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Theoretical analysis of simplified NO-NO_2-O_3 chemistry for near-road NO_2 estimation

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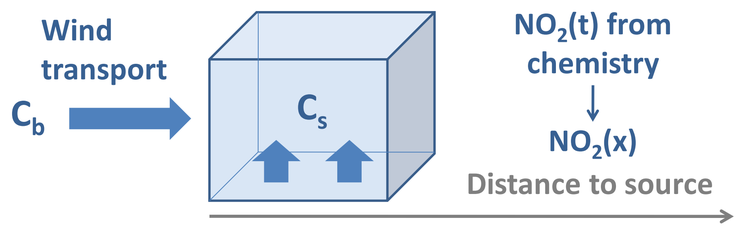
Introduction

Two reactions dominate NO_2 chemistry under local and urban conditions: oxidation of NO and photolysis of NO_2. Atmospheric dispersion models usually include this simplified NO–NO_2–O_3 chemistry in a sequential (modular) approach (e.g., 1,2). Despite the widespread use of simplified schemes, formulations vary in assumptions and parameters (3), and their impact on simulated NO_2 has received little attention. Understanding this is particularly relevant near-road, where residence times can be low and concentrations are higher, often exceeding WHO recommended levels. Sensitivity analyses under designed experiments can help clarify these effects (4).

Objective: To assess how formulations/assumptions and key parameters affect NO_2 under near-road conditions.



Methodology

Basic scheme:

$NO + O_3 \rightarrow NO_2$ (1)
$NO_2 + h\nu \rightarrow NO + O_3$ (2)

Four formulations:

- 1R-stat: one-reaction (1), stationary
- 1R-dyn: one-reaction, dynamic
- 2R-stat: two-reaction, stationary
- 2R-dyn: two-reaction, dynamic

The analysis is divided into:

A. Base Case (BC): chemical evolution of NO_2 vs time/distance, under the 2R-scheme.

B. Sensitivity to formulations under three pollution scenarios: high, moderate, low.

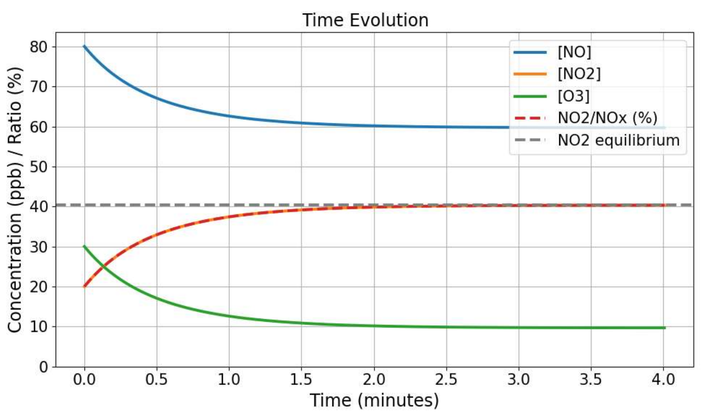
C. Sensitivity (BC) to key parameters: fraction of NO_2 in NOx emissions (f-NO_2: 0.1–0.3), background NO_2 and O_3 (NO_2b, O_3b: 0–40 ppb).

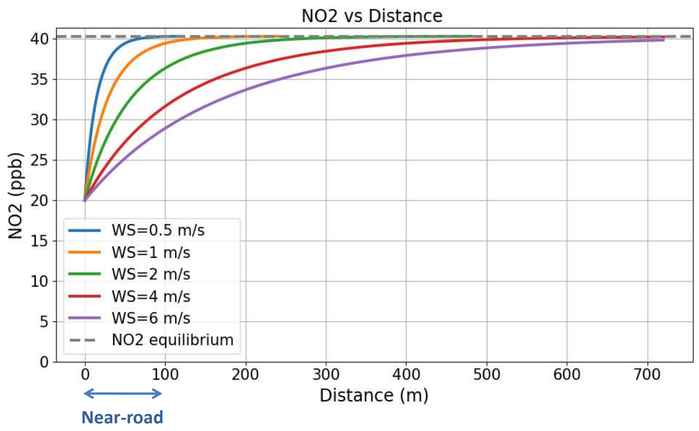
The dynamic schemes are solved using the analytical solution for NO_2(t), obtained from the quadratic formulation of the coupled system. All scenarios consider k = 3.5×10^{-4} $ppb^{-1}.s^{-1}$ and J = 5×10^{-3} s^{-1}.

Scenario	NOx (ppb)	f-NO_2	O_3 (ppb)
BC	100	0.2	30
High	300	0.2	20
Moderate	100	0.4	30
Low	30	0.6	40

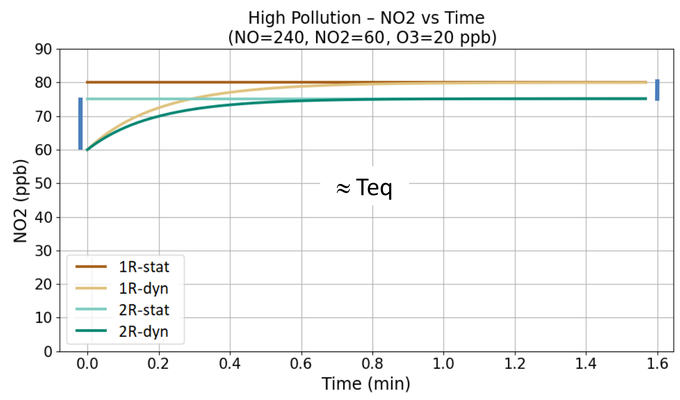
Results

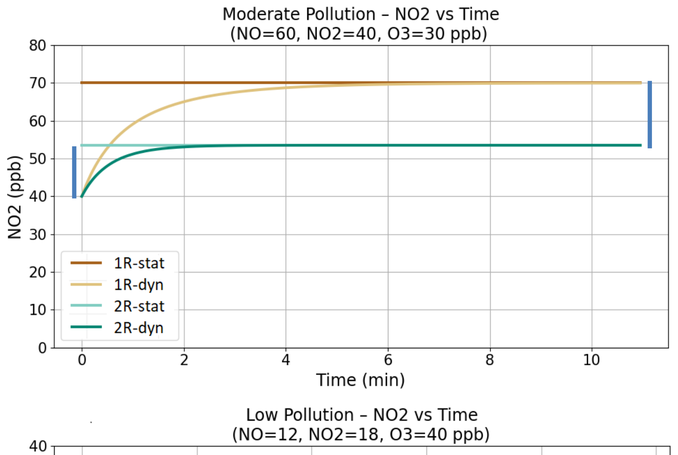
A. Base case dynamics

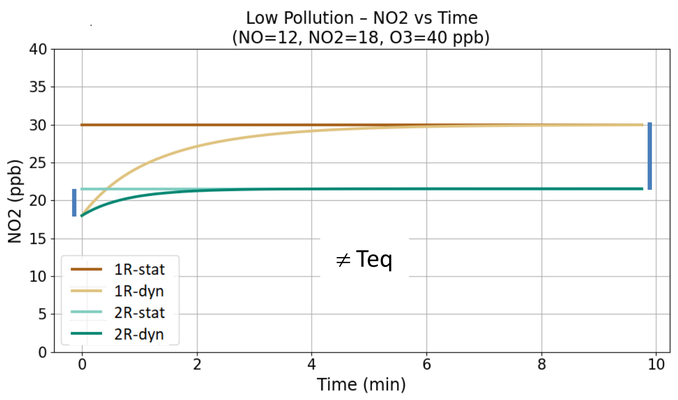




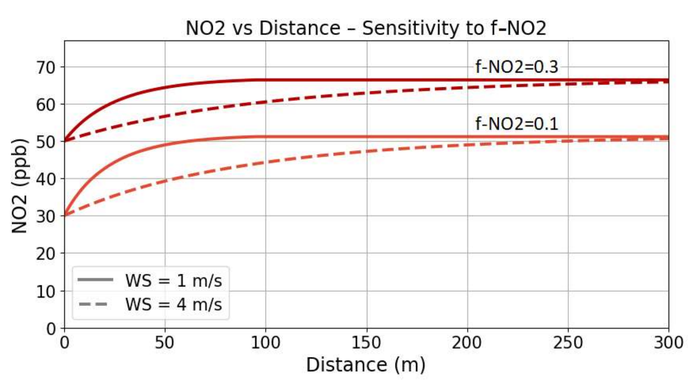
B. Sensitivity to formulation

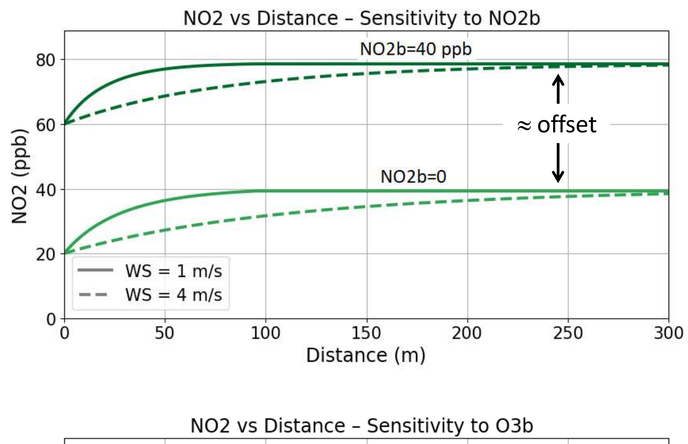


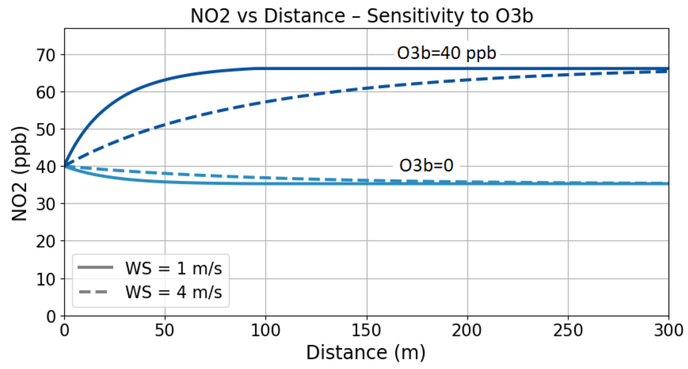




C. Sensitivity to key parameters







Conclusions

- **Formulation choice**: lower influence under high pollution, but under moderate/low NO_2 differences can be comparable to the local chemical contribution.
- **Key parameters**: NO_2b and f-NO_2 set initial NO_2; O_3b controls formation, and their relative importance depends on the initial concentrations of species.
- **Near-road conditions**: NO_2 can remain close to its initial value (except at very low WS), which may help explain the good performance of empirical NO_2–NOx relationships.

References

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