Qatar Photochemical Modeling platform:
A new tool to optimize air pollution control for the Oil and Gas industries

Dr Ali H. Al-Mulla, Dr Azhari F. M. Ahmed, Diane Lecoeur

HARMO Conference

1st June 2010, Bois Colombes
Content of the presentation

- Introduction
- Fundamentals of Photochemical processes
- Architecture of QAQM photochemical platform
- Evaluation
- Overview of results
- Conclusions
Introduction

- In recent history, Qatar witnessed phenomenal economic and industrial growth;

- This led, inadvertently, to an increase in air pollution emissions, including emissions of ozone precursors (NOx and VOCs);

- Significant increases in the level of ambient air ozone over national limits, have been observed;

- Surface ozone, and other photochemical oxidants, are known to have adverse effects on human health and the environment. They represent a serious concern in some highly industrialized regions of the world;

- Faced with this challenge, Qatar Petroleum, in collaboration with experts from TOTAL and ARIA Technologies, has undertaken a joint study to develop a comprehensive national air pollution modeling system, the Qatar Air Quality Model (QAQM) to address the issue.
Fundamentals of Photochemical processes
Fundamentals of Photochemical process

- Ozone is formed in the atmosphere as a result of chemical reactions between VOCs and NOx (precursors) in presence of solar radiation
  - Nitrogen oxides = (NO\textsubscript{x}) = \{ NO ; NO\textsubscript{2} \}
  - Volatile Organic Compounds = VOCs

>> it is a secondary pollutant (not directly emitted)

- Surface Ozone concentration at a given location depends on several factors including:
  - Local emission intensities of precursors,
  - Pollution transport from upwind areas,
  - Meteorological conditions,
  - Solar radiation flux and,
  - Nature of photochemical reactions.

- The chemistry of Ozone formation is generally very complex. It is characterized by highly non-linear relationships between the primary precursor pollutants and the produced photo-oxidants.
Architecture of QAQM photochemical platform
Architecture of QAQM photochemical platform

- Model chain coupling emissions, meteorology, photochemistry

Photochemical model is the core system using input of EM and MM in order to calculate concentrations in 3D for a complete list of substances present in the atmosphere taking into account the full system of chemical reactions that can occur.
Architecture of QAQM photochemical platform

To locally reflect the regional effects, the platform covers three nested (overlapping) scales.

Models:

- Runs over wide scale range with resolution from 100 to 4 km;
- Proceed through the use of nested domain;
- Boundary conditions of LS domain are given by RETRO global measurements (emissions) and NCEP (meteorology);
A/ Meteorological Module MM5

Objective: to simulate meteorological conditions to be used in the photochemical model;

MM5

- Interrogates the Global Weather Forecast Centers which provide the coarse situation
- Produces detailed meteo modeling of large area surrounding Qatar at 3 nested grids;
- It accounts for Gulf topography:
  - To capture the specificity of the gulf region;
  - To take into account long range transport influence.
Objective: to set up a detailed emission inventory of ozone precursors (VOC and NOx)

The inventory includes:
- **Point sources**: stationary sources of emissions identified individually in the inventory.
  - O&G, petrochemicals, power plants, industries etc
- **Mobile sources**: Road, air and ships traffic
- **Area sources**: Other anthropogenic activities (Gas stations, solvent use, dry cleaners...)

Set up at 2 scale levels (Gulf and Qatar)

**Annual NOx emission (2008) including regional contribution**
- **Qatar**: 7%
- **Iran (South)**: 5%
- **Kuwait**: 15%
- **UAE (partial)**: 8%
- **Bahrain**: 6%

**Annual VOCs emission (2008) including regional contribution**
- **Qatar**: 4%
- **Iran (South)**: 10%
- **Kuwait**: 12%
- **UAE (partial)**: 9%
- **Saudi Arabia (East)**: 4.6%

**TOTAL**:
- **NOx**: 4.1 Mt/y
- **VOCs**: 2.5 Mt/y
C/ Chimere Photochemical Model: Grid nesting

Objectives: To configure a multi-scale ozone model specific to Qatar

- Proceed through the use of nested domain down to the scale for which dispersion modeling can be efficiently applied;
- Boundary conditions are given by the coarse simulation;
Model evaluation
Model evaluation (QA/QC)

- Benchmarking is done by comparing CHIMERE modeling output against validated Air Quality monitoring data (9 stations);

- Specific QA/QC protocol used for the validations;

- Validated Air Quality data subjected to statistical analysis to provide valuable information relating to:
  - Regulatory compliance,
  - Temporal and spatial modulation,
  - Analysis of differences / relationships between pollutants & among stations,
  - Identification of specific air pollution episodes;
Based on 2008 data, the MM5 configuration has shown:

- No visible numerical artifacts;
- Good representation of temperature and wind fields over Qatar;
- Good general agreement between observations and simulations for wind direction at most stations (excluding systematic discrepancies due to equipment malfunction);
- Overestimation of wind speed during episodes of synoptic wind (wind from north-west or east), which will be corrected by improved land-use definition;
- The need of more suitable land-use application to improve the model performance.
- The need for further assessment of the model vertical resolution to improve the surface simulation.
Model evaluation:
samples of NO2/O3 modeled output against monitored data

Ras Lafan Camp station
- Modelled output
- Monitored data

Mismatch possibly due to:
- Underestimated peak NOx emission
- Shift in Wind direction
- Uncaptured local effect (sea breeze, topography)
Model evaluation: Nox

For 2008 data set, NOx concentrations are rather well simulated by the model.

However model tends to slightly underestimate the concentrations. The underlining causes for this may be due to the following:

- Underestimation of NOx in the emission inventory e.g. Al Shammal;
- Some episodic industrial events may be missed by the model;
- The model overestimates wind speed during synoptic wind conditions and subsequently underestimates NO2 concentrations especially in RLC-Camps and Al Khor. This issue can be partly corrected by applying the new land-use.
- Model configuration considers NOx emissions within 4*4km grid cells >> lead to dilution of NOx in industrial areas like RLC (further investigation including introduction of “Plume in Grid” and additional nesting levels to improve horizontal grid cell resolution from 4km up to 100 meters).
Model evaluation

Despite its inherent difficulty relative to NOx, Ozone simulations indicate good representations particularly with regard to

- diurnal variations
- background levels.

However, the following constrains have been observed

- in Al Shammal, the diurnal variation is not well reproduced by the model, as a result of the AQS being located in a so called “sea” grid cell
- Underestimation of NOx leads to less ozone titration and subsequently higher ozone simulations
Scenarios
Boundary conditions

Test all emissions emitted in Qatar are removed and only regional emissions remain as an input to the model

• July scenario (NW wind) NO2 importation impacts east coast of Qatar
• February scenario (SE wind) wind does not meet any sources of emission close enough to bring detectable NOx emissions to Qatar
Impact of Qatar activities on O3 production

Test: difference between total simulation (regional + local emissions) and the regional emission only: the difference is equivalent to ozone production due to Qatar activities.

Tests conducted for February (1 to 14) and July (1 to 16) 2008 led to the following results:

- Negative values suggest titration due to Qatar NOx emissions.
- Positive values suggest ozone production due to Qatar activity;
- In Doha, ozone titration accounts for 5 ppb on average;
- Downwind, ozone production accounts for 5 ppb on average, and 10 to 20 ppb maximum i.e. 20% of overall ozone background;
- Production of ozone due to Qatar activity can reach downwind areas located at 100 – 150 km up to 600 km (depending on wind direction: Kuwait and Empty Quarter);
Regulatory emission reduction scenarios

To assess the performance of the platform itself and how it responds to changes in the emissions of NOx and VOCs

- Reduction of precursors at the regional or both local plus regional scales is the most effective solution to reduce ozone in Qatar.
  - Reduction of precursors at the local scale only is unlikely to have an effect on ozone level.
  - Most of the ozone observed in the ambient atmosphere of Qatar is not produced locally. It is formed in areas located upwind from Qatar and is transported with the prevailing wind.

- RLC area (East of Qatar) and Dukhan and Al Shammal area (West and North of Qatar) respond differently to reduction of precursors.
  - At the West and North locations:
    - a reduction of both precursors at local scale would not affect the ozone level, however, a reduction at both scales is likely to have a significant effect.
    - Reduction of VOC at both scales seems to be the most effective solution. This is understood since air quality at Dukhan and Al Shammal is primarily controlled by sources located in the north-west outside of Qatar. In these areas it seems that ozone is VOC driven.
  - RLC area:
    - a reduction of NOx emissions at local scale leads to an increase of ozone level at RLC Camp. This is due to titration by fresh NOx emitted locally. Moreover, a reduction of NOx emissions from regional scale seems to be the most effective solution suggesting a NOx limited situation.

- The above findings give an indication to the complexity of the chemistry of ozone formation in Qatar and how it is influenced by factors of regional nature.
Conclusions
Conclusions

- The QAQM Modeling system designed to investigate photochemical air pollution at Qatar and regional scale, is now operational;

- The way the QAQM platform is currently configured, allows the study of impact scenarios (emission reduction policies, industrial economic development) and retrospective investigation of specific ozone pollution events.

- The major local and regional sources responsible for ozone formation in Qatar are more or less well understood.

- Validation of modeled outputs against observations collected from various monitoring stations produced significant results and conclusions.

- Identified improvement: land-use, additional nesting, better vertical resolution remains to be introduced

- Depending on the prevalent wind, Qatar ozone production can be transported along the Gulf from 100 to 600 km;

- Photochemical system in Qatar is mostly VOCs driven

- Regional collaboration and convention is critical to address this issue.
Utilization

- Results from this study will streamline the strategy for pollution control and contribute to protection of human health and sustainable development.

- **The platform is a tool to assess**
  - the long-term impact, on air quality, of various economic / industrial scenarios for Qatar
  - the cost-benefits of the national regulatory limits and determine the most optimum strategy to roll down surface ozone levels;

- Acquire critical information for QP top management / State to take best decisions (in line with Sustainable Development principles) on industrial and economic development;

- Prospective further work, in this regard, may address future economic development pathways and possible environmental regulatory policies.

- Develop the ozone modeling platform as a forecast tool for a long term objective.
Thank you for your attention
Annexes
Model evaluation (QA/QC step)
Model evaluation (QA/QC)

- Benchmarking is done by comparing CHIMERE modeling output against validated Air Quality and meteorological monitoring data (9 stations);

- Specific QA/QC protocol used for the validations;
  - Validated Air Quality data subjected to statistical analysis to provide valuable information relating to:
    - Regulatory compliance,
    - Temporal and spatial modulation,
    - Analysis of differences / relationships between pollutants & among stations,
    - Identification of specific air pollution episodes;

- Further validation regarding mixing height (MM5 modeled output), using a Radar wind profiler for a one month monitoring, is currently being conducted at four different locations in Qatar by a specialized French company.
Ozone effects on human health and ecosystem
Effects of Ozone on Human Health

- Investigations under ambient conditions have clearly indicated negative impacts on human health. Children, elderly people, and those with chronic respiratory diseases are particularly sensitive.

- Epidemiological research indicates that the effects on human health vary from respiratory system complications to increased mortality at exposure to higher doses.

- The exact mechanism of the impact of ozone on human health is not known, but most likely involve free radicals.

- Due to human health toxicity, specific air quality standards have been established focusing on peak concentrations:
  - The alarm threshold at 120 μg/m³ means that the general population must be warned and that especially sensitive groups, such as children, should be kept indoors,
  - At levels above 235 μg/m³, acute danger exists for the general population.

- The World Health Organisation (WHO) guidelines recommend an updated 8hr threshold of 100 μg/m3. (Recent literature suggests stronger association between 8hr standard & human mortality)
Processes taken into Account

FREE TROPOSPHERE

FREE TROPOSPHERE

MIXING LAYER

Temperature

Inversion

Temperature

Inversion

MIXING LAYER

Winds altitude

2000 m

Winds altitude

2000 m

Winds limit layer

Winds limit layer

Deposition

Deposition

COV

NOx

COV

NOx

COV

NOx

morning

noon

evening