

Atmospheric plume modelling

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Introduction

Consider the transport of a single contaminant whose mass concentration (or density) at location $\mathbf{x} = (x, y, z) \in \mathbb{R}^3$ [m] and time t [s] can be described by a smooth function $C(\mathbf{x}, t)$ [kg m⁻³]. The law of conservation of mass for C may be expressed in differential form as

$$\frac{\partial C}{\partial t} + \nabla \cdot \vec{J} = S \quad (1.1)$$

where $S(\mathbf{x}, t)$ [kg m⁻³s⁻¹] is a source or sink term and the vector function $\vec{J}(\mathbf{x}, t)$ represents the mass flux [kg m⁻²s⁻¹] of contaminant owing to the combined effects of diffusion and advection. The diffusive contribution to the flux arises from turbulent eddy motion in the atmosphere. The main result is that atmospheric diffusion may be assumed to follow Fick's law, which states that the diffusive flux is proportional to the concentration gradient or $\vec{J}_D = -K\nabla C$. The negative sign ensures that the contaminant flows from regions of high concentration to regions of low concentration, and the diffusion coefficient $K(\mathbf{x}) = \text{diag}(K_x, K_y, K_z)$ [m² s⁻¹] is a diagonal matrix whose entries are the turbulent eddy diffusivities that in general are functions of position. The second contribution to the flux is due to simple linear advection by the wind, which can be expressed as $\vec{J}_A = C\vec{u}$, where \vec{u} [ms⁻¹] is the wind velocity. By adding these two contributions together, we obtain the total flux $\vec{J} = \vec{J}_D + \vec{J}_A = C\vec{u} - K\nabla C$, which after substitution into the equation of conservation of mass (1.1) yields the three-dimensional advection-diffusion equation

$$\frac{\partial C}{\partial t} + \nabla \cdot (C\vec{u}) = \nabla \cdot (K\nabla C) + S \quad (1.2)$$

We next make a number of simplifying assumptions that will permit us to derive a closed-form analytical solution.

- The contaminant is emitted at a constant rate Q [kg s⁻¹] from a single point source $\vec{x} = (0, 0, H)$ located at height H above the ground surface, as depicted in Figure 2.1. Then the source term may be written as

$$S(\vec{x}) = Q\delta(x)\delta(y)\delta(z - H)$$

where δ is the Dirac delta function. Note that the units of the delta function are $[\text{m}^{-1}]$.

- The wind velocity is constant and aligned with the positive x-axis so that $\vec{u} = (u, 0, 0)$ for some constant u .
- The solution is steady state, which is reasonable if the wind velocity and all other parameters are independent of time and the time scale of interest is long enough.
- The eddy diffusivities are functions of the downwind distance x only, and diffusion is isotropic so that $K_x(x) = K_y(x) = K_z(x) =: K(x)$.
- The wind velocity is sufficiently large that diffusion in the x-direction is much smaller than advection, then the term $\frac{\partial}{\partial x} \left(K \frac{\partial C}{\partial x} \right)$ can be neglected.
- We are only concerned with the solution for values of $x, z \in [0, \infty)$ and $y \in \mathbb{R}$. In order to obtain a well-posed problem, we must supplement the PDE with an appropriate set of boundary conditions, namely,

$$C(0, y, z) = 0, C(\infty, y, z) = 0, C(x, \pm\infty, z) = 0, C(x, y, \infty) = 0$$

- We assume $C(x, y, z) = 0$ when $x < 0$.
- Pollutant deposition onto the ground occurs at a rate proportional to the local concentration. In many practical situations, contaminant particles are more massive than air and so they tend to settle out of the atmosphere at a well-defined rate known as the settling velocity, w_{set} $[\text{ms}^{-1}]$. To incorporate the effect of settling, we can supplement the advection velocity with a vertical component, $\vec{u} = (u, 0, -w_{set})$.

The first condition is a consequence of the unidirectional wind and the assumption that there are no contaminant sources for $x < 0$. The remaining conditions at infinity are consistent with the requirement that the total mass of contaminant must remain finite. The last assumption leads to the following boundary condition.

$$\left(K \frac{\partial C}{\partial z} + w_{set} C \right) \Big|_{z=0} = w_{dep} C|_{z=0}$$

With our considerations we're trying to solve the following PDE

$$u \frac{\partial C}{\partial x} - w_{set} \frac{\partial C}{\partial z} = K \frac{\partial^2 C}{\partial y^2} + K \frac{\partial^2 C}{\partial z^2} + \delta(x) \delta(y) \delta(z - H) \quad (1.3)$$

which for $x > 0$ takes the form

$$u \frac{\partial C}{\partial x} - w_{set} \frac{\partial C}{\partial z} = K \frac{\partial^2 C}{\partial y^2} + K \frac{\partial^2 C}{\partial z^2} \quad (1.4a)$$

Now integrating (1.4a) over $x \in [-d, d]$ with $d > 0$ we get

$$u[C(d, y, z) - C(-d, y, z)] - w_{set} \frac{\partial}{\partial z} \int_{-d}^d C dx = \left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \int_{-d}^d KC dx + Q\delta(y)\delta(z - H)$$

using measure theoretic version of Leibniz Rule (here C has a jump discontinuity only at $x = 0$ and K is continuous). Define

$$g_d(y, z) = \int_{-d}^d C dx, \quad h_d(y, z) = \int_{-d}^d KC dx$$

As $C(x, y, z) = 0$ for $x < 0$,

$$g_d(y, z) = \int_0^d C dx, \quad h_d(y, z) = \int_0^d KC dx$$

As C is continuous for $x > 0$, $g_d \rightarrow 0$, $h_d \rightarrow 0$ uniformly as $d \rightarrow 0+$ and consequently

$$\lim_{d \rightarrow 0+} \frac{\partial g_d}{\partial z} = 0, \quad \lim_{d \rightarrow 0+} \left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) h_d = 0$$

which leaves us with (after taking limit $d \rightarrow 0+$)

$$C(0+, y, z) = \frac{Q}{u} \delta(y) \delta(z - H)$$

Considering the above a new boundary condition we can write down our re-formed PDE along with its boundary conditions as follows

$$\begin{aligned} u \frac{\partial C}{\partial x} - w_{set} \frac{\partial C}{\partial z} &= K \frac{\partial^2 C}{\partial y^2} + K \frac{\partial^2 C}{\partial z^2} \\ C(0+, y, z) &= \frac{Q}{u} \delta(y) \delta(z - H) \\ C(0, y, z) &= 0, \quad C(\infty, y, z) = 0, \quad C(x, \pm\infty, z) = 0, \quad C(x, y, \infty) = 0 \\ \left(K \frac{\partial C}{\partial z} + w_{set} C \right) \Big|_{z=0} &= w_{dep} C|_{z=0} \end{aligned} \tag{1.4}$$

Solution of (1.4)

In order to simplify (1.4) we make a change of variable by introducing

$$r := \frac{1}{u} \int_0^x K dx, \quad c(r, x, z) := C(x, y, z)$$

which transforms our system into

$$\begin{aligned} \frac{\partial c}{\partial r} - \frac{w_{set}}{K} \frac{\partial c}{\partial z} &= \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2} \\ c(0+, y, z) &= \frac{Q}{u} \delta(y) \delta(z - H) \\ c(\infty, y, z) = c(r, \pm\infty, z) &= w(r, y, \infty) = 0 \\ \left(K \frac{\partial c}{\partial z} + w_{set} c \right) \Big|_{z=0} &= w_{dep} c \Big|_{z=0} \end{aligned} \quad (2)$$

We assume the solution takes the form

$$\begin{aligned} c &= \frac{Q}{u} a(r, y) b(r, z) \exp(p) \\ p &= fr + gy + hz + l \end{aligned}$$

where f, g, h, l are constants to be determined. Plugging our ansatz into the pde we get

$$\frac{\partial a}{\partial r} b + a \frac{\partial b}{\partial r} + fab - \frac{w_{set}}{K} \left(a \frac{\partial b}{\partial z} + hab \right) = \frac{\partial^2 a}{\partial y^2} b + 2g \frac{\partial a}{\partial y} b + g^2 ab + a \frac{\partial^2 b}{\partial z^2} + 2ha \frac{\partial b}{\partial z} + h^2 ab$$

Collecting terms together this can be written as

$$a \left[\frac{\partial b}{\partial r} - \left(\frac{w_{set}}{K} + 2h \right) \frac{\partial b}{\partial z} - \frac{\partial^2 b}{\partial z^2} + \left(f - g^2 - h^2 - \frac{w_{set}h}{K} \right) b \right] + b \left[\frac{\partial a}{\partial r} - 2g \frac{\partial a}{\partial y} - \frac{\partial^2 a}{\partial y^2} \right] = 0$$

To simplify the above equation we set f, g, h in a way such that terms containing

$$\frac{\partial a}{\partial y}, \frac{\partial b}{\partial z}, ab$$

vanish. This implies

$$\begin{aligned} g &= 0 \\ h &= -\frac{w_{set}}{2K} \\ f &= -h^2 = -\frac{w_{set}^2}{4K^2} \end{aligned}$$

And thus our original equation turns into

$$a \left(\frac{\partial b}{\partial r} - \frac{\partial^2 b}{\partial z^2} \right) + b \left(\frac{\partial a}{\partial r} - \frac{\partial^2 a}{\partial y^2} \right) = 0 \quad (2.1)$$

Uniqueness of solution of (2)

Suppose u_1, u_2 solve (2) in the domain $D_+ = \{(r, y, z) : r \in (0, \infty), y \in (-\infty, \infty), z \in (0, \infty)\}$. Set $w = u_1 - u_2$. w also satisfies (2) with the following

boundary conditions

$$w(0+, y, z) = w(\infty, y, z) = w(x, \pm\infty, z) = w(x, y, \infty) = 0$$

$$\left(K \frac{\partial w}{\partial z} + w_{set} w \right) \Big|_{z=0} = w_{dep} w \Big|_{z=0}$$

Define

$$E(r) = \int_0^\infty \int_{-\infty}^\infty w(r, y, z)^2 dy dz$$

Note that $E(r) \geq 0$ and $E(0+) = 0$.

$$\begin{aligned} \frac{\partial E}{\partial r} &= 2 \int_0^\infty \int_{-\infty}^\infty w \left(\frac{w_{set}}{K} \frac{\partial w}{\partial z} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) dy dz \\ &= -\frac{w_{set}}{K} \int_{-\infty}^\infty w^2(r, y, 0) dy - 2 \int_0^\infty \int_{-\infty}^\infty \left[\left(\frac{\partial w}{\partial y} \right)^2 + \left(\frac{\partial w}{\partial z} \right)^2 \right] dy dz \leq 0 \end{aligned}$$

as w_{set}, K are non-negative quantities. So E is a decreasing function of r and $E(0+) = 0$ implies E must be identically zero as it is a non-negative quantity which in turn implies $w \equiv 0$ in D_+ i.e. a solution of (2), if it exists, must be unique.

Solution of (2)

From (2.1) we can say that, (2) is solved if

$$\begin{aligned} \frac{\partial a}{\partial r} &= \frac{\partial^2 a}{\partial y^2} \\ a(0+, y) &= \delta(y), a(\infty, y) = a(r, \pm\infty) = 0 \end{aligned} \tag{2.2}$$

and

$$\begin{aligned} \frac{\partial b}{\partial r} &= \frac{\partial^2 b}{\partial z^2} \\ b(0+, z) &= \delta(z - H), b(\infty, y) = b(r, \infty) = 0 \\ \left(K \frac{\partial b}{\partial z} - w_o b \right) \Big|_{z=0} &= 0 \end{aligned} \tag{2.3}$$

are solved simultaneously where $w_o = w_{dep} - \frac{w_{set}}{2}$. Uniqueness of solution of (2) guarantees the solution obtained like this is the required solution.

Derivation of the last boundary condition

Plugging our ansatz in we get

$$\begin{aligned}
& \left(\frac{Q}{u} K h a b e^p + \frac{Q}{u} K a \frac{\partial b}{\partial z} e^p + \frac{Q}{u} w_{set} a b e^p \right) \Big|_{z=0} = \frac{Q}{u} w_{dep} a b e^p \Big|_{z=0} \\
\Rightarrow & \left(K h b + K \frac{\partial b}{\partial z} + w_{set} b \right) \Big|_{z=0} = w_{dep} b \Big|_{z=0} \\
\Rightarrow & \left(-\frac{w_{set}}{2} b + K \frac{\partial b}{\partial z} + w_{set} b \right) \Big|_{z=0} = w_{dep} b \Big|_{z=0} \\
\Rightarrow & \left(K \frac{\partial b}{\partial z} + \frac{w_{set}}{2} b - w_{dep} b \right) \Big|_{z=0} = 0
\end{aligned}$$

Solution of (2.3)

For the following computations assume $y \in [0, \infty)$. Taking Laplace transform of the pde with respect to r gives us

$$\begin{aligned}
\rho \hat{b} - b(0+, z) &= \frac{\partial^2 \hat{b}}{\partial z^2} \\
\Rightarrow \frac{\partial^2 \hat{b}}{\partial z^2} - \rho \hat{b} &= -\delta(z - H)
\end{aligned}$$

where

$$\hat{b} = \int_0^\infty e^{-\rho r} b(r, z) dr$$

Now taking Laplace transform of the last equation with respect to z we get

$$\begin{aligned}
& -\frac{\partial \hat{b}}{\partial z}(\rho, 0+) - \zeta \hat{b}(\rho, 0+) + \zeta^2 \hat{b} - \rho \hat{b} = -e^{-\zeta H} \\
\Rightarrow & (\zeta^2 - \rho) \hat{b} - \left(\frac{w_o}{K} + \zeta \right) \hat{b}(\rho, 0+) = -e^{-\zeta H} \\
\Rightarrow & \hat{b} = \frac{\left(\frac{w_o}{K} + \zeta \right) B - e^{-\zeta H}}{\zeta^2 - \rho}
\end{aligned}$$

where

$$\hat{b} = \int_0^\infty e^{-\zeta z} \hat{b}(\rho, z) dz, \quad B = \hat{b}(\rho, 0+)$$

Inverting Laplace transform with respect to ζ gives us

$$\hat{b} = \frac{w_0 B u(z)}{K \sqrt{\rho}} \sinh(\sqrt{\rho} z) + B u(z) \cosh(\sqrt{\rho} z) - \frac{u(z - H)}{\sqrt{\rho}} \sinh(\sqrt{\rho}(z - H))$$

where u denotes the Heaviside step function. Therefore,

$$\hat{b} = \begin{cases} \frac{w_0 B}{K \sqrt{\rho}} \sinh(\sqrt{\rho} z) + B \cosh(\sqrt{\rho} z), & 0 \leq z \leq H \\ \frac{w_0 B}{K \sqrt{\rho}} \sinh(\sqrt{\rho} z) + B \cosh(\sqrt{\rho} z) - \frac{1}{\sqrt{\rho}} \sinh(\sqrt{\rho}(z - H)), & z > H \geq 0 \end{cases}$$

In order to make sure $b(r, \infty) = 0 \implies \hat{b}(\rho, \infty) = 0$ we must have

$$\begin{aligned} \lim_{z \rightarrow \infty} \frac{1}{2} \left(B e^{\sqrt{\rho}z} + \frac{w_o B}{K \sqrt{\rho}} e^{\sqrt{\rho}z} - \frac{1}{\sqrt{\rho}} e^{\sqrt{\rho}(z-H)} \right) &= 0 \\ \implies B + \frac{w_o B}{K \sqrt{\rho}} - \frac{e^{-\sqrt{\rho}H}}{\sqrt{\rho}} &= 0 \\ \implies B &= \frac{e^{-\sqrt{\rho}H}}{\sqrt{\rho} + \frac{w_o}{K}} \end{aligned}$$

Setting $q = \frac{w_o}{K}$ and plugging this in gives us

$$2\hat{b} = \begin{cases} \frac{\sqrt{\rho}-q}{\sqrt{\rho}+q} \frac{1}{\sqrt{\rho}} e^{-\sqrt{\rho}(z+H)} + \frac{1}{\sqrt{\rho}} e^{\sqrt{\rho}(z-H)}, & 0 \leq z \leq H \\ \frac{\sqrt{\rho}-q}{\sqrt{\rho}+q} \frac{1}{\sqrt{\rho}} e^{-\sqrt{\rho}(z+H)} + \frac{1}{\sqrt{\rho}} e^{-\sqrt{\rho}(z-H)}, & z > H \geq 0 \end{cases}$$

Or,

$$\begin{aligned} 2\hat{b} &= \frac{\sqrt{\rho}-q}{\sqrt{\rho}+q} \frac{1}{\sqrt{\rho}} e^{-\sqrt{\rho}(z+H)} + \frac{1}{\sqrt{\rho}} e^{-\sqrt{\rho}|z-H|} \\ &= \frac{2}{\sqrt{\rho}+q} e^{-\sqrt{\rho}(z+H)} - \frac{1}{\sqrt{\rho}} e^{-\sqrt{\rho}(z+H)} + \frac{1}{\sqrt{\rho}} e^{-\sqrt{\rho}|z-H|}, \quad z, H \geq 0 \quad \dots (2.4) \end{aligned}$$

We can solve (2.3) if we can compute the inverse Laplace transform of

$$\frac{e^{-\sqrt{\rho}\alpha}}{\sqrt{\rho}} \text{ and } \frac{e^{-\sqrt{\rho}\alpha}}{\sqrt{\rho}+q} \quad \text{with } q, \alpha > 0$$

Inverse Laplace transform of $\frac{e^{-\sqrt{\rho}\alpha}}{\sqrt{\rho}+q}$

Since we can compute

$$\mathcal{L}^{-1} \left(\frac{e^{-\sqrt{\rho}\alpha}}{\sqrt{\rho}} \right) = \frac{e^{-\frac{\alpha^2}{4r}}}{\sqrt{\pi r}}$$

using Bromwich contour fairly easily and

$$\frac{e^{-\sqrt{\rho}\alpha}}{\sqrt{\rho}+q} = \frac{e^{-\sqrt{\rho}\alpha}}{\sqrt{\rho}} \frac{\sqrt{\rho}}{\sqrt{\rho}+q},$$

our strategy for inversion is computing the inverse transform for each term on RHS and then apply convolution theorem. Now,

$$\begin{aligned} \frac{\sqrt{\rho}}{\sqrt{\rho}+q} &= \frac{\sqrt{\rho}(\sqrt{\rho}-q)}{(\sqrt{\rho}+q)(\sqrt{\rho}-q)} = \frac{\rho - \sqrt{\rho}q}{\rho - q^2} = \frac{\rho}{\rho - q^2} - \frac{\rho q}{\sqrt{\rho}(\rho - q^2)} \\ &= \frac{\rho}{\rho - q^2} - \frac{(\rho - q^2 + q^2)q}{\sqrt{\rho}(\rho - q^2)} = \frac{\rho}{\rho - q^2} - \frac{q}{\sqrt{\rho}} - \frac{q^3}{\sqrt{\rho}(\rho - q^2)} \end{aligned} \quad (4.1)$$

For the following computation assume that $\rho > q^2$.

$$\mathcal{L}^{-1}\left(\frac{\rho}{\rho - q^2}\right) = \mathcal{L}^{-1}\left(1 + \frac{q^2}{\rho - q^2}\right) = \delta(r) + q^2 e^{q^2 r} \quad (4.2)$$

$$\begin{aligned} \mathcal{L}\left(\frac{1}{\sqrt{r}}\right) &= \int_0^\infty e^{-\rho r} \frac{dr}{\sqrt{r}} = 2 \int_0^\infty e^{-\rho r^2} dr = \frac{1}{\sqrt{\rho}} \int_{-\infty}^\infty e^{-r^2} dr = \sqrt{\frac{\pi}{\rho}} \\ \Rightarrow \mathcal{L}^{-1}\left(\frac{q}{\sqrt{\rho}}\right) &= \frac{q}{\sqrt{\pi r}} \end{aligned} \quad (4.3)$$

$$\begin{aligned} \mathcal{L}(\text{erf}(\sqrt{r})) &= \frac{2}{\sqrt{\pi}} \int_0^\infty \int_0^{\sqrt{r}} e^{-t^2 - \rho r} dt dr = \frac{2}{\sqrt{\pi}} \int_0^\infty \int_{t^2}^\infty e^{-t^2 - \rho r} dt dr \\ &= \frac{2}{\sqrt{\pi} \rho} \int_0^\infty e^{-t^2 - \rho t^2} dt = \frac{1}{\rho \sqrt{\rho + 1}} \\ \Rightarrow \mathcal{L}(e^r \text{erf}(\sqrt{r})) &= \frac{1}{\sqrt{\rho}(\rho - 1)} \\ \Rightarrow \mathcal{L}^{-1}\left(\frac{q^3}{\sqrt{\rho}(\rho - q^2)}\right) &= \mathcal{L}^{-1}\left(\frac{1}{\sqrt{\frac{\rho}{q^2}}\left(\frac{\rho}{q^2} - 1\right)}\right) = q^2 e^{q^2 r} \text{erf}(q\sqrt{r}) \end{aligned} \quad (4.4)$$

So (4.1), (4.2), (4.3), (4.4) yield

$$\mathcal{L}^{-1}\left(\frac{\sqrt{\rho}}{\sqrt{\rho} + q}\right) = \delta(r) + q^2 e^{q^2 r} - \frac{q}{\sqrt{\pi r}} - q^2 e^{q^2 r} \text{erf}(q\sqrt{r}) \quad (4.5)$$

Therefore,

$$\mathcal{L}^{-1}\left(\frac{e^{-\sqrt{\rho}\alpha}}{\sqrt{\rho} + q}\right) = \left[\delta(r) + q^2 e^{q^2 r} - \frac{q}{\sqrt{\pi r}} - q^2 e^{q^2 r} \text{erf}(q\sqrt{r})\right] * \frac{e^{-\frac{\alpha^2}{4r}}}{\sqrt{\pi r}} \quad (4.6)$$

where $*$ denotes convolution.

$$\int_0^r \delta(r-t) \frac{e^{-\frac{\alpha^2}{4t}}}{\sqrt{\pi t}} dt = \frac{e^{-\frac{\alpha^2}{4r}}}{\sqrt{\pi r}}$$

An useful integral

Before moving on we compute an useful integral below for $a, b, x > 0$.

$$I = \int_0^x e^{-a^2 t^2 - \frac{b^2}{t^2}} dt = e^{-2ab} \int_0^x e^{-(at - \frac{b}{t})^2} dt$$

Set $v = at - \frac{b}{t}$ and note that

$$t = \frac{v + \sqrt{v^2 + 4ab}}{2a}$$

$$2ae^{2ab}I = \int_{-\infty}^{ax - \frac{b}{x}} \left(1 + \frac{v}{\sqrt{v^2 + 4ab}}\right) e^{-v^2} dv$$

Another change of variable $k = \sqrt{v^2 + 4ab}$ gets us to

$$\begin{aligned} 2ae^{2ab}I &= \int_{-\infty}^{ax - \frac{b}{x}} e^{-v^2} dv + e^{4ab} \int_{-\infty}^{ax + \frac{b}{x}} e^{-k^2} dk \\ \implies \int_0^x e^{-a^2t^2 - \frac{b^2}{t^2}} dt &= \frac{\sqrt{\pi}}{4a} \left[e^{-2ab} \operatorname{erf}\left(ax - \frac{b}{x}\right) + e^{2ab} \operatorname{erf}\left(ax + \frac{b}{x}\right) - 2 \sinh(2ab) \right] \end{aligned}$$

This immediately gives us

$$\begin{aligned} \int_0^r q^2 e^{q^2(r-t)} \frac{e^{-\frac{\alpha^2}{4t}}}{\sqrt{\pi t}} dt &= q^2 e^{q^2 r} \int_0^r \frac{e^{-(q^2 t + \frac{\alpha^2}{4t})}}{\sqrt{\pi t}} dt = \frac{2q^2 e^{q^2 r}}{\sqrt{\pi}} \int_0^{\sqrt{r}} e^{-(q^2 t^2 + \frac{\alpha^2}{4t^2})} dt \\ &= \frac{qe^{q^2 r}}{2} \left[e^{q\alpha} \operatorname{erf}\left(q\sqrt{r} + \frac{\alpha}{2\sqrt{r}}\right) + e^{-q\alpha} \operatorname{erf}\left(q\sqrt{r} - \frac{\alpha}{2\sqrt{r}}\right) - 2 \sinh(q\alpha) \right] \end{aligned} \quad (4.7)$$

Now

$$\int_0^r \frac{q}{\sqrt{\pi t(r-t)}} e^{-\frac{\alpha^2}{4t}} dt = \frac{q}{\sqrt{\pi}} \int_{\frac{1}{r}}^{\infty} \frac{e^{-\frac{\alpha^2 t}{4}}}{t\sqrt{rt-1}} dt = \frac{q}{\sqrt{\pi}} \int_1^{\infty} \frac{e^{-\frac{\alpha^2 t}{4r}}}{t\sqrt{t-1}} dt$$

Using the change of variable $k = \sqrt{t-1}$ we get

$$\int_0^r \frac{q}{\sqrt{\pi t(r-t)}} e^{-\frac{\alpha^2}{4t}} dt = \frac{2qe^{-\frac{\alpha^2}{4r}}}{\sqrt{\pi}} \int_0^{\infty} \frac{e^{-\frac{\alpha^2 k^2}{4r}}}{k^2 + 1} dk \quad (4.8)$$

For $\mu \geq 0$ define

$$\begin{aligned} F(\mu) &= \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{e^{-\mu t^2}}{t^2 + 1} dt \\ \implies F'(\mu) &= F(\mu) - \frac{1}{\sqrt{\mu}} \\ \implies e^{-\mu} F(\mu) - F(0) &= - \int_0^{\mu} \frac{e^{-t}}{\sqrt{t}} dt \\ \implies e^{-\mu} F(\mu) - \sqrt{\pi} &= -2 \int_0^{\sqrt{\mu}} e^{-t^2} dt = -\sqrt{\pi} \operatorname{erf}(\sqrt{\mu}) \\ \implies F(\mu) &= \sqrt{\pi} e^{\mu} \operatorname{erfc}(\sqrt{\mu}) \end{aligned}$$

Therefore, (4.8) tells us

$$\int_0^r \frac{q}{\sqrt{\pi t(r-t)}} e^{-\frac{\alpha^2}{4t}} dt = \sqrt{\pi} q \operatorname{erfc}\left(\frac{\alpha}{2\sqrt{r}}\right) \quad (4.9)$$

One more convolution left to compute. But this is where we get stuck. But for large r we can compute the following simple approximation.

$$\begin{aligned}
& \int_0^r q^2 e^{q^2(r-t)} \operatorname{erf}(q\sqrt{r-t}) \frac{e^{-\frac{\alpha^2}{4t}}}{\sqrt{\pi t}} dt = \frac{2q^2 e^{q^2 r}}{\pi} \int_0^r \int_0^{q\sqrt{r-t}} \frac{e^{-q^2 t - \frac{\alpha^2}{4t} - x^2}}{\sqrt{t}} dx dt \\
&= \frac{2q^2 e^{q^2 r}}{\pi} \int_0^{q\sqrt{r}} e^{-x^2} \int_0^{r - \frac{x^2}{q^2}} \frac{e^{-q^2 t - \frac{\alpha^2}{4t}}}{\sqrt{t}} dt dx = \frac{4q^2 e^{q^2 r}}{\pi} \int_0^{q\sqrt{r}} e^{-x^2} \int_0^{\sqrt{r - \frac{x^2}{q^2}}} e^{-q^2 t^2 - \frac{\alpha^2}{4t^2}} dt dx \\
&= \frac{4q^2 e^{q^2 r - q\alpha}}{\pi} \int_0^{q\sqrt{r}} e^{-x^2} \int_0^{\sqrt{r - \frac{x^2}{q^2}}} e^{-q^2(t - \frac{\alpha}{2qt})^2} dt dx \\
&\approx \frac{4q^2 e^{q^2 r - q\alpha}}{\pi} \int_0^{q\sqrt{r}} e^{-x^2} \int_0^{\sqrt{r - \frac{x^2}{q^2}}} e^{-q^2 t^2} dt dx \\
&\approx \frac{4q e^{q^2 r - q\alpha}}{\pi} \int_0^{q\sqrt{r}} e^{-x^2} \int_0^{\sqrt{q^2 r - x^2}} e^{-t^2} dt dx \\
&\approx \frac{2q e^{q^2 r - q\alpha}}{\sqrt{\pi}} \int_0^{q\sqrt{r}} e^{-x^2} \operatorname{erf}(\sqrt{q^2 r - x^2}) dx \tag{4.10}
\end{aligned}$$

For $\mu \geq 0$ define

$$\begin{aligned}
G(\mu) &= \int_0^\mu e^{-x^2} \operatorname{erf}(\sqrt{\mu^2 - x^2}) dx \\
\Rightarrow G'(\mu) &= \frac{2\mu e^{-\mu^2}}{\sqrt{\pi}} \int_0^\mu \frac{dx}{\sqrt{\mu^2 - x^2}} = \sqrt{\pi} \mu e^{-\mu^2} \\
\Rightarrow G(\mu) - G(\infty) &= \sqrt{\pi} \int_\infty^\mu t e^{-t^2} dt \\
\Rightarrow G(\mu) - \int_0^\infty e^{-x^2} dx &= \frac{\sqrt{\pi}}{2} \int_\infty^\mu e^{-t} dt \quad (\text{by dominated convergence theorem}) \\
\Rightarrow G(\mu) &= \frac{\sqrt{\pi}}{2} (1 - e^{-\mu^2})
\end{aligned}$$

Therefore, (4.10) tells us

$$\int_0^r q^2 e^{q^2(r-t)} \operatorname{erf}(q\sqrt{r-t}) \frac{e^{-\frac{\alpha^2}{4t}}}{\sqrt{\pi t}} dt \approx q e^{-q\alpha} (e^{q^2 r} - 1) \tag{4.11}$$

Inversion via Bromwich contour

Consider

$$F(\rho) = \mathcal{L}(f(r)) = \frac{e^{-\sqrt{\rho}\alpha}}{\sqrt{\rho} + q}$$

with $\alpha > 0, q \geq 0$.

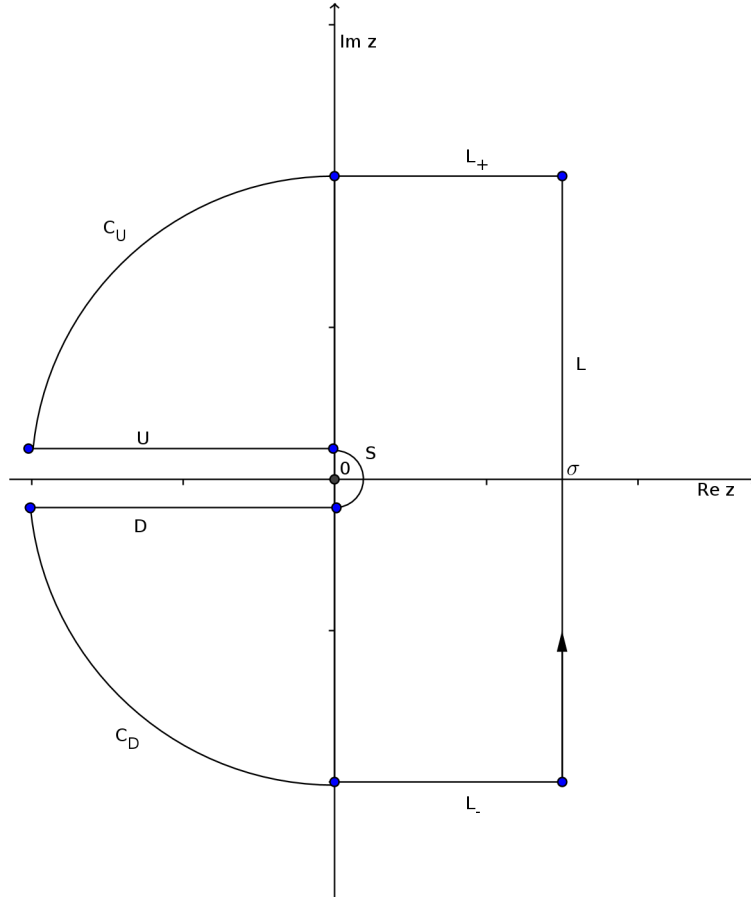


Figure 1: Bromwich contour γ

C_U, C_D are origin-centered circular arcs of radius R , S is an origin-center semi-circle of radius ε . L_+, L_- are horizontal lines represented by $y = \pm R$. U, D are horizontal lines and L is a vertical line represented by $x = \sigma$. We use negative real axis as the branch cut for defining \sqrt{z} with $\arg(z) \in (-\pi, \pi]$. Consider the integral

$$I(C) = \int_C \frac{e^{-\sqrt{\rho}\alpha + \rho r}}{\sqrt{\rho} + q} d\rho$$

We're interested in $I(\gamma)$.

Contribution of L_- as $R \rightarrow \infty$

$$I(L_+) = \int_{\sigma+iR}^{iR} \frac{e^{-\sqrt{\rho}\alpha+\rho r}}{\sqrt{\rho}+q} d\rho = \int_{\sigma}^0 \frac{e^{-\alpha\sqrt{x+iR}+(x+iR)r}}{\sqrt{x+iR}+q} dx$$

$$\Rightarrow |I(L_+)| \leq \frac{1}{\sqrt{R}} \int_0^{\sigma} e^{xr-\alpha\sqrt[4]{R^2+x^2}\cos\frac{\theta}{2}} dx$$

where $\theta = \arg(x+iR)$. As $\theta \in [0, \frac{\pi}{2}]$, $\cos\frac{\theta}{2} > 0$ which implies

$$|I(L_+)| \leq \frac{1}{\sqrt{R}} \int_0^{\sigma} e^{xr} dx \leq \frac{\sigma e^{r\sigma}}{\sqrt{R}}$$

$$\Rightarrow \lim_{R \rightarrow \infty} I(L_+) = 0$$

Contribution of L_- as $R \rightarrow \infty$

$$I(L_-) = \int_{-iR}^{\sigma-iR} \frac{e^{-\sqrt{\rho}\alpha+\rho r}}{\sqrt{\rho}+q} d\rho = \int_0^{\sigma} \frac{e^{-\alpha\sqrt{x-iR}+(x-iR)r}}{\sqrt{x-iR}+q} dx$$

$$\Rightarrow |I(L_-)| \leq \frac{1}{\sqrt{R}-q} \int_0^{\sigma} e^{xr-\alpha\sqrt[4]{R^2+x^2}\cos\frac{\theta}{2}} dx$$

where $\theta = \arg(x-iR)$. As $\theta \in [-\frac{\pi}{2}, 0]$, $\cos\frac{\theta}{2} > 0$ which implies

$$|I(L_-)| \leq \frac{1}{\sqrt{R}-q} \int_0^{\sigma} e^{xr} dx \leq \frac{\sigma e^{r\sigma}}{\sqrt{R}-q}$$

$$\Rightarrow \lim_{R \rightarrow \infty} I(L_-) = 0$$

Contribution of C_U as $R \rightarrow \infty$

$$I(C_U) = iR \int_{\frac{\pi}{2}}^{\phi} \frac{e^{-\alpha\sqrt{Re^{it}}+Rre^{it}+it}}{\sqrt{Re^{it}}+q} dt$$

where $\phi = \arg(-\sqrt{R^2-\varepsilon^2}+i\varepsilon)$. Clearly $\phi \in [\frac{\pi}{2}, \pi]$. Note that $\cos\frac{t}{2} \geq 0$, $\cos t \leq 0$ when $t \in [\frac{\pi}{2}, \pi]$.

$$|I(C_U)| \leq \frac{R}{\sqrt{R}-q} \int_{\frac{\pi}{2}}^{\phi} e^{-\alpha\sqrt{R}\cos\frac{t}{2}+Rr\cos t} dt \leq \frac{R}{\sqrt{R}-q} \int_{\frac{\pi}{2}}^{\phi} e^{-\alpha\sqrt{R}\cos\frac{t}{2}} dt$$

$$\Rightarrow |I(C_U)| \leq \frac{Re^{-\alpha\sqrt{R}\cos\frac{\phi}{2}}(\phi-\frac{\pi}{2})}{\sqrt{R}-q} \Rightarrow \lim_{R \rightarrow \infty} I(C_U) = 0$$

Contribution of C_D as $R \rightarrow \infty$

As cosine is even, identical reasoning shows that

$$\Rightarrow \lim_{R \rightarrow \infty} I(C_D) = 0$$

Contribution of S as $\varepsilon \rightarrow 0$

$$\begin{aligned}
I(S) &= i\varepsilon \int_{-\frac{\pi}{2}}^{-\frac{\pi}{2}} \frac{e^{-\alpha\sqrt{\varepsilon}e^{it}+r\varepsilon e^{it}+it}}{\sqrt{\varepsilon}e^{it}+q} dt \\
\Rightarrow |I(S)| &= \frac{\varepsilon}{q-\sqrt{\varepsilon}} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} e^{-\alpha\sqrt{\varepsilon}\cos\frac{t}{2}+r\varepsilon\cos t} dt \leq \frac{\varepsilon}{q-\sqrt{\varepsilon}} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} e^{r\varepsilon\cos t} dt \leq \frac{\pi\varepsilon e^{r\varepsilon}}{q-\sqrt{\varepsilon}} \\
\Rightarrow \lim_{\varepsilon \rightarrow 0} I(S) &= 0
\end{aligned}$$

Contribution of U as $R \rightarrow \infty, \varepsilon \rightarrow 0$

$$\begin{aligned}
I(U) &= - \int_0^{\sqrt{R^2-\varepsilon^2}} \frac{e^{-\alpha\sqrt{xe^{i\pi}+i\varepsilon}+r(xe^{i\pi}+i\varepsilon)+i\pi}}{\sqrt{xe^{i\pi}+i\varepsilon}+q} dx \\
\Rightarrow |I(U)| &\leq \int_0^{\sqrt{R^2-\varepsilon^2}} \frac{e^{-\alpha\sqrt{x^2+\varepsilon^2}\cos\frac{\phi}{2}-xr}}{|\sqrt{x^2+\varepsilon^2}-q|} dx
\end{aligned}$$

where $\phi = \arg(xe^{i\pi} + i\varepsilon) \in [\frac{\pi}{2}, \pi] \Rightarrow \cos\frac{\phi}{2} \geq 0$.

$$\therefore |I(U)| \leq \int_0^\infty \frac{e^{-xr}}{|\sqrt{x^2+\varepsilon^2}-q|} dx$$

The integrand on RHS behaves as $\frac{e^{-xr}}{\sqrt{x}}$ as $x \rightarrow \infty$ and as $\frac{e^{-xr}}{q-\varepsilon}$ as $x \rightarrow 0$ and therefore the integral on RHS converges. Therefore by dominated convergence theorem,

$$I_U := \lim_{R \rightarrow \infty, \varepsilon \rightarrow 0} I(U) = \int_0^\infty \frac{e^{-i\alpha\sqrt{x}-rx}}{i\sqrt{x}+q} dx$$

Contribution of D as $R \rightarrow \infty, \varepsilon \rightarrow 0$

$$I(D) = \int_0^{\sqrt{R^2-\varepsilon^2}} \frac{e^{-\alpha\sqrt{xe^{-i\pi}-i\varepsilon}+r(xe^{-i\pi}-i\varepsilon)-i\pi}}{\sqrt{xe^{-i\pi}-i\varepsilon}+q} dx$$

Following identical arguments we arrive at

$$I_D := \lim_{R \rightarrow \infty, \varepsilon \rightarrow 0} I(D) = - \int_0^\infty \frac{e^{i\alpha\sqrt{x}-rx}}{-i\sqrt{x}+q} dx$$

Contribution of $U + D$ as $R \rightarrow \infty, \varepsilon \rightarrow 0$

After a little algebra we see

$$\begin{aligned}
I_U + I_D &= -2i \int_0^\infty \frac{e^{-rx}(\sqrt{x}\cos(\alpha\sqrt{x})+q\sin(\alpha\sqrt{x}))}{x+q^2} dx \\
&= -4i \int_0^\infty \frac{e^{-rx^2}(x^2\cos(\alpha x)+qx\sin(\alpha x))}{x^2+q^2} dx
\end{aligned} \tag{5.1}$$

For $p \in \mathbb{R}$, $q \geq 0$, $\mu \geq 0$ define

$$\begin{aligned}
F(\mu) &= \int_{-\infty}^{\infty} \frac{e^{-\mu^2 x^2 + ipx}}{x^2 + q^2} dx \\
\Rightarrow F'(\mu) &= -2\mu \int_{-\infty}^{\infty} e^{-\mu^2 x^2 + ipx} dx + 2\mu q^2 F(\mu) \\
\Rightarrow (e^{-\mu^2 q^2} F)' &= -2\sqrt{\pi} e^{-\mu^2 q^2 - \frac{p^2}{4\mu^2}} \\
\Rightarrow e^{-\mu^2 q^2} F(\mu) - F(0) &= -2\sqrt{\pi} \int_0^\mu e^{-q^2 x^2 - \frac{p^2}{4x^2}} dx
\end{aligned}$$

To compute $F(0)$ we imagine an origin-centered semi-circle of radius R in the upper-half plane and its intercept with x-axis as our contour δ and integrate $\frac{e^{ipz}}{z^2 + q^2}$ over it and take limit as $R \rightarrow \infty$. Contribution of the circular arc vanishes

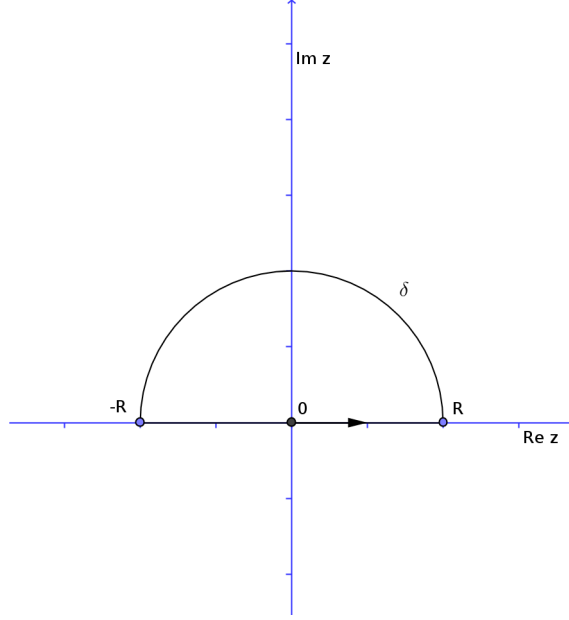


Figure 2: Contour δ

as $R \rightarrow \infty$ and as δ contains one pole of the integrand, namely, iq , using residue theorem we end up with

$$\int_{-\infty}^{\infty} \frac{e^{ipx}}{x^2 + q^2} dx = \frac{\pi e^{-pq}}{q}$$

Therefore, using our "useful" integral we arrive at

$$\begin{aligned} g_1(\mu) &:= \int_{-\infty}^{\infty} \frac{e^{-\mu^2 x^2 + ipx}}{x^2 + q^2} dx = \int_{-\infty}^{\infty} \frac{e^{-\mu^2 x^2} \cos(px)}{x^2 + q^2} dx \\ &= \frac{\pi e^{\mu^2 q^2}}{2q} \left[2 \cosh(pq) - e^{-pq} \operatorname{erf}\left(q\mu - \frac{p}{2\mu}\right) - e^{pq} \operatorname{erf}\left(q\mu + \frac{p}{2\mu}\right) \right] \end{aligned} \quad (5.2)$$

Differentiating (5.2) with respect to p we get

$$\begin{aligned} g_2(\mu) &:= \int_{-\infty}^{\infty} \frac{x e^{-\mu^2 x^2} \sin(px)}{x^2 + q^2} dx \\ &= \frac{\pi e^{\mu^2 q^2}}{2} \left[-2 \sinh(pq) - e^{-pq} \operatorname{erf}\left(q\mu - \frac{p}{2\mu}\right) + e^{pq} \operatorname{erf}\left(q\mu + \frac{p}{2\mu}\right) \right] \end{aligned} \quad (5.3)$$

Using (5.2), (5.3) we see

$$\begin{aligned} I_U + I_D &= -2i \left[\int_{-\infty}^{\infty} e^{-rx^2} \cos(\alpha x) dx - q^2 g_1(\sqrt{r}) + q g_2(\sqrt{r}) \right] \\ &= -2i \left[\int_{-\infty}^{\infty} e^{-rx^2 + i\alpha x} dx - q^2 g_1(\sqrt{r}) + q g_2(\sqrt{r}) \right] \\ &= -2i \left[\frac{\sqrt{\pi} e^{-\frac{\alpha^2}{4r}}}{\sqrt{r}} - \pi q e^{rq^2 + q\alpha} \operatorname{erfc}\left(q\sqrt{r} + \frac{\alpha}{2\sqrt{r}}\right) \right] \end{aligned}$$

Therefore, by Cauchy's theorem

$$\frac{1}{2\pi i} I(L) = \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} \frac{e^{-\alpha\sqrt{\rho} + \rho r}}{\sqrt{\rho} + q} d\rho = \frac{e^{-\frac{\alpha^2}{4r}}}{\sqrt{\pi r}} - q e^{rq^2 + q\alpha} \operatorname{erfc}\left(q\sqrt{r} + \frac{\alpha}{2\sqrt{r}}\right)$$

Therefore,

$$\mathcal{L}^{-1}\left(\frac{e^{-\sqrt{\rho}\alpha}}{\sqrt{\rho} + q}\right) = \frac{e^{-\frac{\alpha^2}{4r}}}{\sqrt{\pi r}} - q e^{rq^2 + \alpha q} \operatorname{erfc}\left(q\sqrt{r} + \frac{\alpha}{2\sqrt{r}}\right) \quad (5.4)$$

which immediately implies,

$$\mathcal{L}^{-1}\left(\frac{e^{-\sqrt{\rho}\alpha}}{\sqrt{\rho}}\right) = \frac{e^{-\frac{\alpha^2}{4r}}}{\sqrt{\pi r}} \quad (5.5)$$

An integral identity

Since all roads lead to Rome, we must have

$$\begin{aligned} q e^{q^2 r} \operatorname{erf}(q\sqrt{r}) * \frac{e^{-\frac{\alpha^2}{4r}}}{\sqrt{\pi r}} &= \int_0^r q e^{q^2(r-t)} \operatorname{erf}(q\sqrt{r-t}) \frac{e^{-\frac{\alpha^2}{4t}}}{\sqrt{\pi t}} dt = e^{q^2 r + \alpha q} - \operatorname{erfc}\left(\frac{\alpha}{2\sqrt{r}}\right) \\ &\quad - \frac{e^{q^2 r}}{2} \left[2 \sinh(q\alpha) - e^{-q\alpha} \operatorname{erf}\left(q\sqrt{r} - \frac{\alpha}{2\sqrt{r}}\right) + e^{q\alpha} \operatorname{erf}\left(q\sqrt{r} + \frac{\alpha}{2\sqrt{r}}\right) \right] \end{aligned} \quad (5.6)$$

Now using (2.4), (5.4), (5.5) we get

$$b = \frac{e^{-\frac{(z+H)^2}{4r}}}{\sqrt{4\pi r}} + \frac{e^{-\frac{(z-H)^2}{4r}}}{\sqrt{4\pi r}} - \frac{w_o}{K} e^{\frac{w_o^2 r}{K^2} + \frac{w_o}{K}(z+H)} \operatorname{erfc}\left(\frac{w_o \sqrt{r}}{K} + \frac{z+H}{2\sqrt{r}}\right) \quad (6.1)$$

Solution of (2)

An identical procedure yields

$$a = -\frac{A e^{-\frac{y^2}{4r}}}{\sqrt{\pi r}}, \quad A = \frac{\partial \hat{a}}{\partial y}(\rho, 0+) - 1, \quad \hat{a} = \int_0^\infty e^{-\rho r} a(r, y) dr$$

Now as

$$a(0+, y) = \delta(y) \text{ and } \lim_{r \rightarrow 0} \frac{e^{-\frac{y^2}{4r}}}{\sqrt{4\pi r}} = \delta(y)$$

we must have $A = -\frac{1}{2}$ and finally,

$$a = \frac{e^{-\frac{y^2}{4r}}}{\sqrt{4\pi r}} \quad (6.2)$$

Combining (6.1), (6.2) we have

$$c(r, y, z) = \frac{Q e^{-\frac{y^2}{4r}}}{4\pi u r} \left[e^{-\frac{(z+H)^2}{4r}} + e^{-\frac{(z-H)^2}{4r}} - \frac{2w_o \sqrt{\pi r}}{K} e^{\frac{w_o^2 r}{K^2} + \frac{w_o}{K}(z+H)} \operatorname{erfc}\left(\frac{w_o \sqrt{r}}{K} + \frac{z+H}{2\sqrt{r}}\right) \right] e^{-\frac{w_{set}^2}{4K^2} r - \frac{w_{set}}{2K} z + l} \quad (6.3)$$

with the constant l yet to be determined. Taking limit $r \rightarrow 0+$ we get

$$\frac{Q}{u} \delta(y) \delta(z-H) = \frac{Q}{u} \delta(y) \delta(z-H) e^{-\frac{w_{set}}{2K} z + l}$$

Note that this solution was obtained by assuming $y \in [0, \infty)$ (so that we could compute Laplace transforms) but symmetry allows us to extend this solution to $y \in (-\infty, \infty)$. Integrating the last equation over $y \in (-\infty, \infty)$ and $z \in [0, \infty)$ we have

$$1 = e^{-\frac{w_{set}}{2K} H + l}$$

which gives us

$$c(r, y, z) = \frac{Q e^{-\frac{w_{set}^2}{4K^2} r - \frac{y^2}{4r} - \frac{w_{set}}{2K}(z-H)}}{4\pi u r} \left[e^{-\frac{(z+H)^2}{4r}} + e^{-\frac{(z-H)^2}{4r}} - \frac{2w_o \sqrt{\pi r}}{K} e^{\frac{w_o^2 r}{K^2} + \frac{w_o}{K}(z+H)} \operatorname{erfc}\left(\frac{w_o \sqrt{r}}{K} + \frac{z+H}{2\sqrt{r}}\right) \right] \quad (6.4)$$

Solution when $H = 0$

(2.4) takes the following form when $H = 0$.

$$\hat{b} = \frac{e^{-\sqrt{\rho}z}}{\sqrt{\rho} + q}$$

and a remains unchanged. So our solution becomes

$$c(r, y, z) = \frac{Qe^{-\frac{w^2}{4K^2}t - \frac{y^2}{4r} - \frac{w_{sgt}}{2K}z}}{2\pi ur} \left[e^{-\frac{z^2}{4r}} - \frac{w_o\sqrt{\pi r}}{K} e^{\frac{w_o^2 r}{K^2} + \frac{w_o z}{K}} \operatorname{erfc} \left(\frac{w_o\sqrt{r}}{K} + \frac{z}{2\sqrt{r}} \right) \right]$$

which is same as the solution that we get from (6.4) by taking limit $H \rightarrow 0$.

Some numerical computations

In this section we try to measure pollutant concentrations due to roads using our simplistic model.

Region of influence for a point source

In this section we compute the region influenced by a point source. To compute the region of influence around a point, we draw a circle of radius R around the point. We have 360 directions, 1 degree apart. We pick a direction and place an emitter on the circle along that direction and compute its effect on the center. Then we shift the emitter away from the center along the same direction until the new effect becomes a certain fraction (called `drop_ratio`) of the old effect and we stop at that point (called `drop_point`). We figure out the `drop_point` for each direction and make a polygon out of them. Below are some figures depicting region of influence for a point source.

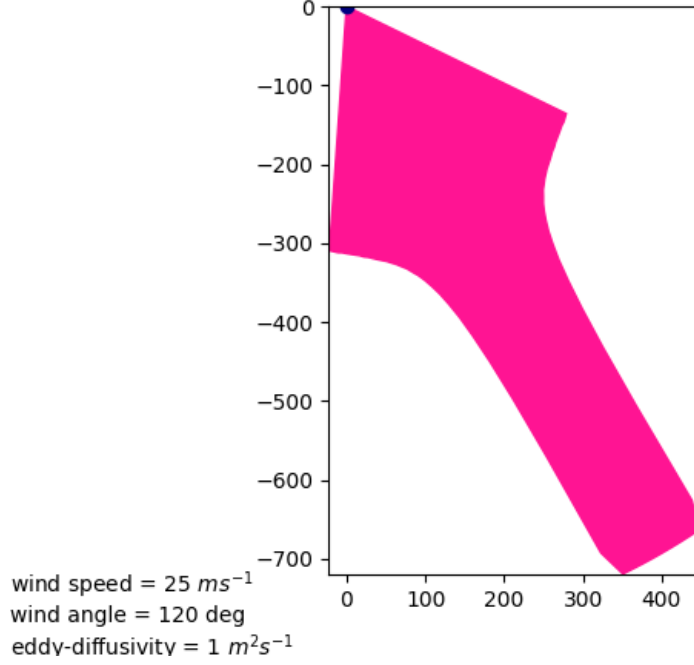


Figure 3: Influence polygon for $R = 300\text{m}$, $w_{set} = w_{dep} = 0 \text{ ms}^{-1}$, $H = 0$ and $\text{drop_ratio} = 10^{-10}$, $u = 25 \text{ ms}^{-1}$

OpenStreetMap^[1]

OpenStreetMap (OSM) is a collaborative project to create a free editable map of the world. We used OSM database to pull out the road network structures we required for this section. When queried for a road network around a location, OSM returns a multigraph with each edge being a straight line. To deal to curvy roads simply more nodes are included in the graph. For example here is the dirvable road network for within 1 kilometer of ICTS with the degree 2 nodes hidden to avoid cluttering.

Pollution Data^[2]

Pollution data for this section were collected from aqicn.org through their application programming interface. There are 5 monitoring centers in Bangalore that upload data pollution data to aqicn. Each of the centers uploads concentration levels for various pollutants e.g. CO, NO₂, PM2.5, PM10, O₃, SO₂. For our computation we'll focus on NO₂ and the monitoring center located at Peenya, one of the biggest industrial areas in Asia.

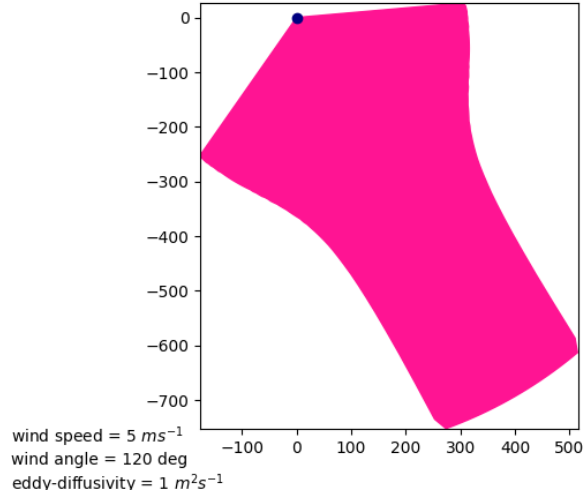


Figure 4: Influence polygon for $R = 300\text{m}$, $w_{set} = w_{dep} = 0 \text{ ms}^{-1}$, $H = 0$ and $\text{drop_ratio} = 10^{-10}$, $u = 5 \text{ ms}^{-1}$

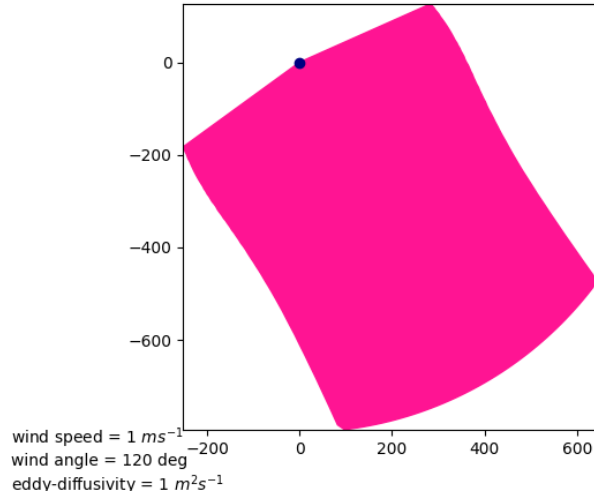


Figure 5: Influence polygon for $R = 300\text{m}$, $w_{set} = w_{dep} = 0 \text{ ms}^{-1}$, $H = 0$ and $\text{drop_ratio} = 10^{-10}$, $u = 1 \text{ ms}^{-1}$

OpenWeatherMap^[3]

OpenWeatherMap is an online service that provides weather data, including current weather data, forecasts, and historical data to the developers of web



Figure 6: Road network within 1 km of ICTS

services and mobile applications. Wind data for this section have been gathered from openweathermap.org.

Road network around Peenya

OpenStreetMap when queried for the road network within 100 km of Peenya returns the following graph. The degree 2 nodes have not been hidden in the figure below. For our analysis we only consider roads categorized in OpenStreetMap as 'motorway', 'primary' and 'trunk'^[4]. These categories are ordered in terms of importance in a descending fashion. Below we provide brief definitions for these categories.

- Motorway: A restricted access major divided highway, normally with 2 or more running lanes plus emergency hard shoulder. Equivalent to the Freeway, Autobahn etc.
- Primary: The most important roads in a country's system that aren't motorways. (Need not necessarily be a divided highway.)

- Trunk: The next most important roads in a country's system. (Often link larger towns.)



Figure 7: Road network within 100 km of Peenya

Deposition and settling velocities of NO_2

If we assume our pollutant particle is a perfect sphere of radius R the total force acting on it due to gravity and buoyancy of air is given by

$$F = \frac{4}{3}\pi R^3(\rho_p - \rho_a)g$$

where ρ_g and ρ_a are respectively the densities of our pollutant and air. According to Stoke's law this force is equal to $6\pi\mu R w_{set}$ where μ is the dynamic viscosity of air, when the pollutant is settling or has achieved terminal velocity. Which gives us

$$w_{set} = \frac{2(\rho_p - \rho_a)R^2g}{9\mu}$$

The bond length between the nitrogen atom and the oxygen atom is 119.7 pm source with the bonds having an angle of 134.3° between them. Therefore for

our purposes,

$$\begin{aligned}
R &\approx 1.20 \times 10^{-10} \text{ m} \\
g &\approx 9.81 \text{ m s}^{-1} \\
\rho_p &\approx 1.45 \times 10^3 \text{ kg m}^{-3} \\
\rho_a &\approx 1.23 \text{ kg m}^{-3} \\
\mu &\approx 1.81 \times 10^{-5} \text{ kg m}^{-1} \text{ s}^{-1}
\end{aligned}$$

Which sets

$$w_{set} \approx 2.51 \times 10^{-12} \text{ m s}^{-1}$$

Therefore, w_{set} for NO_2 is effectively zero which is what we use in our model.

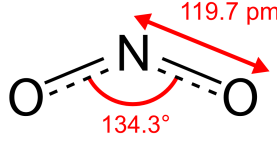


Figure 8: NO_2 bonds

Although data on deposition velocity of NO_2 is hard to come by for Indian cities, a study^[5] on deposition velocities of atmospheric nitrogen in a typical red soil agro-ecosystem in Southeastern China found the average deposition velocity for NO_2 to be $1.2 \times 10^{-3} \text{ m s}^{-1}$. As Bangalore has similar soil type^[6], we set $w_{dep} = 1.2 \times 10^{-3} \text{ m s}^{-1}$ in our model.

Our model for computation

In our model for computing NO_2 concentration at Peenya we assume the following.

- Every part of the of the road network has uniform and identical emission rate.
- The road network entirely lies on the $z = 0$ plane.
- The latitude-longitude of locations have been converted to 2D coordinates using Universal Transverse Mercator projection.
- Pollution sources further than 100 km do not affect the concentration at the point of interest.
- A point source follows equation (6.4) and a line-source follows the line-integrated version of (6.4) with Q being replaced with a quantity Q_s denoting emission rate per unit length with unit $[\text{kg}\cdot\text{m}^{-1}\text{s}^{-1}]$.

- Wind speed and direction are constant over the region in consideration.
- Eddy diffusivity K is a constant over the region of interest.
- We treat Q_s, K as the parameters of our model and try to fit them to the empirical data.
- 22% of NO_2 emissions are due to on road vehicles.^[8]

Range of K, Q_s

According to a 2000 study^[7] on vertical eddy diffusivity in the troposphere, lower stratosphere and mesosphere in Gadanki, Andhra Pradesh, the annual median value of K in $\text{m}^2 \text{s}^{-1}$ is contained in the interval $[e^{-1.3}, e^{0.25}] \subset (0.27, 1.3)$. For our numerical minimization we have used $(0.1, 2)$ as the bounding interval for the value of K in $\text{m}^2 \text{s}^{-1}$.

The bounding interval for Q_s in $\mu\text{g m}^{-1} \text{s}^{-1}$ in our computation was taken to be $(1, 10^7)$.

Results

The pollutant concentration and wind data for this section were recorded on 2018/07/23 at 08 : 00 : 00 am and 08 : 16 : 31 am respectively. Since the wind data does not vary considerably during hourly time-span at the location of interest, 16.5-minute-difference in the observations here is acceptable. Our numerical computation suggests

$$Q_s \approx 32.89 \mu\text{g m}^{-1} \text{s}^{-1}, \quad K \approx 1.00 \text{m}^2 \text{s}^{-1}$$

These values minimize the function $(c_t - c_e)^2$ where c_t and c_e are the theoretical and empirical concentrations with the minimum value being $\approx 4.93 \times 10^{-20} (\mu\text{g})^2 \text{m}^{-6}$.

Informal verification

Due to unavailability of data we try to verify the order of magnitude of our Q_s using some informal calculations in this section. Source-1 (pg-IV) says 36% of the vehicle-related NO_2 comes from heavy goods vehicles (HGV), source-2 (table-2) says emission rate of NO_x for a HGV is $\approx 7 \times 10^{-3} \text{g s}^{-1}$ and source-1 (pg-II, paragraph 3) says NO_2/NO_x ratio for vehicles is ≈ 0.5 . If there are n HGVs per kilometer of the road then disregarding movement of vehicles we get

$$\begin{aligned} (n \times 10^{-3} \text{m}^{-1}) \times (0.5 \times 7 \times 10^{-3} \text{g s}^{-1}) &= (32.89 \times 10^{-6} \text{g m}^{-1} \text{s}^{-1}) \times (0.36) \\ \implies n &\approx 3.39 \end{aligned}$$

In this calculation, we've assumed that all the road-related NO₂ emissions come from major highways which suggests that this is an over-estimation of n . According to source-3 there are 5 vehicles per kilometer road in India. According to source-4 about 50% of these are HGVs. Then assuming these vehicles are uniformly distributed on road, are stationary and constantly emitting pollutants we have

$$n \approx 5 \times 0.5 \approx 2.5$$

The data taken from source-3 were recorded in 2009 which suggests this might be an underestimation of n . These computations suggest our Q_s is most likely of correct order of magnitude.

References

- [1] <https://www.openstreetmap.org>
- [2] <http://aqicn.org/city/bangalore/>
- [3] <https://openweathermap.org/>
- [4] <https://wiki.openstreetmap.org/wiki/Key:highway>
- [5] Dry deposition velocity of atmospheric nitrogen in a typical red soil agro-ecosystem in Southeastern China. Zhou J1, Cui J, Fan JL, Liang JN, Wang TJ.
- [6] https://en.wikipedia.org/wiki/Bangalore_geography_and_environment
- [7] Seasonal variation of vertical eddy diffusivity in the troposphere, lower stratosphere and mesosphere over a tropical station D. Narayana Rao, M. V. Ratnam, T. N. Rao, and S. V. B. Rao.
- [8] <http://www.airqualityontario.com/science/pollutants/nitrogen.php>
- [9] The Mathematics of Atmospheric Dispersion Modeling. John M. Stockie.

Sources used in informal verification

Source-1 : NO₂ emission from the fleet of vehicles in major Norwegian cities. Rolf Hagman, Karl Idar Gjerstad and Astrid H. Amundsen.

Source-2 : NO_x emissions from heavy-duty and light-duty diesel vehicles in the EU: Comparison of real-world performance and current type-approval requirements. The international council on clean transportation.

Source-3 : 2012 World development indicators. The world bank.

Source-4 : 2013 Road Traffic Survey Report. Government of Karnataka Public Works, Ports & Inland Water Transport Department.

Code

Code used in the numerical computation is available at <https://github.com/pinakm9/apm> (although not documented yet).