Chapter 5
Model Validation

A rigorous validation of footprint models is an issue of importance that cannot be overstated. This is so to make sure that their practical applications can be successful. Due to the relative limited amount of robust flux footprint tracer experimental data, emerging models are often compared with other models. Already, the Schuepp et al. (1990) model has been the object of multiple cross-comparisons against airborne flux observations or against the Lagrangian simulations either in its original publication or in a companion paper by Leclerc and Thurtell (1990); the early analytical model proposed by Schuepp et al. (1990) made the object of numerous intercomparisons against other footprint models (Leclerc and Thurtell 1990; Horst and Weil 1992; Schmid 1994; Leclerc et al. 1997; Sogachev et al. 2005). ‘Benchmark’ Lagrangian model by Leclerc and Thurtell (1990) was previously validated against three earlier artificial tracer flux footprint experiments ranging from the simplest outside the roughness layer of smooth homogeneous surfaces to the more difficult rough and within the roughness layer of non-homogeneous rough forest canopies (Finn et al. 1996; Leclerc et al. 2003a; Leclerc et al. 2003b).

There are only a few models which can be selected as reference model. Support for model validations comes to us via the use of LES-based footprint models: such a model reference is invaluable given the wide range of applications of these models to a broad range of atmospheric boundary-layer conditions and over inhomogeneous surfaces. Their application close to the surface is limited due to the validity of the sub-grid scale parameterization. Markkanen et al. (2009) applied such an approach with an LES model deemed to be an “etalon”. In addition to the model intercomparisons with the experimental validation have a high priority. Unfortunately, tracer studies are complex and laborious to realize. Sulfur

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Table 5.1 Comparison of different footprint models against tracers and other models. For models description see Chap. 3 and Table 1.4

Comparison study	Model to compare	Reference tracer/model
Finn et al. (1996)	Leclerc and Thurtell (1990), Horst and Weil (1992, 1994)	SF_6
Leclerc et al. (1997)	Leclerc and Thurtell (1990), Horst and Weil (1992, 1994)	SF_6
Rannik et al. (2000)	Rannik et al. (2000)	Thomson (1987), Kurbanmuradov and Sabelfeld (2000)
Leclerc et al. (2003b)	Horst and Weil (1992, 1994), Leclerc et al. (1997)	SF_6
Kljun et al. (2003)	Kljun et al. (2002)	Kormann and Meixner (2001)
Kljun et al. (2004)	Kljun et al. (2002)	Wind tunnel
Sogachev et al. (2005)	Sogachev et al. (2002, 2004)	Thomson (1987), Kurbanmuradov and Sabelfeld (2000), Schuepp et al. (1990), Kormann and Meixner (2001)
Steinfeld et al. (2008)	Steinfeld et al. (2008)	Leclerc et al. (1997)
Markkanen et al. (2009)	Rannik et al. (2000; 2003), Kljun et al. (2002)	Steinfeld et al. (2008)
Leclerc et al. (unpublished)	Moeng and Sullivan (1994)	Perfluorocarbons (PFTs)

hexafluoride (SF_6), the traditional tracer, is no longer accepted given its high global warming potential. Other tracers such as perfluorocarbons (PFTs) offer an interesting alternative and only mean concentrations can be measured with the current detection methods; in addition, its technology is limited to a few select laboratories. It is in that perspective that Foken and Leclerc (2004) proposed a validation against natural tracers which using different source areas in different field sites as a proxy. The three methods will be discussed in this chapter. We have limited our discussion here to only such papers which have a high impact in this field (Table 5.1), leaving out studies focused mostly intercomparisons between models according to topic.

For a quantitative comparison, the crosswind averaged 1D footprint functions of the concentration or the flux are compared. The relevant quantitative parameters are the position of the peak, the level of the footprint function of the peak and the extension of the footprint. The latter means that the integral of 50 or 90 % of concentration or flux footprint (effect levels) are also assessed. Due to random uncertainties in the Lagrangian models, the extension of the footprint makes only sense for a limited number of particles released or a defined effect level. More often, the location and the footprint in the maximum (peak) of the footprint function were intercompared. A quantitative comparison of locations and footprint functions for a 2D footprint was recently presented by Markkanen et al. (2009, cf. Sect. 5.4).

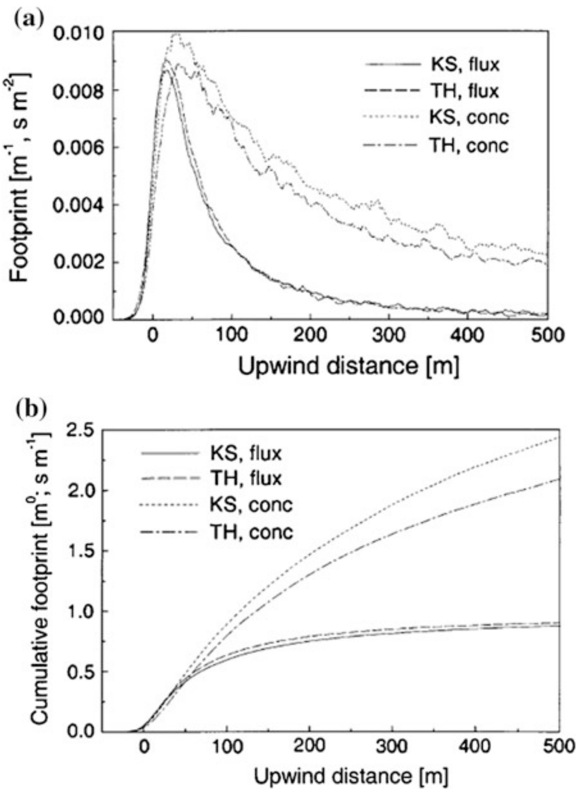


Fig. 5.1 The crosswind integrated **a** footprint function, and **b** its cumulative value, estimated by applying the Lagrangian models of Kurbanmuradov and Sabelfeld (2000, KS) and Thomson (1987, TH), for the observation level 15 m, roughness length 1.5 m, and neutrally stratified flow in the atmospheric surface layer according to Rannik et al. (2000)

5.1 Model Validation Against Other Models

The validation of models against other models is also a very important task. Most of the Lagrangian models based on the well-mixed assumption by Thomson (1987). Therefore, the Kurbanmuradov and Sabelfeld (2000) model, the basis of other models mainly those of Rannik et al. (2000, 2003), was tested against this model. Figure 5.1 shows a good agreement between both models except for the concentration footprint for large upwind distances. This figure also illustrates that the flux footprint is much shorter than the concentration footprint and very well reproduced by both models. The reason is that, close to the measuring point, the trajectories cross the observation level upwards with a positive flux, while for longer distances trajectories moving also downwards leading to a negative contribution to the flux (Rannik et al. 2000).

The comparison against other models was also used to test the model physics. For instance, Rannik et al. (2000) have tested their Lagrangian stochastic simulation with and without along-wind diffusion against the analytical models by Schuepp et al. (1990) and Horst and Weil (1992, 1994). Figure 5.2 shows the

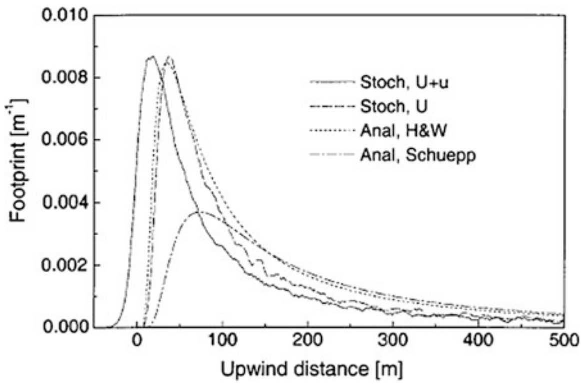


Fig. 5.2 Crosswind integrated flux footprint estimated by the analytical models by Schuepp et al. (1990) and Horst and Weil (1992, 1994, H&W) and stochastic simulation with (U + u) and without (U) along-wind diffusion for the observation level 15 m, roughness length 1.5 m, and neutrally stratified flow in the atmospheric surface layer according to Rannik et al. (2000)

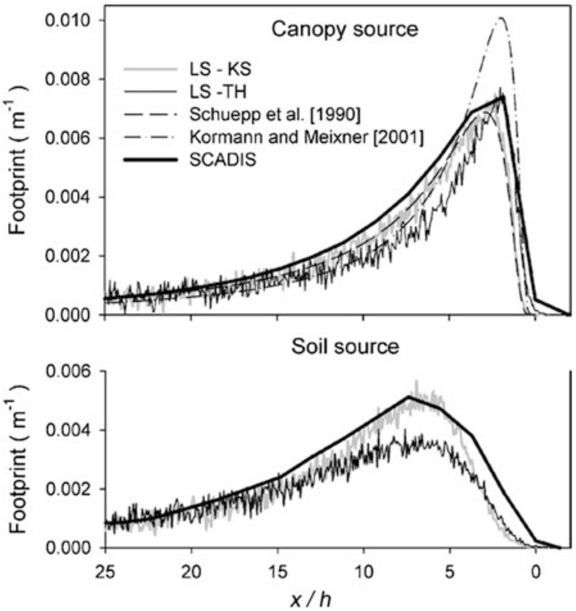


Fig. 5.3 Test of the SCADIS flux footprint model (Sogachev et al. 2002; Sogachev and Lloyd 2004) with footprints derived from both analytical (Schuepp et al. 1990; Kormann and Meixner 2001) and Lagrangian stochastic (Kurbanmuradov and Sabelfeld 2000, LS-KS) and (Thomson 1987, LS-TH) approaches in neutral conditions over a tall homogeneous managed forest ($z = 1.4h_c$) after Sogachev et al. (2005). The distance is normalized by the canopy height x h_c^{-1}, $u_* = 0.46$ m s^{-1}, $d = 9.49$ m, and $z_0 = 1.31$ m, Published with kind permission of © Elsevier, 2005. All Rights Reserved

importance of the along-wind diffusion for a case where the standard deviation of the horizontal wind velocity is of the order of the wind velocity itself, which is the case close to the canopy. Otherwise, the horizontal mean wind velocity is generally much larger than its standard deviation.

The higher-order closure model SCADIS (Sogachev et al. 2002; Sogachev and Lloyd 2004) was compared by Sogachev et al. (2005) with footprints derived from both analytical (Schuepp et al. 1990; Kormann and Meixner 2001) and Lagrangian stochastic (Thomson 1987; Kurbanmuradov and Sabelfeld 2000) approaches in neutral conditions over a tall homogeneous managed pine forest plantation in Florida at a measurement level of 1.4 times of the canopy height. The model footprints exhibit values close to Lagrangian stochastic model results (Fig. 5.3).

Steinfeld et al. (2008) evaluated their Lagrangian simulation (LS) model embedded into an large-eddy simulation code against the work of Leclerc et al. (1997) and found a general agreement when the LS had a subgrid-scale embedded in the turbulence of the LS. They also found that the footprint peak in their model broadly agreed with the results of Leclerc et al. (1997) and the measurements of Finn et al. (1996) with differences in the footprint peak position to be slightly more upstream to the sensor position than the modeled peaks of Leclerc et al. (1997). Steinfeld et al. (2008) attributed this to be possibly because the Leclerc et al. (1997) study did not include the streamwise diffusion on the LS and had a lower resolution. The Steinfeld et al. (2008) model requires that sub-grid scale turbulence be included in the LS for optimum results, as can be seen below in Fig. 5.4. Also Wang and Rotach (2010) compared their LS model with undulating surface against the models by Leclerc et al. (1997) and Steinfeld et al. (2008).

The Steinfeld et al. (2008) study also found that, in neglecting the subgrid-scale parameterisation scheme of turbulent kinetic energy in the embedded Lagrangian simulation model leads, even with the finest resolution, to an underestimation of contributions from near-sensor sources as shown more precise in the cumulative footprint (Fig. 5.5).

Since there is a large demand for results of footprint models in 2D, Markkanen et al. (2009) presented a footprint model validation against the LES which was used as a reference standard (etalon) in a study to evaluate 2D Lagrangian footprints, for observation heights extending throughout the depth of the entire atmospheric boundary layer. As their standard, they used the LES model PALM (Raasch and Schröter 2001) to simulate trajectories of a large number of particles simultaneously with general flow field calculations (Steinfeld et al. 2008). From this data, the footprints are determined in a manner similar to that used in conventional forward Lagrangian models. Markkanen et al. (2009) compared against this Lagrangian footprint model embedded into an LES model the Lagrangian backward simulation footprint model LPDM-B (Kljun et al. 2002) for backward simulations (BW) and the Lagrangian forward simulation model by Rannik et al. (2000, 2003) for forward simulations.

Using the LS forward and backward modes, the models (Rannik et al. 2000; Kljun et al. 2002) examined the sensitivity of the footprint peak with height in the

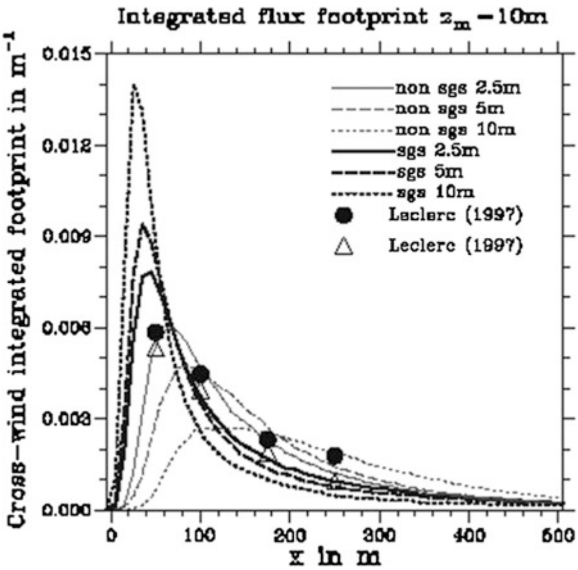
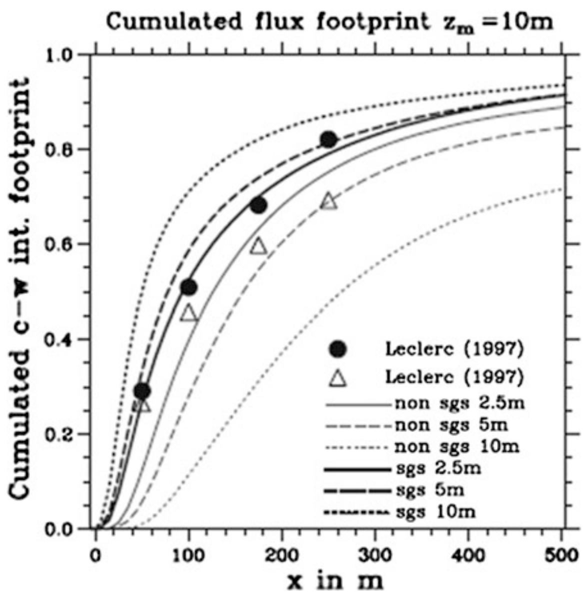


Fig. 5.4 Cross-wind integrated flux footprint for a convective boundary layer similar to that described in Leclerc et al. (1997) for a measurement height of 10 m derived from the six LES runs differing in the application of a subgrid-scale parameterisation scheme (sgs) in the Lagrangian simulation part and in the grid spacing used. For a comparison also the corresponding results derived by Leclerc et al. (1997) from data of the field experiment described in Finn et al. (1996) are shown. (Steinfeld et al. 2008)

Fig. 5.5 Cumulative cross-wind integrated flux footprint for the same case as shown in Fig. 5.4. (Steinfeld et al. 2008)



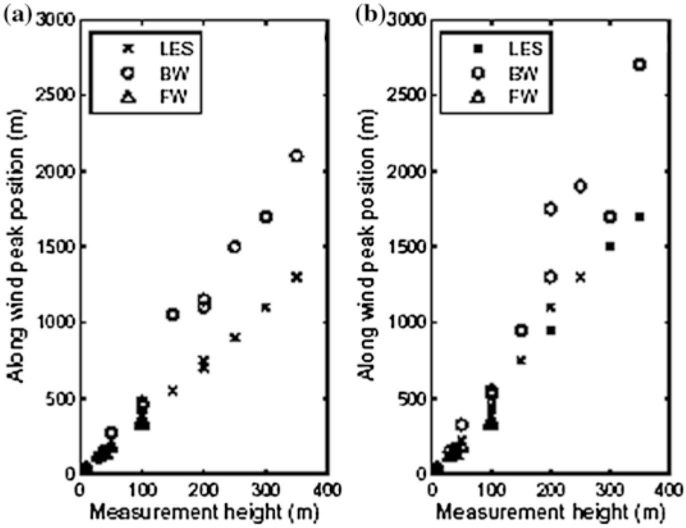


Fig. 5.6 Along-wind peak position of the flux footprint as a function of measurement height for the LES (*crosses*), backward (BW, *circles*) and forward (FW, *triangles*) LS models **a** in the case 1 (*convective*) and **b** in the case 2 (*less unstable*). Results shown only for selected grid resolutions (Markkanen et al. 2009, Published with kind permission of © Copernicus Publications, distributed under the Creative Commons Attribution 3.0 License, 2009. All Rights Reserved)

atmospheric boundary layer, using the LES as their benchmark; they noted that the LS in the backward model's footprint peak departs substantially from their LES counterpart with heights well into the conventional boundary layer. The forward mode, as currently formulated, is a surface layer model so the LS model's peak does not go beyond the top of the surface layer as seen in Fig. 5.6.

5.2 Model Validation and Comparison Against Experimental Data

While much of the efforts related to advance the subject of footprint in a variety of flow over various surfaces i.e. at forest edges, over inhomogeneous surfaces or in complex non-flat terrain have been advancing rapidly, there has been a need to validate the hierarchy of models. The first such study was done by Finn et al. (1996) who conducted a tracer study over a 1–1.5 m tall sagebrush canopy to validate two footprint models. In that experiment, Finn et al. (1996) released sulfur hexafluoride as a passive tracer, and measured the eddy-covariance tracer flux using high-frequency continuous tracer analyzers co-located with sonic anemometers at several distances from a line source and subsequently determined footprint predictions. The tracer flux measurements were made well outside the roughness sub-layer. The measurements were compared against the analytical solution of Horst and Weil (1992, 1994) and the Lagrangian simulation of Leclerc and Thurtell (1990).

Fig. 5.7 Tracer experiment over a peach orchard (*Photograph* by Leclerc)

In a tracer experiment over a peach orchard (Fig. 5.7), Leclerc et al. (2003b) tested several models in the layer outside the roughness sub-layer at the beginning of the summer, and then, due to the rapid orchard growth during summer, for data which were collected within the roughness sub-layer. Both analytical solutions and the Lagrangian simulations of footprints mentioned above tested performed well both within and beyond the roughness sub-layer. In an experiment above a very rough tall managed pine forest plantation, Leclerc et al. (2003a) and Zhang et al. (2010), however, documented that, contributions well outside the footprint envelope contaminate the integrity of flux measurements and that successful footprint modeling applied as long as there are no sharp contrasting temperature differences between the surface of interest (i.e. the pine forest) and the surrounding (the large recently logged swath of land). In these studies, when the wind came from a clearcut located hundreds of meters more than five hundred meters outside the footprint, the tracer fluxes were found to be larger than the modeled footprint fluxes by up to 300 %. Using simultaneously a sodar as a diagnostic tool, the authors noticed that this considerable flux enhancement at the flux tower was accompanied by persistent long lasting vertical motions and both a shift and acceleration of the horizontal flow components during these times. This unexpected flow was part of an organized small-scale circulation—not unlike the land-sea breeze effect—induced by the large fresh hot and bare soil of the clearcut, the latter's temperature (as per the satellite imagery to Landsat records) reaching as much as 20 K higher than the surrounding forest canopy during the day. This result is therefore a tribute to the fortuitous use of fast response continuous eddy-tracer flux measurements, a sodar system, and Landsat maps. Without the combined use of these diagnostic tools, these large errors in the CO_2 flux measurements would normally have gone unnoticed by typical one-point tower CO_2 flux-energy balance measurements alone. This result is of significance since most flux experimentalists work in real, natural, often forested terrain at sites that are less than ideal. The authors therefore recommend that, at many if not most sites, spatial observations of the three-dimensional component of the flow be made in concert with surface-atmosphere exchange point measurements.

5.3 Model Validation with Natural Tracers

The use of a natural tracer experiment over two adjoining surfaces consisting of crops of contrasting fluxes as a means to evaluate footprint models was highlighted earlier by Foken and Leclerc (2004). A schematic layout for a footprint comparison experiment with natural tracers is shown in Fig. 5.8. The fluxes of two contrasting surfaces are measured by single eddy-covariance flux systems. A third system measures the flux from a footprint area, which includes different percentage of the fluxes from the two surfaces depending on the atmospheric stability.

Göckede et al. (2005) used the proposed setup (Fig. 5.8) to validate footprint models using a natural tracer experiment consisting of two dissimilar adjoining surfaces (ploughed field and grassland) with respective fluxes. They tested the FSAM footprint model of Schmid (1997, 2002) and the Lagrangian forward simulation model by Rannik et al. (2000, 2003) and found that the Lagrangian simulation of footprints produce a better performance than the FSAM as shown in the Fig. 5.9 The models vary more dramatically in the near field with the LS performing better. This is due to the natural inclusion of the distance of the sources being included in the trajectories of the particles through the Markov process.

In practice, however, the lack of near-field in the FSAM for the purpose of experiments carried out only a few meters near the ground exerts a minor effect as Göckede et al. (2005) have shown. However, there exists many cases where experiments are carried out using flux systems at greater levels and stable conditions, and in this case the lack of inclusion of the near field in the FSAM could lead to dramatically important errors.

5.4 Classification of the Comparison Results

Most comparisons of footprint models evaluated the crosswind-integrated footprint (Fig. 5.10a). These footprint shapes can be similar despite the fact that the location of the 2D footprint can be very different (Fig. 5.10b). To overcome this deficit, Markkanen et al. (2009) sought to find a more objective way of quantifying similarities and differences. They selected two criteria for this comparison.

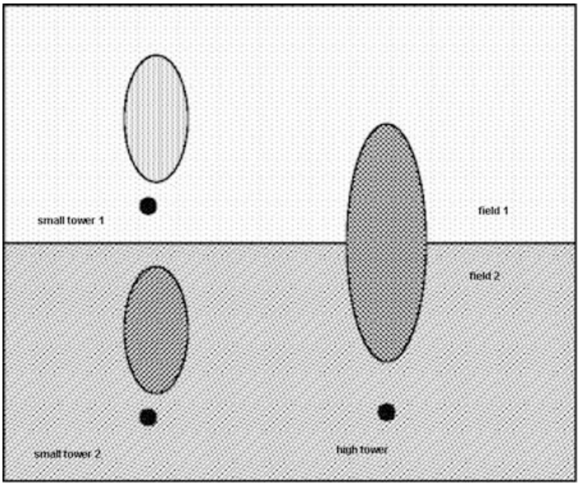


Fig. 5.8 Schematic layout for a footprint comparison experiment with natural tracers according to Foken and Leclerc (2004), Published with kind permission of © Elsevier, 2004. All Rights Reserved

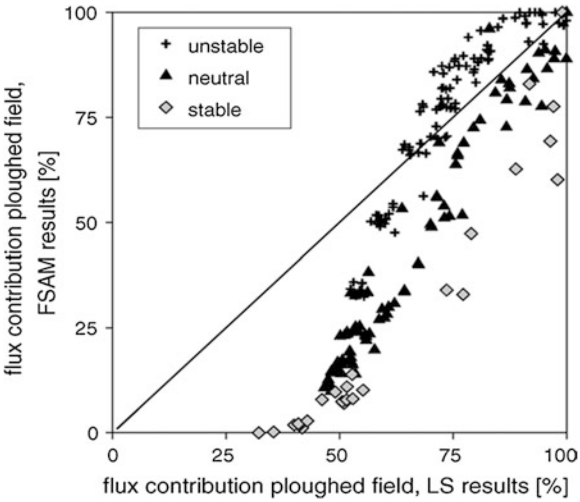


Fig. 5.9 Comparison of the footprint results of the analytic (FSAM, Schmid 1997, 2002) and Lagrangian (LS Rannik et al. 2000, 2003) footprint models for the percentage flux contribution of the ploughed field area at eddy-covariance measurement according to Göckede et al. (2005), Published with kind permission of © Elsevier, 2005. All Rights Reserved

Firstly, for both models, they evaluated the smallest areas contributing 10 (the smallest ellipse in the centre of the footprint), 20, 50 and 80 % (the largest ellipse at the outer border) to the footprints that is $\Omega_p = \Omega_{10}, \Omega_{20}, \Omega_{50}, \Omega_{80}$, respectively. Then they determined the intersection of the two models i.e. both the reference and the validated models ($\Omega_p^{val} \cap \Omega_p^{ref}$) written as $\Omega_p \cap$. In order to compare the equality of predicted footprint functions, the signal predicted by both models originating from $\Omega_p \cap$ can be determined. When both these values are close to or in agreement with the target percentage, the two models agree perfectly. Secondly, of practical relevance, is also the equality of the size of the area of level P by the qualified

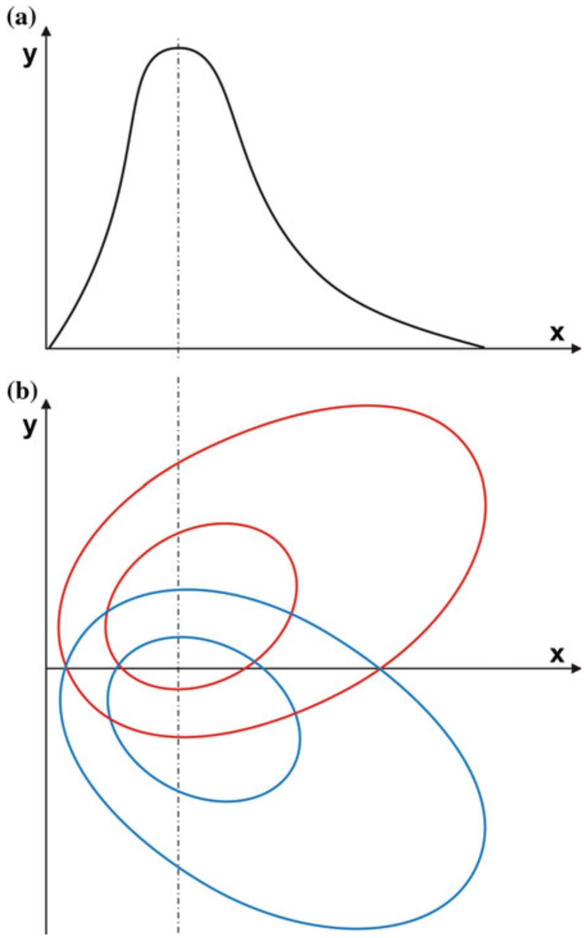


Fig. 5.10 In part **a** the crosswind integrated footprint is shown (1D), which is identical for both 2D footprints shown in part **b**. But the 2D footprints, which are identical in size, cover widely different areas

Table 5.2 Quality categories for footprint comparison according to Markkanen et al. (2009)

Quality comparison	Code	$\frac{\left\|\Omega_p^{val}-\Omega_p^{ref}\right\|}{\Omega_p^{ref}}$ size agreement (%)	$\frac{1-\Omega_p^{\cap}}{\Omega_p^{ref}}$ overlapping agreement (%)
High agreement	3	>60	>70
Moderate agreement	2	>40	>50
Low agreement	1	>20	>30
No agreement	0	<20	<30

model Ω_p^{val} and the reference model Ω_p^{ref}. Also, the footprint size has an influence on the first comparison. Therefore, only a combination of both investigations can provide a good measure for comparison. Accordingly, Markkanen et al. (2009) finally presented a classification of the level of model agreement with the

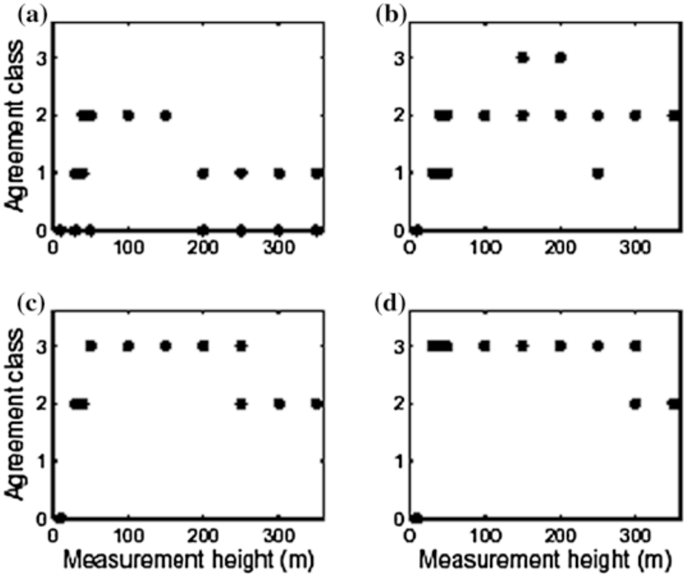


Fig. 5.11 Agreement classes for validation of the flux footprints predicted by the LES parameterization (Steinfeld et al. 2008) without Coriolis force against the parameterization including Coriolis force in the convective case $L = -32$ m. Validations results for (**a**) Ω_{10} (**b**) Ω_{20} (**c**) Ω_{50} and (**d**) Ω_{80}. are shown only for selected grid resolutions ($\Delta x > 0.4\ z_m$) according Markkanen et al. (2009). The small areas around the footprint peak Ω_{10} are often not at the same place and a low quality follows especially for large heights. In contrast the 80 % footprint Ω_{80} overlaps well and a very good quality of agreement is given in nearly all heights. For the classes of agreement see Table 5.2 Published with kind permission of © Copernicus Publications, distributed under the Creative Commons Attribution 3.0 License, 2009. All Rights Reserved

reference. The classification is based both on agreement of sizes of the source areas and on the degree of their overlapping. The size agreement between the examined model and the reference is given as follows:

$$\frac{\left|\Omega_p^{val} - \Omega_p^{ref}\right|}{\Omega_p^{ref}} \tag{5.1}$$

and the degree of overlapping as follows:

$$\frac{1 - \Omega_p^{\cap}}{\Omega_p^{ref}} \tag{5.2}$$

The final agreement class ranging from 0 to 3 (no agreement to good agreement) is consequently determined according to the decision shown in Table 5.2. This method of classification was principally adopted from Rebmann et al. (2005)

and in the updated version by Göckede et al. (2008) for footprint applications for FLUXNET stations. The latter developed a scheme to combine footprints with the land cover data and with the quality check of turbulent fluxes (Foken et al. 2004), for details see Sect. 7.2.4.

An example of the application of this method is given in Fig. 5.11. While for Ω_{80} the agreement of the LES model (Steinfeld et al. 2008) with and without the Coriolis force is very good (high agreement), it was adequate for lower effect levels but low for low and high measuring heights. For the smallest effect level Ω_{10}, the agreement in measuring heights of 100–200 m only class 2. Here, the influence of the first test is more relevant.

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