

Quality and reliability of LES of convective scalar transfer at high Reynolds numbers

Article

Accepted Version

Creative Commons: Attribution-Noncommercial-No Derivative Works 4.0

Li, Q., Bou-Zeid, E., Anderson, W., Grimmond, S. ORCID: https://orcid.org/0000-0002-3166-9415 and Hultmark, M. (2016) Quality and reliability of LES of convective scalar transfer at high Reynolds numbers. International Journal of Heat and Mass Transfer, 102. pp. 959-970. ISSN 0017-9310 doi: https://doi.org/10.1016/j.ijheatmasstransfer.2016.06.093 Available at https://centaur.reading.ac.uk/66168/

It is advisable to refer to the publisher's version if you intend to cite from the work. See <u>Guidance on citing</u>. Published version at: http://dx.doi.org/10.1016/j.ijheatmasstransfer.2016.06.093 To link to this article DOI: http://dx.doi.org/10.1016/j.ijheatmasstransfer.2016.06.093

Publisher: Elsevier

All outputs in CentAUR are protected by Intellectual Property Rights law, including copyright law. Copyright and IPR is retained by the creators or other copyright holders. Terms and conditions for use of this material are defined in the <u>End User Agreement</u>.

www.reading.ac.uk/centaur

CentAUR



Central Archive at the University of Reading

Reading's research outputs online

1 Quality and Reliability of LES of Convective Scalar Transfer at High Reynolds

2 Numbers

- 3 Qi Li¹, Elie Bou-Zeid^{1*}, William Anderson², Sue Grimmond³, Marcus Hultmark⁴
- 4 1 Department of CEE, Princeton University, US
- 5 2 Department of Mechanical Engineering, University of Texas at Dallas, US
- 6 3 Department of Meteorology, University of Reading, UK
- 7 4 Dept. of Mechanical and Aerospace Engineering, Princeton University, US
- 8 * Corresponding author at: CEE-EQuad-E414, Princeton University, Princeton, NJ 08544,
- 9 USA. ebouzeid@princeton.edu

10 Abstract

11 Numerical studies were performed to assess the quality and reliability of wall-modeled 12 large eddy simulation (LES) for studying convective heat and mass transfer over bluff bodies at high Reynolds numbers (Re), with a focus on built structures in the atmospheric 13 14 boundary layer. Detailed comparisons were made with both wind-tunnel experiments and 15 field observations. The LES was shown to correctly capture the spatial patterns of the 16 transfer coefficients around two-dimensional roughness ribs (with a discrepancy of about 17 20%) and the average Nusselt number (Nu) over a single wall mounted cube (with a discrepancy of about 25%) relative to wind tunnel measurements. However, the 18 19 discrepancy in *Re* between the wind tunnel measurements and the real-world applications 20 that the code aims to address influence the comparisons since Nu is a function of Re. 21 Evaluations against field observations are therefore done to overcome this challenge; they 22 reveal that, for applications in urban areas, the wind-tunnel studies result in a much lower range for the exponent m in the classic $Nu \sim Re^m$ relations, compared to field 23

measurements and LES (0.52-0.74 *versus* \approx 0.9). The results underline the importance of conducting experimental or numerical studies for convective scalar transfer problems at a *Re* commensurate with the flow of interest, and support the use of wall-modeled LES as a technique for this problem that can already capture important aspects of the physics, although further development and testing are needed.

29 1 Introduction

Convective heat and mass transfer at high Reynolds numbers ($Re \sim 10^6 - 10^8$) over 30 31 complex surfaces is of interest for many engineering and environmental applications, 32 such as heat exchanger design, agricultural and urban meteorology, and building energy 33 studies. The latter applications are of growing significance due to rapidly expanding 34 urbanization interacting with global climate change to alter the urban environment and 35 the resource intensity of cities in complex ways. The convective heat transfer coefficient 36 over the exterior surfaces of buildings is a key parameter for modeling the exchange of 37 energy between buildings and their environment. This exchange needs to be quantified to 38 calculate accurate heating and cooling loads [1,2], to assess the energy performance of 39 the building envelope [3], and to better simulate the urban environment under a changing 40 climate [4].

In addition, with the heat-mass transfer analogy [5], knowledge on the turbulent transfer
of temperature (under conditions where it can be considered as a passive scalar) is

| 43 | transferable to studies on the exchange of other scalars, especially carbon dioxide and | | | | | |
|----------|---|--|--|--|--|--|
| 44 | moisture [6], which are important for example for assessing the performance of green | | | | | |
| 45 | roofs [7,8]. For urban climatological and meteorological studies, it is crucial to | | | | | |
| 46 | simultaneously capture the turbulent heat and water vapor surface fluxes, which are | | | | | |
| 47 | typically parameterized through an urban canopy model (UCM) [9-12] in coarse | | | | | |
| 48 | geophysical simulations. The transfer coefficients for heat and water vapor are important | | | | | |
| 49 | parameters in these UCMs [13], but their current parameterizations are partially based on | | | | | |
| 50 | experimental results that are over 90 years old [14]. Improved parameterizations would | | | | | |
| 51 | involve environmental turbulent boundary layer flows over large roughness elements the | | | | | |
| 52 | height of which can be a significant fraction of the total boundary layer depth. Such | | | | | |
| 53 | surfaces are termed very rough in Castro et al. [15] and the resulting flow differs from the | | | | | |
| 54 | classic rough-wall boundary layers discussed for example in Jiménez [16] where the | | | | | |
| | | | | | | |
| 55 | height to boundary layer depth ratio is limited to be below 0.025. Advancing our | | | | | |
| 55 56 | | | | | | |
| | height to boundary layer depth ratio is limited to be below 0.025. Advancing our | | | | | |
| 56 | height to boundary layer depth ratio is limited to be below 0.025. Advancing our understanding of the fundamental transport processes of heat and moisture over such | | | | | |
| 56 57 | height to boundary layer depth ratio is limited to be below 0.025. Advancing our understanding of the fundamental transport processes of heat and moisture over such complex surfaces, and how to model them via transfer coefficients beyond the current | | | | | |

Three different approaches have been traditionally taken to gain a better understanding of
 the convective transfer coefficients. The first approach is placing scale models in wind
 tunnels and measuring the convective transfer of either some substance or temperature,

| 63 | while minimizing the effect of buoyancy (which could nonetheless be quite important in |
|----|---|
| 64 | real urban terrain). These studies [17-24] often considered cases at lower Reynolds |
| 65 | numbers $(10^3 - 10^4)$ (due to length scale limitations), with a developing turbulent boundary |
| 66 | layer in a parallel channel flow. Mass transfer experiments, usually with Naphthalene |
| 67 | sublimation techniques [18,25] or water evaporation [23], were performed to study the |
| 68 | mass transfer from surface-mounted cubes in a wind tunnel. These are only some |
| 69 | examples of wind tunnel studies from the extensive literature, which was summarized in |
| 70 | relatively recent reviews [2,3]. One advantage of wind tunnel studies is that the spatial |
| 71 | variation of heat/mass transfer coefficients along the surfaces of the bluff elements can be |
| 72 | accurately measured. The setup of the experiments can also be varied to investigate the |
| 73 | effects of different angles of attack [19] and geometric configuration of the roughness |
| 74 | elements [17,23], among other topographically complexities. However, a simple |
| 75 | extension of these studies to the environment has to be handled with caution. The |
| 76 | Reynolds number of the typical atmospheric boundary layer (ABL) is 3-4 orders of |
| 77 | magnitude higher than that of common wind tunnels. Unlike momentum exchange, which |
| 78 | is fully dominated by form/pressure drag over complex topographies at high Re, heat and |
| 79 | mass exchanges are always performed by molecular conduction or diffusion in the |
| 80 | vicinity of the complex interface and do not lose their dependence on the molecular heat |
| 81 | and mass diffusivities at high <i>Re</i> . Neither the convective to conductive/diffusive scaling |
| 82 | represented by the Nusselt number for heat (Nu) or Sherwood number for mass (Sh), nor |

| 83 | the inertial scaling given by the Stanton number ($St \sim Nu / Re$), become independent of |
|----------------------------------|---|
| 84 | <i>Re</i> in general (See Lienhard and Lienhard[26]). <i>Re</i> -independence for <i>St</i> might be |
| 85 | approached or expected only if the flow over each facet is itself also fully rough [27], |
| 86 | which is not always the case over urban terrain since the surfaces of building facets might |
| 87 | be smooth or transitional. The empirical correlations of Nu, Sh, or St with Re obtained |
| 88 | from these scale model experiments are thus not directly applicable to heat or mass |
| 89 | transfer from buildings [23]. In addition, the usually thin inflow turbulent boundary |
| 90 | layers [2] and the low turbulent intensity levels are further reasons why wind tunnel |
| 91 | studies of heat and mass transfer, although providing very valuable insight, have |
| 92 | limitations that preclude the direct application of their findings to large scale flows at |
| | |
| 93 | high Re, such as flows in the real natural environment [28]. |
| 93 94 | high <i>Re</i> , such as flows in the real natural environment [28]. Another approach that overcomes the problem of low <i>Re</i> in wind tunnel studies is |
| | |
| 94 | Another approach that overcomes the problem of low Re in wind tunnel studies is |
| 94 95 | Another approach that overcomes the problem of low <i>Re</i> in wind tunnel studies is full-scale experiments conducted outdoors on buildings or structures [29-33]. These field |
| 94 95 96 | Another approach that overcomes the problem of low <i>Re</i> in wind tunnel studies is full-scale experiments conducted outdoors on buildings or structures [29-33]. These field experiments give very valuable information especially on the correlation between the |
| 94 95 96 97 | Another approach that overcomes the problem of low <i>Re</i> in wind tunnel studies is full-scale experiments conducted outdoors on buildings or structures [29-33]. These field experiments give very valuable information especially on the correlation between the heat transfer coefficient and wind speed, which can be generalized to a power-law |
| 94 95 96 97 98 | Another approach that overcomes the problem of low <i>Re</i> in wind tunnel studies is full-scale experiments conducted outdoors on buildings or structures [29-33]. These field experiments give very valuable information especially on the correlation between the heat transfer coefficient and wind speed, which can be generalized to a power-law relation between <i>Nu</i> and <i>Re</i> . One manifestation of the continued dependence of heat and |
| 94 95 96 97 98 99 | Another approach that overcomes the problem of low Re in wind tunnel studies is full-scale experiments conducted outdoors on buildings or structures [29-33]. These field experiments give very valuable information especially on the correlation between the heat transfer coefficient and wind speed, which can be generalized to a power-law relation between Nu and Re . One manifestation of the continued dependence of heat and mass exchange on Re is that the exponents in such power laws are themselves Re |

climate studies [1,13]. However, generalization of the findings can also be challenging due to the influence of the exact shapes of the building facets, the texture/roughness of the building surface materials, and the surrounding structures in the outdoor environment. In addition, the positions at which the temperature and wind velocity are measured vary across different field studies, further complicating inter-comparisons between them to extract more universal empirical relations.

109 Numerical simulations are another useful methodology to study this problem. Reynolds 110 averaged Navier-Stokes (RANS), large-eddy simulations (LES) or direct numerical 111 simulations (DNS) have been carried out in the recent years to study the turbulent transfer 112 of momentum and scalars over rough surfaces with roughness elements that mimic 113 buildings or urban canyons [34-37]. Since the computational cost of resolving the viscous 114 layer (i.e. DNS [38-41] or wall-resolved LES [42]) is too high for applications at Re 115 commensurate with the real-world (limiting these techniques to low *Re* where the same 116 challenges discussed above for wind tunnels reemerge), wall modeling is often adopted 117 for RANS or wall-modeled LES studies. The 'law of the wall' or related equilibrium 118 approaches, which are based on the concept of universal behavior of momentum and 119 scalars in the inertial (logarithmic) layer, are often adopted [34,35,43-45]. These types of 120 wall models have some known caveats in complex flow regions [46]; however, good 121 agreement of models using such equilibrium laws with experiments have been found by 122 both Park et al. [34] and Liu et al. [44] in their studies of transfer of scalars over 123 geometrically complex surfaces. The application of such equilibrium wall-models in LES 124 pose additional challenges (compared to RANS) that were very comprehensively 125 assessed by Wyngaard et al. [47]. Various other more sophisticated wall-models that 126 should in principle offer better performance have been proposed such as models that 127 solve the boundary layer equations numerically [48] or analytically [49,50], or models 128 that use a "customized temperature wall function" (CWF) (though based on low Reynolds number results) [51]. Nevertheless, the challenge of wall-modeling in LES 129 130 remains open [52,53], even when the very important influence of buoyancy and how to 131 represent it correctly in wall models (particularly for vertical walls) is ignored. This challenge frames the scope and goals of this paper. 132

133 Given that for studies of turbulent flow and transport over urban-like rough surfaces at 134 high *Re* wall-modeled LES is a feasible and very appealing tool, there is a growing urgent 135 need to assess its skill in capturing turbulent scalar transport. The near-surface 136 performance is more critical for scalars than for momentum (again due to the dominance 137 of form drag, which is partially resolved in LES, for momentum), and as such the role of 138 the wall-model is more prominent. But if the shortcomings of current wall models can be 139 investigated, quantified, and potentially overcome, the impact on future studies that focus 140 on scalar transport under high Re scenarios can be substantial. It is worthwhile to stress 141 again the importance of studying the heat/mass transfer problem at a Reynolds number 142 that is representative of the real problem of interest (which is possible with wall-modeled 143 LES), given that the scalar transfer is inherently *Re*-dependent.

144 Therefore, the objective of this study is to provide a thorough assessment of 145 wall-modeled LES by detailed comparisons to both scale-model and full-scale studies. 146 Knowing the capabilities and limitations of this numerical approach will help to draw 147 more sensible conclusions for future applications in building energy and urban 148 climatology studies. A practical question we seek to answer is: are the errors resulting 149 from the parameterization of unresolved scales (wall and subgrid scale models) in LES 150 larger or smaller than the errors involved in extrapolating from low-Re approaches (DNS 151 or wind tunnels) to high-Re real world flows, for scalar transfer problems? 152 This paper is organized as follows: section two describes the numerical details of the 153 large eddy simulation; section three discusses the comparison of the local scalar transfer 154 coefficient with wind-tunnel studies of two-dimensional roughness; section four 155 considers both the local and average transfer coefficients by comparing to wind-tunnel 156 studies of a single cube; section five focuses on the comparison with full-scale field 157 measurement, section six provides a summary and conclusions.

| Nomenclature | | | | |
|--------------|--|-----------------|--|--|
| c_p | specific heat at constant pressure | Z _{0s} | scalar roughness length | |
| h_c | heat/mass transfer coefficient $q_s / (s_0 - s_{ref})$ | <i>x,y,z</i> | streamwise, cross-stream and vertical coordinate | |
| Н | height of the obstacle (rib or cube) | λ | heat conductivity of solid surface | |

| Li | LES domain size in direction <i>i</i> | Subscripts | | |
|----------|---|--------------|---------------------------------------|--|
| т | power exponent in Nu-Re relation | <i>x,y,z</i> | streamwise, cross-stream and vertical | |
| Re | Reynolds number = $u H / v$ | | directions | |
| S | scalar concentration | LES | quantities from LES | |
| и | characteristic velocity scale | Exp | quantities from experiments | |
| U* | Friction velocity = $(-\tau_w)^{1/2}$, where τ_w is | 0 | quantity at surface | |
| | the total kinematic wall shear stress | | quantity at reference height | |
| Z_{0m} | momentum roughness length | | | |



160 2 Wall-modeled LES and Dynamic Roughness Wall Model

The LES code uses the immersed boundary method (IBM) to account for presence of the roughness elements, in which a discrete time momentum forcing is used to simulate the immersed boundary force [54,55]. The filtered incompressible continuity, Navier-Stokes and scalar conservation equations (Eq.1-3, respectively) are solved assuming hydrostatic equilibrium (we will omit the usual tilde above the variables that denotes filtering for simplicity, but all the variables we will discuss are the filtered/resolved components solved for in LES unless otherwise noted)

168
$$\frac{\partial u_i}{\partial x_i} = 0, \qquad (1)$$

169
$$\frac{\partial u_i}{\partial t} + u_j \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) = -\frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + F_i + B_i, \qquad (2)$$

170
$$\frac{\partial s}{\partial t} + u_i \frac{\partial s}{\partial x_i} = -\frac{\partial q_i^s}{\partial x_i},$$
 (3)

where t denotes time; u_i is the resolved velocity vector; p is the modified pressure; τ_{ij} is 171 the deviatoric part of the subgrid stress tensor; F_i is the body force driving the flow (here 172 173 simply a homogeneous steady horizontal pressure gradient along the x direction); and B_i 174 is the immersed boundary force representing the action of the obstacles (buildings) on the fluid. The density is assumed equal to 1 (all the equations are normalized so the 175 176 numerical value of the density is irrelevant). In Eq.(3), s denotes a passive scalar quantity and q_i^s is the *i*th component of the subgrid scale scalar flux. Although the code can 177 178 simulate active scalars (see [56,57]), the experimental data we identified for code 179 evaluation were under conditions where buoyancy played an insignificant role.

180 The code uses a pseudo-spectral method for computing the horizontal spatial derivatives 181 on a uniform staggered Cartesian grid. To overcome the Gibbs phenomenon that emerges 182 from the combined application of the IBM method with spectral derivatives, a smoothing 183 approach we developed and detailed in Li et al. [58] is adopted. Vertical spatial 184 derivatives are obtained from second-order centered finite difference. Second order 185 Adams-Bashforth time integration is used. The subgrid scale (SGS) stress tensor is 186 modeled using the Lagrangian scale-dependent dynamic Smagorinsky model [59], while 187 the SGS scalar flux model uses the dynamically computed SGS viscosity with a constant 188 SGS Prandtl number (Pr_{SGS}) of 0.4 (this is unrelated to the molecular Pr [60]).

189 In this study, we adopt a new approach for dynamically evaluating the momentum and 190 scalar roughness lengths in the expression of the log-law wall model. The general log-law 191 wall model for momentum and scalars is given by:

192
$$\frac{u}{u_*} = \frac{1}{\kappa} \log\left(\frac{z}{z_{0m}}\right) , \qquad (4)$$

193
$$\frac{s_0 - s}{s_*} = \frac{1}{\kappa} \log\left(\frac{z}{z_{0s}}\right) , \qquad (5)$$

194 where u is the local wall-parallel velocity near the wall; s_0 is the scalar concentration or 195 temperature at the surface; u_* is the friction velocity calculated as the square root of the 196 kinematic wall shear stress τ_w ; s_* is the mass flux concentration or heat flux temperature 197 (defined as the kinematic surface flux divided by u_*); z is distance away from the wall in the wall-normal direction; $\kappa = 0.4$ is the von Kármán constant; and z_{0m} and z_{0s} are the 198 199 roughness lengths for momentum and scalars, respectively. These roughness lengths are 200 often chosen according to the roughness types of the surfaces for hydrodynamically 201 rough walls. However, building facets are often hydrodynamically smooth, including the 202 experiments we compare to. Therefore, instead of adopting a fixed roughness, we 203 dynamically model the roughness lengths for momentum and scalars as a function of the 204 viscous length scale v/u_* . In fact, it has been shown by Kader and Yaglom [61] that 205 similar reasoning to the one that yielded the Prandtl-Nikuradse momentum skin friction 206 law for smooth pipe and channel flow can be applied to scalar transfer in a turbulent flow 207 to obtain heat or mass transfer laws for a smooth wall, with some unknown quantities that 208 can be determined from experiments. Eq.(4) can be rewritten following the 209 Prandtl-Nikuradse skin friction law as

210
$$\left(\frac{u}{u_*}\right) = A \log\left(\frac{z}{v/u_*}\right) + B, \qquad (6)$$

211 which can be further rearranged into

212
$$u_* = \frac{u}{A \log\left(\frac{z \ e^{B/A}}{v \ / \ u_*}\right)} = \frac{u}{A \log\left(\frac{z}{z_{0m}}\right)},$$
(7)

213 where A and B are determined from experiments and z_{0m} is given by

214
$$z_{0m} = \frac{V}{u_*} e^{-B/A}.$$
 (8)

215 The same dimensional analysis can then be similarly developed for scalars:

216
$$s_0 - s(z) = s_* \psi(u_* z / v, v / \chi),$$
 (9)

where χ is the mass or thermal diffusivity, and ψ is a dimensional analysis function to be determined empirically (with the aid of profile-matching as for velocity). Eq.(9) is a general one for turbulent mass or heat transfer in wall-bounded flows. For air, Pr = 0.7and $s_* = q_s / (\rho c_p u_*)$, where q_s is the dynamic heat flux at the wall and c_p the heat capacity of the air. The experiments to determine the form of Eq.(9), as detailed in Kader and Yaglom [61], then yield the log-law for scalar:

223
$$\frac{s_0 - s(z)}{s_*} = \alpha \log\left(\frac{z}{\nu/u_*}\right) + \beta .$$
(10)

For air, α and β can be found from experiments for heat transfer with weak buoyancy. If *s* represents air temperature, then the heat flux at the wall is given by

226
$$\frac{q_s}{\rho c_p} = u_s s_s = u_s \frac{(s_0 - s(z))}{\alpha \log\left(\frac{z \ e^{\beta/\alpha}}{v/u_s}\right)} = u_s \frac{(s_0 - s(z))}{\alpha \log\frac{z}{z_{0s}}} , \qquad (11)$$

227 where z_{0s} for the scalar can be written as:

$$z_{0s} = \frac{v}{u_*} e^{-\beta/\alpha} \,. \tag{12}$$

The roughness length expressions in Eq.(8) and Eq.(12) should be universal for smooth walls, and thus we can adopt the constants determined by Kader and Yaglom from experiments for fully turbulent flows [61,62] (Table 1 in Kader and Yaglom[61]; *A* can be viewed as the inverse of the von Kármán number, but only the ratios B/A and β/α influence the results and here we select the same ratio of 3.9/1.8 for both momentum and scalars, which effectively yield

235
$$z_{0m} = z_{0s} = \frac{V}{8.73u_*} \simeq \frac{V}{9u_*} \quad . \tag{13}$$

236 This result applies for molecular Prandtl of Schmidt numbers ~ 1 , which is a reasonable 237 approximation for all the tests we conduct in this study. These length scales depend on u_* 238 which varies in space and time over complex geometries. We thus use an explicit approach where u_* form the previous time step is used in Eq. (13) to determine z_{0m} at 239 240 every wall location, and then the updated z_{0m} is used to compute u_* from Eq.(7). This 241 dynamic equilibrium wall-model controls the fluxes at the solid-fluid interface, and 242 therefore is important to determine if the LES is able to capture the physics of the flow 243 and reproduce experimental observations. It is important to note here that this model, by construction since it assumes smooth facets, yields a Stanton number that is Re dependent. On the other hand, if the facets were assumed fully rough with constant z_{0m} and z_{0s} , the heat transfer regime would become Re independent. We assume the presence of a logarithmic form at the first grid point away from the wall of the solid, which is commonly done in direct forcing immersed boundary method as adopted here.

249

250 3 Spatial variation of the transfer coefficient compared to a wind tunnel study

251 3.1 Experimental setup of mass transfer over two-dimensional ribs

252 The dimensional (e.g. in W K $^{-1}$ m $^{-2}$) local heat or mass transfer coefficient is defined as

253
$$h_c = \frac{q_s}{s_0 - s_{ref}} , \qquad (14)$$

where s_{ref} is some reference scalar quantity in the fluid. The distributions of the local heat and mass transfer coefficients obtained from detailed scale-model measurements have large spatial variations over the surface of roughness elements due to the highly complex flow patterns involving separations and reattachments in the flow. It is therefore desirable to assess the capability of the wall-modeled LES in predicting these spatial patterns of local heat and mass transfer coefficients.

Nevertheless, one here again faces the challenge that the magnitudes of h_c in scaled-model experiments at lower *Re* and LES at larger *Re* are not directly comparable due to the dependence of h_c on *Re*. However, since the momentum dynamics are less sensitive to Re, the spatial flow patterns should match as long as the scaled-model Reexceeds ~ 10⁵, and therefore the resulting spatial variation patterns of h_c should be comparable. Therefore, to overcome the magnitude discrepancy and still compare the spatial variabilities, the heat or mass transfer coefficients from different scale-model experiments and numerical simulations are usually normalized for appropriate comparison [13].

269 The measurement of mass transfer coefficient from a wind-tunnel study on evaporation of 270 water from two-dimensional roughness (ribs) by Narita [23] is used here as a benchmark 271 case to assess the LES. The roughness elements, made of acrylic resin of 1mm thickness, 272 were covered with wetted filter paper. A fine thermistor sensor was inserted just below 273 the paper surface to monitor the surface temperature. The evaporating surface is assumed 274 to be at saturation. A weighing method was used to obtain the evaporation rate and thus 275 the mass transfer coefficient can be estimated by knowing the ambient water vapor 276 concentration. Measurements were conducted at a low relative humidity to keep the 277 experimental error of the transfer coefficient to within 4%.

Note that the sharp edges of these 2D ribs fix the separation points to the downstream top corners of each rib, and thus strengthen the insensitivity of the flow patterns to *Re* and improve the flow simulation results [63].

281 3.2 Numerical model of mass transfer

282 We considered configurations with three different separation distances between the 283 two-dimensional ribs. Figure 1 is a side view of the basic configuration. The rib height H284 is represented with 16 grid points. We use a horizontally periodic boundary condition for 285 momentum and mass (thus we are simulating infinite repetitions of the patterns shown in 286 Figure 1). The longer section behind the ribs is used to ensure that the inflow velocity at the first rib is free of the wake influence from the fifth element. It also mimics the test 287 288 section surface upstream of the ribs in the open circuit wind tunnel [23]. The 289 experimental Reynolds number is 16000, where velocity is fixed at 4m/s at the top of the 290 boundary layer and length scale is the rib height. The experiment did not precisely 291 control the humidity in the incoming air in the wind tunnel. Instead, during each run 292 where the evaporation rate was measured, the evaporation rate from a flat plate placed in 293 the free stream was simultaneously recorded for normalizing the measurements. 294 Therefore, we could not replicate the exact details of the mass inflow, but again these 295 only affect the magnitude and not the spatial patterns of the transfer coefficient that we 296 seek to investigate here.

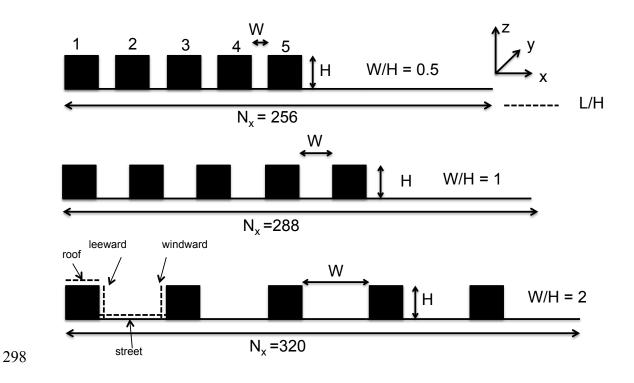
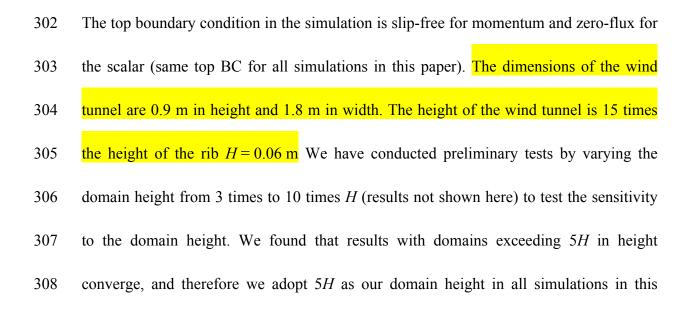
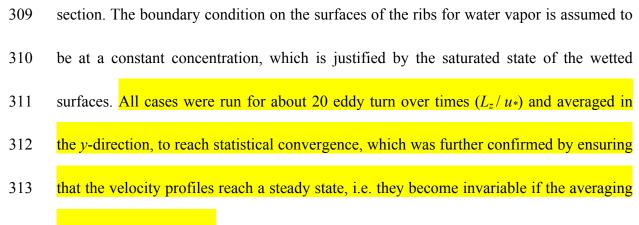


Fig. 1. Side view of the geometric configuration of the numerical simulations. The cases of W/H=0.5, 1 and 2 are shown in the figure from top to bottom. Inflow is from left to right. N_x is the number of grid points in x-direction. $N_z = 80$ total vertical grid points for all three cases.





314 time is further increased.

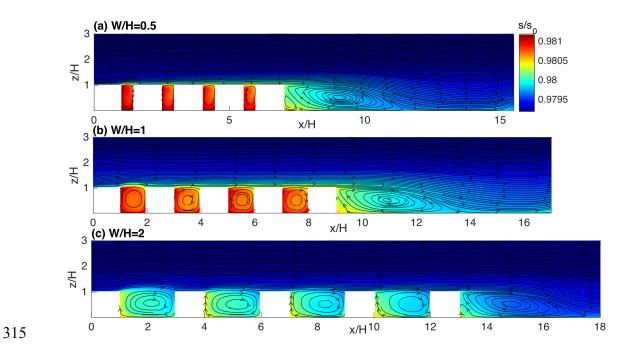


Fig. 2 Mean (time- and *y*-averaged) contour plots of s/s_0 and streamlines. The wind is from left to right. The white spaces represent the transect areas occupied by the solid 2-dimensional ribs. Color scale for the normalized scalar concentration is the same for all three cases.

Figure. 2 (a)-(c) shows the pseudocolor plots of the scalar concentration normalized by
the surface scalar concentration, together with the streamlines. The central vortices in the

321 W/H = 0.5 and 1 cases are characteristic of the 'skimming flow' regime and explain the 322 high concentrations of scalar in the space between the ribs ("the street canyon"), whereas 323 the slightly asymmetric flow field in case W/H = 2 is evidence of more complex flow 324 interactions in the 'wake interference regime' [64,65] that allows more exchange between 325 the canyon and the air aloft. The flow patterns are consistent with the regime expected for 326 this geometry. In addition to the more intensive exchanges for the widest canyon, the reduced "emitting surface" to "canyon volume" ratio, (W + 2H) / (HW) = H + 2/W, 327 when W increases and H is maintained constant, further explains the reduced 328 329 concentrations in the canyon.

330 Figure. 3 (a)-(c) shows instantaneous contour of the scalar concentration normalized by the surface scalar concentration, together with the streamlines along one xz-slice at a 331 332 fixed y. The instantaneous structures in the scalar concentration field, as well as the 333 streamlines, are generally distinct from their averaged counterparts shown in figure 2, 334 particularly for the W/H = 2 case. The depicted turbulent structures are important for the 335 vertical exchange; for example, one can observe the strong ejection from the last canyon 336 in Figure 3(c) for the W/H = 2 case. This is consistent with general observations for such kind of type-k roughness where the eddies of scale H are shed out of the cavity, resulting 337 in the more complex flow interactions. The instantaneous vortices inside the canyons for 338 339 the two other cases, especially W/H = 1 in 3(b), are somewhat more similar to their time

and space averaged counterparts in figure 2(b). This dominant mean circulation inside the
canyons for these cases might hinder ejections and sweeps near the top of the canyons
and reduce the instantaneous exchange between canyons and air above. While we show
only one snapshot here; other snapshots we analyzed conveyed the same information.

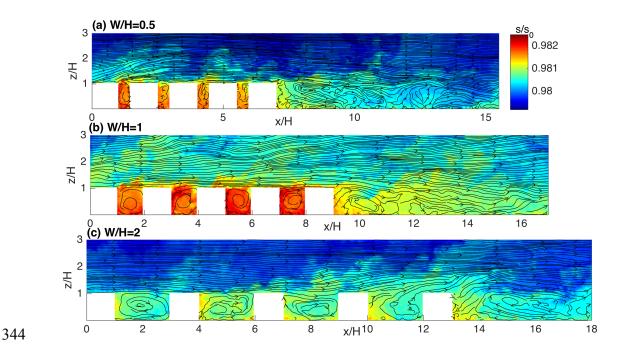


Fig. 3 Snapshots of instantaneous s/s_0 and streamlines. The wind is from left to right. The white spaces represent the transect areas occupied by the solid 2-dimensional ribs. Color scale for the normalized scalar concentration is the same for all three cases.

Figure. 4 shows the comparisons between the experimental and LES results for the three rib separations, while Table 1 lists the absolute percentage deviation of the LES from the experiments. All quantities are normalized by the average mass transfer coefficient on the floor in between two consecutive ribs. The experimental data are averaged over multiple

352 ribs starting where the transfer coefficient over subsequent ribs converge. To best mimic 353 the experimental data, we average the LES result using relevant quantities from the 354 second to the fifth rib, where the transfer coefficients become independent of location of 355 the ribs. We tested different averaging ranges and the impact on the results is minimal 356 The resulting general spatial trends for each case, as well as the changes in transfer 357 coefficient patterns as a result of the variation in the separation distance, are adequately 358 captured by the LES. Despite the fact that the leeward transfer coefficient varies quite 359 considerably across different cases, its variation is captured well: for example, the peak 360 for W/H=1 was observed to occur at about 0.4H from the bottom and this maximum is 361 also clear in LES. Both the experiment and the LES also show that the decrease along 362 that face at W/H=0.5 is more pronounced than W/H=2. The variation on the street face 363 (floor between two ribs) is also reasonably captured by the LES. The maximum of the 364 transfer coefficient on the street occurs at about 0.5H in the experiments for cases W/H=1365 and W/H=2, which is also the location predicted by the LES. This peak matches the 366 location of the highest wall-parallel velocity produced by the recirculating flow in the 367 canyon. Given the complexity of the wakes and recirculation inside the canyon, the 368 matching of the observed time-averaged transfer coefficients that are modulated by these 369 flow patterns indicate that the wall-modeled LES is capable of reproducing them, as well 370 as the spatial distributions of the local mass transfer they generate inside the canyon.

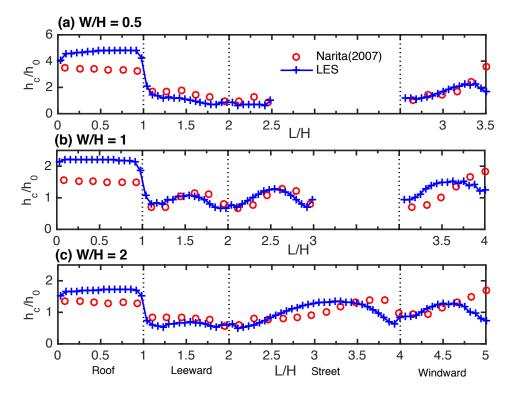
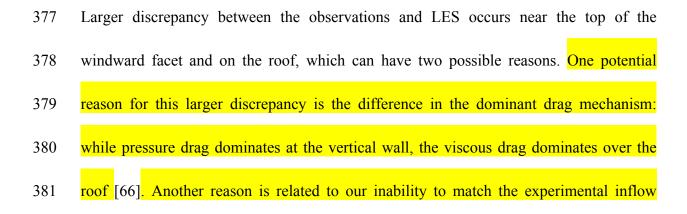




Fig. 4. The normalized mass transfer coefficient for different positions across the canyon. L is the path length along the interface, and a unit L/H is the length of the dotted line indicated in Fig. 1 for case W/H=2 as an example. The white space with no data for the cases in (a) and (b) does not reflect a data gap, but the fact that the street widths are shorter in these cases compared to the case in (c), which we adopt to fix the overall width of the figure.



| 382 | conditions in LES exactly, as shown in Figure 5. The inflow vertical profiles of the |
|-----|---|
| 383 | normalized mean streamwise velocity and turbulent intensity (TI) at the upstream of |
| 384 | location $x = 0$ are shown in Figure 5. The mean velocity in both LES and experiment is |
| 385 | normalized by its value at $z=H$, while the TI is computed locally. The mass transfer from |
| 386 | the roof surface and upper part of the front/windward wall are more dependent on the |
| 387 | inflow profile (mean velocity as well as turbulence intensity) than the bottom and the |
| 388 | leeward faces. To test the sensitivity of the mass transfer for the different faces to inflow |
| 389 | conditions, another test was conducted also assuming a fully periodic domain but without |
| 390 | the long extension. This implies an infinite array of ribs, and is further removed from the |
| 391 | actual setup in the wind tunnel. The results from this test (not shown here) indicate that |
| 392 | while the absolute value of the error defined as $ (h_{LES}-h_{Exp})/h_{Exp} $ remained similar for the |
| 393 | leeward and bottom faces, the errors on the front and top faces were 3-5 times larger |
| 394 | compared to the values presented in Table 1, which correspond to the basic setup. This |
| 395 | further confirms the importance of characterizing the inflow in experiments accurately |
| 396 | and reporting it in the associated paper to allow the data to be used for model validation, |
| 397 | and supports our explanation that the higher discrepancy in the upper part of the |
| 398 | windward facet and on the roof are related to a mismatch in the inflow. |
| | |

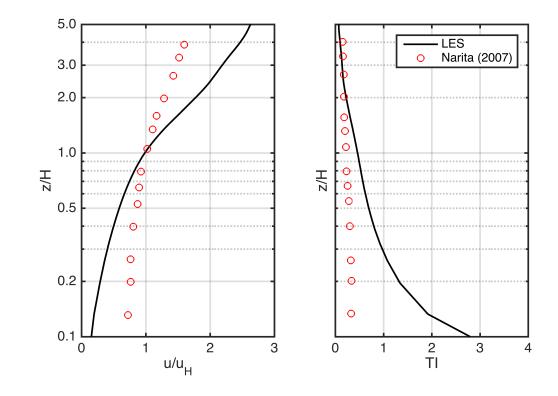
| | Leeward | Street | Windward | Roof | Average |
|-----------------|---------|--------|----------|------|---------|
| <i>W/H</i> =1/2 | 18.2 | 15.5 | 20.3 | 42.3 | 25.5 |
| <i>W/H</i> =1 | 11.1 | 12.0 | 30.2 | 35.5 | 22.5 |
| <i>W/H</i> =2 | 20.2 | 22.5 | 17.4 | 27.8 | 22.0 |

401 Table 1. The absolute percentage deviation (%), $|(h_{LES} - h_{Exp})/h_{Exp}| \times 100$, of the averaged transfer

402

403

coefficient over each facet and all facets combined.



404 Fig. 5 The comparison between the mean streamwise velocity and turbulent intensity TI at the405 inflow section between LES and experiment.

406 4 Facet-averaged heat transfer from a cube compared to a wind tunnel study

407 *4.1 Experimental set-up of heat transfer from a single cube*

408 The turbulent forced convective heat transfer over a wall-mounted cube at relatively low 409 Reynolds number has been quite extensively studied as discussed in the introduction. In 410 particular, we will focus on the study by Nakamura et al. [22] since their experiment was 411 conducted at a relatively high Re - from 4,200 to 33,000 - despite the fact that is remains 412 orders of magnitude lower than for real buildings. Furthermore, relations between Nu and 413 *Re* for different faces of the cube were proposed in that study, and they will be useful for our comparisons. In this experiment, a copper cube was heated by an embedded heater to 414 415 maintain the surface temperature approximately constant (within \pm 0.5 °C). The cube, 416 with a dimension of 30 mm, was placed in a low-speed wind tunnel of 4 m height. 3 m width, and 8 m length. A turbulent boundary layer is achieved by placing a horizontal 417 circular cylinder 500 mm upstream from the cube to act as a trip. The diameter of the 418 419 circular cylinder is 10 mm and the boundary layer depth to cube height ratio varies from **1.5 to 1.83.** A temperature difference of approximately 10 °C is maintained between the 420 421 surface of the cube and the air temperature. Re, defined based on the cube height and the 422 bulk velocity upstream of the cube, was varied to assess how it is related to Nu. 423

._.

425 **4.2** Numerical model of heat transfer from a single cube

426 For all simulations in this section, a horizontally periodic domain is used. Figure 6 is the 427 schematic drawing of the setup of the numerical simulation. 30 grid points are used along 428 each side of the cube. The domain height is 4H, where H is dimension of the cube. The upper boundary condition is impermeable with a free-slip for momentum and 429 430 zero-gradient (no flux) for temperature. Five different simulations were performed at 431 different Reynolds number in our LES by varying the horizontal pressure forcing, which is equivalent to changing the bulk velocity in the inflow. The Reynolds number is defined 432 433 as Re = UH/v, where U is the free stream velocity in the wind tunnel. The LES velocity used in *Re* is taken at the location (x,z)=(0, 1.5H), which provides a reasonable match to 434 435 the experimental definition. Notice that in the LES setup the wall model defines an inner scale (since we are using a smooth-wall roughness length parameterization that depends 436 437 on v), and the nominal *Re* of the simulations can therefore be determined; viscous stresses 438 are neglected in the numerical integration of the momentum and scalar equations.

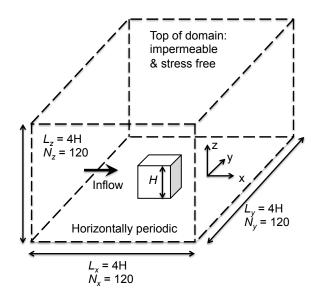


Fig.6. Schematic drawing of the setup of the numerical simulation. A heated cube of size *H* is placed in the middle of the domain. The grid consists of 120^3 nodes, and the domain size is $L_x = L_y = L_z = 4H$.

- 443 For all simulated cases, a constant temperature wall boundary condition is implemented
- 444 in the wall model. All cases were simulated for a total of 100 eddy turnover times,
- 445 defined as L_z/u_* (this corresponds to 400 eddy turnover times defined based on the cube
- 446 scale). After a transient of 50 eddy turnovers, all time-averaged statistics reported were
- 447 computed using the last 50 eddy turnovers times.
- 448 Figure 7(a) shows a vertical x-z transect along y = 2H (middle of the cube), where both
- 449 the contour of temperature deviation from the inflow temperature, defined as $(\theta \theta_i)/\theta_i$,
- 450 and the velocity streamlines are shown. Similarly, figure 7(b) is a horizontal transect at
- 451 z = 0.015H (near the floor). The temperature deviation contours depict large spatial

gradients around the cube. The separation near z = H/2, and the reattachment zone near the lower corner of the front face of the cube (figure 7(a)) compare well with experimental visualizations [22,67]. The separation zone and the two counter-rotating vortices shown in figure 7(b) near the rear face are also some well-known features of flow around a single cube, as seen for example in flow visualizations in Nakamura *et al.* [22] and Martinuzzi and Tropea [67].

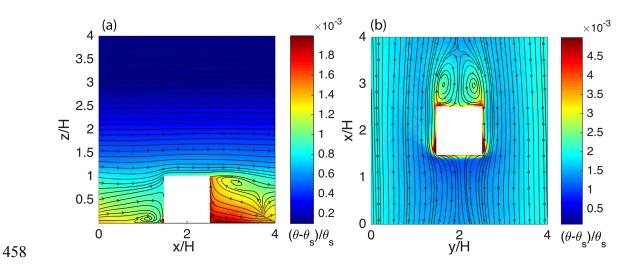


Fig.7. Mean flow field (streamlines) and contour plot of the temperature deviation from θ_{inflow} along (a) a vertical *x-z* plane at y = 2H; and (b) a horizontal plane close to the floor at z = 0.015H.

462 The *Nu-Re* relation obtained from experimental measurements of Nakamura *et al.* [22]
463 follow the classic power law

the coefficients of which are given in Table 2. Due to the difference in *Re*, these

464

 $Nu = a Re^{m}$

(15)

| 466 | experimental Nu-Re relations of Nakamura et al. are extrapolated to the Re of the LES for |
|-----|--|
| 467 | comparison. This ignores the well-known dependence of m on Re , a caveat we will revisit |
| 468 | in the next section. However, this approach was necessary since reducing our Re further |
| 469 | to match the experiment would place our first grid point in the viscous or buffer layers |
| 470 | and preclude us from testing the wall-modeled LES configurations that we aim to use for |
| 471 | full-scale (real-world) applications. |

472

| | а | т |
|--------------|-------|------|
| front | 0.71 | 0.52 |
| side | 0.12 | 0.70 |
| rear | 0.11 | 0.67 |
| top | 0.071 | 0.74 |
| cube average | 0.138 | 0.68 |

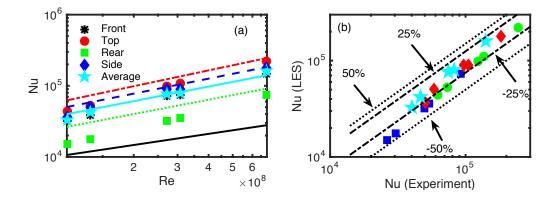
473 Table 2. The coefficients and exponents in Eq.(15) as determined in Nakamura *et al.* [22].

Figure 8(a) shows the comparisons between the relations proposed by Nakamura *et al.* [22], extrapolated to the LES *Re*, for the averaged *Nu* on different facets and the LES results. Although these experimental relationships were found at *Re* orders of magnitude smaller, the match between predicted values according to Eq.(15) and those obtained from LES is in fact reasonable. The front and leeward faces show higher errors than the other faces, but errors cancel out and cube-averaged fluxes match quite well. This can be

480 interpreted either as giving confidence in the performance of LES, or alternatively in the 481 applicability of extrapolations from low Re studies to the higher Re flows in the 482 real-world. Figure 8(b) shows that the ratio of deviation R_d defined as:

$$R_d = N u_{LES} / N u_{Exp} \quad , \tag{16}$$

where the experimental results are the values predicted from Eq.(15) and table 2, at 484 485 different *Re*. Except for the front face which is excluded from this comparison, exchanges from the other faces remain within 50% of the measurements. The most likely reason 486 why the front face deviates the most from the experimental result is that the experimental 487 flow over that face could still be in a regime of laminar or transitional flow. This is 488 489 strongly suggested by the small experimental exponent, 0.52, which is considerably lower 490 than that expected in turbulent flows, and rather very close to the 0.5 limit expected for 491 laminar flows [68]. In addition, the turbulent boundary layer depth in the experiment is 492 1.5 δ/H , which is different than the fully developed one in LES of $4\delta/H$.

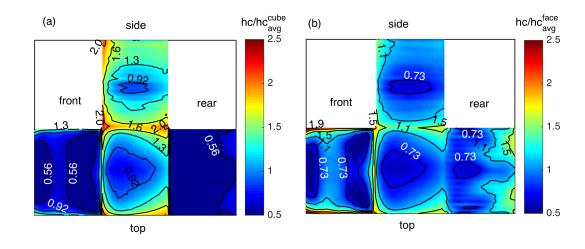


494 Fig.8.(a): Nu-Re relation for different faces using empirical results from Nakamura et al.[22] i.e.
495 using m and a from Table 2 and extrapolating to the Re of the LES. (b):Nusselt number of the

496 experiment vs. that from LES. The black lines denote the quantities Nu_{exp} (1+ R_d), where 497 $R_d = \pm 25$ and $\pm 50\%$. The front face is excluded in (b) since its errors are much higher due to the 498 *Re* discrepancy.

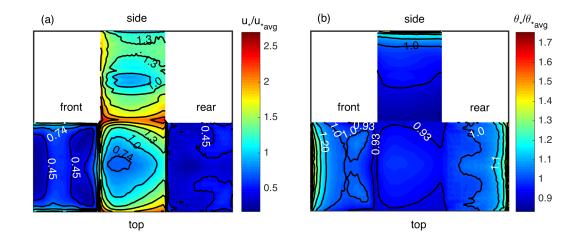
499 It is often of practical interest to use the cube-averaged or facet-averaged value of the 500 heat transfer coefficient when considering the bulk heat exchange between a building envelope and the surrounding air, despite the high spatial variability. Figure 9(a) shows 501 502 the contours of the heat transfer coefficient normalized by the cube average. Only one 503 side-face is shown because of symmetry. Large deviations from the cube-averaged value 504 occur on the edges as expected. The spatial variation at the intersections between front, 505 top and rear faces is the most prominent. Figure 9(b) depicts the heat transfer coefficient 506 normalized by the respective face-averaged values. Despite the large spatial variability at 507 the intersections between difference faces, the cyan contour of value 1.1 indicates that the 508 deviation over a large area of each face is only moderate. This implies that for practical 509 applications, point-measured values in the center of a facet or numerically-determined 510 face-averaged values give good estimates of the transfer over larger portions of each facet, 511 despite some loss of information on the higher values near the corners. However, 512 cube-averaged values should not be applied to individual facets. The contour plots in 513 figure 9 also compare well qualitatively with results in the experiments of Nakamura et al. 514 [22].

515 The wall friction velocity u_* and temperature scale θ_* , where $\theta_* = q_0/(u_*\rho cp)$, are shown 516 in figure 10(a) and (b) respectively. The spatial variability patterns of u_* are strongly 517 correlated with those of h_c , indicating that the friction velocity has a strong impact on 518 heat transfer as expected. The patterns of θ_* on the other hand are distinct, with strong 519 heat exchange near the bottom of the all faces due to the horseshoe vortex depicted in 520 figure 7.



522 Fig.9. (a): Local heat transfer coefficient normalized by the cube-averaged value on all four facets.

523 (b): Local heat transfer coefficient normalized by each facet average value.



525 Fig.10. (a): Spatial distribution of the wall friction velocity u_* normalized by the cube average 526 value. (b): Spatial distribution of the wall temperature scale θ_* normalized by cube average value.

Separate sensitivity tests with varying domain heights of 1.7*H* and 3*H* were also conducted and yielded markedly different results due to the increased flow blockage resulting in higher velocities around the cube. As shown in Table 3, the shorter domains result in higher *Nu* as a consequence of these higher velocities. The much smaller difference between 3H and 4*H* compared to 1.7*H* and 4*H* nevertheless indicated that convergence occurs when $L_z \approx 4H$.

533

| Percentage difference between surface averaged Nu compared to case L_z =4 H | | | | | |
|---|-------|-------|-------|-------|---------|
| L_z | Front | Тор | Rear | Side | Average |
| 1.7 <i>H</i> | +43.8 | +54.1 | +34.5 | +15.0 | +32.5 |
| 3 <i>H</i> | +10.8 | +5.60 | +6.76 | +6.78 | +7.34 |

Table 3 Percentage difference between surface averaged Nu compared to case $L_z=4H$

535 5 Comparison to full-scale field measurements

Field measurements of heat transfer coefficients provide valuable information to evaluate 536 537 high-Re numerical models with minimal discrepancy in the Reynolds number. We 538 considered the measurement performed by Hagishima et al. [69] in detail for comparison. This outdoor measurement campaign was conducted over two sites: one was on a 539 540 building roof, and the other on a vertical wall of a cubical extension mounted on a roof. 541 We selected the building roof case for comparison, in which there is a better similarity in 542 the setup between our numerical simulation and the field experiment. The roof surface 543 energy balance equation, together with the temperature difference between the building 544 surface and air temperature measurement, were used in the experiment to calculate the 545 convective heat transfer coefficient h_c . The temperature and wind speed measurements on 546 the roof were positioned at about 10% and 6% of the height of the building respectively. 547 The general Nu-Re relation was deduced from the experimental data and found to follow the power law relation 548

549

$$Nu = 0.023 \,\mathrm{Re}^{0.891} \tag{17}$$

with R-square value of 0.964, irrespective of wind direction variability. The length scale in the Reynolds number is defined as the length from the roof edge considering the wind direction, while the velocity scale is $u_0 = \sqrt{u^2 + v^2 + w^2}$, with the wind components measured by the anemometers.

554 For the comparison between these field measurements and the LES in terms of the fitted

555 relation between the Nusselt and Reynolds numbers, we estimate the Reynolds number 556 based on the same definition of the characteristic length and velocity scales used by 557 Hagishima et al. [69]. The same five sets of simulations presented in section 4 are used to estimate the Nu-Re relation. The h_c on the building roof is spatially variable as we 558 showed in previous sections; this affects the field experimental results fitted from 559 560 measurements at a few points. For accurate comparison, we extract the h_c from the LES 561 roof at the same locations where Hagishima et al. acquired measurements on the 562 experimental roof. Figure 11 depicts the distribution of the exponent m and coefficient a 563 in $Nu = a Re^{m}$, found from linear-regression of the LES results at different Re over the 564 roof facet. The red marks denote where the experimental measuring points were 565 positioned, approximately. On average, the spatial variation of the exponent m is about 566 11%, while a much greater variation is seen in the coefficient a, the values of which 567 varied by one order of magnitude.

From the roof-averaged LES results and the ones averaged over the 4 experimental points,we respectively obtain

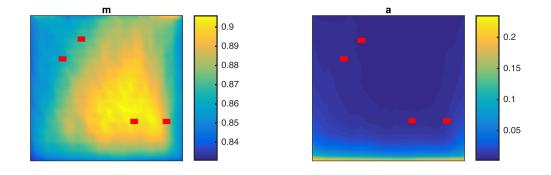
570
$$Nu_{LES}^{\text{roof-average}} = 0.013 Re_{LES}^{0.88}$$
, $Nu_{LES}^{4\text{points-average}} = 0.075 Re_{LES}^{0.88}$. (18)

571 The strong similarity in the exponent values in Eq.(17) and Eq.(18) indicates that our 572 wall-modeled LES is able to capture the change in heat transfer coefficient well even as 573 the wind speed (i.e. Re) varies. The LES values of a (0.013 and 0.075) bracket the 574 experimental value (0.023). We do not anticipate being able to exactly capture the 575 experimental value of a, as well as we capture m, for several reasons including:

Setup conditions in the field experiment and the LES cannot be exactly matched, and
 a is highly sensitive to these conditions unlike *m*. For example, according to a report
 by Hagishima et al. [69], the 0.25 m protrusion around the building edge induces
 separation and backflow. The measuring height was 0.60 m above the roof-top but the
 wake caused by these intrusions can affect the exact magnitude of heat transfer
 reflected in *a* (but not its scaling with *Re* reflected by *m*).

582 2. The wall-model imposes a thermal roughness length in LES by assuming a smooth 583 wall, but the actual smoothness of the roof used in the Hagishima *et al.* study is not 584 characterized. Some building walls could very well be transitionally or 585 hydrodynamically rough such that the actual roughness length z_0 of these surfaces is 586 needed to match *a*, although we point out that this would have also caused 587 discrepancy in *m*.

Therefore, the LES can be expected to quantitatively predict the scaling represented by min the relation between the wind speed and forced convective heat transfer with high accuracy, but the exact magnitude of h_c for a given wall also requires matching a and is highly dependent on fine details such as wall texture and material, and surrounding obstructions.



593

Fig.11. Spatial distribution of the best-fit results of m and a on the building roof, where the wind is blowing from bottom to top of the figure. The red dots are the location of the experimental measurements of Hagishima et al. [69].

597 Table 4 gives a summary of results from other field experiments that attempt to relate the 598 heat transfer to change in wind velocity (i.e. Nu-Re relation). Although the experimental 599 conditions and measurement techniques vary across these campaigns, and certainly 600 discrepancies exist among them, there seems to be a consistent power law relation 601 between the forced convective heat transfer and the wind speed with an exponent in the 602 range of 0.67-0.89. The wall-modeled LES considered in this paper is shown to give results that consistently fall within the experimental range. All of the exponents are <1, 603 604 suggesting that the flow over the surfaces is not in the fully rough regime where the 605 Stanton number would become independent of Re. 606

| Experimental LES | | |
|-------------------------|------------------------------------|------|
| Emmel et al.[30] | 0.85 (Roof) | 0.88 |
| Clear et al.[32] | 0.8 (Roof) | 0.88 |
| Yazdamian and Klems[31] | 0.89 (Windward, low-rise building) | 0.89 |
| | 0.671 (Leeward, low-rise building) | 0.90 |

Table 4. The exponent in the *Nu-Re* relation for different experiments and corresponding valuesfrom LES.

610 6 Discussion and Conclusions

611 This study assessed the capability of the wall-modeled LES approach to capture the 612 physics of forced convective heat/mass transfer between the surfaces of buildings and the 613 atmosphere. Through detailed comparisons to both wind-tunnel studies and field 614 experiment, we have shown that our LES is able to reasonably predict i) the spatial 615 variation of the heat/mass transfer coefficient over the different facets of 2D ribs; ii) the 616 average Nusselt number for a single cube (with larger discrepancy relative to 617 measurements over the windward face very likely related to the *Re* discrepancy); and iii) 618 the power law relation between the Nusselt and Reynolds numbers compared to field 619 measurements. The excellent match of the power law exponent *m* is largely attributable to 620 the dynamic wall model we proposed and implemented here.

Returning to the motivating question we asked: "are the errors resulting from theparameterization of unresolved scales (wall and subgrid scale models) in LES larger or

smaller than the errors involved in extrapolating from low-*Re* approaches (DNS or wind
tunnels) to high-*Re* real world flows, for scalar transfer problems?", the overall
conclusion from out study indicates that the LES, despite its inherent parameterizations,
is more suitable for studying real-world buildings:

1) Wind-tunnel studies result in $Nu \sim Re^{-0.52-0.74}$, a significantly lower exponent 627 628 range than the ≈ 0.9 observed in field measurements and LES. This is consistent 629 with the expected trend of a lower *m* when *Re* is lower, and suggests that the 630 low-Re effects in the wind tunnel are biasing the findings and would make them not suitable for extrapolation to the real-world (yet as mentioned in the 631 632 introduction some current models rely on such coefficients empirically determined from water channel studies from 1924 [14]). As such, when LES-wind 633 634 tunnel discrepancies arise, it seem more likely that the errors are related to the 635 extrapolation of wind tunnel Nu-Re relations outside their range of validity.

636 2) There is a strong sensitivity of the heat transfer exchange coefficient to inflow
637 conditions, and the inflow is wind tunnel studies (or many simulations for that
638 matter) do not represent realistic upwind conditions in the real world.

For building models and urban microclimate models that often use averaged value for modeling turbulent heat exchange, based on our simulation results, the use of facet-averaged values seem to be appropriate, but the relatively large differences among different facets preclude the use of a single coefficient for the whole building since this

| 643 | would not capture the large facet-to-facet variations. In addition, we have documented |
|-----|--|
| 644 | (not surprisingly) that it is important in numerical simulation like LES to match the |
| 645 | experimental inflow conditions, especially for the windward faces that are affected the |
| 646 | most. For future experimental studies in wind tunnels or field experiments, details such as |
| 647 | the inflow profiles in a wind tunnel, measuring positions of wind and temperature, and |
| 648 | wind directions should be included so that further validation studies can be conducted |
| 649 | with more details of the experimental setup. For the types of numerical experiments |
| 650 | considered here, the suitable domain height should be greater than 4 times the height of |
| 651 | the obstacle. Another point to note is that the exponent <i>m</i> in $Nu \sim Re^m$ being close to 1.0 |
| 652 | (both in building-scale field measurement and LES) is a manifestation of approaching the |
| 653 | fully rough limit[27], in which the Stanton number is independent of <i>Re</i> . However, this |
| 654 | limit is not reached suggesting that transitional effects persist. This should not be |
| 655 | confused with the building canopy scale flow, which is clearly in the fully rough regime. |
| 656 | Going forward, the results gives us confidence in the capability of LES and the potential |
| 657 | for using the technique to develop a better understanding of coupled scalar and |
| 658 | momentum transfer at high-Re over complex topographies, and to formulate improved |
| 659 | spatially-averaged surface exchange models to be used in coarse atmospheric models |
| 660 | (weather or climate) where the buildings cannot be resolved. |

663 Acknowledgement

| 664 | This study | was funded by the US National Science Foundation's Sustainability Research |
|---|--|---|
| 665 | Network C | ooperative Agreement # 1444758 and Water Sustainability and Climate |
| 666 | program (| Grant # CBET-1058027. The simulations were performed on the |
| 667 | supercompu | ting clusters of the National Center for Atmospheric Research through |
| 668 | project P36 | 861020. W.A. was supported by the Army Research Office Environmental |
| 669 | Sciences Directorate (Grant # W911NF-15-1-0231; PM: Dr. J. Parker). | |
| 670 | | |
| 671 | | |
| 672 | References | |
| 673 674 675 | [1] | M. Mirsadeghi, D. Cóstola, B. Blocken, J.L.M. Hensen, Review of external convective heat transfer coefficient models in building energy simulation programs: Implementation and uncertainty, Applied Thermal Engineering. |
| 676 677 678 679 | [2] | 56 (2013) 134–151. T. Defraeye, B. Blocken, J. Carmeliet, Convective heat transfer coefficients for exterior building surfaces: Existing correlations and CFD modelling, Energy Conversion and Management. 52 (2011) 512–522. dai:10.1016/i anagement.2010.07.026 |
| 680681682683 | [3] | doi:10.1016/j.enconman.2010.07.026. J.A. Palyvos, A survey of wind convection coefficient correlations for building envelope energy systems' modeling, Applied Thermal Engineering. 28 (2008) 801–808. doi:10.1016/j.applthermaleng.2007.12.005. |
| 684 685 | [4] | D. Li, E. Bou-Zeid, Quality and sensitivity of high-resolution numerical simulation of urban heat islands, Environ. Res. Lett. 9 (2014). |
| 686 687 688 | [5] | T.H. Chilton, A.P. Colburn, Mass Transfer (Absorption) Coefficients Prediction from Data on Heat Transfer and Fluid Friction, Ind. Eng. Chem. 26 (1934) 1183–1187. doi:10.1021/ie50299a012. |
| 689 690 691 | [6] | B. Blocken, J. Carmeliet, The influence of the wind-blocking effect by a building on its wind-driven rain exposure, Journal of Wind Engineering and Industrial Aerodynamics. 94 (2006) 101–127. |

| 692 693 | [7] | T. Sun, E. Bou-Zeid, ZH. Wang, E. Zerba, GH. Ni, Hydrometeorological determinants of green roof performance via a vertically-resolved model for |
|------------|------|---|
| 694 | | heat and water transport, Building and Environment. 60 (2013) 211–224. |
| 695 | | doi:10.1016/j.buildenv.2012.10.018. |
| 696 | [8] | T. Sun, E. Bou-Zeid, GH. Ni, To irrigate or not to irrigate: Analysis of |
| 697 | | green roof performance via a vertically-resolved hygrothermal model, |
| 698 | | Building and Environment. 73 (2014) 127–137. |
| 699 | | doi:10.1016/j.buildenv.2013.12.004. |
| 700 | [9] | V. Masson, A physically-based scheme for the urban energy budget in |
| 701 | | atmospheric models, Boundary-Layer Meteorol. 94 (2000) 357–397. |
| 702 | | doi:10.1023/A:1002463829265. |
| 703 | [10] | ZH. Wang, E. Bou-Zeid, J.A. Smith, A coupled energy transport and |
| 704 | | hydrological model for urban canopies evaluated using a wireless sensor |
| 705 | | network, Quarterly Journal of the Royal Meteorological Society. 139 (2013) |
| 706 | | 1643–1657. doi:10.1002/qj.2032. |
| 707 | [11] | C.S.B. Grimmond, M. Blackett, M.J. Best, J.J. Baik, S.E. Belcher, J. |
| 708 | | Beringer, et al., Initial results from Phase 2 of the international urban energy |
| 709 | | balance model comparison, International Journal of Climatology. 31 (2011) |
| 710 | | 244–272. doi:10.1002/joc.2227. |
| 711 | [12] | C.S.B. Grimmond, T.R. Oke, D.G. Steyn, Urban Water Balance 1. A Model |
| 712 | | for Daily Totals, (1986). |
| 713 | [13] | A. Hagishima, J. Tanimoto, K.I. Narita, Intercomparisons of experimental |
| 714 | | convective heat transfer coefficients and mass transfer coefficients of urban |
| 715 | | surfaces, Boundary-Layer Meteorol. 117 (2005) 551–576. |
| 716 | [14] | W. Jürges, Der Wärmeübergang an einer ebenen Wand, 1924. |
| 717 | [15] | I.P. Castro, H. Cheng, R. Reynolds, Turbulence Over Urban-type Roughness: |
| 718 | | Deductions from Wind-tunnel Measurements, Boundary-Layer Meteorol. |
| 719 | | 118 (2006) 109–131. doi:10.1007/s10546-005-5747-7. |
| 720 | [16] | J. Jiménez, TURBULENT FLOWS OVER ROUGH WALLS, |
| 721 | | Http://Dx.Doi.org/10.1146/Annurev.Fluid.36.050802.122103. 36 (2004) |
| 722 | | 173-196. doi:10.1146/annurev.fluid.36.050802.122103. |
| 723 | [17] | D.A. Aliaga, J.P. Lamb, D.E. Klein, Convection heat transfer distributions |
| 724 | | over plates with square ribs from infrared thermography measurements, |
| 725 | | International Journal of Heat and Mass Transfer. 37 (1994) 363–374. |
| 726 | | doi:10.1016/0017-9310(94)90071-X. |
| 727 | [18] | M.K. Chyu, V. Natarajan, Local heat/mass transfer distributions on the |
| 728 | | surface of a wall- mounted cube, Transections of the ASME. Journal of Heat |
| 729 | | Transfer. 113 (1991) 851–857. doi:10.1115/1.2911213. |

| 730 731 | [19] | T. Igarashi, Heat transfer from a square prism to an air stream, International Journal of Heat and Mass Transfer. 28 (1985) 175–181. |
|------------|-------|--|
| 732 | [20] | doi:10.1016/0017-9310(85)90019-5. |
| 733 | [20] | E.R. Meinders, T.H. Van Der Meer, K. Hanjalić, Local convective heat |
| 734 725 | | transfer from an array of wall-mounted cubes, International Journal of Heat |
| 735 736 | | and Mass Transfer. 41 (1998) 335–346. |
| | [21] | doi:10.1016/S0017-9310(97)00148-8. |
| 737 | [21] | E.R. Meinders, K. Hanjalić, Vortex structure and heat transfer in turbulent |
| 738 | | flow over a wall-mounted matrix of cubes, International Journal of Heat and |
| 739 740 | [22] | Mass Transfer. 20 (1999) 255–267. doi:10.1016/S0142-727X(99)00016-8. |
| 740 | [22] | H. Nakamura, T. Igarashi, T. Tsutsui, Local heat transfer around a |
| 741 | | wall-mounted cube in the turbulent boundary layer, International Journal of |
| 742 | | Heat and Mass Transfer. 44 (2001) 3385–3395. |
| 743 | [00] | doi:10.1016/S0017-9310(01)00009-6. |
| 744 | [23] | K.I. Narita, Experimental study of the transfer velocity for urban surfaces |
| 745 | | with a water evaporation method, Boundary-Layer Meteorol. 122 (2007) |
| 746 | F. 43 | 293–320. |
| 747 | [24] | F. Pascheke, J.F. Barlow, A. Robins, Wind-tunnel Modelling of Dispersion |
| 748 | | from a Scalar Area Source in Urban-Like Roughness, Boundary-Layer |
| 749 | | Meteorol. 126 (2007) 103–124. doi:10.1007/s10546-007-9222-5. |
| 750 | [25] | J.F. Barlow, I.N. Harman, S.E. Belcher, Scalar fluxes from urban street |
| 751 | | canyons. Part I: Laboratory simulation, Boundary-Layer Meteorol. 113 |
| 752 | | (2004) 369–385. doi:10.1007/s10546-004-6204-8. |
| 753 | [26] | J.H. Lienhard, A Heat Transfer Textbook, Courier Corporation, 2013. |
| 754 | [27] | R.L. Webb, E.R.G. Eckert, R.J. Goldstein, Heat transfer and friction in tubes |
| 755 | | with repeated-rib roughness, International Journal of Heat and Mass Transfer. |
| 756 | | 14 (1971) 601–617. doi:10.1016/0017-9310(71)90009-3. |
| 757 | [28] | F.L. Test, R.C. Lessmann, A. Johary, Heat transfer during wind flow over |
| 758 | | rectangular bodies in the natural environment, Transections of the ASME. |
| 759 | | Journal of Heat Transfer. 103 (1981) 262-267. doi:10.1115/1.3244451. |
| 760 | [29] | D.L. Loveday, A.H. Taki, Convective heat transfer coefficients at a plane |
| 761 | | surface on a full-scale building facade, International Journal of Heat and |
| 762 | | Mass Transfer. 39 (1996) 1729-1742. doi:10.1016/0017-9310(95)00268-5. |
| 763 | [30] | M.G. Emmel, M.O. Abadie, N. Mendes, New external convective heat |
| 764 | | transfer coefficient correlations for isolated low-rise buildings, Energy and |
| 765 | | Buildings. 39 (2007) 335–342. |
| 766 | [31] | M. Yazdanian, J.H. Klems, Measurement of the exterior convective film |
| 767 | | coefficient for windows in low-rise buildings, ASHRAE Transactions. 100 |
| 768 | | (1994) 1087–1096. |
| | | |

| 769 770 771 | [32] | R.D. Clear, L. Gartland, F.C. Winkelmann, An empirical correlation for the outside convective air-film coefficient for horizontal roofs, Energy and Buildings. 35 (2003) 797–811. |
|-------------------|------|---|
| 772 | [33] | Y. Liu, D.J. Harris, Full-scale measurements of convective coefficient on |
| 773 | | external surface of a low-rise building in sheltered conditions, Building and |
| 774 | | Environment. 42 (2007) 2718–2736. |
| 775 | [34] | S.B. Park, J.J. Baik, A large-eddy simulation study of thermal effects on |
| 776 | | turbulence coherent structures in and above a building array, J. Appl. Meteor. |
| 777 | | Climatol. 52 (2013) 1348–1365. |
| 778 | [35] | V.B.L. Boppana, ZT. Xie, I.P. Castro, Large-Eddy Simulation of Heat |
| 779 | | Transfer from a Single Cube Mounted on a Very Rough Wall, |
| 780 | | Boundary-Layer Meteorol. 147 (2012) 347-368. |
| 781 | | doi:10.1007/s10546-012-9793-7. |
| 782 | [36] | T. Defraeye, B. Blocken, J. Carmeliet, CFD simulation of heat transfer at |
| 783 | | surfaces of bluff bodies in turbulent boundary layers: Evaluation of a |
| 784 | | forced-convective temperature wall function for mixed convection, Journal |
| 785 | | of Wind Engineering and Industrial Aerodynamics. 104-106 (2012) 439- |
| 786 | | 446. |
| 787 | [37] | J. Liu, J. Srebric, N. Yu, Numerical simulation of convective heat transfer |
| 788 | | coefficients at the external surfaces of building arrays immersed in a |
| 789 | | turbulent boundary layer, International Journal of Heat and Mass Transfer. |
| 790 | | 61 (2013) 209–225. doi:10.1016/j.ijheatmasstransfer.2013.02.005. |
| 791 | [38] | S. Leonardi, P. Orlandi, R.J. Smalley, L. Djenidi, R.A. Antonia, Direct |
| 792 | | numerical simulations of turbulent channel flow with transverse square bars |
| 793 | | on one wall, Journal of Fluid Mechanics. 491 (n.d.) 229-238. |
| 794 | [39] | S. Leonardi, L. Djenidi, P. Orlandi, R.A. Antonia, Heat transfer in a |
| 795 | | turublent channel flow with square bars and circular rods on one wall, |
| 796 | | Journal of Fluid Mechanics. 776 (n.d.) 512–530. |
| 797 | [40] | O. Coceal, T.G. Thomas, I.P. Castro, S.E. Belcher, Mean Flow and |
| 798 | | Turbulence Statistics Over Groups of Urban-like Cubical Obstacles, |
| 799 | | Boundary-Layer Meteorol. 121 (2006) 491–519. |
| 800 | | doi:10.1007/s10546-006-9076-2. |
| 801 | [41] | O. Coceal, T.G. Thomas, S.E. Belcher, Spatial Variability of Flow Statistics |
| 802 | | within Regular Building Arrays, Boundary-Layer Meteorol. 125 (2007) 537- |
| 803 | | 552. doi:10.1007/s10546-007-9206-5. |
| 804 | [42] | S.B. Pope, Turbulent Flows, Cambridge University Press, 2000. |
| 805 | [43] | D.B. Spalding, A new analytical expression for the drag of a flat plate valid |
| 806 | | for both the turbulent and laminar regimes, International Journal of Heat and |
| 807 | | Mass Transfer. 5 (1962) 1133–1138. doi:10.1016/0017-9310(62)90189-8. |

| 808 809 810 | [44] | C.H. Liu, T.N.H. Chung, Forced convective heat transfer over ribs at various separation, International Journal of Heat and Mass Transfer. 55 (2012) 5111–5119. doi:10.1016/j.ijheatmasstransfer.2012.05.012. |
|-------------------|-------|--|
| 811 | [45] | M.G. Giometto, A. Christen, C. Meneveau, J. Fang, M. Krafczyk, M.B. |
| 812 | | Parlange, Spatial Characteristics of Roughness Sublayer Mean Flow and |
| 813 | | Turbulence Over a Realistic Urban Surface, Boundary-Layer Meteorol. |
| 814 | | (2016) 1–28. doi:10.1007/s10546-016-0157-6. |
| 815 | [46] | B.E. Launder, On the Computation of Convective Heat-Transfer in Complex |
| 816 | L - J | Turbulent Flows, Journal of Heat Transfer-Transactions of the Asme. 110 |
| 817 | | (1988) 1112–1128. |
| 818 | [47] | J.C. Wyngaard, L.J. Peltier, S. Khanna, LES in the surface layer: Surface |
| 819 | | fluxes, scaling, and SGS modeling, J. Atmos. Sci. 55 (1998) 1733–1754. |
| 820 | | doi:10.1175/1520-0469(1998)055<1733:LITSLS>2.0.CO;2. |
| 821 | [48] | W. Cabot, P. Moin, Approximate wall boundary conditions in the large-eddy |
| 822 | | simulation of high Reynolds number flow, Flow, Turbulence and |
| 823 | | Combustion. 63 (2000) 269–291. doi:10.1023/A:1009958917113. |
| 824 | [49] | X.I.A. Yang, J. Sadique, R. Mittal, C. Meneveau, Integral wall model for |
| 825 | | large eddy simulations of wall-bounded turbulent flows, Physics of Fluids |
| 826 | | (1994-Present). 27 (2015) 025112. doi:10.1063/1.4908072. |
| 827 | [50] | X. Yang, J. Sadique, R. Mittal, C. Meneveau, Exponential roughness layer |
| 828 | | and analytical model for turbulent bounday layer flow over |
| 829 | | rectangular-prism roughness elements, Journal of Fluid Mechanics. 789 (n.d.) |
| 830 | | 127–165. |
| 831 | [51] | T. Defraeye, B. Blocken, J. Carmeliet, An adjusted temperature wall function |
| 832 | | for turbulent forced convective heat transfer for bluff bodies in the |
| 833 | | atmospheric boundary layer, Building and Environment. 46 (2011) 2130- |
| 834 | | 2141. doi:10.1016/j.buildenv.2011.04.013. |
| 835 | [52] | S.B. Pope, Ten questions concerning the large-eddy simulation of turbulent |
| 836 | | flows, New Journal of Physics. 6 (2004) –35. |
| 837 | | doi:10.1088/1367-2630/6/1/035. |
| 838 | [53] | J. Slotnick, CFD Vision 2030 Study, 2014. |
| 839 | [54] | S. Chester, C. Meneveau, M.B. Parlange, Modeling turbulent flow over |
| 840 | | fractal trees with renormalized numerical simulation, Journal of |
| 841 | | Computational Physics. 225 (2007) 427-448. doi:10.1016/j.jcp.2006.12.009. |
| 842 | [55] | Y.H. Tseng, C. Meneveau, M.B. Parlange, Modeling flow around bluff |
| 843 | | bodies and predicting urban dispersion using large eddy simulation, |
| 844 | | Environmental Science & Technology. 40 (2006) 2653-2662. |
| 845 | | doi:10.1021/es051708m. |

| 846 847 848 849 | [56] | V. Kumar, J. Kleissl, C. Meneveau, M.B. Parlange, Large-eddy simulation of a diurnal cycle of the atmospheric boundary layer: Atmospheric stability and scaling issues, Water Resources Research. 42 (2006) n/a–n/a. doi:10.1029/2005WR004651. |
|--------------------------|--------------|--|
| 850 | [57] | S. Shah, E. Bou-Zeid, Very-Large-Scale Motions in the Atmospheric |
| 851 | | Boundary Layer Educed by Snapshot Proper Orthogonal Decomposition, |
| 852 | | Boundary-Layer Meteorol. 153 (2014) 355–387. |
| 853 | | doi:10.1007/s10546-014-9950-2. |
| 854 | [58] | Q. Li, E. Bou-Zeid, W. Anderson, The impact and treatment of the Gibbs |
| 855 | | phenomenon in immersed boundary method simulations of momentum and |
| 856 | | scalar transport |
| 857 | , Journal of | f Computational Physics. (n.d.). |
| 858 | [59] | E. Bou-Zeid, C. Meneveau, M. Parlange, A scale-dependent Lagrangian |
| 859 | | dynamic model for large eddy simulation of complex turbulent flows, |
| 860 | | Physics of Fluids. 17 (2005). doi:10.1063/1.1839152. |
| 861 | [60] | W. Anderson, Passive scalar roughness lengths for atmospheric boundary |
| 862 | | layer flow over complex, fractal topographies, Environ Fluid Mech. 13 (2013) |
| 863 | | 479-501. doi:10.1007/s10652-013-9272-9. |
| 864 | [61] | B.A. Kader, A.M. Yaglom, Heat and mass transfer laws for fully turbulent |
| 865 | | wall flows, International Journal of Heat and Mass Transfer. 15 (1972) |
| 866 | | 2329-2351. doi:10.1016/0017-9310(72)90131-7. |
| 867 | [62] | A.E. Perry, J.B. Bell, P.N. Joubert, Velocity and temperature profiles in |
| 868 | | adverse pressure gradient turbulent boundary layers, Journal of Fluid |
| 869 | | Mechanics. 25 (1966) 299-320. doi:10.1017/S0022112066001666. |
| 870 | [63] | L. Temmerman, M.A. Leschziner, C.P. Mellen, J. Fröhlich, Investigation of |
| 871 | | wall-function approximations and subgrid-scale models in large eddy |
| 872 | | simulation of separated flow in a channel with streamwise periodic |
| 873 | | constrictions, International Journal of Heat and Mass Transfer. 24 (2003) |
| 874 | | 157-180. doi:10.1016/S0142-727X(02)00222-9. |
| 875 | [64] | T.R. Oke, Boundary Layer Climates, Routledge, 1978. |
| 876 | [65] | A.E. Perry, W.H. Schofield, P.N. Joubert, Rough wall turbulent boundary |
| 877 | | layers, Journal of Fluid Mechanics. 37 (1969) 383-413. |
| 878 | | doi:10.1017/S0022112069000619. |
| 879 | [66] | S. Leonardi, I.P. Castro, Journal of Fluid Mechanics - Abstract - Channel |
| 880 | | flow over large cube roughness: a direct numerical simulation study, Journal |
| 881 | | of Fluid Mechanics. (2010). |
| 882 | [67] | R. Martinuzzi, C. Tropea, The Flow Around Surface-Mounted, Prismatic |
| 883 | | Obstacles Placed in a Fully Developed Channel Flow (Data Bank |
| 884 | | Contribution), J. Fluids Eng. 115 (1993) 85-92. doi:10.1115/1.2910118. |
| | | |

| 885 886 | [68] | F.P. Incropera, Introduction to Heat Transfer Fourth Edition Wie, Wiley, 2002. |
|--------------------------|------|---|
| 887 888 889 890 | [69] | A. Hagishima, J. Tanimoto, Field measurements for estimating the convective heat transfer coefficient at building surfaces, Building and Environment. 38 (2003) 873–881. doi:10.1016/S0360-1323(03)00033-7. |