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# 1 **An adjoint approach for the analysis of RANS** 2 **closure using pressure measurements on a high-rise** 3 **building**

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9 In this study we investigate the closure of a common turbulence model for Reynolds  
10 averaged Navier–Stokes (RANS) in the framework of variational data assimilation prediction  
11 of wind flows around big structures. This study considers practical experimental settings  
12 where only sparse wall-pressure data, measured in a wind tunnel, are available. The evaluation  
13 of the data model coupling cost functional gradient is efficiently carried out with the exact  
14 continuous adjoint of the RANS model. Particular attention is given to the derivation of  
15 the adjoint turbulence model and the adjoint wall law. Given the dual description of the  
16 dynamics, composed of the RANS model and its adjoint, some methodological settings that  
17 enable diagnosis of the turbulence closure are explored here. They range from adjoint maps  
18 analysis to global constants calibration and finally consider the adjunction of a distributed  
19 parameter. Numerical results on a high-rise building reveal a high reconstruction ability of  
20 the adjoint method. A good agreement in wind load and wake extension was obtained. As  
21 with sparse observations, the sensitivity field is generally not very regular for distributed  
22 parameters, seeking these parameters in a space of more regular functions belonging to the  
23 Sobolev space ( $H^1$ ) is also proposed to strengthen the efficiency of the method. This has  
24 been shown to lead to a very efficient data assimilation procedure as it provides an efficient  
25 descent direction as well as a useful regularisation mechanism. Beyond providing an efficient  
26 data-driven reconstruction technique, the proposed adjoint methodology enables an in-depth  
27 analysis of the turbulence closure and finally improves it significantly.

28 **Key words:**

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29 **MSC Codes** (*Optional*) Please enter your MSC Codes here

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**Abstract must not spill onto p.2**

## 30 1. Introduction

31 During their lifetime, buildings are continuously exposed to wind coming from all directions.  
32 Particularly, due to their extended exposed surface, high-rise buildings and high slender  
33 structures undergo extremely strong lateral aerodynamic forces. As a consequence, large  
34 lateral deflections or, even worse, some problematic tearing affecting security may be  
35 observed. Yet, by having a prior understanding of the airflow surrounding these big structures,  
36 wind loads can be predicted and such issues avoided. To understand how these turbulent  
37 flows affect the structures, physical models along with numerical simulations are usually  
38 deployed. On the one hand, for more than a century, experiments with scaled models of  
39 buildings have been carried out in wind tunnels (Cermak & Koloseus 1954; Jensen 1958).  
40 After years of advancement on measurement techniques together with an increased knowledge  
41 on wind dynamics, tunnel experiments have proven their reliability for loads prediction issues  
42 (Surry 1999; Cochran & Derickson 2011). High-Frequency Force Balance method (HFFB)  
43 (Tschanz & Davenport 1983) and High-Frequency Pressure Integration (HFPI) (Irwin &  
44 Kochanski 1995) are two examples of techniques employed for such force measurements.  
45 Despite many improvements brought to deal with turbulent flows, such techniques provide  
46 only partial information of the complex wind-structure interactions involved. For instance,  
47 when the structure has a complex geometrical shape, the very sparse nature of the cladding  
48 pressure measurements brought by HFPI techniques may lead to a misrepresentation of the  
49 local pressure field.

50 On the other hand, more recently, thanks to the significant progress of computational  
51 capabilities, computational fluid dynamics (CFD) techniques have proven their value to give  
52 a complete representation of these flows, enabling a better understanding of the relation  
53 between the flow structures and the wind loads. However, since an accurate description  
54 of such turbulent flows requires a fine enough resolution, this technique may rapidly  
55 become impractical due to the large computational resources required. To go beyond  
56 this computational limitation, turbulence model closures associated with the Reynolds  
57 averaged Navier–Stokes (RANS) simulation were widely adopted to give some insight  
58 into the time-averaged flow profile. With such models, turbulence characteristics can be  
59 reasonably represented at lower computational costs. Over the years, motivated by the  
60 available computational wind engineering guidelines (Tominaga *et al.* 2008; EN 2005),  
61 several established turbulence models have been deeply investigated (Cochran & Derickson  
62 2011; Meroney & Derickson 2014). While RANS simulations offer good qualitative results  
63 that are physically relevant, due to their inherent assumptions built from accumulated  
64 knowledge on real turbulent flows, close inspection on wind loads reveals typical failures in  
65 their prediction. For instance, early studies by Murakami (1990, 1997) compared the standard  
66  $k - \epsilon$  model (Launder & Sharma 1974) with unsteady large-eddy simulations (LES) and wind  
67 tunnel experiments. They revealed the model's poor accuracy resulting in an over-production  
68 of turbulent kinetic energy in the flow impingement region. Various revisions of the model  
69 (*e.g.*, RNG by Yakhot *et al.* (1992), realizable by Shih *et al.* (1994), MMK by Tsuchiya *et al.*  
70 (1997)) have provided results close to measurements obtained in wind tunnels. Yet, recent  
71 studies have shown that such models still fail to reproduce an accurate recirculation region  
72 behind the building (Yoshie *et al.* 2007; Tominaga & Stathopoulos 2010, 2017).  
73 This accuracy issue may strongly hinder the model predictive skill when compared to  
74 real-world measurements. One way to correct this deficiency consists in devising methods  
75 allowing to couple turbulence modelling with measurements.

76 Indeed, during the last decades, a wide variety of coupling techniques has been increasingly  
77 considered in fluid mechanics applications. Such techniques, commonly referred-to as data  
78 assimilation (DA), have been employed to estimate an optimal flow state provided by a

79 given dynamical model such that it remains close enough to observations. So far, two  
80 different classes of DA techniques have been applied to that end. On the one hand, Bayesian  
81 techniques, often referred to as sequential DA techniques, have been used to estimate  
82 optimal flow parameters from data affected by a high uncertainty level (Meldi & Poux  
83 2017; Mons *et al.* 2016). On the other hand, optimal control techniques, like variational  
84 DA or ensemble-variational DA, have been proposed for direct and large eddy numerical  
85 description models (Mons *et al.* 2016; Gronsksis *et al.* 2013; Yang *et al.* 2015; Mons *et al.*  
86 2017; Li *et al.* 2020; Chandramouli *et al.* 2020; Mons *et al.* 2021). In this latter kind of  
87 approaches, DA is formulated as a constrained optimisation problem (Bryson & Ho 2018).  
88 A cost functional, reflecting the discrepancies between some (incomplete) measurements  
89 of the flow variables and a numerical representation of the flow dynamics, is minimised  
90 using a gradient-based descent method. In such an optimisation problem, the functional  
91 gradient's evaluation is efficiently carried out through the dynamical model's adjoint instead  
92 of a costly finite difference approach (Errico 1997; Plessix 2006). At this point, these  
93 DA methods were often used to reconstruct initial conditions and/or boundary conditions  
94 for nonstationary flow simulation issues (such as large eddy simulations). In the last few  
95 years, mean flow reconstruction problems have also been considered with data assimilation  
96 techniques. In some studies (Foures *et al.* 2014; Symon *et al.* 2017), built from variational DA  
97 techniques, the authors considered laminar steady Navier–Stokes equations corrected by an  
98 unknown volume-force to directly model the turbulence effects. These studies showed that, in  
99 laminar or transitional flows, such models perform well to assimilate synthetic particle image  
100 velocimetry (PIV) data. Other DA studies at high Reynolds number were performed with  
101 RANS turbulence models (Li *et al.* 2017; Singh & Duraisamy 2016; Franceschini *et al.* 2020).  
102 In these works, mean flow DA approaches exploited the turbulence models' structure, which  
103 results from a trade-off between asymptotic theories on turbulence mixing and empirical  
104 tuning to fit experimental data. This was expressed through a calibration process of the  
105 closure constants or of a corrective source term added to the turbulence model. Experimental  
106 knowledge plays here a crucial role. Such studies dealt mainly with fundamental and industrial  
107 oriented flow configurations in which turbulence is often generated at a unique integral  
108 scale. However, to the authors' knowledge, for flow configurations involving complex flow  
109 interactions as in the case of an atmospheric boundary layer around a bluff-body, turbulence  
110 closure structure analysis using DA techniques are still largely unexplored. Nevertheless, it  
111 is noteworthy that formal uncertainty quantification (UQ) techniques have been employed to  
112 interpret these closure models in probabilistic terms (Etling *et al.* 1985; Duynkerke 1988;  
113 Tavoularis & Karnik 1989; Edeling *et al.* 2014; Margheri *et al.* 2014). For example, in a  
114 recent work by Shirzadi *et al.* (2017), global coefficients of the standard  $k - \epsilon$  model were  
115 adapted for unstable atmospheric boundary layer (ABL) flow around high-rise buildings  
116 using a forward UQ technique (*e.g.*, Monte Carlo simulations).

117 In the present work, we propose investigating one of the most common turbulence closure  
118 models for RANS modelling in a variational data assimilation procedure framework. A  
119 continuous adjoint approach is considered and then discretised using a 3D finite volume  
120 scheme.

121 A special attention has been paid to the wall treatment during the derivation of the  
122 ajoint RANS model in order to ensure consistency between the two dual dynamics. One  
123 way of tackling this can be found in the work of Zymaris *et al.* (2010) in the context of  
124 shape optimization. However, in the present work, the second-order finite volume numerical  
125 scheme implies specificities of the formulation of atmospheric boundary layer wall law at  
126 the continuous level. Especially, relationships at the wall boundary expressed at the ground  
127 (face value), and within the logarithmic layer (cell-centered value) coexist. Since atmospheric  
128 boundary layer interacts with the building, wall law is crucial and we propose a fully consistent

129 continuous adjoint approach for this model. Without loss of generality, we will, first, use  
 130 this methodology to investigate the sensitivity fields of the global closure coefficients of the  
 131 high Reynolds realizable revision of the  $k - \epsilon$  model (Shih *et al.* 1994). Their physical  
 132 interpretation will enable us to point out limits on such closure models' applicability for  
 133 data-model coupling purposes, particularly for wind flows around buildings.

134 Contrary to previous data-model studies in which velocity measurements were considered  
 135 on significant parts of the flow domain, we only rely on sparse pressure data measured on  
 136 the building surface. This difference is far from being cosmetic as it leads so far to a much  
 137 more practical experimental setting for large-scale volumetric measurements. Besides, we  
 138 point out some difficulties faced in the literature in coupling RANS modeled 3D flows with  
 139 only parietal experimental measurements. Within that framework we will discuss limitations  
 140 and improvements in estimating wind loads and mean velocities surrounding a high-rise  
 141 building. To address the limitations of common turbulence modelling more efficiently, we  
 142 will then relax the model rigidity by considering a distributed additive control parameter in  
 143 the turbulent dissipation transport equation, where the closure is performed. Beyond the fact  
 144 that it provides a better agreement with real flow data due to the richer control parameter space  
 145 and avoids overfitting to the data thanks to the prior information brought by the RANS model  
 146 structure, the optimal control parameter enables us to identify features that are missing in the  
 147 initial RANS closure hypotheses. To that end, a modified dissipation rate equation and its  
 148 adjoint equation are introduced. A physical interpretation of the reconstructed field will then  
 149 be addressed to point out the limits of models' closure applicability for data-model coupling  
 150 purposes. In the optimisation procedure, the adjoint sensitivity field and the associated cost  
 151 functional gradient is generally irregular for distributed control parameters due to the lack  
 152 of specific treatment. This lack of regularity often even hinders a proper estimation of the  
 153 sensitivity map and requires the adjunction of regularisation terms whose calibration is not  
 154 straightforward. In contrast to this conventional approach, searching the control parameters in  
 155 a space of regular functions: the Sobolev space  $H^1(\Omega)$ , is proposed to regularise the descent  
 156 direction. As will be shown, this leads to a very efficient data assimilation procedure.

157 The paper is organised as follows. We first describe the adjoint-based turbulence model and  
 158 wall-pressure measurements coupling for flow reconstruction around a high-rise building.  
 159 The next section improves the adjoint-based turbulence models' sensitivity analysis tool and  
 160 proposes a corrective turbulence model. Then, the case studied is described. The models'  
 161 sensitivities are discussed, and their performances for flow reconstruction from wall-pressure  
 162 data are presented. Finally, a summary and further outlook are given.

## 163 2. Development for an adjoint-based diagnostics

164 In this section, we set up the variational data-model coupling framework, based on optimal  
 165 control techniques. A particular attention is given to the analytical derivation of the adjoint  
 166 model of one of the most common turbulence models, the realizable revision of  $k - \epsilon$ , coupled  
 167 with near wall closure.

### 168 2.1. Variational approach

169 A generic variational data-coupling problem can be formally described by the following  
 170 optimisation problem :

$$\begin{aligned}
 & \min_{\alpha} \quad \mathcal{J}(\alpha, \mathbf{X}(\alpha), \mathbf{Y}_{\text{obs}}) \\
 & \text{subject to} \quad M_i(\alpha, \mathbf{X}(\alpha)) = 0 \quad i = 1, \dots, N
 \end{aligned}
 \tag{2.1}$$

173 where  $\mathcal{J}()$  is the cost function that quantifies the misfit between observations and the model,  
 174 *i.e.* here measurements and CFD solution respectively, penalised by an *a priori* statistical  
 175 knowledge of these discrepancies in the form of a covariance matrix. Here we refer to the  
 176 flow measurements  $\mathbf{Y}_{\text{obs}}$ , and the predicted flow  $\mathbf{X}$ . The bound  $N$  stands for the number  
 177 of independent variables necessary for a full description of the flow. The minimisation of  
 178 this function is constrained by the set of flow governing equations  $M_i$ . Such problem may  
 179 be solved using a gradient-based algorithm. It consists in iteratively evaluating the cost  
 180 functional and its sensitivity derivatives in order to find the minimum by successive updates  
 of the control variables  $\alpha$ . The sketch of the procedure is given in algorithm 1.

---

**Algorithm 1**  $\min_{\alpha} \mathcal{J}(\alpha, \mathbf{X}(\alpha), \mathbf{Y}_{\text{obs}})$

---

**Initialisation:**  $\alpha^m = \alpha_b$  and  $m=0$

**repeat**

Solve  $\mathbf{M}(\mathbf{X}^m, \alpha^m) = 0$

Compute sensitivity  $\frac{\partial \mathcal{J}}{\partial \alpha}(\mathbf{X}^m, \alpha^m)$

update  $\alpha \rightarrow \alpha^{m+1}$ ;  $m + 1 \rightarrow m$

**until**  $\|\mathcal{J}^m - \mathcal{J}^{m-1}\| < \varepsilon$

---

181

182 In order to properly define the cost function, one may proceed as follows. The only available  
 183 experimental inputs are wall-pressure measurements. Ideally, the discrepancy between the  
 184 experimental pressure measure and the model wall-pressure can be expressed as  $\delta P^w =$   
 185  $P_{\text{obs}}^w - \mathcal{H}(P^w)$  where  $\mathcal{H}(\cdot)$  restricts the pressure fields,  $P$ , at the measurement positions (the  
 186 subscript  $w$  stands for wall). However, due to measurement errors, this difference must be  
 187 weighted by their associated uncertainties. Having no access to the real pressure values, these  
 188 uncertainties have to be estimated. By assuming a normal distribution around the measured  
 189 value, this can be introduced by means of an empirical covariance matrix. Concerning the  
 190 operator  $\mathcal{H}(\cdot)$ , in this work, we have considered interpolation by a Gaussian kernel of half size  
 191 of the building width  $D$ , from the computational grid to the position of the measurements  
 192 to ensure consistency between estimated observation and pressure measurements. So far,  
 193 it should be pointed out that under the assumption of incompressible flow, the pressure  
 194 solved numerically is only defined up to a constant. Thus, the experimental and numerical  
 195 pressures can be compared through respective pressure coefficient  $C_p = \frac{P - P_{\text{ref}}}{1/2\rho U_{\text{ref}}^2}$  with  $P_{\text{ref}}$   
 196 denoting the reference static pressure at the inlet of the domain and  $U_{\text{ref}}$  stands for the inflow  
 197 velocity. We note the difference between numerical and experimental wall pressure values  
 198 by  $\delta C_p^w = C_{p_{\text{obs}}}^w - C_p^w$ .

199 To ensure that the set of parameters  $\alpha$  remains in a realistic set of values, we define a  
 200 physically likely range for each component  $\alpha_i$ . This can be formalised by a penalisation term  
 201 on the cost functional, leading to

$$202 \quad \mathcal{J}(P, \alpha) = \left\| \frac{1}{2} \rho U_{\text{ref}}^2 \delta C_p^w \right\|_{R^{-1}}^2 + \|\alpha - \alpha_b\|_{B^{-1}}^2, \quad (2.2)$$

203 We note the Mahalanobis norm  $\|f\|_{A^{-1}}^2 = \langle f, A^{-1}f \rangle$ , in which  $A^{-1}$  is an inverse covariance  
 204 matrix and  $\langle \cdot, \cdot \rangle$  is the  $L^2$  inner product. Note here that  $R$  is the covariance matrix defined  
 205 from measurement's uncertainties,  $B$  is the covariance matrix associated to the parameter  
 206 validity range. Without loss of generality, a diagonal measurement covariance with a constant  
 207 standard deviation  $\sqrt{R_{ii}} = 1$  is used. This uniformity represents an equal degree of confidence  
 208 for each measurement, and the diagonal structure ensues from an assumption of spatially  
 209 uncorrelated errors, which can be assumed for sufficiently distant measurements. Matrix  $B$

210 corresponds to *a priori* knowledge on the range of values of the parameters. In practice, it  
 211 is worth noting that the role of  $B$  matrix is twofold. In the one hand, it imposes a realistic  
 212 interval in which the parameters can be optimised; while, on the other hand, it ensures a  
 213 consistent scaling between inhomogeneous terms.

## 214 2.2. A RANS model

215 The incompressible airflow surrounding the building can be fully described by its velocity  $\mathbf{u}$   
 216 and pressure  $p$ . This unsteady state, solution of the Navier–Stokes equations, can be further  
 217 decomposed in terms of its mean,  $(\mathbf{U}, P_\phi)$ , that will be resolved and a modeled fluctuation  
 218  $(\mathbf{u}', p')$ . By applying time averaging to the Navier–Stokes equations, one can obtain the  
 219 partial differential equations (PDEs) of the RANS equations in a conservative form, whose  
 220 solution provides the mean wind flow :

$$221 \quad \frac{\partial(\rho U_j U_i)}{\partial x_j} = -\frac{\partial P_\phi}{\partial x_i} + \mu \frac{\partial}{\partial x_j} \left[ \frac{\partial U_i}{\partial x_j} \right] - \frac{\partial}{\partial x_j} \left( \overline{\rho u'_i u'_j} \right), \quad (2.3)$$

$$222 \quad \frac{\partial U_j}{\partial x_j} = 0.$$

224 , where  $\rho$  stands for the fluid density and  $\mu$  the kinematic viscosity. Due to the non-linear  
 225 term, the averaging procedure leads to a second-order moment  $\overline{u'_i u'_j}$ , called the Reynolds  
 226 stress. Since all the unsteadiness and turbulence effects of the wind flow are contained in this  
 227 term, without *a priori* specification of this term, the above system is not closed and cannot  
 228 be solved. The immediate solution for the closure is to include additional transport equations  
 229 to predict the turbulence second-order statistics. Relying on the Boussinesq analogy between  
 230 large-scale dissipation and molecular friction, Reynolds stresses are commonly modeled  
 231 using a turbulent diffusion-like term, so-called eddy viscosity model. Several models have  
 232 been proposed to relate quantities describing turbulent fluctuations. A common practice  
 233 associates the turbulent kinetic energy  $k = 1/2 \sum_i \{u'_i u'_i\}$ , representing the isotropic part of  
 234 the exact Reynolds stress, with the turbulence length scale  $l$ . Due to their simple structures,  
 235 these models often require empirical closure functions or constants which are established and  
 236 determined from experimental knowledge, with an attempt to ensure their widest possible  
 237 applications. For instance, the steady realizable  $k - \epsilon$  turbulence model (Shih *et al.* 1994), in  
 238 which  $\epsilon \sim \frac{k^{3/2}}{l}$  models the turbulence dissipation rate at the viscous scale, is often adopted  
 239 for wind flow expertise around real-world buildings. The Reynolds stress is assumed linearly  
 240 linked to the mean shear stress by an eddy viscosity as follows:

$$241 \quad -\overline{\rho u'_i u'_j} = \mu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \rho k, \quad (2.4)$$

242 where  $\mu_t$  stands for the isotropic (*i.e.* assuming that length and time scales of turbulence are  
 243 smaller than those of the mean flow with no preferential direction) eddy viscosity coefficient.  
 244 Its value is calculated using the relation

$$245 \quad \mu_t = C_\mu \rho \frac{k^2}{\epsilon}. \quad (2.5)$$

246 The coefficient  $C_\mu$ , following the work of Shih *et al.* (1994), is a non uniform constant defined  
 247 by

$$248 \quad C_\mu = \frac{1}{A_0 + A_s U_s \frac{k}{\epsilon}}, \quad (2.6)$$

249 where  $A_s$  and  $U_s$  are functions of the mean strain and rotation rates and  $A_0$  is a closure tuning  
 250 coefficient. Substituting the Reynolds stress model (2.4) in the mean momentum equation  
 251 (2.3) yields to

$$252 \quad \frac{\partial(\rho U_j U_i)}{\partial x_j} = -\frac{\partial}{\partial x_i} \left( P_\phi + \frac{2}{3} \rho k \right) + \frac{\partial}{\partial x_j} \left[ \mu_{eff} \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \right], \quad (2.7)$$

253 where  $\mu_{eff} = (\mu_t + \mu)$  stands for an effective viscosity. It can be noted that the isotropic  
 254 component  $\frac{2}{3} \rho k$  is absorbed in a modified mean pressure  $P = P_\phi + \frac{2}{3} \rho k$  and only the  
 255 anisotropic part of the Reynolds stress plays an effective role in transporting momentum.  
 256 It is worth noting that anisotropy here arises only from the mean flow strain and does not  
 257 depend on the turbulent fluctuations. Moreover, in the computation of the pressure coefficient  
 258 (required for the observation error in the cost functional (2.2)), we subtract the isotropic part  
 259 to obtain  $C_p = \frac{P - \frac{2}{3} \rho k - P_{ref} + \frac{2}{3} \rho k_{ref}}{1/2 \rho U_{ref}^2}$  where  $k_{ref}$  stands for the inflow kinetic energy. With regards  
 260 to the turbulence closure model, the transport of mean turbulent kinetic energy,  $k$ , is described  
 261 by

$$262 \quad \frac{\partial(\rho U_j k)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + \mu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_j} - \rho \epsilon, \quad (2.8)$$

263 where  $\sigma_k$  is a closure constant that enables the scalar mixing of  $k$  to be affected by other  
 264 mechanisms than eddy viscosity. The hypothesis, associated to the value  $\sigma_k = 1$ , in which  
 265 the eddy diffusion affects in the same way the momentum and the turbulent kinetic energy  
 266  $k$ , is analysed in section 5.2.

267 The turbulent dissipation rate transport is described by the model proposed by Shih *et al.*  
 268 (1994)

$$269 \quad \frac{\partial(\rho U_j \epsilon)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_i} \right] + C_1(S, k, \epsilon) S \epsilon - C_2 \frac{\epsilon^2}{k + \sqrt{\mu \epsilon}}, \quad (2.9)$$

270 where  $S = 2(S_{ij} S_{ij})^{\frac{1}{2}}$  is the magnitude of mean strain rate where  $S_{ij} = \frac{1}{2} \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right)$  and  
 271  $C_1 = \max(0.43, \eta / (5 + \eta))$  where  $\eta = Sk / \epsilon$  is the normalised strain rate. The constants  $\sigma_\epsilon$   
 272 and  $C_2$  are closure coefficients that need to be calibrated. Assuming that the generation of  
 273  $\epsilon$  is linked to its redistribution everywhere, as it is established in the log-layer, leads to a  
 274 relationship between these coefficients (details in section 5.2.2). This closure hypothesis is  
 275 analysed as well in section 5.2.

276 To properly close this set of equations (since the model is valid only for high Reynolds  
 277 regimes), an asymptotic behaviour has to be imposed near the wall. Indeed, for large scale  
 278 configurations (*i.e.*, ABL, high-rise buildings), the first grid centre of the finite volume  
 279 discretisation closest to the wall usually falls in the logarithmic layer. The domain covered  
 280 by the first grid cell is noted  $\Omega_c$ , and the values of the flow variables taken at the center of  
 281 these cells are marked  $|_c$ . The wall boundary at the ground and on the tower are respectively  
 282  $\partial\Omega_{gr}$  and  $\partial\Omega_{tower}$ . Following Pope (2001) and recommendations specific to ABL flows in  
 283 Richards & Norris (2011), we consider the following wall-law

$$284 \quad u_\tau = C_\mu^{1/4} k|_c^{1/2}, \quad (2.10)$$

$$285 \quad y^+|_c = \frac{\rho u_\tau y|_c}{\mu}, \quad (2.11)$$

$$286 \quad U^+|_c = \frac{1}{\kappa} f(y^+|_c), \quad (2.12)$$

$$287 \quad U_i t_i|_c = u_\tau U^+|_c, \quad (2.13)$$

$$288 \quad P_k|_c = \rho \epsilon|_c = \frac{\rho u_\tau^3}{\kappa y|_c}, \quad (2.14)$$

$$289 \quad \frac{\partial k}{\partial x_j} n_j = 0 \quad \text{at} \quad \partial\Omega_{\text{tower}} \cup \partial\Omega_{\text{gr}}, \quad (2.15)$$

291 where  $U^+$ ,  $y^+$  are the dimensionless wall unit tangential velocity component and distance  
 292 from wall, respectively,  $n_i$  and  $t_i = 1 - n_i$  are the projections of normal and tangential unit  
 293 vectors onto the boundary face in the orthonormal frame  $(x, y, z)$ . The log function  $f$  is  
 294 an empirical function parametrised by constants which depends on the wall type (such as  
 295 smooth or rough); and  $\kappa = 0.41$  is the Von Kármán constant. The expression of  $f$  is different  
 296 at the ground and on the tower. At the ground rugosity is considered, while the tower is  
 297 assumed to be smooth. This leads to the following wall law

$$298 \quad U^+|_c = \frac{1}{\kappa} \ln(E y^+|_c) \quad \text{at} \quad \partial\Omega_{\text{tower}}, \quad (2.16)$$

299 and

$$300 \quad U^+|_c = \frac{1}{\kappa} \ln\left(\frac{y|_c + z_0}{z_0}\right) \quad \text{at} \quad \partial\Omega_{\text{gr}}, \quad (2.17)$$

301 the eddy viscosity in the cell closest to the wall is then defined such that

$$302 \quad \mu_t = \mu \left( \frac{1}{\frac{\partial U^+}{\partial y^+}|_c} - 1 \right) \quad \text{at} \quad \partial\Omega_{\text{gr}} \cup \partial\Omega_{\text{tower}}, \quad (2.18)$$

303 where  $E = 9.8$  is the roughness parameter for smooth walls (Versteeg & Malalasekera 2007)  
 304 and  $z_0 = 0.02$  m is the roughness length which is relevant for an ABL flow scale.

305 In the first grid cell within the log-region, viscous effects are neglected ( $y^+ \gg \mathcal{O}(1)$ ), and  
 306 then the friction velocity  $u_\tau$  is scaled by the square root of the fluctuations, following the  
 307 empirical expression  $u_\tau = C_\mu^{1/4} k^{1/2}$  with  $C_\mu = 0.09$  in (2.10). In this region, production  
 308 and dissipation balance leads to (2.14). In this equation, the exact expression for a rough  
 309 wall is  $\epsilon|_c = \frac{u_\tau^3}{\kappa(y|_c + z_0)}$ , and we have neglected the roughness length since  $z_0 \approx 0.02 y|_c$ .  
 310 In addition to enforcing the value of  $\epsilon$  at the boundary, equation (2.14) specifies the value  
 311 of production  $P_k$  in  $\Omega_c$ , which corresponds to the second term of the RHS in (2.8). In  
 312 the transport equation of  $k$ , the diffusion term is zero in the log-layer, which implies, under  
 313 energy balance assumption, that  $k$  is uniform. This constitutes a good physical approximation  
 314 (Pope 2001), and leads to (2.15). Finally, constant shear stress assumption across the wall-  
 315 normal direction allows to deduce the eddy viscosity in the first grid cell from the logarithmic  
 316 velocity profile (equation (2.18)), consistently with Kalitzin *et al.* (2005).

317 A similar boundary condition is considered in Zymaris *et al.* (2010), but considering the  
 318 possibility to have a first grid point within the viscous layer (that is in practice never the case  
 319 for ABL flows). In this latter formulation, a Dirichlet boundary condition is considered for  
 320  $k$  through (2.10). For wind engineering applications, a well documented unphysical peak of

321 turbulent kinetic energy close to the wall can be observed and some more advanced near-  
 322 wall modelling formulations have been proposed to reduce this artefact (see for instance  
 323 Hargreaves & Wright 2007; Parente *et al.* 2011; Richards & Norris 2011). Since we need  
 324 to derive the adjoint equations, we have chosen to focus on a more simple and general  
 325 formulation, where the Neumann boundary condition for  $k$  is enforced in equation (2.15)  
 326 (since  $k$  is constant in  $y$  within the log-layer), and equation (2.10) is used to obtain  $u_\tau$ . Let  
 327 us note that this implementation is designed for high Reynolds numbers. It is standard in  
 328 OpenFOAM and is used for instance in Tominaga *et al.* (2008).

### 329 2.3. A continuous adjoint RANS model

330 The optimisation problem (2.1) can be solved increasing the cost function with the constraint,  
 331 *i.e.* the RANS model. This is done through Lagrange multipliers also called adjoint variables.  
 332 The resulting unconstrained optimisation problem can be written in a compact form as

$$333 \quad \mathcal{L}(\mathbf{X}, \mathbf{X}^*, \alpha) = \mathcal{J}(P, \alpha) + \langle \mathbf{X}^*, \mathbf{M}(\mathbf{X}, \alpha) \rangle_\Omega, \quad (2.19)$$

334 where  $\langle \cdot, \cdot \rangle_\Omega$  stands for the spatial  $L^2$  inner-product in the flow domain  $\Omega$ . The mean flow  
 335 state  $\mathbf{X}$  is defined by the set  $(\mathbf{U}, P, k, \epsilon, \mu_t)$ . As for the adjoint state  $\mathbf{X}^*$ , we define it as  
 336  $(\mathbf{U}^*, P^*, k^*, \epsilon^*, \mu_t^*)$ . The term  $\mathbf{U}^*$  stands for the adjoint velocity,  $P^*$  is the adjoint pressure  
 337 field,  $k^*$  is the adjoint turbulent kinetic energy,  $\epsilon^*$  the adjoint kinetic dissipation rate and  $\mu_t^*$   
 338 the adjoint eddy-viscosity.

339 Solving the optimisation problem implies to find the set of parameters, the state vector  
 340 and the adjoint state such that the derivatives of  $\mathcal{L}$  with respect to all variables vanish. To  
 341 this end, based on the application of the Green-Gauss theorem and the use of integrations  
 342 by parts – see the Appendix and the work of Othmer (2008) – the adjoint system reads as  
 343 follows:

$$344 \quad -\rho \frac{\partial U_j U_i^*}{\partial x_j} - \rho U_j \frac{\partial U_j^*}{\partial x_i} - \frac{\partial}{\partial x_j} \left[ \mu_{eff} \left( \frac{\partial U_i^*}{\partial x_j} + \frac{\partial U_j^*}{\partial x_i} \right) \right] + \frac{\partial P^*}{\partial x_i} = D_{U^*,i} \quad (2.20)$$

$$345 \quad \frac{\partial U_j^*}{\partial x_j} = 0 \quad (2.21)$$

$$346 \quad -\frac{\partial \rho U_j k^*}{\partial x_j} - \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k^*}{\partial x_j} \right] - \rho \frac{2}{3} \frac{\partial U_i}{\partial x_i} k^* = D_{k^*} \quad (2.22)$$

$$347 \quad -\frac{\partial \rho U_j \epsilon^*}{\partial x_j} - \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon^*}{\partial x_j} \right] - \rho \frac{\partial P_\epsilon}{\partial \epsilon} \epsilon^* + \rho \frac{\partial s_\epsilon}{\partial \epsilon} \epsilon^* = D_{\epsilon^*} \quad (2.23)$$

$$348 \quad \frac{\partial P_k}{\partial \mu_t} k^* - \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_j^*}{\partial x_i} - \frac{1}{\sigma_k} \frac{\partial k}{\partial x_i} \frac{\partial k^*}{\partial x_i} - \frac{1}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_i} \frac{\partial \epsilon^*}{\partial x_i} = \mu_t^*. \quad (2.24)$$

The right-hand sides are expressed as

$$\begin{aligned} D_{U^*,i} &= \rho k \frac{\partial k^*}{\partial x_i} + \rho \epsilon \frac{\partial \epsilon^*}{\partial x_i} + \rho \frac{2}{3} \frac{\partial k k^*}{\partial x_i} - \frac{\partial P_\epsilon}{\partial U_i} \epsilon^* - \frac{\partial P_k}{\partial U_i} k^* - \frac{\partial}{\partial x_i} \left( \frac{\partial \mu_t}{\partial U_i} \mu_t^* \right) \\ D_{k^*} &= \rho \frac{\partial P_\epsilon}{\partial k} \epsilon^* - \rho \frac{\partial s_\epsilon}{\partial k} \epsilon^* - \frac{\partial \mu_t}{\partial k} \mu_t^* \\ D_{\epsilon^*} &= -\frac{\partial \mu_t}{\partial \epsilon} \mu_t^*, \end{aligned}$$

350 where  $P_k$  and  $P_\epsilon$  stand for the production terms of turbulent energy (second term in the  
 351 RHS of (2.8)) and for the turbulence dissipation rate (second term in the RHS of (2.9)),

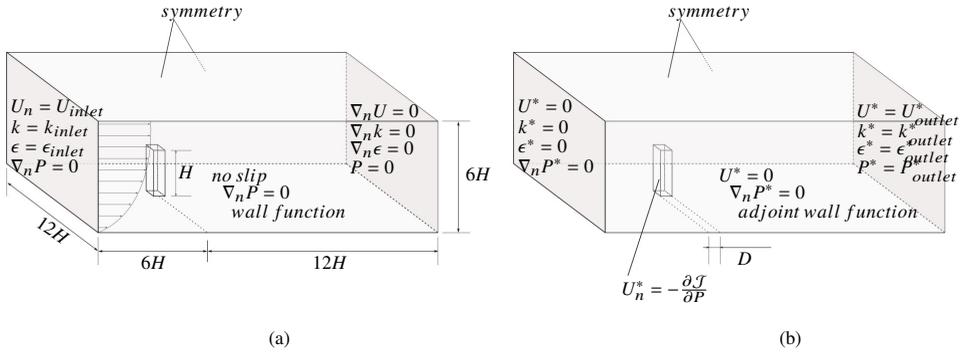


Figure 1: Settings and boundary conditions of the direct (a) and adjoint (b) problems.

352 respectively. As for  $s_\epsilon$ , it denotes the modeled sink of turbulence dissipation rate (third term  
353 in the RHS of (2.9)).

354 Note that as both production terms are functions of the velocity, then chain rule allows to  
355 obtain  $\partial P_\epsilon / \partial U_i$  and  $\partial P_k / \partial U_i$ , see the appendix. Moreover, the system (2.20-2.23) is quite  
356 similar to the one obtained in Zymaris *et al.* (2010), yet, with some differences arising from  
357 the realizability condition of the eddy viscosity expression (last term of  $D_{U_i}$ ). Furthermore,  
358 unlike the derivation of Zymaris *et al.* (2010) in which the eddy viscosity expression is  
359 directly replaced in the RANS equations, the augmentation of the Lagrangian with (2.5),  
360 leading to equation (2.24), has shown to offer better numerical stability in solving the adjoint  
361 system. Indeed, similarly as the iterative computation of the direct RANS system,  $\mu_i^*$  is  
362 updated at each step after solving the equations for  $k^*$  and  $\epsilon^*$ . To solve this adjoint system,  
363 adjoint boundary conditions have to be derived consistently with the boundary conditions of  
364 the direct problem. The next section is dedicated to this crucial point.

#### 2.4. Adjoint boundary conditions

365  
366 The treatment of the adjoint boundary conditions is a central piece in adjoint methods in order  
367 to obtain consistency in the gradient computation. In our case with the transport equations  
368 of turbulent quantities, some treatments are not standard, particularly at the adjoint wall  
369 law. Moreover, some specific treatments are performed at the discrete level of the finite  
370 volume formulation. In this section, we propose to recall the general procedure to obtain  
371 adjoint boundary conditions, and then to detail the conditions to enforce at each boundary.  
372 Boundary conditions for the flow and adjoint fields are summarised in figure 1.

373 Derivation of (2.19) leads, in addition to system (2.20)-(2.23), to a system of boundary  
374 terms. Directional derivative with respect to  $P$ , leads to

$$375 \quad [U_i^* n_i \delta P]_{\partial\Omega} = -\frac{\partial \mathcal{J}}{\partial P} \delta P, \quad (2.25)$$

376 where the boundary integral is defined as  $[\cdot]_{\partial\Omega} = \int_{\partial\Omega} (\cdot) d\partial\Omega$ .

377 Note that differentiation of the cost function, (2.2), w.r.t.  $P$  is computed through the

379 definition of the pressure coefficient. By differentiating with respect to  $U_i$ , we obtain

$$\begin{aligned}
& [P^* \delta U_i n_i]_{\delta \Omega} - \left[ \rho \left( (U_i^* n_i)(U_i n_i) + U_j U_j^* n_i \right) \delta U_i n_i \right]_{\delta \Omega} - \left[ \mu_{eff} (U_i^* n_i + U_j^* n_j) \frac{\partial \delta U_i}{\partial x_j} \right]_{\delta \Omega} \\
& - \left[ \delta U_i \mu_{eff} \left( \frac{\partial U_i^* n_i}{\partial x_j} n_i + \frac{\partial U_j^* n_j}{\partial x_i} n_i \right) \right]_{\delta \Omega} \\
& - \left[ \delta U_i \left( \frac{5}{3} \rho k k^* n_i + \left( \frac{\partial P_k}{\partial U_j} n_i \right) k^* + \rho \epsilon \epsilon^* n_i + \left( \frac{\partial P_\epsilon}{\partial U_j} n_i \right) \epsilon^* + \left( \frac{\partial \mu_t}{\partial U_j} n_i \right) \mu_t^* \right) \right]_{\delta \Omega}.
\end{aligned} \tag{2.26}$$

381 Derivative with respect to  $k$ , leads to

$$\left[ -\frac{2}{3} \rho U_i^* n_i \delta k \right]_{\delta \Omega} + [\rho U_i n_i k^* \delta k]_{\delta \Omega} - \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) k^* \frac{\partial \delta k}{\partial x_j} n_j \right]_{\delta \Omega} + \left[ \frac{\partial \left( \mu + \frac{\mu_t}{\sigma_k} \right) k^*}{\partial x_j} n_j \delta k \right]_{\delta \Omega}, \tag{2.27}$$

383 and with respect to  $\epsilon$  to

$$[\rho U_i n_i \epsilon^* \delta \epsilon]_{\delta \Omega} - \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \epsilon^* \frac{\partial \delta \epsilon}{\partial x_j} n_j \right]_{\delta \Omega} + \left[ \frac{\partial \left( \mu + \frac{\mu_t}{\sigma_k} \right) \epsilon^*}{\partial x_j} n_j \delta \epsilon \right]_{\delta \Omega}. \tag{2.28}$$

385 Finally by deriving with respect to  $\mu_t$ , we obtain

$$\left[ \delta \mu_t \left( \mu_t^* - \left( \frac{\partial U_j}{\partial x_i} n_j + \frac{\partial U_i}{\partial x_j} n_j \right) U_i^* - \frac{\rho}{\sigma_k} k^* \frac{\partial k}{\partial x_j} n_j - \frac{\rho}{\sigma_\epsilon} \epsilon^* \frac{\partial \epsilon}{\partial x_j} n_j \right) \right]_{\delta \Omega}. \tag{2.29}$$

387 Then at each boarder, variations of the direct boundary conditions are injected in the  
388 system (2.25)–(2.29), to obtain the corresponding adjoint boundary conditions.

#### 389 2.4.1. Inlet

390 At the inlet, the direct boundary conditions lead to

$$391 \quad \delta U_i t_i = 0 \quad ; \quad \delta U_i n_i = 0 \quad ; \quad \delta k = 0 \quad ; \quad \delta \epsilon = 0. \tag{2.30}$$

392 Substituting this in (2.25)–(2.28), the system reduces to

$$393 \quad U_i^* t_i = 0 \quad ; \quad U_i^* n_i = 0 \quad ; \quad k^* = 0 \quad ; \quad \epsilon^* = 0. \tag{2.31}$$

394 This quite standard result at the continuous level is not straightforward to implement in the  
395 finite volume formulation. No condition is imposed on  $P^*$  and the inlet boundary condition  
396 for the adjoint pressure is left arbitrary. But, in accordance with (Zymaris *et al.* 2010;  
397 Othmer 2008) and identically as the numerical treatment of the direct inlet pressure  $P$ , zero  
398 Neumann condition on  $P^*$  is imposed to ensure numerical stability. To obtain the other  
399 boundary conditions, the same approach is employed.

#### 400 2.4.2. Outlet

401 At the outlet, the pressure value is prescribed while the other flow variables have their normal  
402 gradient imposed, leading to

$$403 \quad P^* n_i = (U_i^* n_i)(U_i n_i) + (U_j^* U_j) n_i + \mu_{eff} \frac{\partial (U_j^* n_j)}{\partial x_i} n_i + \frac{5}{3} \rho k k^* n_i + \rho \epsilon \epsilon^* n_i + \left( \frac{\partial \mu_t}{\partial U_j} n_j \right) n_i \mu_t^*. \tag{2.32}$$

404 This provides a constraint on the boundary condition to determine the adjoint pressure at the  
 405 outlet. In equation (2.32), the adjoint pressure at the next iteration is determined explicitly by  
 406 evaluating  $U^*$  at the previous iteration. Projecting then the fluxes on the outlet tangent plane,  
 407 we obtain:

$$408 \quad \mu_{eff} \frac{\partial(U_j^* t_j)}{\partial x_i} n_i + (U_i^* t_i)(U_i n_i) = - \left( \frac{\partial \mu_t}{\partial U_i} n_i \right) t_i \mu_t^* - \left( \frac{\partial P_k}{\partial U_j} n_j \right) t_i k^* - \left( \frac{\partial P_\epsilon}{\partial U_j} n_j \right) t_i \epsilon^*. \quad (2.33)$$

409 This equation provides a boundary condition for the tangential component of the adjoint  
 410 velocity.

411 It is worth noting that, instead, an alternative choice could be made by imposing  $P^* = 0$   
 412 and determining the adjoint velocity by solving equations (2.32) and (2.33). Previous works,  
 413 for a different turbulence model (Zymaris *et al.* 2010) or for frozen turbulence assumption  
 414 (Othmer 2008), showed that both implementations yields to identical sensitivities.

415 Derivation w.r.t.  $k$ ,  $\epsilon$  and  $\mu_t$  leads, respectively, to

$$416 \quad \rho k^* U_i n_i + \rho D_k \frac{\partial k^*}{\partial x_i} n_i = \frac{\partial \mu_t}{\partial k} \mu_t^*, \quad (2.34)$$

$$417 \quad \rho \epsilon^* U_i n_i + \rho D_\epsilon \frac{\partial \epsilon^*}{\partial x_i} n_i = \frac{\partial \mu_t}{\partial \epsilon} \mu_t^*, \quad (2.35)$$

$$418 \quad \left( \frac{\partial U_j}{\partial x_i} n_j + \frac{\partial U_i}{\partial x_j} n_j \right) U_i^* = \mu_t^*. \quad (2.36)$$

420 Therefore, for known outlet direct and adjoint velocities, the adjoint eddy viscosity is updated  
 421 through equation (2.36). Then, conditions (2.34) and (2.35) can be imposed to solve  $k^*$  and  
 422  $\epsilon^*$  respectively.

### 423 2.4.3. Symmetry

424 As for the side and top free-stream boundaries under symmetry condition, we assume a zero  
 425 flux of all flow variables,

$$426 \quad \frac{\partial P}{\partial x_i} n_i = \frac{\partial(U_j t_j)}{\partial x_i} n_i = \frac{\partial k}{\partial x_i} n_i = \frac{\partial \epsilon}{\partial x_i} n_i = 0, \quad (2.37)$$

427 and zero normal velocity,

$$428 \quad U_i n_i = 0. \quad (2.38)$$

429 We thus obtain the following boundary conditions for the adjoint variables:

$$430 \quad U_i^* n_i = 0, \quad \frac{\partial(U_i^* t_i)}{\partial x_j} n_j = 0, \quad \frac{\partial k^*}{\partial x_i} n_i = 0, \quad \frac{\partial \epsilon^*}{\partial x_i} n_i = 0, \quad \mu_t^* = 0. \quad (2.39)$$

431 This shows that symmetric boundary conditions are conserved with the adjoint model.

### 432 2.4.4. Walls

433 The wall boundaries are split into two parts, namely  $\partial\Omega_{\text{tower}}$  for the part where data are  
 434 provided, *i.e.* the tower, and  $\partial\Omega_{\text{gr}}$  for the walls at the ground modelling the surrounding  
 435 environment, for which there is no data. Based on equation (2.25) we have

$$436 \quad U_i^* n_i = \frac{\partial \mathcal{J}}{\partial P} \quad \text{at} \quad \partial\Omega_{\text{tower}}, \quad (2.40)$$

$$437 \quad U_i^* n_i = 0 \quad \text{at} \quad \partial\Omega_{\text{gr}}, \quad (2.41)$$

$$438 \quad U_i^* t_i = 0 \quad \text{at} \quad \partial\Omega_{\text{tower}} \cup \partial\Omega_{\text{gr}}. \quad (2.42)$$

440 Therefore exactly in the same way as for the inlet, the no-slip condition on the velocity,  
 441 associated with a zero Neumann condition on the mean pressure, implies a homogeneous  
 442 Dirichlet boundary condition for the adjoint velocity and a zero Neumann condition for  
 443 the adjoint pressure at the ground walls  $\partial\Omega_{\text{gr}}$ . Let us note that due to the wall-pressure  
 444 measurements, the Dirichlet condition on the adjoint variable  $U^*$  is inhomogeneous on the  
 445 normal component along  $\partial\Omega_{\text{tower}}$  at the sensor positions.

446 Considering the adjoint turbulence variables  $(k^*, \epsilon^*, \mu_t^*)$ , it is important to consider the  
 447 expression of the wall-law in order to derive their boundary conditions. As we impose a  
 448 homogeneous Neumann boundary condition for  $k$  in equation (2.15), it can be observed that  
 449 this leads to the same set of conditions as in the outlet (equations (2.34), (2.35) and (2.36)).  
 450 Moreover, with the no slip condition and the set of conditions for the adjoint velocity ((2.40),  
 451 (2.41), (2.42)), the wall boundary conditions for the adjoint kinetic energy, dissipation rate  
 452 and eddy viscosity read as

$$453 \quad k^*|_c = \frac{\partial\mu_t}{\partial k} \frac{\mu_t^*}{\rho U_i n_i} \quad \text{at} \quad \partial\Omega_{\text{tower}} \cup \partial\Omega_{\text{gr}} \quad (2.43)$$

$$454 \quad \frac{\partial\epsilon^*}{\partial x_i} n_i = 0 \quad \text{at} \quad \partial\Omega_{\text{tower}} \cup \partial\Omega_{\text{gr}}, \quad (2.44)$$

$$455 \quad \mu_t^* = 2 \left( \frac{\partial(U_i n_i)}{\partial x_j} n_j \right) U_i^* n_i \quad \text{at} \quad \partial\Omega_{\text{tower}}, \quad (2.45)$$

$$456 \quad \mu_t^* = 0 \quad \text{at} \quad \partial\Omega_{\text{gr}}. \quad (2.46)$$

458 Here,  $\frac{\partial\mu_t}{\partial k}$  is obtained by differentiating the algebraic equation (2.18) using chain rule  
 459 formulae.

460 Furthermore in the direct model, inertial energy balance (2.14) leads to a modification of  
 461 the source terms in (2.8) within the first cell in  $\Omega_c$ . A similar procedure has to be performed  
 462 in the adjoint equation:

$$D_{k^*} = \rho \frac{\partial P_\epsilon}{\partial k} \epsilon^* - \rho \frac{\partial s_\epsilon}{\partial k} \epsilon^* + \rho \left( \frac{\partial P_k}{\partial k} \Big|_c - \frac{\partial \epsilon}{\partial k} \Big|_c \right) k^* \Big|_c \quad \text{and} \quad D_{\epsilon^*} = 0 \quad \text{in} \quad \Omega_c. \quad (2.47)$$

464 At the boundary, the wall law allows to express  $P_k$ ,  $\epsilon$ ,  $P_\epsilon$  and  $s_\epsilon$  as an explicit function of  $k$   
 465 and then to evaluate explicitly the derivatives with respect to  $k$  (not shown here for sake of  
 466 compactness).

467 Hence, with this treatment, wall conditions for the adjoint system are now fully consistent  
 468 with the initial RANS model and leads us thus to a consistent minimisation procedure.

469 Now that we have at our disposal a dual description of the dynamics composed of a  
 470 RANS direct model and the adjoint of its tangent linear representation, we explore three  
 471 methodological settings for an in-depth diagnosis of the turbulence closure. The first tool at  
 472 hand consists simply to inspect the adjoint state maps. The second one consists in optimising  
 473 global constants parameters of the turbulence model for reducing the observation error; and  
 474 to relax/enforce constraints on these parameters to test physical hypotheses. The last one,  
 475 goes one step further and considers the adjunction of distributed unknowns which enables  
 476 to identify a missing term in the equation where the turbulence closure is performed, i.e., in  
 477 the transport equation for the energy dissipation rate in the model considered here. In order  
 478 to conduct an efficient structural inspection, the distributed parameter is sought in a Sobolev  
 479 space and further estimated through a data-assimilation procedure. These three settings are  
 480 described in section 3 and applied then to a high-rise building case study described section  
 481 4. The numerical results on this case study for the three different sensitivity analyses are  
 482 presented in section 5.

### 483 3. Adjoint-based diagnostic tool for turbulence models

484 In the previous section we detailed the construction of a continuous adjoint model (together  
 485 with its consistent boundary conditions) of the tangent linear operator of a RANS model for  
 486 very high Reynolds flow, associated with large integral/body length scales. In this section, we  
 487 present some methodological tools derived from this adjoint operator. Beyond providing a  
 488 data-driven flow reconstruction, it enables us an in-depth analysis of the turbulence closure.

#### 489 3.1. Adjoint state as a basis for sensitivity analysis

While in general, adjoint variables are usually considered as a purely mathematical object, they do have physical meaning as shown in several works (Hall & Cacuci 1983; Giles & Pierce 2000; Gunzburger 2003). Although we know that RANS models (at least with Boussinesq eddy viscosity hypothesis for its closure) does not allow an accurate representation of complex flows, they nevertheless provide some usefull global insights on the flow state. With this in mind, the reconstructed adjoint state enables to highlight a misrepresentation of the turbulent flow by the RANS model, hence, pointing where it is possible to optimise the RANS model parameters to optimally reduce the difference between the CFD state and a given experimental dataset. Moreover, from an optimisation perspective, one may interpret them as a steepest descent direction of an objective cost function, for a particular control parameter. For instance, the adjoint velocity can be seen as the influence of an arbitrary forcing  $\mathbf{f}_u$  acting on the mean momentum equation. This can be shown when deriving an optimality condition by a perturbation of this force,

$$\begin{aligned} \mathbf{M}_u(\mathbf{X}, \alpha) = \mathbf{f}_u &\quad \rightarrow \quad \frac{\partial \mathcal{J}}{\partial \mathbf{f}_u} = \mathbf{U}^*. \\ \text{Momentum equation} &\quad \rightarrow \quad \text{Optimality condition.} \end{aligned}$$

490 Then, as we perform a first update of this forcing by a gradient-descent minimisation  
 491 algorithm, one obtain

$$492 \quad \mathbf{f}_u^{it_1} = (\mathbf{f}_u^{it_0} = 0) - \lambda \mathbf{U}^*,$$

while  $\lambda$  is a positive non-dimensional marching step factor. Through dimensional analysis, one may scale  $\mathbf{U}^*$ , which has the dimension of an acceleration, as  $U^* \sim \frac{U_{\text{ref}}^2}{H_{\text{ref}}}$ . The adjoint velocity features are thus immediately representing a missing term, that can be interpreted as a correction of the Reynolds stress. Examining the adjoint turbulence variables of a  $k - \epsilon$  model, namely  $k^*$ ,  $\epsilon^*$  and  $\mu_t^*$ , similar interpretations can be drawn as we consider arbitrary forcing such as

$$\begin{aligned} M_k(\mathbf{X}, \alpha) = f_k &\quad \rightarrow \quad \frac{\partial \mathcal{J}}{\partial f_k} = k^*, \\ M_\epsilon(\mathbf{X}, \alpha) = f_\epsilon &\quad \rightarrow \quad \frac{\partial \mathcal{J}}{\partial f_\epsilon} = \epsilon^*, \\ M_{\mu_t}(\mathbf{X}, \alpha) = f_{\mu_t} &\quad \rightarrow \quad \frac{\partial \mathcal{J}}{\partial f_{\mu_t}} = \mu_t^*. \end{aligned}$$

493 The adjoint variables shed some light on the flow regions that are sensitive to an eventual  
 494 correction of the turbulence model. As this will be shown in the case study of section 5,  
 495 this interpretation is very helpfull to analyze the incorporation of additional variables to  
 496 define efficient data-driven turbulence closure. These forcings can indeed be associated to  
 497 any of modeled terms meant to adress a particular turbulence modelling error (e.g. energy

498 production, backscattering, redistribution or dissipation). The sensitivity of the associated  
 499 parametric shapes and hyper-parameter can be efficiently obtained and inspected through the  
 500 adjoint operator.

### 501 3.2. Adjoint diagnosis on global closure coefficients

502 Given the adjoint dynamics, the sensitivity of any parameter can be obtained from the  
 503 optimality condition (6.4). Free constants of the RANS model can be finely tuned knowing  
 504 their sensitivities. As we will show for a particular turbulence model (realizable  $k - \epsilon$ ), the  
 505 quality of the associated numerical reconstructions appears to be quite restricted, for a range  
 506 of physically acceptable values of these parameters. The reason of the inefficiency of the  
 507 calibration procedure is interpreted below in terms of a too strong model ‘‘rigidity’’. This  
 508 hindering facts will be later illustrated when we will perform the sensitivity analysis and data  
 509 assimilation on the high-rise building case.

#### 510 3.2.1. A sensitivity field

511 Considering the vector  $\alpha = (A_0, C_2, \sigma_k, \sigma_\epsilon)$  of closure parameters, the optimality con-  
 512 dition (6.4) is obtained by differentiating the Lagrangian (2.19) in the directions  $\delta\alpha =$   
 513  $(\delta A_0, \delta C_2, \delta\sigma_k, \delta\sigma_\epsilon)$ :

$$\begin{aligned}
 \frac{\partial \mathcal{L}}{\partial A_0} \delta A_0 &= \left\langle \frac{\partial M_{\mu_t}}{\partial A_0} \delta A_0, \mu_t^* \right\rangle_\Omega = \langle -\mu_t C_\mu \delta A_0, \mu_t^* \rangle_\Omega = \langle -\mu_t C_\mu, \mu_t^* \rangle_\Omega \delta A_0 \\
 \frac{\partial \mathcal{L}}{\partial C_2} \delta C_2 &= \left\langle \frac{\epsilon^2}{k + \sqrt{\mu} \epsilon}, \epsilon^* \right\rangle_\Omega \delta C_2 \\
 \frac{\partial \mathcal{L}}{\partial \sigma_k} \delta \sigma_k &= \left\langle -\frac{\partial}{\partial x_j} \left[ \frac{\mu_t}{\sigma_k^2} \frac{\partial k}{\partial x_i} \right], k^* \right\rangle_\Omega \delta \sigma_k \\
 \frac{\partial \mathcal{L}}{\partial \sigma_\epsilon} \delta \sigma_\epsilon &= \left\langle -\frac{\partial}{\partial x_j} \left[ \frac{\mu_t}{\sigma_\epsilon^2} \frac{\partial \epsilon}{\partial x_i} \right], \epsilon^* \right\rangle_\Omega \delta \sigma_\epsilon.
 \end{aligned} \tag{3.1}$$

515 So far, this does not include any explicit dependency of the cost on the set of parameters, such  
 516 as a penalisation term. It can be observed that the optimality conditions reduce drastically  
 517 the high dimensional dependency of the model to the lower dimensional parameter space.  
 518 This reduction, performed via the inner product  $\langle \cdot, \cdot \rangle_\Omega$ , does reflect the global compromising  
 519 character of the closure coefficients. This results in a rather rigid situation when seeking data-  
 520 model fitting. However, this rigidity can be understood as a strong confidence in the model  
 521 structure. This strongly constrains the solutions but enables, on the other hand, to assimilate  
 522 very sparse measurements. The examination of the spatially varying adjoint variables to  
 523 diagnose the parameter sensitivity provides useful piece of information even though we deal  
 524 with a rigid parametric model for the reconstruction. This type of analysis will be exploited  
 525 in our case study.

#### 526 3.2.2. Penalty range

527 To ensure realistic numerical solutions, relevant physical range for each of the closure  
 528 coefficients is defined. These constraints are introduced via penalty terms on the control  
 529 parameters through an error covariance matrix, in cost function (2.2). Values of the parameters  
 530 outside of a range defined by the standard deviation are hence strongly penalised. These  
 531 standard deviations are in practice fixed from experiments on prototypical configurations  
 532 of boundary layer or decaying turbulence. This may become questionable in regions where  
 533 the fluid and building interact and near flow separations associated with strong shears. As

534 a matter of fact, the assumptions underlying the concept of eddy viscosity starts to be less  
 535 reasonable in these regions (Pope 2001). Thus, as a compromise, the range limits are fixed  
 536 from experiments as intervals  $\Delta\alpha_i$  centered around the background a priori value. The  
 537 covariance matrix is finally expressed as follows

$$538 \quad B_{ii}^{-1} = \zeta_i \left( \frac{|\frac{\partial \mathcal{J}_0}{\partial \alpha}|}{\Delta\alpha_i} \right).$$

539 As mentioned earlier, this covariance has two roles: first, to impose the trusted (or recom-  
 540 mended) ranges  $\Delta\alpha_i$  and secondly, to ensure a dimensional homogeneity of the cost function  
 541 through the norm of the sensitivity derivative given at the first minimisation iteration  $|\frac{\partial \mathcal{J}_0}{\partial \alpha}|$ .  
 542 The importance of control variables with high values of sensitivity derivatives is strengthened  
 543 in the objective function in comparison to less sensitive parameters. The parameters  $\zeta_i$  are  
 544 dimensionless free parameters allowing to give more or less global *a priori* confidence on  
 545 each parameter. In practice these parameters can be fixed from a priori considerations.

### 546 3.3. Adjoint diagnosis on spatially distributed closure: correction in the dissipation 547 transport equation

548 In contrast to the previous section, we consider now the adjoint system as a basis for  
 549 the inspection of the model misrepresentations through a distributed parameter. Instead of  
 550 correcting coefficients of the model, we consider here the adjunction of a force to one of  
 551 the model equations. We consider a corrective forcing term at the level of the dissipation  
 552 transport equation, where the closure takes place. Then, with the aim to further investigate  
 553 such a closure through a data-assimilation procedure, a specific optimisation in the  $H^1(\Omega)$   
 554 Sobolev space is proposed in order to provide a regularisation procedure that guaranties an  
 555 efficient descent direction as well as an implicit spatial smoothing of the forcing. With this  
 556 regularisation, a significant improvement of the results will be shown in our study case.

#### 557 3.3.1. A corrective model

558 As it was noted in the previous section, due to the model rigidity arising from the drastically  
 559 small parameter space, the flow is not free to visit a sufficiently large domain of the state  
 560 space that is too far from the basic RANS model. To overcome such restrictions, one  
 561 may straightforwardly consider a set of closure parameters with a higher dimension. Still  
 562 maintaining the validity of the Boussinesq approximation, a strategy consists in enriching  
 563 the turbulence model structure. We choose to add a forcing term in the transport equation  
 564 of  $\epsilon$  (equation (2.9)) in order to correct what we may call structural errors, *i.e.* error arising  
 565 from the choice of the turbulence model equation. We could have considered as well a  
 566 control parameter defined directly as the forcing of equation (2.9), however, we preferred to  
 567 introduce some dependency of this forcing to the state variable. We choose a forcing term of  
 568 the form  $-\frac{\rho U_{\text{ref}}}{H_{\text{ref}}} \epsilon f_\epsilon$ , where  $f_\epsilon$  is the dimensionless control parameter. The sign convention  
 569 is chosen so as the added forcing corresponds to a sink of dissipation. The objective of the  
 570 pre-multiplication by  $\epsilon$  is to prevent unphysical dissipation corrections at locations where  
 571 there is no turbulence and to focus specifically on relevant regions such as the shear layers  
 572 and the wake. The constant term  $\frac{\rho U_{\text{ref}}}{H_{\text{ref}}}$  ensures the proper physical dimension. Numerical  
 573 tests presented in section 5.3.1, demonstrate that this term behaves indeed much better than a  
 574 direct forcing term. With this additional forcing, the dissipation transport equation becomes

$$575 \quad \frac{\partial \rho U_j \epsilon}{\partial x_j} - \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_i} \right] - C_1(S, k, \epsilon) S \epsilon + C_2 \frac{\epsilon^2}{k + \sqrt{\mu \epsilon}} = -\frac{\rho U_{\text{ref}}}{H_{\text{ref}}} \epsilon f_\epsilon. \quad (3.2)$$

576 This model remains close to the RANS structure as to avoid overfitting effects in the context  
577 of severe differences between the state space and measurements.

### 578 3.3.2. Sensitivity field

579 The fact that the added distributed parameter depends on the state variable  $\epsilon$ , requires some  
580 modifications of the adjoint equations. In compact form, the adjoint equation on  $\epsilon^*$  reads  
581 now as

$$582 \quad M_{\epsilon^*} = -\frac{\rho U_{\text{ref}}}{H_{\text{ref}}} f_{\epsilon} \epsilon^*, \quad (3.3)$$

where  $M_{\epsilon^*}$  contains all the adjoint terms derived from equation (2.23). Regarding the adjoint  
boundary conditions, since no face flux are involved through the additive term, no changes  
have to be made. The optimality condition associated with the control parameter  $f_{\epsilon}$  is  
obtained by considering the directional derivative

$$\left\langle \frac{\partial \mathcal{L}}{\partial f_{\epsilon}}, \delta f_{\epsilon} \right\rangle_{\Omega} = \left\langle \frac{\rho U_{\text{ref}}}{H_{\text{ref}}} \epsilon \delta f_{\epsilon}, \epsilon^* \right\rangle_{\Omega},$$

583 leading straightforwardly to express the Lagrangian sensitivity to  $f_{\epsilon}$  as

$$584 \quad \frac{\partial \mathcal{L}}{\partial f_{\epsilon}} = \frac{\rho U_{\text{ref}}}{H_{\text{ref}}} \epsilon \epsilon^*. \quad (3.4)$$

585

### 586 3.3.3. Descent direction

With very sparse partial observations and the consideration of spatially distributed control  
parameters, the risks of obtaining local minima or unphysical flow reconstructions is much  
stronger. The control parameter can be any function of  $L^2(\Omega)$ , which allows highly irregular  
functions. Regularisation is a classical way to reduce the number of local minima eventually  
associated to unphysical solutions. To that purpose, penalty of the spatial gradients of  
the control parameter is often considered (Franceschini *et al.* 2020). Such regularisations  
introduces a smoothing penalty parameter on which the solution strongly depends and whose  
value is in general non-trivial to choose. In the following, we consider as an alternative a  
Sobolev gradient regularisation (Protas *et al.* 2004; Tissot *et al.* 2020). It consists to define  
the control parameter in the Sobolev space  $H^1(\Omega)$  which is more regular than  $L^2(\Omega)$ . With  
this approach the functional is still defined in its basic form as

$$\mathcal{J}(P) = \frac{1}{2} \|\rho U_{\text{ref}}^2 \delta C_p^w\|_{R^{-1}}^2.$$

587 Provided the optimality condition (3.4) and for an arbitrary functions  $\psi$  and  $\phi$  in  $H^1(\Omega)$ , the  
588 Sobolev gradient is defined such that

$$589 \quad \left\langle \frac{\partial \mathcal{L}}{\partial f_{\epsilon}}, \psi \right\rangle_{\Omega} = \left\langle \frac{\partial \mathcal{L}}{\partial f_{\epsilon}}^{H^1}, \psi \right\rangle_{H^1}, \quad (3.5)$$

590

with the inner product definition

$$\langle \phi, \psi \rangle_{H^1} = \int_{\Omega} \phi \psi + l_{sob}^2 (\nabla \phi \cdot \nabla \psi) d\Omega,$$

591 in which  $l_{sob}$  is a free parameter homogeneous to a length scale. Through integration by part  
592 of the second term of the inner product (involving the function at gradients), the equality

593 (3.5) leads to the new optimality condition

$$594 \quad \frac{\partial \mathcal{L}}{\partial f_\epsilon}{}^{H^1} = \left( \frac{1}{1 + l_{sob}^2} (\mathbb{I} - l_{sob}^2 \nabla^2) \right)^{-1} \frac{\partial \mathcal{L}}{\partial f_\epsilon}, \quad (3.6)$$

595

596 in which  $\nabla^2$  stands for the Laplacian operator. Equation (3.6) is a filtering of the sensitivity  
 597 in  $L^2(\Omega)$  to the Sobolev space. With this approach, the sensitivity field is consequently  
 598 regularised through the solution of a modified Helmholtz equation. Since matrix inversion  
 599 is not an option in such large system, the Poisson equation (3.6) is here solved through an  
 600 iterative technique expressed within the same finite volume scheme as for the direct RANS  
 601 equations. The additional cost is of the order of magnitude of one additional iteration of  
 602 the RANS solver, but as we shall see it, this clearly leads overall to a gain due to a faster  
 603 convergence of the outer loop optimisation problem. It is worth to mention that this type of  
 604 formulation offers two main advantages compared to classical regularisation terms. In the  
 605 one hand, as opposed to the global penalty coefficient introduced in those latter, the free  
 606 parameter involved in the Sobolev gradient approach is a physical quantity. As a matter of  
 607 fact, this parameter can be seen as a filtering length scale below which the sensitivity field  
 608 is smoothed. It provides us a way to introduce a characteristic length scale relevant with  
 609 the flow (*e.g.*, the building width for instance). In the other hand, the Sobolev gradient does  
 610 ensure a descent direction. Indeed, applying a Taylor expansion of the cost function around  
 611 an initial guess  $f_\epsilon$  in the direction  $\delta f_{\epsilon ps} = -\frac{\partial \mathcal{L}}{\partial f_\epsilon}{}^{H^1}$  can be expressed as follows

$$612 \quad \mathcal{J}(f_\epsilon + h\delta f_\epsilon) = \mathcal{J}(f_\epsilon) + h \left\langle \frac{\partial \mathcal{L}}{\partial f_\epsilon}, \delta f_\epsilon \right\rangle_\Omega + \mathcal{O}(h^2).$$

613 Substituting the second term in the RHS and by using the equality (3.5) yields to

$$614 \quad \mathcal{J}(f_\epsilon + h\delta f_\epsilon) = \mathcal{J}(f_\epsilon) - h \left\| \frac{\partial \mathcal{L}}{\partial f_\epsilon}{}^{H^1} \right\|_{H^1}^2 + \mathcal{O}(h^2),$$

615 in which we define the norm  $\|a\|_{H^1}^2 = \langle a, a \rangle_{H^1}$ . Thus, for a small enough perturbation  $h\delta f_\epsilon$ ,  
 616 we have  $\mathcal{J}(f_\epsilon + h\delta f_\epsilon) < \mathcal{J}(f_\epsilon)$ . Now, injecting this optimality condition into a steepest  
 617 descent algorithm, an update of the forcing at an iteration  $n$  reads:

$$618 \quad f_\epsilon^{n+1} = f_\epsilon^n - \lambda \left. \frac{\partial \mathcal{L}}{\partial f_\epsilon}{}^{H^1} \right|_n, \quad (3.7)$$

619

620 in which the step size is constrained by  $\lambda = \beta / \max(\frac{\partial \mathcal{L}}{\partial f_\epsilon}{}^{H^1})|_{n=0}$  where  $\beta = 2 \cdot 10^{-2}$  is chosen  
 621 based on the sensitivity validation. In the next section, we present some numerical results  
 622 obtained on a realistic case study in terms of the turbulence model parameters estimation and  
 623 in terms of their sensitivity analysis, with the objective of analysing the closure hypotheses  
 624 of a given RANS model using the data assimilation framework.

#### 625 4. Case study

626 In this section, we first describe the wind tunnel experiments. Then, we present the numerical  
 627 setup.

#### 4.1. Description of the wind tunnel experiment

628

629 Experimental data were provided by the CSTB (Nantes, France) from the work of Sheng  
 630 *et al.* (2018). Measurements were performed in the atmospheric boundary layer wind tunnel  
 631 (NSA) with a test section of 20 m long, 4 m wide and 2 m high. Upstream of the isolated  
 632 building, roughness elements and turbulence generator were set to reproduce the wind profile  
 633 perceived by the full scale building. The floor of the wind tunnel is equipped with a turntable  
 634 that enables the flow incidence to vary from 0 to 360°. In the present paper, only one wind  
 635 direction is considered. In these experiments, the building was modeled with a wall-mounted  
 636 prism of square cross-section with the dimensions: 10 cm × 10 cm × 49 cm which corresponds  
 637 to a tower of height  $H = 147$  m and a width  $D = 30$  m at full scale. To perform measurements,  
 638 two tower models were built. The first model was made of Plexiglas which allows for optical  
 639 access and, thus, to use particle image velocimetry (PIV). The second model was equipped  
 640 with 265 pressure taps to measure the unsteady pressure distribution on the modeled building.

641

#### 4.2. Numerical setup

642 The open source library OpenFOAM (5th version of the OpenFOAM foundation) (Weller  
 643 *et al.* 1998) was used to implement the CFD and adjoint governing equations. The library  
 644 utilizes a second order finite volume discretisation approach (Moukalled *et al.* 2016) and a  
 645 fully implicit first order method for time integration. A prediction-correction procedure is  
 646 used for the pressure-velocity coupling based on the Rhie-Chow interpolation (Rhie & Chow  
 647 1983). Correction for mesh non orthogonality was applied for the Poisson solver. A full scale  
 648 building is modeled and a neutral atmospheric boundary model was used (Richards & Hoxey  
 649 1993) to enforce the inlet wind profiles. Profiles for  $U$ ,  $k$  and  $\epsilon$  are defined as

$$650 \quad U_{in} = \frac{u_{\tau}^{ABL} \ln\left(\frac{z+z_0}{z_0}\right)}{\kappa}, \quad k_{in} = \frac{(u_{\tau}^{ABL})^2}{\sqrt{C_{\mu}}} \quad \text{and} \quad \epsilon_{in} = \frac{(u_{\tau}^{ABL})^3}{\kappa(z+z_0)}, \quad (4.1)$$

651 where  $u_{\tau}^{ABL}$  is the friction velocity associated with the constant shear stress along the ABL  
 652 width

$$653 \quad u_{\tau}^{ABL} = \frac{\kappa U_{ref}}{\ln\left(\frac{H_{ref}+z_0}{z_0}\right)}$$

654 in which  $U_{ref}$  and  $H_{ref} = \frac{2}{3}H$  are, respectively, reference velocity and height chosen to  
 655 match with the experimental profiles (and thus the eurocode (EN 2005)) (see figure 2). These  
 656 profiles are consistent with the wall treatment as we prescribe eddy viscosity's ground-value  
 657 by (2.18), such that  $u_{\tau} = u_{\tau}^{ABL}$ . As for the roughness height  $z_0$ , it was set to 0.02, as an  
 658 intermediate between the roughness class I and class II (EN 2005).

659 The size of the computational domain was fixed to ensure that the blockage effects are  
 660 inferior to 3% (Tominaga *et al.* 2008; EN 2005). Grid refinement was chosen to ensure a  
 661 good representation of the wind gradient at the inlet. Unstructured grid was then adopted  
 662 with the minimum distance of the centroid of the cell adjacent to the building walls set to  
 663 0.001  $H$ . This grid refinement reached approximately 3.5 million cells.

664 The adjoint differential equations were discretised using the same CFD library as for the  
 665 direct equations. As for the direct simulation, the adjoint pressure and velocity were iteratively  
 666 solved using a prediction-correction procedure. The discretisation schemes used for the flow  
 667 equations were maintained. Moreover, we note that the derivation of the non-linear terms  
 668 leads to an explicit dependency of the adjoint solution on the direct flow solutions that  
 669 prevents a parallel computation of the two solvers.

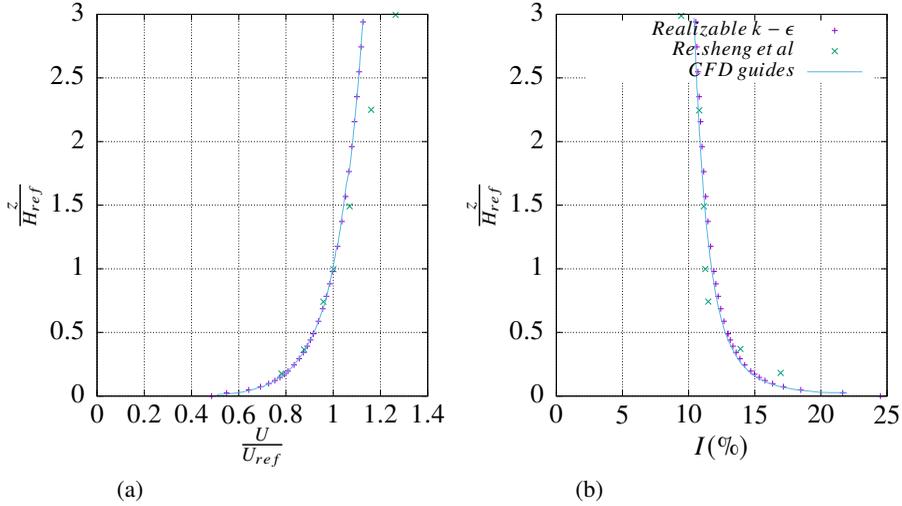


Figure 2: Profile of the neutral atmospheric boundary layer: (a), mean wind velocity; (b), turbulent intensity  $I$  as defined in (EN 2005).

## 670 5. Results

671 In this section, we validate the proposed data assimilation scheme for global and distributed  
 672 turbulence model parameters. An adjoint state analysis is conducted to obtain the sensitivities  
 673 to both model control closure parameters, global and distributed coefficients. We assess the  
 674 limits of global closure optimization performances and exhibit the ability of the proposed  
 675 distributed closure method not only to reconstruct wall-pressure-driven wake flow accurately  
 676 but also to enable turbulence closure analysis.

677

### 5.1. Adjoint state analysis

678 The normalised adjoint fields (by their maximum in-plane values), shown in figures 3, 4 and 5,  
 679 highlight the areas of interest in terms of turbulence modelling on two horizontal plans (at  
 680 normalised height  $z/H_{ref} = \{0.19, 1\}$ ) and on the symmetry plane (at  $y/D = 0$ ). These areas  
 681 correspond to regions, whose state is observable by the sensors, and where the turbulence  
 682 closure model fails to reproduce the physical behaviour of the flow; this corresponds to the  
 683 recirculation regions behind and at the top of the building (as seen in the centered streamwise  
 684 vertical plans on figure 5), the area of the vortex shedding due to flow separation (seen in  
 685 the horizontal plans on figure 3 and 4) and the flow impingement region of the building.  
 686 Based on these adjoint fields, the cost functional's sensitivity to any control parameter (be  
 687 distributed or not) can be obtained through its associated optimality condition.

688

### 5.2. Results for the global coefficients

689 This section exhibits the adjoint approach's capability to provide a complete information  
 690 on the cost sensitivity to the model's global coefficients. First, we analyse the sensitivity  
 691 fields to highlight the spatial locations where a modification of these global coefficients  
 692 could efficiently correct the model errors. Then, we discuss the results of a data assimilation  
 693 procedure. The data assimilation is performed to investigate some closure hypotheses validity  
 694 in the RANS modelling.

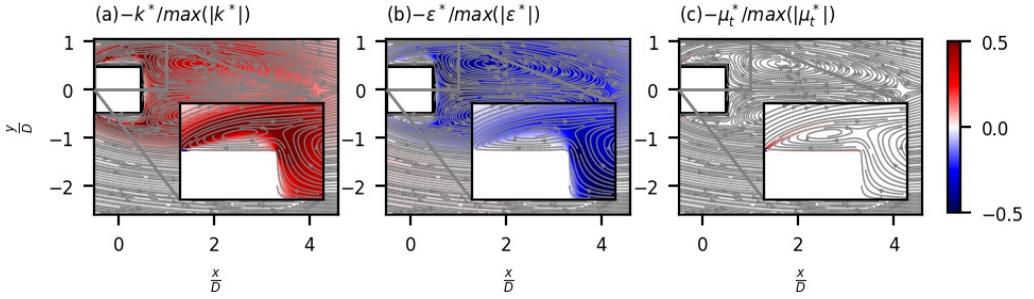


Figure 3: Adjoint turbulence variables at horizontal plane with normalised height  $z/H_{ref} = 0.19$ :(a),  $\epsilon^*$ ; (b),  $k^*$ ; (c),  $\mu_t^*$ . Variables are normalised by their in-plane peak values.

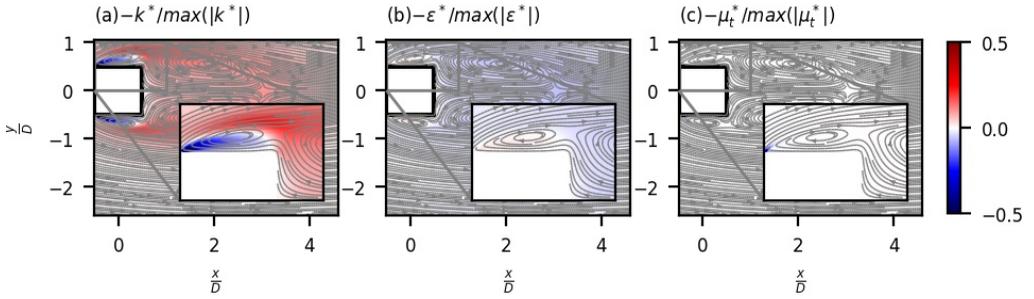


Figure 4: Adjoint turbulence variables at horizontal plane with normalised height  $z/H_{ref} = 1$ :(a),  $\epsilon^*$ ; (b),  $k^*$ ; (c),  $\mu_t^*$ . Variables are normalised by their in-plane peak values.

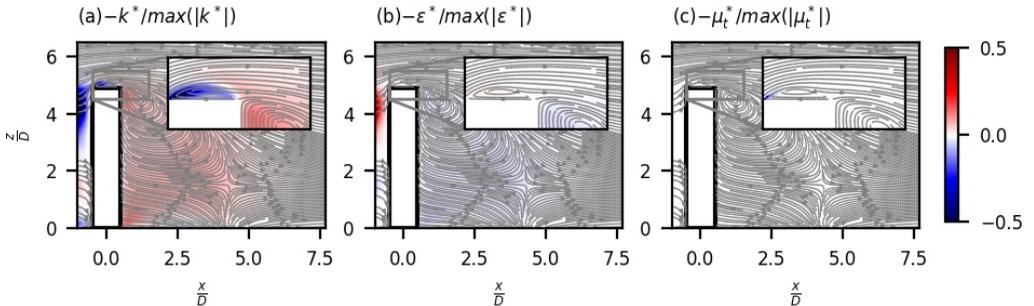


Figure 5: Adjoint turbulence variables at symmetry plane :(a),  $\epsilon^*$ ; (b),  $k^*$ ; (c),  $\mu_t^*$ . Variables are normalised by their in-plane peak values.

### 695 5.2.1. Sensitivity analysis

696 In order to explore the effect of the turbulence model's global coefficients, their associated  
 697 sensitivity maps (plotted in figure 6, 7, and 8, and defined by the spatially distributed operand  
 698 inside the integral in the optimality condition (3.1)) are discussed. Sensitivities have been  
 699 validated with finite differences, leading to a good agreement.

700 We can see that there is a high interest in optimising these coefficients at the shear  
 701 layers resulting from flow separations at the leading lateral edges and on top of the building.  
 702 However, there is very little sensitivity in the bulk of the recirculation wake region. Moreover,  
 703 with regards to the regularity of the sensitivity fields,  $\frac{\partial \mathcal{J}}{\partial \sigma_k}$  and  $\frac{\partial \mathcal{J}}{\partial \sigma_\epsilon}$  (Figures 6 and 7 (a)  
 704 and (b)) have the largest local variations compared to the others. In fact, this is explained by

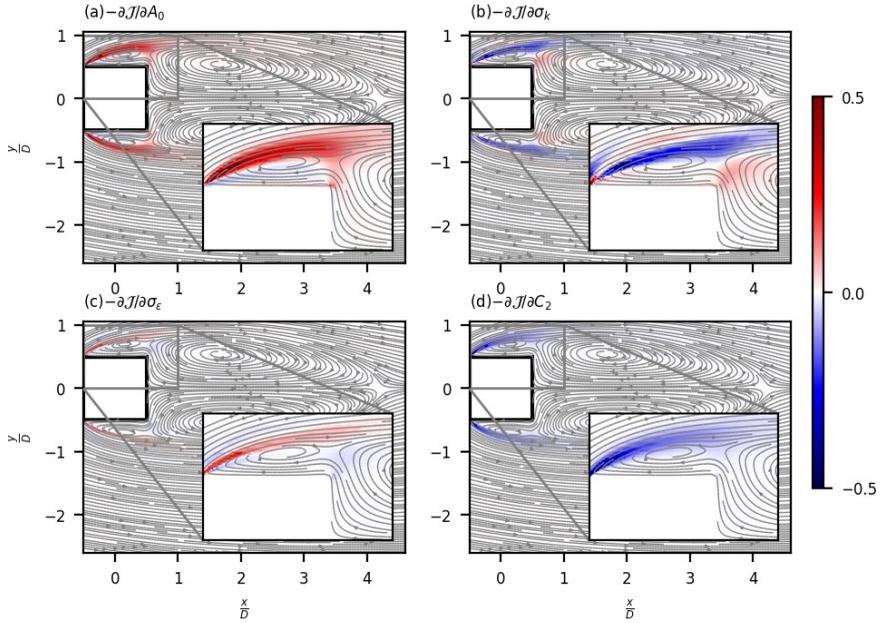


Figure 6: Closure coefficient sensitivities at horizontal plane with normalised height  $z/H_{ref} = 0.19$ : (a), sensitivity to  $A_0$ , (b),  $\sigma_k$ ,  $\sigma_\epsilon$  (c), and, (d),  $C_2$  (d). Sensitivities are normalised by their in-plane peak values.

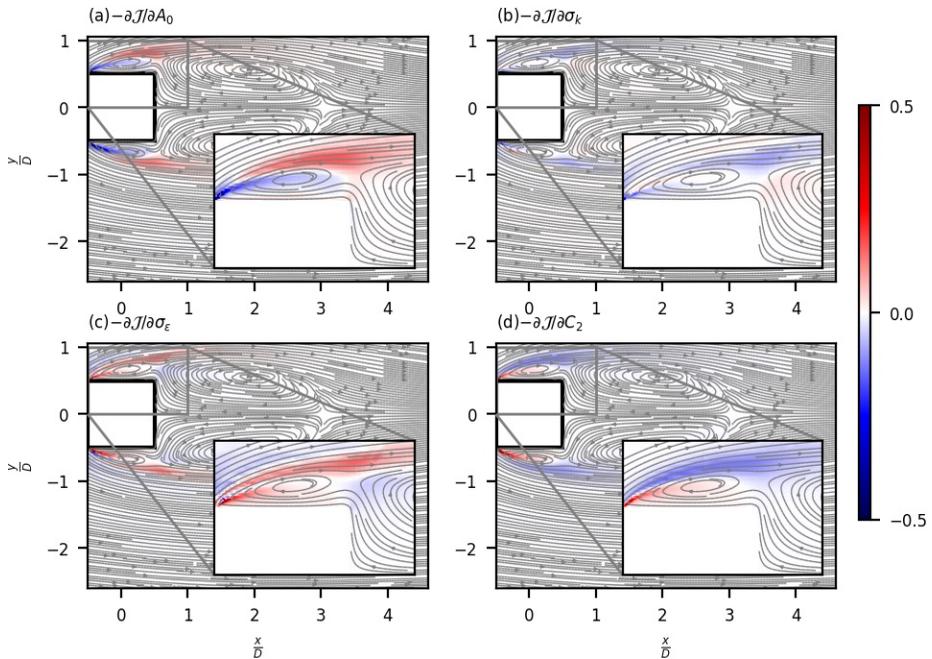


Figure 7: Closure coefficient sensitivities at horizontal plane with normalised height  $z/H_{ref} = 1$ : (a), sensitivity to  $A_0$ , (b),  $\sigma_k$ ,  $\sigma_\epsilon$  (c), and, (d),  $C_2$  (d). Sensitivities are normalised by their in-plane peak values.

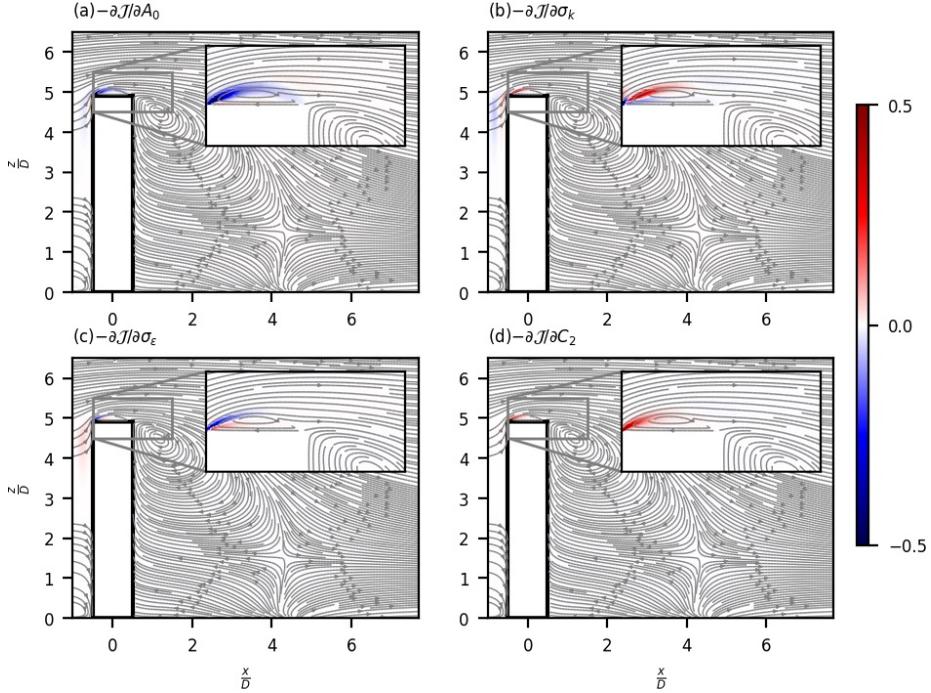


Figure 8: Closure coefficient sensitivities on the symmetry plane with normalised: (a), sensitivity to  $A_0$ , (b),  $\sigma_k$ ,  $\sigma_\epsilon$  (c), and, (d),  $C_2$  (d). Sensitivities are normalised by their in-plane peak values.

705 the high (second) order derivative associated with the diffusion of  $k$  and  $\epsilon$ , in the optimality  
 706 conditions. Now, regarding the local signs and overall values of each sensitivity field, we  
 707 observe systematic change of sign over the domain. The  $L^2$  inner product in (3.1) leads to  
 708 an averaged compromise solution over the whole domain for the global coefficient values.  
 709 This compromise is likely to provide a far too weak amplitude for these coefficients in key  
 710 regions of the flow.

### 711 5.2.2. Closure hypothesis analysis through data assimilation

712 In this section, the optimisation problem is solved iteratively by following Algorithm 1, and  
 713 we discuss the data assimilation procedure's ability to estimate the flow state. Guided by the  
 714 work of Shih *et al.* (1994), we intend here to devise some penalty ranges for the coefficients.  
 715 Concerning the coefficients which are involved in the energy dissipation rate budget, referring  
 716 to the work (Shih *et al.* 1994), the  $C_2$  coefficient is actually expressed as  $C_2 = \beta/\eta$ , in which  
 717  $\beta = \eta + 1$  is the dissipation decay rate (such as  $\epsilon/\epsilon_{t_0} = (t/t_0)^{-\beta}$  where  $t_0$  is an initial time)  
 718 and  $\eta$  is the energy decay exponent (such as  $k/k_{t_0} = (t/t_0)^{-\eta}$ ) that varies from 1.08 to 1.3  
 719 in decaying homogeneous turbulence experiments (Shih *et al.* 1994). Thus, a range for this  
 720 coefficient can be set as  $C_2 \in [1.76, 1.93]$ , where the background value is 1.9.  
 721 For  $\sigma_\epsilon$ , the inertial turbulence assumption near the wall allows to establish

$$722 \quad \sigma_\epsilon = \frac{\kappa^2}{C_2 \sqrt{C_\mu} - C_1} \quad (5.1)$$

723 were the von Kármán constant  $\kappa = 0,41$ , the eddy viscosity coefficient  $C_\mu = 0.09$  and  
 724  $C_1 = 0.43$ . Assuming a quasi-linear dependency between the two constants (see figure 10),  
 725 knowing the range on  $C_2$  we obtain  $\sigma_\epsilon \in [1.14, 1.71]$ . To possibly relax the underlying

---

Scenario	$\sigma_k$	$\sigma_\epsilon$	$C_2$	$A_0$	$\frac{\mathcal{J}-\mathcal{J}_0}{\mathcal{J}_0}$
Default value	1.0	1.2	1.9	4.0	
<b>A</b>	1.10	1.07	1.95	4.03	10.6%
<b>B</b>	1.0	0.92	1.98	4.05	13.2%
<b>C</b>	1.04	1.05	1.97	3.99	10.7%

---

Table 1: Summary of the optimisation results, closure coefficients and the relative decrease of cost function.

---

726 assumption of decaying turbulence for this range, two cases study will be considered for this  
727 constant. In the first scenario, it will be assumed that relation (5.1) holds beyond the inertial  
728 layer, as established by Shih *et al.* (1994). On the second scenario, this constraint is relaxed  
729 and coefficient  $\sigma_\epsilon$  is assumed to be an independent control parameter. In that case, the closure  
730 is thus performed by the data. The second case is expected to bring more degree of freedom  
731 in the optimisation process, due to the independent adaptation of the two coefficients.

732 In the transport equation of  $k$ , the coefficient  $\sigma_k$ , which adjusts the level of turbulent energy  
733 mixing with respect to the momentum eddy diffusivity, is commonly fixed to unity (as in  
734 any  $k - \epsilon$  turbulent model). This generally assumes a quasi-equality between the scalar and  
735 the momentum mixing. Due to the lack of comparative studies in the literature between the  
736 *realizable* model results and experiments, estimating a physical range for this coefficient is  
737 not possible. Therefore, we considered two optimisation procedures where in the first one  
738 we maintain  $\sigma_k = 1$  while in the other case we relax this constraint letting  $\sigma_k$  evolve in the  
739 arbitrary chosen range:  $\sigma_k \in [0.9, 1.1]$ . Similarly, for the bounds on  $A_0$ , without any *a priori*  
740 informations on its physical range, we fixed a larger range of possible value:  $A_0 \in [3.6, 4.4]$ ,  
741 where the background usual value is 4.0.

742 Based on the remarks of the previous section, the results of three data-assimilation  
743 scenarios are discussed and compared. A first straightforward approach corresponds to the  
744 optimisation of the four coefficients independently. This is referred to as scenario **A**. Then, two  
745 scenarios are considered to investigate the two closure assumptions mentioned in the previous  
746 section. First, we consider the equality between the mixing of turbulent kinetic energy and  
747 momentum, referred as scenario **B**. Secondly, keeping  $\sigma_k$  a free parameter, the scenario **C**  
748 consists in enforcing the inertial constraint and defining  $\sigma_\epsilon$  using (5.1). Three criteria are  
749 considered to evaluate the agreement between the CFD results and the measurements. The  
750 first is the relative reduction of cost function  $\frac{\mathcal{J}-\mathcal{J}_0}{\mathcal{J}_0}$ ,  $\mathcal{J}_0$  being the initial cost. This depicts  
751 the improvement of the global effect of wind on the building. Next,  $C_p$ , the dimensionless  
752 pressure, is compared locally on the facades of the building. Third, to quantify the accuracy  
753 of the recovered mean flow field, the streamwise length of the recirculation region behind  
754 the building is compared to the one observed from the PIV plans.

755 Regarding the update of the coefficients, a steepest descent algorithm is used with an adaptive  
756 step. A maximum step size is set to  $10^{-2}$  while a minimum step size inferior to  $10^{-4}$   
757 is considered as an optimisation convergence criteria. The confidence coefficients are all  
758 set to  $\zeta_i = 5 \times 10^{-2}$ . This low uniform values represent a relative degree of confidence  
759 on the background closure values. The variations of the closure coefficients along the  
760 optimisation iterations are shown in figure 9. The maximum reduction of the cost and the  
761 optimal coefficients values for the three considered scenarios are summarised in table 1. In  
762 terms of mismatch between CFD and experimental mean pressure, it is shown that the highest  
763 reduction can be achieved through the optimisation scenario **B**. Conversely, scenario **C** leads  
764 to the least improvement in the cost function. However, we note a faster convergence rate for

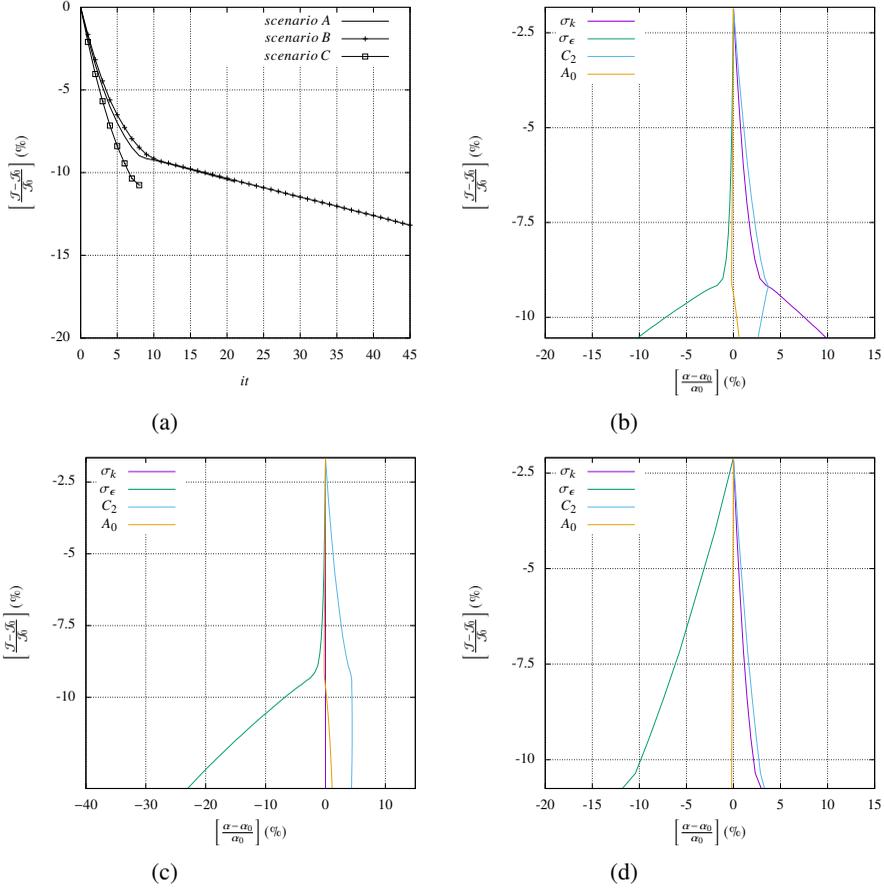


Figure 9: Cost function reduction, (a), and closure coefficient variations: (b), scenario **A**; (c), scenario **B**; (d), scenario **C**.

765 **C**, for which the optimal solution is reached 5 times faster than for **B**. Furthermore, a shift  
 766 between the two regimes can be noticed in scenarios **A** and **B**. Indeed, this shifting occurs  
 767 when the penalisation on the variation of  $C_2$  becomes of the same order of magnitude than the  
 768 required advancement for the cost minimisation. Whereas in **B**,  $\sigma_k$  is not optimised and the  
 769 trend on  $C_2$  until convergence is mainly dominated by its penalisation. In all scenarios, the  
 770 optimal value of  $C_2$  increases while it stays within 5% of the background value. Considering  
 771  $A_0$ , a minor variation is observed during optimisation in all scenarios. On the contrary, a  
 772 higher variation of  $\sigma_\epsilon$  below the recommended range is necessary to reduce the cost function.  
 773 In figure 10, we show the variation of  $\sigma_\epsilon$  with respect to  $C_2$ . In scenario **C**, a quasi-linear  
 774 dependency is established through relation (5.1). However, we retrieve the two regimes in **B**  
 775 and **A** where this dependency is broken.

776 In general, it can be concluded that a better agreement between the turbulence model (e.g  
 777 *realizable*  $k - \epsilon$ ) and wind tunnel experiments, in terms of wind load on the facades of  
 778 high-rise buildings, can be achieved through optimisation of the closure coefficients. Even  
 779 if it offers less degrees of freedom in the optimisation, better results are obtained when  
 780 enforcing the constraint that equals turbulence mixing in the equation of transport of  $k$  to  
 781 momentum mixing by the eddy viscosity (scenario **B**). This suggests that it is a physically  
 782 valid hypothesis in our case study. It helps structuring the data assimilation process and

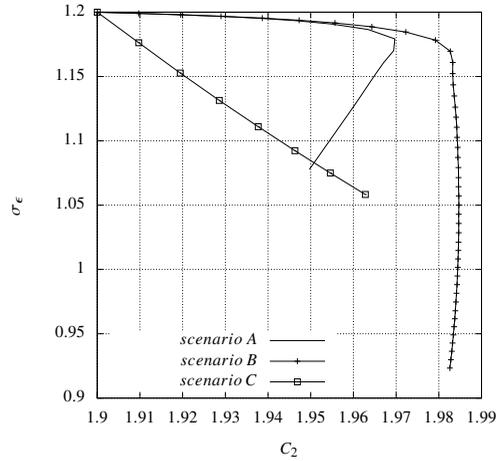


Figure 10:  $\sigma_\epsilon$  variations with respect to  $C_2$  for all scenarios.

783 leads to a robust procedure. It states that the turbulent mixing of the momentum and kinetic  
 784 energy are of same nature. At the opposite, by relaxing the constraint and establishing  
 785 relation (5.1) as valid out of the inertial layer (scenario **C**) may lead to lower agreement  
 786 with measurements. Indeed, this assumption may hold reasonably in flows where turbulence  
 787 behaviour is isotropic. However, in the presence of bluff body, e.g flows with separation  
 788 and recirculation dynamics, this assumption is undoubtedly unrealistic. Scenario **B** might be  
 789 considered as the best optimisation choice to get better wind load representation on high-rise  
 790 building given the considered turbulence closure (*i.e.* realizable  $k - \epsilon$ ). Following the best  
 791 optimisation scenario, 13% gain on the overall predicted loads are obtained. Furthermore, a  
 792 comparison of the predicted pressure coefficient at the building facades (see figure 11) this  
 793 gain is associated to the slight improvement observed especially along the side facades.

794 Nearly no change at the front facade and along the upfront corners is observed. As a matter of  
 795 fact, this observations confirms what was earlier mentioned in the sensitivity analysis  
 796 where the rigidity of the considered turbulence model is shown to play a major role on the  
 797 degree of improvement that can be achieved to fit with measurements.

798 With regard to the mean flow reconstruction, adopting the best optimisation scenario  
 799 (scenario **B**), the contours of the mean velocity field are compared with the available PIV  
 800 plans reported from the work of Sheng *et al.* (2018). It is a strong validation since these  
 801 measurements are not used in the data assimilation. Figures 12, 13 and 14 show the normalised  
 802 streamwise velocity at the streamwise central plane (top) and at two horizontal plans, *i.e.*  
 803  $z/H_{ref} = 0.19$  and  $z/H_{ref} = 1$ . The CFD with background values and optimised values  
 804 following **B** are compared with the PIV measurements.

805 In order to show the effect of data assimilation, velocity contours are superimposed  
 806 (right column) and thicker lines are plotted to track the size of the recirculation region.  
 807 The reattachment length on the ground, is reported in table 2. After optimisation, velocity  
 808 contours show a better estimation of the recirculation region length which is shorter compared  
 809 to the non-optimised model. This improvement is more affirmed near the ground, where the  
 810 relative error of reattachment length  $Y$  with respect to PIV,  $\epsilon_Y = \frac{\delta Y_0}{\delta Y_{end}}$ , with the default  
 811 ( $Y_0$ ) and the optimised ( $Y_{end}$ ), is reduced by 26%. Despite this enhancement, it should be  
 812 pointed out that CFD model still under-predicts the flow in the wake region. This is the  
 813 best improvement of this specific turbulence model we obtained by assimilating the pressure  
 814 measurements. The two limiting ingredients are the model rigidity and the partial sparse

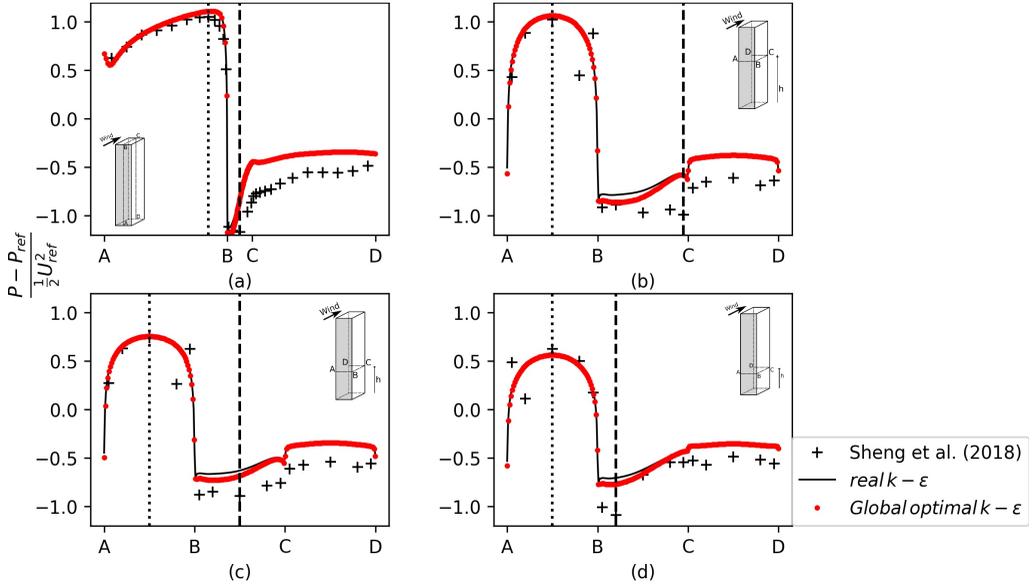


Figure 11: Comparison of pressure coefficient profiles between CFD (scenario **B**) and experimental results along building facades. Contours are taken at building symmetry plane, (a) and three horizontal plans at  $z/H_{ref} = 1$ , (b),  $z/H_{ref} = 0.27$ , (c) and  $z/H_{ref} = 0.19$ , (d), respectively.

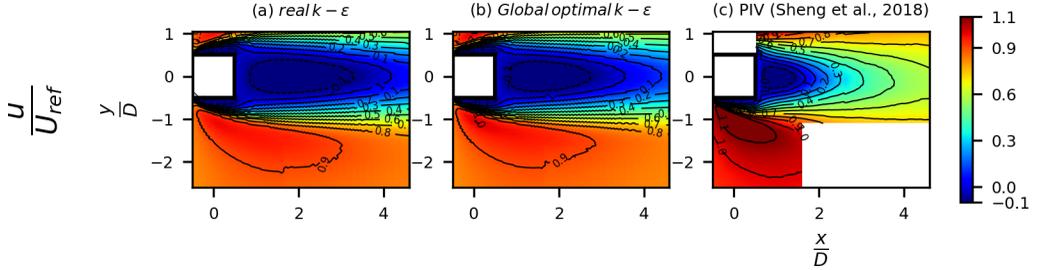


Figure 12: Comparison of mean stream-wise contour between CFD (scenario **B**) and Re. Sheng (PIV) experiments at horizontal plane with normalised height  $\frac{z}{H_{ref}} = 0.19$ .

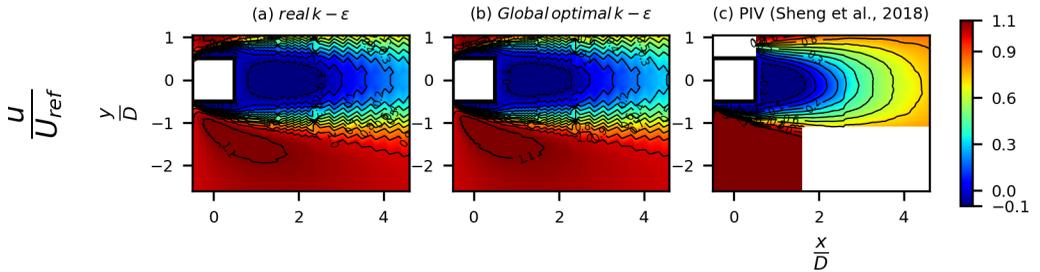


Figure 13: Comparison of mean stream-wise contour between CFD (scenario **B**) and Re. Sheng (PIV) experiments at horizontal plane with normalised height  $\frac{z}{H_{ref}} = 1$ .

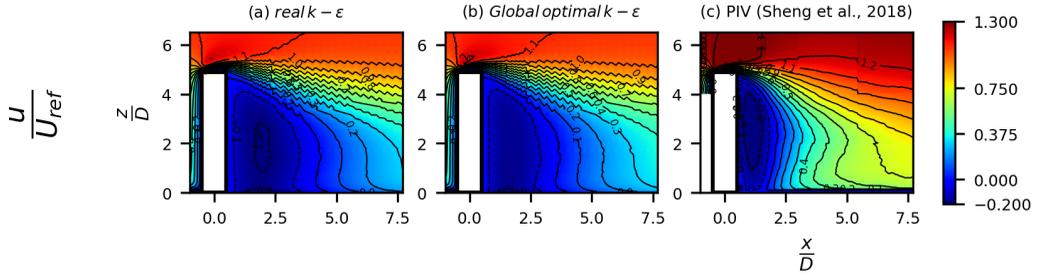


Figure 14: Comparison of mean stream-wise contour between CFD (scenario **B**) and Re. Sheng (PIV) experiments at symmetry plane with normalised height  $\frac{z}{H_{ref}} = 1$ .

---

	Exp	realizable $k - \epsilon$	optimised
$Y^f (m)$	$\sim 50$	139.8	116.1
$Y^r (m)$	-	13.6	11.7

---

Table 2: Comparison of the (dimensional) reattachment lengths on the roof and floor, CFD optimised with global constant calibration (scenario **B**).

815 observations (pressure at the boundary) of the complex flow. In the next section, spatially  
 816 distributed control parameters in the transport equation of dissipation are considered in order  
 817 to relax this structural constraint.

### 818 5.3. Distributed closure parameter in the energy dissipation budget

819 This section is dedicated to the results related to the investigation of the adjunction on  $k - \epsilon$   
 820 (realizable) model of a distributed control parameter in the energy dissipation rate budget.  
 821 First, we analyse the sensitivity fields to highlight the spatial locations where the closure  
 822 form of  $\epsilon$  budget appears inadequate to reproduce the measurements and would require a  
 823 structural correction. Then, the data-assimilation results of this spatially corrected model are  
 824 analysed.

#### 825 5.3.1. Sensitivity analysis

826 We analyse the parameter sensitivity fields given by the proposed closure model, which  
 827 corresponds to the first iteration step of the data assimilation procedure. Indeed, we are  
 828 interested in the gradient of the cost functional with respect to the distributed control  
 829 parameters for  $f_\epsilon = 0$ . Figures 15, 16, and 17 compare the sensitivity maps for the added  
 830 control parameter against a direct forcing (which corresponds to the adjoint variable on  $\epsilon^*$ ).  
 831 Globally, sensitivity to the proposed parameter  $f_\epsilon$  shows a strong response in a restricted  
 832 flow area. In contrast with very diffused sensitivity maps for the direct forcing, the sensitivity  
 833 maps of the additional forcing do highlight the regions of great relevance for the model  
 834 improvement. They correspond to the same regions as those designated by the sensitivity  
 835 maps of the global constants in the previous section. For instance, we note a tendency to  
 836 bring significant dissipation rate adjustments starting from the leading edges and continuing  
 837 into the lateral shear layers and more downstream at the wake region edges. Let us note that  
 838 multiplication by the variable  $\epsilon$  has damped sensitivities at regions nonrelevant for turbulence  
 839 energy budget, such as the high peaks of sensitivity observed around the wake centerline  
 840 for the direct forcing (see figure 15). As we span upward, as shown at height  $z/H_{ref} = 1$   
 841 in figure 16, the maps actually reveal a step function tendency as we go from separated

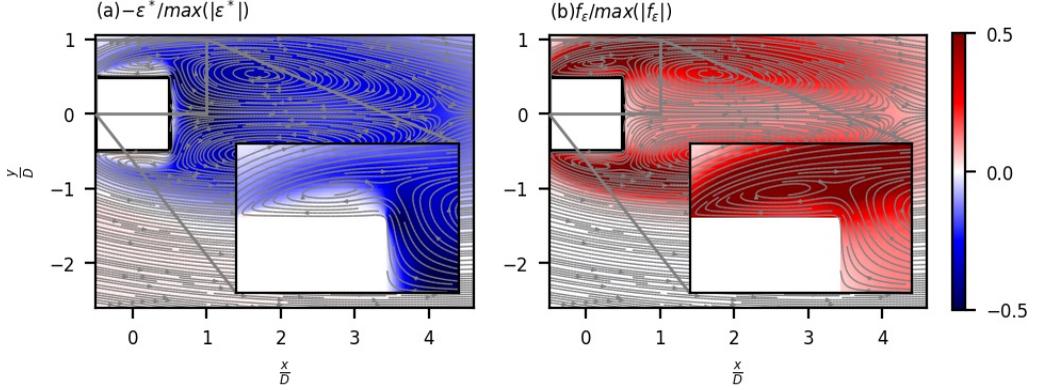


Figure 15: Adjoint turbulence dissipation and the constrained control at horizontal plane with normalised height  $\frac{z}{H_{ref}} = 0.19$ . Variables are normalised by their in-plane peak values.

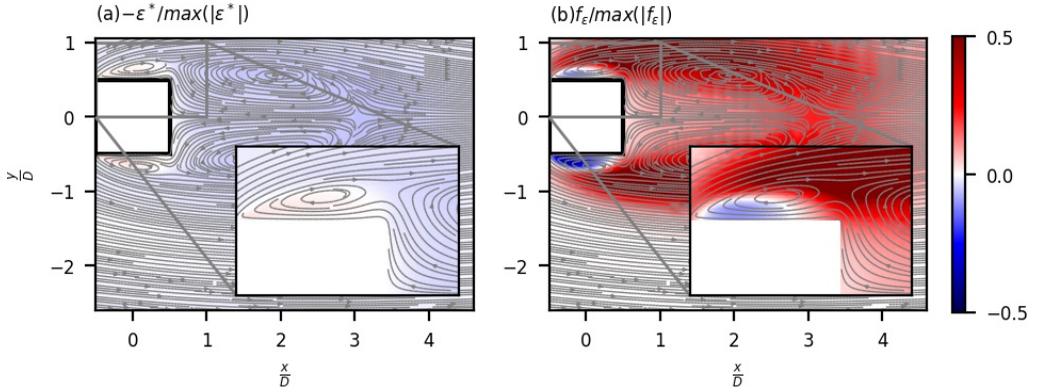


Figure 16: Adjoint turbulence dissipation and the constrained control at horizontal plane with normalised height  $\frac{z}{H_{ref}} = 1$ . Variables are normalised by their in-plane peak values.

842 flow regions, *i.e.*, the lateral and top shear layers, toward the wake region. Furthermore,  
 843 with regard to the sign, eventual contributions to the  $\epsilon$  budget are interpreted as follows.  
 844 A negative value of  $f_\epsilon$  would tend to increase the dissipation rate, while a positive value  
 845 would instead decrease it. Hence, on both lateral and top separated flows, the parameter  
 846 suggests there an increase of the dissipation rate. The sensitivity analysis points here an  
 847 over-production of turbulent kinetic energy, which is a known common default of the  $k - \epsilon$   
 848 closure models in such flow configurations reported, for instance, in (Murakami 1990, 1997;  
 849 Shirzadi *et al.* 2017). Moreover, along the outer edges of the lateral shears toward the wake  
 850 edges, the sensitivity maps suggest reducing the dissipation rate. This tendency is consistent  
 851 with a rather under-predicted turbulent mixing, resulting in the overly extended wake region  
 852 behind the building (Shirzadi *et al.* 2017).

### 853 5.3.2. Closure analysis through data-assimilation

854 We consider now the solution of a data-model coupling using the modified closure equation  
 855 (3.2). Regarding the assimilation procedure's setting, the steepest descent algorithm is used  
 856 with the Sobolev gradient computed in (3.6) as a descent direction. Regarding the filtering  
 857 choice, two values  $l_{sob} = 0.1D$  and  $0.2D$  were tested. Let us note that with  $l_{sob} = 0$ , *i.e.*

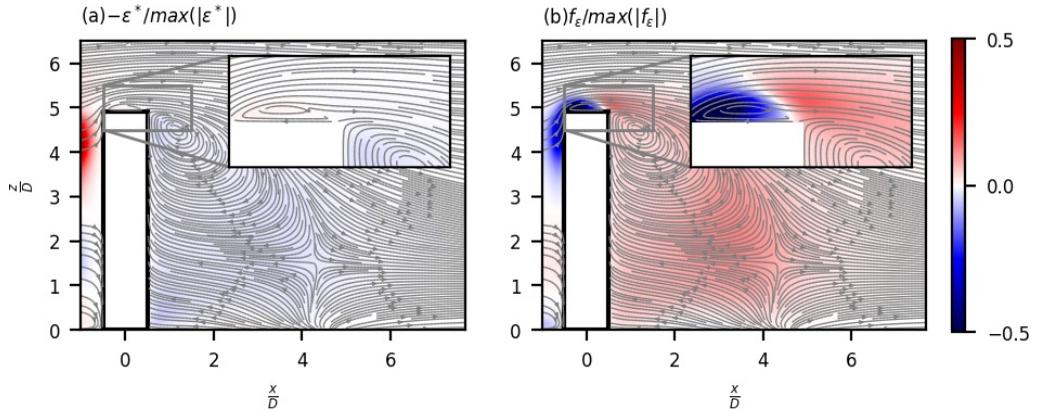


Figure 17: Adjoint turbulence dissipation and the constrained control at symmetry plan. Variables are normalised by their in-plane peak values.

858 no smoothing of the  $L^2$  gradient, the procedure was notably unstable, showing the need for  
 859 regularisation. As for a higher value of  $l_{sob} = 0.2D = 6$  m, this choice yielded to an over  
 860 smoothing. As the sensitivity varies by length scales that are quite small in comparison to  
 861 this length, this advocates a value of  $l_{sob} \sim$  lateral recirculation width. Therefore, a filtering  
 862 length scale equivalent to 10% of the building's width seems to give a good compromise to  
 863 filter the small-scales, as suggested also in Tissot *et al.* (2020).

864 Sobolev gradient regularisation has been compared with standard  $l^2$ -norm penalty (results  
 865 not shown here for sake of conciseness), the latter requiring an *a posteriori* tuning of the  
 866 hyper parameter. Sobolev gradient leads to the lowest discrepancy ( $\frac{\mathcal{J}}{\mathcal{J}_0} \simeq 0.42$ ) compared to  
 867 the best gradient penalisation ( $\frac{\mathcal{J}}{\mathcal{J}_0} \simeq 0.56$ ), the hyper parameter value being selected using  
 868 L-curve criteria (Hansen 1992). Moreover, Sobolev gradient requires 3 times less iterations  
 869 than penalty method. A too large value of the  $l^2$ -penalty parameter leads a drastic increase of  
 870 the number of iterations with a slight loss of performances with respect to the best  $l^2$ -penalty  
 871 parameter, while a too low penalty leads to a premature cessation of iterations with poor  
 872 performances.

873 **Wind load profiles** The reconstructed pressure loads are compared with the experimental  
 874 data (Sheng *et al.* 2018) and the non-assimilated model in figure 18. We can see that, in  
 875 comparison with the coefficient calibration, the modified closure model produces far better  
 876 results in most of the building's wall regions. In terms of pressure discrepancy, the modified  
 877 closure model manages to capture well suction at both top leading edge in the symmetry  
 878 plane (point B in sub-figure(a)) and lateral leading edges (see figure 18(b), (c), and (d)).  
 879 However, while a good agreement with the data is obtained along the lateral facades, minor  
 880 to important deviations are apparent as we get closer to the trailing edges and especially  
 881 when we approach the high-end. This gradually leads to poorer pressure interpolation as the  
 882 discrepancy reaches a maximum value at the upper back facade around  $H_{ref}$  (sub-figure(a)  
 883 and (b)). Yet, the modified closure model shows a slightly better prediction near the top-  
 884 trailing edge than the calibrated default model. Therefore, at this level of comparison, such  
 885 closure model does improve the data-model capability. The remaining regions where no  
 886 improvement is seen might reflect the limited controllability of such turbulence model with  
 887 wall pressure measurement.

888 **Flow topology** Regarding the spanwise flow structure, figures 19 and 20 show sectional  
 889 streamlines at both  $z/H_{ref} = 0.19$  and  $z/H_{ref} = 1$  height, respectively. Here it is noteworthy  
 890 to mention that these sectional streamlines are computed for in-plane velocity components.

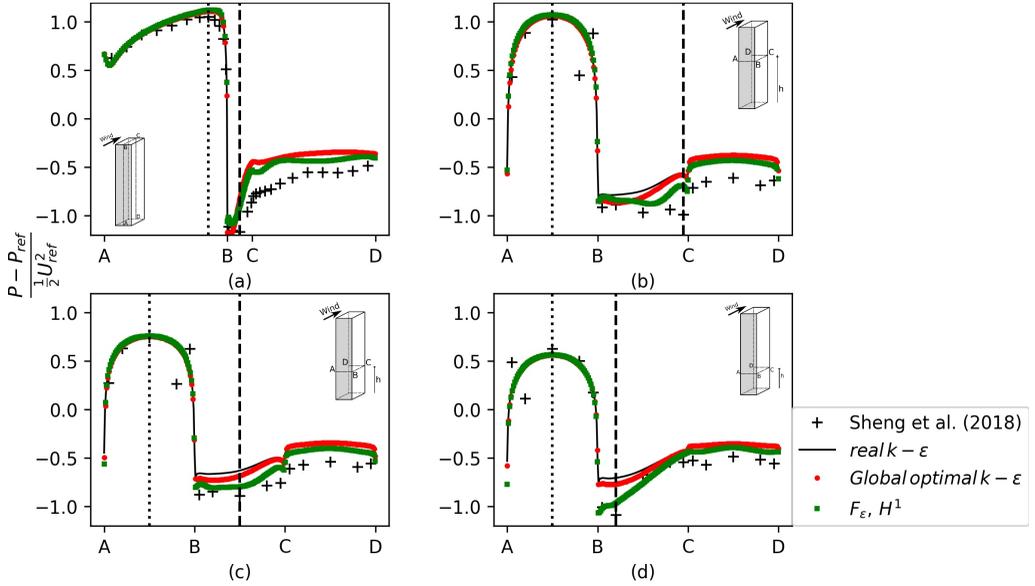


Figure 18: Pressure coefficient profiles along building facades. Comparison is made between an  $\epsilon$  budget correction and global calibration using scenario **B**. Contours are taken at building symmetry plan, (a) and three horizontal plans at  $z/H_{ref} = 1$ , (b),  $z/H_{ref} = 0.27$ , (c) and  $z/H_{ref} = 0.19$ , (d), respectively.

891 In each sub-figure, streamlines predicted with the non-assimilated model (sub-figure (a)) is  
 892 compared with the calibrated model (scenario **B**) (b), with  $f_\epsilon$  closure correction (c) and PIV  
 893 experiments from Sheng *et al.* (2018) (d). At both levels, the model's reconstructed flow ( $f_\epsilon$ )  
 894 still preserves the symmetry of the two distinct pairs of averaged vortex structure. Moreover,  
 895 an excellent agreement with experiments is obtained in the wake transverse extension and  
 896 the vortices focal point positions in comparison with the calibrated model.

897 Figure 21 shows time-averaged sectional streamlines at the  $y/D = 0$  symmetry plane in  
 898 the transverse-wise structure. As can be seen from figure 21, the two distinct types of average  
 899 streamlines are also observed on both reconstructed flows ((b) and (c)). It is constituted by an  
 900 upper recirculation starting at the roof-top and a lower recirculation region raised from the  
 901 ground wall, separated by a saddle point. Thus, regarding the wake's extension, the modified  
 902 closure model leads to a drastic reduction of the recirculating flow compared to the calibrated  
 903 mode, thus reaching a realistic size. This can be quantified by the position of the saddle point  
 904 ( $x/D = 4, z/D = 2$ ) in the RANS model which has been moved around ( $x/D = 2, z/D = 2$ ).  
 905 This striking result is mitigated by the fact that this saddle point has been pulled slightly too  
 906 far upstream. It should be recalled that only pressure measurements in the facade have been  
 907 available and that PIV measurements are used here only for validation. This good agreement  
 908 with external data proves that we are neither in overfitting nor in an over-constrained situation.  
 909 Indeed, the two-dimensional vortices at both elevations ( $\frac{z}{H_{ref}} = 0.19, 1$ ) are a transverse  
 910 projections of the three-dimensional rolls, one on each side of the wake symmetry plan, which  
 911 connects near the free end. Such structure is consistent with some model descriptions brought  
 912 on wakes of finite length square cylinders, with similar height/width ratio, that are subject to  
 913 boundary layer flows of various thickness (Kawamura *et al.* 1984; Wang & Zhou 2009). A  
 914 global three-dimensional picture gathering the two-dimensional previous plots is shown in  
 915 figure 22). Examining the optimal forcing fields in figure 23, we retrieve the same tendencies  
 916 observed in the sensitivity analysis before the reconstruction. After the optimisation, the

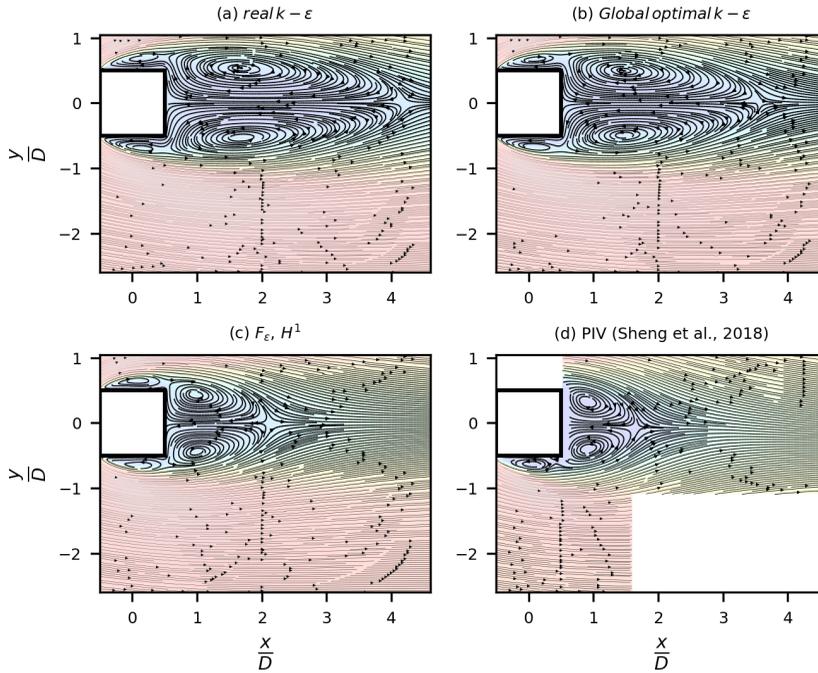


Figure 19: Flow topology (2D) on horizontal plane at normalized height  $\frac{z}{H_{ref}} = 0.19$  with local constraint correction. Comparison is made between an  $\epsilon$  budget correction and global calibration using scenario **B**.

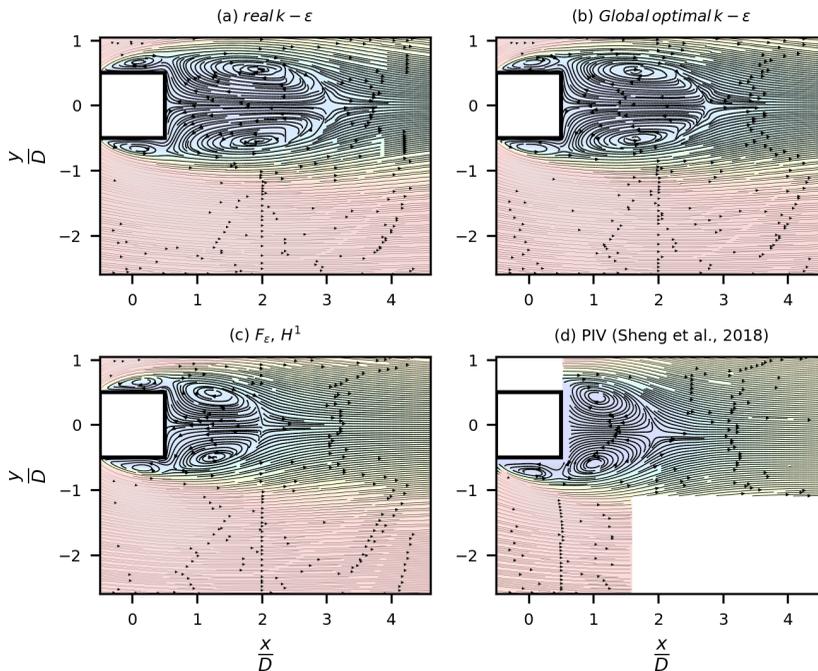


Figure 20: Flow topology (2D) on horizontal plane at normalized height  $\frac{z}{H_{ref}} = 1$  with local constraint correction. Comparison is made between an  $\epsilon$  budget correction and global calibration using scenario **B**.

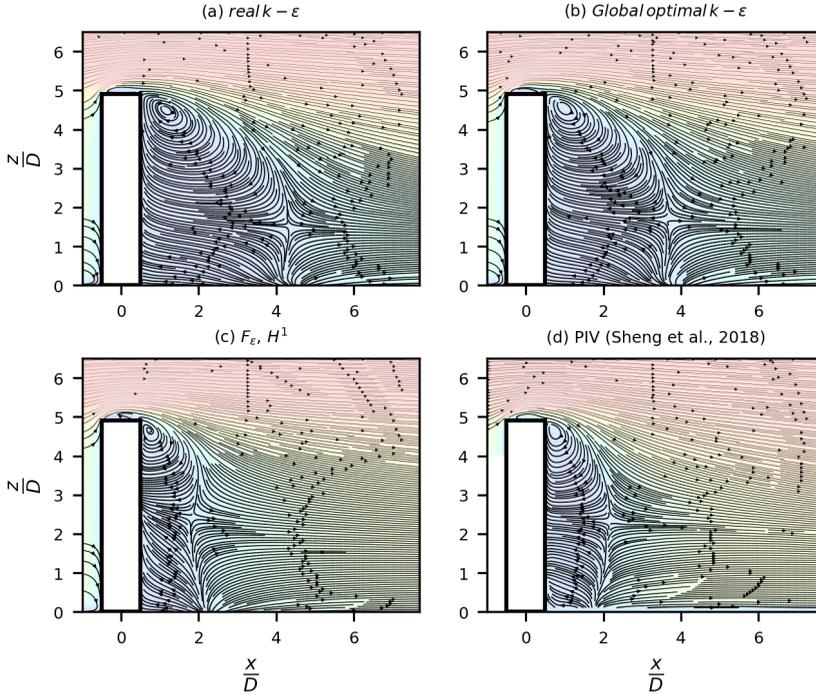


Figure 21: Flow topology (2D) on symmetry plane with local constraint correction. Comparison is made between an  $\epsilon$  budget correction and global calibration using scenario **B**.

917 parameter  $f_\epsilon$  still keeps advocating less turbulence production in the shear layers of the  
 918 lateral separated flow (see 23(a) and (b)), while, conversely, more mixing at the edges of the  
 919 wake downstream. Corrections are performed where strong turbulence inhomogeneity and  
 920 anisotropy occur. It acts in a way to redistribute dissipation rate, by the means of sources  
 921 and sinks, from the upstream region toward the downstream region. When considering only  
 922 calibration of the global coefficients, the model structure prevents this redistribution. This  
 923 suggests that some turbulence mechanisms related to anisotropy and inhomogeneity effects  
 924 are not properly taken into account in the model closure and need to be included to represent  
 925 accurately some key regions of the flow.

## 926 6. Conclusions

927 The use of steady RANS models under the eddy viscosity hypothesis is known to be inaccurate  
 928 for practical applications such as micro-climate studies (at urban scale). For instance, in the  
 929 prediction of wind-loads on a high-rise building, most of the state-of-the-art  $k - \epsilon$  turbulence  
 930 models (including the realizable revision studied here) tend to give poor wake flow accuracy  
 931 estimations, as well as an inaccurate wall-pressure value, when compared to wind tunnel  
 932 experiments. One way to tackle this deficiency consists in adopting data-model coupling  
 933 techniques such as the variational DA approach based on optimal control. To set up such a  
 934 framework in our context we devised a consistent analytical derivation of one of the most  
 935 common turbulence models (*i.e.* realizable revision of  $k - \epsilon$ ) coupled with near wall closure.  
 936 This has resulted in the definition of a continuous adjoint model (together with its consistent  
 937 boundary conditions) of the tangent linear operator of the RANS model. Given the dual  
 938 description of the dynamics composed of the RANS direct model and the adjoint of its

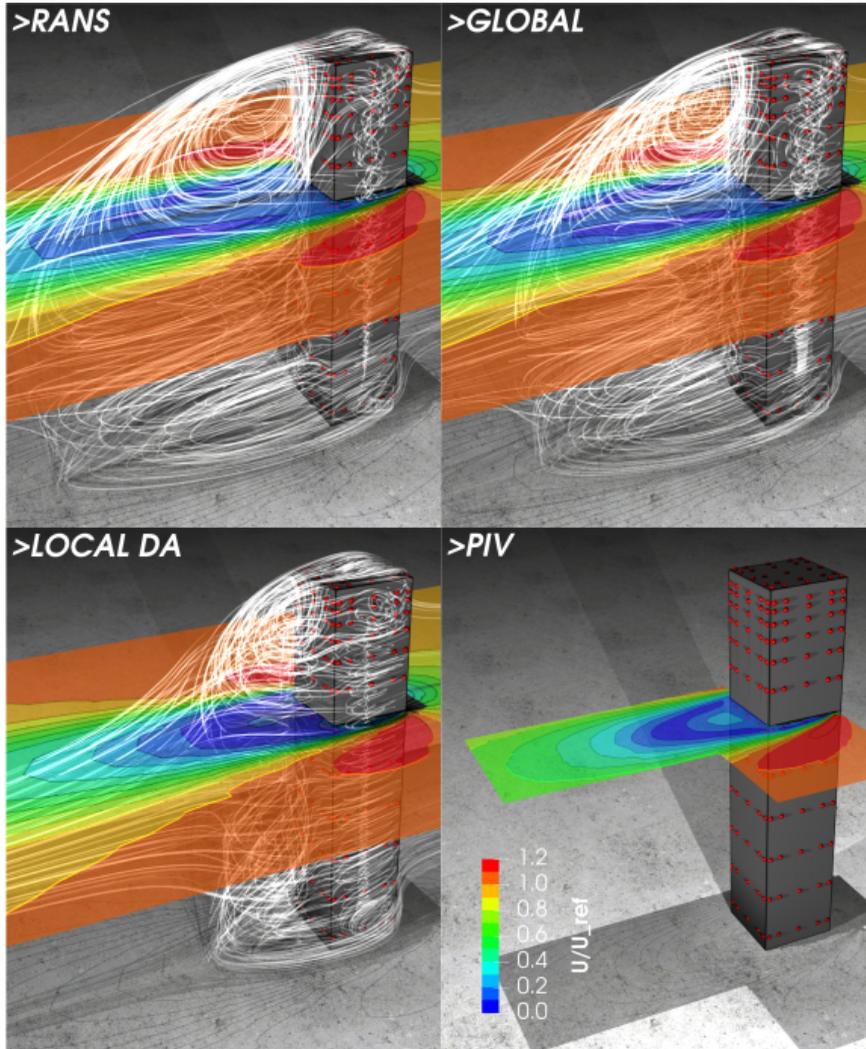


Figure 22: Flow topology (3D) of the realizable  $k - \epsilon$  model, global coefficient calibration and  $\epsilon$  budget correction against PIV plane at  $z/H_{ref} = 1$ .

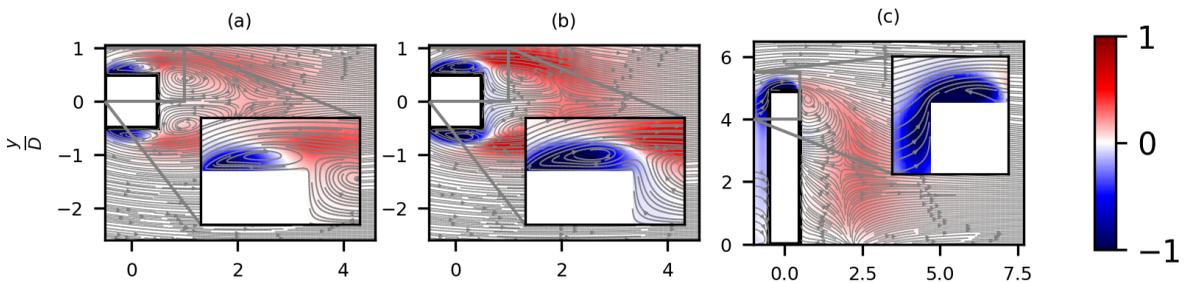


Figure 23: Converged parameter  $f_\epsilon$ , with Sobolev gradient ( $l_{sob} = 0.1D$ ); (a), at horizontal plane at  $z/H_{ref} = 0.19$ , (b)  $z/H_{ref} = 1$  and, (c) at symmetry plane  $y/D = 0$ .

939 tangent linear representation, we have explored three methodological settings that provides  
940 an efficient sensitivity analysis and an in-depth diagnosis of the turbulence closure adopted  
941 on such flows.

942 The first tool consisted in the inspection of the adjoint state variables in relation with their  
943 physical meaning. The second one was dedicated to providing a better understanding of the  
944 model output's variabilities in terms of the model's closure global constants. With the last  
945 one, we went one step further. We considered the adjunction of a distributed parameter which  
946 enables the reanalysis of the closure at a structural level (such as the choice of the transport  
947 equation for the energy dissipation rate on the  $k - \epsilon$  model as considered here). To conduct an  
948 efficient structural inspection, a distributed parameter is sought in a Sobolev space and further  
949 estimated through a data-assimilation procedure. As a sensitivity field is generally not very  
950 regular for distributed parameters, the use of Sobolev gradient was proposed here for both  
951 a regularisation purpose and to define an improved descent direction for the minimisation  
952 technique. These three settings have then been applied to a high-rise building case study.

953 Sensitivity maps of the  $k - \epsilon$  global coefficients had revealed high interest in optimising  
954 them mainly at the shear layers resulting from flow separations at the leading lateral edges and  
955 on top of the building. Moreover, little sensitivity in the bulk of the recirculation wake region  
956 was observed. Despite all the spatial variability of the sensitivity fields, it was shown that  
957 the optimality condition drastically reduces the high dimensional dependency of the model  
958 to each coefficient. Regarding the model hypotheses which guided the choice for closed  
959 default values, a better data coupling is obtained by enforcing the constraint that equates  
960 turbulence energy mixing to momentum mixing, even if it offers fewer degrees of freedom in  
961 the optimisation. This suggests that it is a physically valid hypothesis that structures the model  
962 and then helps for convergence. Conversely, by relaxing this constraint and establishing the  
963 relation (5.1), which dictates a strong bound limiting the production of energy dissipation  
964 rate to its redistribution (supposedly valid in the inertial layer near the wall), this leads to  
965 lower agreement with experiments. As both assumptions constitute a common practice for  
966 closure to most eddy viscosity models, it is expected that these results extend to several  
967 other models of similar forms. The limited performance of the DA procedure, achieved when  
968 controlling global turbulence parameters, points out the rigidity of the considered turbulence  
969 model when used with realistic wall pressure measurements.

970 Considering a distributed parameter to the  $\epsilon$  budget, in order to complement the model in  
971 terms of local source/sink process, sensitivity maps highlight regions where global constants  
972 are not too sensitive (for instance, the wake region) and exhibit relatively less variability in  
973 term of sign changes. Maps had actually revealed binary tendencies, separating the lateral and  
974 top shear regions and the wake flow. Regarding the regularisation, a comparison of the cost  
975 reduction results with a conventional penalisation approach showed that Sobolev gradient  
976 yields a much faster convergence and lower discrepancy levels. Let us note that, along with the  
977 Sobolev gradient, the robustness of the DA procedure was enabled as a first order numerical  
978 scheme to solve the dual dynamics. Regarding the reconstruction ability, compared with  
979 coefficient calibration, the modified closure model produced better results in most of the  
980 building's wall regions in terms of wind load profiles, yet, results suggest some remaining  
981 restrictions as reconstructed profiles tend toward the original model in some regions. An  
982 excellent agreement with PIV experiments was obtained in wake transverse extension. It  
983 should be recalled that only pressure measurements in the facade have been assimilated.  
984 This good agreement with measurements of different nature and that have not been used in  
985 the assimilation proved that we are neither overfitting the data nor in an over-constrained  
986 situation.

987 This work thus illustrates the capabilities of adjoint methods. Beyond providing a data-  
988 driven flow reconstruction, they enable an in-depth analysis of the turbulence closure. Indeed,

989 by regarding adjoint fields as a physical forcing, rather than as a purely mathematical object,  
 990 these data-driven reconstructed fields allows to highlight a misrepresentation of the turbulent  
 991 flow by the RANS model, and hence, to address errors within a particular turbulence  
 992 modelling form (*e.g.* energy production, backscattering, redistribution or dissipation).  
 993 Although the results presented were for a particular turbulence model and on a specific  
 994 bluff-body-like case, over-estimation of the recirculation length in bluff bodies is a common  
 995 features in RANS models, and the proposed methodology could be employed without loss  
 996 of generality. Provided sparse wall pressure measurements, the technique can be directly  
 997 applied to any complex wake flow embedded in the atmospheric boundary layer.

998 Beyond the demonstration of an efficient data assimilation method, the results show  
 999 that in a 3D wake flow immersed in an atmospheric boundary layer, sparse wall pressure  
 1000 measurements located on the building facades carry enough information to perform relevant  
 1001 estimations of the wake velocity field, while RANS simulations alone systematically  
 1002 overestimate the recirculation length.

### 1003 **Acknowledgements**

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 1007 providing us the experimental data.

### 1008 **Declaration of Interests**

1009 The authors report no conflict of interest.

### 1010 **APPENDIX**

1011 Under differentiability condition, it can be shown (Le Dimet & Talagrand 1986; Gunzburger  
 1012 2003) that the problem of determining the optimal set of flow state variables,

$$1013 \quad \mathbf{X} = (U_x, U_y, U_z, P, k, \epsilon, \mu_t)$$

1014 and the set of parameters  $\alpha$ , of the cost function  $\mathcal{J}(\mathbf{X}, \alpha)$  under the constraint

$$1015 \quad \mathbf{M}(\mathbf{X}, \alpha) = 0$$

1016 is equivalent to the problem of determining the optimal set of these variables in addition to  
 1017 an adjoint state

$$1018 \quad \mathbf{X}^* = (U_x^*, U_y^*, U_z^*, P^*, k^*, \epsilon^*, \mu_t^*)$$

1019 of the Lagrangian functional  $\mathcal{L}(\mathbf{X}, \mathbf{X}^*, \alpha)$ . With the inner product defined as  $\langle \psi, \phi \rangle_\Omega =$   
 1020  $\int_\Omega \psi^T \phi \, d\Omega$  where  $\psi$  and  $\phi$  are any two regular vectorial functions defined on the domain  $\Omega$ ,  
 1021 the Lagrangian, is

$$1022 \quad \mathcal{L}(\mathbf{X}, \mathbf{X}^*, \alpha) = \mathcal{J}(P, \alpha) + \int_\Omega (\mathbf{X}^*)^T \mathbf{M}(\mathbf{X}, \alpha) \, d\Omega. \quad (6.1)$$

1023

1024 The first order variation  $\delta\mathcal{L}$  resulting from perturbation  $(\delta\mathbf{X}, \delta\mathbf{X}^*, \delta\alpha)$  of  $(\mathbf{X}, \mathbf{X}^*, \alpha)$ , in  
 1025 compact form, is equal to

$$\begin{aligned}
 1026 \quad \delta\mathcal{L} &= \frac{\partial\mathcal{J}}{\partial P}\delta P + \frac{\partial\mathcal{J}}{\partial\alpha}\delta\alpha + \int_{\Omega} (\mathbf{X}^*)^T \left( \frac{\partial\mathbf{M}}{\partial U_x} \delta U_x \right) d\Omega + \int_{\Omega} (\mathbf{X}^*)^T \left( \frac{\partial\mathbf{M}}{\partial U_y} \delta U_y \right) d\Omega \\
 1027 \quad &+ \int_{\Omega} (\mathbf{X}^*)^T \left( \frac{\partial\mathbf{M}}{\partial U_z} \delta U_z \right) d\Omega + \int_{\Omega} (\mathbf{X}^*)^T \left( \frac{\partial\mathbf{M}}{\partial P} \delta P \right) d\Omega + \int_{\Omega} (\mathbf{X}^*)^T \left( \frac{\partial\mathbf{M}}{\partial k} \delta k \right) d\Omega \\
 1028 \quad &+ \int_{\Omega} (\mathbf{X}^*)^T \left( \frac{\partial\mathbf{M}}{\partial\epsilon} \delta\epsilon \right) d\Omega + \int_{\Omega} (\mathbf{X}^*)^T \left( \frac{\partial\mathbf{M}}{\partial\mu_t} \delta\mu_t \right) d\Omega + \int_{\Omega} (\delta\mathbf{X}^*)^T \mathbf{M}(\mathbf{X}, \alpha) d\Omega. \quad (6.2) \\
 1029
 \end{aligned}$$

1030 Using the duality identity defined as

$$1031 \quad \int_{\Omega} (\mathbf{L}\phi) \psi d\Omega = \int_{\partial\Omega} (\mathbf{B}\phi) (\mathbf{C}\psi) d\partial\Omega - \int_{\Omega} \phi (\mathbf{L}^*\psi) d\Omega$$

where  $\mathbf{L}$  is a linear differential operator and  $(\mathbf{B}, \mathbf{C})$  are lower order differential operators, resulting from the integration by part, that embed the natural boundary condition,  $\delta\mathcal{L}$  becomes

$$\begin{aligned}
 \delta\mathcal{L} &= \frac{\partial\mathcal{J}}{\partial P}\delta P + \frac{\partial\mathcal{J}}{\partial\alpha}\delta\alpha - \int_{\Omega} \left( \frac{\partial\mathbf{M}^*}{\partial U_x} \mathbf{X}^* \right)^T \delta U_x d\Omega - \int_{\Omega} \left( \frac{\partial\mathbf{M}^*}{\partial U_y} \mathbf{X}^* \right)^T \delta U_y d\Omega \\
 &- \int_{\Omega} \left( \frac{\partial\mathbf{M}^*}{\partial U_z} \mathbf{X}^* \right)^T \delta U_z d\Omega - \int_{\Omega} \left( \frac{\partial\mathbf{M}^*}{\partial P} \mathbf{X}^* \right)^T \delta P d\Omega - \int_{\Omega} \left( \frac{\partial\mathbf{M}^*}{\partial k} \mathbf{X}^* \right)^T \delta k d\Omega \\
 &- \int_{\Omega} \left( \frac{\partial\mathbf{M}^*}{\partial\epsilon} \mathbf{X}^* \right)^T \delta\epsilon d\Omega - \int_{\Omega} \left( \frac{\partial\mathbf{M}^*}{\partial\mu_t} \mathbf{X}^* \right)^T \delta\mu_t d\Omega + \int_{\Omega} (\delta\mathbf{X}^*)^T \mathbf{M}(\mathbf{X}, \alpha) d\Omega \\
 &\quad + \int_{\partial\Omega} (\delta\mathbf{X})^T (\mathbf{C}\mathbf{X}^*) d\partial\Omega + \int_{\partial\Omega} (\mathbf{B}\delta\mathbf{X})^T \mathbf{X}^* d\partial\Omega.
 \end{aligned}$$

Since the perturbations are arbitrary, setting the first variation of  $\mathcal{L}$  with respect to the Lagrangian arguments equal to zero leads to an optimality system. With respect to an arbitrary variation of the adjoint state, we recover the constraint equations; while for an arbitrary variation of the state  $\mathbf{X}$  all the terms that include the product of adjoint state to the tangent linear of the constraint has to vanish. Further, with respect to the set of parameters, vanishing the total variation leads to an optimality condition that enclose the optimality system. Collecting these results yields to

$$\begin{aligned}
 \text{state equations} &\quad \Rightarrow \quad \mathbf{M}(\mathbf{X}, \alpha) = 0 \\
 \text{adjoint equations} &\quad \Rightarrow \quad \left( \frac{\partial\mathbf{M}}{\partial\mathbf{X}} \right)^* \mathbf{X}^* = 0 \\
 \text{optimality condition} &\quad \Rightarrow \quad \frac{\partial\mathcal{J}}{\partial\alpha} + \left( \frac{\partial\mathbf{M}}{\partial\alpha} \right)^* \mathbf{X}^* = 0,
 \end{aligned}$$

1032 where  $\left( \frac{\partial\mathbf{M}}{\partial\alpha} \right)^*$  is the adjoint of the model derivative with respect to the parameters. If it is  
 1033 possible to solve this coupled optimality system through one-shot methods, then optimal  
 1034 states and parameters can be obtained without an optimisation iteration. However, due to  
 1035 non linearity and the very large size of this system ( $\sim 3 \times \text{size}(\mathbf{X})$ ) one still have to iterate  
 1036 in order to solve the optimality system. Thus, having solved the state equations for  $\mathbf{X}$  and  
 1037 then  $\mathbf{X}^*$  solution of the adjoint system, model parameters can be iterated by a gradient based  
 1038 optimisation algorithm until optimality condition is satisfied. In a steepest descent algorithm,

1039 the parameter is updated at an iteration  $n$  according to:

$$1040 \quad \alpha^{n+1} = \alpha^n - \lambda_n d_n \quad (6.3)$$

1042 where  $d_n$  is the descent direction which is defined recursively by:

$$1043 \quad d_n = \frac{\partial \mathcal{L}}{\partial \alpha} = \left( \frac{\partial \mathbf{M}}{\partial \alpha} \right)^* \mathbf{X}^* + \frac{\partial \mathcal{J}}{\partial \alpha}, \quad (6.4)$$

1044 Concerning adjoint based optimisation methods, we refer the reader to (Gunzburger 2003;  
1045 Gronsks *et al.* 2013).

#### 1046 *Duality with the realizable $k - \epsilon$*

1047 In this section, more details regarding the derivation of the adjoint model are brought. We  
1048 illustrate the manner in which model specificities are treated in the adjoint procedure. Thus,  
1049 expanding the integrands, the expression (6.1) is rewritten as follow,

$$1050 \quad \mathcal{L}(\mathbf{X}, \mathbf{X}^*, \alpha) = \mathcal{J}(P, \alpha) + \int_{\Omega} \sum_{i=1}^3 U_i^* \underbrace{\left( \frac{\partial(\rho U_j U_i)}{\partial x_j} + \frac{\partial}{\partial x_i} P - \frac{\partial}{\partial x_j} \left[ \mu_{eff} \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \right] \right)}_{M_{U_i}} d\Omega$$

$$1051 \quad + \int_{\Omega} \underbrace{P^* \left( \frac{\partial U_j}{\partial x_j} \right)}_{M_P} d\Omega + \int_{\Omega} \underbrace{k^* \left( \frac{\partial \rho U_j k}{\partial x_j} - \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] - \mu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_j} + \rho \epsilon \right)}_{M_k} d\Omega$$

$$1052 \quad + \int_{\Omega} \underbrace{\epsilon^* \left( \frac{\partial \rho U_j \epsilon}{\partial x_j} - \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_i} \right] - \underbrace{C_1(S, k, \epsilon) S \epsilon}_{P_\epsilon} + \underbrace{C_2 \frac{\epsilon^2}{k + \sqrt{\mu \epsilon}}}_{S_\epsilon} \right)}_{M_\epsilon} d\Omega$$

$$1053 \quad + \int_{\Omega} \underbrace{\mu_t^* \left( \mu_t - C_\mu(U_i, k, \epsilon) \rho \frac{k^2}{\epsilon} \right)}_{M_{\mu_t}} d\Omega. \quad (6.5)$$

1054

1055 In fact, upon a first variation of the Lagrangian w.r.t each state component, each one of  
1056 the terms in (6.2) is indeed the weighted sum of partial derivative of the designated terms  
1057 ( $M_{U_i} - M_{\mu_t}$ ) in (6.5). For the sake of concisness, in what follows, directional derivatives of  
1058 (6.5) are only expressed upon perturbation of the velocity. Indeed, we intend her to point  
1059 out the differentiation of the turbulence sources terms w.r.t. the velocity. Thus, the partial

1060 derivative of (6.5) in direction  $\delta U_i$  leads to the following:

$$\begin{aligned}
 1061 \quad \left\langle \frac{\partial \mathcal{L}}{\partial U_i}, \delta U_i \right\rangle_{\Omega} &= \int_{\Omega} \left[ \sum_{i=1}^3 U_i^* \left( \underbrace{\frac{\partial(\rho \delta U_j U_i + U_j \delta U_i)}{\partial x_j}}_{\frac{\partial M_{U_i}}{\partial U_i}} - \frac{\partial}{\partial x_j} \left[ \mu_{eff} \left( \frac{\partial \delta U_i}{\partial x_j} + \frac{\partial \delta U_j}{\partial x_i} \right) \right] \right) \right. \\
 1062 \quad &+ P^* \underbrace{\left( \frac{\partial \delta U_j}{\partial x_j} \right)}_{\frac{\partial M_P}{\partial U_i}} + k^* \underbrace{\left( \frac{\partial \rho \delta U_{jk}}{\partial x_j} - \mu_t \left( \frac{\partial \delta U_i}{\partial x_j} + \frac{\partial \delta U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_j} - \mu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial \delta U_i}{\partial x_j} \right)}_{\frac{\partial M_k}{\partial U_i}} \\
 1063 \quad &+ \epsilon^* \underbrace{\left( \frac{\partial \rho \delta U_j \epsilon}{\partial x_j} - \frac{\partial P_{\epsilon}}{\partial U_i} \delta U_i \right)}_{\frac{\partial M_{\epsilon}}{\partial U_i}} - \mu_t^* \underbrace{\left( \frac{\partial C_{\mu}}{\partial U_i} \delta U_i \rho \frac{k^2}{\epsilon} \right)}_{\frac{\partial M_{\mu t}}{\partial U_i}} \Big] d\Omega \quad (6.6) \\
 1064 \quad &
 \end{aligned}$$

where

$$\begin{aligned}
 \frac{\partial P_{\epsilon}}{\partial U_i} \delta U_i &= \frac{\partial C_1}{\partial U_i} \delta U_i S \epsilon + C_1 \frac{\partial S}{\partial U_i} \delta U_i \epsilon \\
 &= \left( \frac{5k}{\epsilon(5+\eta)^2} + 1 \right) \frac{\partial S}{\partial U_i} \delta U_i \\
 &= \frac{1}{2S} \left( \frac{5k}{\epsilon(5+\eta)^2} + 1 \right) S_{ij} \left( \frac{\partial \delta U_i}{\partial x_j} + \frac{\partial \delta U_j}{\partial x_i} \right),
 \end{aligned}$$

while

$$\frac{\partial C_{\mu}}{\partial U_i} \delta U_i = -C_{\mu}^2 \frac{k}{\epsilon} \left( \frac{\partial A_s}{\partial U_i} \delta U_i U_s + A_s \frac{\partial U_s}{\partial U_i} \delta U_i \right),$$

which, after applying the chain rule, can be rewritten as

$$\frac{\partial C_{\mu}}{\partial U_i} \delta U_i = -C_{\mu}^2 \frac{k}{\epsilon} \left( \underbrace{\frac{\partial A_s}{\partial \phi} \frac{\partial \phi}{\partial W} \frac{\partial W}{\partial S_{ij}}}_{\frac{\partial A_s}{\partial S_{ij}}} \underbrace{\frac{\partial S_{ij}}{\partial U_i} \delta U_i}_{\delta S_{ij}} + A_s \left[ \frac{\partial U_s}{\partial S_{ij}} \delta S_{ij} + \frac{\partial U_s}{\partial \tilde{\Omega}_{ij}} \underbrace{\frac{\partial \tilde{\Omega}_{ij}}{\partial U_i} \delta U_i}_{\delta \tilde{\Omega}_{ij}} \right] \right),$$

for which

$$\begin{aligned}
 \frac{\partial A_s}{\partial S_{ij}} &= \left( -\sqrt{6} \sin(\phi) \right) \left( -\frac{\sqrt{6}}{6} \frac{\left[ \tanh(s(\sqrt{6}W+1)) - \tanh(s(\sqrt{6}W-1)) \right]}{\sqrt{1 - \min(\max(\sqrt{6}W, -1), 1)}} \right) \\
 &\quad \left( 2\sqrt{2} \left[ \frac{3S_{ij}S_{jk}S^3 - S_{ij}S_{jk}S_{kl}(2S+4)S_{ij}}{S^6} \right] \right),
 \end{aligned}$$

and

$$\begin{aligned}
 \frac{\partial U_s}{\partial S_{ij}} &= \frac{S_{ij}}{U_s}, \\
 \frac{\partial U_s}{\partial \tilde{\Omega}_{ij}} &= \frac{\tilde{\Omega}_{ij} + \tilde{\Omega}_{ji}}{2U_s}.
 \end{aligned}$$

Note that  $s \gg 1$  is a free parameter to the hyperbolic step function, thus dealing with local discontinuity resulting from min/max operators. As  $S_{ij}$  and  $\tilde{\Omega}_{ij}$  being linear operators of  $U_i$ ,

their total variations are straightforward,

$$\delta\tilde{\Omega}_{ij} = \frac{\partial\tilde{\Omega}_{ij}}{\partial U_i} \delta U_i = \frac{1}{2} \left( \frac{\partial\delta U_i}{\partial x_j} - \frac{\partial\delta U_j}{\partial x_i} \right),$$

$$\delta S_{ij} = \frac{\partial\tilde{\Omega}_{ij}}{\partial U_i} \delta U_i = \frac{1}{2} \left( \frac{\partial\delta U_i}{\partial x_j} + \frac{\partial\delta U_j}{\partial x_i} \right).$$

1065 It is worth mentioning that  $\partial M_{\mu_t} / \partial U_i$  in (6.6) arises from the so called "realizable form"  
 1066 of the eddy viscosity relation in (Shih *et al.* 1994), which for other revisions of  $k - \epsilon$  model  
 1067 vanishes naturally.

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