An Optimised Method to Couple Meteorological and Photochemical Models for Air Quality Applications

Abstract

Air quality numerical studies require coupling of meteorological and photochemical forecast. Most of the time, this coupling is realised in a non-simultaneous way, i.e. first a meteorology model is run, data are stored, and photo-chemistry is simulated. This study shows that significant errors may be generated in gas-phase photochemical modeling if meteorological field update intervals are too coarse to resolve wind-field time variations. Three different coupling methods are compared. Differences between a decoupled method using hourly updates and a fully coupled calculation, are shown to be on the same order of magnitude as the disagreement between observations and model predictions in current applications. A so-called hybrid method in which meteorology updates are performed after a well defined time lag (CFL limit, i.e. few minutes) is presented and is shown to be a good compromise between the full coupled (updates based on the time step of the meteorological resolution, i.e. each 20s) and decoupled (hourly updates) methods. Indeed this hybrid method keeps a level of accuracy very close to full coupling while CPU time is kept similar to the decoupled method. The impact of different transport time step on the accuracy of the results is also investigated. Concentrations resulting from three different time-steps calculations are compared showing that smaller transport time steps significantly improve results for the hybrid method but only slightly for the decoupled method.
1. Introduction.

The numerical study of air quality with photochemical models requires meteorological data (at various scales). These meteorological data either result from observations which are extrapolated over the whole domain to obtain mass-consistent wind fields (Sistla et al. 1996, Goodin et al. 1980) or through prognostic models. These latter may sometimes include links with observations through nudging techniques (Stauffer et al. 1990 and Stauffer et al. 1991).

Whatever the followed methodology, a wind-flow field is always required to start photochemical calculations and final results will crucially depend on the quality of this data. Since observations are generally available only at discrete times (e.g. hourly), photochemical models coupled with diagnostic wind-fields (based on observations) are fed at those particular times. This approach is limiting since it does not incorporate the effect of atmospheric motions having smaller time-scale variations than the update time interval. For prognostic meteorological models, this constraint is removed but other problems arise. If the two models (meteorological and photochemical) are run independently (i.e., first meteo and afterwards photochemistry), a higher updating frequency can be problematic because all the meteorological information must be stored. On the other hand, if the two models are run simultaneously, the CPU time increases for a single simulation. Since air quality modeling studies generally require testing of several different emission scenario, the need of re-running the meteorological model for each of these scenario may lead to CPU time problems. This explains why most of the existing models use relatively large updating time increments; (Chang et al. 1987), except for a few authors who applied a direct simultaneous coupling (Vogel et al. 1991, Svensson 1995).

In this paper, a quantitative analysis of the error generated in air quality modeling by different meteorology update frequency is carried out for the special case of a bi-dimensional sea-breeze over complex terrain. These errors are estimated for both passive and reactive species. The two methods of coupling described above, i.e. coupled (run simultaneously) or decoupled (discrete update time) are discussed and a compromise which combines the advantages of low CPU and storage costs is developed and compared to the two others.

The impact of chemistry and meteorology update time increment on air quality results is investigated here by use of the TVM/LCC model. This model is based on the nonhydrostatic incompressible TVM (Thermal Vorticity Mesoscale model) (Schayes et al. 1996, Thunis 1995) coupled with the chemical solver of the air quality model CIT (Mac Rae et al. 1982, Young and Boris 1977). The chemistry is based on the chemical mechanism LCC which includes prognostic equations for 35 species involved in 106 reactions (Lurmann et al. 1987, Harley et al. 1993). Both chemical species, thermodynamic and dynamic variables are advected by the Piecewise Parabolic Method (PPM) (Collela and Woodward 1984) corrected for multidimensional modeling by Clappier (1998). TVM/LCC applies an operator splitting technique, i.e. advection is integrated separately from the chemistry.

In order to study the impact of the meteorology update frequency, i.e. the frequency with which the air quality model is fed by meteorological data, three strategies can be differentiated (Fig. 1):

1) **Decoupled**: The photochemical module and the meteorological module are run independently. Meteorology is run first with an internal time step determined by the interactions between thermodynamic and dynamic fields. For the 2-D case selected here, the time step was 20s. The meteorological parameters are provided to the photochemical module every chosen time intervals (in the following, a one hour interval time updating has been selected). The transport of the chemical species then operates with an internal time step limited by the CFL condition, i.e. between 100 and 1000s depending on the wind field intensity. Note that this methodology is currently followed by most air quality models.

2) **Full coupling**: The meteorology and transport of the chemical species are solved simultaneously using the same time-step. The latter is then fixed as the minimum of the two previously discussed internal time-steps, i.e. the one limited by meteorology (20s). This methodology provides the most accurate results since species transport is always calculated using the most recent meteorological data; it will therefore serve as reference in the discussion hereafter.

3) **Hybrid coupling**: The meteorological module is run with its 20s time-step until it reaches the CFL criteria of the transport. At this specific time, the resulting meteorology is provided to update transport. In order to compare this methodology with the previous one, a smooth transition between the two methods will be obtained by selecting update intervals equal to fractions of the CFL. In the following section, three simulations are carried out using transport time steps set to 0.1, 0.5 and 1 times the CFL limit.
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Fig.1: Schematic representation of the three coupling techniques: decoupled, full-coupled and hybrid. $\Delta t_d$ is the time step of the meteorological module (resolution of the dynamic), $\Delta t_c$ is the time step of the photochemical module (resolution of the transport and the chemistry).

For the three methods described above, only the frequency of meteorological updates is considered. The chemical solver restarts operating each time transport is updated i.e. the same time-step is used for both species transport and chemistry although for the latter, internal time-steps may obviously be different. Although the two last methods may seem relatively similar, their CPU requirements may be very different. For one full coupled case, the chemical solver restarts calculations each 20s while it is only the case each 100 to 1000s (i.e. CFL limit) for hybrid coupling. This can create an important CPU difference since the chemical solver usually starts its calculations with a time-step of a fraction of second which then increases during the integration of the chemistry. A repetition each 20s of the small chemical time-steps may become very costly.
3. Results.

a. Description of the test case.

An idealised 2D case consisting of a Gaussian shape mountain (height: 500m, half width: 10 km) bounded on its left side by a 25 km wide water surface is studied here. The modeling domain is 86 km long by 8 km high and is divided into 57 horizontal by 10 vertical grids. In the horizontal direction the finest resolution is 1 km in the central part of the domain and the grid is horizontally stretched at the two borders. In the vertical direction the grid is stretched up the model top. Simulations start at 6:00 LST and last for 24 hours. Fig. 2 shows the flow-field pattern at 12 (2a), 17 (2b) and 19 LST (2c), with the typical features expected from differential heating are reproduced: land/sea breeze and anabatic-katabatic winds on both sides of the mountain. This complex flow field which evolves rapidly with time is well suited to study the impact of updating frequency on air quality modeling results. Note that there is no feedback mechanism between chemistry and meteorology, i.e. the meteorological field remains unchanged for each test case. Two test cases are hereafter studied. First, a passive tracer is considered to understand the impact of meteorology update on the various coupling methods. Secondly, gas phase chemistry is included.

![Flow-field pattern at different times](image)

**Fig.2**: Vertical cross sections of the horizontal wind field at different times. Solid and dotted lines are for positive and negative values, respectively. Values located on the left of abscissa 0 are in sea.
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**b. Passive tracer.**

In this case, a puff of passive tracer (a dimensionless concentration of 100 at 2 km from the coast, 150 m above the surface and background concentration set to 1) is emitted at 15:00 LST between the shoreline and the mountain. Results for the three coupling methods at 20:00 LST are shown in Fig.3 for CFL=1 (update each time CFL is reached). From this figure, the hybrid results are very similar to those obtained with full coupling while some local differences are observed in the case of the decoupled technique. Note that for updating frequency smaller than the CFL, i.e. CFL=0.1 and 0.5, the results (not shown) are very similar.

![Fig.3: Puff position for the passive tracer 5 hours after release for the different coupling methods.](image-url)
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In Table 1 are given the maximum and mean differences between the fully and other coupling cases using the following definitions: the normalised difference $\text{diff}$, is computed via:

\[
\text{diff} = 100 \cdot \left| \frac{c_{ij} - c'_{ij}}{c_{\text{max}}} \right|
\]  

(1)

where $c_{ij}$ is the concentration at the point $i,j$ for the test case, $c'_{ij}$ is the concentration for the fully coupled case, $c_{\text{max}} = \max_{i=1, nx} \ max_{j=1, nz} \left( |c_{ij} - cb|, |c'_{ij} - cb| \right)$, $cb$ is the background value and $nx$ and $nz$ the number of points in horizontal and vertical direction respectively.

The maximum normalised difference is

\[
\text{diff}_{\text{max}} = \max_{i=1, nx} \ max_{j=1, nz} \left( \text{diff} \right)
\]  

(2)

The root mean square normalised difference is computed by mean of the normalised difference (1):

\[
\text{rmsdiff} = \frac{1}{nx \cdot nz} \sum_{i=1, nx} \sum_{j=1, nz} \left( \text{diff} \right)^2
\]  

(3)

Table 1 shows that difference between the decoupled (with hourly interval) and the full coupled method (RMS of 12.3 for CFL=1) is much larger than the difference between the hybrid and fully coupled method (RMS of 2.2). It is interesting to note that this RMS error increases with the size of the time step for the hybrid method while it is not the case for the decoupled one. Indeed, in the latter case, most of the error is due to the poor frequency of meteorology updates and the numerical error generated by the different CFL time-steps conditions only slightly modulate this error. On the contrary, in the case of the hybrid method, most of the error is now only due to the numeric since the meteorology update frequency is relatively high. In Fig.4 are represented the spatial differences between the fully coupled and decoupled results (4a), and between the hybrid and fully coupled method (4b), both with a time step fixed at CFL=1. From this figure, the greatest differences in percentage are found in vicinity of the puff borders where transport is important and concentration gradients are large.
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![Decoupled -Full Coupling](image1)

![Hybrid -Full Coupling](image2)

**Fig.4:** Difference cross-sections between a) full and decoupled and b) hybrid and full, for the passive tracer concentrations after 5 hours of simulated time.

<table>
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<th>Passive tracer</th>
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<th></th>
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<td></td>
<td>Max.</td>
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<td>Max.</td>
<td>RMS Diff.</td>
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<td>RMS Diff.</td>
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1 Root mean square difference

**Table 1:** Maximum (left column) and mean (right column) differences for the passive tracer test for different techniques and different fraction of CFL. Values are in percent.

c. Reactive tracer.

In this case, a source is located between the shoreline and the mountain. It emits volatile organic compounds (VOC), nitrogen oxides (NO\textsubscript{x}) and CO at a rate typical of an urban area. The evolution of both primary and secondary (e.g. ozone) species is here followed. Simulations start at 8:00 LST. Figs. 5, 6 and 7 show the resulting O\textsubscript{3}, NO\textsubscript{x} and VOC concentrations, respectively after 12 hours of simulation (at 20:00 LST). The maximum difference between the decoupled and fully coupled method reaches 57% for ozone and 74% for NO\textsubscript{x} (Table 2) while they are drastically reduced to 4.7% and 1.5% respectively, for the hybrid method. These maximum differences are all observed in vicinity of the surface where wind time variations are the more dramatic. The RMS differences illustrate the same trend, i.e. evolving from 10.9% (O\textsubscript{3}) and 5.6% (NO\textsubscript{x}) for the decoupled results to 0.5 and 0.1% for the hybrid one. Results for the VOC concentrations are almost similar to those obtained for NO\textsubscript{x}. It is important to realise that this 10% error generated by the decoupled method for O\textsubscript{3} is of the same order of magnitude as the difference generally found between measurements.
and model results (e.g. CARB, 1990). The impact of coupling methodologies becomes therefore important for complex terrain areas in which rapidly evolving winds are observed.
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<table>
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<th></th>
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<th>CFL=0.1 RMS Diff.</th>
<th>CFL=0.1 RMS Diff.</th>
<th>CFL=0.5 Max.</th>
<th>CFL=0.5 RMS Diff.</th>
<th>CFL=0.5 RMS Diff.</th>
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<th>CFL=0.1 RMS Diff.</th>
<th>CFL=0.1 RMS Diff.</th>
<th>CFL=0.5 Max.</th>
<th>CFL=0.5 RMS Diff.</th>
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<th>CFL=1.0 RMS Diff.</th>
<th>CFL=1.0 RMS Diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hybrid</td>
<td>0.1</td>
<td>0.01</td>
<td>0.5</td>
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<td>5.1</td>
<td>63.7</td>
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<td>64.4</td>
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</table>

1 Root mean square difference

Table 2: Maximum (left column) and mean (right column) errors for Ozone, $NO_x$ and VOC for the reactive tracer test for different techniques and different fraction of CFL. Values are in percent.
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**Fig. 5:** Ozone concentration in ppm at 20:00 LST for the different coupling methods.

**Fig. 6:** NO\(_x\) concentration in ppm at 20:00 LST for the different coupling methods.
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Fig. 7: VOC concentration in ppm at 20:00 LST for the different coupling methods.
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For both reactive and passive tracers, important differences which appear where pollutant gradients are large are then advected throughout the domain. This means that if one looks at the predicted temporal evolution of a pollutant at one location, the greatest differences occur only during a relatively short time period while afterwards, the different methods give similar results (Fig. 8). This does not mean that the error suddenly dissipated; it was instead advected to another downwind location.

![Ozone time evolution](image)

**Fig.8:** Time evolution of the ozone concentration at a specific location (mountain slope opposite to emission source) for the different coupling techniques.

While the hybrid and decoupled methods produce quite different results compared to the reference fully coupled case, the CPU time required by each method (Fig. 9) is approximately on an order of magnitude smaller than that required by the fully coupled method (all test cases were run on a SUN SPARC 10). This dramatic decrease in CPU requirement between the hybrid and fully coupled method arises from the way the chemical solver typically works. As shown schematically in Figure 10, the chemical solver (Young and Boris 1977) uses very short time steps at the beginning of a calculation (the time step then increases as calculation proceeds), and this is repeated after each transport step. This creates then a major CPU penalty whenever chemical integration has to be repeated too often (e.g. McRae et al. 1982). This CPU penalty can even be larger for other methods, e.g. Gear-type solvers like LSODE (Hindmarsh 1974) or SMVGEAR (Jacobson and Turco 1995). On the other hand, QSSA (Hessdvelt et al. 1978) types of solver would not lead to this kind of problem since their constant time-step through the whole calculation does not enable them to take advantage of larger transport time steps.
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**Fig. 9:** Required simulation time for the different coupling techniques.

The previous arguments explain why the hybrid method is much faster than the fully coupled one. We have yet to explain why the hybrid and decoupled methods require similar CPU time. For decoupled simulations, even if the wind fields are only hourly updated, the transport of species is limited by the CFL condition. This means that if only transport of a chemical tracer is considered, full coupling (i.e. using the meteorological model time-step for transport species) would require only a CPU increase proportional to the ratio between the fraction of CFL and the meteorological time-step. Note that if the time-step is chosen such that the fraction of CFL is based on the maximum velocity anywhere in the domain, most of the domain will have a local fraction of CFL less than one. Note also that time-steps larger than the CFL limit could lead to advection of a pollutant air mass over a grid without its possible interaction with emissions or deposition within that grid. In areas with a very heterogeneous mixture of emissions, this could lead to significant errors and concentration waves would be observed in the results.

**Decoupled method:**

- **Transport time step:** 100-1000s (CFL)
- **Chemical time step:** 10^{-5}s to 100s

**Full coupling method:**

- **Transport time step:** 20s (dynamics)
- **Chemical time step:** 10^{-5}s to 10s

*Fig. 10:* Schematic evolution of the Young and Boris solver time step
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The choice of the transport time-step alter both CPU requirements and model accuracy. Clappier (1998) suggested that a transport time-step equal to the CFL limit was acceptable for standard test cases in which chemistry and emissions are not included, and wind field is steady. As already discussed in the passive tracer section, the use of different transport time step (0.1, 0.5 and 1 times the CFL) was shown to lead only to slight changes in model accuracy (Table 2) but the CPU required for these three simulations is significantly modified (Fig. 9). Indeed, the 0.1 CFL case requires approximately ten times more CPU than the two other cases (0.5 and 1 CFL). The hybrid method is therefore time efficient only for large time-steps.

The above results are derived for gas-phase modeling. Clouds and their chemistry poses additional challenges since the variable fields (e.g. liquid water content) can be much more irregular. In this case, some strategies, such as interpolation in time can lead to poor results (Muller et al. 1996). For example, advection of a cloud and the corresponding liquid water over two computational grids leads to an artificial diffusion of the cloud that increases interactions between gas and aqueous phases. This can, in turn, lead to increased oxidation of sulphur dioxide and other species, and depletion of hydrogen peroxide.


Air quality numerical studies require the coupling of meteorological data to photochemical models. Most of the time, this coupling is realised in a non-simultaneous way, i.e. first meteorology and then chemistry. This study has shown that significant errors may be generated in gas-phase photochemical modeling if meteorological field update intervals are too coarse to resolve wind-field time variations. Differences between a decoupled method using hourly updates and a fully coupled calculation, were shown to be on the same order of magnitude than disagreement between observations and model predictions in current applications (CARB, 1990). It was demonstrated that the so-called hybrid method in which meteorology updates are made each few minutes (CFL limit) was a good compromise between the full coupled (updates each 20 s) and decoupled (hourly updates) methods. Indeed this method proved to keep a level of accuracy very close to full coupling while CPU time was kept similar to the decoupled method. The hybrid method may also work in a decoupled way but storage of the meteorological data will then soon become unreasonable. Note, the main disadvantage of the hybrid method lies in the fact that, for each tested emission scenario, meteorology must be calculated again. But it seems to be an acceptable price to correctly simulate the effect of rapidly changing wind-fields.
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The impact of different transport time step on results accuracy was also investigated. Concentrations resulting of three different time-steps calculations were compared and it showed that smaller transport time steps improve results significantly for the hybrid method but only slightly for the decoupled method. Most part of the error was due not to the loss of accuracy of the numerical advection scheme for longer time-steps but to the updating frequency. Results obtained with a time-step equal to the CFL, although they were the worse of the three results, were still very similar to the reference fully coupled results. This hybrid method constitute therefore a good compromise between the full coupled and decoupled method. It is as accurate as the full coupled method and as computationally efficient as the decoupled method. These results also suggest that fully coupled meteorological and air quality models could be accurate but would not use computational resources efficiently. Note finally that all simulations were carried out only for bi-dimensional cases since interpretation of the results was facilitated and since conclusions qualitatively remains unchanged for three-dimensional cases.
REFERENCES


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