# Supplementary Materials

## Development of the city-scale chemistry transport model CityChem – EPISODE and its application to the city of Hamburg

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## S1. Standard method for calculation of the vertical eddy diffusivity

The standard method for calculation of the vertical eddy diffusivity is based upon the description in Byun et al. (1999). The non-dimensional profile functions of the vertical gradient of potential temperature, $\Theta$, are expressed as:

$$\phi_H = \mathrm{Pr}_0\left(1 + \beta_H \frac{z}{L}\right) \qquad \text{for moderately stable } \left(1 \geq \frac{z}{L} > 0\right) \qquad \text{(S.1a)}$$

$$\phi_H = \left(1 - \gamma_H \frac{z}{L}\right) \qquad \text{for unstable and neutral } \left(\frac{z}{L} \leq 0\right) \qquad \text{(S.1b)}$$

Where Pr0 is the Prandtl number for neutral stability and $\beta_H$ and $\gamma_H$ are coefficients of the profile functions determined through field experiments. For very stable conditions ($z/L$ > 1) the expression suggested by Holtslag et al. (1990) is used to extend the applicability of the surface similarity:

$$\phi_H = \mathrm{Pr}_0\left(\beta_H + \frac{z}{L}\right) \qquad \text{(S.1c)}$$

Within the planetary boundary layer (PBL), vertical eddy diffusivity is parameterized with:

$$K_*^{(z)} = \frac{\kappa u_* z(1 - z/h_{mix})^{3/2}}{\phi_H(z/L)} \qquad \text{for } \frac{z}{L} > 0 \ \text{(stable)} \qquad \text{(S.2a)}$$

$$K_*^{(z)} = \kappa w_* z(1 - z/h_{mix}) \qquad \text{for } \frac{z}{L} \leq 0 \ \text{(unstable and neutral)} \qquad \text{(S.2b)}$$

Where $w*$ is the convective velocity, $h_{mix}$ is the height of the PBL (mixing height) above the urban area. For each vertical model layer, the eddy diffusivity is calculated iteratively within 5 sub-layers. The vertical eddy diffusivity of the respective layer is obtained as vertical average of the sub-layer diffusivities.

## S2. Sub-grid model for point sources (SEGPLU)

The Gaussian segmented plume model SEGPLU (Walker and Grønskei, 1992) computes and keeps record of the subsequent positions of the plume segments and the pollutant concentration within each of the plume segments released from a point source. SEGPLU treats the emission from individual point sources as a temporal sequence of instantaneous releases of a specified pollutant mass. The finite length plume segments are emitted at discrete time intervals $\Delta T$ given by $\Delta T$ = 3600(s) /2N, where N is an integer value. $N$ depends on the meteorological conditions and becomes larger as the wind speed increases. The segments are redirected at every grid point and every simulation hour according to changes of the wind flow field. The subsequent position of plume segments and pollutant concentration within each of the plume segments is then calculated.

The initial horizontal position of the plume segment corresponds to the (x, y)-coordinates of the point source and the initial vertical position is estimated from plume rise formulas, where the plume rise is determined by stack height, stack exit velocity of the emitted pollutant and buoyancy of the effluent. The length of the plume segment is prescribed as $L_{seg} = u \cdot \Delta t$ and the direction of the plume is set equal to the wind direction at the point source. The mass of a pollutant $M_{seg,i}$ in the plume segment depends on the point source emission rate $Q_{p,i}$, as $M_{seg,i} = Q_{p,i} \cdot \Delta t$. While the plume segments are transported by horizontal advection, the new position of the plume segment ($Xseg$, $Yseg$) as function of the travel time $t$ (time since release) is calculated as:

$$X_{seg}(t + \Delta t) = X_{seg}(t) + \mathrm{u}\Delta t \qquad \text{and}$$
$$Y_{seg}(t + \Delta t) = Y_{seg}(t) + \mathrm{v}\Delta t \tag{S.3}$$

The cross-wind dispersion of each plume segment is calculated according to (Irwin, 1983):

$$\sigma_y(t) = \sigma_v \cdot t \cdot \left(1/\left(1 + 0.9\sqrt{t/1000}\right)\right) \tag{S.4}$$

The vertical dispersion of the plume segments is calculated according to the expression by Venkatram et al. (1984):

$$\sigma_z(t) = \sigma_w \cdot t \cdot \sqrt{1 + \frac{t}{2T_L}} \tag{S.5}$$

The standard deviation of the horizontal wind fluctuations, $\sigma_v$, and the vertical wind fluctuations, $\sigma_w$, are calculated using the profile method (as described in Slørdal et al. (2003); section 2.1). The Lagrangian timescale $T_L$ is defined as:

$$T_L = \frac{\lambda}{\sigma_w} \tag{S.6}$$

The dispersion length $\lambda$ is specified as $\lambda^{-1} = \lambda_s^{-1} + \lambda_n^{-1}$ with:

$$\lambda_s = \frac{\gamma^2 \sigma_w}{N} \quad \text{and} \quad \lambda_n = \alpha \cdot z \tag{S.7}$$

Where $\gamma$ and $\alpha$ are empirical coefficients with values of 0.52 and 0.36, respectively, and $N$ is the Brunt-Vaisala frequency, defined as:

$$N = \sqrt{\frac{\mathrm{g}}{T} \frac{d\theta}{dz}} \tag{S.8}$$

Where g is the gravitational constant (9.80665 m $s^{-2}$) and $d\theta/dz$ is the gradient of the potential temperature. For neutral or unstable conditions, ($d\theta/dz$ is zero or negative) the Brunt-Vaisala frequency is set equal to zero, and $T_L$ is calculated using $\lambda = \lambda n$. A consequence of Eq. (S.4) and (S.5) is, that the dispersion parameters for the plume segment dispersion are proportional to $t$ for short travel time and proportional to $\sqrt{t}$ for long travel time.

The ground level concentration contribution $C_{point,p}$ from the plume segment released from a specific point source $p$ to a certain receptor point is calculated using the Gaussian plume dispersion equation:

$$C_{point,p} = \frac{Q_p \cdot e^{-\lambda_w T_{add}}}{2\pi \cdot \mathrm{u} \cdot \sigma_y \cdot \sigma_z} \cdot \exp\left[-\frac{y_r^2}{2\sigma_y^2}\right] \cdot \left\{\exp\left[-\frac{\left(z_r - H_{eff}\right)^2}{2\sigma_z^2}\right] + \alpha_p \cdot \exp\left[-\frac{\left(z_r + H_{eff}\right)^2}{2\sigma_z^2}\right]\right\} \tag{S.9}$$

where

$x_r$, $y_r$, $z_r$ : rececptor point location (x-axis is parallel with the wind direction),

$Q_p$ : emission rate (g $s^{-1}$) for the point source, corresponding to the plume segment,

$H_{eff}$ : effective emission height (m),

$\alpha_p$ : partial reflection coefficient due to dry deposition,

$\lambda_w$ : wet scavenging coefficient ($s^{-1}$),

$T_{add}$ : advection time from start of the plume segment to the receptor point (s).

Dry deposition from plume segments is calculated using the partial reflection approach (Hanna et al., 1982). Wet deposition is calculated using predefined scavenging rates and the (grid-cell average) precipitation rate. When the plume segment reaches a predefined horizontal or vertical extent or when the segmented plume experiences a large change in wind direction (larger than the redirection limit), it is inserted into the (Eulerian) main grid cell containing its centre of mass. The size of the critical extent is optimally set as $\sigma_y/\Delta y = 4$ or $\sigma_z/\Delta z = 4$, where $\sigma_y$ and $\sigma_z$ are the horizontal and vertical length scales of the plume segment, and $\Delta y$ and $\Delta z$ are the grid spacing in the horizontal and vertical direction, respectively. Once the plume segment is transported outside of the model domain, its mass is lost. The model user can define (1) the maximum horizontal size (as grid cell fraction, default: 0.25) of the plume segments in each vertical model layer, (2) the redirection limit angle (default: 30°), and (3) the minimum wind speed (default: 0.4 m $s^{-1}$) in SEGPLU.

## S3. Sub-grid model for line sources (HIWAY-2)

The HIWAY-2 model (Petersen, 1980) is applicable for any wind direction, street orientation, and receptor location at distances tens to hundreds of meters downwind of the line source, given that the terrain is relatively uncomplicated. HIWAY-2 computes the concentration of a pollutant by numerically integrating the Gaussian plume point source equation over a finite length of the road. Each street lane (or lane segment) with vehicle traffic is simulated as a straight, continuous, finite length, line source with a uniform emission rate. The emission intensity on each of the lanes is assumed to be uniform along the line source. Pollutant concentrations caused by vehicle traffic are found by interpretation of the line source as a finite sum of simple Gaussian point-source plumes, and the total line source contribution is then derived by numerical integration (i.e. summation) over the length of the line source, thinking of the line source as a line-of-points.

The concentration contribution $C_{line}$ at the receptor point $r^*$ from traffic emissions is found by integrating the concentration contributions from each of the infinitesimal point sources along the line source $s$, according to:

$$C_{line,s} = \left(\frac{Q_s}{\mathrm{u}}\right) \cdot \int_0^L \mathrm{f} ds \tag{S.10}$$

where $Q_s$ (in g $\mathrm{m}^{-1}$ $\mathrm{s}^{-1}$) is the emission intensity from the line source, $L$ is the source length (in m), $ds$ is an infinitesimal line segment (in m), and $\mathrm{f}$ is the point source dispersion function (in $\mathrm{m}^{-2}$). Each of the point sources is placed in the middle of the lane, $m_l$, with distance of a half lane width, $w_l/2$, from the middle of the street.

The integral in Eq. (S.10) is approximated by use of Richardson extrapolation of the trapezoidal rule. Estimates are made dividing the line source into a number of intervals equal to 3, 6, …, $3 \cdot (2)^9$.

Calculations are successively repeated for each partition class until the concentration estimates converge to within 2 percent of the previous estimate (Petersen, 1980).

The sub-grid model for line sources distinguishes between four classes of atmospheric stability by evaluating the temperature difference between a lower height ($z_1$) and an upper height ($z_2$) in the two lowest model layers, $\Delta T = (z_2 - z_1) \cdot dT/dz$. Table S.1 shows how the stability classes are related to the Pasquill-Gifford (P-G) classes.

For stable conditions or when the diffusion in the vertical is unlimited, the ordinary point source Gaussian dispersion function is used in Eq. (S.10), given by:

$$\mathrm{f} = \frac{1}{2\pi \cdot \sigma_y \cdot \sigma_z} \cdot \exp\left[-\frac{y_r^2}{2\sigma_y^2}\right] \cdot \left\{\exp\left[-\frac{(z_r - H_{tr})^2}{2\sigma_z^2}\right] + \exp\left[-\frac{(z_r + H_{tr})^2}{2\sigma_z^2}\right]\right\} \tag{S.11}$$

where $H_{tr}$ is effective emission height (m) from traffic, assumed to be zero, $z_r$ is the receptor height above ground (m), set to 2 m. The calculation of the crosswind and vertical dispersion parameters $\sigma_y$ and $\sigma_z$ is described below.

For unstable or neutral conditions, given that $\sigma_z$ is larger than 1.6 times the mixing layer height $h_{mix}$, the concentration distribution below the mixing layer is considered to be uniform with height, regardless of either source or receptor height:

$$\mathrm{f} = \frac{1}{\sqrt{2\pi} \cdot \sigma_y \cdot h_{mix}} \cdot \exp\left[-\frac{y^2}{2\sigma_y^2}\right] \tag{S.12}$$

For all other unstable or neutral conditions, multiple reflections at the ground are taken into account, and the following Gaussian dispersion function is used:

$$\begin{aligned} \mathrm{f} = {} & \frac{1}{2\pi\cdot\sigma_y\cdot\sigma_z}\cdot\exp\left[-\frac{y_r^2}{2\sigma_y^2}\right]\cdot\left\{\exp\left[-\frac{(z_r-H_{tr})^2}{2\sigma_z^2}\right]+\exp\left[-\frac{(z_r+H_{tr})^2}{2\sigma_z^2}\right]\right. \\ & +\sum_{n=1}^{\infty}\left(\exp\left[-\frac{1}{2}\left(\frac{z-H_{tr}-2n\cdot h_{mix}}{\sigma_z}\right)^2\right]+\exp\left[-\frac{1}{2}\left(\frac{z+H_{tr}-2n\cdot h_{mix}}{\sigma_z}\right)^2\right]\right. \\ & \left.\left.+\exp\left[-\frac{1}{2}\left(\frac{z-H_{tr}+2n\cdot h_{mix}}{\sigma_z}\right)^2\right]+\exp\left[-\frac{1}{2}\left(\frac{z+H_{tr}+2n\cdot h_{mix}}{\sigma_z}\right)^2\right]\right)\right\} \end{aligned} \qquad \text{(S.13)}$$

The infinite sum series in Eq. (S.13) converges rapidly, more than five summations ($n$ = 5) of the four sum terms are seldom required (Petersen, 1980). In Equations (S.11) to (S.13) the dispersion parameters are evaluated for the given atmospheric stability class and downwind distance $x$.

In the sub-grid line source model component, the dispersion parameters are generally defined as:

$$\sigma_y = \sqrt{\sigma_{ya}^2 + \sigma_{y0}^2} \qquad \text{(S.14a)}$$

$$\sigma_z = \sqrt{\sigma_{za}^2 + \sigma_{z0}^2} \qquad \text{(S.14b)}$$

where $\sigma_{ya}$ is the crosswind dispersion and $\sigma_{za}$ is the vertical dispersion, respectively, resulting from ambient turbulence, $\sigma_{y0}$ is the initial crosswind dispersion and $\sigma_{z0}$ is the initial vertical dispersion.

The initial spread of the plume from traffic due to vehicle induced turbulence depends on the wind speed (Slørdal et al., 2003):

$$\begin{cases} \sigma_{y0} = 3 & ;\ \mathrm{u} > 3.0\ ms^{-1} \\ \sigma_{y0} = 10 & ;\ \mathrm{u} < 1.0\ ms^{-1} \\ \sigma_{y0} = 10 - \left(7\cdot\frac{u-1.0}{2.0}\right) & ;\ 1.0\ ms^{-1} \leq \mathrm{u} \leq 3.0\ ms^{-1} \end{cases} \qquad \text{(S.15a)}$$

$$\begin{cases} \sigma_{z0} = 1.5 & ;\ \mathrm{u} > 3.0\ ms^{-1} \\ \sigma_{z0} = 5 & ;\ \mathrm{u} < 1.0\ ms^{-1} \\ \sigma_{z0} = 5 - \left(3.5 \cdot \frac{u-1.0}{2.0}\right) & ;\ 1.0\ ms^{-1} \leq \mathrm{u} \leq 3.0\ ms^{-1} \end{cases} \tag{S.15b}$$

The crosswind dispersion due to ambient turbulence is given by (Petersen, 1980):

$$\sigma_{ya} = 1000 \cdot x \cdot \frac{\sin \theta_p}{2.15 \cdot \cos \theta_p} \tag{S.16}$$

where $x$ is the downwind distance (in km) and $\theta_p$ is the half angle of the crosswind plume spreading, given by:

$$\theta_p = \mathrm{c} - \mathrm{d} \cdot \ln\left(\frac{x}{x_0}\right) \tag{S.17}$$

In Eq. (S.17), c and d are constants depending on stability and $x_0$ is the normalizing distance (here 1 km is used). The vertical dispersion due to ambient turbulence is given by (Petersen, 1980):

$$\sigma_{za} = \mathrm{a} \cdot x^{\mathrm{b}} \tag{S.18}$$

The empirical constants a and b depend on the stability. Values of a, b, c, and d are tabulated in Table S.1. Sufficiently far downwind the atmospheric dispersion process dominates. At 300 m downwind the above described dispersion curves are merged into the P-G dispersion curves.

At present deposition (dry or wet) is not explicitly included as a sink term in the line source model component.

## S4. Simplified street canyon model

A Gaussian plume model is used for the calculation of the direct contribution to the concentration at the receptor point located at distance $x$ from the line source, i.e. from the mid-line of the street, by integrating along the wind path at street level; the integration path depending on wind direction, extension of the recirculation zone and the street canyon length (Hertel and Berkowicz, 1989):

$$\int_{x_{start}}^{x_{end}} \frac{dC_{scdir,s}}{dx} dx = \sqrt{\frac{2}{\pi}} \cdot \frac{Q_s}{W_{sc}\sigma_w} \cdot \int_{x_{start}}^{x_{end}} \frac{1}{x+\frac{\mathrm{u}_{street} \cdot h_0}{\sigma_w}} dx \qquad (S.19)$$

Where $h_0$ is a constant that accounts for the height of the initial pollutant dispersion ($h_0$ = 2 m is used here, i.e. equal to the height of the receptor), $\sigma_w$ is the vertical velocity fluctuation due to mechanical turbulence generated by wind and vehicle traffic in the street, and $u_{street}$ is the wind speed at street level, calculated assuming a logarithmic reduction of the wind speed at roof top towards the bottom of the street (Berkowicz et al., 1997). Note that the wind direction at street level in the recirculation zone is mirrored compared to the roof level wind direction. Outside the recirculation zone, the wind direction is the same as at roof level. The vertical velocity fluctuation is calculated as a function of the street level wind speed, and the traffic produced turbulence by the following relationship (Berkowicz et al., 1997):

$$\sigma_w = \sqrt{(\alpha_s \mathrm{u}_{street})^2 + (\sigma_{w0})^2} \qquad (S.20)$$

where $\alpha_s$ is a proportionality constant, empirically assigned a value of 0.1, and $\sigma_{w0}$ is the traffic-induced turbulence, assigned a value of 0.25 m $s^{-1}$, typical for traffic on working days between 8 a.m. and 7 p.m. in situations where traffic-induced turbulence dominates (Kastner-Klein et al., 2000; fig. 6 therein). Traffic-induced turbulence plays an important role in the dispersion of pollutants in a street, particularly in low wind-speed conditions.

The integration path for Eq. (S.19) begins from $x_{start}$ which is defined as the distance from the receptor point where the plume has the same height as the receptor, which is zero in the case that $h_0$ is smaller or equal to the height of the receptor. The upper integration limit is $x_{end}$ defined as tabular values in Ottosen et al. (2015; Table 3 therein). The integration is performed along a straight line path against the wind direction. The calculation of the maximum integration path, $L_{max}$, depends on the wind direction with respect to the street axis, $\theta_{street}$ , i.e. angle between the street and the street level wind direction (Ottosen et al., 2015). When the integration path is long, as usually the case for near parallel flow, the plume from the traffic within the canyon will start dispersing out of the canyon at the top. It is assumed that this takes place when the plume height $\sigma_z$ becomes equal to the general canyon building height, $H_{sc}$, defined as distance $x_{esc}$. From this point onwards, the contribution to the concentration at the receptor is assumed to decay exponentially with the rate given by $k_{esc} = \sigma_{wt}/H_{sc}$ (Hertel and Berkowicz, 1989).

The length of the recirculation zone, $L_{rec}$, is estimated as being twice the average building height of the canyon and limited by $W_{sc}$. The recirculation zone is modelled as a trapezium with the upper length $L_{top}$ being half of the baseline length $L_{base}$, where $L_{base}$, is defined as min($L_{rec}$, $L_{max}$). The length of the hypotenuse of the trapezium is calculated as $L_{hyp} = \sqrt{(L_{base}/2)^2 + H_{sc}^2}$, assuming the leeward side edge of the recirculation zone to be the vertical building wall, with length of the building height. It is further assumed that the slant edge of the recirculation zone towards the opposite street side is not intercepted by buildings; $L_{base}$ is therefore limited to the street canyon width $W_{sc}$.

The contribution from recirculation is computed using a simple box model and concentrations are computed assuming equality of the inflow and outflow of the pollutant. This is expressed by the relationship (Berkowicz et al., 1997):

$$C_{screc,s} = \frac{Q_s}{W_{sc}} \cdot \frac{L_{base}}{\sigma_{wt} L_{top} + \sigma_{hyp} L_{hyp}} \qquad \text{(S.21)}$$

Where $\sigma_{wt}$ is the ventilation velocity of the canyon as given by Hertel and Berkowicz (1989) and $\sigma_{hyp}$ is the average turbulence of the hypotenuse of the trapezium (slant edge towards the opposite street side).

## S5. Numerical solver for chemistry

The photochemistry operator is used alternately with the transport (advection and diffusion) operator in the CityChem model for every model time step $dt$ in the model. Each transport operator (advection and diffusion) has a timing of $\Delta t$ seconds, while the photochemistry operator has a timing of $2\Delta t$ seconds. Hence for one model time step $dt$ the full sequence transport/chemistry/ transport is performed.

The atmospheric photochemistry equations form a stiff non-linear system of ordinary differential equations (ODE):

$$\frac{dy}{dt} = P(t,y) - L(t,y) \cdot y\,, \quad k = 1, \dots, m \tag{S.22}$$

Where $y$ is the solution vector containing the 3-D grid concentration field of $m$ chemical species. $P$ and $L$ describe the photochemistry production and loss terms, respectively. Here $P(t, y)$ is a vector of size $m$, and $L(t, y)$ is a diagonal matrix of size $m \times m$. To integrate the system of equations a numerical solver based on the TWOSTEP algorithm defined by Verwer and Simpson (1995) has been implemented in CityChem. The further development of the chemistry scheme is flexible in the sense that additional compounds and reactions can be included using the chemical pre-processor GenChem (Simpson et al., 2012).

Following Verwer and Simpson (1995), a Gauss-Seidel integration procedure is used, where for each reactive species $k$, the production rate $P_k$, the loss rate $L_k$ and then the updated concentrations $y_k^{n+1}$ are calculated in turn.

The updated concentration for the iteration is obtained using a Padé approximation of a variable-step 2nd order Backward Differentiation Formula (BDF):

$$y_k^{n+1} = \frac{Y_k^n + \gamma \cdot \tau \cdot P_k(t_{n+1}, y^{n+1})}{1 + \gamma \cdot \tau \cdot L_k(t_{n+1}, y^{n+1})} \tag{S.23}$$

where $\tau$ is the time step between the solutions $y^n$ and $y^{n+1}$, and $\gamma = (d+1)/(d+2)$, with $d = (t_n - t_{n-1})/(t_{n+1} - t_n)$; and $Y^n = [(d+1)^2 y^n - y^{n-1}]/(d^2 + 2d)$. $P_k$ is the $k$'th element of the vector $P$ and $L_k$ is the $k$'th element on the diagonal of the matrix $L$.

An initial iterate is calculated by the following extrapolation formula (Verwer and Simpson, 1995):

$$y^{(0)} = y^n + \frac{1}{d}(y^n - y^{n-1}) \tag{S.24}$$

During one iteration of the Gauss-Seidel method the initial iterate is used to calculate the estimate of the first species, which is then used to replace the initial iterate for the second species and so forth until all m species of the solution vector are calculated. At each iteration stage the latest values of concentrations are used for all reactants. As shown in Verwer and Simpson (1995), the Gauss-Seidel iterative method converges rapidly for gas-phase photochemistry schemes, suggesting that two iterations are sufficient. Consequently, the method implemented here uses only two iterations per time step.

In order to retain accuracy in the solution of the stiff ODE system, a weighted error norm is calculated as follows:

$$\|E^{n+1}\|_w = \max\left(\frac{|E_k^{n+1}|}{W_k^n}\right), \quad \text{with } W_k^n = \mathrm{atol}_k + \mathrm{rtol}_k \cdot |y_k^n| \tag{S.25}$$

Where $\mathrm{atol}_k$ and $\mathrm{rtol}_k$ for the absolute and relative error tolerance defined for all species of “CC45”. The integration step is accepted if the weighted error norm fulfils the condition $\|E^{n+1}\|_w \leq 1.0$ , whereas the integration is rejected if not. The relative tolerances for all species were set to 0.1 (i.e. 10 % relative error).

If two successive rejections occur the process is restarted. The missing starting value after a restart, or at the beginning of the simulation period, is calculated by the implicit Euler method:

$$y_k^{n+1} = \frac{Y_k^n + \tau \cdot P_k(t_{n+1}, y^{n+1})}{1 + \tau \cdot L_k(t_{n+1}, y^{n+1})} \qquad \text{(S.26)}$$

which is treated with the Gauss-Seidel iterative method in the same way as the second order BDF (Eq. (S.23)), using two iterations per time step. However, as initial iterate $y^{(0)}$ the initial value $y^0$ is used instead of the value from the extrapolation formula in Eq. (S.24).

The new time step, $\tau_{new}$, is estimated by the expression:

$$\tau_{new} = \max\left(0.5, \min\left(2.0, \frac{0.8}{\sqrt{\|E^{n+1}\|_w}}\right)\right) \cdot \tau_{old} \qquad \text{(S.27)}$$

The time step is further constrained by a prescribed minimum time step of 0.1 s and a maximum time step of $2dt$.

**Table S1:** Atmospheric stability classes in the sub-grid model components.

| Stability class | Name | Temperature difference $\Delta T$ between 10 m and 25 m | Mapping to P-G class | Line-source parameterization of ambient turbulence | | | |
|---|---|---|---|---|---|---|---|
| | | | | a | b | c | d |
| 1 | Unstable | $\Delta T$ < -0.5° | A, B, C | 110.62 | 0.932 | 18.333 | 1.8096 |
| 2 | Neutral | -0.5° < $\Delta T$ < 0.0° | D | 86.49 | 0.923 | 14.333 | 1.7706 |
| 3 | Moderately stable | 0.0° < $\Delta T$ < 0.5° | E | 61.14 | 0.915 | 12.5 | 1.0857 |
| 4 | Stable | $\Delta T$ > 0.5° | F | 61.14 | 0.915 | 12.5 | 1.0857 |

**Table S2:** Chemical reactions and photo-dissociation reactions of the “CC45” scheme. Give constants ε1, ε2, ε3 and ε4 for the photolysis reactions. For notes see end of Table.

| Reaction no. | Educts | Products | Rate coefficient |
|---|---|---|---|
| *Inorganic chemistry* | | | |
| IN-1 | OP + O2 + M | ⟶ O3 | 5.67E-34 × M × O2 × (*T*/300)$^{-2.8}$ |
| IN-2 | OD + M | ⟶ OP | 1.8E-11 exp(107/*T*) × N2 + 3.2E-11 exp(67/*T*) × O2 |
| IN-3 | OP + NO + M | ⟶ NO2 | *ktr*(NO + OP) |
| IN-4 | OD + H2O | ⟶ 2. OH | 2.2E-10 × H2O |
| IN-5 | O3 + NO | ⟶ NO2 + O2 | 1.4E-12 exp(-1310/*T*) |
| IN-6 | O3 + NO2 | ⟶ NO3 + O2 | 1.4E-12 exp(-2470/*T*) |
| IN-7 | O3 + OH | ⟶ HO2 + O2 | 1.7E-12 exp(-940/*T*) |
| IN-8 | O3 + HO2 | ⟶ OH + 2 O2 | 2.03E-16 × (300/*T*)$^{-4.57}$ exp(693/*T*) |
| IN-9 | NO + NO3 | ⟶ NO2 + NO2 | 1.8E-11 exp(110/*T*) |
| IN-10 | NO + HO2 | ⟶ NO2 + OH | 3.6E-12 exp(270/*T*) |
| IN-11 | NO3 + HO2 | ⟶ NO2 + OH + O2 | 3.5E-12 |
| IN-12 | NO2 + NO3 | ⟶ N2O5 | *ktr*(NO2 + NO3) |
| IN-13 | NO2 + OH + M | ⟶ HNO3 | *ktr*(NO2 + OH) |
| IN-14 | N2O5 | ⟶ NO2 + NO3 | *ktr*(N2O5) |
| IN-15 | OH + H2 | ⟶ HO2 + H2O | 7.7E-12 exp(-2100/*T*) |
| IN-16 | HO2 + HO2 | ⟶ H2O2 | *FH2O* × 2.2E-13 exp(600/*T*) |
| IN-17 | HO2 + HO2 + M | ⟶ H2O2 | *FH2O* × 1.9E-33 exp(980/*T*) |
| IN-18 | OH + HNO3 | ⟶ NO3 + H2O | *k*(OH + HNO3) |
| IN-19 | SO2 + OH | ⟶ HO2 + H2SO4 | *ktr*(SO2 + OH) |

|  |  |  |  |  |
|---|---|---|---|---|
| IN-20 | SO2 + CH3O2 | ⟶ | H2SO4 + HCHO + HO2 | 4.0E-17 |
| IN-21 | OH + HONO | ⟶ | NO2 | 2.5E-12 exp(-260/$T$) |
| IN-22 | OH + NO | ⟶ | HONO | *ktr*(OH + NO) |
| *Heterogeneous chemistry* |  |  |  |  |
| HE-1 | H2SO4 | ⟶ | aerosol sink | 5.0E-6 × M / 2.55E19 |
| *Methane chemistry* |  |  |  |  |
| MA-1 | OH + CH4 | ⟶ | CH3O2 | 1.85E-20 × $T^{2.8}$ × exp(-987/$T$) |
| MA-2 | CH3O2 + NO | ⟶ | HCHO + HO2 + NO2 | 2.3E-12 exp(360/$T$) |
| MA-3 | CH3O2 + NO3 | ⟶ | HCHO + HO2 + NO2 | 1.3E-12 |
| MA-4 | OH + CH3OH | ⟶ | HO2 + HCHO + H2O | 6.38E-18 exp(144/$T$) × $T^2$ |
| MA-5 | HO2 + CH3O2 | ⟶ | 0.9 CH3O2H + 0.1 HCHO | 3.8E-13 exp(780/$T$) |
| MA-6 | CH3O2H + OH | ⟶ | HCHO + OH | 1.0E-12 exp(190/$T$) |
| MA-7 | CH3O2H + OH | ⟶ | CH3O2 + H2O | 1.9E-12 exp(190/$T$) |
| MA-8 | OH + HCHO | ⟶ | CO + HO2 + HO2 | 1.25E-17 × $T^2$ × exp(615/$T$) |
| MA-9 | NO3 + HCHO | ⟶ | HNO3 + CO + HO2 | 2.0E-12 exp(-2440/$T$) |
| MA-10 | OH + CO | ⟶ | HO2 + CO2 | 1.44E-13 + 3.43E-33 × M |
| *Ethane and ethanol chemistry* |  |  |  |  |
| EA-1 | OH + C2H6 | ⟶ | C2H5O2 + H2O | 6.9E-12 exp(-1000/$T$) |
| EA-2 | C2H5O2 + NO | ⟶ | HO2 + CH3CHO + NO2 | 2.55E-12 exp(380/$T$) |
| EA-3 | C2H5O2 + NO3 | ⟶ | HO2 + CH3CHO + NO2 | 2.3E-12 |
| EA-4 | OH + CH3CHO | ⟶ | 0.95 CH3COO2 + 0.05 CH3O2 + 0.05 CO | 4.4E-12 exp(365/$T$) |
| EA-5 | CH3COO2 + NO2 + M | ⟶ | PAN | *ktr*(CH3OO2 + NO2) |
| EA-6 | PAN + M | ⟶ | CH3COO2 + NO2 | *ktr*(PAN) |
| EA-7 | CH3COO2 + NO | ⟶ | NO2 + CH3O2 + CO2 | 7.5E-12 exp(290/$T$) |

| | | | | |
|---|---|---|---|---|
| EA-8 | OH + C2H5OH | ⟶ | CH3CHO + HO2 | 6.7E-18 exp(511/$T$) × $T^2$ |
| *n-butane chemistry* | | | | |
| NB-1 | OH + NC4H10 | ⟶ | SECC4H9O2 | 2.03E-17 exp(78/$T$) × $T^2$ |
| NB-2 | NO + SECC4H9O2 | ⟶ | NO2 + 0.65 HO2 + 0.65 CH3COC2H5 + 0.35 CH3CHO + 0.35 C2H5O2 | 2.54E-12 exp(360/$T$) |
| NB-3 | OH + CH3COC2H5 | ⟶ | CH3COCHO2CH3 | 2.53E-18 exp(503/$T$) × $T^2$ |
| NB-4 | CH3COCHO2CH3 + NO | ⟶ | NO2 + CH3COO2 + CH3CHO | 2.54E-12 exp(360/$T$) |
| *Ethene chemistry* | | | | |
| EE-1 | C2H4 + OH +M | ⟶ | CH2O2CH2OH | $ktr$ (OH + C2H4) |
| EE-2 | CH2O2CH2OH + NO | ⟶ | NO2 + 2 HCHO + HO2 | 2.54E-12 exp(360/$T$) |
| EE-3 | C2H4 + O3 | ⟶ | 1.14 HCHO + 0.63 CO + 0.13 HO2 + 0.13 OH + 0.14 H2O2 | 9.1E-15 exp(-2580/$T$) |
| *Propene chemistry* | | | | |
| PE-1 | OH + C3H6 + M | ⟶ | CH3CHO2CH2OH | $ktr$ (OH + C3H6) |
| PE-2 | NO + CH3CHO2CH2OH | ⟶ | NO2 + CH3CHO + HCHO + HO2 | 2.54E-12 exp(360/$T$) |
| PE-3 | O3 + C3H6 | ⟶ | 0.545 HCHO + 0.545 CH3CHO + 0.56 CO + 0.36 OH + 0.28 HO2 + 0.09 H2O2 + 0.1 CH4 + 0.28 CH3O2 | 5.5E-15 exp(-1880/$T$) |
| *o-xylene chemistry* | | | | |
| OX-1 | OXYL + OH | ⟶ | OXYLOHO2 | 1.36E-11 |
| OX-2 | OXYLOHO2 + NO | ⟶ | NO2 + CH3COCHO + MEMALDIAL + HO2 | 2.54E-12 exp(360/$T$) |
| OX-3 | MEMALDIAL + OH | ⟶ | MEMALO2 | 5.58E-11 |
| OX-4 | MEMALO2 + NO | ⟶ | NO2 + HO2 + CH3COCHO + HCOCHO | 2.54E-12 exp(360/$T$) |
| OX-5 | OH + CH3COCHO | ⟶ | CH3COO2 + CO | 1.9E-12 exp(575/$T$) |
| OX-6 | OH + HCOCHO | ⟶ | HO2 + 2 CO | 6.6E-18 exp(820/$T$) × $T^2$ |

*Isoprene chemistry*

| | | | | |
|---|---|---|---|---|
| IS-1 | C5H8 + OH | ⟶ | ISOPO2 | 2.7E-11 exp(390/$T$) |
| IS-2 | ISOPO2 + NO | ⟶ | MVK + HCHO + HO2 + NO2 | 2.54E-12 exp(360/$T$) |
| IS-3 | MVK + OH | ⟶ | MVKO2 | 4.1E-12 exp(453/$T$) |
| IS-4 | MVKO2 + NO | ⟶ | CH3COCHO + HCHO + HO2 + NO2 | 1.4E-12 exp(-180/$T$) |

| Reaction no. | Educts | | Products | $\varepsilon_1$ | $\varepsilon_2$ | $\varepsilon_3$ | $\varepsilon_4$ |
|---|---|---|---|---|---|---|---|
| *Photolysis reactions* | | | | | | | |
| PH-1 | O3 | ⟶ | OD | 2.00E-04 | 1.400 | 0.86 | 0.33 |
| PH-2 | O3 | ⟶ | OP | 1.23E-03 | 0.600 | 0.92 | 0.41 |
| PH-3 | NO2 | ⟶ | OP + NO | 1.45E-02 | 0.400 | 0.91 | 0.38 |
| PH-4 | H2O2 | ⟶ | 2 OH | 2.20E-05 | 0.750 | 0.88 | 0.35 |
| PH-5 | HNO3 | ⟶ | NO2 + OH | 3.00E-06 | 1.250 | 0.87 | 0.33 |
| PH-6 | HCHO | ⟶ | CO + 2 HO2 | 5.40E-05 | 0.790 | 0.88 | 0.34 |
| PH-7 | HCHO | ⟶ | CO + H2 | 6.65E-05 | 0.600 | 0.89 | 0.35 |
| PH-8 | CH3CHO | ⟶ | CH3O2 + HO2 + CO | 1.35E-05 | 0.940 | 0.87 | 0.33 |
| PH-9 | CH3COC2H5 | ⟶ | CH3COO2 + C2H5O2 | 2.43E-05 | 0.877 | 0.92 | 0.41 |
| PH-10 | CH3COCHO | ⟶ | CH3COO2 + CO + HO2 | 9.72E-05 | 0.877 | 0.92 | 0.41 |
| PH-11 | HCOCHO | ⟶ | 1.9 CO + 0.1 HCHO + 0.5 HO2 | 5.40E-04 | 0.790 | 0.92 | 0.41 |
| PH-12 | NO3 | ⟶ | NO + O2 | 3.53E-02 | 0.081 | 0.92 | 0.42 |
| PH-13 | NO3 | ⟶ | NO2 + OP | 8.94E-02 | 0.059 | 0.92 | 0.42 |
| PH-14 | N2O5 | ⟶ | NO2 + NO3 | 3.32E-05 | 0.567 | 0.88 | 0.35 |
| PH-15 | CH3O2H | ⟶ | HCHO + OH + HO2 | 2.27E-05 | 0.620 | 0.88 | 0.35 |
| PH-16 | HONO | ⟶ | OH + NO | 3.22E-03 | 0.400 | 0.91 | 0.38 |

Notes:
Special rate constants and reaction parameters:

$FH2O$ = 1 + 1.4E-21 exp(2200/$T$) × H2O;
$k$(OH + HNO3) = $K_1$ + ($K_3$ × M)/(1.0 + ($K_3$ × M/$K_4$) with $K_1$ = 2.4E-14 exp(460/$T$), $K_3$ = 6.5E-34 exp(1335/$T$), $K_4$ = 2.7E-17 exp(2199/$T$);

Rate coefficients for three-body reactions using the Troe expression (e.g. Atkinson et al., 2006), where the reaction rates are calculated as: $ktr = \frac{k_0 k_\infty}{k_0 + k_\infty} F$, with the broadening factor $F$ calculated using the approximate expression: $log_{10}F \cong \frac{log_{10}F_c}{1+[log_{10}(k_0/k_\infty)/N]^2}$, where $N = [0.75 - 1.27 log_{10}F_c]$, are given as follows:

$ktr$(NO+OP): $k_0$/M = 1.0E-31 $(300/T)^{1.6}$, $k_\infty$ = 3.0E-11 $(300/T)^{-0.3}$, $F_c$ = 0.85;
$ktr$(NO2+NO3): $k_0$/M = 3.6E-30 $(300/T)^{4.1}$, $k_\infty$ = 9.7E-12 $(300/T)^{-0.2}$, $F_c$ = 0.35;
$ktr$(NO2+OH): $k_0$/M = 3.3E-30 $(300/T)^{3.0}$, $k_\infty$ = 4.1E-11, $F_c$ = 0.40;
$ktr$(N2O5): $k_0$/M = 1.3E-3 $(300/T)^{3.5}$ exp(-11000/$T$), $k_\infty$ = 9.7E14 $(300/T)^{-0.1}$ exp(-11080/$T$);
$ktr$(OH+NO): $k_0$/M = 7.4E-31 $(300/T)^{2.4}$, $k_\infty$ = 3.3E-11 $(300/T)^{0.3}$, $F_c$ = exp(-$T$/1420);
$ktr$(CH3OO2 + NO2): $k_0$/M = 2.7E-28 $(300/T)^{7.1}$, $k_\infty$ = 1.2-11 $(300/T)^{0.9}$, $F_c$ = 0.3;
$ktr$(PAN): $k_0$/M = 4.9E-3 $(300/T)^{-12100}$, $k_\infty$ = 5.4E16 exp(-13830/$T$), $F_c$ = 0.3;
$ktr$(OH+C2H4): $k_0$/M = 8.6E-29 $(300/T)^{3.1}$, $k_\infty$ = 9.0E-12 $(300/T)^{0.85}$, $F_c$ = 0.48;
$ktr$(OH+C3H6): $k_0$/M = 8.0E-27 $(300/T)^{3.5}$, $k_\infty$ = 3.0E-11 (300/$T$), $F_c$ = 0.5;
$ktr$(SO2+OH): $k_0$/M = 4.0E-31 $(300/T)^{-3.3}$, $k_\infty$ = 2.0E-12, $F = 0.45^{1/(1 + log_{10}(k_0/k_\infty)^2)}$

**Table S3:** Statistical comparison of meteorological variables modelled with TAPM and observations for 2012 based on hourly values. Statistical parameters: number of observations ($N$), mean (observed, modelled), standard deviation (STD; observed, modelled), overall bias (Bias), correlation (Corr), root mean square error (RMSE), and index of agreement (IOA).

| Station | Meteorological variable | $N$ | $\bar{O}$ | $\bar{M}$ | $\mathrm{STD_O}$ | $\mathrm{STD_M}$ | Bias | Corr | RMSE | IOA |
|---|---|---|---|---|---|---|---|---|---|---|
| Hamburg weather mast (10 m) | Temperature [°C] | 8691 | 9.71 | 10.17 | 5.92 | 5.95 | 0.15 | 0.96 | 1.55 | 0.98 |
| | Wind speed [m $s^{-1}$] | 8605 | 3.03 | 3.02 | 1.53 | 1.34 | 0.01 | 0.79 | 0.94 | 0.88 |
| | Wind direction [°] | 8605 | 185.6 | 204.0 | 88.0 | 83.6 | 18.37 | 0.73 | 65.7 | 0.85 |
| | Tot. solar radiation [W $m^{-2}$] | 8690 | 113.5 | 144.5 | 175.0 | 206.2 | 31.05 | 0.81 | 122.8 | 0.89 |
| Hamburg weather mast (50 m) | Temperature [°C] | 8683 | 9.40 | 9.91 | 5.85 | 5.91 | 0.12 | 0.97 | 1.49 | 0.98 |
| | Wind speed [m $s^{-1}$] | 8745 | 4.93 | 4.94 | 2.31 | 2.11 | 0.01 | 0.76 | 1.54 | 0.87 |
| | Wind direction [°] | 8745 | 198.5 | 206.8 | 87.7 | 83.4 | 8.27 | 0.75 | 61.1 | 0.87 |
| DWD Hamburg Airport (10 m) | Temperature [°C] | 8785 | 9.36 | 9.91 | 5.82 | 5.80 | 0.15 | 0.95 | 1.73 | 0.98 |
| | Relative humidity [fraction] | 8785 | 0.806 | 0.797 | 0.149 | 0.148 | -0.01 | 0.70 | 0.116 | 0.83 |
| | Wind speed [m $s^{-1}$] | 8785 | 3.94 | 3.07 | 2.01 | 1.44 | -0.87 | 0.81 | 1.48 | 0.82 |
| | Wind direction [°] | 8785 | 203.5 | 205.5 | 86.5 | 83.5 | 2.02 | 0.72 | 64.1 | 0.85 |

**Table S4:** Stations of the Hamburg air quality monitoring network included in the comparison. Available pollutant measurements for 2012 are indicated by X. Station types: traffic (tra), industrial (ind), urban background (ubg).

| Station code | Station name | Coordinates (UTM 32N); height (a.s.l.) | Station type | $O_3$ | $SO_2$ | NO | $NO_2$ | $PM_{2.5}$ | $PM_{10}$ |
|---|---|---|---|---|---|---|---|---|---|
| 80KT | Altona-Elbhang | 562611 E;<br>5933342 N;<br>25 m | ubg |  | X | X | X |  | X |
| 21BI | Billbrook | 571730 E;<br>5931713 N;<br>5 m | ind |  | X | X | X |  | X |
| 51BF | Bramfeld | 573434 E;<br>5943029 N;<br>31 m | ubg | X |  | X | X |  |  |
| 72FI | Finkenwerder West | 555949 E;<br>5932255 N;<br>0 m | ind |  |  | X | X |  | X |
| 68HB | Habichtstrasse | 569743 E;<br>5938684 N;<br>12 m | tra |  |  | X | X | X | X |
| 64KS | Kieler Strasse | 562563 E;<br>5935470 N;<br>16 m | tra |  |  | X | X | X |  |
| 70MB | Max-Brauer Allee | 562473 E;<br>5934507 N;<br>25 m | tra |  |  | X | X |  | X |
| 17SM | Stresemannstrasse | 563414 E;<br>5935091 N;<br>20 m | tra |  |  | X | X |  | X |
| 52NG | Neugraben | 556885 E;<br>5926120 N;<br>3 m | ubg | X |  | X | X |  |  |
| 13ST | Sternschanze | 564134 E;<br>5935504 N;<br>15 m | ubg | X | X | X | X | X | X |
| 20VE | Veddel | 567752 E;<br>5930928 N;<br>5 m | ind |  | X | X | X | X | X |
| 61WB | Wilhelmsburg | 565692 E;<br>5929231 N;<br>3 m | ubg |  | X | X | X | X | X |
| 54BL | Blankenese | 552066 E;<br>5935753 N;<br>75 m | ubg | X |  | X | X |  |  |
| 27TA | Tatenberg | 571900 E;<br>5927121 N;<br>2 m | ubg | X |  | X | X |  |  |
| 74BT | Billstedt | 573088 E;<br>5932744 N;<br>18 m | ubg |  |  | X | X |  |  |

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