Dispersion of Pollutants based on a Reaction – Diffusion model

D. Quesada

School of Science, Technology and Engineering Management, St. Thomas University, Miami Gardens, FL 33054

Abstract

In this communication, a reaction – diffusion model consisting of three interacting species is discussed. Reaction-diffusion mathematical models combine in a single framework the local chemical reactions between species in which substances are transformed into each other and diffusion, which cause them to spread out over a surface in space. In urban biometeorology reaction-diffusion models in bounded regions are very important in order to analyze the impact of urban canyons on the spatial distribution of chemical species. In this communication CO, NO_x, and O_3 were selected as model species. Even though, it is a very simplified model for the chemistry of the atmosphere, as well as for the entire dynamics of the atmosphere it focuses on the different diffusivity of species, their reactivity, and the non – linear character of the processes. Three models are explored: Fisher's equation, Newell-Whitehead-Segel equation, and Zeldovich equation. The current state of the atmosphere is introduced via external forcing to the equation with different amplitudes and frequencies.

1. Motivations

Dispersion of pollutants is a central topic in atmospheric modeling as well as in environmental weather hazards management. A considerable body of evidences exists in the scientific literature regarding the impact of different chemical species and particulate matter on human health (cardio-respiratory diseases). Approaches based on meso-scale models as WRF-Chem and CMAQ have provided very good insights about the spreading and the reactivity of different chemical species within the atmosphere. However, the downscaling of these calculations to urban environments is still pending to be solved. Computational Fluid Dynamics (CFD) calculations are very good at these scales, and some hybrid approaches overlapping these two limits are in use. On the other end, the solution of the linear equation of diffusion has permitted to track the concentration of pollutants in the form of a Gaussian function and understand the overall spatial distribution of them in flat homogenous geometries.

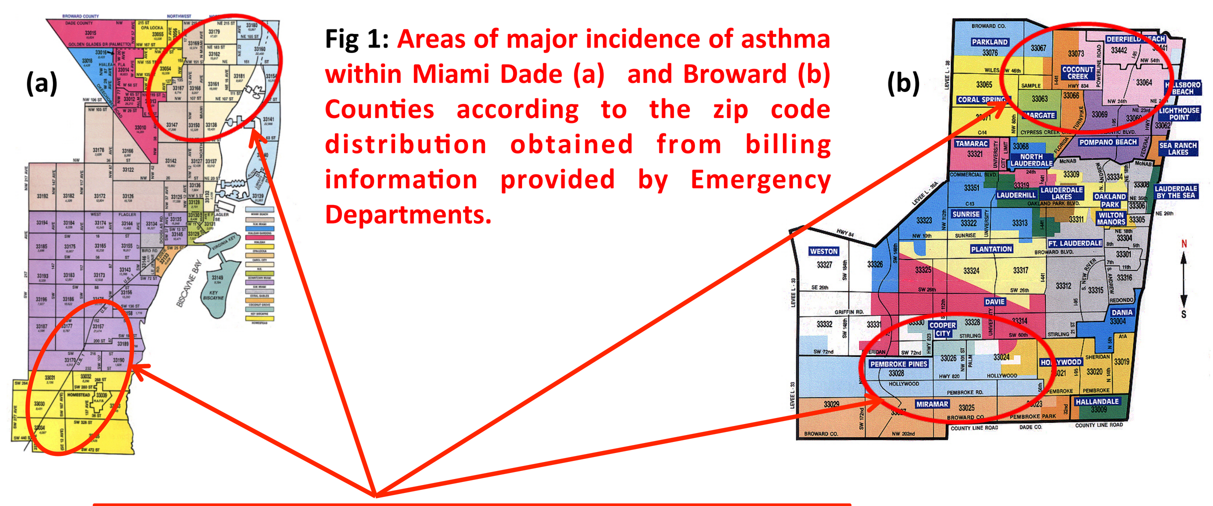

Fig 1: Areas of major incidence of asthma within Miami Dade (a) and Broward (b) Counties according to the zip code distribution obtained from billing information provided by Emergency Departments.

Features of Circled Areas
- Very close to highly transited roads and/or Expressways
- High motor load, due to connecting bridges
- Low income population
- Predominant ethnicity African – American

Challenges and Pre-conditions

- Spatial distribution of asthma cases mixes different variables (physicochemical and socio-economic) which are difficult to unify in a single model. While the physicochemical variability happens at time intervals from hours to days, socio-economic variables last for days, even years. This fact allows a separation of them. The presentation focuses of the physicochemical component only.
- Information about the concentration of chemical species very sparse, few ground – based measuring sites re operational at this moment. WRF + Chem and CMAQ results might be used for guidance.
- Very irregular landscape geometry.

Objectives of this Presentation

- To implement a Reaction – Advection – Diffusion model for three chemical species within the atmosphere.
- To evaluate the extent landscape's geometry might affect the reactivity and trapping of pollutants.
- To compare obtained solutions with the spatial distribution (zip code distribution) of cases of asthma in Miami Dade County.
- To evaluate the feasibility of using these solutions as an operational guidance for more WRF + Chem simulations.

2. Model implementation

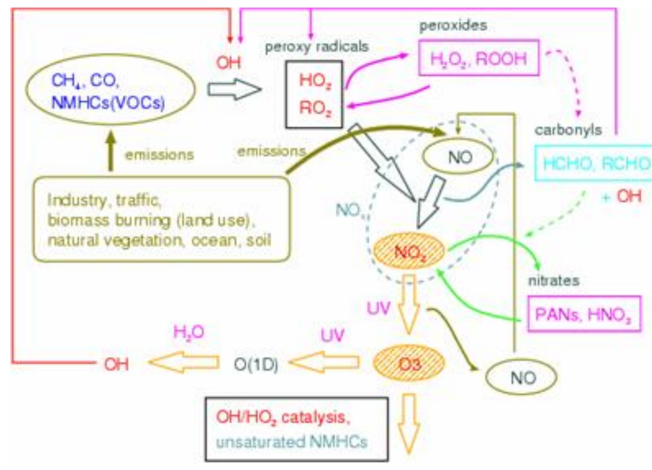

Fig 2: Schematic representation of the feedback involved in the production and transformation of CO, NO_x, and O_3 within the atmosphere.

- Due to the existence of a large amount of chemical species continuously reacting within the atmosphere, their physical kinetics will demand a large system of non – linear differential equations.
- A coarse – grained approach might be used on the other hand by appealing to some "effective", "mean - field" constants of reaction and reduce the analysis to three important chemical compounds: CO, NO_x, and O_3.
- In order to consider the possibility of diffusion while these reactions take place, a reaction – diffusion model is a good starting point.
- If sources are mobile, or there is an external influence of the wind, then a reaction – advection – diffusion model is a good starting point.

Reaction Kinetics

C_1 – concentration of CO
C_2 – concentration of NO_x
C_3 - concentration of O_3

Single Specie Models

$$\frac{dC}{dt} = F(C)$$
$$F(C) = kC \quad \textit{exponential growth}$$
$$F(C) = aC\left(1 - \frac{C}{K}\right) \quad \textit{logistic model}$$

Multi Species Models

Lotka – Volterra type models

$$\frac{dC_1}{dt} = aC_1 - bC_1C_2$$
$$\frac{dC_2}{dt} = cC_1C_2 - dC_2$$

Michaelis – Menten type models
Substrate inhibition system

$$\frac{dC_1}{dt} = k_1 - k_2C_1 - H(C_1, C_2)$$
$$\frac{dC_2}{dt} = k_3 - k_4C_2 - H(C_1, C_2)$$
$$H(C_1, C_2) = \frac{k_5C_1C_2}{k_6 + k_7C_1 + k_8C_1^2}$$

What do we know about pollution?

- Too little NO_x: O_3 loss rather than radical cycling leading to net O_3 chemical destruction.
- Intermediate NO_x: efficient O_3 production via cycling of HO_x and NO_x radicals.
- Too much NO_x: Radical termination by alternate route (e.g. OH + NO_2)
- CO stimulates NO_x through kind of "symbiosis"
- NO_x and O_3 dynamics might be treated as a Michaelis – Menten substrate – inhibition model

$$\frac{dC_1}{dt} = a_1C_1\left(1 - \frac{C_1 - b_{12}C_2}{K_1}\right)$$
$$\frac{dC_2}{dt} = a_2C_2\left(1 - \frac{C_2 - b_{21}C_1}{K_2}\right) - H(C_2, C_3)$$
$$\frac{dC_3}{dt} = k_3 - k_4C_3 - H(C_2, C_3)$$

Reaction Kinetics Model

Advection – Diffusion Model

$$\frac{\partial C}{\partial t} - D\,\Delta C + \vec{V}\cdot\vec{\nabla}C = F(C) + f(x,y,z,t)$$

$$\Delta C \equiv \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}$$

$$\vec{V} = (u(x,y,t), v(x,y,t), w(x,y,t) - w_g)$$

D is the coefficient of diffusion of the chemical specie C.
V is the wind speed vector, where w_g refers to the falling speed of the chemical by gravity.
F(C) is the kinetic term responsible for the mechanism of reaction.
f(x,y,z,t) is the power of the source.

Single specie Models

- Fisher Model – F(C) – Logistic growth – Each chemical is treated independently with its own carrying capacity.

$$\frac{\partial C_i}{\partial t} - D_i\,\Delta C_i + \vec{V}\cdot\vec{\nabla}C_i = aC_i\left(1 - \frac{C_i}{K_i}\right) + f_i(x,y,z,t)$$

The solution is a propagating front, separating two non-equilibrium homogeneous states, one of which is stable and another one is unstable.

- Newell-Whitehead-Segel Model – Cubic non linear diffusion equation.

$$\frac{\partial C_i}{\partial t} - D_i\,\Delta C_i + \vec{V}\cdot\vec{\nabla}C_i = aC_i\left(1 - \frac{C_i^2}{K_i}\right) + f_i(x,y,z,t)$$

The model has been used to simulate the Rayleigh-Benard convection instability.

- Zeldovich Model – modeling of bistable systems. It contains two stable states separated by an unstable state. It has been used in modeling combustion.

$$\frac{\partial C_i}{\partial t} - D_i\,\Delta C_i + \vec{V}\cdot\vec{\nabla}C_i = C_i(1 - C_i)(C_i - \beta) + f_i(x,y,z,t)$$

Three Species Model

$$\frac{\partial C_1}{\partial t} - D_1\,\Delta C_1 + \vec{V}\cdot\vec{\nabla}C_1 = F(C_1, C_2, C_3) + f_1(x,y,z,t)$$
$$\frac{\partial C_2}{\partial t} - D_2\,\Delta C_2 + \vec{V}\cdot\vec{\nabla}C_2 = F(C_1, C_2, C_3) + f_2(x,y,z,t)$$
$$\frac{\partial C_3}{\partial t} - D_3\,\Delta C_3 + \vec{V}\cdot\vec{\nabla}C_3 = F(C_1, C_2, C_3) + f_3(x,y,z,t)$$

3. Numerical Solutions

Numerical solutions were done using the software Mathematica 9.0

Wolfram Mathematica 9

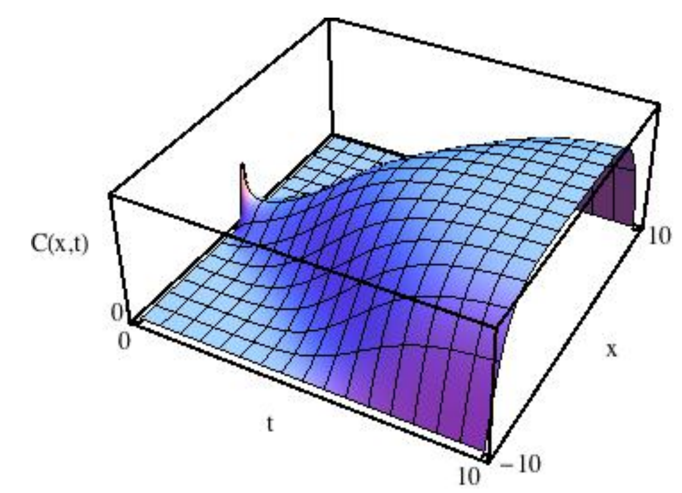

Fig. 3: Solution of the one-dimensional reaction diffusion equation with the Fisher model. The equation was solved with zero wind components and in a dimensionless format with:
- time scaled to the growth rate "a" τ = a t,
- distance scaled to diffusion length z = x $(a/D)^{1/2}$
- Concentration scaled to carrying capacity c = C(x,t)/K
- Dirichlet boundary conditions C(-10,t) = C(10,t) = 0

Notice that the small initial fluctuation leads to an instability, that develops in a nonlinear way: a front propagating away from the initial perturbation. Finally the uniform stable state is established on the whole space interval.

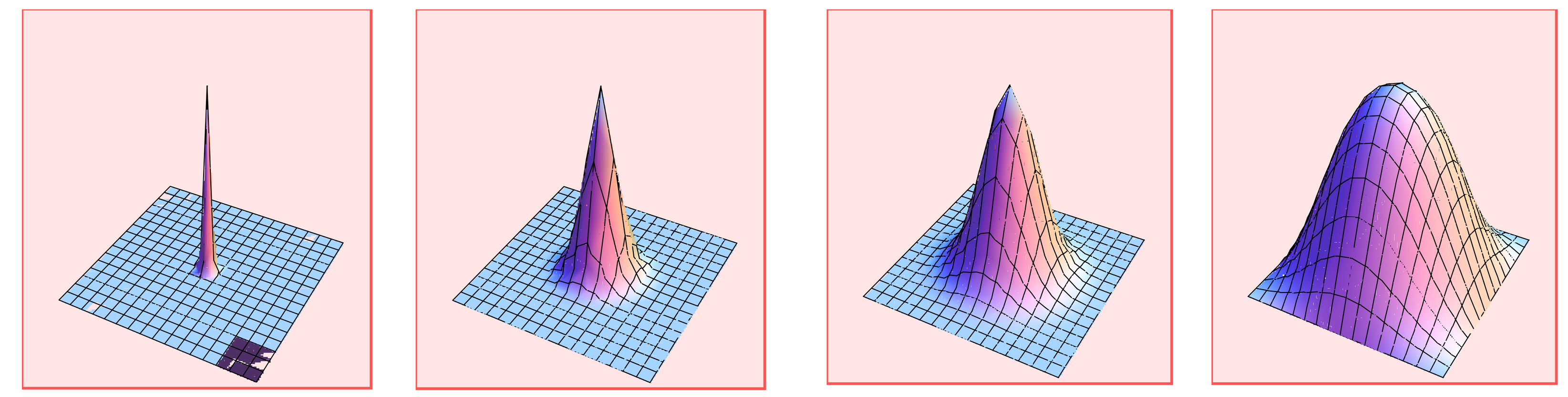

Fig. 4: Solution of the two-dimensional reaction diffusion equation with the Fisher model. The equation was solved with zero wind components and with the same dimensionless scheme as before. Notice the same front propagation observed in the one-dimensional situation.

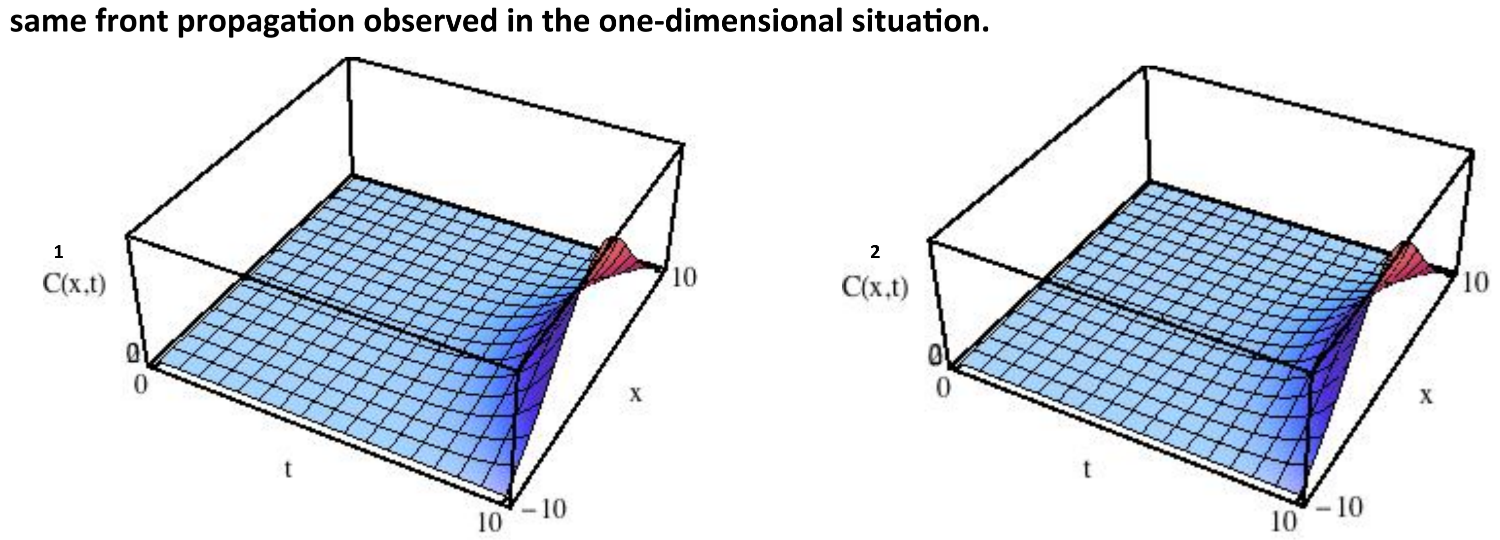

Fig. 5: Solution of the one-dimensional reaction diffusion equation with the Fisher model for two interacting chemical species. The reaction function was selected as a Lotka – Volterra model with symbiosis (mutual enhancement). The equation was solved with zero wind components and with the same dimensionless scheme as before. Notice the same front propagation observed in the single specie situation; however delayed because of the competition.

Conclusions

- The use of advection – diffusion – reaction models in pollution dispersal is feasible and might help to understand the role of nonlinearities.
- The model might be solved for different geometries, including complex terrains.
- Three species models are rich in phenomena of pattern formation, including those from two species, typically found in Turing-like modes of morphogenesis.
- The inclusion of wind patterns interacting with competing species might explain the hot spots for respiratory diseases found on the downwind direction around the heavy loaded transportation areas.

Acknowledgments

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