On the evaluation of pollutant gas dispersion around complex sources by means of a Lattice gas model

R. Cipollone & A. Sciarretta
Department of Energetics, University of L'Aquila, Italy.

Abstract

For the prediction of local and transient diffusion of pollutant gases from power plants and traffic sources, the Lattice Gas approach is proposed in this paper. The model was parameterised by some non-dimensional numbers that, together with physical data, define completely the case to study. The influence of such numbers is explored and a comparison is made with usual parameterisation of the turbulence in diffusional models. Several simulation tests allow to verify if the results of the model are, in the steady-state limit, coherent with the ones offered by the well validated and universally adopted Gaussian plume equation.

1 Introduction

The study of the environmental impact of power plants and traffic sources requires predictive tools that can deal with a large variety of source types, surrounding conditions and diffusional processes. Most of the air quality models used for technical and regulatory purposes and suggested by environmental agencies adopt the steady-state Gaussian plume equation (GPE) as the modelling core. This choice does not allow for taking into account space- and time-variable conditions, since GPE is a steady-state model and merges all the next-to-source effects in the plume rise height term.

Even the most recent and complex EPA models (such as AERMOD), that still introduce refinements of the air turbulence parameterisation, terrain description and plume rise calculation, do not remove such limitations. The EPA puff model CALPUFF does take into account transient effects, but is still not adequate to study local effects, since it keeps the use of plume rise height as a way to simulate air-emission interaction. The same can be said of transient Gaussian models, that simulate a continuous emission as a sequence of impulsive puffs.
Therefore, to include both transient and local effects into an engineering analysis, the only way currently available is the direct numerical solution of the dispersion equation using CFD techniques (finite-volume or grid models, e.g. REMSAD, PANACHE, WYNDVALLEY). Unfortunately, the implementation and use of such models are not immediate and require a specific background in computational fluid-dynamics. Moreover, CFD results are largely affected by the values assigned to an usually large number of parameters, and by the description of the boundary conditions, that are not always exactly known. Also, the randomness of the processes involved is a further aspect that may limit the effectiveness of this, though accurate and physically-consistent, approach.

An alternative approach to CFD was first proposed in the early 90s [1],[2] and recently developed by the authors [3]. It is the Lattice Gas approach, in which the diffusion of pollutant gas in the atmosphere is simulated by means of particles moving on the sites of a lattice with square cells. Many physical phenomena, such as wind transport, momentum and heat exchange, deposition, can be described by simple rules, easy to implement and manage. Moreover,
- transient situations can be studied, without the need for a special description,
- the lattice can be fitted to study next-to-source phenomena,
- the lattice can be built in such a way to represent realistic landscape,
- the model set-up requires the definition of a limited number of parameters,
- an inherent randomness is introduced, without additional complexity.

In spite of such promising features, this approach was relatively unexplored for the specific field of interest. The main contribution of the authors [3] was to obtain from it quantitative - rather then only qualitative - predictions, by having introduced three non-dimensional parameters to evaluate operational quantities (cell dimension, solution time step, etc.), and by having related them to actual physical quantities (wind velocity, pollutant mass flow rates, etc.). Now, a detailed parametric analysis, concerning the mentioned non-dimensional parameters and their effect on the solution, appears of great interest, in order to provide information on how to select their values to represent different scenarios.

In the paper, first the two-dimensional Lattice Gas Model (LGM) is presented, with the basic model architecture and the fundamental equations. Particular attention is given to the definition of the three non-dimensional parameters – namely, number ratio, time ratio and mass ratio – that define completely the model. A sensitivity analysis is reported in the results section for these three parameter, and an equivalence is found in the steady-state limit, between their values and the GPE diffusional parameters. Finally, the simulation of transient effects and of ground pollutant concentrations are explored.

2 The model

The general structure of the LGM is represented in the flowchart of Fig.1, where a time-cycle is sketched, along with the single submodels for air motion field (Sec. 2.3), and pollutant motion rules (transport, collisions, sources, buoyancy, boundaries, Sec. 2.4). Before the start of the cycle, and according to the specific
case studied, the lattice has to be defined (Sec. 2.1) and a sequence representing the pollutant emission over time has to be prepared for each source (Sec. 2.2).

### 2.1 Definition of the lattice

The space domain is described by a two-dimensional lattice, with square cells of fixed dimension $\Delta r$. The fluid-dynamic process of pollutant dispersion in air is represented by fluid particles moving across the lattice sites. A fixed mass $\Delta m$ is associated to each particle.

![Flowchart of the model](image1)

![Lattice schematics](image2)

The motion of the particles follows a basic rule: a particle is allowed to move only to the nearest neighbour sites $(k = 1,\ldots,4)$ or be at rest $(k = 5)$. Consequently, the particle velocity is quantized to five values (see Fig. 2):

$$
\begin{align*}
    c_x(k) &= \begin{cases} 
    1 & k = 1 \\
    0 & k = 2, 4, 5 \\
    -1 & k = 3 
\end{cases}  \\
    c_z(k) &= \begin{cases} 
    1 & k = 1, 3, 5 \\
    -1 & k = 4 
\end{cases}
\end{align*}
$$

Velocity $c$ in eqn (1) is non-dimensional, or in lattice units. To obtain actual fluid velocity, $c$ has to be multiplied by the “lattice velocity” $\Delta r/\Delta t$, $\Delta t$ being the fixed time step of the model.

Instead of assigning values directly to the dimensional quantities $\Delta r$, $\Delta m$ and $\Delta t$, a set of non-dimensional parameters is introduced. They are $X_u$ (velocity ratio), $X_n$ (number ratio), and $X_t$ (time ratio), defined as:

$$
X_u = \frac{u_{\text{max}}}{\Delta r/\Delta t}, \quad X_n = \frac{\rho_{\text{max}}}{\Delta m/\Delta t^2}, \quad X_t = \frac{\Delta m/\Delta t}{m_{\text{max}}}.
$$

The suffix "max" refers to the maximum value of the corresponding variable (velocity, density or mass flow rate) that has to be represented for the specific study. Since the values for the three parameters in eqn (2) can be arbitrarily assigned, some guidelines for their selection are necessary. For this purpose, a detailed sensitivity analysis will be shown in the results section.
2.2 The pollutant emission
For each source, a sequence of particles is pre-defined (see Fig. 1) to represent the pollutant emission over a time $t_f$, during which the emission velocity and temperature $(u_{e0}, T_{e0})$ are considered constant. The number of particles in the sequence $N_e$, their total momentum and kinetic energy (in the lattice units) are assigned as follows in order to be coherent with emission and lattice data:

$$N_e = \frac{t_f}{X_t \Delta t}$$  

(3)

$$P_{xe} = \frac{u_{e0} N_e \Delta t}{\Delta r}$$  

(4)

$$E_{ke} = N_e k T_e T_{e0}$$  

(5)

Every $X_t$ time steps – eqn (2) –, a new pollutant particle is randomly selected in the sequence and released at the lattice site corresponding to the source.

2.3 The air motion field
At each time step, a set of particles is distributed over the lattice in such a way to represent the air field. The number of particles to be distributed, their total momentum and kinetic energy (in the lattice units) are assigned as follows in order to be coherent with actual air properties and lattice data:

$$N_a(z) = \frac{P_a(z) L_x \Delta r}{\Delta m}$$  

(6)

$$P_{xa}(z) = \frac{u(z) N_a(z) \Delta t}{\Delta r}$$  

(7)

$$E_{ka}(z) = N_a(z) k T_a T_e(z)$$  

(8)

The distribution of air particles is made in a random way over the lattice sites. According to the principle of exclusion, at each site there can only be one particle for each direction.

2.4 Pollutant motion rules
At each time step, the pollutant particles present in the lattice are moved according to their velocity. A particle in the site $[i,j]$ is transferred to the new site $[i + c_x(k), j + c_z(k)]$, with the same direction $k$. Applying the exclusion principle, if the new site is occupied by an air particle with the same direction, this one is moved to the nearest free site at the same height.

Then, for each site it is evaluated if there is more than one pollutant particle. If it is so, a collision occurs, during which the total number of particles, the total momentum and the total kinetic energy before the collision have to be conserved. For this purpose, a table that contains all the possible collisions of 2 up to 5 particles has been prepared. The solution is randomly selected among the possible ones.

When a pollutant particle reaches the upwind or downwind boundaries of the lattice, it is simply removed. Other boundary conditions can be described in the LGM with high accuracy and versatility: flat or complex terrain, as well as a

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mixing height, are represented by a given sequence of lattice sites. The interaction between particles and boundaries can reflect many physical phenomena. Here, the soil is considered as absorbing (a particle that reaches it, is removed from the lattice), while the mixing height is considered as reflecting (a particle that reaches it, has the vertical component of its velocity inverted), but several other scenarios can be easily implemented.

A Boolean matrix $E(i,j,k,t)$ is used to summarise the pollutant particle distribution at each time $t$. The matrix values can be either 1 or 0, according to the presence/absence at the site $[i,j]$ of a particle moving along the direction $k$.

### 2.5 Evaluation of the pollutant concentration

The pollutant concentration at the various sites is evaluated as a time average, from the beginning of the simulation to the current time, by summing the number of particles given by the state matrix. To obtain concentration units, the mean number of pollutant particles has to be multiplied by the mean number of air particles per site, that is to say the parameter $X_n$. The resulting equation has been finally derived:

$$c(i,j) = \frac{X_n}{t_f} \sum_{t=0}^{t_f} \sum_{k=1}^{5} E(i,j,k,t)$$  \hspace{1cm} (9)

### 3 Results

The simulation tests reported in this section have been carried out to verify the ability of the LGM approach to simulate local and transient diffusion and provide evaluations comparable with the Gaussian equation in the steady-state limit. Moreover, a sensitivity analysis will be presented, in order to show the influence of the three dimensionless parameters on the solution.

The base test case selected for these purposes is an emission from a single stack with the characteristics shown in Table 1.

<table>
<thead>
<tr>
<th>Table 1: Process parameters for base test case</th>
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<tbody>
<tr>
<td><strong>Emission</strong></td>
</tr>
<tr>
<td>$u_{0}$</td>
</tr>
<tr>
<td>$T_{0}$</td>
</tr>
<tr>
<td>poll. mass flow rate</td>
</tr>
<tr>
<td>poll. conc. in emission</td>
</tr>
<tr>
<td>stack height</td>
</tr>
</tbody>
</table>

For this case, a space domain of $600 \times 80$ m around the source (placed at 30 m downwind) has been considered, with a mixing height at 80 m acting as a totally reflecting boundary. The result in terms of pollutant concentration obtained with the application of the LGM is reported in Fig. 3a as a contour plot, for a final time of 10 min. The non-dimensional parameters defined in Sec. 2.1 have been
given the values: \( X_u = 0.75, X_n = 1.2, X_I = 1.2 \). The kinetic and thermal plume rise have not been simulated, in order to separate the calculation of the plume rise height from the simulation of the diffusion process. For the same reason, the wind velocity was set constant with the height, and therefore the basic Gaussian equation was used as a comparison.

In Fig. 3b the result obtained with the Gaussian equation is shown. In order to match the LGM result, the values \( \gamma = 0.32, \delta = 0.73 \) have been adopted for the vertical diffusion coefficient \( \sigma_z = \gamma x^\delta \). For the horizontal diffusion coefficient, a constant value equal to \( \sigma_y = \alpha = 0.4 \text{ [m]} \) was used, as the pollutant is uniformly confined into a region of constant width along the \( y \)-direction.

The values selected for the parameters are very close to the ones used in [3] for a lower wind and in absence of the mixing height, which gave an analogous agreement with LMG results. In [3], it was shown how these values are fully coherent with what is proposed in technical literature, and it was concluded that, in the steady-state limit, the LMG gives quantitative and qualitative results quite comparable with conventional procedures based on the Gaussian equation. The fact that the comparison is also valid when boundary conditions are modified (mixing height), is another proof of the validity of the proposed approach.

Starting from the basic test case of Fig. 3, the non-dimensional parameters were varied in order to explore their influence on the solution. For the parameter \( X_n = 1.4 \) and 1.0 (base case \( X_n = 1.2 \)), the steady results are shown in Fig. 4a-b. It can be seen that an increase of \( X_n \) also increases the diffusion both along the horizontal and the vertical direction. Similar steady conditions can be obtained with the Gaussian equation, by setting proper values for the parameters that lead to the evaluation of diffusion coefficients. An attempt to find such values led to the concentration plots shown in Fig. 4c-d, obtained with the parameters summarized in Table 2. While \( \alpha \) requires substantial variations in order to fit the LGM data, \( \gamma \) and \( \delta \) are constant in the three cases. This means that \( X_n \) has the same effect on the diffusion process as the parameter \( \sigma_y \).
The same analysis has been made for the variations of the non-dimensional parameter \( X_t \). For the same values 1.4 and 1.0 (base case \( X_t = 1.2 \)), the results are shown in Fig. 5a-b. No substantial variation can be observed in the vertical diffusion, and only weak variations in the horizontal diffusion. These data can be obtained by Gaussian equation (Fig. 5c-d) with constant values for \( \alpha \) and \( \delta \), while \( \gamma \) varies slightly, still assuming values that are typical of the stability class selected (Table 3). This analysis shows how the parameters \( X_t \) and \( \gamma \) play the same role in the simulation of the diffusion process.

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**Figure 4**: Results for varying \( X_n \), with a-b) LGM, c-d) Gaussian equation

**Figure 5**: Results for varying \( X_t \), with a-b) LGM, c-d) Gaussian equation
Table 2: Equivalence between LGM and GPE for varying $X_n$

<table>
<thead>
<tr>
<th>$X_n$</th>
<th>$\alpha$</th>
<th>$\gamma$</th>
<th>$\delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.4</td>
<td>0.33</td>
<td>0.32</td>
<td>0.73</td>
</tr>
<tr>
<td>1.2</td>
<td>0.40</td>
<td>0.32</td>
<td>0.73</td>
</tr>
<tr>
<td>1.0</td>
<td>0.55</td>
<td>0.32</td>
<td>0.73</td>
</tr>
</tbody>
</table>

Table 3: Equivalence between LGM and GPE for varying $X_n$

<table>
<thead>
<tr>
<th>$X_n$</th>
<th>$\alpha$</th>
<th>$\gamma$</th>
<th>$\delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.4</td>
<td>0.40</td>
<td>0.32</td>
<td>0.75</td>
</tr>
<tr>
<td>1.2</td>
<td>0.40</td>
<td>0.32</td>
<td>0.73</td>
</tr>
<tr>
<td>1.0</td>
<td>0.40</td>
<td>0.32</td>
<td>0.72</td>
</tr>
</tbody>
</table>

The variation of the third dimensionless parameter, $X_u$, leads to the plots shown in Fig. 6, for the values 0.85 and 0.65 (base case $X_u = 0.75$). The three scenarios appear to be quite close to each other, leading to the conclusion that $X_u$ does not significantly affect the solution, and has only an influence on the computational complexity and time.

Another result presented here concerns the evaluation of the pollutant concentrations at the soil level, that are of fundamental importance due to their effects on human life and their immediate comparability to the air quality limits.

The equivalence of the LGM and the Gaussian model in the steady limit is evident in Fig. 7, that shows the pollutant concentration evaluated near the soil as a function of the downwind distance, for the base case (Fig. 1) and for $X_n = 1.0$. The agreement between the two models (LMG, irregular curve, GPE, smooth curve) is impressive from a distance of around 170 m from the source. For points situated upwind, the LMG evaluates concentrations due to local effects near the source, that the Gaussian equation does not take into account.

The appearance of local and transient effects is better illustrated in Fig. 8. For the case of $X_n = 1.4$, the sequence of concentration contour plots for subsequent times is shown. The sequence starts at 100 s (Fig. 8a) with the plume still
confined around the source. This is one instance in which the LGM shows the best potential compared to GPE, and also puff models that do require a predefined plume rise to simulate the plume-air interaction along z-direction. Increasing the observation time (Fig. 8b-e), the effect of increasing contour smoothing is evident. It can also be seen that the sequence smoothly converges to the steady-state concentration field (Fig. 8f), already presented in Fig. 2.

Figure 7: Concentration at soil, for a) base case, and b) $X_n = 1.0$

Figure 8: Evolution of the plume after
a) 100 s, b) 200 s, c) 300 s, d) 400 s, e) 500 s, f) 600 s
4 Conclusions

The LGM has been shown to be a promising method for the evaluation of transient and local diffusion around pollutant sources. Therefore, the LGM is an approach able to model those phenomena that are impossible to simulate with standard GPE-based diffusional models, or only partially possible with puff models or transient Gaussian models. At the same time, it has been shown how in the steady-state limit, when the GPE is valid, the results obtained with the LGM are quite comparable, if a proper selection is made for the turbulence parameters. This should be regarded also as an indirect proof of the validity of the proposed model.

The equivalence between LPG and GPE parameters has been deepened in the paper. The results of such an analysis can be summarized as:

- the role played by the number ratio, that has the meaning of mean number of particles per lattice site, is the inverse of that of the horizontal diffusion coefficient in the GPE.
- the role played by the time ratio, that has the meaning of mean time between subsequent emissions, can be compared with that of $\delta$, or of the variation of vertical diffusion along the downwind distance.
- the velocity ratio seems not to have a significant influence on the simulation of the diffusional process. Different values of this parameter actually lead to very similar results.

When the LGM has to be applied to environmental impact studies, a selection of proper values for these three parameters can be therefore made according to the data available in the literature for the Gaussian diffusional parameters. Based on the steady-state comparison between LGM and GPE, and given the proved reliability of GPE under steady conditions, an agreement between LGM transient and local predictions and actual data for a number of scenarios can also be reasonably expected. However, a validation of the model for simple transient conditions that can be described using puff- or transient Gaussian models will be the subject of a further study.

References

