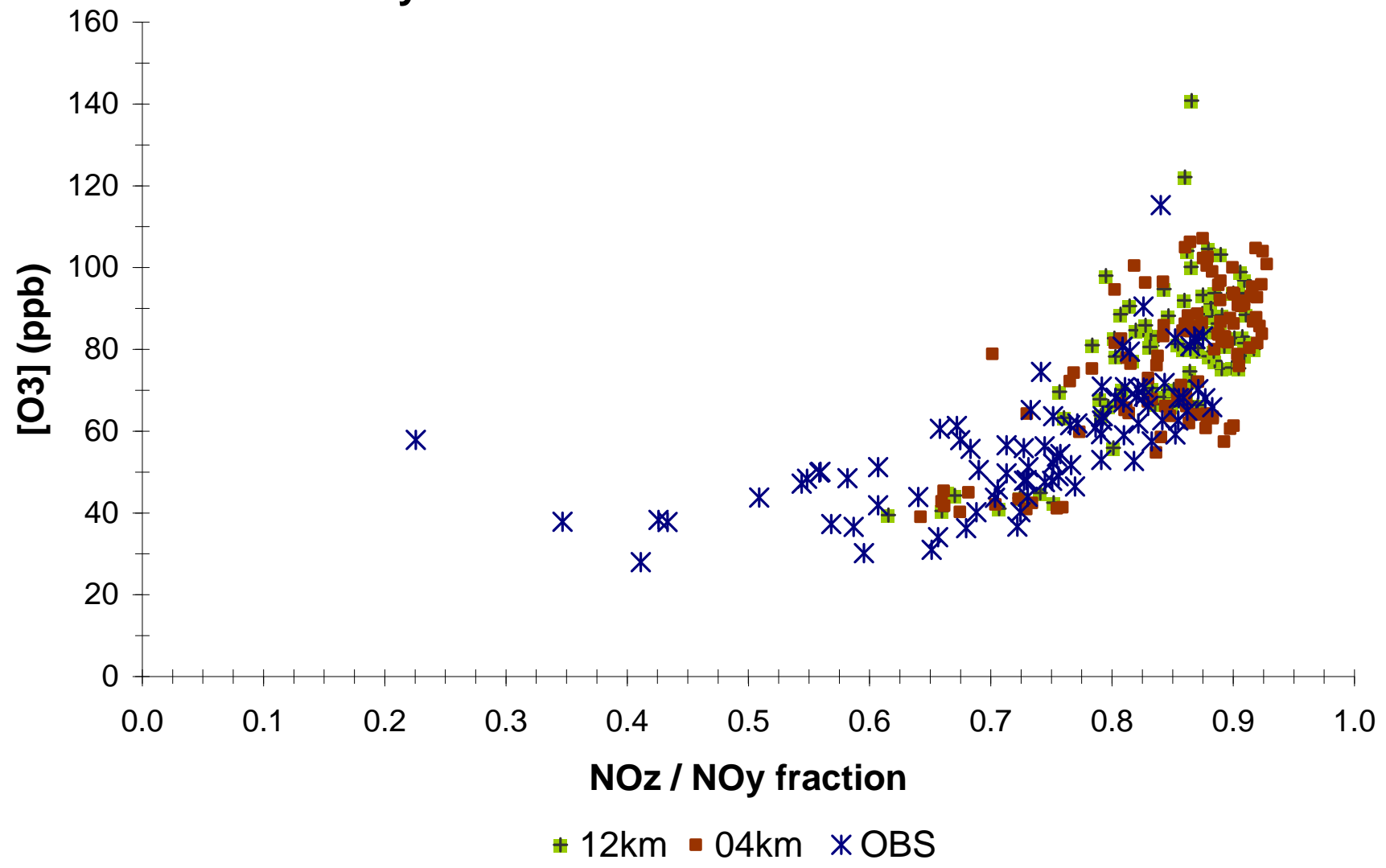
SOS site Dickson
CMAQ Re-eval RADM2 vs OBS
5 - 18 July 1995 OBS-limited Hours (217 hrs)



SOS site Dickson
CMAQ CB4 vs OBS
5 - 18 July 1995 OBS-limited Hours with O3 / NO_x >46



**SOS site Dickson
CMAQ RADM2 vs OBS
5 - 18 July 1995 OBS-limited Hours with O3 / NOx >46**



Individual Components Diagnostic Probe *(cont'd)*

Air Mass Aging Results

Aging comparisons are consistent with information from O_3 / NO_x values in showing good behavior of CMAQ in the NO_x -limited region of the response space

- confirming the presence of large, very fresh NO_x plumes arriving at Dickson throughout the photochemically active period of some days to which the grid model does not respond correctly
- suggesting slightly better performance of the 4km models over the 12km
- indicating some apparent differences between the chemistries, the precise cause and potential consequences of which are still being evaluated

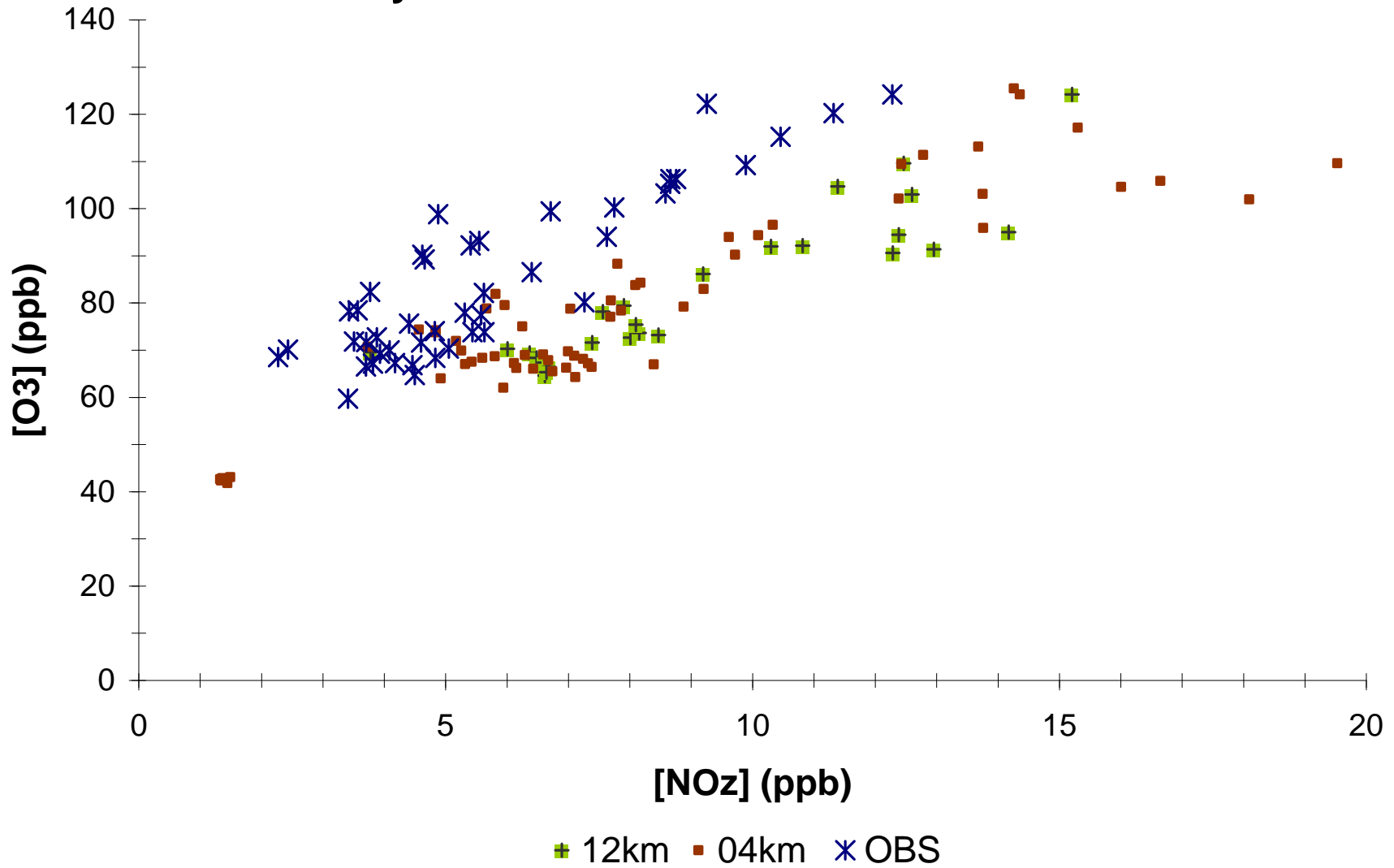
Process Diagnostic Probe

O₃ Production Efficiency : [O₃] to [NO_Z]

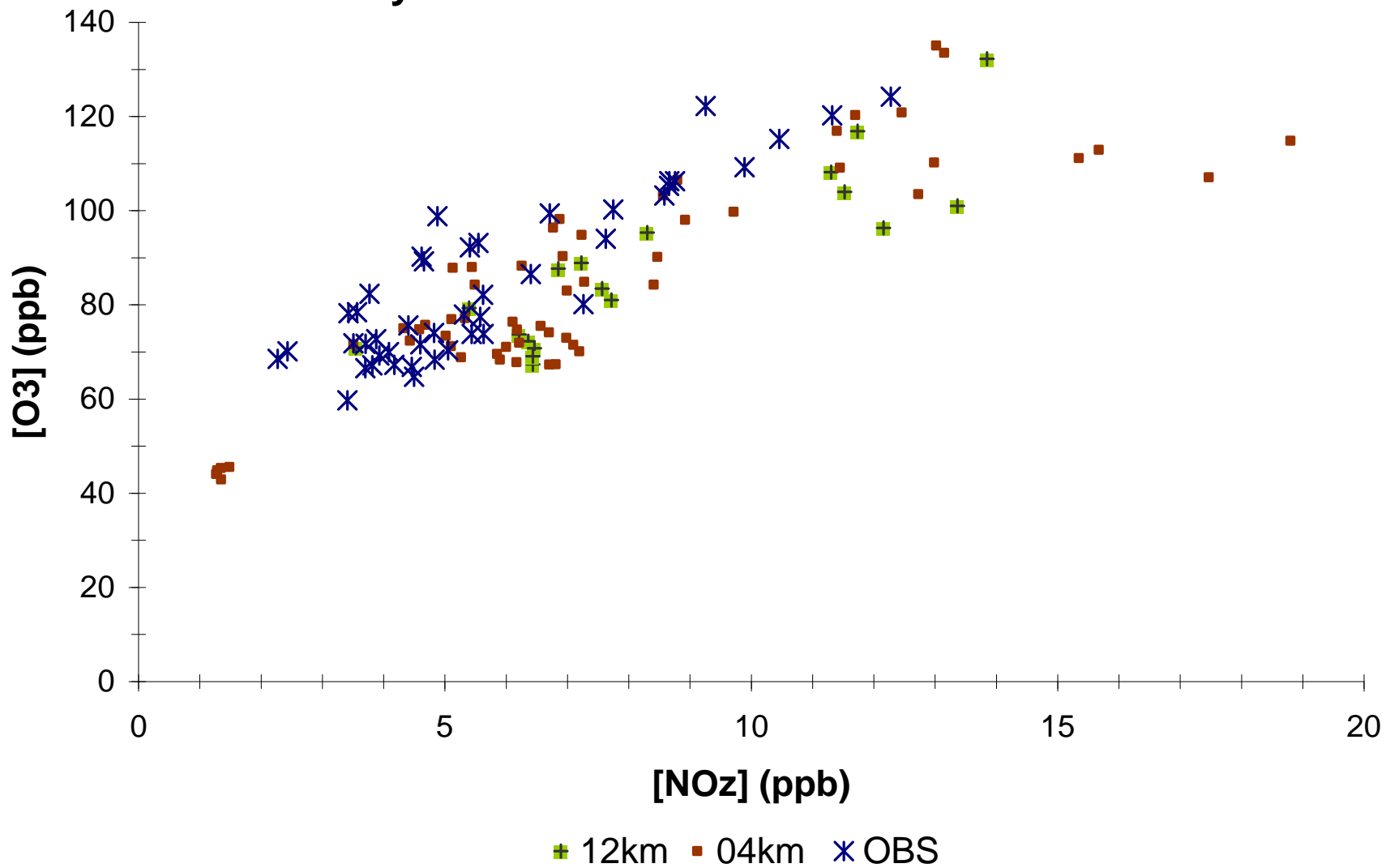
The slope of the line produced with comparisons of [O₃] to [NO_Z] provides a measure of the photochemical processing of NO_X referred to as the O₃ production efficiency, or the number of O₃ molecules produced for each NO_X processed to NO_Z

- often presented with observations, or in a few cases with results from a constrained model, for all hours observed or in the simulation
- however, that complicates interpretation of the test by mixing together production rates from very different parts of the diurnal O₃ production cycle, determined by the relative availabilities of NO_X and radicals changing through time
- plots shown here are selected for hours in the observations and in the models filtered by [O₃] / [NO_X] for the range >46, well into the NO_X-limited region of the response space

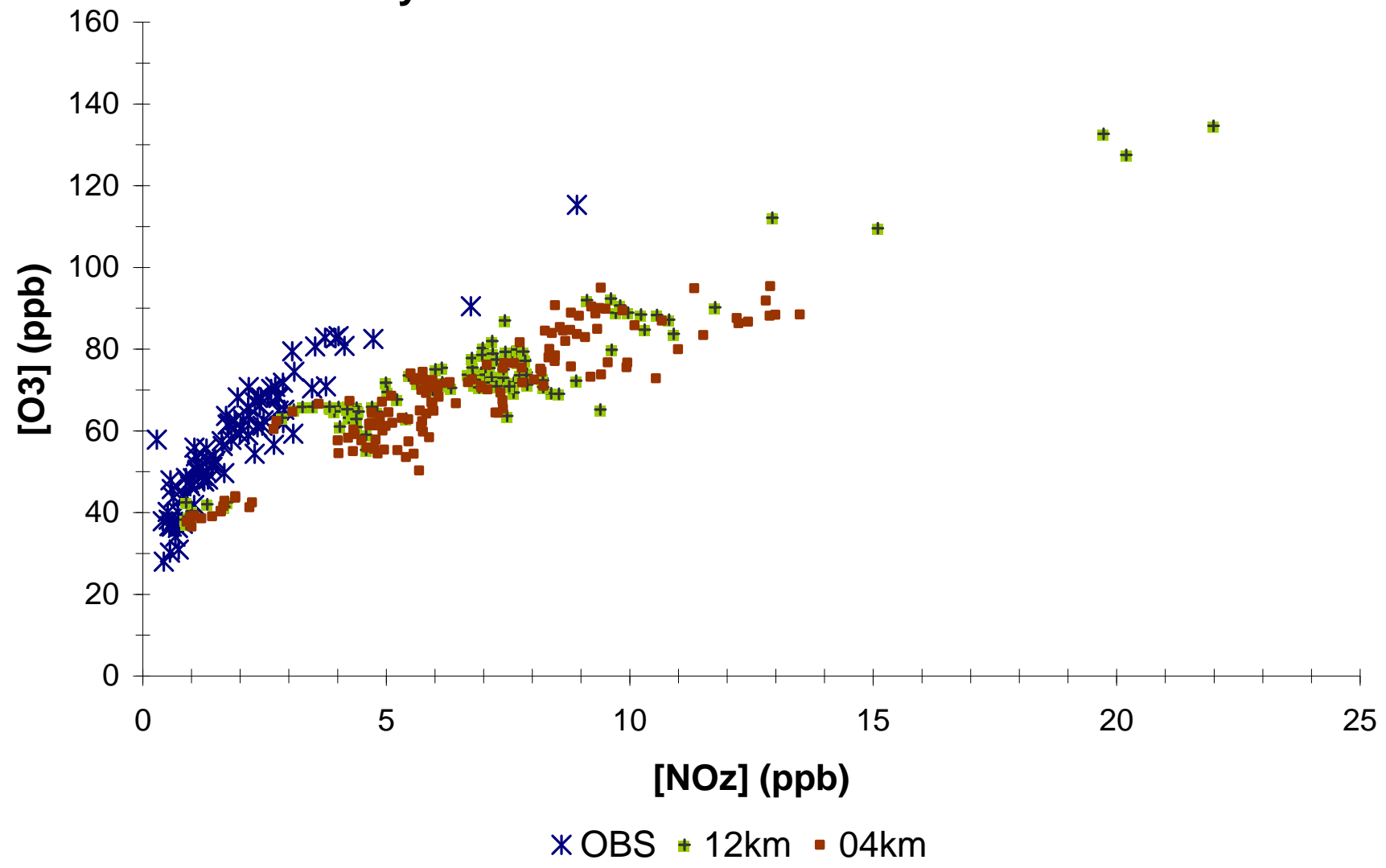
SOS site Youth
CMAQ CB4 vs. OBS
5 - 18 July 1995 OBS-limited Hours with O3 / NOx >46



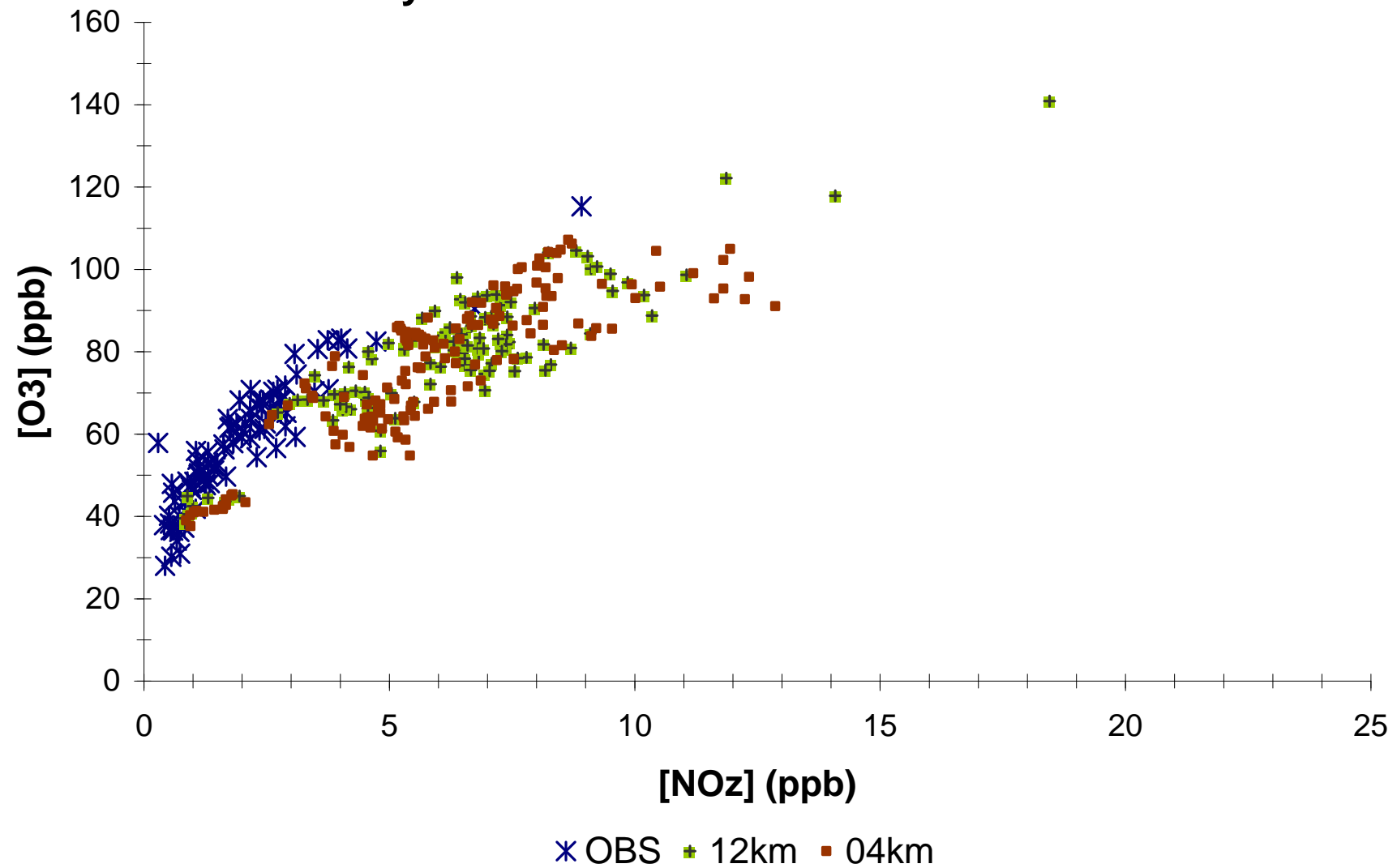
SOS site Youth
CMAQ RADM2 vs. OBS
5 - 18 July 1995 OBS-limited Hours with O3 / NOx >46



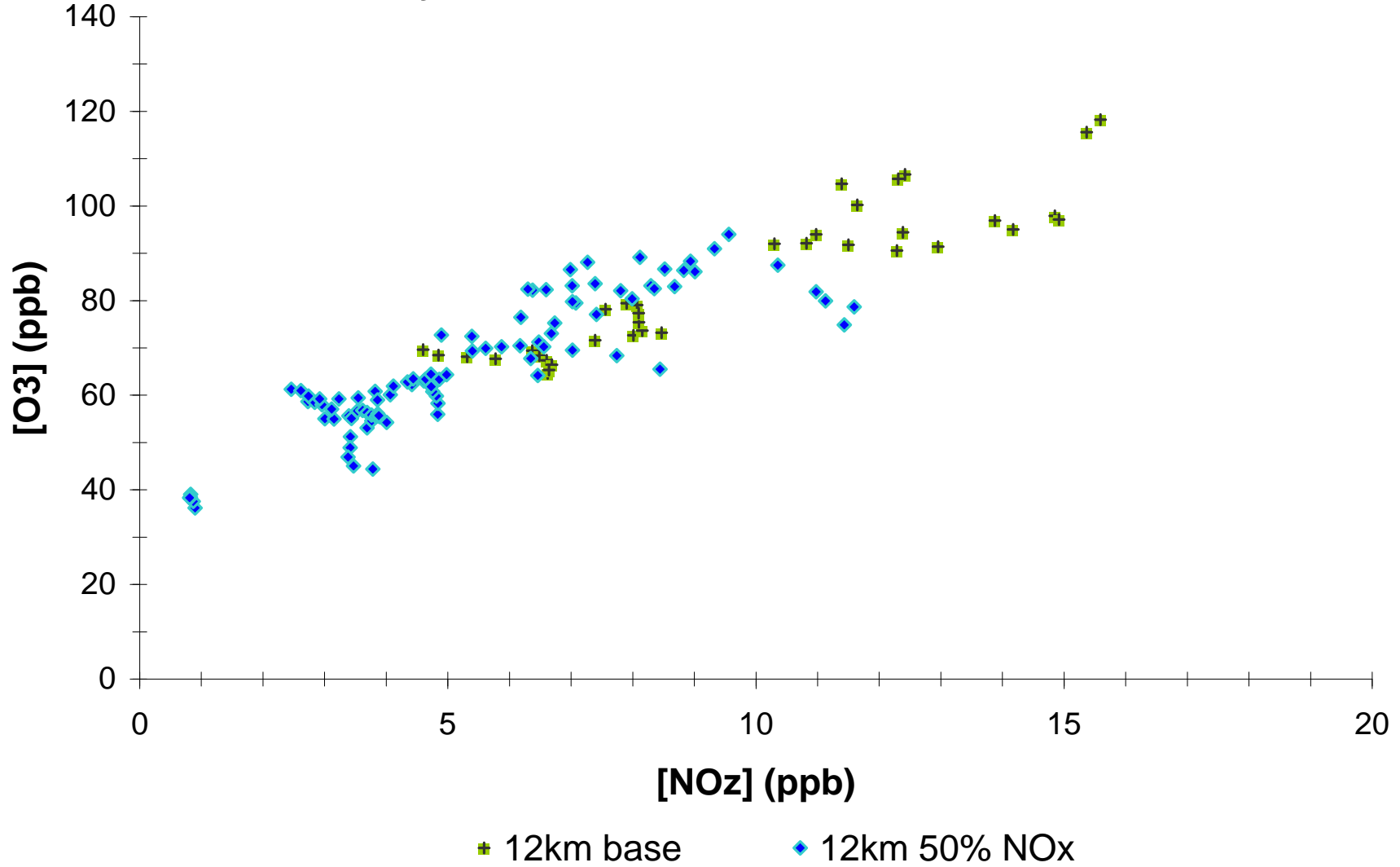
**SOS site Dickson
CMAQ CB4 vs. OBS
5 - 18 July 1995 OBS-limited Hours with O3 / NOx >46**



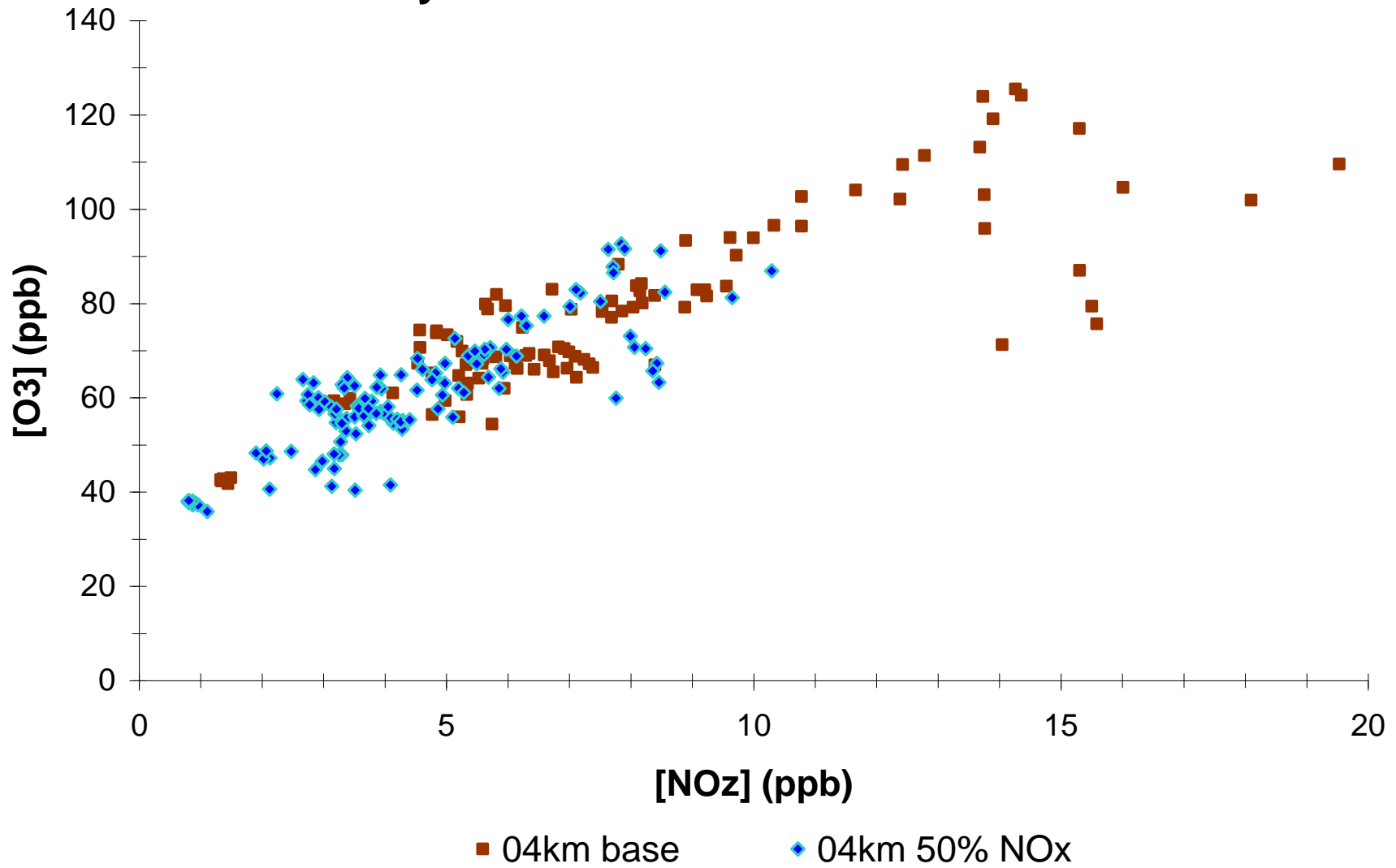
SOS site Dickson
CMAQ RADM2 vs. OBS
5 - 18 July 1995 OBS-limited Hours with O3 / NOx >46



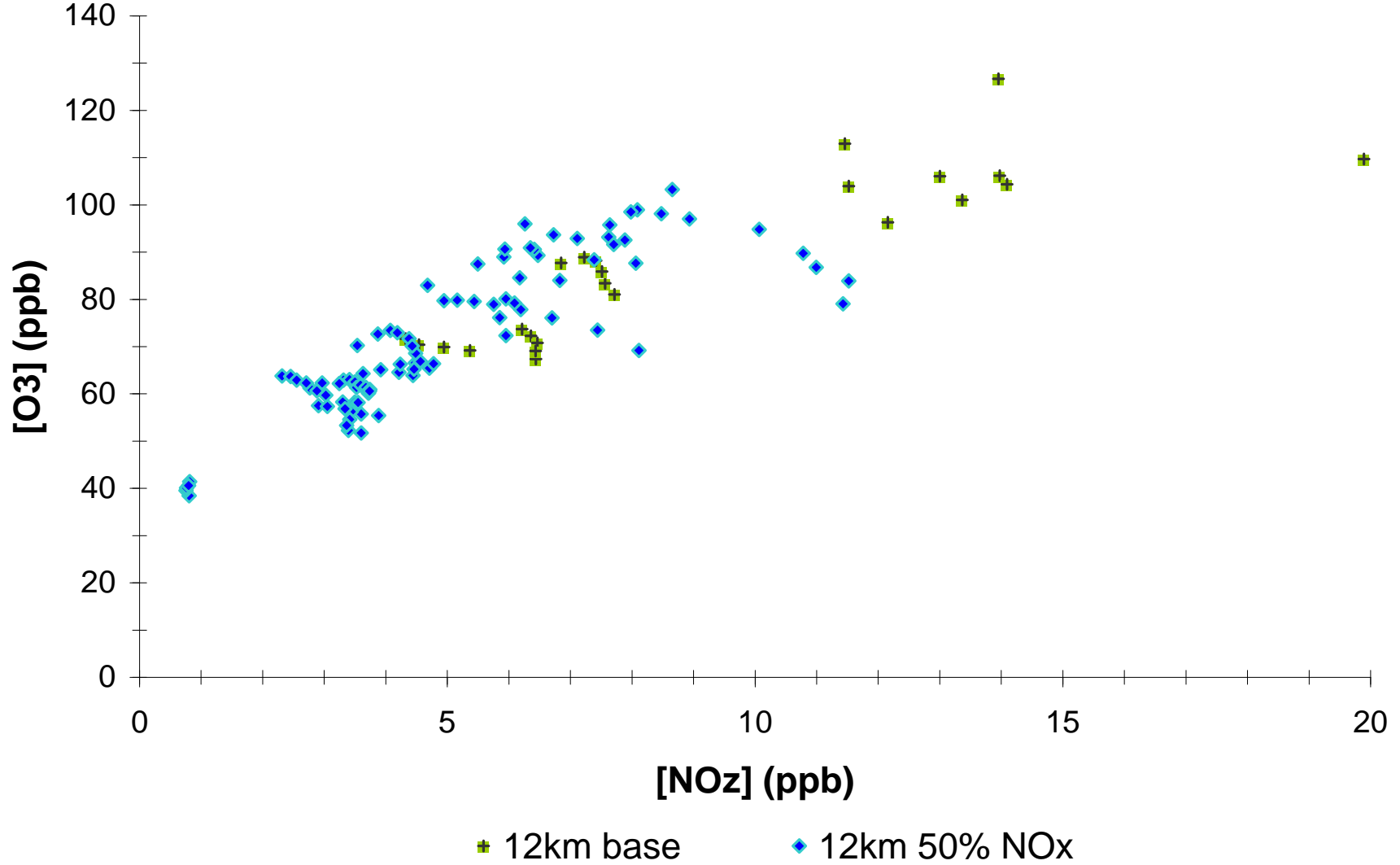
SOS site Youth
CMAQ CB4 Base Case and 50% NOx Control
5 - 18 July 1995 All Model Hours with O3 / NOx >46



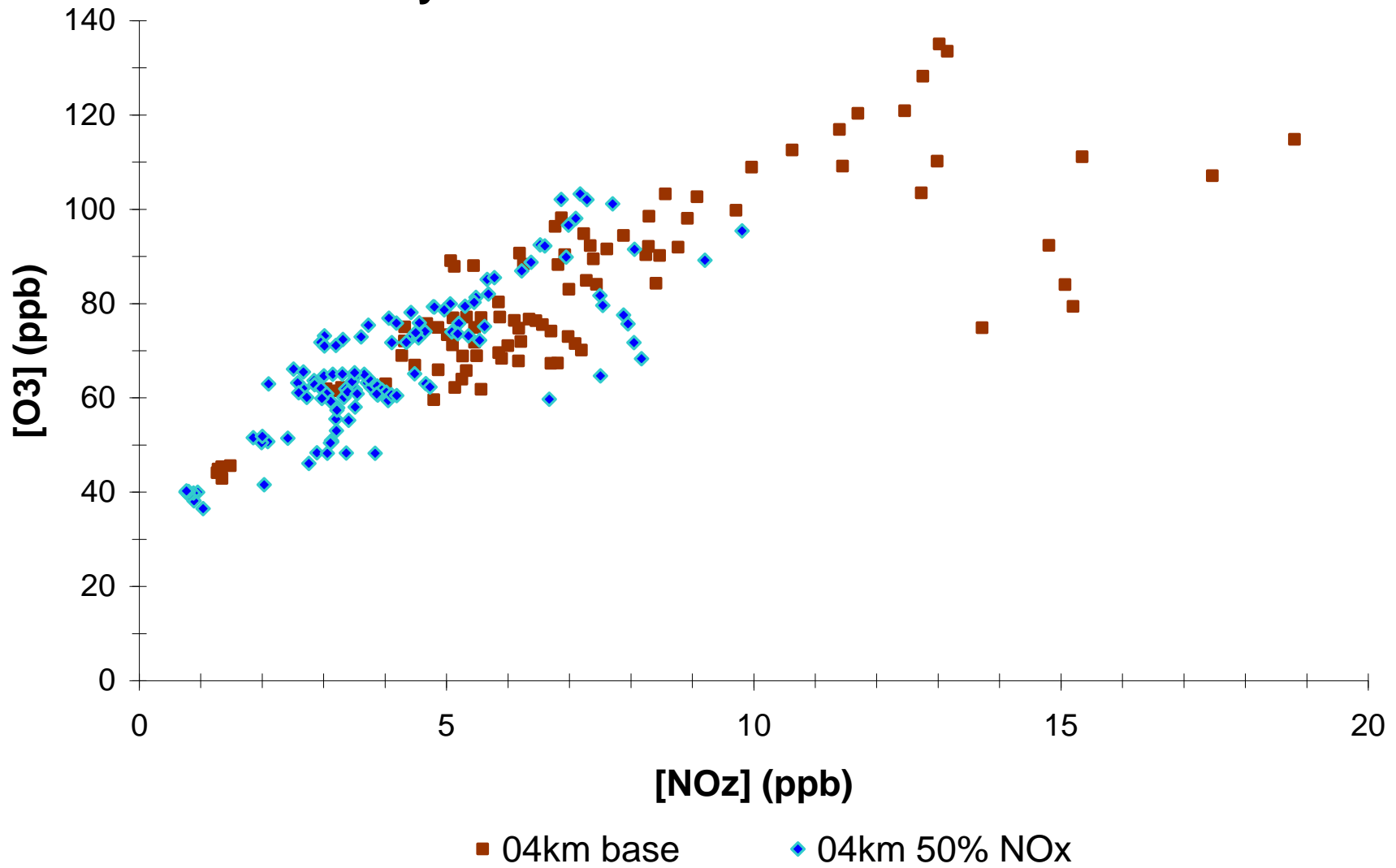
SOS site Youth
CMAQ CB4 Base Case and 50% NOx Control
5 - 18 July 1995 All Model Hours with O3 / NOx >46



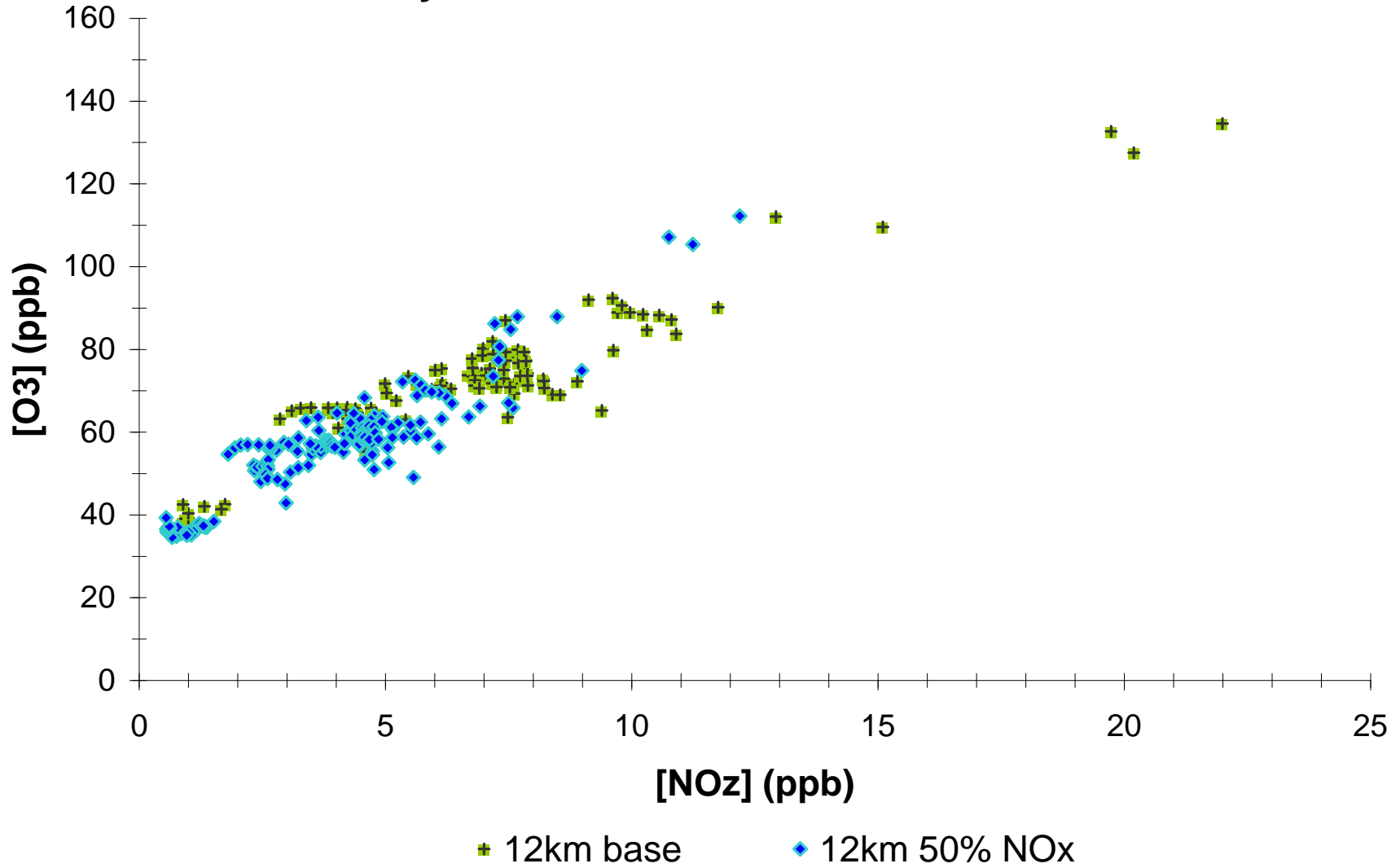
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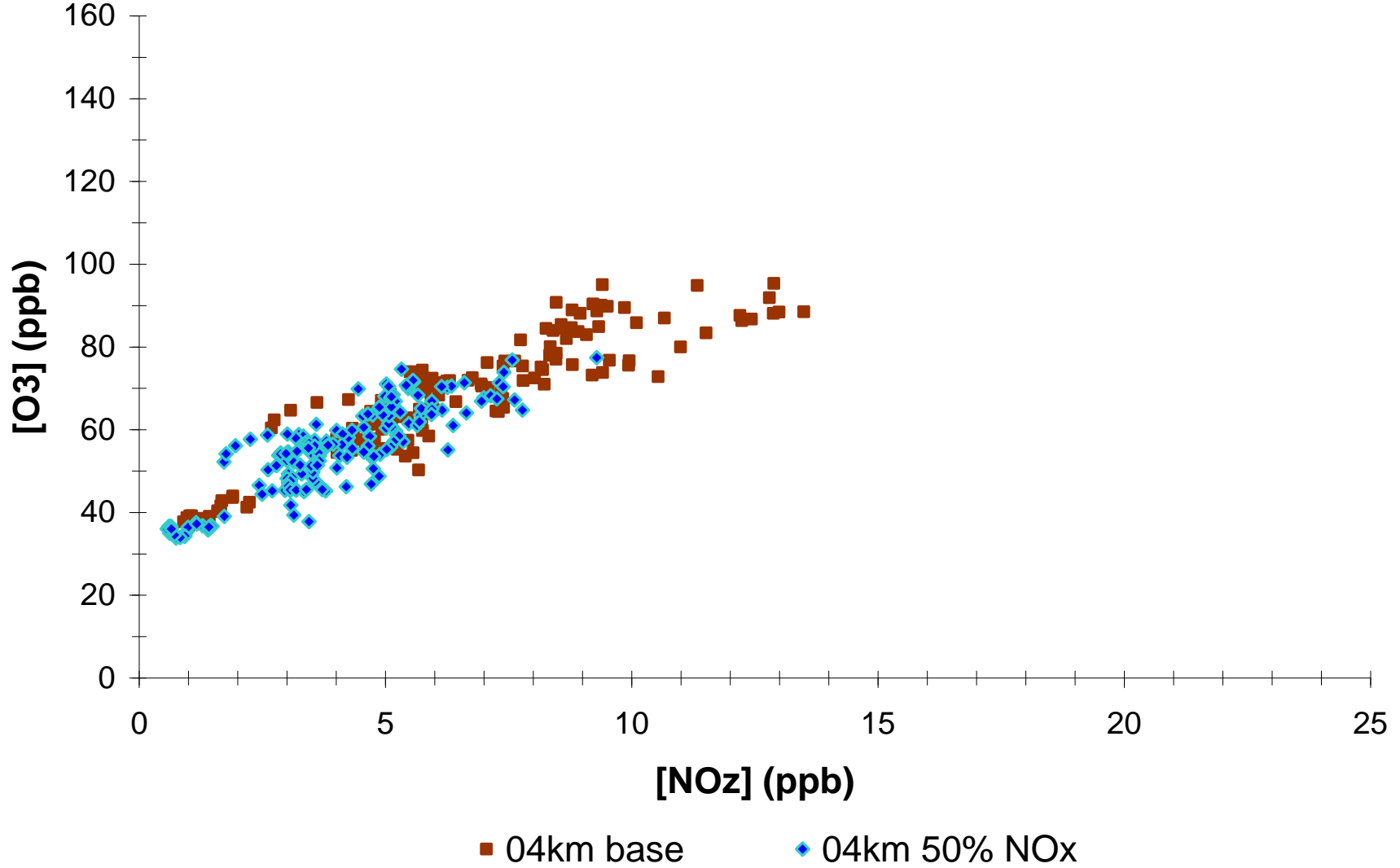
SOS site Youth
CMAQ RADM2 Base Case and 50% NOx Control
5 - 18 July 1995 All Model Hours with O3 / NOx >46



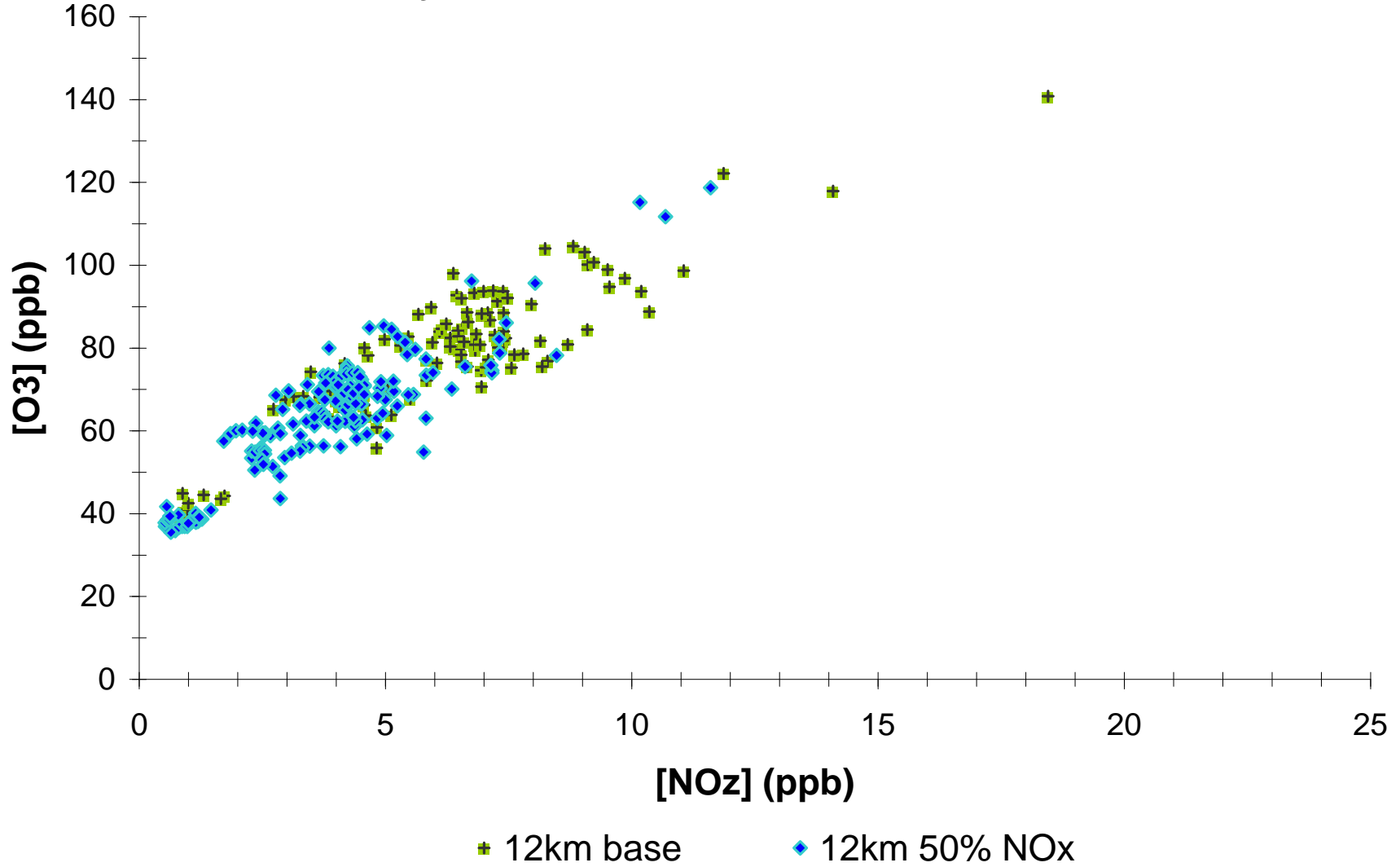
SOS site Dickson
CMAQ CB4 Base Case and 50% NOx Control
5 - 18 July 1995 All Model Hours with O3 / NOx >46



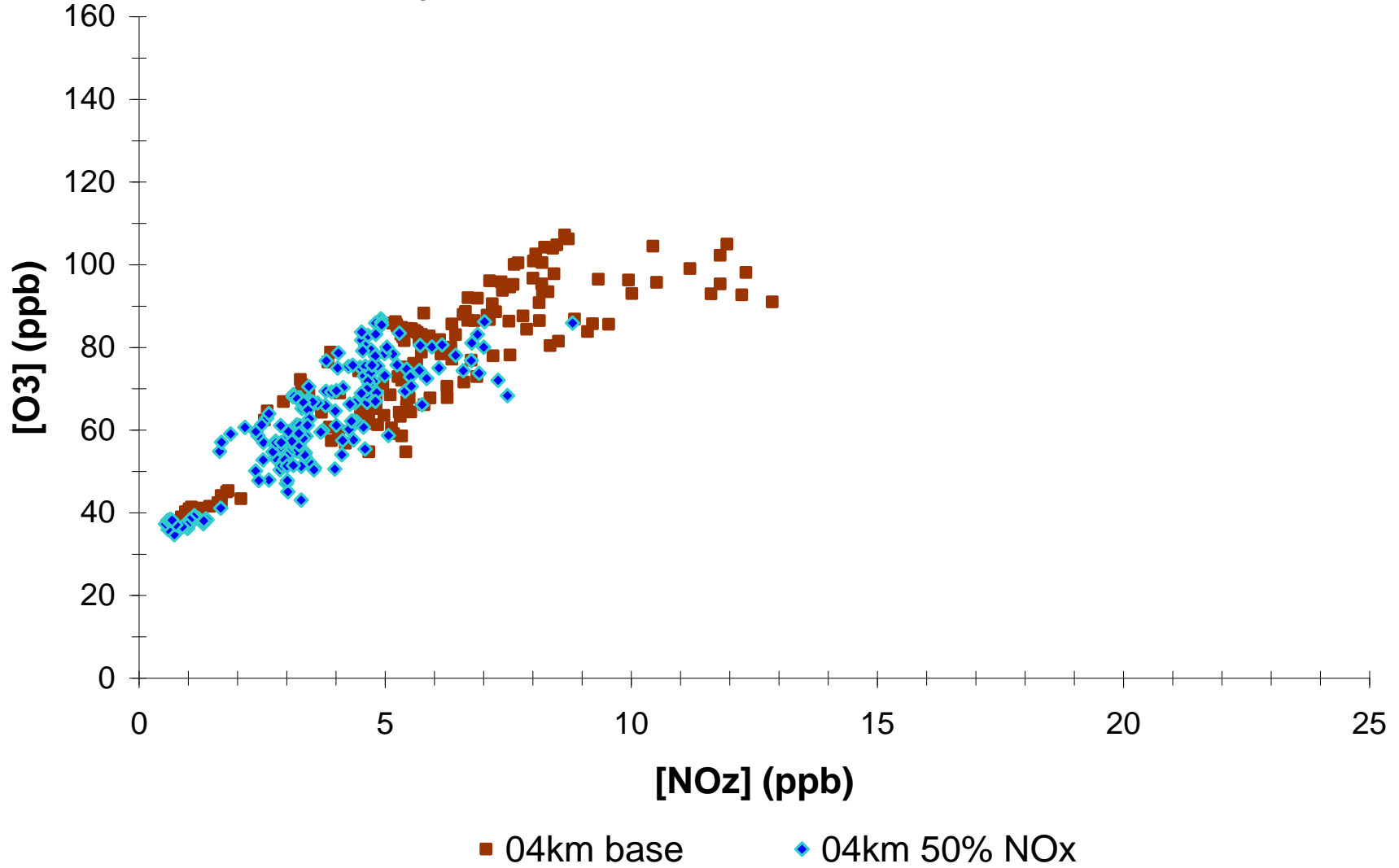
SOS site Dickson
CMAQ CB4 Base Case and 50% NOx Control
5 - 18 July 1995 All Model Hours with O3 / NOx >46



SOS site Dickson
CMAQ RADM2 Base Case and 50% NOx Control
5 - 18 July 1995 All Model Hours with O3 / NOx >46



SOS site Dickson
CMAQ RADM2 Base Case and 50% NO_x Control
5 - 18 July 1995 All Model Hours with O₃ / NO_x >46



Process Diagnostic Probe (*cont'd*)

O₃ Production Efficiency Results

- CMAQ appears to track the production efficiency line traced out by the [O₃] to [NO_z] observations in the NO_z-limited region well, though values from the grid model can be displaced along that line for sites like Dickson that are influenced by large-scale fresh NO_x plumes; preliminary results (not shown) indicate that PinG will show improvement here
- the models behave as expected for the 50% NO_x control runs, bringing the hourly points back along the curve toward the origin
- differences between the chemistries are initially apparent, with CB4 appearing rather flatter against the line of the observations – *i.e.*, lower O₃ production efficiencies; however, the cause and potential significance of this apparent difference are still being investigated
- traditional regression statistics cannot be used to interpret the nonlinear relationship between O₃ and NO_z since both are independent variables and substantial curvature exists in the line; we are pursuing nontraditional statistical tests for assessing the apparent differences we see across the chemistries, the grid spacings, and the sites

Diagnostic Probes of Photochemical Dynamics : Summary Findings

The three diagnostic probes tested here provide **robust and reliable process information separately and when used together about the aggregate production rate of O₃** and some details of NO_x cycling in determining that rate

- (1) **[O₃] / [NO_x]** segregates the radical-limited, NO_x-limited, and the near-ridgeline regions of the response surface effectively across the sites examined here
- (2) **CMAQ correctly reproduces most of the relevant distributions** of observed [O₃] / [NO_x] values where photochemistry appears to be the dominant determinant
- (3) for the urban-influenced site at Youth, **4km models demonstrate substantially better fits to the observations of the [O₃] / [NO_x] ratios, predict an [O₃] to [NO_z] slope closer to that of the observations, and predicted a more appropriate number of hours each day in the NO_x-limited range of [O₃] / [NO_x] >46**
- (4) **air mass aging comparisons, such as the ratio [NO_z] / [NO_y] and [O₃] as a function of NO_x aging, are useful complements to the ridgeline indicator** and provide a check on interpretations derived from that response surface probe
- (5) in general, **CMAQ appears to be aging NO_x appropriately** where the photochemistry is not confounded by emissions or meteorology error

Diagnostic Probes of Photochemical Dynamics : Summary Findings (*cont'd*)

- (6) CMAQ (grid model) reproduces the curve of observed O₃ production efficiency reasonably well, though model values can be displaced along that line for sites influenced by large-scale NO_x plumes like Dickson; PinG results show improvement here
- (7) CMAQ's predicted O₃ production efficiency appears to respond correctly to simulated NO_x emissions control
- (8) differences between CB4 and RADM2 are not apparent in the distributions of the ridgeline indicator, but may be apparent in the [O₃] to [NO_z] slopes where CB4 appears rather flatter against the line of the observations