CFD Modeling of Reactive Pollutants in an Urban Street Canyon using Different Chemical Mechanisms

iCUC9
20th-24th July 2015
Toulouse France

B Sanchez[a,b], JL Santiago[a], A Martilli[a], M Palacios[a], F Kirchner[c]

[a] Center for Energy, Environment and Technology (CIEMAT), Madrid, Spain
[b] Engineering and Economy of transport (INECO), Madrid, Spain
[c] GAIASENS Technologies. Sarl, Switzerland

e-mail: beatriz.sanchez@externos.ciemat.es

GOBIERNO DE ESPAÑA
MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD
Ciemat
Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas
MiNOx street
Life

Introduction

- At microscale the atmosphere and urban distributions interaction generates a complex flow and heterogeneous dispersion of pollutants within the canopy

- An accurate understanding of Urban Air Quality requires considering a coupled behavior between dispersion of reactive pollutants and atmospheric dynamics

- Urban Air Pollution → Traffic emissions

- Nitrogen Oxide (NO)
- Nitrogen dioxide (NO_2)
- Volatile Organic Compounds (VOCs)

Limitations

- In a real and complex geometry, the required computational time is large

- Implementing chemical reactions in a CFD model increase the CPU time considerably due to the coupling of pollutant transport equations

Objectives

To simulate the pollutants dispersion considering chemistry:

- To reproduce reactive pollutant distribution using the simplest chemical mechanism minimizing CPU time

- Analyze the conditions in which the implementation of a complex chemical mechanism is necessary

Structure

To model in 2D and 3D idealized urban geometries:

- The chemical and dynamic coupling under different chemical approaches:

  (a) Passive tracer (non-reactive)

  (b) NOx-O_3 photostationary state (PSS)

  (c) Complex chemical mechanism (CCM)

- Evaluation of the influence of atmospheric parameters (wind speed and ozone concentration)

Quantify the variation on NO and NO_2 concentration with the use of chemical mechanism

Chemical Mechanisms

Passive Tracer → Considering NO and NO_2 non-reactive

Photostationary State →

$$NO_2 + h\nu \longrightarrow NO + O_3$$
$$O + O_2 + M \longrightarrow O_3 + M$$
$$O_3 + NO \longrightarrow NO_2 + O_2$$

Complex Chemical Mechanism → 23 chemical species
25 chemical reactions

Due to the limitation of CPU time, CCM has been reduced based on Regional Atmospheric Chemistry Mechanism (RACM) using CHEMATA program software (Kirchner, 2005)

Study scenarios

Ozone

- $O_3 = 10$ ppb
- $O_3 = 40$ ppb

Geometry

- 2D
- 3D

Wind Speed

- $\mathrm{u}(z = 2\mathrm{H}) = 2\ m\ s^{-1}$
- $\mathrm{u}(z = 2\mathrm{H}) = 4\ m\ s^{-1}$

- Passive tracer (non-reactive)
- NOx-O_3 photostationary state (PSS)
- Complex chemical mechanism (CCM) → Different ratios of VOCs-to-NOx emission:
  - VOCs/NOx=1/5
  - VOCs/NOx=1/2

CFD Model description

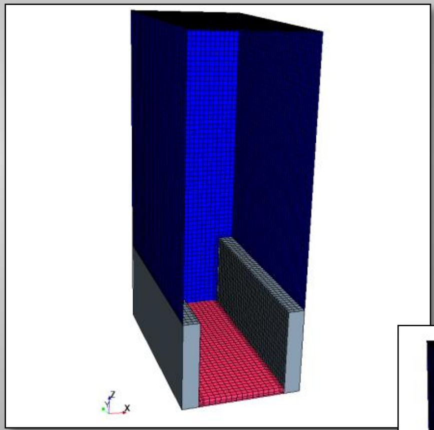
- Reynolds-averaged Navier-Stokes (RANS) equations with a k-ϵ turbulence model
- Transport equations of chemical species

$$\frac{\partial C_i}{\partial t} + U_i \frac{\partial C_i}{\partial x_j} = D \frac{\partial^2 C_i}{\partial x_j \partial x_j} + \frac{\partial}{\partial x_j}\left(K_c \frac{\partial C_i}{\partial x_j}\right) + \left[\Delta C_i\right]_{Chem} + S_{C_i}$$

- Computational domains

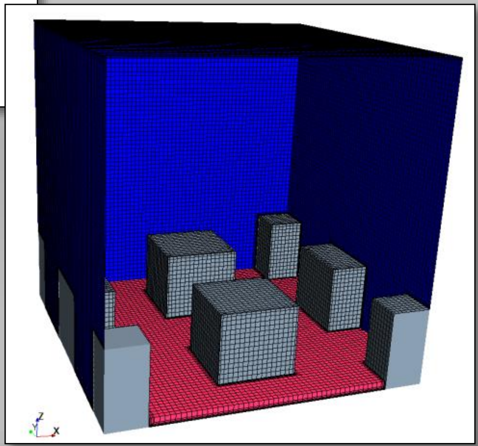
  2D-geometry: Street-Canyon

  - 24x40x64 m



  3D-geometry: Staggered Array of cubes:

  - 64x64x64 m
  - $\lambda_p = 0.25$



Simulation Set up

❖ **Boundary conditions for momentum equations**

- Simulating an infinite number of streets

u_τ: Reference velocity
H: Buildings height

y-direction → zero gradient boundary conditions

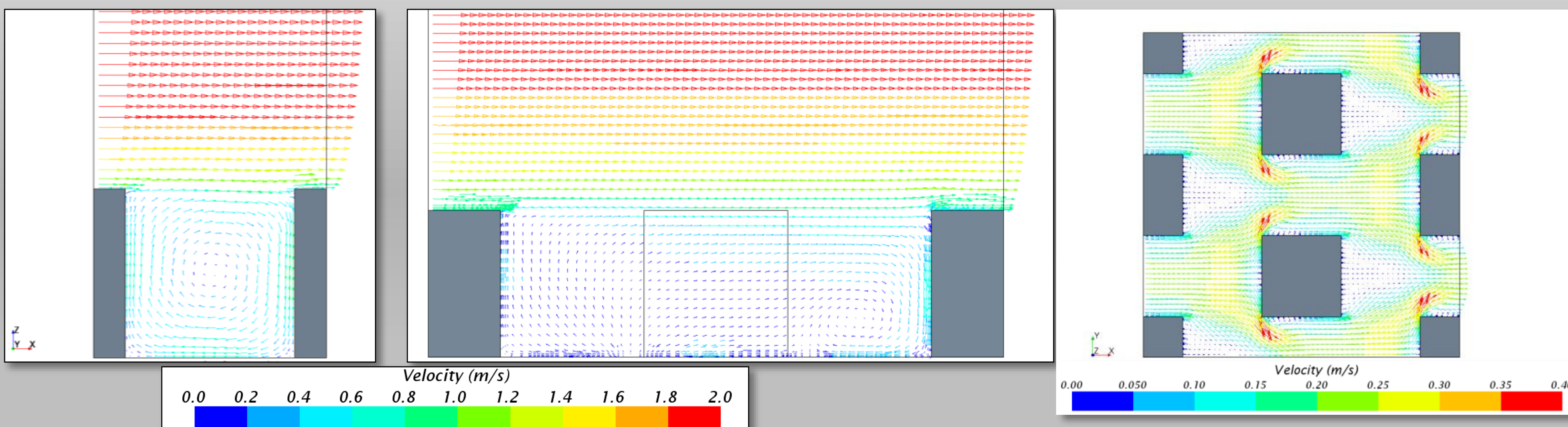
x-direction → Periodic Conditions: $\partial P / \partial x = \rho\, u_\tau^{2} / 4H$

$u_\tau = 0.45\ m\ s^{-1}$

$u_\tau = 0.225\ m\ s^{-1}$

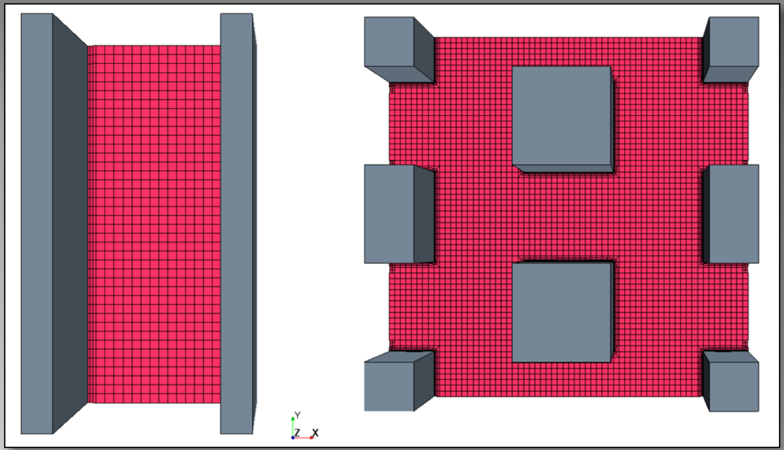
Flow field:

2D-Geometry *3D-Geometry*



Simulation Set up

❖ **Traffic Emissions**



- Located at the bottom

- NOx fixed emissions:

$$\begin{cases} S_{NO} = 112\ \mu g\ m^{-1} s^{-1} \\ S_{NO_2} = 17\ \mu g\ m^{-1} s^{-1} \end{cases} \longrightarrow \text{For all emissions cases}$$

- VOCs emissions ⟶ Complex Chemical Mechanism

- VOCs-to-NOx emissions :

$$\begin{cases} VOCs/NOx = 1/5 \quad \textbf{(CCM5)} \\ VOCs/NOx = 1/2 \quad \textbf{(CCM2)} \end{cases}$$

Simulation Set up

❖ **Top Conditions**

- Constant concentration at the top → Important role within the canyon

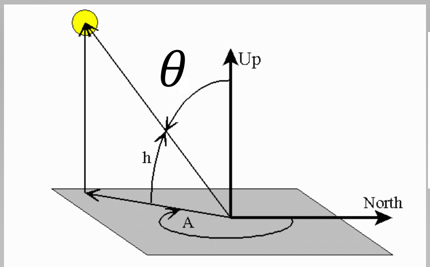
NO	16 ppb
NO2	35 ppb

- VOCs concentration at the top change with emission ratio
- $[O_3]$ is computed using photostationary equilibrium and is dependent on zenith angle (θ)

$\theta = 45°$, $\theta = 78°$ → $J_{NO_2} = A \exp(B/\cos(\theta))$ (A and B are constant)

$$[O_3] = \frac{J_{NO_2}[NO_2]}{k\,[NO]}$$

→ $O_3 = 40$ ppb, $O_3 = 10$ ppb



Evaluation of Atmospheric Parameters

Study scenarios

Ozone

- $O_3 = 10$ ppb ***(Low O_3)***
- $O_3 = 40$ ppb ***(High O_3)***

Geometry

- 2D
- 3D

Wind Speed

- $\mathrm{u}(z = 2\mathrm{H}) = 2\ m\ s^{-1}$ ***(Ut0225)***
- $\mathrm{u}(\mathrm{z} = 2\mathrm{H}) = 4\ m\ s^{-1}$ **(Ut045)**

- Passive tracer (non-reactive) ***(P)***
- NOx-O_3 photostationary state ***(PSS)***
- Complex chemical mechanism (CCM) →

VOCs-to-NOx emission

- VOCs/NOx=1/5 ***(CCM5)***
- VOCs/NOx=1/2 ***(CCM2)***

Evaluation of Atmospheric Parameters

- In order to compare the scenarios, the concentration is normalized:

$$C_{norm} = \frac{C\ u_\tau\ W}{Q}$$ *(Street Canyon)*

$$C_{norm} = \frac{C\ u_\tau\ A_{Em}^2}{Q}$$ *(Staggered Array of cubes)*

W: Street width
L: Street length
Q: Source emission rate $(\mu g\ m^{-1} s^{-1})$

- The difference with respect to Passive tracer is quantify using:

$$\delta C\ (\%) = \frac{C_{norm} - C_{norm}(P)}{C_{norm}(P)} \times 100$$

Evaluation of Atmospheric Parameters

Study scenarios

Geometry

2D 3D

Wind Speed

$u(z = 2H) = 2\ m\ s^{-1}$

(Ut0225)

$u(z = 2H) = 4\ m\ s^{-1}$

(Ut045)

- Passive tracer (non-reactive) ***(P)***
- NOx-O_3 photostationary state ***(PSS)***
- Complex chemical mechanism (CCM) →

VOCs-to-NOx emission

VOCs/NOx=1/5 ***(CCM5)***

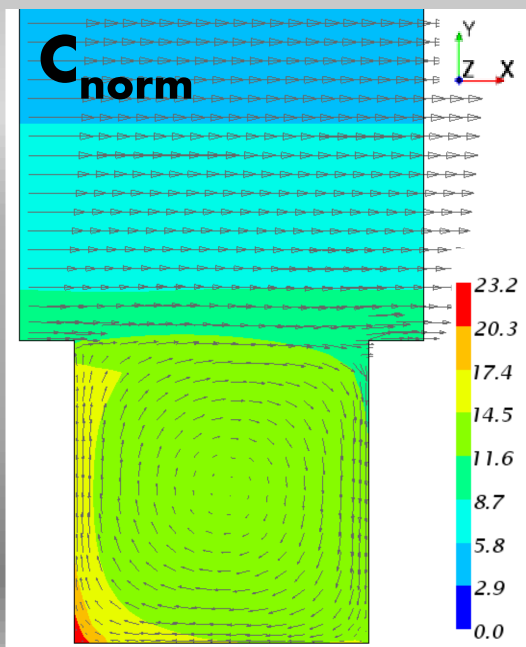
VOCs/NOx=1/2 ***(CCM2)***

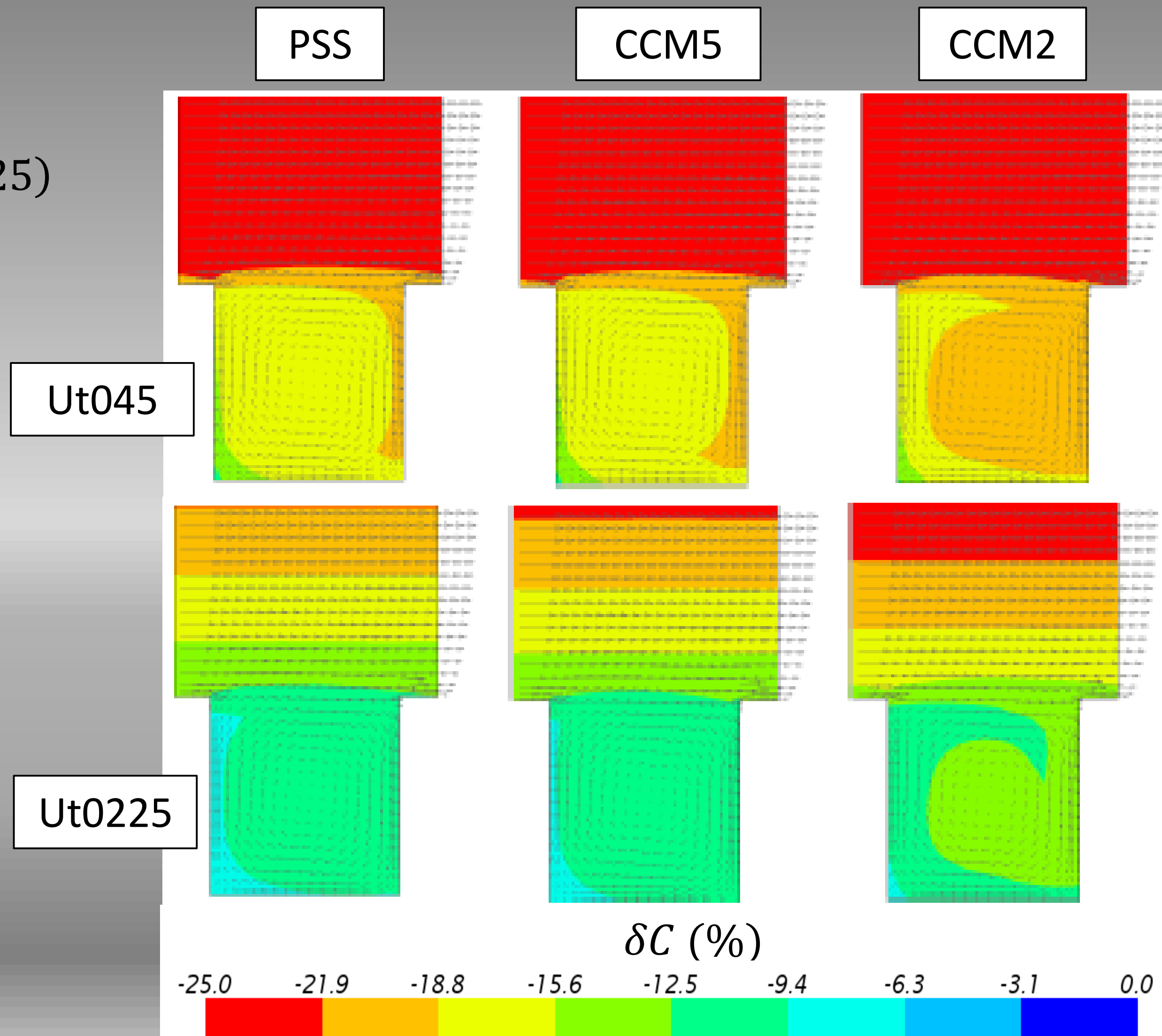
Wind Speed

$$\delta C\ (\%) = \frac{C_{norm} - C_{norm}(P)}{C_{norm}(P)} \times 100$$

δ[NO]

- $\delta C\ (Ut045) > \delta C(Ut0225)$
- Bigger differences with higher VOCs emissions

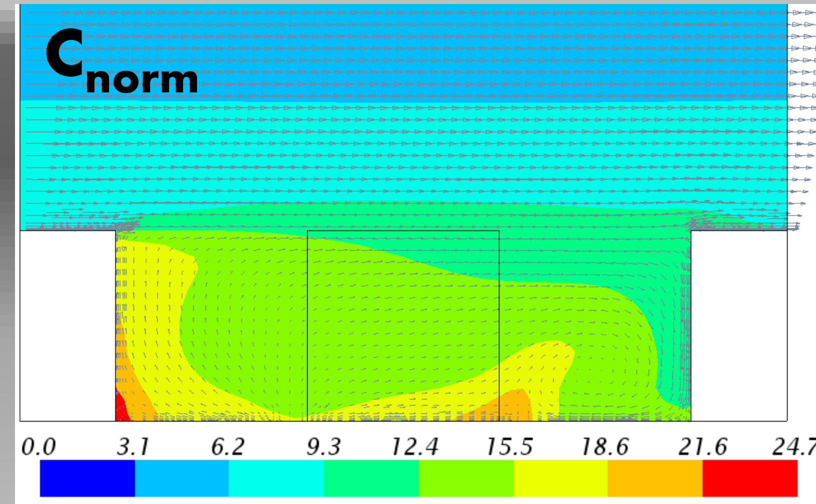


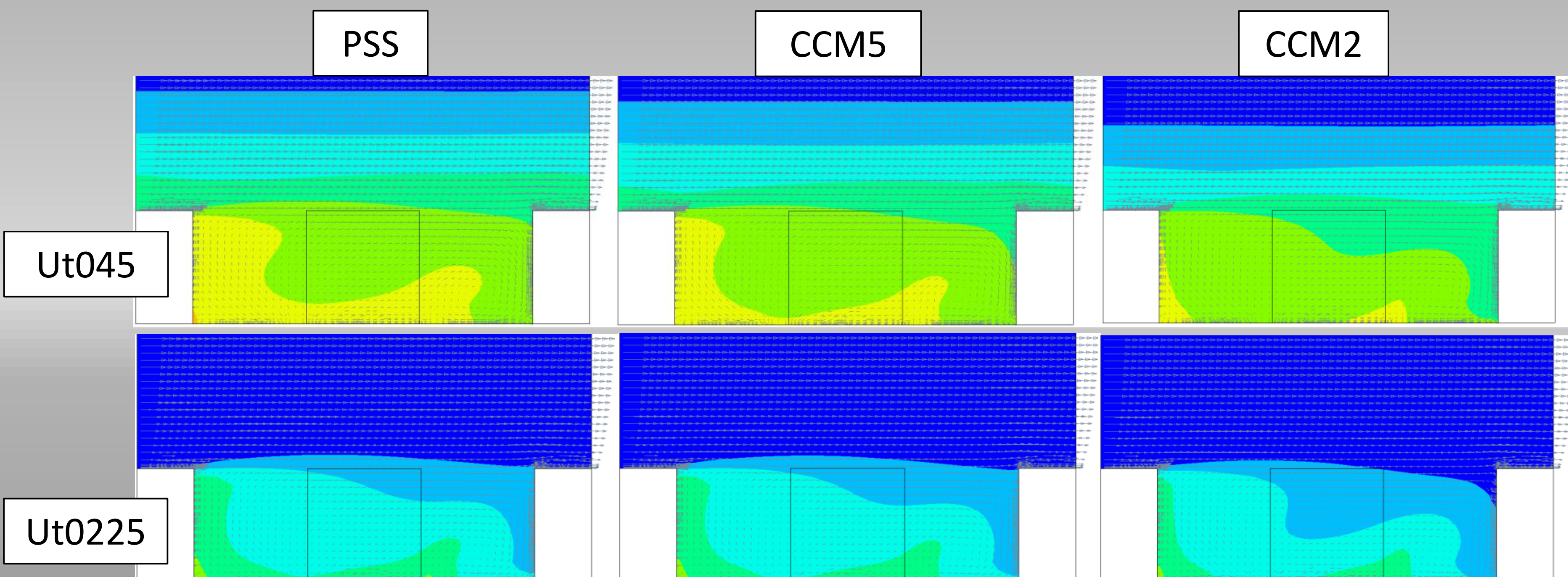


Wind Speed

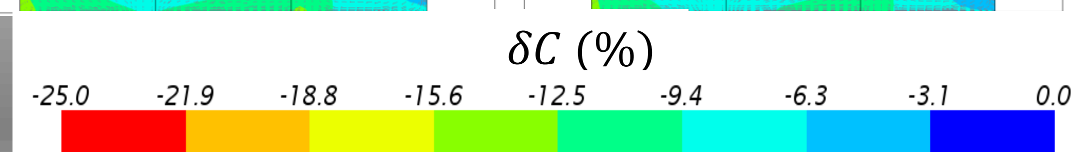
δ[NO]

- More ventilation implies less differences between chemical mechanisms





$$\delta C\ (\%) = \frac{C_{norm} - C_{norm}(P)}{C_{norm}(P)} \times 100$$

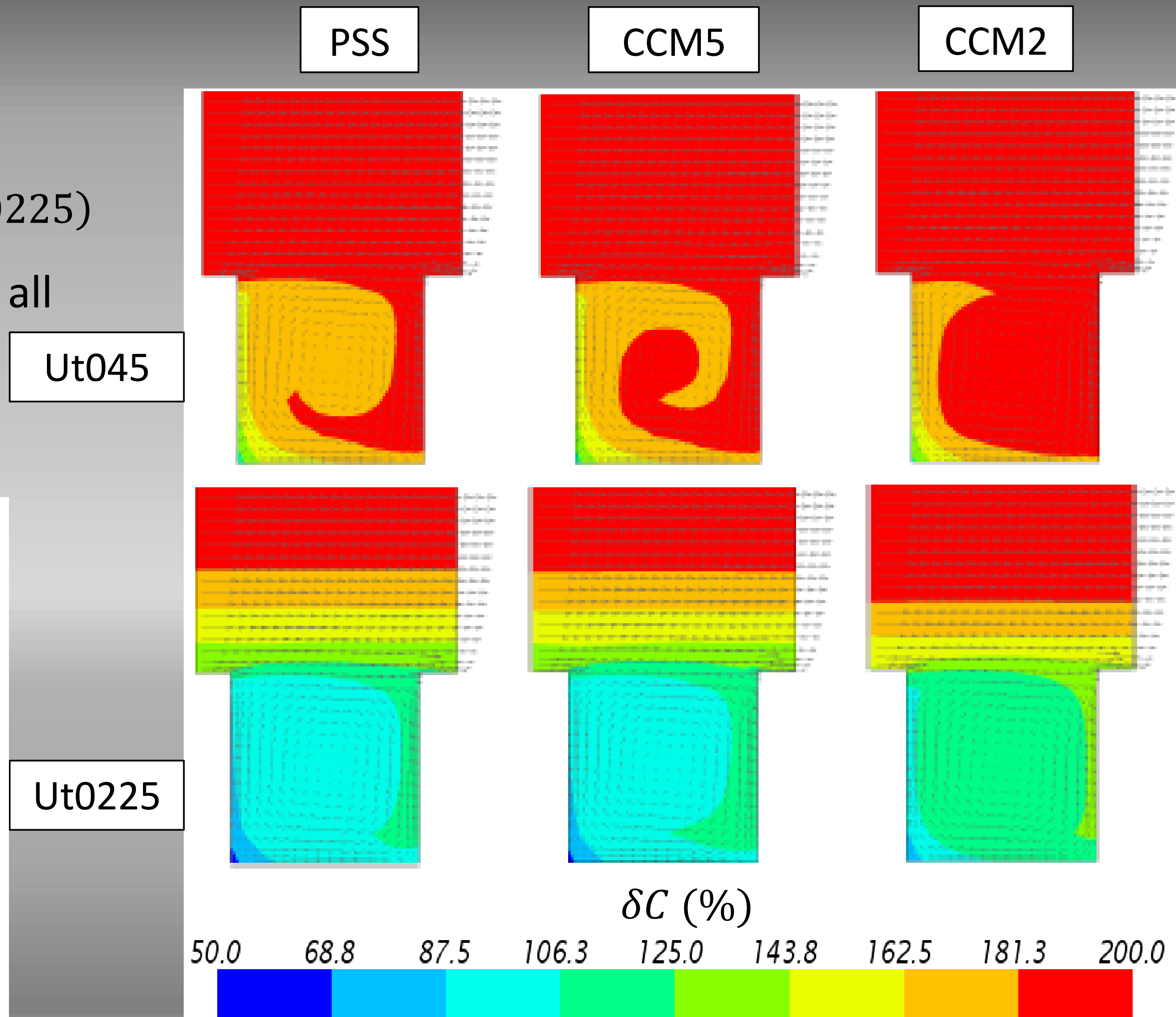


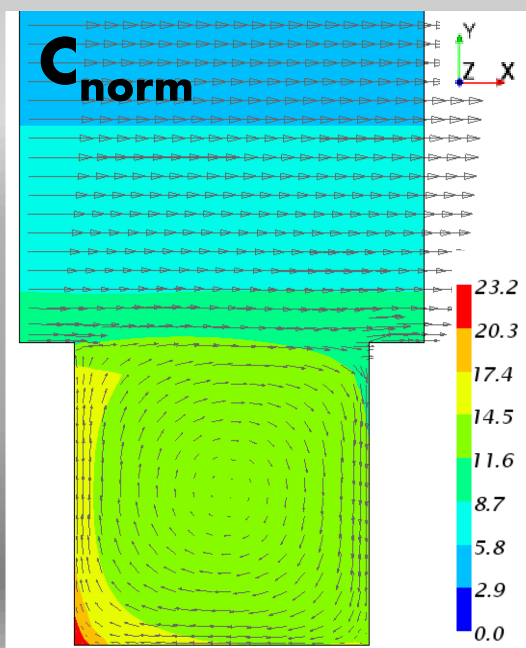
$$\delta C\ (\%) = \frac{C_{norm} - C_{norm}(P)}{C_{norm}(P)} \times 100$$

Wind Speed

$\delta[NO_2]$

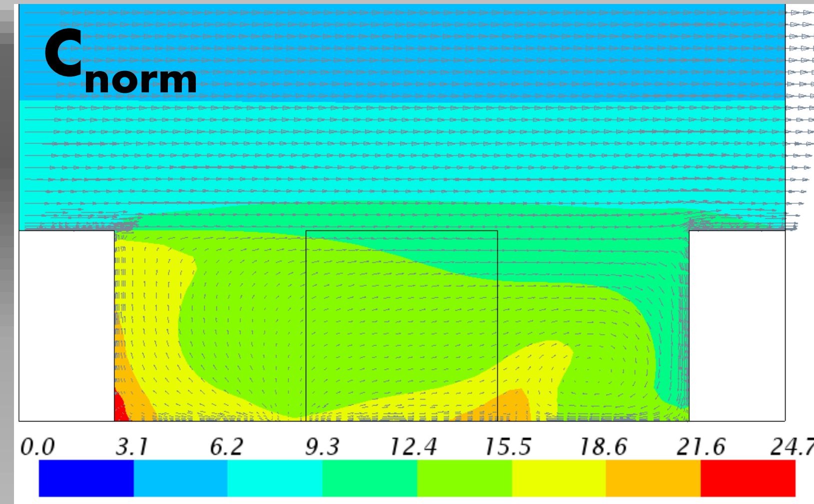
- $\delta C\ (Ut045) > \delta C(Ut0225)$
- Differences between all chemical systems





Wind Speed

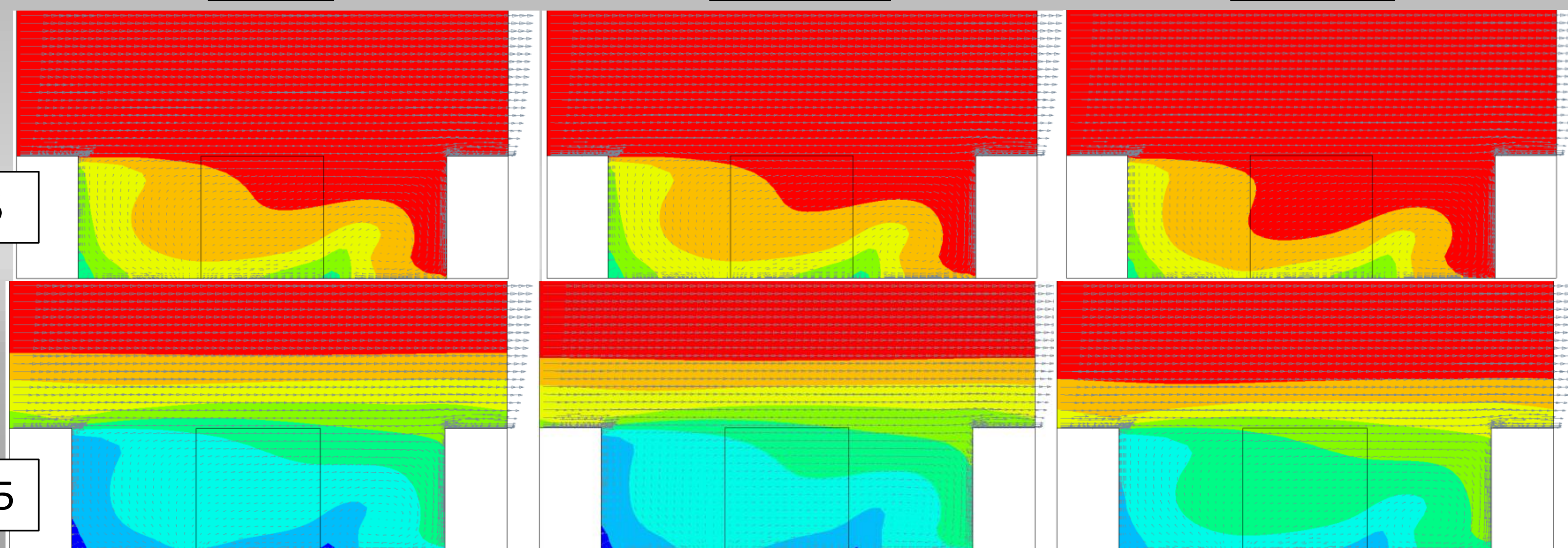
δ[NO2]



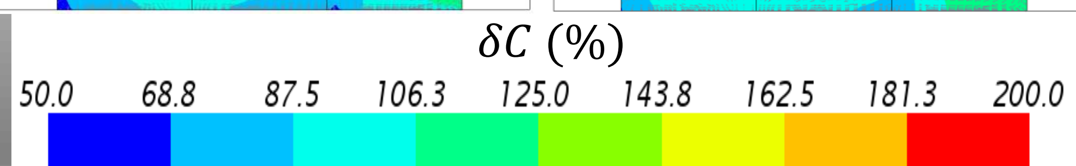
PSS | CCM5 | CCM2

Ut045

Ut0225



$$\delta C\ (\%) = \frac{C_{norm} - C_{norm}(P)}{C_{norm}(P)} \times 100$$



Wind Speed

Vertical profiles

$$C_{norm} = \frac{C\, u_\tau\, W}{Q}$$

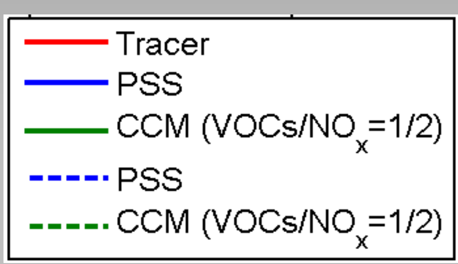
$$C_{norm} = \frac{C\, u_\tau\, A^2{}_{Em}}{Q}$$

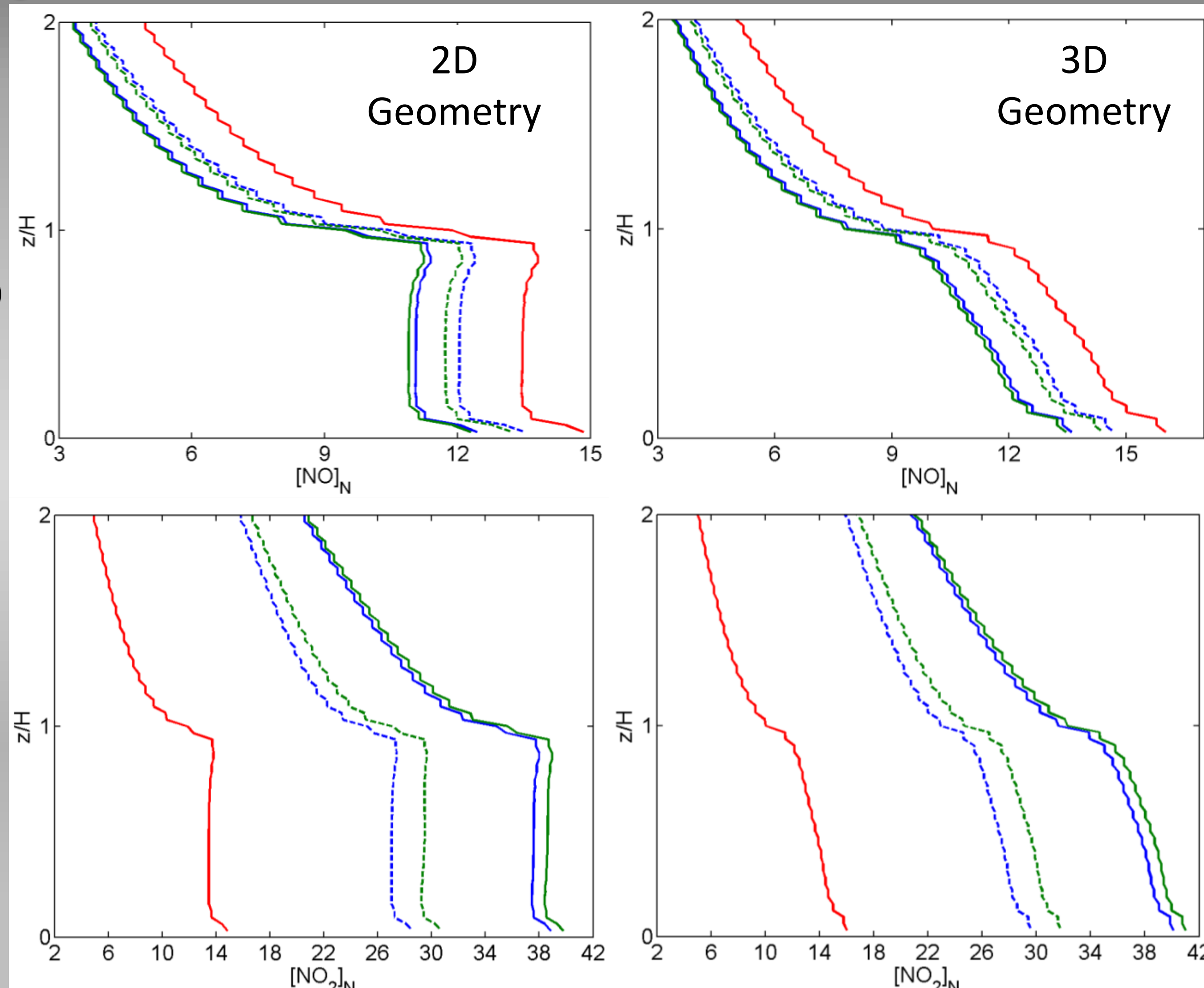
- Horizontal spatial averaged of $[NO]_N$ and $[NO_2]_N$

$\delta C\ (Ut045) > \delta C(Ut0225)$

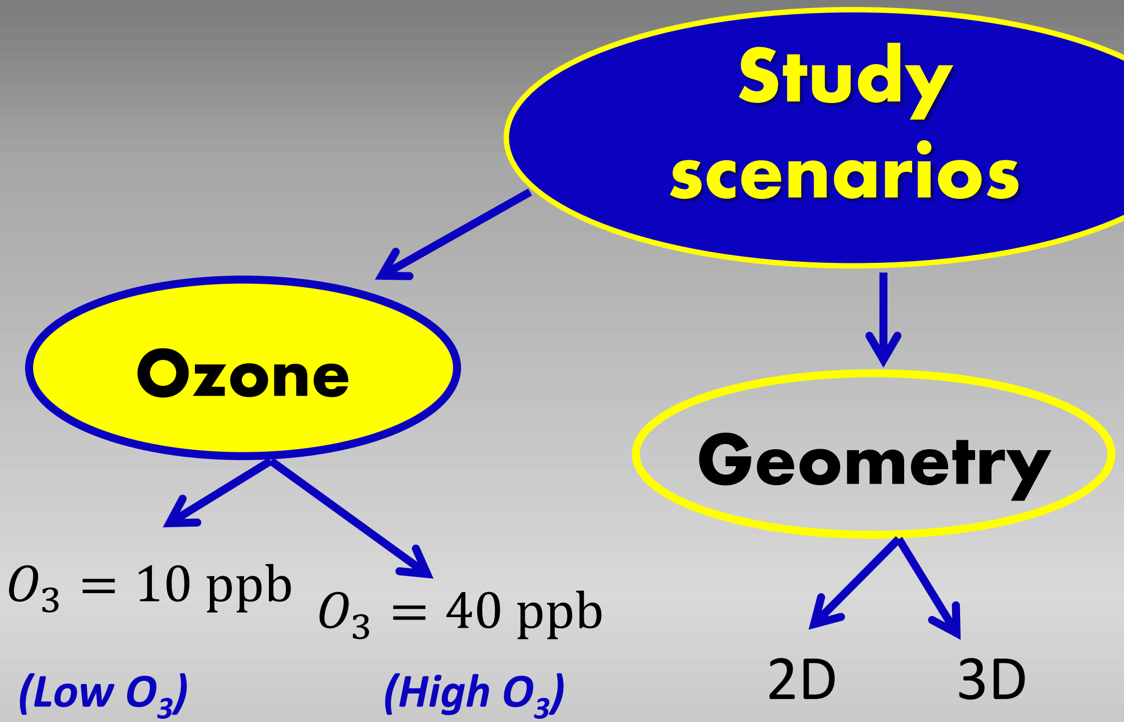
- Lower velocity implies more differences between chemical systems

(*solid line*): Ut045
(*dashed line*): Ut0225





Evaluation of Atmospheric Parameters



- Passive tracer (non-reactive) ***(P)***
- NOx-O_3 photostationary state ***(PSS)***
- Complex chemical mechanism (CCM) →

VOCs-to-NOx emission

VOCs/NOx=1/5 ***(CCM5)***

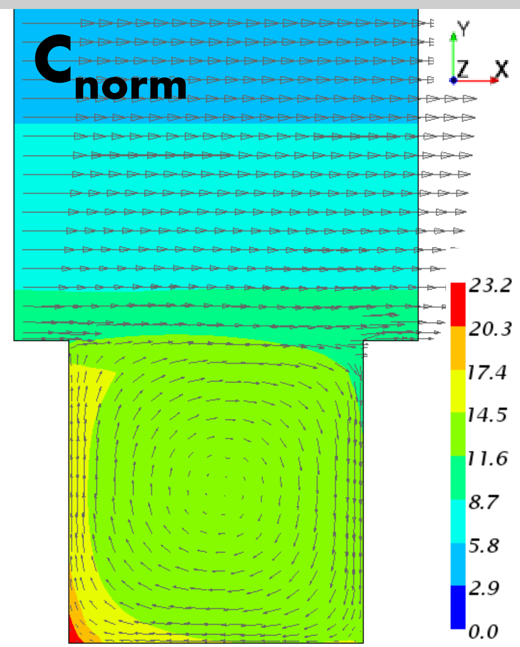
VOCs/NOx=1/2 ***(CCM2)***

Ozone

$$\delta C\ (\%) = \frac{C_{norm} - C_{norm}(P)}{C_{norm}(P)} \times 100$$

δ[NO]

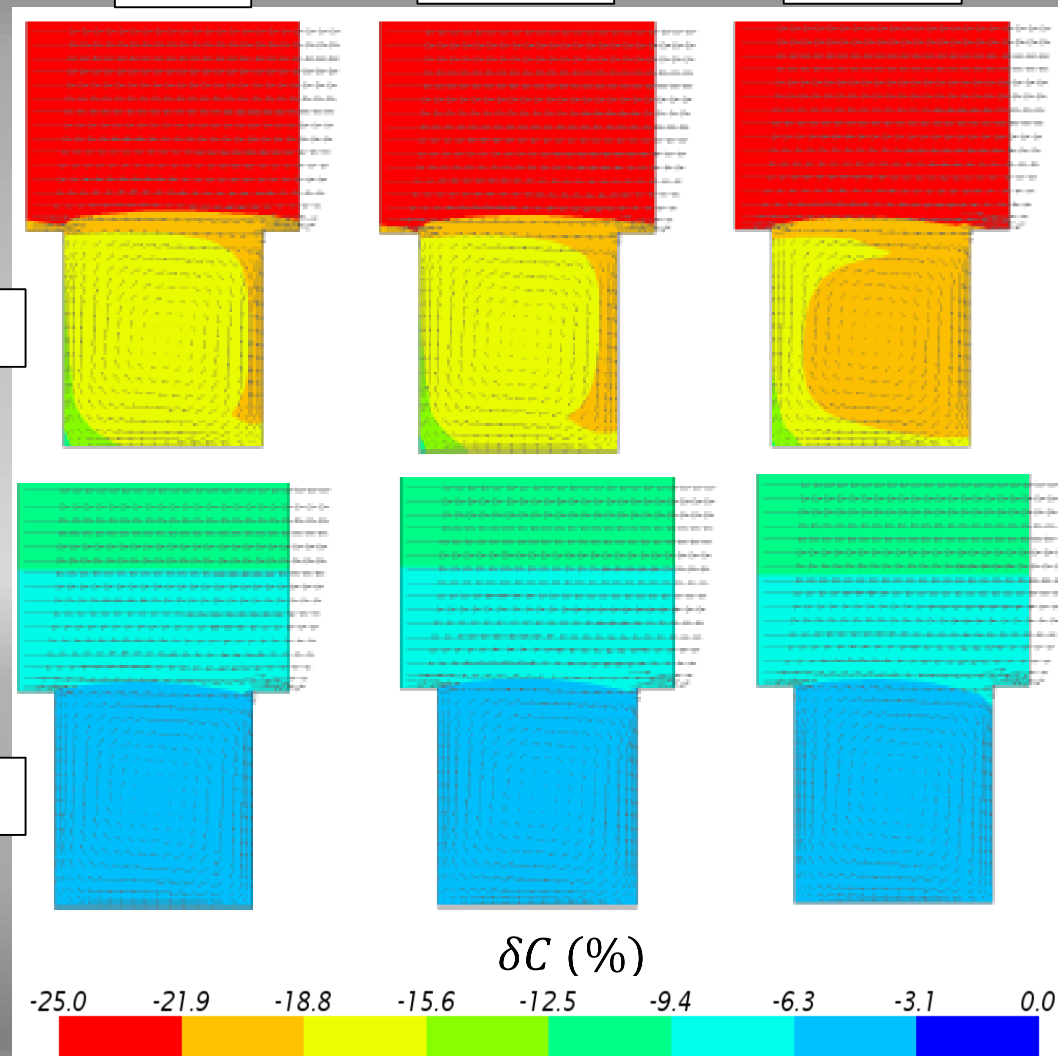
- $\delta C\ (\text{High}\ O_3) > \delta C(\text{Low}\ O_3)$
- Differences between all chemical systems with high O_3



PSS CCM5 CCM2

High O_3

Low O_3

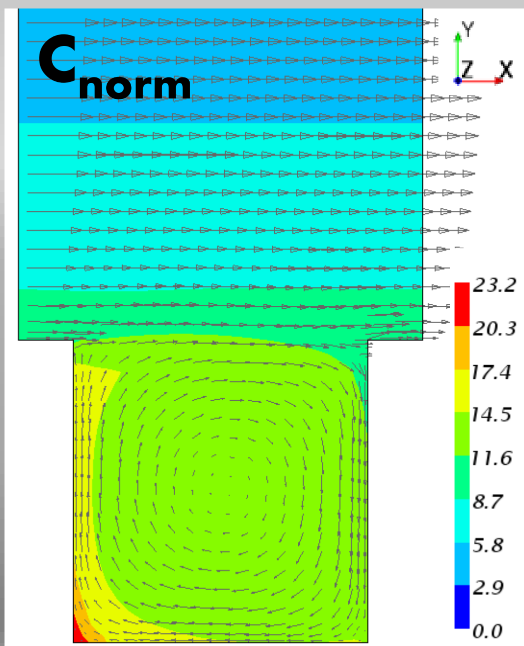


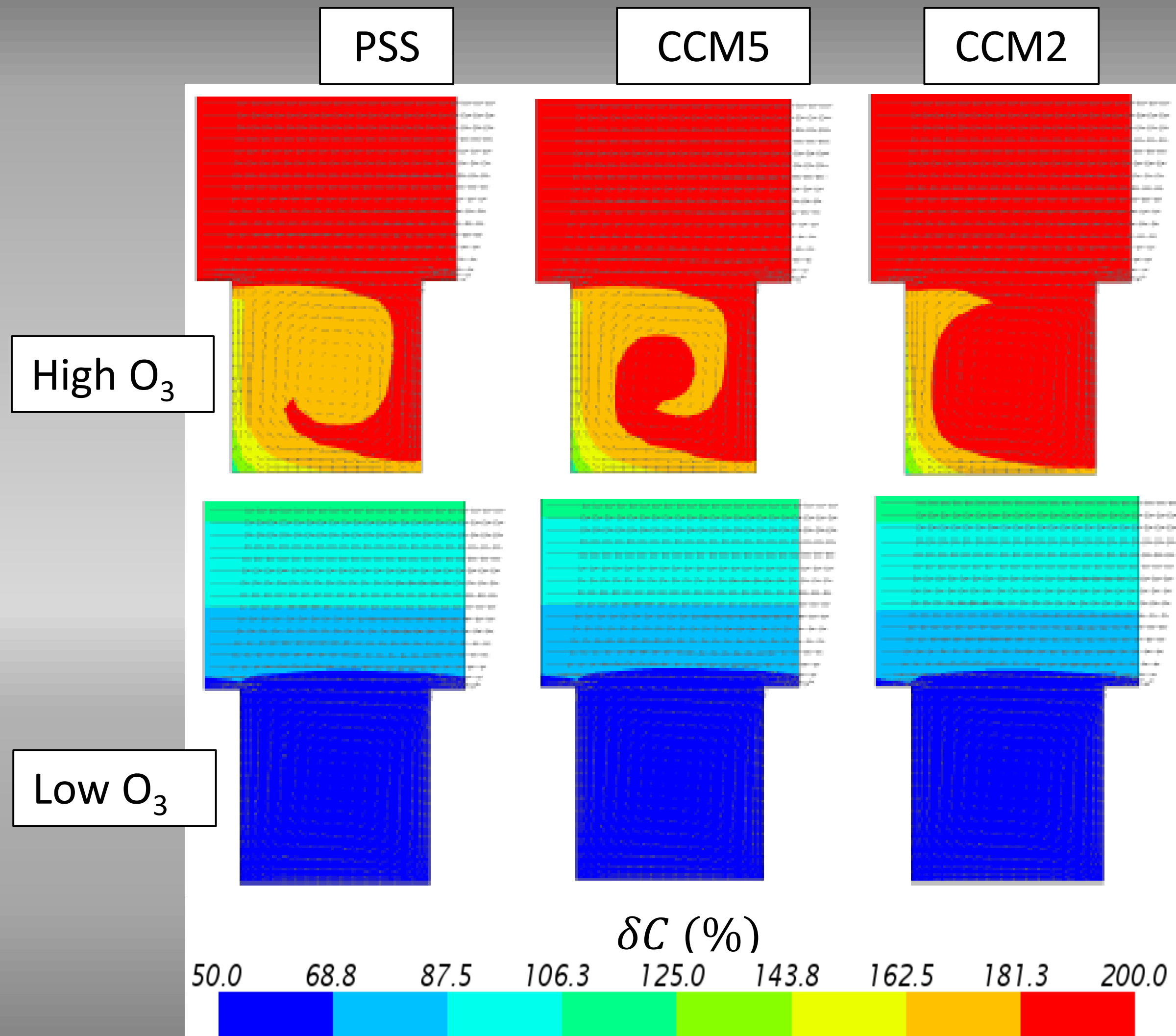
Ozone

$$\delta C\ (\%) = \frac{C_{norm} - C_{norm}(P)}{C_{norm}(P)} \times 100$$

δ[NO2]

- $\delta C\ (\text{High } O_3) > \delta C(\text{Low } O_3)$
- Differences between all chemical systems with high O_3

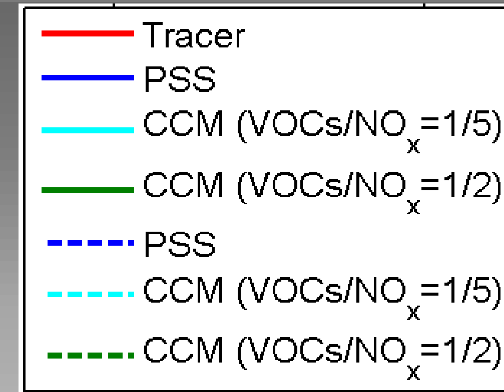


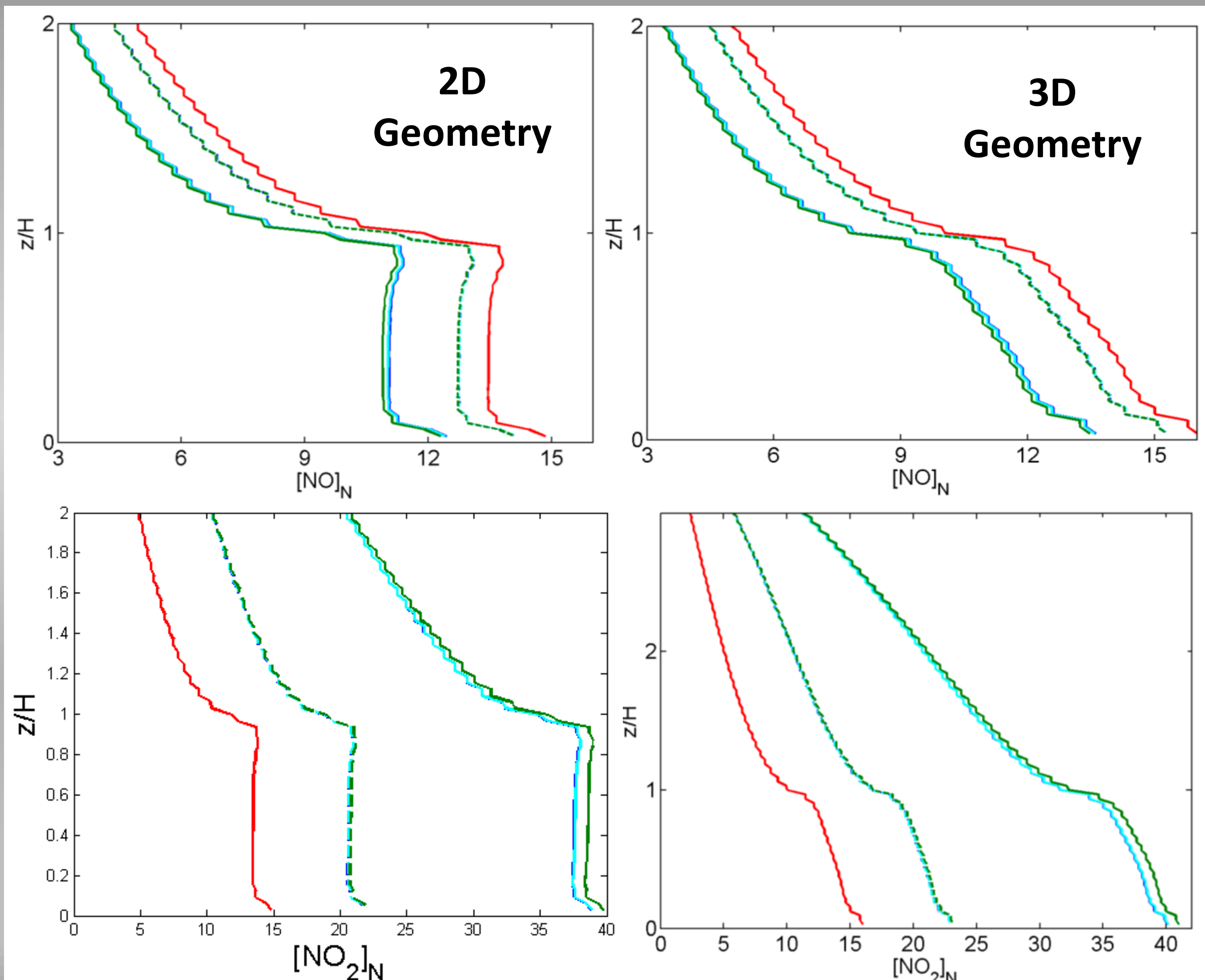


Ozone

Vertical profiles

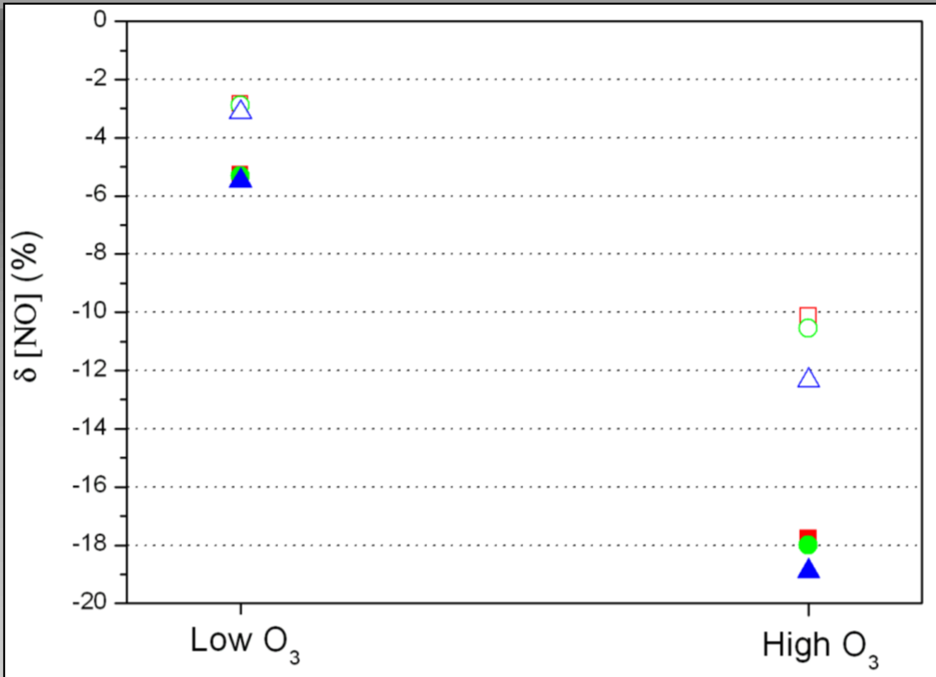
(*solid line*): High Ozone
(*dashed line*): Low Ozone

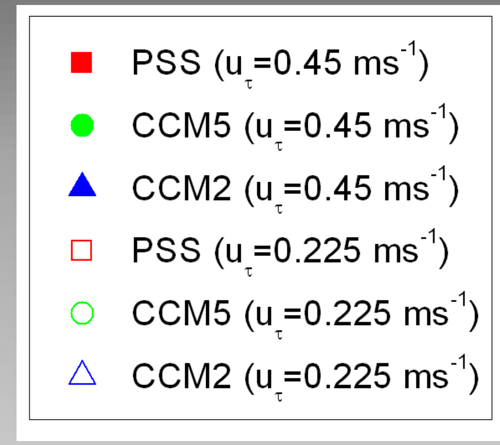




- Horizontal spatial average of $[NO]_N$ and $[NO_2]_N$
- The same vertical profile: PSS and CCM5
- High O_3: Importance of NOx/VOCs emission ($[NO_2]_N$)
- Low O_3: the difference between chemical mechanism is insignificant

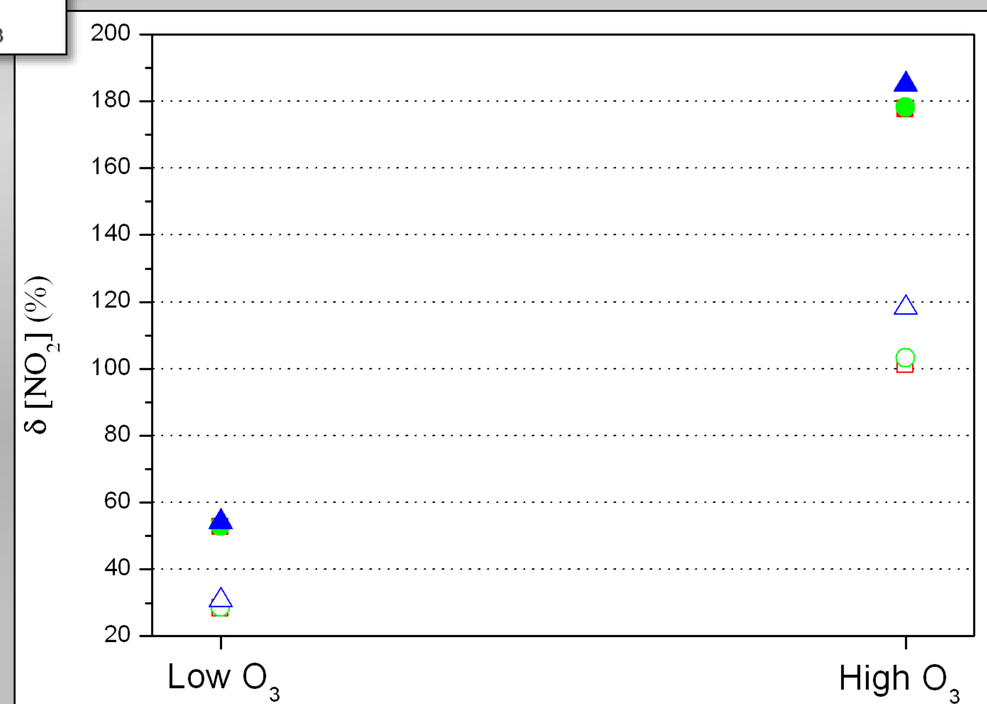
2D Geometry





- The average of δC below the canopy

$$\delta C = \frac{C_{norm} - C_{norm}(PS)}{C_{norm}(PS)}$$



Conclusions

- ✓ The biggest change in [NO] and [NO_2] is obtained between chemical mechanisms and tracer (non-reactive)
- ✓ In the case of high [O_3], the errors induced by the use of PSS are lager when the VOCs-to-NOx emission ratio increases → Lower [NO]
  Higher [NO_2]
- ✓ With lower [O_3] at the top of the domain, [NO] and [NO_2] can be simulated by a simple or complex chemical mechanisms due to the differences between mechanisms are negligible.
- ✓ The influence of a complex chemical mechanism is slightly smaller in 3D than 2D geometry since major ventilation is produced within the street.

Thank you
for your attention

Aditional Slides

Simulation Set up

- **Top Conditions**

- Constant concentration at the top → Important role within the canyon

NO	16 ppb
NO2	35 ppb
CO	200 ppb
SO2	2 ppb

- **Ozone concentration** is computed using photostationary equilibrium and is dependent on zenith angle (θ)

$$\left\{ \begin{array}{l} \theta = 45° \\ \theta = 78° \end{array} \right. \rightarrow J_{NO_2} = A \exp(B/\cos(\theta))$$

(A and B are constant)

$$\downarrow$$

$$[O_3] = \frac{J_{NO_2}[NO_2]}{k\,[NO]} \rightarrow \left\{ \begin{array}{l} O_3 = 39.8 \text{ ppb} \\ O_3 = 10.2 \text{ ppb} \end{array} \right.$$

Simulation Set up

❖ Top Conditions

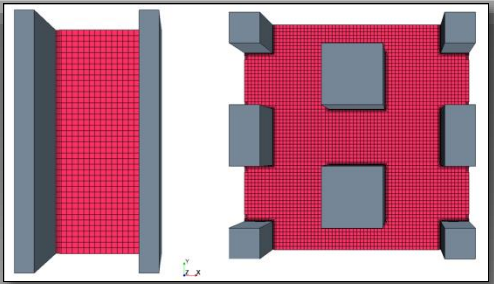
- **VOCs concentration** at the top change with emission ratio

	Emission scenarios	
	VOCs-to-NOx=1/5	**VOCs-to-NOx=1/2**
NO	16 ppb	16 ppb
NO2	35 ppb	35 ppb
VOCs	10.2 pbb	25.5 pbb

- Volumetric proportion within VOCs group are:

OLE	28.6 %
ARO	23.1 %
ALK	38.6%
ALD	4.0 %
HCHO	5.6 %

Simulation Set up



- **Traffic Emissions**
  - NOx fixed emissions: $S_{NO} = 112\ \mu g\ m^{-1} s^{-1}$, $S_{NO_2} = 17\ \mu g\ m^{-1} s^{-1}$
  - VOCs emissions ⟶ Complex Chemical Mechanism
  - Some VOCs are joined in specific chemical groups
  - VOCs-to-NOx emissions : $VOCs/NOx = 1/5$ **(in ppb)**; $VOCs/NOx = 1/2$ **(in ppb)**
  - Volumetric proportion within VOCs group are:

OLE	28.6 %
ARO	23.1 %
ALK	38.6%
ALD	4.0 %
HCHO	5.6 %

Validation

- **CFD Model**

- Validated previously with tunnel measurements in:
  - Papers

- **Complex Chemical Mechanism**

- Validated previously with results of box model

- Experimental measurements