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Development of a New Meteorological Ventilation Index for Urban Air Quality Studies



Marie Haeger-Eugensson¹, Katarina Borne², Deliang Chen^{1,2}, Karin Persson¹

¹IVL Swedish Environmental Research Ltd ²Earth Sciences Center, Gothenburg University

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Abstract

Experience from many years of measurements in urban areas in Sweden shows that high concentrations of various air pollutant components occur not only in large cities but also in small towns. One possible reason is variation in the local meteorological conditions causing poor ventilation facilities. For some years IVL has used an empirical statistical calculation method (the so called "URBAN-model") developed by IVL. The model has primarily been used for estimating the risk of exceeding different national standard values of air pollution concentrations in small and medium sized towns in Sweden.

The purpose of this investigation was to develop a method in a test area to improve the calculations of air pollution concentrations used in the former URBAN-model. This was achieved by reproducing the local meteorological variations better in a new ventilation index and a dispersion-adjusting constant and also with better temporal and spatial resolution of the parameters. By using an advanced numerical model, TAPM (The Air Pollution Model), the old ventilation factor was improved by using the output parameters mixing height and wind-speed respectively, for calculating new ventilation parameters with high time and spatial resolution (1 month and 1x1 km). The results were then included in an improved calculation routine/model implemented into the URBAN model. Since the TAPM model previously has only been validated in Asia and as the circumstances are rather different in northern Europe (rain, soil moisture day length etc) it was necessary to verify the model's performance on meteorology modelling, before using the output of the model to develop new ventilation parameters. The validation showed that the model performs well in simulating air temperature and wind, which are the two most important fields to drive air pollution modelling. Also, TAPM was confirmed to have strong ability in simulating thermally driven mesoscale systems, such as sea-land breeze and urban heat island effects. It is thus concluded that TAPM is a very useful tool for local meteorological air pollution applications.

A comparison between monthly averages of measured and calculated NO_2 concentrations (with the new model) shows a fair accordance. When comparing NO_2 calculated with the old and the new URBAN-model and NO_2 measurements, the new model shows a much better agreement with measured data. Consequently, the need of evaluation of the air quality in communities and small cities can be better met by using this improved URBAN model. Since the time consuming and complicated meteorological modelling is only used to generate the new ventilation parameters, the actual NO_2 calculations with the new URBAN model can still remain rather simple compare to other dispersion models.

The method developed for the test area can be developed for whole Sweden and thus meets the extended demands of accurate air pollution calculations in small communities.

1. Introduction

1.1 Background

Experience from many years of measurements in urban areas in Sweden shows that high concentration of various air pollution components occur not only in large cities but also in small towns. One possible reason is variations of the local meteorological conditions causing poor ventilation. According to the investigation performed by The Parliament Committee on Environmental Objectives (Miljömålskommittén) about 10% of the communities in the country are going to exceed the threshold values of NO₂ even if proposed reductions of emissions are being carried through. In areas where there are no information about the air quality or meteorology, it is a very expensive and timeconsuming procedure to obtain reliable data from either long-term measurements or advanced modelling. Thus, there will be a continuous need of reliable, cost effective and rapid calculations of the air quality in the future, in order to meet the EU air quality directives in both small and medium sized towns. Until recently IVL has used an empirical statistical calculation method, i.e. the "URBAN-model" developed by IVL, for estimating the risk of exceeding different national standard values of the concentration of air pollutant in these locations. The dispersion possibility in the model is based on a ventilation index calculated from the mixing height and wind speed (Holzwoth, 1972 and Krieg and Olsson, 1977). Similar methods have recently been used in the United States, especially in determining the ventilation potential for smoke from wildland fires (Hardy et al 2002), with a further development by adding a locally developed inversion potential (Fergeson, 2002 and Fergeson et al., 2003).

1.2 The URBAN-model

The URBAN-model has primarily been used for estimating the risk of exceeding different national standard values of the concentration of air pollutant in small and medium sized towns in Sweden. The scale of the calculation area is about a Swedish medium sized community. Percentile calculation and street level concentrations are estimated from the urban background concentration with a statistical relationship based on measurements (Persson et al. 2002).

The URBAN model (equation 1) is thus based on measured air pollution concentration in urban background, C_t , collected at the national URBAN measuring network (Persson 2002), minus rural background concentration, C_b , and a ventilation factor, F_V .

C_t - C_b =log(population)* F_V

(1)

The logarithmic function in the model is based on the assumption that the emission of

air pollutants in a region is proportional to the population in the area. Even though this method of calculating the emissions are rather rough there is a clear connection between the two parameters. This can be explained as the activity of each person produces a certain amount of air pollution (traffic, heating etc.) which is distributed over the area. The relation between NO_x emission and population from 35 different communities in Sweden from 1995 has been tested and is shown in *Figure 1*. The logarithmic correlation is valid for small to medium sized communities (straight line in a logarithmetic scale) but for larger communities that relation is less accurate (exponential line in a logarithmic scale).



Figure 1. Relation between population (logarithmic scale) and emission of NO_x (linear scale).

The determination of ventilation index in Sweden was developed by SMHI (Krieg and Olsson. 1977) and is derived from calculations of the mixing height¹ (H) and the ground level wind speed (U) (2).

V=U*H

(2)

¹ The mixing height is defined as that level where the temperature of the adiabatically lifted parcel becomes less than the measured ambient temperature. This means that the mixing height is the height from ground to the top of the mixing layer. In the mixing layer the turbulence is rather uniform resulting in fairly good dispersion of air pollutants. However, at the mixing height the turbulence is suppressed causing difficulties for pollutants to penetrate. The vertical limitation can be caused by for example an inversion layer.

For the calculation of H the vertical temperature from balloon soundings is used. The wind profile is thus not taken into consideration. Since there are very few radio soundings in the country, both in time (at 00 and 12 GMT) and place, these calculations only show a mixing height that is assumed to represent large areas. The partition of

Sweden into zones with different ventilation indexes is therefore very approximate (*Figure 2*) without consideration of local variations (SOU, 1979). This is also true for the calculated ventilation factor, F_v .

From the calculated F_v (Equation 1) it is possible to derive air pollution concentrations of towns without measurements (of air quality and/or meteorology), by first determine in which zone of ventilation index the town is located (*Figure 2*) and then use the calculated F_v for that region. The background concentrations for all regions are already specified in the model.



Figure 2. The former ventilation index (V)(SOU 1979) based on calculations of mixing height and wind speed (Krieg and Olsson. 1977).

1.3 Purpose

In order to improve the calculations of concentration of air pollution in towns with the former URBAN model, the local meteorological variations needs to be represented better in a new improved calculation routine. The aim of this study is to develop the method and to demonstrate its usefulness in southwestern Sweden. The long-term goal is to apply the method for whole Sweden, which will help meeting extended demands of calculations in small communities.

2 Methods

Improved mixing parameters has been developed and tested in the southwestern part of

Sweden, in order to improve the calculations of the concentration of air pollutants in small cities without meteorological and/or air quality measurements. The mixing parameters are a new ventilation index (V) combined with a dispersion-adjusting constant (C_d). V_i is based on similar method as SMHI have used (Krieg and Olsson, 1977) but with higher time and spatial resolution, since the circumstances for ventilation differs rather much during different seasons, especially in northern Sweden. The mixing parameters are then used to improve the calculations of the air pollution concentrations in the URBAN-model.

2.1 New Mixing Height calculation

In order to improve the old ventilation factor used in the URBAN-model, a higher time and spatial resolution in the calculation of mixing height was essential. This was completed by using an advanced numerical model, TAPM, (The Air Pollution Model) developed by Australian CSIRO Atmospheric Research Division (see further Appendix 1). This model system integrates meteorology and air dispersion and air chemistry (Hurley, 1999b), but in this case only the meteorology was used. Here the spatial resolution of 1x1 km and the time resolution 1-month are used to represent the ventilation conditions for two years (1999 and 2000). The investigated area is southwestern Sweden including 6 urban areas, Alingsås, Borås, Göteborg, Kungälv, Vänersborg and Trollhättan (*Figure 3*).



Figure 3. Map over the investigated area with the 6 cities marked with circles.

A very important feature of TAPM is its ability to explicitly deal with surface energy budget and temperature, which allows simulation of thermally driven wind systems and also a properly modelled mixing height. The development presented in shows the distinct diurnal variation of mixing height, which is strong at the day time due to the unstable atmosphere and weak at the nigh time due to the stable stratification of the atmosphere. More information about the validation is found in appendix 2 and in Chen et al. (2002).





Figure 4. The modelled mixing height (m) during night and day on the 12th of June

The output parameter from TAPM used here is mixing height (H) with a resolution of 1x1 km. This is calculated for each hour using boundary layer variables including temperature and wind profile, also calculated by TAPM. The monthly mean H is then calculated for each town by integrating the hourly values.

2.1.1 Short description of TAPM

Air pollution models typically use either observed data from a surface based meteorological station or a diagnostic wind field model based on available observations. TAPM is different from these approaches in that it solves the fundamental fluid dynamics and scalar transport equations to predict meteorology and pollutant concentration for a range of pollutants important for air pollution applications. It eliminates the need of site-specific meteorological observations. Instead, the model predicts the flows important to local-scale air pollution transport, such as sea breezes and terrain induced flows, against a background of larger-scale meteorology provided by synoptic analyses. It predicts meteorological and pollution parameters directly on local, city or inter-regional scales.

The model was designed to be run in a nestable way so that the spatial resolution can be as fine as ~ 100 m. In addition, it can be run for one year or longer, which provides a means to deal with statistics of meteorological and pollutant variables (further information on TAPM in appendix 1).

2.1.2 Validation of the TAPM-model

The model has previously been validated in different parts of Asia (appendix 2). However, since the circumstances are rather different in northern Europe (rain, soil moisture day length etc.) it was necessary to verify the model's performance on meteorology modelling before using the output of the model in calculating a new ventilation index. For this purpose, TAPM was run with three nestings that have spatial resolution of 9 km, 3 km and 1 km. There are 90*90 grid points in horizontal dimensions (see Figure 1) and 20 levels in vertical (from 10 to 8000 meters).

Based on the comparisons between the TAPM output from the two years run and the surface/profile measurements on air temperature and wind, it has been found that TAPM performs well in simulating air temperature and wind for Swedish conditions. These parameters are the two most important fields to drive the air pollution modelling. In addition, TAPM has strong ability in modelling sea-land breeze and urban heat island effect (see Appendix 2). As such, it is concluded that in the future TAPM can be applied in meteorological modelling and environmental impact assessment in Sweden with confidence. (Further results from the validation in Appendix 2).

2.2 Calculation of H with Holzworth algorithm

The Holzworth algorithm is the method which have been used for many years and was also used by SMHI 1977 to calculate H for developing the ventilation index V. Here an attempt is made to validate the mixing height (H) from TAPM at Landvetter airport by comparing it with H calculated using Holzworth algorithm (1972) based on balloon sounding data (*Figure 9*).

The calculation of H was made twice a day based on synoptic observations as well as data from a radiosonde sounding. To compute the morning mixing height, the minimum temperature from 0200 to 0600 (LST) is determined. To this value 5°C is added. Holzworth developed his algorithm for an urban environment in order to estimate urban air pollution. He established this adjustment to account for temperature differences between rural and urban environments and for some initial surface heating just after sunrise. To estimate the morning H, the adjusted minimum surface temperature follows the dry adiabatic lapse rate up to the intersection with the observed 1200 (GMT) temperature radio sounding.

A similar computation is made using the maximum temperature from 1200 to 1600 (LST) and the 1200 (GMT) radio sounding, except that the surface temperature is not adjusted. The assumption made by Holzworth was that afternoon H in urban and nearby rural areas does not differ significantly, whereas the nocturnal H is often very different.



Figure 9. Comparison between calculation of mixing height by TAPM and by Holzworth algorithm.

However, the agreement, visualised in *Figure 9*, is rather poor, possibly due to the difference in the calculation techniques and the quality of the substitute input data to the

Holzworth method (Hozworth 1972).

2.3 Calculation of the new mixing parameters

The new mixing parameters are a new ventilation index (V) and a dispersion-adjusting constant (C_d) which are substituting F_v from the old URBAN-model (C_d*V=F_v). The calculation of V are based on the calculation in equation 2 but includes calculation of wind speed (U) and a new types of calculations of mixing height (H) both performed with TAPM in a grid resolution of 1x1 km.

To determine C_d , measurements of monthly average of NO₂ minus the background concentration and the monthly average of V (or H*U). C_d is thus calculated according to equation 3, which are based on equation (1).

 C_t - C_b =log(population)* V* C_d

(3)

At all sites and times where measurements of NO₂-concentrations (C_t) existed, C_d was calculated separately at each site and months for the two years. Those calculations were then used to determine the NO₂ concentration in towns where there were no measurements, by assuming that C_d is similar for towns with similar V's.

3. Results

3.1 Mixing height

3.1.1 Mixing height in the investigated area

The mixing height calculation in TAPM is performed in each grid (1x1 km) over the investigated area. An example from January 1999 is presented in *Figure 10*.



Figure 10. The distribution of mixing height (H) in the investigated area during January 1999 calculated by the TAPM-model.

The distribution of mixing height is closely linked to surface characteristics and topography. This is visualised in *Figure 11* where the mixing height increase rapidly along the coast line and further inland continue to increase due to topography but in the valleys H is still low. However, in the highest eastern part of the area, the mixing height becomes less again despite the high terrain. The reason for low mixing heights here is possibly caused by the more inland and thus more stable mixing conditions during night.



Figure 11. The distribution of mixing height from January overlayed the topography in the investigated area.

The result of the mixing height calculations at each site is presented as monthly means in Figure 12a) for 1999 and b) for 2000. The result in Figure 12a) shows a distinct seasonal cycle where the height difference between winter and summer is about 200-250m at four of the sites (Alingsås, Borås, Trollhättan and Vänersborg) with a variation of about 50 m. The mixing height from the other two sites (Göteborg and Kungälv) is rather similar all year around, with a variation of 50-75 m.

In 2000 (Figure 12 b) the pattern of the yearly mixing heights is similar, even though the elevation during summertime is not as clear as in 1999. The wintertime in year 2000 shows a larger diversity between the different sites than during the previous winter 1999. However, at these latitudes the weather is very changing from year to year and since the mixing height is dependent on many of the varying processes such as wind speed (horizontal and vertical), surface and vertical temperature, soil moisture (especially during summer), sea temperature etc such yearly differences are to be expected.





Figure 12 a) The monthly mean mixing height from 1999 and b) from 2000, separated for each site.

From the results of the mixing height calculations, presented in Figure 12 a) and b), it becomes clear that there are two different developments of the mixing heights. One at the two sites (Göteborg, Kungälv) located close to the coast, and one at the other four sites, (Alingsås, Borås, Trollhättan and Vänersborg) located inland. In order to generalise and simplify the further calculations in the new URBAN-model, a classification of the values of mixing height was made into a coastal and an inland group. This is assumed to be relevant since the variability between the inland and coastal sites respectively, as well as between the years, is rather moderate. The monthly means of the two years and groups have been calculated and are presented in *Figure 13*.

The mean mixing height during the six winter months (Oct-Mar) from the inland sites varies between 225-260 m, and from the coastal sites between 200-250 m. During summer (May-Sep) the mixing height at the inland sites is stable located at around 325 m but it descend in September to 250 m.



Figure 13. The monthly mean mixing height from 1999 and 2000. The dotted line represents the four inland sites and the grey line the coastal sites. The thick line is a mean of all six.

3.2 The new ventilation index, V

In the calculations of V the wind speed and the mixing height is used (according to equation 2). The mean wind speed during the two years from the inland and coastal sites is presented in *Figure 14* below. The difference between the wind speed at the inland and the coastal sites are rather small and thus not what would be expected with higher wind speeds near the coast. This may be explained that non of the coastal sites are located straight at the coastline, but instead about 10 and 15 km from the coast while the inland sites are located about 55-70 km from the coast.



Figure 14. The mean wind speed for the inland and coastal sites during 1999 and 2000.

The monthly mean of the new V presented in *Figure 15* is calculated for the two years from the inland and coastal sites respectively and also as an average of all sites.



Figure 15. Mean calculations of the new the ventilation index, V, for the inland, coastal and all sites.

High values of V indicate poor dispersion facilities and varies both between the seasons and locations with the lowest values during summer and highest during winter, except for April at the coastal sites, which performs a very high V.

When comparing the results in *Figure 13* and *Figure 14* it becomes clear that the mixing height is the parameter that has the greatest influence on V resulting in the difference between the locations. However, the high value of V in April is possibly derived from the low wind speed in April. Further, the difference of V, between the inland and coastal sites is derived from the mixing height, since there is not much difference between the wind speed at the different locations.

3.3 The dispersion-adjusting constant C_d

The monthly means of C_d was calculated according to equation 3 for each month at each site for the two years. Since there was a rather large difference between the inland and the coastal sites both in terms of V and H, the calculation of C_d was also separated into inland and coastal, (Figure 16). Similar to V high C_d indicates poor dispersion conditions. (*Figure 16*).



Figure 16. Monthly mean calculation for 1999 and 2000 of C_d separated into inland and coastal sites compared with the mean C_b of all sites.

The shapes of the curves in *Figure 16* are similar to the shapes of curves of V but with a modification, mainly during the winter season. These adjustments are depending on the urban background concentrations of NO_2 , which are also included in the equation. The values of C_d 's are thus adjusted by the air pollution concentration in the various cities which will improved the reflection of local conditions resulting in further tuning of the model.

3.4 The NO₂ concentrations calculated by the new URBAN model

For calculating the concentration of NO_2 in cities without measurements, the new model (equation 3) can be used. Here either $C_{b-inland}$ or $C_{b-coastal}$ is used, depending on the location of the city. However, the mixing height and wind speed used in the calculation was not taken as an average of an inland or coastal location. They were instead derived from the monthly means for the specific grid in TAPM where the city is located.

Following this procedure, a comparison is done between monthly mean measured and calculated concentration of NO₂ (*Figure 17*) which shows a good agreement (with a R^2 of 0.6 and N=68).



Figure 17. Comparison between monthly mean of measured and calculated concentration of NO_2 for the two years (99-00). $C_{b-inland}$ and $C_{b-coasta}l$ is used depending on the location of the town.

According to *Figure 17* the calculated concentrations are in general slightly overestimated when the concentrations are below 20 μ g/m³ and somewhat underestimated when the concentrations are higher than 20 μ g/m³. The measured concentration of NO₂ and the ratio between measured and calculated concentrations are presented in *Figure 18*.



Figure 18. Comparison between measured NO_2 and the ratio of measured/calculated NO_2 .

The above comparison shows that between 17-27 μ g/m³ the calculated NO₂ values are approximately in a ratio of 1 and with an accuracy of ±0.2 μ g/m³. The calculated concentrations are therefore well modelled in this interval. For concentrations higher than about 27 μ g/m³ the ratio is about 0.8, indicating a slight underestimation of the concentration. However, in this range there are to few observations and thus why the result becomes more uncertain. For lower concentrations than 17 μ g/m³ the ratio is 1.3, resulting in somewhat overestimating of the modelled concentrations. The accuracy here is about ±0.3 μ g/m³. Consequently, the results presented in Figure 17 and Figure 18 show that the agreements between measured and calculated monthly means of NO₂ are generally good.

3.5 Comparison between old and new calculations and measurements.

The old URBAN-model only calculates mean concentration over six months during the wintertime. The monthly mean concentration calculated by the new URBAN-model is thus converted into six month means and then compared with the calculations by the old URBAN model for the same period. The result of that comparison is presented in *Figure 19*.



Figure 19. Comparison between measurements (red squares) of the six month mean of the NO_2 concentration and calculated six month means by the old (dotted line) and the new URBAN-model (black line) at each site.

The comparison between NO_2 calculations by the old and the new URBAN-model shows that the new model calculates NO_2 concentrations with a much better accuracy in all cases but one (Kungälv), according to the measured concentration. The monitoring

point in Kungälv is suspected not to be located in a representative urban background spot. Thus, this might be one reason why the calculated NO_2 concentration in Kungälv is not performing a fit as good as for the others sites.

4. Discussion and conclusions

The problem with dispersion modelling of today is that if all the important processes should be included into the calculation, the model becomes difficult to run (a decent knowledge in meteorology is required to run the models properly) and they often require long computation time. By calculating some of the main parameters for dispersion (H and U) with the advanced model TAPM and using this result in a simple model, some of these problems are solved. Consequently, the high demands of the simple model being able to reproduce a site specific climatology is thus being fulfilled, by the calculation of V (H*U) in the high resolution and in combination with the dispersion-adjusting constant, C_b . This is thus resulting in improved calculations compared to the performance of the URBAN-model. The reason why the urban background concentration is appropriate to use when calculating the C_b , is that the result of all dispersion processes in an area (in combination with the regional background concentration) are representing the "correct" answers, provided that the measurements are located at comparable urban background sites.

Is it relevant to use the population as an estimation of the emissions? The test presented in *Figure 1* shows that the connection is rather apparent for NO₂. The idea is that each person is generating about the same amount of air pollutants from vehicles, heating a.s.o. resulting in a rather good valuation of the emission in a community, as long as the population remains in the community most of the time. One can therefore assume this is a relevant approach at least for air pollutants mainly generated from local sources. One other possible improvement of the emission calculations in the new URBAN-model could be a separate calculation for each town and city, instead of the whole community. As the new URBAN-model calculates in a much higher geographical resolution than the old version, this change would be relevant to perform. It has not yet been tested if the connection is as good between population and other pollutants as it is for NO₂. This requires further investigations.

Another possibility is to use other types of emission inputs such as the new Swedish national emission inventory, which have been updated during the last year. When the resolution of this emission data is better it might be used to improve the calculations further and also for adding other pollutants.

The relevance of using a simple model

This type of rather simple empirical, statistical calculation of the concentrations of air pollutants, the old URBAN-model, has been used for some years by IVL and the

Swedish road administration as a screening method to indicate if the concentration of air pollution is exceeding the threshold values in small communities. However, since the requirements of more accurate estimations are rising even for small towns an improvement of the calculations has been done. This improvement results in:

- a dispersion-related constant, C_b, is calculated from measurements of monthly means of concentration of air pollution at different geographical locations.
- a better description of the meteorological site-specific dispersion processes, described in the new ventilation index, V, including mixing height, wind speed in combination with C_b. All parameters are calculated with better time and geographical resolution than for the old F_v.
- the emissions are, like in the old model, still derived from the amount of the population in the communities (Figure 1), but its accordance has been verified here.
- the background concentration is upgraded, when needed, from the databases at IVL
- the new empirical calculation method implemented into the new URBAN-model, which meet the increasing demands of air pollution modelling, especially in small cities.

The need of a valuation of the air quality in small cities is thus assumed to be fulfilled by using this rather simple but appropriate model rather than using a more advanced model. The reason is that the result does not become better with an advanced model than with a simple, if the input emissions are not performed with good resolution both according to time and geographical resolution. So far the model has been tested in the southwestern part of Sweden with promising result why the next step is to continue similar development for the whole Sweden. However, in accordance to the Swedish standards, the percentiles are to be calculated for some parameters. Thus, in the old URBAN-model the urban background concentration is transferred into different percentiles and also street level concentration. For applying these relations into the new URBAN-model they may have to be recalculated into monthly means.

Since the result from this investigation is very promising the method should be possible to apply for the whole Sweden in the future. This will not necessarily result in more groups of V than the old V's, but instead a more detailed gridded information of V and C_b like a mosaic for the whole of Sweden.

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Appendix 1 Description of the model -TAPM

The TAPM model

Recently, TAPM (The Air Pollution Model) developed by Australian CSIRO Atmospheric Research Division, appeared as an attractive model system since it integrates meteorology and air chemistry (Hurley, 1999b). This model was designed to be run in a nestable way so that the spatial resolution can be as fine as ~ 100 m. In addition, it can be run for one year or longer, which provides a means to deal with statistics of meteorological and pollutant variables.

Essentials of the Model

Air pollution models that can be used to predict pollution concentrations for periods of up to a year, are generally semi-empirical/analytic approaches based on Gaussian plumes or puffs. Typically, these models use either observed data from a surface based meteorological station or a diagnostic wind field model based on available observations. TAPM is different from these approaches in that it solves the fundamental fluid dynamics and scalar transport equations to predict meteorology and pollutant concentration for a range of pollutants important for air pollution applications. It consists of coupled prognostic meteorological and air pollution concentration components, eliminating the need to have site-specific meteorological observations. Instead, the model predicts the flows important to local-scale air pollution transport, such as sea breezes and terrain induced flows, against a background of larger-scale meteorology provided by synoptic analyses. It predicts meteorological and pollution parameters directly (including some photochemistry) on local, city or inter-regional scales.

Meteorology model

The meteorological component of TAPM is an incompressible, non-hydrostatic, primitive equation model with a terrain-following vertical co-ordinate for threedimensional simulations. The model solves the momentum equations for horizontal wind components, the incompressible continuity equation for vertical velocity, and scalar equations for potential virtual temperature and specific humidity of water vapour, cloud water and rainwater. Explicit cloud microphysical processes are included. Turbulence kinetic energy and eddy dissipation rates are calculated for determining the turbulence terms and the vertical fluxes. Further, surface energy budget is considered to computer the surface temperature. A vegetative canopy and soil scheme is used at the surface. Radiative fluxes at the surface and at upper levels are also calculated.

Air pollution model

The air pollution component of TAPM, which uses predicted meteorology and turbulence from the meteorological component, includes three modules. The Eulerian Grid Module (EGM) solves prognostic equations for concentration and for cross-correlation of concentration and virtual potential temperature. The Lagrangian Particle Module (LPM) can be used to represent near-source dispersion more accurately, while the Plume Rise Module is used to account for plume momentum and buoyancy effects for point sources. The model also has gas-phase photochemical reactions based on the Generic Reaction Set, and gas- and aqueous-phase chemical reactions for sulphur dioxide and particles. In addition, wet and dry deposition effects are also included.

Graphical user interface

The model is driven by a graphical user interface, which is used to:

(1) select all model input and configuration options, including access to supplied databases of terrain height, vegetation and soil type (USGS), synoptic-scale meteorology (CSIRO), and sea-surface temperature (NOAA)

(2) run the model

(3) choose and process model output, including options for visualisation, extraction of time-series, production of static 1-D and 2-D plots and summary statistics using common packages such as EXCEL.

Comments on use of TAPM

Model limitations

Although TAPM performs well in many aspects, it has some major limitations as the following:

(1) TAPM should not be used for larger domains than 1000 km by 1000 km, due to curvature of the earth.

(2) The GRS photochemistry option in the model may not be suitable for examining small perturbations in emissions inventories, particularly in VOC emissions, due to the highly lumped approach taken for VOC's in this mechanism. VOC reactivates should also be chosen carefully for each region of application.

Soil moisture setting

The soil moisture is an import parameter in determining the surface energy balance. Based on our experience, a seasonal variable should be used. The following soil moisture (Table 1:1) is recommended for the model running for the Swedish West Coast. This table is based on NCEP reanalysis of 1999 over the area. Further study may be needed to specify it in a better way.

Table 1:1 Deep soil volumetric moisture in content $m^3 m^{-3}$ (i.e. the volume of water per volume of soil) used in model run

Mon	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Value	0.29	0.30	0.28	0.24	0.21	0.19	0.18	0.19	0.21	0.23	0.26	0.28

Model outputs

The output of TAPM is rich, covering both 2D and 3D fields. The 2D fields are:

• total solar radiation, net radiation, sensible heat flux, evaporative heat flux, friction velocity, potential virtual temperature, potential temperature, convective velocity, mixing height, screen-level temperature, screen-level relative humidity, surface temperature and rainfall,

The 3D fields are:

• horizontal wind speed, horizontal wind direction, vertical velocity, temperature, relative humidity, and potential temperature and turbulence kinetic energy.

A very important feature of TAPM is its ability to explicitly deal with surface energy budget and temperature, which allows simulation of thermally driven wind systems. As examples, Figures 1:1-1:2 give snapshots of modelled surface temperature wind during one day and one night. The figures show distinct diurnal variations both in temperature and wind patterns.

The figure 1:1 show that during the daytime, solar radiation heats the ground faster than the sea, which results in higher air temperature over land compared to the sea. Therefore, air with lower density ascends over land and air with higher density descends over sea. Near the surface, air flow (figure 1:2) from the sea to the land, leading to development of sea breeze. During clear nights, the cooling of land is faster than the sea, hence air blow from land to sea over the surface, leading to formation of land breeze.

Figure 1:3 is a snap shot of the vertical wind during day and night. The return flow of the sea breeze can be seen at the model level 9 (750 m).







Figure 1:2. The modelled surface wind during night and day on 12 June 1999 a) at 03:00 local time; b) at 15:00 local time (figure from Deliang et al 2002).



Figure 1:3. The modelled cross section (X-Z or u-10w) of wind during night and day on 12 June 1999 a) at 03:00 local time; b) at 15:00 local time. Unit of u and w m/s (figure from Deliang et al 2002).

Appendix 2 Validation of the model system

In this part there is a short description of the validation of the TAPM model only presenting data from 1999. The full description (of all stations and both years) is described in Chen et al (2002).

TAPM has previously been used and verified for regions in Australia and other parts of the world (e.g. Hurley, 1999a). CSIRO has applied the model to meteorological (and some air pollution) verification studies for Kwinana and the Pilbara (WA), Cape Grim and Launceston (TAS) (Hurley, 1999a), Melbourne (VIC), Newcastle and Sydney (NSW), and Mt Isa (QLD), as well as for Kuala Lumpur (Malaysia). However, to our knowledge, the use of TAPM in Europe has not been documented before. For its wide application in environmental impact assessments in Europe and in Sweden, it is necessary to perform a model validation using the observational data. In this report, a comparison will be made between the model results and the measurement to quantify TAPM's ability and performance for Sweden.

Validation

Model set-up and methodology

Since meteorological factors play an important role in air pollution modeling, it is necessary to verify the model's performance on meteorology modeling first. For this purpose, TAPM was run with three nestings that have spatial resolution of 9 km, 3 km and 1 km. There were 90*90 grid points in horizontal dimensions (see Figure 2:1) and 20 levels in vertical (10, 50, 100, 150, 200, 300, 400, 500, 750, 1000, 1250, 1500, 2000, 2500, 3000, 4000, 5000, 6000, 7000, and 8000 meters). The model was integrated for consecutive five-day intervals covering the years 1999 and 2000. This approach is chosen because 1) the output for five days can be saved in one CD, which makes the output data manageable; 2) the five day simulation takes about two days for a normal PC to run, which is a reasonable time interval. A disadvantage with this approach is that the simulation is interrupted every five days, which implies that the small-scale variations may not be well developed in the beginning of every five-day simulation. Therefore, the model performance could well be better if the simulated data in the beginning (say the first day) would have been ignored.

The modeled air temperature at 2 m and wind at 10 m were selected as the two important fields for model validation. These levels are named modeled surface temperature and modeled surface wind respectively. The conventional statistical measures were adopted to determine the difference and correlation between the modeled

results and the measurements. All comparisons were made for 1999 and 2000 respectively, in order to determine eventual differences from year to year.



Figure 2:1. Model domains of the three nestings. The three surfaces stations (circles) and two Sodar stations (squares) used in the comparisons are shown in the last nesting.

Observational Data

The observational data used for model validation are from NCDC/NOAA in the TD9956-Datsav III variable length ASCII format. The TD9956 data contain all hourly records as well as any observations taken in-between hours.

The stations used in the validation are GOTEBORG (Göteborg), LANDVETTER and SAVE (Säve), as indicated by bold letters. The time period of the data is from 1 January 1999 to 31 December 2000. The three stations provide meteorological data from various levels above the ground (Göteborg ≈ 50 m, Landvetter ≈ 10 m and Säve ≈ 10 m) characterising the urban and suburban surface in the area. These levels are all named observed surface temperature and observed surface wind respectively.

In addition, upper level wind data from two sound radar stations (Hunneberg, Borås, see figure 2:1) were selected for profiles comparisons. Compared with the surface data, the Sodar data is rather incomplete. The details about the measurements can be found in Deliang et al. (2002). The instruments provide wind profiles from 50 m height up to maximum 475 m height. Generally, data is collected up to a level of approximately 175 m, but very seldom above 400 m. The horizontal wind range is 35 m/s, the vertical wind range is ± 10 m/s. The wind accuracy is 0.2 m/s or better for the horizontal and 0.05 m/s for the vertical wind.

To make the direct comparison possible, sodar measurements at different levels are interpolated to the model levels. Missing values appear in both the surface and upper air measurement occasionally. Simulated values are omitted if the corresponding observations are missing. Thus, the numbers of data available for different comparisons vary always and need to be indicated in the statistics.

Some of the results

Surface comparison

The scatter plots of the observed and modelled hourly near ground air temperature, horizontal wind (u, v component) at the Göteborg station are displayed in Figures 2:2-2:4 for 1999. Plotts from the other stations and for 2000 are found in Deliang (2002). The related statistics can be found in Table 2:1.





Figure 2:2. Scatter plot of the observed and modelled hourly surface air temperature at Göteborg station for 1999.

Figure 2:3. Scatter plot of the observed and modelled hourly surface wind (u component) at the Göteborg station for 1999.



Figure 4. Scatter plot of the observed and modelled hourly surface wind (v component) at the Göteborg station for 1999.

The statistics listed in the Tables 2:1, shows that TAPM has been successfully in modelling the near surface temperature and horizontal wind, although the skills for temperature and wind are varying.

For surface temperature, high correlation (greater than 0.92) and small square error (0.03 to 0.05°C) were found between the model results and the measurements. In general, the model systematically underestimated surface temperature by about 1°C. The surface wind (Table 2:1) was also well simulated, but the correlation coefficients were somewhat lower compared to those of temperature. The modelled horizontal wind was thus overestimated at urban site (Göteborg) and underestimated at non-urban sites (Landvetter as well as Säve) in 1999. There were considerable changes in the statistics between 1999 and 2000, indicating that year-to-year changes are important for this region. However, here only 1999 comparison are presented. The full comparison is

presented in Chen et al. (2002).

*	Correlation	Modeled	Observed	Bias	RMSE
	coefficient	average	average		
(a)Göteborg (2085*)					
Surface air temperature (°C)	0.94	9.8	10.4	-0.6	0.2
Surface wind u component (m/s)	0.71	0.4	0.3	0.1	0.2
Surface wind v component (m/s)	0.60	0.7	0.7	0.0	0.2
Surface wind speed (m/s)	0.38	2.8	2.5	0.3	0.2
(b) Landvetter (8711*)					
Surface air temperature (°C)	0.93	6.9	7.6	-0.7	0.2
Surface wind, u component (m/s)	0.82	0.7	0.4	0.3	0.2
Surface wind, v component (m/s)	0.75	1.0	1.6	-0.6	0.2
Surface wind speed (m/s)	0.67	3.9	4.4	-0.5	0.2
(c) Säve (8765*)					
Surface air temperature (°C)	0.94	7.9	8.2	-0.3	0.2
Surface wind, u component (m/s)	0.78	0.8	0.6	0.2	0.2
Surface wind, v component (m/s)	0.75	1.1	1.4	-0.3	0.2
Surface wind speed (m/s)	0.65	3.9	4.1	-0.2	0.2

Table 2:1. Comparison between the modeled and observed variables for 1999

* sample number for statistics

The diurnal variations, seasonal variations and daily averages of the observed and simulated surface air temperature are presented in Figures 2:5 for 1999. The slight underestimate of the surface temperature in Göteborg appears to be systematic with respect to time, as shown by Figures 2:5. However, the seasonal variations indicate that the underestimates mainly occur during cold months. This may be partly due to the neglect of the anthropogenic heating in the city.

The diurnal variations, seasonal variations and daily averages of the observed and simulated surface wind direction (Figure 2:6) and speed (Figure 2:7) are displayed for 1999. In general, the simulations for wind direction follow the evolution of the observations well, although there are fairly systematic differences. For wind speed, the differences between 1999 and 2000 were fairly large especially for Göteborg (Chen et al. 2002).

The model has a strong ability to simulate urban heat island effect, which can be seen in Figure 2:8. The figure shows that the temperature difference between the urban (Göteborg) and the suburban (Landvetter and Säve) stations can reach 1.4-3.4 \Box C (Göteborg-Landvetter) and 1.5-3.8 \Box C) (Göteborg-Säve) on the hourly basis for modeled results and for measurements. The simulations follow the observations well, though the difference varies with year.

A very important feature of TAPM is its ability to explicitly deal with surface energy budget and temperature, which allows simulation of thermally driven wind systems. An examination of the modeled results reveals that the model performs well in modeling meso-scale wind system, such as land-sea breeze circulation.





Profile comparison

The statistics of observed and modelled wind profiles at selected levels at Hunneberg and Borås are listed in Table 2:2 and Table 2:3, respectively.

From the results following features are obvious:

1) The evolution of the simulated upper winds follows those of the observed fairly well, as reflected in the correlation coefficients that are comparable to those in the surface comparison.

2) The agreements at the two sites are comparable.

3) The Sodar measurements at the two sites have a persistent bias, pointing to a systematic error in the measurements or in simulations.

4) Difference between results in 1999 and 2000 are considerable, with results in 1999 being better than those in 2000 are. One possible reason could be poorer quality of synoptic data in 2000.

Component	Height	Correlation	Modeled	Observed	Bias	RMSE
-	C C	coefficient	average	average		
wind-u	50m (7672*)	0.78				0.2
wind-v		0.66				0.2
wind speed		0.54	6.0	3.5	2.5	0.2
wind-u	100m	0.81				0.2
	(7674*)					
wind-v		0.70				0.2
wind speed		0.60	7.0	5.5	1.5	0.3
wind-u	150m	0.82				0.2
	(7658*)					
wind-v		0.70				0.2
wind speed		0.62	7.8	6.6	1.2	0.3
wind-u	200m	0.81				0.2
	(7015*)					
wind-v		0.70				0.2
wind speed		0.57	8.5	7.2	1.3	0.3
wind-u	300m	0.76				0.3
	(3908*)					
wind-v		0.69				0.3
wind speed		0.50	9.5	7.8	1.7	0.4

Table 2:2. Comparison between the modeled and observed wind profiles at Hunneberg in 1999. Unit of wind speed: m/s.

wind-u	400m	0.73				0.4
	(1253*)					
wind-v		0.68				0.4
wind speed		0.51	10.5	8.2	2.3	0.5

* sample number for statistics

Table 2:3. Comparison between the modeled and observed wind profiles at Borås in 1999. Unit of wind speed: m/s.

Component	Height	Correlation	Modeled	Observed	Bias	RMSE
-		coefficient	average	average		
Wind-u	50m (7297*)	0.80				0.2
Wind-v		0.71				0.2
Wind speed		0.60	5.3	3.8	1.5	0.2
Wind-u	100m (7851)	0.83				0.2
Wind-v		0.72				0.2
Wind speed		0.64	6.6	5.0	1.6	0.2
wind-u	150m (7364*)	0.77				0.2
wind-v		0.71				0.2
wind speed		0.49	7.5	5.5	2.0	0.3
wind-u	200m (5013*)	0.77				0.3
wind-v		0.71				0.2
wind speed		0.51	8.0	6.1	1.9	0.3
wind-u	300m (1544*)	0.81				0.4
wind-v		0.67				0.4
wind speed		0.45	9.8	8.0	1.8	0.4
wind-u	400m (298*)	0.87				0.5
wind-v		0.70				0.5
wind speed		0.56	11.7	9.6	2.1	0.6

* sample number for statistics

Appendix 3 Calculation of mixing height using Holzworth algorithm

A brief description of the theoretical background and calculation procedure of calculation of mixing height (H) at Landvetter uses Holzworth algorithm (1967).

The algorithm

The algorithm is used to calculate a twice-daily H based on synoptic observations as well as data from a radio sonde sounding. To compute the morning mixing height, the minimum temperature from 0200 to 0600 (LST) is determined. To this value 5°C is added. Holzworth developed his algorithm for an urban environment in order to estimate urban air pollution. He established this adjustment to account for temperature differences between rural and urban environments and for some initial surface heating just after sunrise. To estimate the morning H, the adjusted minimum surface temperature follows the dry adiabatic lapse rate up to the intersection with the observed 1200 (GMT) temperature radio sounding.

A similar computation is made using the maximum temperature from 1200 to 1600 (LST) and the 1200 (GMT) radio sounding, except that the surface temperature is not adjusted. The assumption made by Holzworth was that afternoon H in urban and nearby rural areas does not differ significantly, whereas the nocturnal H is often very different.

Calculation procedure

Before calculating the H the temperature at 925 hPa level are converted in to potential temperature $\theta = T[P_0/P]^{0.286}$ where P_0 =air pressure at the surface level and P=air pressure at 925 hPa level.

The surface potential temperature should be computed from the minimum temperature (in the morning) and the pressure at the first level in the 1200 (GMT) radio sounding (Why use pressure data several hours later?). Unless the data are missing, the first level in a sounding is representative of the surface (check the height of the field station to verify the true first level of sounding, at Landvetter 155 m.a.s.l and after moving the position 164 m.a.s.l). In this calculation the surface potential temperature is equal to the surface absolute temperature. Since potential temperature generally increases with height in the atmosphere, the linearly interpolation that is assumed in the calculation is acceptable.

H is calculated by plotting two linear gradients (one based on surface temperature and the dry adiabatic lapse rate and one based on radio sound measurements at 1200 (GMT). The gradients are described using the equation $y_1=k_1x+m_1$ and $y_2=k_2x+m_2$ where

y₁=temperature gradient based on radio sound observations

y₂=temperature gradient based on surface observations and the dry adiabatic lapse rate

m₁=radiosound measured surface temperature (for Landvetter: at 155 m or 164 m level)

 m_2 =surface minimum temperature (+5°C) during 0100-0500 (UTC, this is equal to 0200-0600 LST) respectively surface maximum temperature during 1100-1500 (UTC).

 k_1 =radiosound mesured temperature gradient (using temperature at 155 m.a.s.l (or 164 m.a.s.l.) and temperature at 925 hPa level)

k₂=dry adiabatic lapse rate (=0,0098 K/m)

The height x where the two linear equation cross each other is expressed:

 $k_1x+m_1=k_2x+m_2$

 $(k_1 - k_2)x = m_1 - m_2$

 $x=m_1-m_2/k_1-k_2$

x=mixing height (m)

From this easy way of calculating the H, sensible values are only achieved if a.) The radiosond gradient is smaller than the dry adiabatic lapse rate and the radiosond surface temperature is higher than the observed surface temperature during the morning, or b.) The radiosond gradient is larger than the dry adiabatic lapse rate and the radiosond surface temperature is lower than the observed surface temperature during the morning. If these conditions do not occur there will be no crossing of the gradients or the crossing will occur at a level less than the surface height above sea level. These situations are labelled XXX in the file MIXING.TXT (which show date and the calculated H (m)) and occur most frequently during the winter months. In the file TEMPGRAD.TXT data from the radiosoundings with date, time (UTC), temperature at ground level, height above ground at 925 hPa (m), and calculated temperature gradient (K/m) are shown. The file TMINMAX.TXT includes observations from the surface field station with date, minimum temperature at 2m during 0100-0500 (UTC), and maximum temperature at 2m during 1100-1500 (UTC).

Detailed information of the field stations, instruments and data

Detailed information of the field stations, instruments and data used for calculation of the mixing height (MH) in the Swedish west coast area during 1999 - 2000, are presented in this chapter.

Location

- Radiosond data from Landvetter (lat. 57.67N lon. 12.30E height 155 m.a.s.l.)
- Synoptic meteorological station Säve (lat. 57.47 N lon. 11.53E height 53 m.a.s.l.)
- Synoptic meteorological station Göteborg (lat. 57.42 N lon. 12.00E height 5 m.a.s.l.)
- Synoptic meteorological station Landvetter (lat. 57.40 N lon. 12.18E height 169

m.a.s.l.)

Sampling

Radiosond data are measured continuously at hour: 0, 6, 12, 18 during Jan 1999 – Jun 2000; at hour: 0, 12 during Jul - 17 Sep 2000; and at approximate hour: 11, 23 (really the hour the radiosonde is launched) during 18 Sep – Dec 2000.

The radiosonde takes measurements at intervals of approximately 2 seconds. The high-resolution data files contain all such data. Though, Landvetter measures standard resolution and the data files contain measurements taken at particular levels of the atmosphere. Measurements are reported to the Met. Office at standard and significant pressures levels. The standard pressure levels are 1000, 925, 850, 700, 500, 400, 300, 250, 200, 150, 100, 70, 50, 30, 20 and 10 mb.

The radiosonde parameters are pressure (hPa), height above sea level (m), dry-bulb temperature (° K), dew-point temperature (° K), wind direction (°), wind speed (m/s).

The synoptic meteorological station Göteborg (WMO number 025130) is run by SMHI and measures data every third hour. Station Landvetter (WMO number 025260, ESGG) run by the Landvetter airport and station Säve (WMO number 025120, ESGP) run by the Swedish Military Weather Service measures continuously every hour.

Instrumentation

The radiosonde at Landvetter (WMOnumber 02527) uses a radiosonde called VRS80N, ground equipment called DIGICORA, and the windfinding method: OMEGA/LORAN.

The RS80 radiosonde, manufactured by the Finnish Company Vaisala, has been routinely used in many countries. Powered by a water-activated battery, the instrument takes measurements at approximately 1.3 second intervals during the ascent. Pressure, temperature (and humidity) are measured using three capacitative sensors. A schematic diagram of the layout of the RS80 is shown in the figure below.

General technical specifications of Vaisala RS80 are:

PTU sensors are individually factories calibrated.

Pressure:	BAROCAP® Capacitive aneroid
Measuring range:	1060 hPa to 3hPa (mb)
Resolution:	0.1 hPa
Accuracy:	Reproducibility (1): 0.5 hPa
	Repeatability of calibration (2): 0.5 hPa
Temperature:	THERMOCAP® Capacitive bead
Measuring range:	+60 °C to - 90 °C

Resolution:	0.1 °C		
Accuracy:	Reproducibility (1): 0.2 °C up to 50 hPa, 0.3 °C for 50-15 hPa,		
	0.4°C above 15 hPa level		
	Repeatability of calibration (2): 0.2 °C		
Lag:	< 2.5 s (6 m/s flow at 1000 hPa)		
Humidity:	HUMICAP® Thin film capacitor		
Measuring range:	0 to 100 % RH		
Resolution:	1 % RH		
Lag:	1 s (6 m/s flow at 1000 hPa, +20 °C)		
Accuracy:	Reproducibility (1): <3 %RH		
	Repeatability of calibration (2): 2 %RH		

Wind speed and direction are not directly measured by the radiosonde. These parameters are calculated from the position of the sonde at successive time intervals.

The LORAN-C Radio Navigation System:

This system uses a network of *LO*ng *RA*nge *N*avigation beacons, which transmit radio signals at known frequencies. In addition to the sensors of the RS80 already described, the RS80L radiosonde carries a radio receiver to detect the LORAN signals.

The receiver measures the difference in time taken for the signals from two beacons of known position to reach the sonde. Such points of equal time difference form the loci of a set of rectangular hyperbolae. Signals are received from three pairs of beacons. The difference in the time of signal reception from each pair identifies a hyperbola. The radiosonde is thus located at the intersection of these hyperbolae, a known distance from the fixed LORAN beacons. The wind speed and direction can then be calculated from the difference between successive positions of the sonde. The ground station equipment performs these calculations.

The LORAN-C method calculates the position of the radisonde with an accuracy of approximately +/-300m. Wind speeds are calculated with an accuracy of +/-1 to 2m/s.

The instrumentation on the three synoptic meteorological stations is standard equipments.

The station at Säve measures at the level of 2 m above the ground, wind speed and direction using Vaisala cup anemometer WAA 15 (accuracy: +/- 0.1 m/s, threshold value: 0.4 m/s) and wind vaneWAV 15 (accuracy: +/- 2.8 °, threshold value: 0.3 m/s, resolution: 5.6 °), temperature using a thermistor (accuracy +/- 0.2 °C) and cloud cover using visual observations.

The station at Landvetter measures temperature at the level of 1.5 m and wind at the level of 10 m above the ground. Similar equipment (including measuring accuracy and units)

as at Säve are used here.

The station at Göteborg measures at the level of a 10 m height mast positioned on the roof of an approximately 40 m high building. On the mast the temperature sensor is positioned at the 1.5 m level and wind anemometer and wind vane at the 10 m level. Similar equipment (including measuring accuracy and units) as at Säve are used here.

Miscellaneous

Further information on radiosond instrumentation may be find at <u>http://www.badc.rl.ac.uk/data/radiosonde/radhelp.html#wind</u>