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A note on the distribution function of density fluctuations in the model COFIN

Eine Notiz zur Verteilungsfunktion der Dichtefluktuationen im Modell COFIN

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Abstract

In the model COFIN the density fluctuations in a plume are derived from LIDAR measurements. However, the distribution function given is neither normalized nor non-negative. It is shown how these deficiencies can be removed.

Preface to second edition

The only change with respect to the first edition is a correction of the graphical representation of the Weibull distribution.

1 Analysis of the COFIN model

The report Risø-R-1329(EN)[1] on the model COFIN describes in chapter 3.11 a model for the probability density function (pdf) $P(c, y)$ of concentration fluctuations in the moving system of a plume. c is the concentration and y the (horizontal) distance from the plume axis. We cite from this report. A pdf is normalized, i.e. it has to fullfill the equation

$$\int_0^\infty P(c, y)\, dc = 1 \,. \tag{1}$$

The following definitions are made:

$$c_n(y) = \int_0^\infty P(c, y)\, c^n\, dc \ \text{ for } \ n = 1, 2, \ldots, \tag{2}$$

$$c_{n,0} = c_n(0) \,, \tag{3}$$

$$c_0 = c_{1,0} \,, \tag{4}$$

$$\sigma_n^2 = \int_{-\infty}^{+\infty} c_n(y)\, y^2\, dy \Big/ \int_{-\infty}^{+\infty} c_n(y)\, dy \,. \tag{5}$$

The following relations have been observed analysing LIDAR measurements:

$$c_n(y) = A_n f(y/\sigma_n) \,, \tag{6}$$

$$\frac{\sigma_1}{\sigma_n} = \frac{n + \beta}{1 + \beta} \text{ with } \beta \approx 1.9 \,, \tag{7}$$

$$P(c, 0) = g_2(c) \,, \tag{8}$$

$$g_p(c) = \frac{p}{c_0 \Gamma(p)} \left(\frac{pc}{c_0}\right)^{p-1} \exp(-pc/c_0) \,. \tag{9}$$

From these relations the following pdf is deduced:

$$P(c, y) = [1 - \gamma(y)]\, \delta(c) + \gamma(y) P_c(c, y) \,, \tag{10}$$

$$P_c(c, y) = \frac{4c}{c_0^2} \frac{1 + 2s(\beta - 2) + 4se^{2s}c/c_0}{1 + 2s\beta} \exp\left[-e^{2s}2c/c_0 + 2s(3 - \beta)\right] \,, \tag{11}$$

$$\gamma(y) = \left(1 + 2\frac{|y|}{\sigma_0}\right) \exp(-2|y|/\sigma_0) \,, \tag{12}$$

$$\sigma_0 = \frac{1 + \beta}{\beta} \sigma_1 \,, \tag{13}$$

$$s = \frac{|y|}{\sigma_1(1 + \beta)} \,. \tag{14}$$

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[1] M.Nielsen, P.C.Chatwin, H.E. Jørgensen, N.Mole, R.J.Munro, S.Ott: *Concentration Fluctuations in Gas Releases by Industrial Accidents — Final Report.* Risø-R-1329(EN), Risø National Laboratory, Roskilde, Denmark (May 2002)

The general structure of $P_c(c, y)$ is

$$P_c(c, y) = a_1(y)c[1 + a_2(y)c] \exp[-a_3(y)c], \tag{15}$$

$$a_1(y) = \frac{4}{c_0^2} \frac{1 + 2s(\beta - 2)}{1 + 2s\beta} \exp[2s(3 - \beta)], \tag{16}$$

$$a_2(y) = \frac{4se^{2s}}{c_0[1 + 2s(\beta - 2)]}, \tag{17}$$

$$a_3(y) = \frac{2e^{2s}}{c_0}. \tag{18}$$

Equation (1) applied to equation (10) yields

$$1 - \gamma(y) + \gamma(y) \int_0^\infty P_c(c, y) \, dc = 1. \tag{19}$$

That means P_c itself must be normalized. We try to verify this condition in the following. Using the relations

$$\int_0^\infty c \exp(-a_3 c) \, dc = a_3^{-2}, \tag{20}$$

$$\int_0^\infty c^2 \exp(-a_3 c) \, dc = 2a_3^{-3} \tag{21}$$

we get:

$$\int_0^\infty P_c(c, y) \, dc = \frac{a_1}{a_3^2} + \frac{2a_1 a_2}{a_3^3}, \tag{22}$$

$$= \frac{a_1}{a_3^3}(a_3 + 2a_2), \tag{23}$$

$$= \frac{a_1}{a_3^3} \left\{ \frac{2e^{2s}}{c_0} + \frac{8se^{2s}}{c_0[1 + 2s(\beta - 2)]} \right\}, \tag{24}$$

$$= \frac{a_1}{a_3^3} \frac{2e^{2s}}{c_0} \frac{1 + 2s(\beta - 2) + 4s}{1 + 2s(\beta - 2)}, \tag{25}$$

$$= \frac{4}{c_0^2} \frac{1 + 2s(\beta - 2)}{1 + 2s\beta} \frac{c_0^3}{8} \frac{2}{c_0} \frac{1 + 2s\beta}{1 + 2s(\beta - 2)} \exp[2s(3 - \beta) - 6s + 2s], \tag{26}$$

$$= \exp[2s(1 - \beta)]. \tag{27}$$

Therefore, the pdf $P_c(c, y)$ is correctly normalized only if $s = 0$, i.e. on the plume axis.

2 Correction of the deficiencies

The deficiency seems to have its origin in a typing error in equation (COFIN.163) which correctly should read

$$
\begin{aligned}
P(c,y) =& [1 - \gamma(y)]\,\delta(c) \\
&+ \exp[2s(1-\beta)]H(\zeta)[1 - 2s(1-\beta)] - 2cs\exp[2s(2-\beta)]H'(\zeta)\,,
\end{aligned}
\tag{28}
$$

$$
\zeta = ce^{2s}\,.
\tag{29}
$$

This can be written as

$$
P(c,y) = [1 - \gamma(y)]\,\delta(c) + \gamma(y)e^{2s}\frac{(1 - 2s + 2s\beta)H - 2s\zeta H'}{1 + 2\beta s}
\tag{30}
$$

using

$$
\gamma(y) = (1 + 2\beta s)\exp(-2\beta s)\,.
\tag{31}
$$

Therefore, we have

$$
P_c(c,y) = e^{2s}\left\{H(\zeta) - \frac{2s}{1 + 2\beta s}[H(\zeta) + \zeta H'(\zeta)]\right\}\,.
\tag{32}
$$

The function $H(\zeta)$ is normalized, therefore

$$
\int_0^\infty P_c(c,y)\,\mathrm{d}c = \int_0^\infty \left\{H(\zeta) - \frac{2s}{1 + 2\beta s}[H(\zeta) + \zeta H'(\zeta)]\right\}\,\mathrm{d}\zeta\,,
\tag{33}
$$

$$
= 1 - \frac{2s}{1 + 2\beta s}[1 - 1]\,,
\tag{34}
$$

$$
= 1
\tag{35}
$$

using partial integration for the evaluation of $\int \zeta H'(\zeta)\,\mathrm{d}\zeta$. Starting from equation (32), also the higher moments of the pdf can be checked:

$$
c_n = \int_0^\infty P(c,y)c^n\,\mathrm{d}c\,,
\tag{36}
$$

$$
= \gamma(y)\int_0^\infty P_c(c,y)c^n\,\mathrm{d}c \ \text{ for } \ n > 1\,,
\tag{37}
$$

$$
= \gamma(y)e^{-2ns}\int_0^\infty \left\{\zeta^n H(\zeta) - \frac{2s}{1 + 2\beta s}[\zeta^n H(\zeta) + \zeta^{n+1}H'(\zeta)]\right\}\,\mathrm{d}\zeta\,,
\tag{38}
$$

$$
= \exp[-2s(\beta + n)]\left\{(1 + 2\beta s)H_n - 2s[H_n - (n+1)H_n]\right\}\,,
\tag{39}
$$

$$
\text{with } \ H_n = \int_0^\infty H(\zeta)\zeta^n\,\mathrm{d}\zeta\,,
\tag{40}
$$

$$
= H_n[1 + 2s(\beta + n)]\exp[-2s(\beta + n)]\,,
\tag{41}
$$

$$
= H_n[1 + 2|y|/\sigma_n]\exp[-2|y|/\sigma_n]\,.
\tag{42}
$$

This is the required expression of equation (6).

Replacing $H(\zeta)$ in equation (32) by the Gamma distribution $g_2(\zeta)$ of equation (9)

$$g_2(\zeta) = \frac{4\zeta}{c_0^2} \exp(-2\zeta/c_0)\,, \tag{43}$$

$$\zeta g_2'(\zeta) = \zeta \left[\frac{4}{c_0^2} \exp(-2\zeta/c_0) - \frac{8\zeta}{c_0^3} \exp(-2\zeta/c_0) \right]\,, \tag{44}$$

$$= g_2(\zeta) \left[1 - \frac{2\zeta}{c_0} \right] \tag{45}$$

yields the pdf

$$P_c(c, y) = e^{2s} g_2(\zeta) \left\{ 1 - \frac{2s}{1 + 2\beta s} \left[2 - 2\frac{c}{c_0} e^{2s} \right] \right\}\,, \tag{46}$$

$$P_c(c, y) = \frac{2}{c_0} e^{2s} \varphi e^{-\varphi} \left\{ 1 - \frac{2s}{1 + 2\beta s} (2 - \varphi) \right\}\,, \tag{47}$$

$$\varphi = 2\frac{c}{c_0} e^{2s}\,. \tag{48}$$

It is easily verified that this form of $P_c(c, y)$ is normalized:

$$\int_0^\infty P_c(c, y)\, \mathrm{d}c = \int_0^\infty \varphi e^{-\varphi} \left\{ 1 - \frac{2s}{1 + 2\beta s} (2 - \varphi) \right\} \mathrm{d}\varphi\,, \tag{49}$$

$$= 1\,. \tag{50}$$

However, P_c is not always non-negative. From equation (47) it can be seen, that P_c is negative if $1 + 2s[\beta - 2 + \varphi]$ is negative. This occurs for small values of c (small φ) and large values of s because $\beta < 2$. The same holds for the P_c of equation (COFIN.166).

This deficiency can be avoided if the general form of the Gamma distribution with $p < 2$ is used. If we replace $H(\zeta)$ in equation (32) by

$$g_p(\zeta) = \frac{p}{c_0 \Gamma(p)} \varphi^{p-1} \exp(-\varphi)\,, \tag{51}$$

$$\text{with}\ \ \varphi = p\zeta/c_0\,, \tag{52}$$

$$\zeta g_p'(\zeta) = \frac{p}{c_0 \Gamma(p)} \left(\frac{p\zeta}{c_0} \right)^{p-1} [p - 1 - p\zeta/c_0] \exp(-p\zeta/c_0)\,, \tag{53}$$

$$= \frac{p}{c_0 \Gamma(p)} \varphi^{p-1} [p - 1 - \varphi] \exp(-\varphi) \tag{54}$$

we get the following relation

$$P_c(c, y) = e^{2s} \frac{p\varphi^{p-1}}{c_0 \Gamma(p)} \frac{1 + 2s[\beta - p + \varphi]}{1 + 2\beta s} \exp(-\varphi)\,. \tag{55}$$

It can be seen that P_c is non-negative only if $p \leq \beta \approx 1.9$. It might be possible on the base of the available data to adjust the value of p or β appropriately. A better solution probably is to replace the Gamma distribution by a Weibull distribution $w(c)$:

$$w_p(c) = \frac{p}{\hat{c}} \left(\frac{c}{\hat{c}}\right)^{p-1} \exp\left[-\left(\frac{c}{\hat{c}}\right)^p\right], \tag{56}$$

$$\hat{c} = c_0/\Gamma(1 + 1/p), \tag{57}$$

$$cw'_p(c) = \frac{p}{\hat{c}} \left(\frac{c}{\hat{c}}\right)^{p-1} \exp\left[-\left(\frac{c}{\hat{c}}\right)^p\right]\left[p - 1 - p\left(\frac{c}{\hat{c}}\right)^p\right]. \tag{58}$$
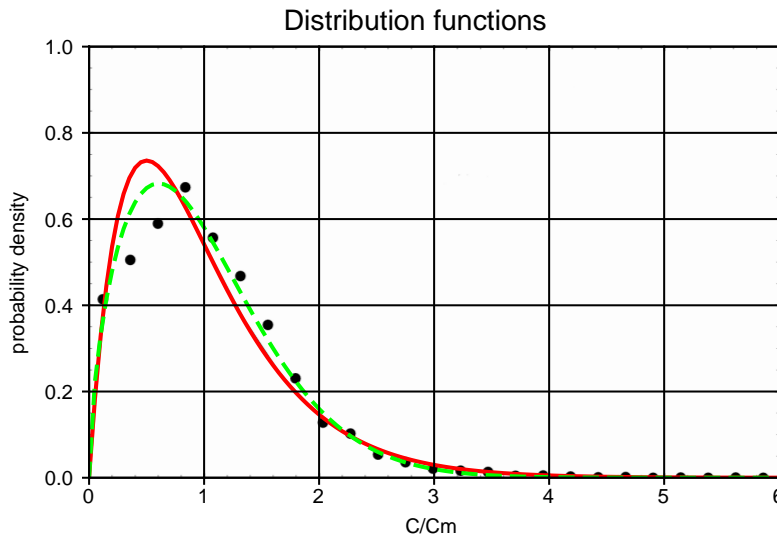
In this case, equation (32) takes the form

$$P_c(c, y) = e^{2s} \frac{p}{\hat{c}} \frac{\psi^{p-1}}{1 + 2\beta s} \exp\left(-\psi^p\right)[1 + 2\beta s - 2s(1 + p - 1 - p\psi^p)], \tag{59}$$

$$\text{with } \psi = \frac{\zeta}{\hat{c}} = \frac{c}{c_0} e^{2s}\Gamma(1 + 1/p), \tag{60}$$

$$= e^{2s} \frac{p}{c_0} \frac{\psi^{p-1}\Gamma(1 + 1/p)}{1 + 2\beta s} \exp\left(-\psi^p\right)[1 + 2s(\beta - p + p\psi^p)]. \tag{61}$$

The distribution of the concentration fluctuations on the plume axis in the moving frame is well approximated by a Weibull distribution with $p \approx 1.6$, as can be seen from the following picture:

Comparison of distribution functions: Gamma distribution with $p = 2$ (solid, red), Weibull distribution with $p = 1.6$ (dashed, green) and experimental data (dots).

Using this Weibull distribution the pdf P_c is non-negative.