Detailed final report

Air quality oriented urban design strategies

/Levegőminőség-orientált várostervezési stratégiák/

K124439

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Execution of the research plan

I. model development

GPU-based LES [1]

In the framework of the project, we developed a modeling workflow based on thermal analogy, which enables the investigation of the dispersion of passive air pollutants using a GPU-based CFD model (ANSYS Discovery Live). With the new method, the execution of Large-Eddy Simulation models can be accelerated by two orders of magnitude compared to commonly used CPU-based models. The new process can significantly contribute to the practical application of dispersion studies based on large-eddy simulation and the extension of the investigated parameter range.

Inlet for limited-range LES [1, 8]

To produce realistic inflow turbulence, we developed an intake configuration based on passive turbulence generators, through which the average velocity and turbulence intensity characteristic of the urban boundary layer can be set with sufficient accuracy in the large-eddy simulation model, even when using a short computational domain. In addition to the vertical mean velocity and turbulence intensity profiles, the adequacy of the artificial boundary layer was also supported by the good agreement of point velocity-power spectra.

The velocity field provided by the GPU-based LES was validated based on Christof Gromke's (2007) wind tunnel measurements on a street canyon model. The results were in good agreement with the measurement data. After that, we carried out dispersion studies in the case of a single street canyon and the wind direction perpendicular to its longitudinal axis, the results of which (in terms of concentration distribution) were compared with the wind tunnel measurements of Gromke (2016). Compared to standard modeling methods, the new model showed excellent agreement with the measurement data.

Analysis of dynamic wind load with a GPU-based LES model [8]

The GPU-based boundary layer wind tunnel model also enables the examination of the dynamic wind load on buildings. We made further investigations with the University of Karlsruhe (KIT) to validate this application. KIT conducted new wind tunnel experiments to determine the time-dependent surface pressure on a cube-shaped building model set at 90° and 45° angles with the flow at 175 measurement points. The accuracy of the GPU-based numerical model was evaluated using the COST 732 indicators compared with the measurement data. The model showed sufficient accuracy for engineering practice, with a correlation factor of 0.90 for averages and 0.73 for fluctuations. The method developed in this research can be used not only for dispersion tests but also for analyzing static and dynamic wind loads affecting buildings. Due to the technical limitations of currently available graphics cards, the accuracy of the numerical wind tunnel model does not yet reach the accuracy of wind tunnel measurements. Still, it is swift compared to the experimental method. In possession of a CAD model, the dispersion tests can be performed in a few (2-6) hours, even in the case of complex geometric arrangements, so that the method can be recommended for preliminary tests and geometric optimization in addition to wind tunnel tests. We detailed the method's expected accuracy and application limitations in our related publication.

Coupled heat and pollutant transport in a periodic domain [10]

In the ANSYS FLUENT simulation system, we developed a coupled heat and pollutant transport model operating in the periodic domain. The effect of natural convection on the transport of air pollutants was investigated as a function of the bulk Richardson number, i.e., the $Ri_b = Gr/Re^2$ parameter formed from the Grashof number and the Reynolds number, in the geometric arrangement used in the field experiments of Sun Yat-sen University (SYSU). We have demonstrated the model's suitability for examining pollution transport over long distances (up to 20-50 streets). We investigated the impact of the mass Richardson number (Ri_b), expressing the intensity of solar irradiation, on the mass Stanton number (k^*), which describes the ventilation efficiency.

Our results indicate that the effect of natural ventilation caused by local solar irradiation in a high-rise building environment becomes significant in the $Rib>3$ range. In the $Ri_b>10$ range, typical in windless summer conditions, solar radiation is the dominant driving force for ventilation. Our model opens up the opportunity to investigate and develop buildings that make better use of solar energy (for example, with suitable exterior painting) and thus avoid critical episodes of air pollution in summer. For the practical application of the model, it is also necessary to validate the method with field measurements; therefore, in our related article, we stated our intention to cooperate with working groups performing field measurements and described the requirements for comparable measurements in detail.

OpenFOAM implementation [11]

The non-hydrostatic atmospheric model published by Kristóf et al. (2009) was further developed and implemented in the OpenFOAM software environment along with the original version. In the new model, by numerically calculating the derivatives, thus omitting certain simplifying conditions, it is possible to examine atmospheres with arbitrary temperature stratification and composition. The advantage of the new model is that it can be flexibly adapted to the simulation tasks that arise in engineering practice by specifying the model parameters independently of the code. In the validation case developed by Straka et al. (1993), the results of the new model and the EULAG model used as a reference agree well. The comparison was carried out at several mesh resolutions. For extrapolated mesh-independent results, the deviation of the front position is smaller than the mesh resolution.

We also implemented the periodic dispersion model of Kristóf et al. (2017) in the OpenFOAM environment. The OpenFOAM version showed an exact match with the results in our previous publication.

Measurement-driven LES (TWF-LES) [5]

We have developed a model for the effects of wind shear occurring at the upper part of the large eddy simulation domain and turbulent structures larger than the size of the domain. In previous similar model studies, the flow was induced by a constant pressure gradient. In the proposed model, we use a driving force of variable direction and magnitude (Transient Wind Forcing, TWF), controlled so that the wind speed follows the measured velocity-time series in the reference point above the buildings. The TWF method may model the effect of turbulent scales exceeding the size of the periodic domain, which mainly causes deviations from standard models due to the big changes in wind direction. The direction of the artificial wind produced in laboratory experiments displays less variation than natural wind. The reasons for this are that the dimensions of the wind tunnel limit the size of the flow structures that can be produced and that some essential effects - such as the Ekman layer, thermal convection, density stratification, and the synoptic pressure gradient - cannot be modeled in wind tunnels. By taking into account the effect of macroscopic turbulence, the air pollutant dispersion studies with the TWF model can even exceed the accuracy limits of wind tunnel experiments. The relaxation time of the force control is chosen so that the propulsion force does not prevent the LES model from creating mesoscopic turbulence. To describe microscopic turbulence, we apply the well-known Smagorinsky-Lilly SGS model.

Another difference compared to previous LES models is that we assume a driving force with vertically varying intensity. The intensity of the driving force decreases moving away from the reference point, so the formation of an excessive pressure drop in the direction of the wind speed can be avoided, and the coherence distance related to the time scale of macroscopic turbulence can also be taken into account.

To verify the accuracy of TWF-LES, we used the results of field experiments at Sun Yat-sen University (SYSU) on a series of quasi-periodic street canyons built from 1.2-meter-high concrete modules. We used the time series of horizontal velocity components recorded at twice the height of the building model to drive the TWF-LES model. The model validation was carried out based on the time averages and RMSs of the horizontal velocity components measured at four different heights in the middle plane of the street canyon according to the validation metrics of COST Action 732 (Franke, 2009). For the initial model version, the correlation coefficient (r) was 0.94 for average speeds and 0.84 for fluctuations. We also demonstrated that the model accuracy can be further improved by optimizing the model parameters of the method. Through partial optimization, the value of the correlation coefficient for average values was increased to 0.975 and, in the case of speed fluctuations, to 0.98.

Unbounded aperiodic dispersion model in a periodic model domain [5]

We developed a new air pollutant transport model combining the TWF-LES model and the Lagrangian particle tracking method. An essential element of the process is that the number of periodic jumps along both horizontal directions is detected and stored among the unique characteristics of the particles during the calculations of the particle trajectory, which enables the determination of the actual (distant) positions of particles emitted by a given source. Using the model, we investigated the pollutant plumes emitted from a point source located in the center line of a street canyon in natural wind corresponding to the velocity data of the SYSU experiment. By comparing the results of LES models with transient and static wind forcing, significant (even qualitative) differences were found, which point in the direction of the field measurements.

By applying the periodic particle tracking method, the computing cost and time requirements of dispersion studies for the idealized urban surfaces can be substantially reduced (by orders of magnitude). The new method can be embedded in larger-scale transient dispersion models and provides high-resolution results so that it can be a realistic alternative to porous city models in later practical applications. Therefore, instead of developing porous models, we focused on the further development and validation of the new periodic particle tracking method for large-eddy simulations.

LES-based atmospheric boundary-layer database [13, 14, 19]

Our measurement-driven LES studies pointed out some of the limitations of wind tunnel tests and standard microscale numerical dispersion models. The atmospheric stratification and the wind direction changes caused by the Coriolis force in the atmospheric boundary layer - which are not taken into account by traditional models - significantly influence the near-ground wind statistics and, consequently, urban heat and air pollution transport processes. To address this issue, we investigated the atmospheric boundary layer with an explicit resolution of the surface roughness, considering the mesoscale atmospheric effects, using large-eddy simulations in periodic domains. In two different domain sizes (240m x 240m x 500m and 80m x 80m x 120m), we performed LES and a dispersion study using our new particle tracking method. In both models, we used identical mesh resolution and simplified the urban structure in square columns. The effect of atmospheric stability and the Coriolis force was taken into account using the transformation method developed by Kristóf et al. (2008). The larger domain included the entire atmospheric boundary layer, so the flow could be produced by prescribing a constant geostrophic pressure gradient. Assuming different building heights, atmospheric stability conditions, and geographic latitudes in the large domain, we generated a total of 16 realistic atmospheric boundary layers. The small domain contained only approx. 1/40 of the volume of the large domain, therefore the main driving force of the flow was the turbulent shear stress (wind shear) formed near the upper boundary of the domain, which was taken into account in the LES using the TWF model. In the examined cases, the wind speed, wind direction, turbulence, and concentration fields determined in the small domain showed a good agreement with the reference data extracted from the large domain, which supports the applicability of the TWF model in atmospheric transport studies. A good match with the reference data (especially in terms of wind directions) was only achieved if we took into account the effect of the Coriolis force and the synoptic pressure gradient (corresponding to the geostrophic wind) in the small-scale model, which suggests that these "mesoscale" effects were also relevant to the small-scale periodic models, which actually represent an infinite space.

Development of a special surface modelling and meshing tool [15, 20]

Creating a high-quality numerical mesh is one of the critical steps in Computational Fluid Dynamics (CFD). In the case of urban flows, this is a very complex task, during which the flow features, the available computing capacity, and as many details as possible of the geometry (topography, buildings, surface coverage, etc.) must be taken into account. This task is almost impossible to perform manually, so it was necessary to develop a software tool that automatically creates the geometry of the domain and the numerical mesh based on the available GIS data and the domain parameters specified by the user. We used the Shuttle Radar Topography Mission database to describe the surface shape, the Copernicus Land Monitoring Service data to parameterize the surface coverage, and the OpenStreetMap database to parameterize the built-up area geometrically. The method allows for explicit or porous roughness and vegetation modeling.

In cooperation with the Department of Analytical Chemistry of ELTE, we investigated the dispersion of urban air pollutants following an extreme particulate emission event using the new surface modelling and meshing tool. Based on observations made at the BpART observatory during five years of August 20 fireworks events, 2021 showed exceptionally high particle numbers. In order to reveal the cause of the phenomenon, we carried out a high-resolution transport study in the OpenFOAM system for the area between Erzsébet Bridge and Lágymányosi Bridge in Budapest. In the vicinity of the observation point, the particle concentration history determined by the Lagrange model - despite the uncertainties in the location and intensity of the sources - showed good agreement with the measurement data.

II. Wind tunnel tests and model validation [7, 12, 18]

We carried out wind field and dispersion tests for three different installation forms, on rows of parallel street canyons, in the wind direction perpendicular to the streets. We kept the total volume of the building models constant, as well as the width of the streets and building models in the direction of flow. The three different installation forms were selected based on the preliminary CFD modeling: installation with uniform height, 1:3 height-alternating with closed-row installation in a square grid (matrix) layout, and 1:3 height-alternating with closed-row installation in a chessboard (staggered) layout. The building height - street width ratio is the same in all three cases. The wind field and turbulence were investigated using two-component laser Doppler velocimetry (LDA), which also enabled the determination of local turbulent fluctuations. The dispersion tests were carried out with methane tracer gas emitted from point sources placed in the center line of street surfaces. The concentration measurements were made with a fast flame ionization detector (FFID) suitable for transient testing. The measuring devices were moved with the help of an automatic positioning system along profiles in various directions, with a spatial resolution of 0.2 mm.

The experimental data were used to validate the TWF-LES model and the dispersion model based on the aperiodic particle trajectory calculation.

We performed a statistical analysis based on the experimental database to characterize the concentration fluctuations. Concentration fluctuations measured in street canyons and above roof level can be described by gamma distribution or exponentially modified Gaussian distribution. Along the length of the trace gas plumes, the concentration distributions shift from exponential to Gaussian, and the Coefficient of Variation continuously decreases, which indicates the progress of homogenization. The results will be used to develop numerical models suitable for describing concentration fluctuations, which can push the boundaries of modeling the harmful effects of toxic, infectious, explosive, and unpleasant-smelling gases.

III. Practical applications in urban air quality control

Low Boundary Walls [1]

The effect of the LBWs placed in the street canyon on the dispersion of pollutants was investigated using three approaches:

A. using the periodic transport model implemented in OpenFOAM in street canyons with aspect ratios of 1, 1.25, and 1.5 H/W for three different LBW heights;
B. in the case of multiple LBWs placed between two building blocks of finite length, using LES, and
C. in quasi-periodic street canyon models of 0.5, 0.67, 1, 1.5, and 2 H/W aspect ratios and L/H = 10 with GPU-based LES.

Based on the results of the (periodic) model of an infinite series of street canyons without cross streets, LBWs have a negative effect on air quality in terms of the total street-level pollutant concentration. This is because the LBWs reduce the intensity of the street canyon vortex, thereby reducing its ability to dilute pollution. In the case of a periodic arrangement, we obtained an increasing concentration with increasing boundary wall height by applying the Reynolds-averaged turbulence model. The adverse effect can also be observed in the case of a wind direction perpendicular to the axis of the street and at 45° and increases with street width. A similar, negative result was also obtained in the case of LBWs placed on the roads between square building blocks.

Our tests using GPU-based large-eddy simulation showed that the air quality improvement effect of the knee wall placed in the middle of the street loses its positive impact in the case of street canyon series for the wind direction perpendicular to the longitudinal axis: while in the first street canyon, 40-70% concentration reduction can be observed, in the last (3dr of 6th, depending on the aspect ratio) the concentration decrease was only 15-40%.

Buildings with open foundations [16]

Based on the results of the LES, by using open building foundations (while maintaining a constant useful building volume), a concentration reduction of about 30-60% can be achieved with an opening size of 3-6 m (in the case of a building height of 18 meters) in the average of the first 5 street canyons. The degree of concentration reduction in the windward direction decreases rapidly as it progresses. Determining the effective street canyon number requires further investigation.

Based on our investigations with the periodic dispersion model, the opening of the foundations of the buildings arranged in an infinite plane grid is not expected to improve the air quality if the useful volume of the buildings is kept at a constant value.

Varying building height [2, 3, 4, 7, 16]

We investigated the ventilation of 15 different building layouts using GPU-based LES. Keeping the useful building volume constant, we examined the concentration of pollutants at street level in 5 consecutive street canyons. A 52% improvement in the dimensionless mass transfer coefficient (k*) was found compared to the simple street canyon row layout, using square-based buildings arranged in a checkerboard pattern. The results of the tests were used to design the wind tunnel model experiments. Bálint Papp won first place in the National Scientific Student Competition (OTDK) with his related presentation.

In our wind tunnel experiments with buildings of alternating height along the length of the building - in an asymmetrical (checkerboard) arrangement on both sides of the street - we observed a concentration reduction of about 45% at street level if the building height ratio was greater than 3. The advantage of this installation form is that the (more valuable) area on the ground floor of buildings does not decrease compared to the constant height installation form. It also enables the installation of a larger window area.

Miskolc Újgyőr main square area [9]

We investigated the impact of the reconstruction of a district of Miskolc (around Újgyőr main square) on the air pollution dispersion using a GPU-based LES, taking into account the current building layout and four different concept plans. All four plan versions (installation of taller buildings than the existing one on the north side of Andrássy Gyula utca, as well as E-W layout strip houses, N-S layout strip houses, and point houses installed on the south side of the main road) proved to be more favorable than the current installation form in terms of air quality. The CFD model showed a significant difference between the individual alternatives. In the value of the dilution factor (k*) taken at pedestrian head height, the unique concept plan versions showed an improvement of 11-32%.

Deviations from the original research plan

The vast majority of the planned research tasks were implemented and the results were published.

By the end of the project, we were not able to reach publishable results in the case of the research goals set out in points II.c and III.d-f. The main reason for this is that in Jing et al.'s latest publication (Jing, Y., Zhong, H. Y., Wang, W. W., He, Y., Zhao, F. Y., & Li, Y. (2021). Quantitative city ventilation evaluation for urban canopy under heat island circulation without geostrophic winds: Multi-scale CFD model and parametric investigations. Building and Environment, 196, 107793.) presents a detailed study of the parameter dependence of urban heat island convection and its effect on urban air quality. Therefore the points listed above in the work plan have lost their novelty. To analyze the phenomenon, Jing et al. (2021) used the transformation method developed by Kristóf et al. (2009), which is also consistent with the research method planned in the framework of the research project.

Compared to the research plan, many unplanned, significant results appear in our publications, which can serve as starting points for further research. Our results beyond the original work plan:

a) Application of GPU-based large-eddy simulation in air pollutant dispersion tests using a thermal analogy.
b) Modeling the effect of wind shear and macroscopic turbulence in dispersion models based on LES (TWF model coupling).
c) Lagrangian modeling of aperiodic transport in unbounded space with a wind field determined by LES in a small periodic domain.
d) Application of GPU-based large-eddy simulation to swiftly determine the dynamic wind load on buildings.

e) Wind tunnel dispersion tests with a fine temporal resolution and statistical analysis of concentration fluctuations in the case of three different building layouts.

Publications, scientific public impact

Out of the 5 international journal publications undertaken in the work plan, four were published by the end of the reporting period [1, 5, 7, 8], and one Hungarian-language journal article was also published [11]. Shortly after the end of the reporting period, we submitted three more manuscripts [18, 19, 20] to international journals classified as Q1/D1.

Instead of the promised 6 conference publications, 10 presentations were given [2, 3, 6, 9, 10, 12, 13, 14, 15, 16].

The principal investigator submitted his MTA doctoral thesis entitled "Urban Wind" [17] and defended it with 100% success. Two of the 7 theses points presented in the DSc thesis are based on the results of this research project. The results achieved in the project also form the basis of the PhD thesis of Bálint Papp and Márton Koren, which are expected to be submitted after the reporting period.

In connection with the project, two TDK theses were prepared. Two first places and a special prize were achieved in the university competition, and one first and one second place in the national competition.

Publications

Publications in the reporting period:

[1] KRISTÓF, Gergely; PAPP, Bálint. Application of GPU-based Large Eddy Simulation in urban dispersion studies. Atmosphere, 2018, 9.11: 442.

[2] KRISTÓF, Gergely; PAPP, Bálint. Optimization of Building Patterns for Better Air Quality Using GPU-Based Large Eddy Simulation, Geophysical Research Abstracts Vol. 21, EGU2019 General Assembly, 2019.

[3] PAPP, Bálint; KRISTÓF, Gergely. Épületmintázatok optimalizálása a levegőminőség javításának érdekében GPU alapú nagyörvény szimulációval. OGÉT 2019 proceedings.

[4] PAPP, Bálint. Városi szennyezőanyag-terjedés vizsgálata nagyörvény szimulációval numerikus szélcsatornában. OTDK dolgozat és előadás. Műszaki Tudományi szekció (Környezetmérnöki I. tagozat), 2019, I. helyezés. Témavezető: KRISTÓF, Gergely.

[5] Kristóf, G.; Papp, B.; Wang, H.; Hang, J. Investigation of the flow and dispersion characteristics of repeated orographic structures by assuming transient wind forcing. Journal of Wind Engineering and Industrial Aerodynamics, 2020, 197, 104087. https://doi.org/10.1016/j.jweia.2019.104087

[6] Papp, B., Kristóf, G., Gromke, C. (2020). Épületek szélterhelésének becslése GPU alapú nagyörvény szimulációval numerikus szélcsatornában. XXVIII. Nemzetközi Gépészeti Konferencia – OGÉT, 161-165.

[7] Papp, B., Kristóf, G., Istók, B., Koren, M., Balczó, M., Balogh, M. (2021). Measurement-driven Large Eddy Simulation of dispersion in street canyons of variable building height. Journal of Wind Engineering and Industrial Aerodynamics, 211, 104495. https://doi.org/10.1016/j.jweia.2020.104495

[8] Papp, B., Kristóf, G., Gromke, C. (2021). Application and assessment of a GPU-based LES method for predicting dynamic wind loads on buildings. Journal of Wind Engineering and Industrial Aerodynamics. https://doi.org/10.1016/j.jweia.2021.104739

[9] Szilágyi, M. Á., Papp, B. (2021). Miskolc átszellőzésének vizsgálata GPU alapú nagyörvény szimulációval. XXVIIII. Nemzetközi Gépészeti Konferencia (OGÉT 2021) kiadványkötete (ISSN 2668-9685), 80-83. https://ojs.emt.ro/index.php/oget/article/view/471/397

[10] Papp, B., Kristóf, G. (2021). The role of thermal convection in the dispersion of traffic-induced air pollutants in the urban environment. 20th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes. https://www.researchgate.net/publication/352560131_The_role_of_thermal_convection_in_the_dispersion_of_traffic-induced_air_pollutants_in_the_urban_environment

[11] Koren, M., Balogh, M. (2020). Kis léptékű nem-hidrosztatikus légköri áramlások numerikus modellezése mérnöki célokra. Légkör: Az Országos Meteorológiai Intézet szakmai tájékoztatója 65(3), 130-135.

[12] Papp, B., Istók, B., Koren, M., Balczó, M., Kristóf, G. (2022). Statistical assessment of the ventilation of street canyons based on time-resolved wind tunnel experiments. PHYSMOD 2022 – International Workshop on Flow and Dispersion Phenomena, Book of extended abstracts (ISBN 978-80-87012-81-9), 143-155.

[13] Koren, M., Balogh, M., Kristóf, G. (2022). Transient Wind Forcing: a method for modelling wind shear in building-scale Large Eddy Simulations, PHYSMOD 2022 – International Workshop on Flow and Dispersion Phenomena, Book of extended abstracts (ISBN 978-80-87012-81-9), pp 123.

[14] Koren, M., Kristóf, G (2022) Wind-shear coupling method to implicate large turbulent structures in a building-scale large eddy simulation, Conference on Modelling Fluid Flow (CMFF'22), WORKSHOP 5 - Coupling techniques in multiscale atmospheric models: Microphysics, local scale simulations, PBL structure. Oral presentation.

[15] Balogh, M., Farkas, Á., Weidinger, T., Salma, I., Dispersion simulation of firework-related aerosols, Conference on Modelling Fluid Flow (CMFF'22), WORKSHOP 5 - Coupling techniques in multiscale atmospheric models: Microphysics, local scale simulations, PBL structure. Oral presentation.

[16] Papp, B., Kristóf, G. (2022). Building Patterns Favorable for Air Quality: A Parameter Study Using LES. Proceedings of the Conference on Modelling Fluid Flow CMFF'22 (ISBN 978-963-421-881-4), 443-456. https://www.cmff.hu/pdf/CMFF22_Conference_Proceedings.pdf

[17] Kristóf, G (2021). The Urban Wind. Thesis points of the DSc thesis submitted to the Hungarian Academy of Science. http://real-d.mtak.hu/1402/

Further publications submitted shortly after the end of the reporting period:

[18] Papp, B., Istók, B., Koren, M., Balczó, Kristóf, G. (2022). Statistical assessment of the concentration fluctuations in street canyons with homogeneous and variable roof height. Building and Environment. Benyújtva: 2022.09.15

[19] Koren, M., Kristóf, G. (2022). Shear-driven LES using the Transient Wind Forcing model. Journal of Wind Engineering and Industrial Aerodynamics. Benyújtva: 2022.09.30

[20] Salma, I., Farkas, Á., Weidinger, T., Balogh, M., Firework smoke and its consequences on urban air quality and deposition in the human respiratory system, Environment International, (D1, IF=13.352), Submitted: 2022.09.1.