An Introduction

to

Ozone Modeling

Presented by:

Dick Karp

Air Quality Division

TCEQ

July 22, 2008

Why Model Ozone?

- Section 182 of the 1990 Federal Clean Air Act Amendments lists SIP Requirements:
  - For areas classified as Serious…
  - Develop an Attainment Demonstration SIP…
  - Based on photochemical grid modeling
- EPA Guidance Documents
  - "Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals…." (April, 2007)

Ground-level Ozone Formation

Ozone is a secondary pollutant

- Not emitted directly into atmosphere
- Forms via a complex chemical process

Photochemical reaction

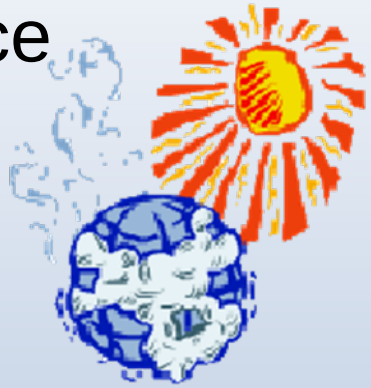
- Requires UV energy from sunlight, so
- Ozone forms during daytime, decreases at night

Complex chemical reaction between

- NOx - Nitrogen Oxides (NO, NO_2)
- VOCs - Volatile Organic Compounds
- CO - Carbon Monoxide

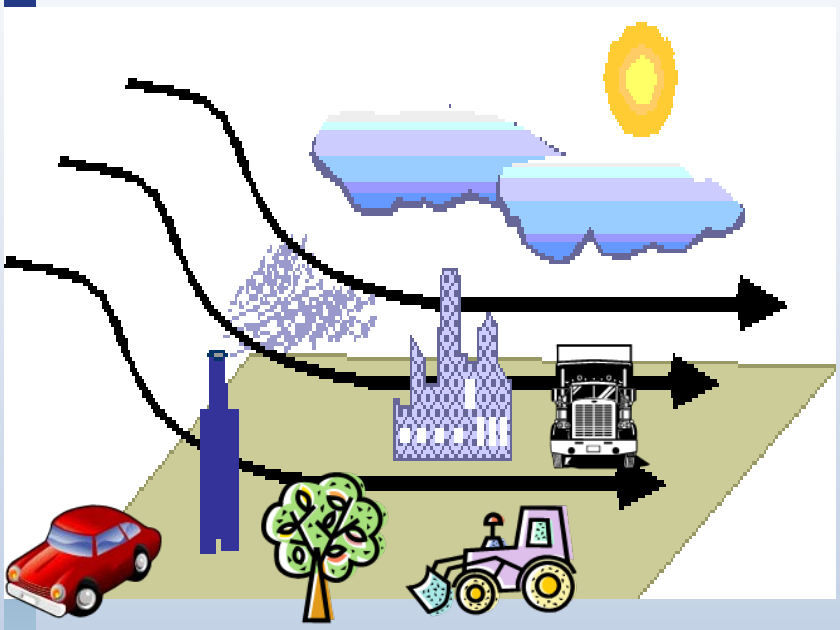
Ground-level Ozone Formation

Ground-level ozone forms when nitrogen oxides (NO_X) and volatile organic compounds (VOC) mix in the presence of sunlight

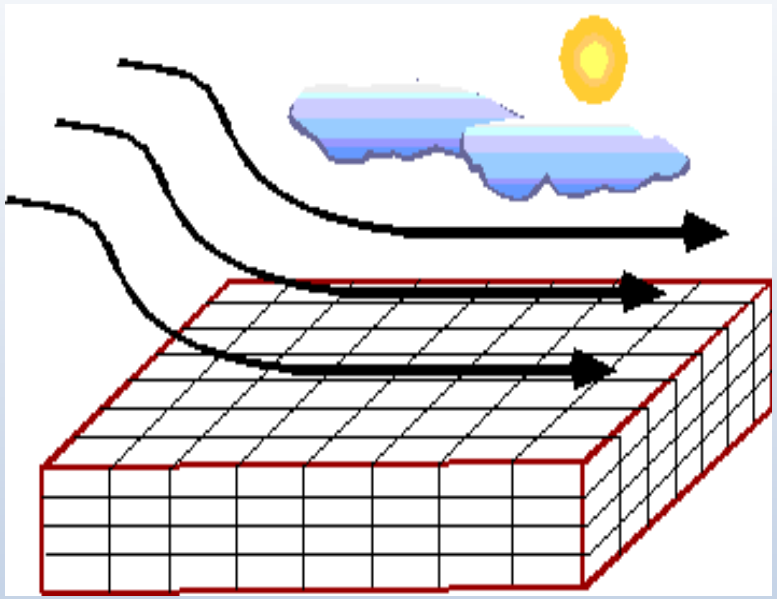


NO_X + VOC +  ⟶ Ozone

Photochemical Grid Models

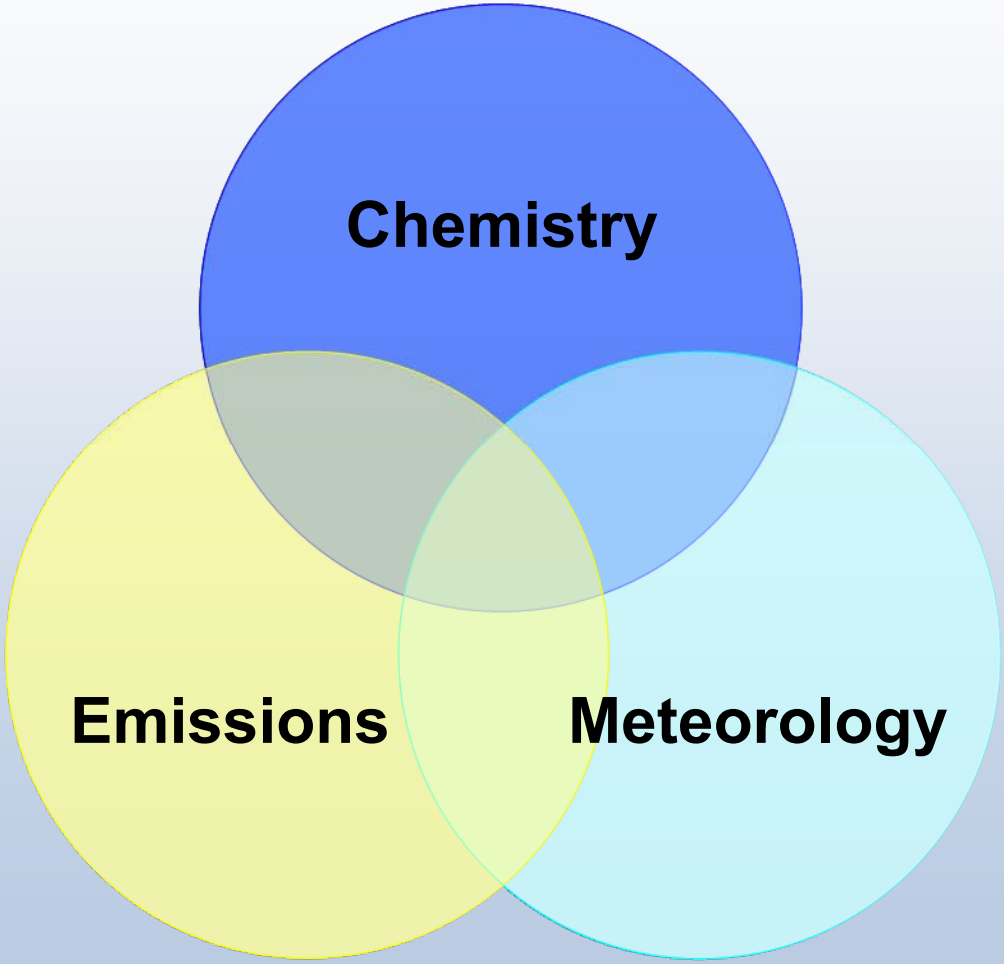


Real World Situation



Computer Grid Simulation

Photochemical Modeling Inputs



Photochemical Modeling Inputs

- Chemistry Equations
  - Chemistry changes during day and night
  - 51 chemical groups, 156 reactions
  - Complex system of differential equations
- Meteorological Data
  - Wind transports and mixes pollutants
  - Temperature affects reaction rates
  - Sunlight provides energy (ultraviolet radiation)
- Emissions Inventory
  - Emissions from cars, planes, factories, power plants
  - Nitrogen Oxides and Volatile Organic Compounds (VOC)
  - Speciation - Separate NO_X and VOC emissions into chemical components

Ozone Meteorology

- Clear (or slightly cloudy) skies,
  - Limited clouds allows solar energy to reach the surface,
  - Lots of Ultraviolet energy to make ozone
- High Temperatures
  - Mix the air vertically
  - Accelerate the chemistry and
  - Speed up ozone formation
- Low Wind Speeds
  - Weak Winds → limited dispersion, dilution
  - Air stays in one place for a long time
  - Coastal areas get flow reversal

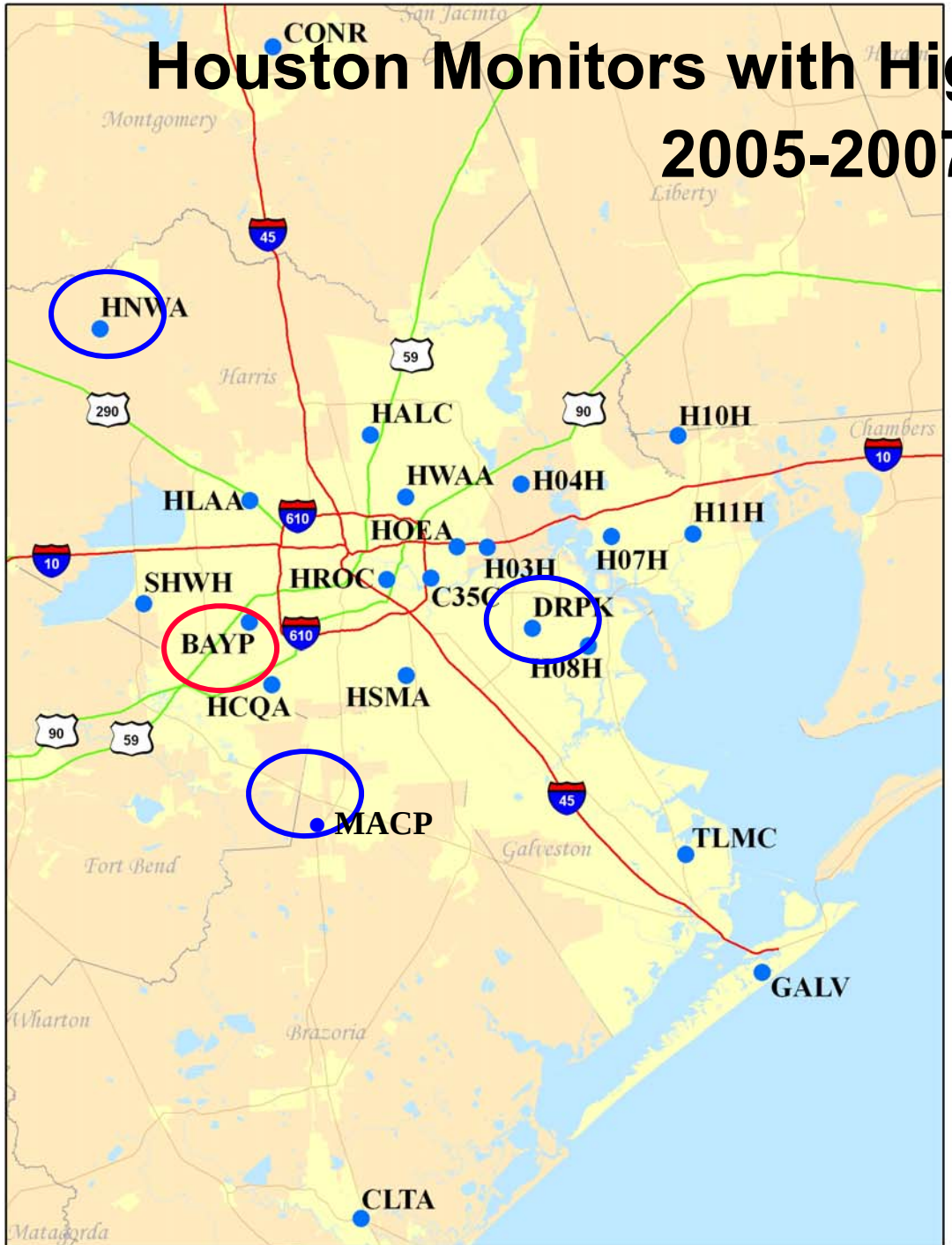
Sources of Precursor Chemicals

- Nitrogen Oxides come from combustion
  - Cars, trucks, ships, trains, planes
  - Construction and commercial equipment
  - Industrial boilers, heaters, compressors, pumps, flares
  - Electrical power plants
  - Forest and wild fires
- VOCs come from evaporation and incomplete combustion
  - Industrial/petrochemical facilities
  - Architectural and surface coating
  - Solvents evaporation
  - Gasoline and other fuels
  - Plants, particularly oak trees

Emissions Inventory Categories

- Point Sources
  - Industrial sources (Petrochemical and Electric Generating)
- On-Road Mobile sources
  - Cars, trucks, buses, motor cycles, 18 wheelers
- Non-Road sources
  - Trains, planes, ships, construction and commercial equipment, compressors, pumps etc
- Area Sources
  - Oil and gas production, architectural and surface coating, gas stations, etc
- Biogenic Sources
  - Oak and Pine Trees, Vegetation, Farming

Houston Monitors with High Design Values 2005-2007



BAYP	BAYLAND PARK	96
C35C	CLINTON DRIVE	
CLTA	CLUTE	
CONR	CONROE	
DRPK	DEER PARK	93
GALV	GALVESTON	
HALC	ALDINE	
HCQA	CROQUET	
HLAA	LANG	
HNWA	NW HARRIS CO	91
HOEA	HOUSTON EAST	
HROC	HOUSTON REGIONAL OFFICE	
HSMA	SWISS & MONROE	
HWAA	NORTH WAYSIDE	
SHWH	SHELL WESTHOLLOW	
TLMC	TEXAS CITY/LA MARQUE	
H03H	HRM 3 HADEN ROAD	
H04H	HRM 4 SHEDLON ROAD	
H07H	HRM 7 WEST BAYTOWN	
H08H	HRM 8 LA PORTE	
H10H	HRM 10 MONT BELVIEU	
H11H	HRM 11 EAST BAYTOWN	
MACP	MANVEL-CROIX PARK	91

Protecting Texas by Reducing and Preventing Pollution

TCEQ
Texas Commission on Environmental Quality
Chief Engineer's Office
Air Quality Division
PO Box 13087 (Mail Code 164)
Austin, Texas 78711-3087

December 12, 2006 Raj Nadkarni, (512) 239-1934

Ozone Modeling in SIP Development

Base Case	Day-specific emissions and meteorology; must replicate what was actually monitored during episode
Future Base Case	Apply future growth and on-the-books controls to estimate future emissions and day-specific meteorology
Test Control Strategies	Determine the additional control strategies and reductions that will effectively reduce ozone at monitors
Write SIP	Document modeling procedures, control strategy modeling, and corroborative analyses

Modeling Episodes

- 2005
  - Episode0: May 19 - June 3, 2005
  - Episode1: June 17 - June 30, 2005
  - Episode2: July 27 - August 8, 2005
- 2006
  - Episode 0: May 31-June 15, 2006
  - Episode 1: August 13- September 15, 2006
  - Episode 2: October 3 – October 11, 2006

Goal of Ozone Modeling

- Get the right ozone concentrations at:
  - The right time
  - The right place
  - For the right reasons
- Get enough valid modeling days so the results are reliable